UNIVERSIDAD DE GUANAJUATO

Universitat de Girona

Theoretical Insights of p-Block Compounds in Ring Expansion Reactions and Catalysis

Thesis to obtain a double Master of Science degree in Chemistry (University of Guanajuato) and Advanced Catalysis and Molecular Modelling (University of Girona)

Victor Alonso Lucas Rosales

Supervisor:
Dr. José Oscar Carlos Jiménez Halla
Departamento de Química, DCNE, Universidad de Guanajuato

Co-supervisor:
Dr. Albert Poater i Teixidor
Departament de Química, IQCC, Universitat de Girona

Guanajuato, Guanajuato
August 2025

Evaluation Committee Members

President

Dr. Marco Antonio García Revilla

Departamento de Química, DCNE, Universidad de Guanajuato

Secretary

Dr. Gerardo González García

Departamento de Química, DCNE, Universidad de Guanajuato

Member

Dr. Oracio Serrano Torres

Departamento de Química, DCNE, Universidad de Guanajuato

Substitute

Dr. Crispín Silviano Cristóbal Gasga

Departamento de Química, DCNE, Universidad de Guanajuato

UNIVERSIDAD DE GUANAJUATO

DEPARTAMENTO DE QUÍMICA

DIVISIÓN DE CIENCIAS NATURALES Y EXACTAS

The undersigned hereby certifies that the research work reported in this thesis, entitled ***Theoretical Insights of p-Block Compounds in Ring Expansion Reactions and Catalysis***, submitted in fulfillment of the requirements for the degree of Master of Science in Chemistry, has been carried out under my supervision and that of Dr. Albert Poater i Teixidor from the *Institut de Química Computacional i Catàlisi* at University of Girona, Catalonia, Spain. This work is original and is being presented for the first time for the purpose of obtaining an academic degree.

Dr. José Oscar Carlos Jiménez Halla

Supervisor of Thesis

A mi madre,

Jakline Rosales Saucedo

Y a mi padre,

Abel Lucas Hernández

List of Publications

Part of the results of this thesis has been published in the following peer-reviewed international journal:

V. A. Lucas-Rosales, M. A. Vázquez, G. Merino, A. Poater, J. O. C. Jiménez-Halla, Electrophilic Insertion and Ring Growth in 1,2,5-Azadiborolidines: Theoretical Evidence for Boron-Driven Expansion, *Organic Chemistry Frontiers*, 2025, *in press*.

Other collaborations:

I. A. E. Cruz-Jiménez, P. A. Argumedo-Castrejón, J. B. Mateus-Ruiz, **V. A. Lucas-Rosales**, O. A. Valle-González, J. O. C. Jiménez-Halla, J. A. Luján-Montelongo, Deoxygenation of heterocyclic *N*-oxides employing iodide and formic acid as a sustainable reductant, *New J. Chem.*, 2024, **48**, 9424–9428.

II. L. I. Lugo-Fuentes, **V. A. Lucas-Rosales**, J. A. Sandoval-Mendoza, R. Shang, J. P. Martínez, J. O. C. Jiménez-Halla, Different Reaction Modes Operating in *ansa*-Half-Sandwich Magnesium Catalysts, *Chem. Eur. J.*, 2024, **30**, e202304130.

List of Congresses

Part of the results of this thesis were defended in the following presentations:

I. **V. A. Lucas-Rosales**, G. Merino, M. A. Vázquez-Guevara, A. Poater, J. O. C. Jiménez-Halla, "Estudio teórico sobre la inserción de CO en la 1,2,5-azadiborolidina" (poster), 9º Simposio Latinoamericano de Química de Coordinación y Organometálica, La Habana, Cuba, 2024.

II. **V. A. Lucas-Rosales**, G. Merino, M. A. Vázquez-Guevara, A. Poater, J. O. C. Jiménez-Halla, "Estudio teórico sobre la inserción de CO en la 1,2,5-azadiborolidina" (poster), 6º Simposio Mexicano de Química Supramolecular, CDMX, México, 2024.

III. **V. A. Lucas-Rosales**, J. O. C. Jiménez-Halla, A. Poater, G. Merino, M. A. Vázquez-Guevara, "Inserción de CO en la 1,2,5-azadiborolidina: una predicción teórica" (talk), LII Simposio Jacobo Gómez Lara, Guanajuato, México, 2024.

IV. **V. A. Lucas-Rosales**, J. O. C. Jiménez-Halla, A. Poater, G. Merino, M. A. Vázquez-Guevara, "Efecto de la retrodonación π sobre la inserción de CO en diferentes boraciclos" (poster), LIII Simposio Jacobo Gómez Lara, Guanajuato, México, 2025.

V. **V. A. Lucas-Rosales**, J. O. C. Jiménez-Halla, A. Poater, G. Merino, M. A. Vázquez-Guevara, "Estudio computacional sobre la expansión de anillo en azadiborolidinas empleando CO" (poster), LI Simposio Jacobo Gómez Lara, Guanajuato, México, 2024.

In July 2025, the first chapter of this thesis was defended at the Faculty of Sciences in the University of Girona to obtain a Master Science degree in Advanced Catalysis and Molecular Modelling.

List of Schemes

List of Charts

List of Tables

List of Figures

Summary

Chapter 1 illustrates the potential applications of ring expansion reactions in boron chemistry. We start with a computational analysis regarding the carbon monoxide (CO) insertion reaction in borole derivatives that has already been validated experimentally. We then use isosterism to transpose this type of reactivity to the 1,2,5-azadiborolidine ring, a boracycle that has not previously been investigated in this context. Here, we demonstrate that CO insertion occurs via a ring expansion mechanism governed by electronic, not steric, factors. Furthermore, we predict the ease of this reaction under mild conditions for 1,2,5-tri-*tert*-butyl-1,2,5-azadiborolidine in a solution of *n*-pentane.

In **Chapter 2**, we investigate triethanolamine borate, a polycyclic compound characterised by a transannular bond between a boronic acid fragment and a tertiary amine. This atrane is known to catalyse the cycloaddition of epoxides and carbon dioxide (CO_2). In this study, we computationally elucidate the reaction mechanism of this transformation and clarify the roles played by the catalyst and cocatalysts. Having revealed the catalyst's mechanism of action, we proceeded to enhance its catalytic activity by atom substitutions, thus performing predictive catalysis. This results in the construction of a new family of atranes with potential applications in the ring-opening reaction of epoxides.

Contents

Description of the Project

Ring expansion reactions play a crucial role in organic synthesis, offering a versatile strategy for constructing complex molecular structures. These reactions involve the enlargement of cyclic structures, often leading to the formation of larger rings or fused ring systems.[1–3] The importance of ring expansion reactions lies in their ability to efficiently generate diverse molecular architectures, enabling the synthesis of a wide range of biologically active compounds, pharmaceuticals, and materials.[4]

The first report on ring expansion reactions dates to the mid-20th century when researchers began exploring the potential of these transformations in the context of organic synthesis.[5] This pioneering work laid the foundation for subsequent developments in the field, with chemists leveraging ring expansion reactions to streamline the synthesis of complex molecules and address synthetic challenges.

In the realm of boron-containing compounds, the exploration of ring expansion reactions has gained particular attention. Boron-containing compounds exhibit unique reactivity patterns and incorporating them into ring expansion strategies introduces an additional dimension to the synthetic toolbox. The use of boron-containing substrates in ring expansion reactions allows for the selective functionalization of molecules, providing access to novel compounds with diverse applications.[6–8]

While the field continues to evolve, the study of ring expansion reactions, especially in the context of boron chemistry, holds great promise for advancing the synthesis of valuable compounds with applications in medicine, materials science, and beyond. Understanding the intricacies of these reactions paves the way for innovative and efficient synthetic routes, contributing to the broader landscape of organic chemistry.[9,10]

On the other hand, boron-guided catalysis plays a key role in research and industrial processes.[11] Boron compounds exhibit catalytic activity primarily due to their unique acidic properties, which can be adjusted according to the groups to which the boron atom is bonded. Furthermore, boron compounds are attractive due to their alignment with the principles of green chemistry and their strong metal-mimetic behaviour.[12,13] These two factors mean that boron-based catalysts, which are generally environmentally friendly, can achieve results that, until a few decades ago, were only possible using transition metals (e.g. Pd, Rh, Ru, Sc, Y). These results include C-C bond formation, hydrogenation, hydroboration, among others.[14] These new synthetic methods are known as metal-free and have the advantage of reducing production costs while ensuring high reaction yields.

The aim of this computational work is to shed new light on ring expansion reactions and boron-based catalysis. The project is therefore divided into two parts. Introduction, hypothesis, objectives, methods, results and conclusions are presented in a particular way for each project, developing a chapter for each one.

References

1. D. Orr, N. Yousefi and T. G. Minehan, *Org. Lett.*, 2018, **20**, 2839–2843.
2. S. Jana, Z. Yang, C. Pei, X. Xu and R. M. Koenigs, *Chem. Sci.*, 2019, **10**, 10129–10134.
3. W. Wang, X. Cui, J. Ma, Y. Li and X. Wang, *Chin. J. Org. Chem.*, 2021, **41**, 2715.
4. J. R. Donald and W. P. Unsworth, *Chem. Eur. J.*, 2017, **23**, 8780–8799.
5. D. Redmore and C. D. Gutsche, *Carbocyclic Ring Expansion Reactions*, Academic Press, NY, 1968.
6. H. Wang, J. Zhang and Z. Xie, *Chem. Sci.*, 2021, **12**, 13187–13192.
7. Z. Güven, L. Denker, H. Dolati, D. Wullschläger, B. Trzaskowski and R. Frank, *Chem. Eur. J.*, 2022, **28**, e202200673.
8. T. Bischof, L. Beßler, I. Krummenacher, L. Erhard, H. Braunschweig and M. Finze, *Chem. Eur. J.*, 2023, **29**, e202300210.
9. J. F. Araneda, W. E. Piers, M. J. Sgro and M. Parvez, *Organometallics*, 2015, **34**, 3408–3413.
10. K. R. Bluer, L. E. Laperriere, A. Pujol, S. Yruegas, V. A. K. Adiraju and C. D. Martin, *Organometallics*, 2018, **37**, 2917–2927.
11. X. Tan and H. Wang, *Chem. Soc. Rev.*, 2022, **51**, 2583–2600.
12. V. Nori, F. Pesciaioli, A. Sinibaldi, G. Giorgianni and A. Carlone, *Catalysts*, 2021, **12**, 5.
13. B. J. Graham and R. T. Raines, *J. Org. Chem.*, 2024, **89**, 2069–2089.
14. Y. Ma, S.-J. Lou and Z. Hou, *Chem. Soc. Rev.*, 2021, **50**, 1945–1967.

CHAPTER 1

"New molecules incite theory, which is the unifying,

framework-building way the chemist makes connections"

Roald Hoffmann,

Nobel Prize in Chemistry 1981

Electrophilic Insertion and Ring Growth in 1,2,5-Azadiborolidines: Theoretical Evidence for Boron-Driven Expansion

Victor A. Lucas-Rosales,[a,b] Miguel A. Vázquez,[a] Gabriel Merino,[*c] Albert Poater,[*b] and J. Oscar C. Jiménez-Halla[*a]

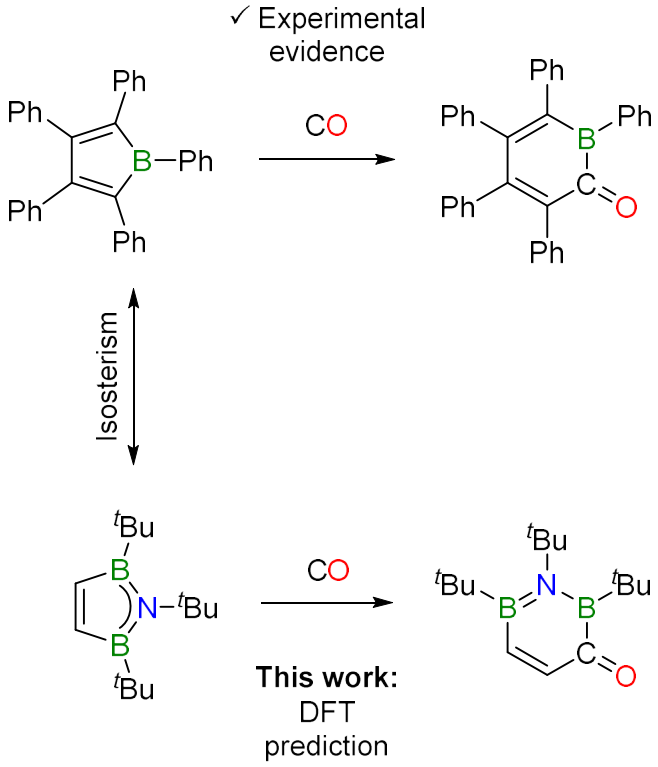
[a.] Departamento de Química, División de Ciencias Naturales y Exactas, Universidad de Guanajuato, Noria Alta S/N 36050, Guanajuato, Guanajuato, México. E-mail: jjimenez@ugto.mx

[b.] Institut de Química Computacional i Catàlisi, Departament de Química, Universitat de Girona, C/ Mª Aurèlia Capmany 69, 17003 Girona, Catalonia, Spain. E-mail: albert.poater@udg.edu

[c.] Departamento de Física Aplicada, Centro de Investigación y de Estudios Avanzados, Unidad Mérida, Km 6 Antigua Carretera a Progreso. Apdo. Postal 73, Cordemex, 97310, Mérida, Yucatán, México. E-mail: gmerino@cinvestav.mx

1.1. Abstract

This study computationally investigates the reactivity of 1,2,5-azadiborolidine derivatives towards carbon monoxide (CO), extending ring-expansion mechanisms from borole chemistry. Establishing structural and electronic analogy through isosterism, we propose that endocyclic CO insertion operates in this new class of boron heterocycles. Boracycle 1,2,5-tri-*tert*-butyl-1,2,5-azadiborolidine emerged as the optimal candidate, exhibiting a favourable three-step pathway: CO insertion, dimerization of the ring-expanded intermediate, and subsequent double [1,2]-migration. Thermochemical analysis confirms viability under mild conditions, with solvents (DCM, *n*-pentane, THF) enhancing stability; *n*-pentane affords optimal kinetics. Key reactivity indicators include B–C(O) and C–O bond lengths, while correlations between kinetic barriers and π-backbonding-like energy provide predictive insight. This work broadens boron-based reactivity by proposing a *fourth* class of CO-inserting boracycles and highlights 1,2,5-azadiborolidines as versatile, metal-free frameworks for small-molecule activation.



1.2. Introduction

Ring expansion reactions remain indispensable tools in synthetic organic chemistry, offering direct access to medium- and large-sized ring systems that are often challenging to construct via conventional cyclization methods. These reactions provide a strategic advantage by increasing ring size without dismantling pre-existing molecular complexity, a concept widely embraced in natural product synthesis and drug design.[1] Notably, recent work by Chouraqui and co-workers emphasized the growing utility of ring expansion methodologies for synthesizing structurally diverse and conformationally rich scaffolds, frequently with enhanced biological relevance and physicochemical properties.[2]

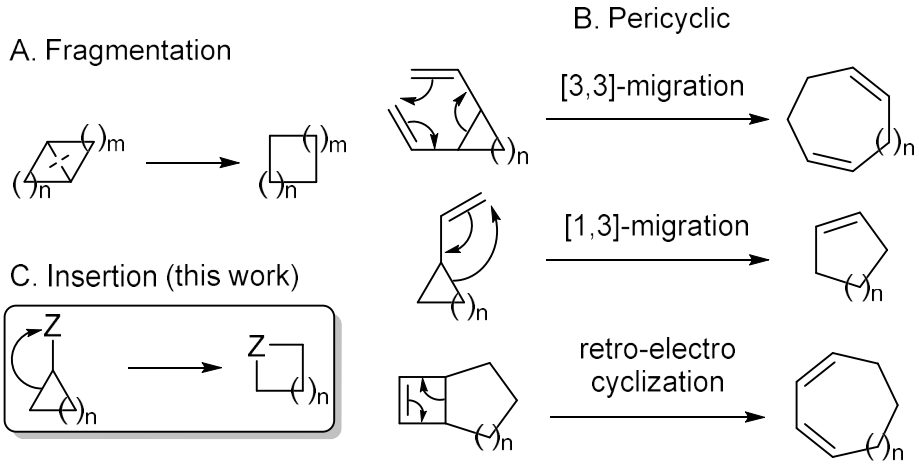


Chart 1.1. Classification of ring expansion reactions.

Ring expansions can be broadly classified into three mechanistic categories, defined by the transformation driving the ring-size increase (**Chart 1.1**).[2,3] A) Fragmentation reactions typically involve cleavage of a small ring or leaving group, followed by rearrangement or migration to form a larger ring. These processes often proceed through carbocationic or radical intermediates and are broadly applied in skeletal editing. B) Pericyclic reactions (e.g., electrocyclic ring openings, sigmatropic rearrangements, cycloadditions) proceed via concerted mechanisms governed by orbital symmetry and have been central in synthesizing polycyclic and strained architectures. C) Insertion reactions, the focus of this study, entail the formal incorporation of an external atom or functional group into a cyclic framework. These transformations frequently proceed under mild conditions

with high regiochemical and stereochemical control, rendering them particularly attractive for constructing complex, functionalized ring systems.

Among the elements used in insertion strategies, boron stands out due to its unique electron-deficient character, which enables distinctive bonding modes and electrophilic reactivity not typically observed in classic organic systems.[4–9] The incorporation of boron atoms into molecular frameworks facilitates the development of advanced materials with potential applications across diverse fields, including energy storage,[10–17] optoelectronics,[17–21] drug design,[22–24] and small molecule activation.[9,17,25–27]

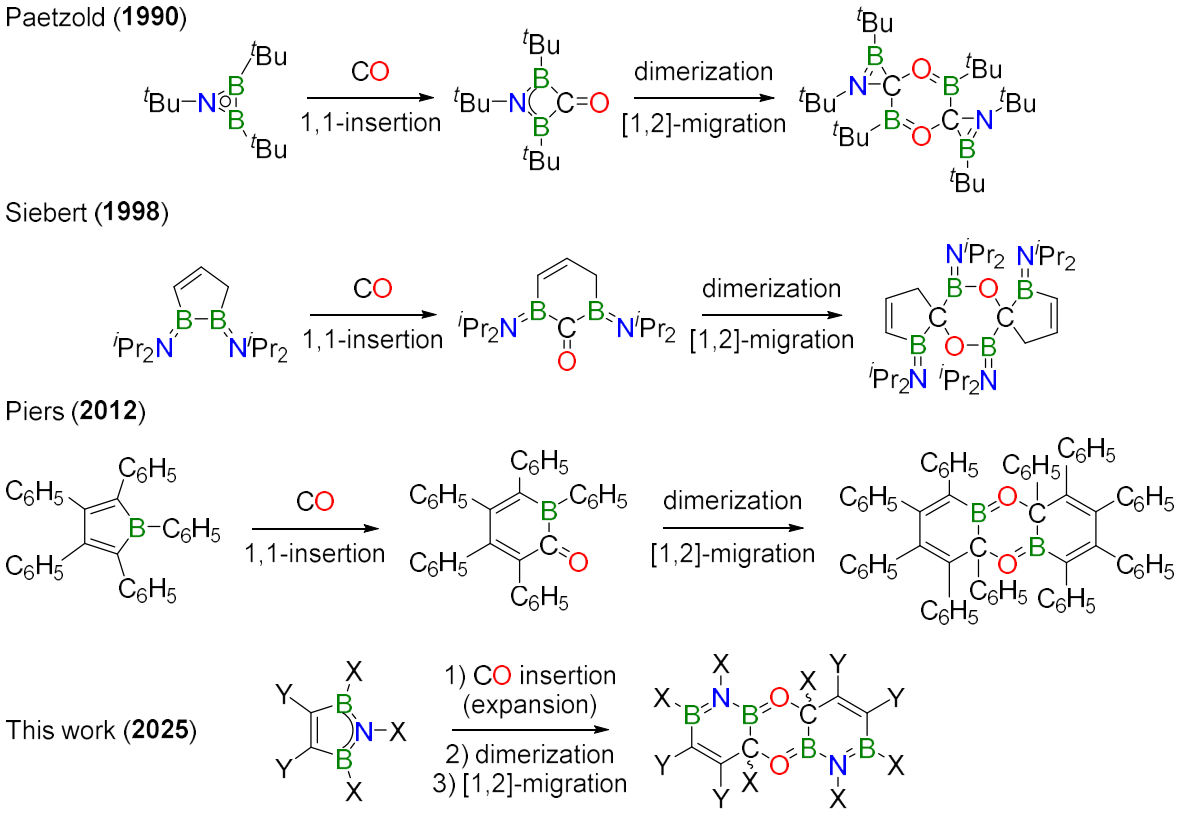


Chart 1.2. CO insertion-induced ring expansion reactions in boracycles.

Within this landscape, ring expansion reactions in boracycles constitute a powerful subclass, enabling access to structurally diverse and electronically tuneable organoboron architectures (**Chart 1.2**). Early work by Paetzold and Boese showed that a *tert*-butyl-substituted azadiboriridine (NB_2R_3) undergoes 1,1-insertion with carbon monoxide (CO), followed by dimerization and a [1,2]-migration to afford a six-membered diboroxan

heterocycle.[28] Siebert subsequently provided mechanistic insights into a related boron-mediated ring expansion via CO insertion, dimerization, and rearrangement.[29] More recently, Piers and co-workers expanded the synthetic utility of such transformations by developing transition-metal-free ring expansion of boroles, yielding larger boracycles with improved stability and applications in materials chemistry.[30]

Given that borole and 1,2,5-azadiborolidine share analogous structural and electronic features, they can be viewed as isosteres. We thus envisaged that azadiborolidines might exhibit similar reactivity toward CO insertion, ring expansion, or dimerization. Frontier molecular orbitals (particularly the LUMO centred on boron) could likewise behave analogously in electrophilic or π-system reactions, as shown for boroles. However, early experimental studies revealed different reactivity for azadiborolidines due to adjacent electron-deficient boron centres and a lone pair-bearing nitrogen.[31–35]

Recent work highlights azadiborolidines as tuneable reactivity platforms: Brown[36] and Hu and Cui[37] showed strategic functionalization to modulate their reactivity with small molecules like CO, enabling ring-expanded heterocycles and synthetically relevant boron–heteroatom linkages. These transformations underscore the flexibility of the B–N–B core as both a structural and reactive unit.

Beyond small-molecule activation, azadiborolidines and related BN-heterocycles exhibit promising electronic and optical properties. Studies by Wu, Zeng and co-workers[38] and Narita and Müllen[39] explain how N–B incorporation into π-conjugated systems influences aromaticity, stability, and electronic delocalization, highlighting their potential in organic electronic and optoelectronic applications. The polar N–B bond facilitates fine-tuning of HOMO–LUMO gaps while maintaining planarity and delocalization essential for conjugated systems.

Herein, we employed Density Functional Theory (DFT) to investigate the viability of CO-induced ring expansion reactions in 1,2,5-azadiborolidine, specifically addressing substituent effects. Given that borole and 1,2,5-azadiborolidine rings are isoelectronic compounds, and in principle, isosteres, it is hypothesised that they exhibit similar reactivity towards CO-promoted ring expansion. Hence, the main objective of this study is to predict the CO insertion reaction in any of the 1,2,5-azadiborolidine derivatives already reported experimentally. As secondary objectives, the research seeks to identify reactivity descriptors capable of predicting and explaining such reactivity.

1.3. Computational Methods

DFT calculations were performed using Gaussian 09.[40] The long-range hybrid functional ωB97X-D was employed with the Ahlrichs split-valence def2-SVP basis set for all atoms.[41,42] Geometry optimizations were conducted in the gas phase without constraints and assuming singlet electronic configurations. Initial coordinates were extracted from crystallographic data where available. Harmonic frequency calculations characterized stationary points. Thermal corrections to Gibbs free energy were obtained under the ideal gas approximation at 298.15 K and 1 atm. Electronic energies were refined via single-point calculations using the def2-TZVPP basis set.[42] Solvent effects were incorporated via the polarizable continuum model (PCM) with SMD parameters, using dichloromethane (DCM), *n*-pentane, and tetrahydrofuran (THF) as representative solvents common in the synthesis of such molecules.[43] Gibbs free energies thus correspond to the ωB97X-D/def2-TZVPP//ωB97X-D/def2-SVP level. This approach provides an effective balance between accuracy and computational cost.[44,45]

The global electrophilicity index (ω),[46] defined as $\omega = \mu^2/2\eta$, where μ is the chemical potential and η hardness, serves as a reactivity descriptor. Within the ground-state parabolic model, μ and η were approximated using the vertical ionization potential (I) and electron affinity (A), yielding $\omega = (I+A)^2/8(I-A)$. Applying Pearson[47] and using Koopmans' theorem,[48] I and A can be approximated as the negative values of the HOMO and LUMO energies, ε_{HOMO} and ε_{LUMO}, respectively. This leads to the working equation: $\omega = (\varepsilon_{HOMO}+\varepsilon_{LUMO})^2/8(\varepsilon_{LUMO}-\varepsilon_{HOMO})$. Though strictly valid for Hartree-Fock theory, the utility of this approximation in conceptual DFT is well-established.[49–52] Frontier orbital energies were computed at the gas-phase single-point refinement level.

Geometrical descriptors, specifically the molecular planarity parameter (MPP) and the span of deviation from planarity (SDP),[53] were calculated for the starting heterocycles. Additionally, steric hindrance was evaluated by calculating buried volumes ($\%V_{Bur}$) and generating steric maps using SambVca 2.1.[54–57]

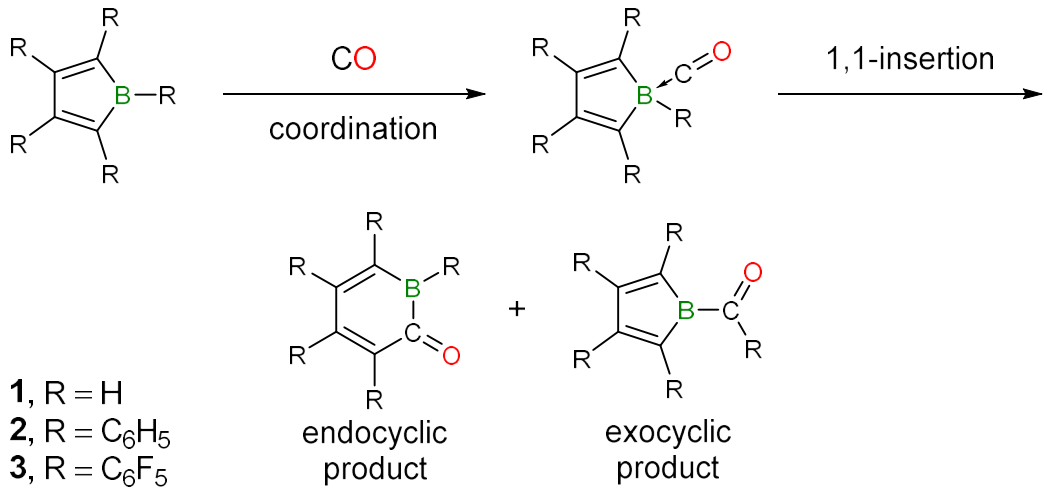
Further wavefunction analysis used NBO and Multiwfn software.[58,59] The multicentre index (MCI) was computed within the natural atomic orbital (NAO) framework,[60–63] while π-backbonding interactions were quantified via second-order perturbation theory analysis of the Fock matrix in the NBO basis. Due to the delocalized nature of these interactions, diffusion functions were essential, and analyses were therefore performed at the ωB97X-D/def2-TZVPPD level on optimized gas-phase geometries.[64]

1.4. Results and Discussion

1.4.1. CO-induced ring expansion reactions in boroles.

We initially explored the ring expansion reactivity of borole derivatives with CO, focusing on the parent borole (**1**), pentaphenylborole (**2**), and perfluoropentaphenylborole (**3**). Compounds **2** and **3** were previously studied experimentally by Piers and co-workers,[30] providing a benchmark to assess electronic and steric effects on the thermodynamics and kinetics of CO-mediated ring expansion. These boroles were later compared with 1,2,5-azadiborolidines to quantify energetic requirements for analogous pathways.

The proposed mechanism comprises two key steps (**Scheme 1.1**). First, the formation of Lewis adducts through CO coordination to boron, followed by 1,1-insertion of CO via *endocyclic* (ring B–C bond) or *exocyclic* (exterior B–C bond) pathways.



Scheme 1.1. A plausible reaction mechanism for the CO insertion to borole (R = –H, $–C_6H_5$, $–C_6F_5$). The endocyclic product refers to the ring expansion reaction.

As shown in **Figure 1.1**, CO coordination is spontaneous for all the boroles ($\Delta G_{R\rightarrow I\text{-}1}$) with low energy barriers ($\Delta G^{\ddagger}_{R\rightarrow TS\text{-}1}$). However, substituents reduce the exergonic character: electron-withdrawing (EW) groups (e.g., R = $–C_6F_5$) favour Lewis adduct formation thermodynamically over electron-donating (ED) groups (e.g., R = $–C_6H_5$). Nevertheless, neither EW nor ED groups universally lower the energy cost of this step. The energetic analysis indicates reversible CO coordination for **2** ($\Delta G_{R\rightarrow I\text{-}1}$ = –1.8 kcal mol^{-1}) and **3** ($\Delta G_{R\rightarrow I\text{-}1}$ = –5.4 kcal mol^{-1}), aligning with experimental findings.[30]

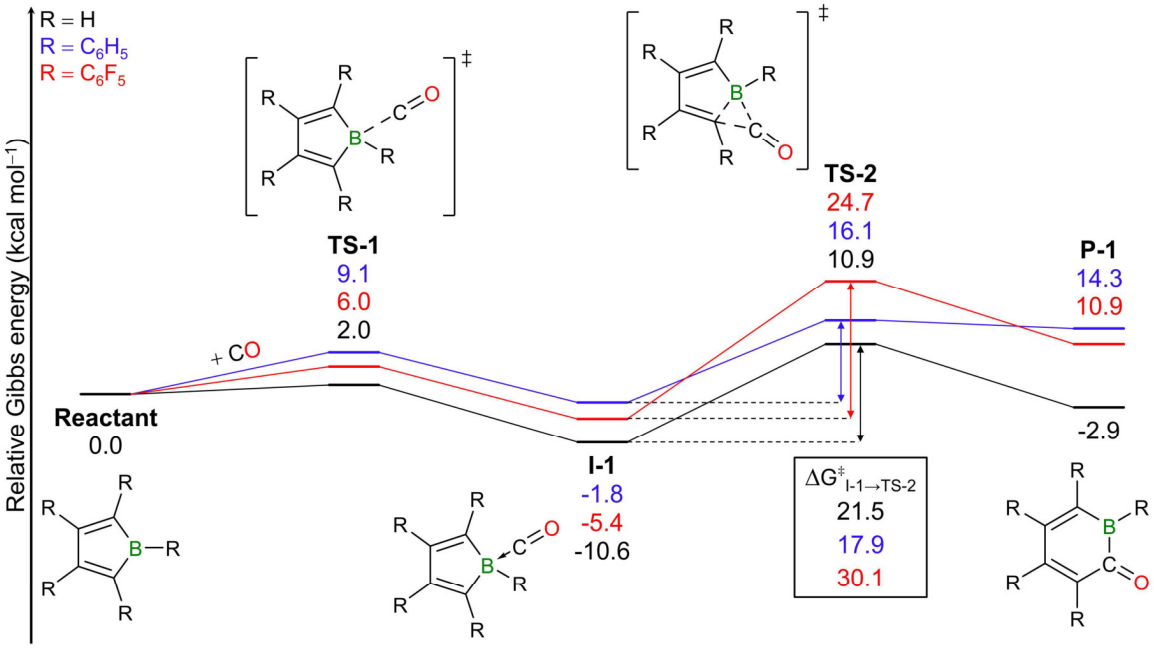


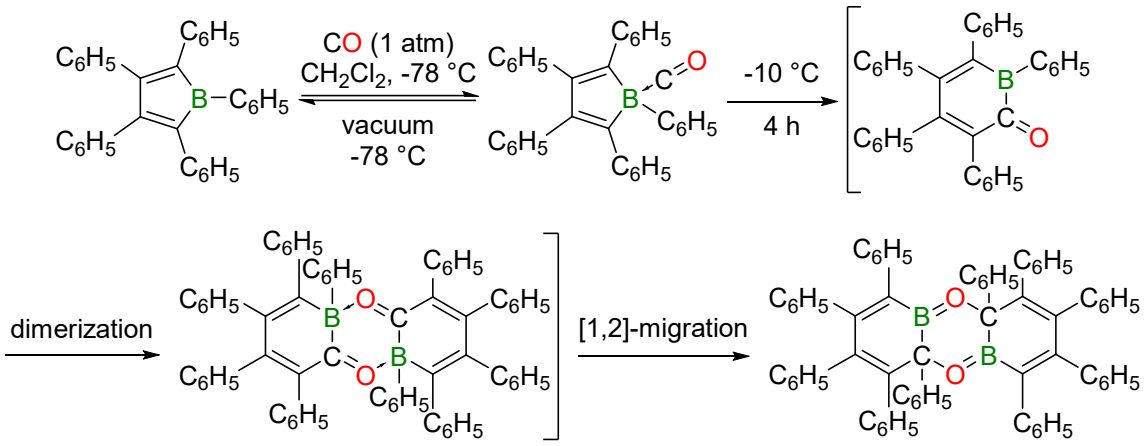
Figure 1.1. Relative Gibbs free energy profiles for the ring expansion reaction of selected borole derivatives with CO. Gas-phase energy values (kcal mol^{-1}) were calculated at the ωB97X-D/def2-TZVPP//ωB97X-D/def2-SVP level.

Subsequent CO insertion barriers ($\Delta G^{\ddagger}_{I\text{-}1\rightarrow TS\text{-}2}$) are 21.5 (**1**), 17.9 (**2**), and 30.1 (**3**) kcal mol^{-1}. Note that the endocyclic insertion is kinetically feasible at room temperature for **1** and **2**, though only **1** affords a thermodynamically stable product ($\Delta G_{R\rightarrow P\text{-}1}$ = –2.9 kcal mol^{-1}). Crucially, ED groups significantly reduce the insertion barrier in comparison to EW groups, highlighting substituent effects: EW groups facilitate CO coordination, while ED groups promote the insertion. Steric modulation likely also contributes.[65] Exocyclic pathways exhibit higher barriers and endergonic profiles (Figure S1).

Regarding reactivity, the ω values are 1.519 (**1**), 1.446 (**2**), and 2.479 (**3**) eV. The trend **2** < **1** < **3** correlates with the insertion barrier heights ($\Delta G^{\ddagger}_{I\text{-}1\rightarrow TS\text{-}2}$), suggesting electrophilicity critically influences kinetics beyond steric/electronic effects. Notably, global electrophilicity appears to play a key role in determining the kinetic accessibility of the insertion step.

These computational findings align with experimental results reported by Piers and co-workers.[30] Compound **2** forms the Lewis adduct **I-1** in CH_2Cl_2 at –78 °C. Upon warming to –10 °C, NMR spectroscopy reveals primarily the dimerized ring-expansion product rather than the monomer (**Chart 1.3a**). The absence of a monomer agrees with thermochemical data

(a) Reaction scheme for the dimerization process after the ring expansion of **2**.



(b) Reversible formation of the Lewis adduct when **3** is used.

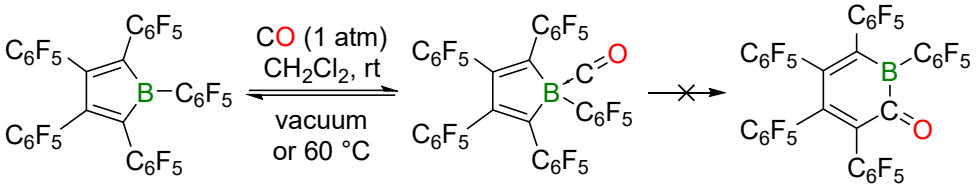


Chart 1.3. Experimental evidence for the CO insertion reactions of **2** and **3**.

identifying the ring-expansion intermediate as unstable ($\Delta G_{R\rightarrow P\text{-}1}$ = 14.3 kcal mol^{-1}). For **3**, the Lewis adduct is well-characterized by X-ray crystallography (CCDC Number: 863188), yet no insertion product is formed even at high temperatures (**Chart 1.3b**), consistent with the high energy barrier for the endocyclic CO insertion ($\Delta G^{\ddagger}_{I\text{-}1\rightarrow TS\text{-}2}$ = 30.1 kcal mol^{-1}). In contrast, while experimental data for **1** remain unavailable, our results suggest its ring expansion is feasible under appropriate thermal control. Moreover, these results show excellent agreement with the energy profiles of Lin, including dimerization pathways and solvent effects.[65]

1.4.2. Building bridges: isosterism between borole and 1,2,5-azadiborolidine.

Given the shared central heterocyclic framework of boroles **1**–**3**, we focus on **1** for detailed discussion. Note that 1,2,5-azadiborolidine (**4**) exhibits structural similarity to borole, theoretically derived by replacing a C=C double bond with an isoelectronic N=B double bond adjacent to the ring boron atom. This substitution, termed as heteroatom doping, is a well-

established strategy for tuning electronic properties,[66–71] primarily altering the electronic structure of the ring and related features.

As shown in **Figure 1.2**, both **1** and **4** adopt C_{2v} symmetry and $^1A_1$ singlet ground state. Their adiabatic singlet-triplet energy gaps, ΔE_{ST} = 20.9 (**1**) and 51.0 (**4**) kcal mol^{-1}, confirming the singlet as the ground state for both cases. As 4π-electron systems, they display antiaromatic character, as evidenced by their low multicentre indices (MCI).[72–74] Notably, **4** shows greater electronic delocalization across the ring, reflected in its higher MCI value relative to **1**. This enhanced delocalization in **4** correlates with a lower global electrophilicity index, indicating a reduced electrophilic character compared to **1**. MCI analysis of the lowest-lying triplet states (C_{2v}, $^3B_2$) reveals increased delocalization in both molecules, in agreement with Baird's rule, which predicts aromaticity in triplet-state 4π-systems.[75–77] Accordingly, while **1** is more antiaromatic in the singlet state, it becomes more aromatic than **4** in the triplet state. This shift in aromatic character helps to explain the significantly lower ΔE_{ST} observed in **1**, as aromatic stabilization in the triplet state contributes to its energetic favourability.[78,79]

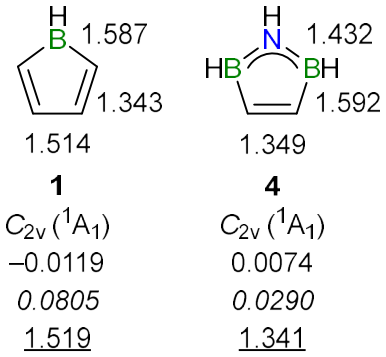


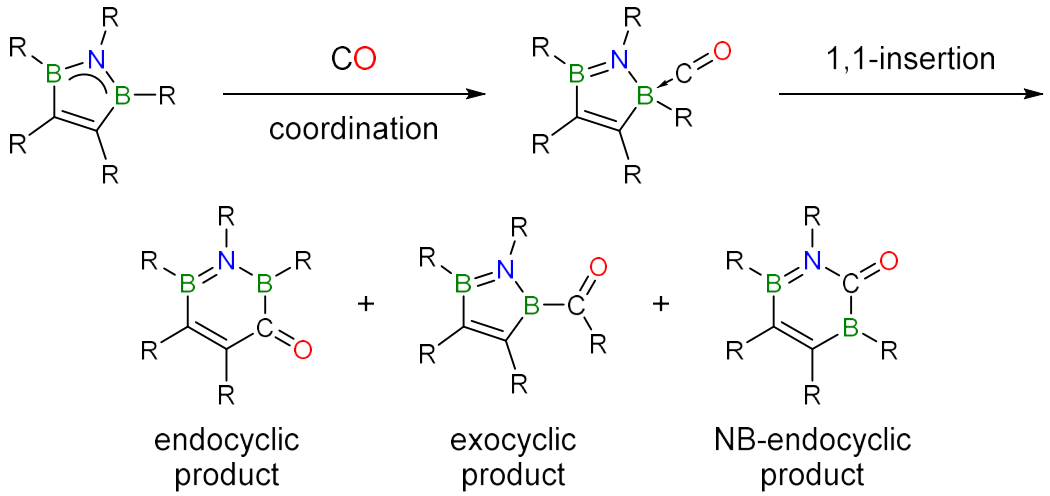
Figure 1.2. Comparison of structural, symmetric, reactivity, and electronic features between borole and 1,2,5-azadiborolidine. Bond lengths are expressed in Å, singlet- and triplet-state (italics) MCI values in electrons, and global electrophilicity (underline) in eV.

Geometric analysis reveals similar B–C (1.587–1.592 Å) and C=C (1.343–1.349 Å) bond lengths in compounds **1** and **4**. In 1,2,5-azadiborolidine, the N–B bonds are fully equalized, with bond length (1.432 Å) closely matching borazine values from X-ray crystallography (1.429 Å,[80] and 1.427–1.429 Å[81]). This supports a borazine-like bonding structure in the B–N–B fragment, consistent with Yáñez's computational studies,[82] indicating nitrogen lone-pair delocalization over the B–N–B moiety as the optimal Lewis representation (**Figure 1.2**).

Frontier molecular orbital analysis (Figure S2) reveals a key distinction: while HOMOs and LUMOs of **1** and **4** share identical symmetry, shape, and comparable energies, their ordering is reversed, **1**-HOMO resembles **4**-LUMO, and *vice versa*. Consequently, these systems are not isolobal; however, they constitute isosteres under current IUPAC definitions.[83,84]

1.4.3. Towards CO insertion into 1,2,5-azadiborolidines.

Despite lacking isolobal equivalence, the isosteric properties shared between borole and 1,2,5-azadiborolidine suggest analogous reactivity. Therefore, we examined the two-step CO reaction mechanism (coordination followed by 1,1-insertion) for **4**. Given asymmetric endocyclic bonds adjacent to boron (N–B *vs.* B–C), we evaluated insertion at the N–B bond—termed NB-endocyclic insertion (**Scheme 1.2**).



Scheme 1.2. A plausible reaction mechanism between 1,2,5-azadiborolidine derivatives and CO. The endocyclic products refer to the ring expansion reaction.

We used previously synthesized azadiborolidines as starting materials (**Chart 1.4**). Haubold and co-workers reported the first synthesis in 1980 (1,2,3,4,5-pentamethyl derivative **5**),[31] followed months later by Siebert's 3,4-diethyl-1,2,5-trimethyl-1,2,5-azadiborolidine (**6**).[32] Köster and co-workers advanced the field in 1994 by introducing trimethylsilyl substituents (e.g., **7**).[34] Paetzold's pioneering work on azadiboriridine reactivity subsequently enabled derivatives 1,2,5-tri-*tert*-butyl-1,2,5-azadiborolidine (**8**) and

1,2,5-tri-*tert*-butyl-3,4-dimethyl-1,2,5-azadiborolidine (**9**).[33,35] These compounds have only been characterized by NMR and MS to date.

Hypothetical pentaphenyl (**10**) and fluorinated pentaphenyl (**11**) analogues, designed by similarity to boroles **2** and **3**, were also computationally examined. Conversely, compounds **12**–**15** have been structurally authenticated: **12** by Müllen (CCDC Number: 1412367);[39] dianion $\mathbf{13}^{2-}$ by Zeng (CCDC Number: 1555140);[38] **14** by Cui (CCDC Number: 2045630),[37] and **15** by Lindley (CCDC Number: 2122486).[36] Beyond these, only the 1,2,5-azadiborolidines by Piers, in 2004, and Li, in 2020, have been reported.[85,86]

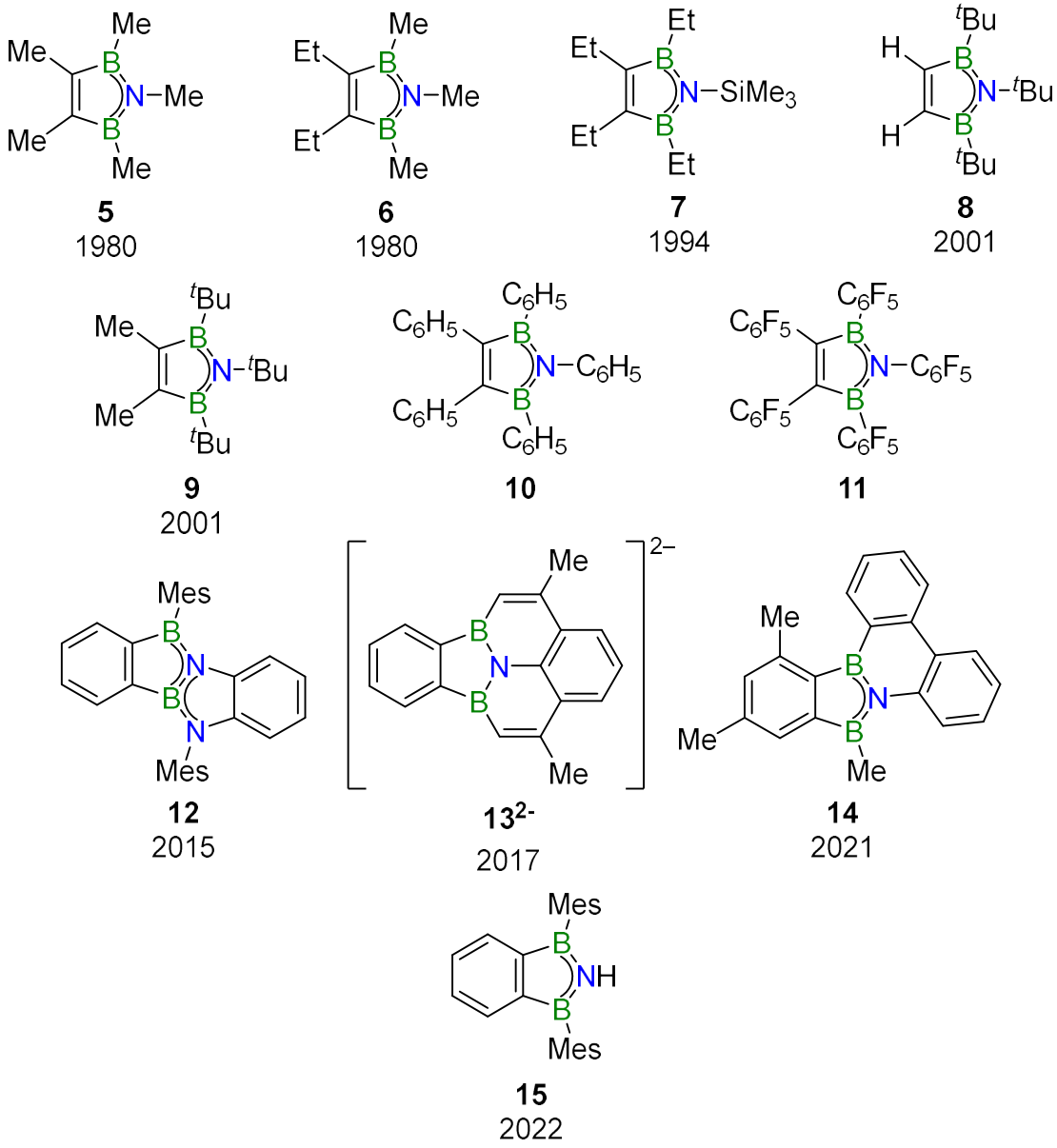
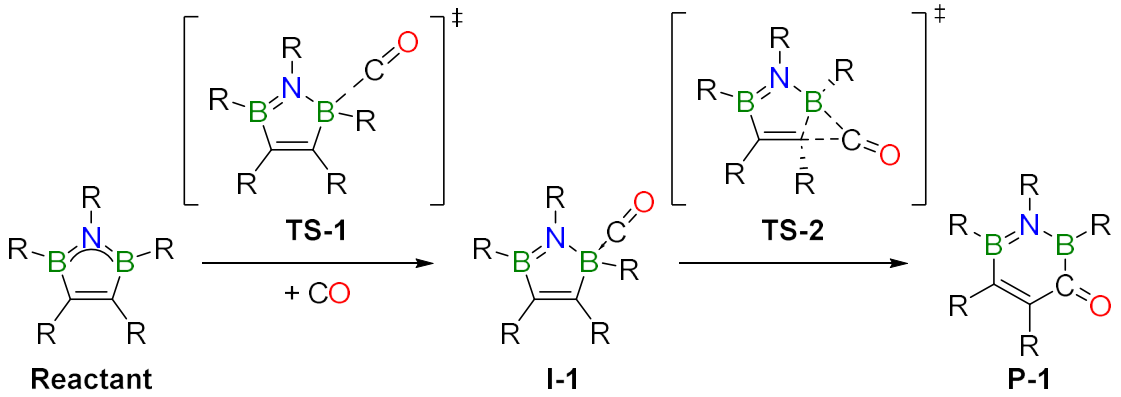


Chart 1.4. Overview of synthesized 1,2,5-azadiborolidine derivatives used in this work.

Table 1.1. Relative Gibbs energy values (kcal mol^{-1}), calculated at the ωB97X-D/def2-TZVPP//ωB97X-D/def2-SVP level of theory in gas-phase, for the ring expansion reaction between different 1,2,5-azadiborolidine derivatives and CO.



Entry	Reactant	TS-1	I-1	TS-2	P-1
1	**8**	15.2	11.2	23.9	11.4
2	**9**	17.4	14.2	26.8	11.0
3	**4**	11.8	8.2	30.0	0.1
4	**7**	15.1	12.3	30.5	7.1
5	**10**	15.9	13.7	31.9	13.9
6	**5**	16.4	15.9	33.8	4.7
7	**6**	16.3	15.7	34.9	5.2
8	**15**	22.5	21.6	37.5	4.8
9	**12**	22.0	21.4	37.8	–0.4
10	**14**	14.8	14.2	39.2	6.6
11	**11**	12.4	10.1	41.1	12.3
12	**13**	22.4	22.1	45.9	1.3

Given experimental confirmation that borole **2** undergoes ring expansion while **3** does not, we now evaluate CO insertion feasibility in 1,2,5-azadiborolidines using previously derived kinetic and thermodynamic profiles.

In contrast to boroles **2** and **3**, CO coordination for 1,2,5-azadiborolidine derivatives is endergonic, exhibiting higher energy barriers in all cases (**Table 1.1**). The rate-determining step remains ring expansion (**R→TS-2**), yet the reaction Gibbs energy ($\Delta G_{R\rightarrow P\text{-}1}$) is consistently lower than for borole **2** ($\Delta G_{R\rightarrow P\text{-}1}$ = 14.3 kcal mol^{-1}). This indicates thermodynamic favourability upon replacing borole with a 1,2,5-azadiborolidine unit. For

instance, compounds **4**, **12**, and **13** show $\Delta G_{R\rightarrow P\text{-}1}$ values near equilibrium (0.1, –0.4, and 1.3 kcal mol^{-1}, respectively). Kinetically, however, endocyclic CO insertion faces higher barriers than **2**. Particularly, heterocycles **8** and **9** show barriers ($\Delta G^{\ddagger}_{R\rightarrow TS\text{-}2}$ = 23.9 and 26.8 kcal mol^{-1}, respectively) exceeding **2** but below **3**, suggesting ring expansion at increased temperatures or extended reaction times. In contrast, **4** and **7** exhibit barriers near 30.0 kcal mol^{-1}, rendering ring expansion unlikely under standard conditions. The remaining derivatives (entries 5–12) display even higher barriers ($\Delta G^{\ddagger}_{R\rightarrow TS\text{-}2}$ > 30.1 kcal mol^{-1}), substantially diminishing the prospect of CO insertion under experimental conditions.

Exocyclic insertion is noncompetitive for **5**–**7**, **11**–**12**, and **15**, yet yields the kinetic product for **4** and **13**–**14** (Table S1). Conversely, it affords the thermodynamic product for **8**–**10**. NB-endocyclic insertion, tested representatively for **4**, **5**, **8**, and **10**, proved noncompetitive (Table S2), likely due to cleavage of the delocalized B–N–B bond during insertion, which compromises ring stability. This underscores the greater strength of the N–B bond relative to the inherently labile B–C bond in boroles.[87,88]

The electron-rich nitrogen and electron-deficient boron in 1,2,5-azadiborolidine advise plausible dimerization. Calculations for all derivatives (Figure S3), except **12**–**15** (whose X-ray structures preclude dimerization), reveal favourable dimerization only for **4**. For **5**, the reaction Gibbs energy (5.9 kcal mol^{-1}) and barrier (17.1 kcal mol^{-1}) align with experimental detection of only trace dimer by NMR.[31] Increasing substituent size elevates both energy and barrier, confirming high steric sensitivity.

1.4.4. Statistical analysis of geometrical and reactivity descriptors.

Across the examined 1,2,5-azadiborolidines (**Chart 1.4**), optimized geometries reveal an average N–B bond length of 1.446 Å (σ = 0.009 Å). Despite lost bond equalization in the B–N–B moiety, N–B lengths remain borazine-like, supporting similar electronic character. Notice that most rings are planar, except **8**, **9**, and **14**, as revealed by large MPP and SDP values (Table S3); their out-of-plane distortions relieve steric strain from bulky substituents (e.g., *tert*-butyl groups in **8** and **9**). For adduct **I-1**, average B–C(O) and C–O bond lengths are 1.622 Å (σ = 0.043 Å) and 1.129 Å (σ = 0.003 Å), respectively (Table S4).

A systematic analysis quantified key thermochemical correlations across azadiborolidine and borole derivatives (**Figure 1.3**). The strongest correlation (R^2 = 0.9544) was found between the energy barrier for CO coordination ($\Delta G^{\ddagger}_{R\rightarrow TS\text{-}1}$) and its reaction Gibbs energy ($\Delta G_{R\rightarrow I\text{-}1}$), yielding a Brønsted-Evans-Polanyi (BEP) equation.[89–94] A secondary

correlation ($R^2 = 0.8487$) was found between ring expansion barrier and B–C(O) bond length. Second-order perturbation analysis of **I-1** quantified π-backbonding-like energy (stabilization from donor→π*(CO) interactions). Total energetic stabilization performed by the two endocyclic σ-MOs related to the boron centre reveals a significant correlation with B–C(O) bond length ($R^2 = 0.8491$) and with the total barrier ($R^2 = 0.8539$). Notably, using average π-backbonding energy (cf. Piers et al.[30]) substantially reduced correlation coefficients (Figure S4). We thus recommend employing *total* (not average) π-backbonding energy for future studies of such adducts.

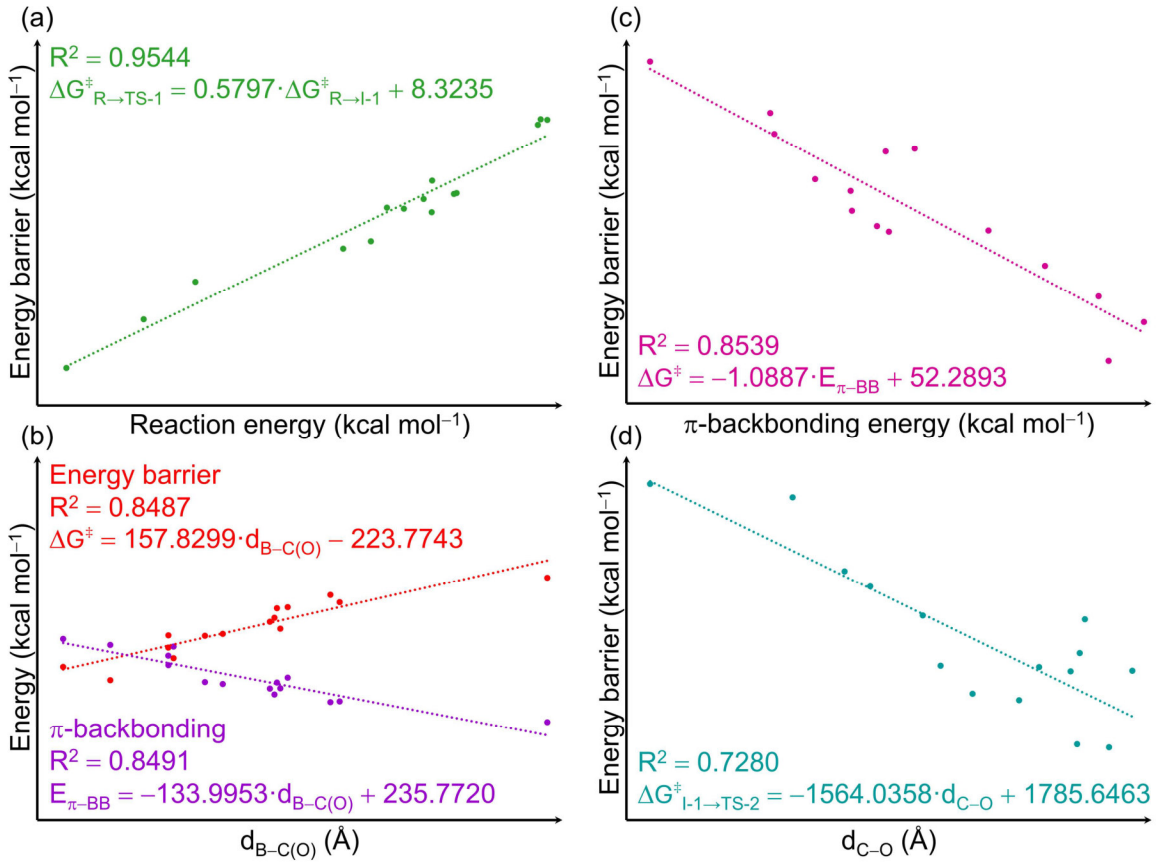


Figure 1.3. Analysis of linear correlations from gas-phase thermochemistry data for the endocyclic CO insertion among compounds **1**–**15**. (a) Energy barrier and reaction energy of the CO coordination step. (b) Total energy barrier (in red) and π-backbonding energy (in purple) related to the B–C(O) bond length. (c) Total energy barrier and π-backbonding energy. (d) Energy barrier of the second reaction step and the C–O bond length. The π-backbonding energy and the B–C(O) and C–O bond lengths were calculated for adduct **I-1**.

A moderate correlation was found between the CO insertion barrier ($\Delta G^{\ddagger}_{I\text{-}1\rightarrow TS\text{-}2}$) and the C–O bond length ($R^2 = 0.7280$). However, no meaningful correlations emerged between C–O bond length and either the B–C(O) bond length or π-backbonding energy. A weak correlation was also noted between ω and the ring expansion barrier ($R^2 = 0.6950$, Figure S4c). This trend contradicts Parr's principle, which states that higher ω values correspond to greater electron-accepting ability and, therefore, higher reactivity.[46] Piers previously identified this apparent *paradox*,[30] suggesting that the dependency of π-backbonding stabilization on the initial electrophilicity of the ring may explain it. However, our computations indicate that the correlation between ω and π-backbonding is negligible (Figure S4d), and weaker than those shown in **Figure 1.3**. Complete π-backbonding and electrophilicity data are provided in Tables S3–S5.

Additional insights were obtained from the analysis of the steric environment in **I-1** (Figure S5). First, steric hindrance remains largely unchanged upon replacing borole ring with a 1,2,5-azadiborolidine core. Second, $\%V_{Bur}$ is more sensitive to the substituent size at positions 1, 2, and 5 than at positions 3 and 4 of the heterocycle. Third, substitution of hydrogen with fluorine significantly increases the $\%V_{Bur}$. Although fluorination is often employed to enhance ring electrophilicity, it may also compromise the steric environment of the Lewis adduct. Nonetheless, neither the planarity of the starting ring (e.g., MPP and SDP indices) nor the steric hindrance (e.g., $\%V_{Bur}$ values) in **I-1** were found to be significant predictors of the thermochemistry of the CO-induced ring-expansion reaction.

1.4.5. Complete energy profile for the most suitable preliminary candidate.

Given that the experimental final product of borole **2** is its dimer rather than the ring-expanded monomer (**Chart 1.3a**), we explored the dimerization energy profile for 1,2,5-azadiborolidine derivatives. Focusing on **8**, the most promising candidate based on ring expansion energetics, we calculated the extended profile (**Figure 1.4**). Following CO-induced ring expansion of **8** (**R→P-1**), viable dimerization (**P-1→I-2**) occurs, succeeded by double [1,2]-migration of boron substituents (**I-2→P-2**). Here, **P-1** is the kinetic while **P-2** is the thermodynamic product. Dimerization proceeds concertedly through **TS-3**, aligning with product hierarchy of borole **2**[30] but differing mechanistically: **8** dimerizes concertedly, whereas **2** follows stepwise pathways.[65] The transformation is highly exergonic ($\Delta G_{R\rightarrow P\text{-}2}$ = –62.2 kcal mol^{-1}) with a thermally accessible total barrier ($\Delta G_{R\rightarrow TS\text{-}3}$ = 25.3 kcal mol^{-1}).

To better approximate experimental conditions (where 1,2,5-azadiborolidine syntheses typically employ DCM, *n*-pentane, or THF), we analysed solvent effects. For

compound **8**, the energetic impact is most pronounced during 1,1-endocyclic CO insertion (**R→P-1**). The barrier $\Delta G^{\ddagger}_{R\rightarrow TS\text{-}2}$ decreases from 23.9 kcal mol^{-1} (gas-phase) to 19.0 kcal mol^{-1} in THF, while $\Delta G_{R\rightarrow P\text{-}1}$ drops from 11.4 kcal mol^{-1} to 4.8 kcal mol^{-1} in DCM. Thus, THF optimally lowers the kinetic barrier, whereas DCM provides superior thermodynamic stabilization. For the full profile, dimerization of expanded ring **P-1** remains rate-determining. The barrier $\Delta G^{\ddagger}_{R\rightarrow TS\text{-}3}$ is consistent across solvent environments: 25.9 (THF), 25.4 (DCM), 25.3 (gas), and 25.3 kcal mol^{-1} (*n*-pentane). Though solvents slightly destabilize the overall reaction ($\Delta G_{R\rightarrow P\text{-}2}$ = –60.6 to –62.2 kcal mol^{-1}) deviations are minimal. *n*-Pentane emerges as optimal, combining the lowest barrier with favourable thermodynamics.

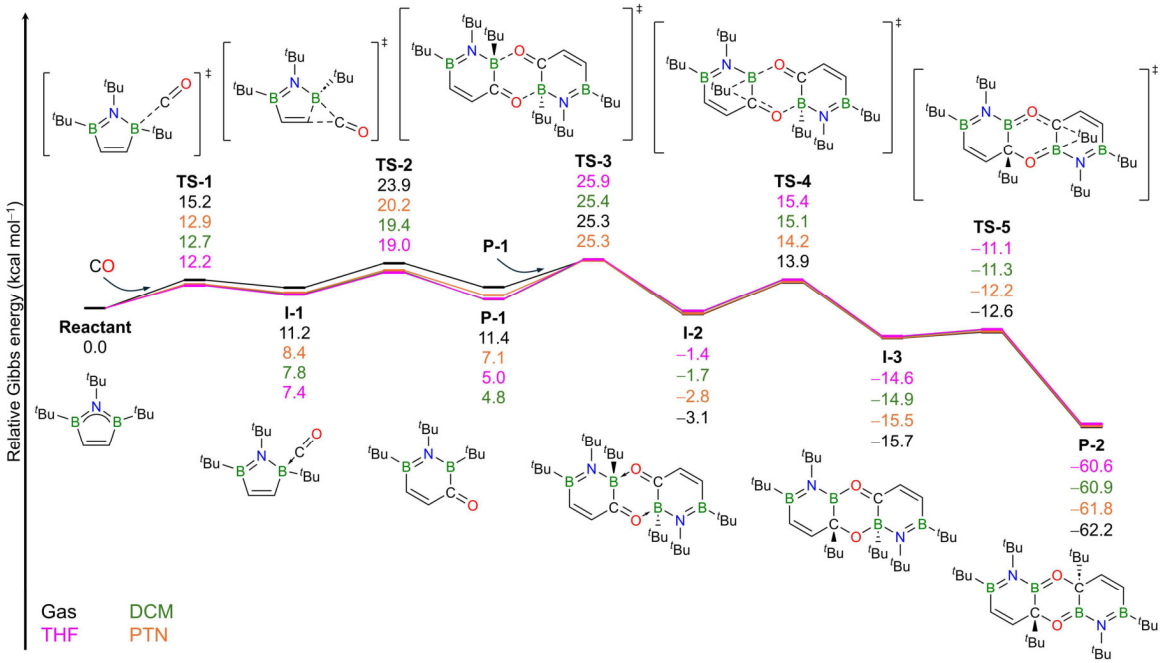


Figure 1.4. Relative Gibbs free energy profile for the ring expansion of **8** with CO, followed by a dimerization process and a subsequent [1,2]-migration of the central *tert*-butyl substituents. Energy values (kcal mol^{-1}) were calculated at the ωB97X-D/def2-TZVPP//ωB97X-D/def2-SVP level in gas-phase and three solvents: dichloromethane (DCM), *n*-pentane (PTN), and tetrahydrofuran (THF).

1.4.6. A comparative study with other DFT protocols.

The number of coordination complexes between boron and CO that have been isolated and well characterized is limited. A seminal example is the work reported by Willner and

Oberhammer in 2002.[95] In this study, the single-crystal (**Figure 1.5**) of the Lewis adduct $(CF_3)_3B–C(O)$ (**16**) and the kinetics of the CO coordination process were elucidated. The similarity of the atoms that constitute **16**, in conjunction with the same coordination process discussed throughout our study, provides a rigorous frame of reference for evaluating the quality of the computational method employed herein.

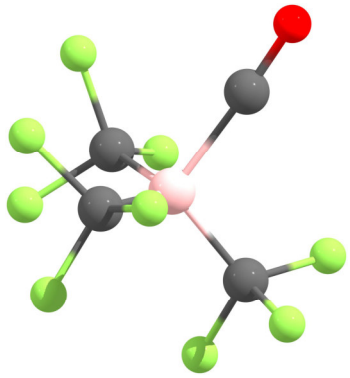


Figure 1.5. Molecular structure of tris(trifluoromethyl)borane carbonyl (**16**) obtained from X-ray crystallographic data (CCDC Number: 201824).

Firstly, compound **16**, contrary to the previously discussed findings, is not synthesized by direct coordination of CO. Instead, it is produced by the solvolysis of the salt $K[B(CF_3)_4]$ in concentrated sulfuric acid. The point group symmetry of **16** is C_3, which deviates slightly from the C_{3v} group due to a rotation in the trifluoromethyl ($–CF_3$) fragments. The B–C(O) and C–O bond lengths are 1.69 Å and 1.11 Å in solid state, whereas 1.617 Å and 1.124 Å in gas phase, respectively. It was established that, at room temperature, the complex compound in question exists as a colourless liquid and as a vapor, with a decomposition half-time of 45 minutes. In the presence of ^{13}CO, the carbonyl group exchange occurs via a ligand association/dissociation equilibrium, which follows a temperature-dependent first-order rate law. The latter feature facilitated the determination of the activation energy (26.8 kcal mol^{-1}) associated to the CO dissociation process in gas-phase. Moreover, DFT computations at the B3LYP/6-31G(d) level indicate that the activation energy is nearly identical to the B–C(O) bond energy.[95] Consequently, the activation energy can be estimated by considering the corresponding reaction energy.

In this regard, the previously used methodology (see **Section 1.3**) was applied to study relevant properties of compound **16**. The results obtained were compared with those already

reported as a benchmark. An examination of the gas-phase geometry of **16** at ωB97X-D/def2-SVP level revealed lengths of 1.593 Å and 1.119 Å for B–C(O) and C–O bonds, respectively. The deviations are 0.024 Å and 0.005 Å compared to the experimental data. The gas-phase reaction energy of the CO dissociation process was calculated to be 27.1 kcal mol^{-1} (**Table 1.2**). This amount represents a modest improvement over the previously calculated value of 27.3 kcal mol^{-1} obtained at B3LYP/6-31G(d) level. Furthermore, following the reaction pathway through a relaxed scan of the potential energy surface (PES) along the B–C(O) length in **16**, the presence of a transition state was not observed in gas phase (**Figure 1.6**). This finding supports the statement of the similarity between the activation and reaction energies.

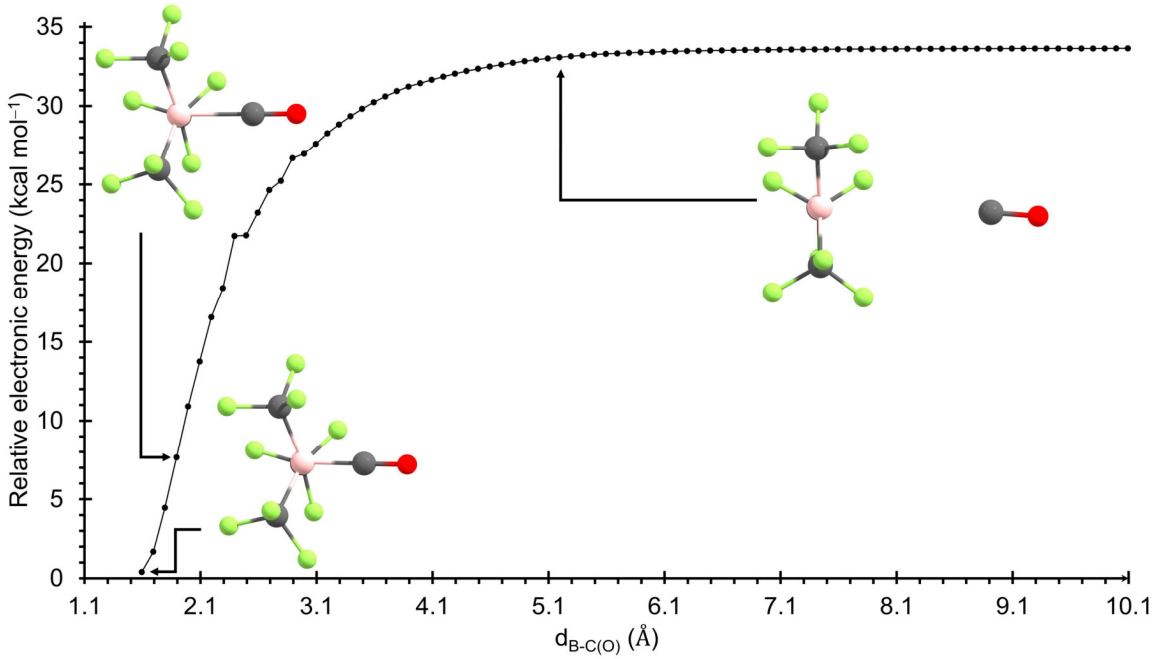


Figure 1.6. Relaxed PES scan over the B–C(O) length in **16**. Energy values (kcal mol^{-1}) were calculated at the ωB97X-D/def2-SVP level in gas-phase.

The computation of the B–C(O) and C–O bond lengths, in conjunction with the reaction energy related to the CO dissociation process, were performed again. This time, we used the hybrid functional M06-2X as well as ωB97X-D together with Ahlrichs' and Pople's basis sets, as displayed in **Table 1.2**. M06-2X is a Minnesota functional, also popular and recommended for applications involving main-group thermochemistry and kinetics.[96] We also implemented Ahlrichs def2-TZVPP and Pople's basis sets such as 6-311+G(d,p) and 6-

311G(d,p), looking for a more accurate description employing a triple-ζ basis sets.[97,98] Diffusion functions were implemented given that the B–C(O) bond is relatively weak and there are π-backbonding-type interactions, as demonstrated previously (see **Section 1.4.4**).

Table 1.2. Comparative DFT study of relevant bond lengths and energies for **16**.

B–C(O) bond length (Å)	**M06-2X**	**ωB97X-D**	**Experimental[95]**
def2-SVP	1.611	1.593	1.617
def2-TZVPP	1.606	1.587	
6-311G(d,p)	1.605	1.589	
6-311+G(d,p)	1.609	1.592	
C–O bond length (Å)			
def2-SVP	1.114	1.119	1.124
def2-TZVPP	1.109	1.113	
6-311G(d,p)	1.111	1.115	
6-311+G(d,p)	1.111	1.114	
B–C(O) bond energy (kcal mol^{-1})			
def2-TZVPP/def2-SVP	28.9	27.1	26.8 ± 0.2
def2-TZVPP	29.0	27.2	
6-311G(d,p)	30.0	27.8	
6-311+G(d,p)	30.1	28.1	

It can be concluded that the M06-2X functional provides a more accurate reproduction of the B–C(O) bond length in the gas-phase. The def2-SVP basis set was the most effective in this regard, thereby indicating that the implementation of larger basis sets is not essential for the attainment of adequate geometries. On the other hand, ωB97X-D functional reproduces the C–O bond length in **16** with greater accuracy. Along the different basis sets used, the same observation is replicated: the simpler basis set def2-SVP exhibits a higher concordance with the known experimental bond lengths. From a thermochemical perspective, the discrepancy is more pronounced. M06-2X overestimates the energy value associated with CO dissociation by around 2–4 kcal mol^{-1}. Similarly, Pople's basis sets generate outcomes that overrate the reference value more than Ahlrichs' basis sets. It is emphasized that the measurement which corresponds most closely to the experimental energy

value is that calculated utilizing the DFT method used in this work (see **Section 1.3**). Hence, the analysis developed herein corroborates the quality of the thermochemical results discussed in preceding sections. Unfortunately, the relevant transition state regarding the CO dissociation process in **16** could not be characterized by any of the methods proposed. This makes computational characterization of the energy barrier difficult. Consequently, it is challenging to ascertain which level of theory best reproduces the reaction kinetics.

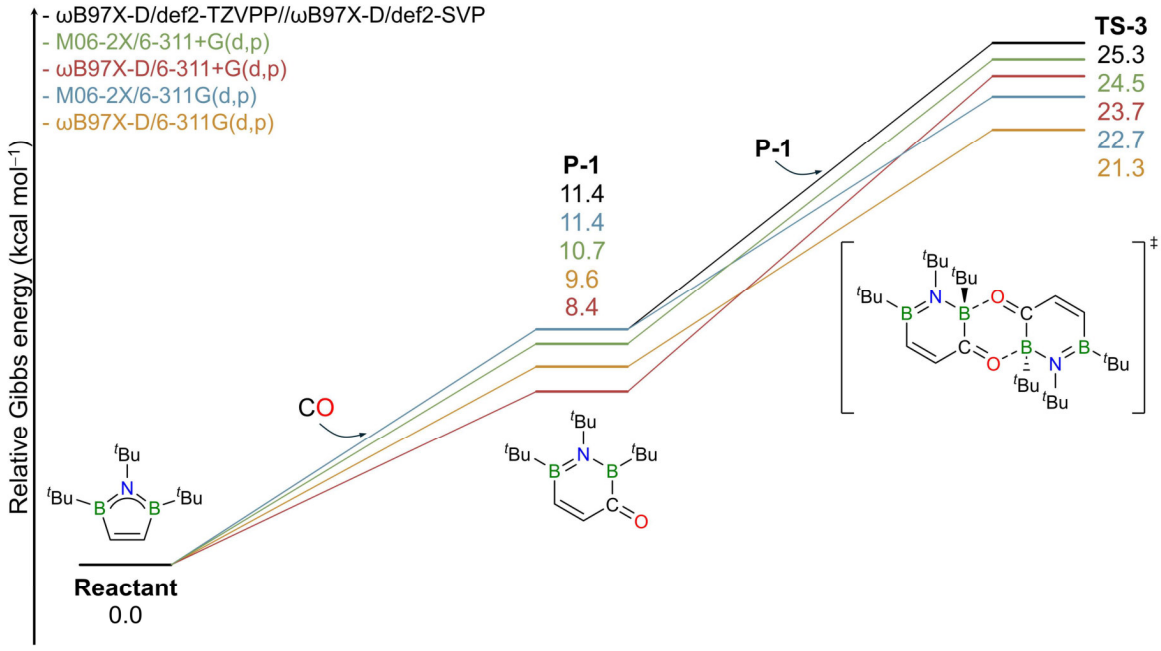


Figure 1.7. Gas-phase thermochemistry data (kcal mol^{-1}) related to the dimerization of **P-1** considering the collection of functionals and basis sets shown in the colour code.

Nevertheless, the total energy barrier ($\Delta G^{\ddagger}_{R\rightarrow TS\text{-}3}$, **Figure 1.4**), which is related to the rate-determining step for the overall reaction of **8** with CO, was recalculated (**Figure 1.7**). The same functionals and basis sets mentioned above were utilized. In accordance with the preceding analysis, results obtained with M06-2X predict higher energies in comparison to those obtain with ωB97X-D. Regarding Gibbs energy of **P-1** formation, it is clear that the inclusion of diffuse functions on Pople's basis sets results in a reduction of the Gibbs energy value ($\Delta G_{R\rightarrow P\text{-}1}$ = 10.7 and 8.4 kcal mol^{-1} for M06-2X and ωB97X-D) in contrast to the exclusion of them ($\Delta G_{R\rightarrow P\text{-}1}$ = 11.4 and 9.6 kcal mol^{-1} for M06-2X and ωB97X-D). A similar examination conducted on the relative energies of **TS-3** leads to the opposite effect. Despite numerous attempts, it was not possible to optimize **TS-3** using the M06-2X/def2-SVP level.

The high dependence on the integration grid in Minnesota functionals is likely the cause of this failure. Nevertheless, it is important to note that the range of the energy barrier is between 21.3–25.3 kcal mol^{-1} in the gas-phase when comparing all computational methods utilized herein. This outcome is significant as it indicates that, despite the variations in the level of theory, the kinetics result remains within the limits of processes achievable at mild temperatures.

Finally, the rate-determining step under consideration was recalculated by performing geometry optimizations in solvent-phase at the (SMD: *n*-pentane)ωB97X-D/def2-TZVPP//ωB97X-D/def2-SVP level. This resulted in a Gibbs energy of 7.1 kcal mol^{-1} related to the ring-expanded product formation ($\Delta G_{R\rightarrow P\text{-}1}$), and a barrier height of 24.7 kcal mol^{-1} concerning the transition state **TS-3**. Once more, a thermally accessible barrier is obtained, supporting the kinetic feasibility of the polyheterocycle **P-2** produced through the overall reaction of **8** and CO in a *n*-pentane solution.

1.5. Conclusions

We performed a computational study to elucidate the mechanism of endocyclic CO insertion into borole rings. Establishing structural analogy via isosterism between borole and 1,2,5-azadiborolidine enabled the transposition of CO ring expansion to this unexplored boron heterocycle. For the optimal candidate (**8**), the overall pathway comprises: (1) CO-induced ring expansion, (2) dimerization, and (3) double [1,2]-migration, mirroring borole mechanisms. These results confirm that **8** exhibits comparable CO reactivity alongside structural similarity to boroles. Computations predicted viable CO insertion for **8**, yielding polycyclic **P-2**. Solvent screening (DCM, *n*-pentane, THF) revealed favourable thermochemical effects, with *n*-pentane offering optimal kinetics and exergonicity.

Mechanistically, B–C(O) and C–O bond lengths in Lewis adducts correlate with ring expansion kinetics. Significant correlation between π-backbonding energy and reaction barrier highlights its utility as predictive descriptor for boron systems. We encourage experimental validation to establish 1,2,5-azadiborolidine as the *fourth* boron heterocycle undergoing CO insertion, advancing boron's metal-mimetic role and enabling design of novel functional materials.

1.6. Supporting Information

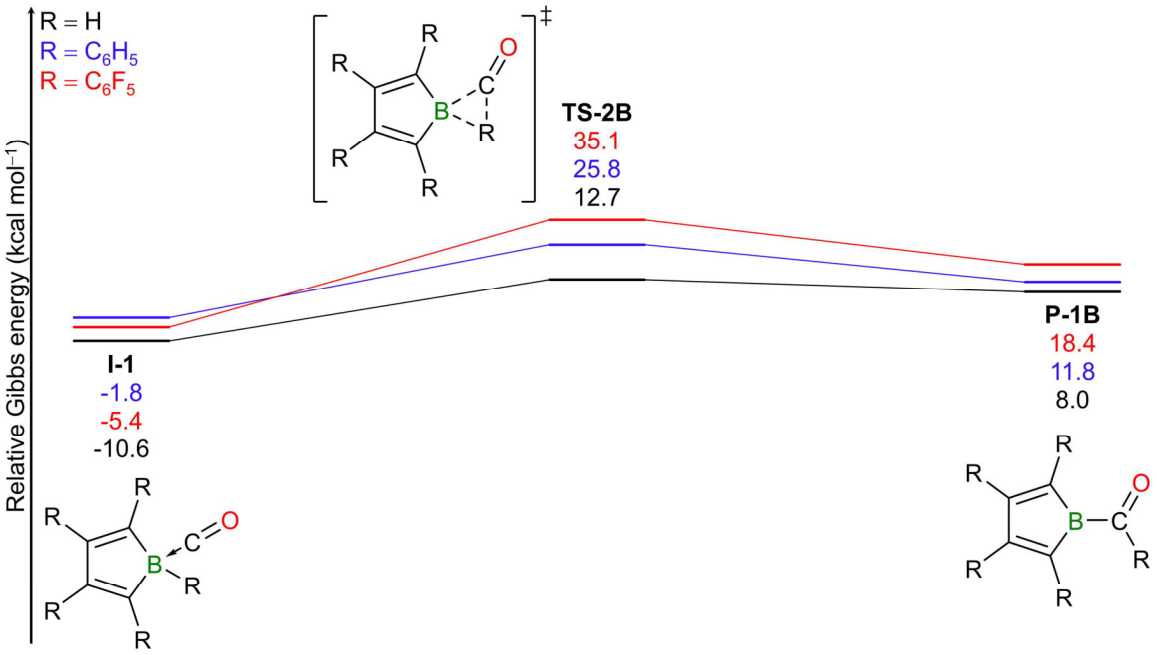


Figure S1. Relative Gibbs free energy profiles for the exocyclic CO insertion of selected borole derivatives. Gas-phase energy data (kcal mol^{-1}) were calculated at the ωB97X-D/def2-TZVPP//ωB97X-D/def2-SVP level.

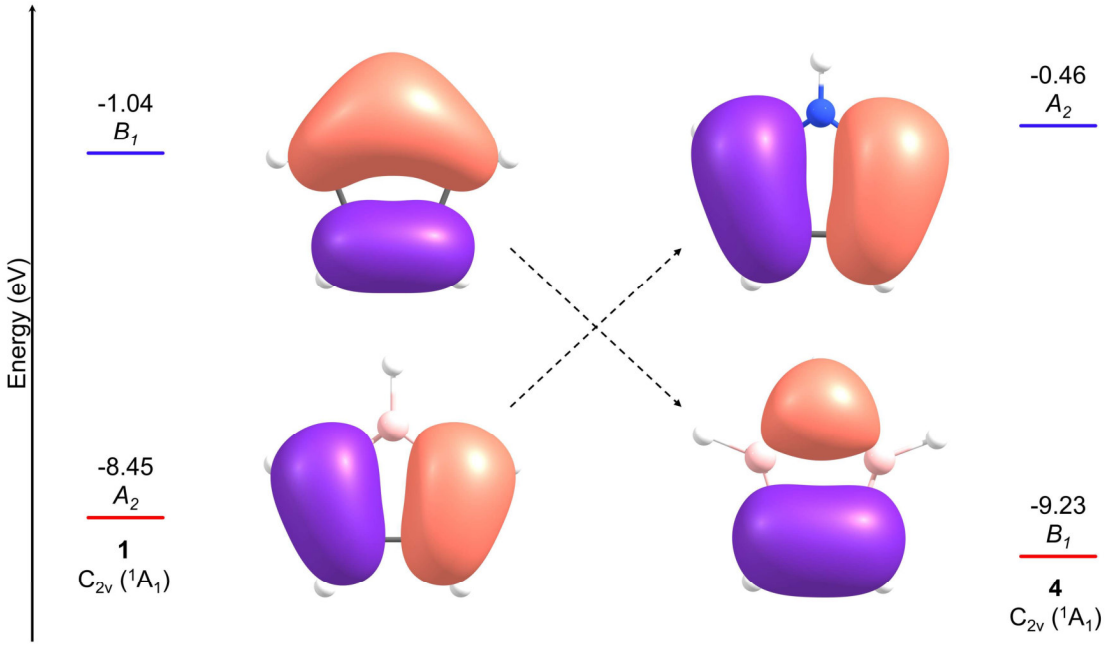


Figure S2. HOMO (red) and LUMO (blue) gas-phase energy values (eV) for borole (**1**) and 1,2,5-azadiborolidine (**4**). Orbital symmetry (italics) is printed at each point. Orbital isosurfaces are shown at the centre. Data were obtained at the ωB97X-D/def2-TZVPP//ωB97X-D/def2-SVP level.

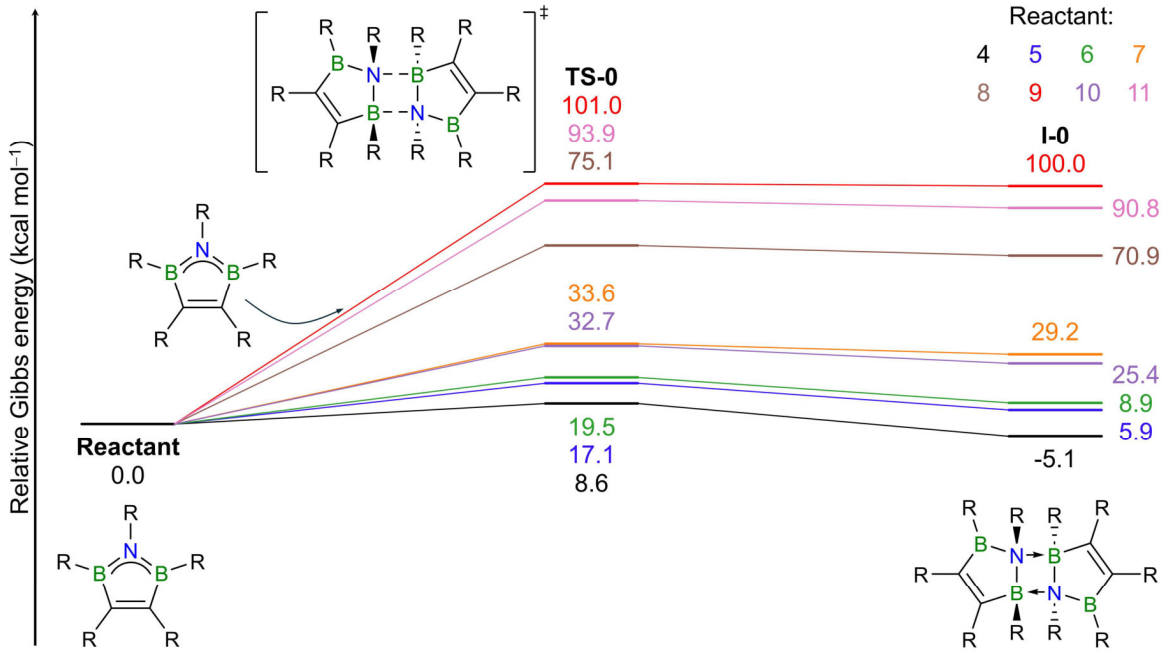


Figure S3. Relative Gibbs energy profiles concerning the dimerization process of the starting heterocycles **4**–**11**. Gas-phase energy values (kcal mol^{-1}) were calculated at the ωB97X-D/def2-TZVPP//ωB97X-D/def2 SVP level.

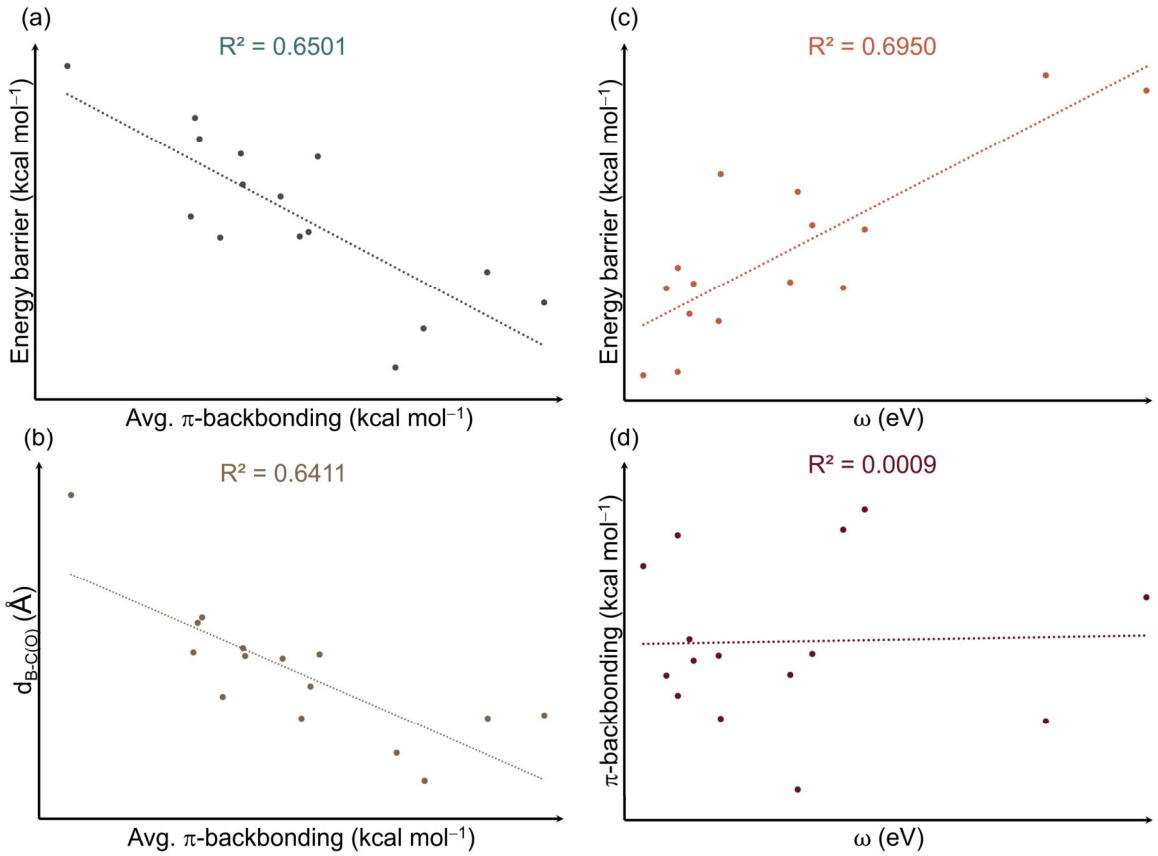


Figure S4. Analysis of linear correlations from gas-phase thermochemistry data for the endocyclic CO insertion among compounds **1**–**15**. Average π-backbonding energy alongside with (a) total barrier, and (b) B–C(O) bond length. Correlation of global electrophilicity with (c) energy barrier of the second reaction step, and (d) π-backbonding energy. The π-backbonding energies and B–C(O) bond length were calculated for adducts **I-1**, while the ω value is measured on the starting heterocycles.

Steric maps and $\%V_{Bur}$ of adduct **I-1**(Figure S5) were calculated defining, as centre, the carbon atom of the CO moiety; boron atom in which the coordination occurs was utilized to define the Z axis; and the carbon atom inside the ring responsible for the CO insertion was used to define the XZ plane. Then, the following analysis reflects the most relevant results.

Firstly, a straightforward comparison can be made between compounds **1** and **4**, as they only contain hydrogen atoms surrounding the rings. The adducts formed by these compounds have almost identical total $\%V_{Bur}$ and $\%V_{Bur}$ components per quadrant, demonstrating the isosterism of these heterocycles once again.

Secondly, by comparing the structures of the Lewis adduct produced from boracycles **2** and **3**, we can see that replacing hydrogen with fluorine atoms as substituents in the phenyl moieties results in a higher $\%V_{Bur}$. This is expected given that fluorine is a larger atom than hydrogen and therefore occupies more space.

Thirdly, in compounds **5** and **6** the only structural difference is an increase in the substituents' volume by switching from methyl (–Me) to ethyl (–Et) groups in positions 3 and 4 along the ring. This increase is insignificant in the steric maps, as reflected by the nearly equal values of $\%V_{Bur}$. A similar observation can be established by comparing molecules **8** and **9**. Notice that when substituents' volume in positions 1, 2, and 5 increases, so does the $\%V_{Bur}$, as demonstrated by comparing molecules **5**–**6** with **7**–**9**.

Fourthly, the replacement of borole by 1,2,5-azadiborolidine ring facilitates a comparison of **10**–**11** with **2**–**3**, as was previously conducted for **1** and **4**. Similar observations are reached. For instance, the steric hindrance in **2** is virtually identical to that in **10**, as it is for **3** and **11**, or **1** and **4**. Furthermore, a comparison of **10** and **11** revealed a consistent increase in $\%V_{Bur}$, attributable to the transition from a perproteo to a perfluoro derivative, analogous to the shift from **2** to **3**.

Finally, in the case of molecules **12**–**15**, we highlight the steric hindrance produced by the mesitylene (–Mes) groups, which is the reason for the higher $\%V_{Bur}$ values shown in **12** and **15** compared to **13** and **14**.

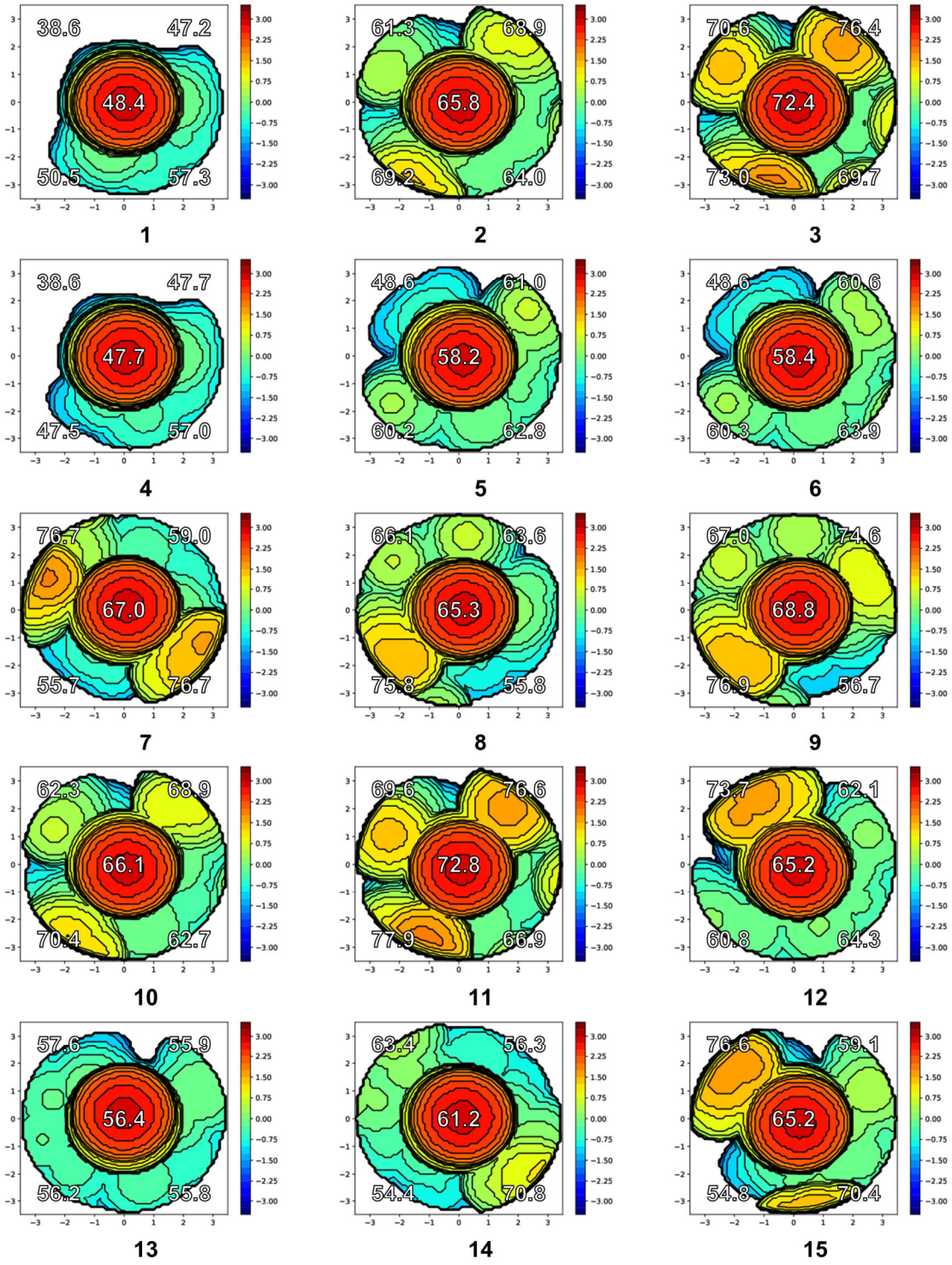
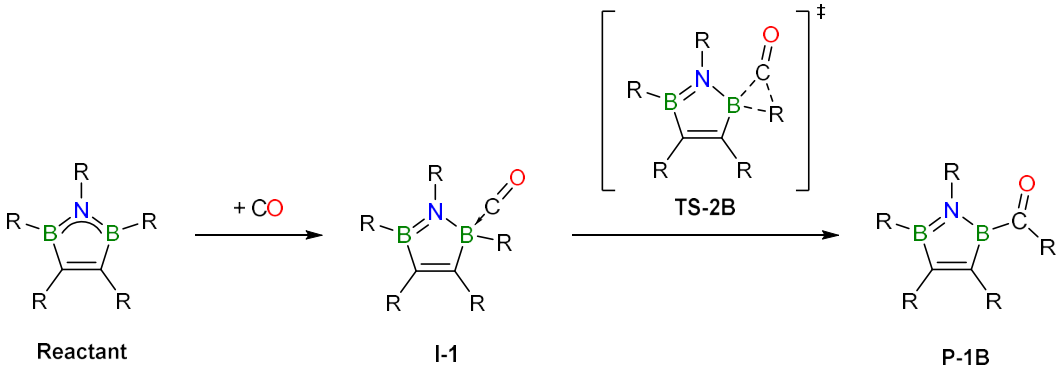


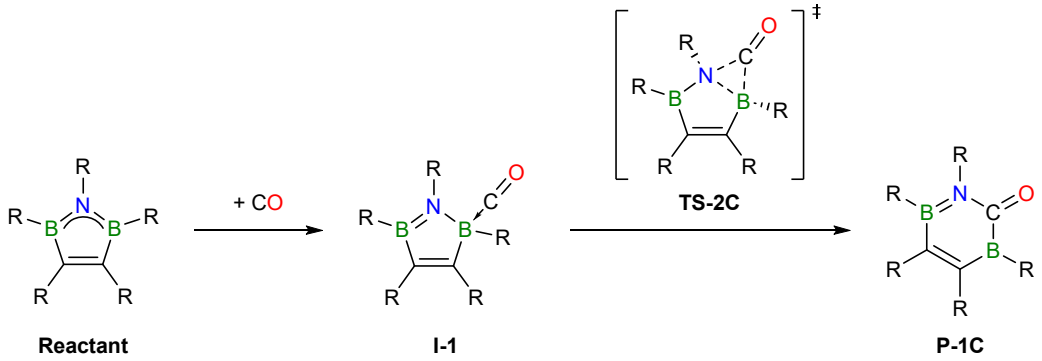
Figure S5. Steric maps of adduct **I-1**, produced from CO coordination in boracycles **1**–**15**. The isocontour scheme in Å is shown at right for each compound. Red and blue zones indicate more and less hindered zones in the coordination sphere. Total $\%V_{Bur}$ at the centre and its contributions per quadrant are printed.

Table S1. Relative Gibbs energy values (kcal mol^{-1}), calculated at the ωB97X-D/def2-TZVPP//ωB97X-D/def2-SVP level of theory in gas-phase, for the exocyclic insertion between different 1,2,5-azadiborolidine derivatives and CO.



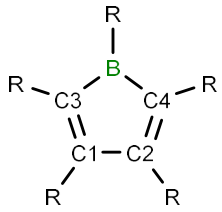
Entry	Reactant	I-1	TS-2B	P-1B
1	**8**	11.2	28.8	1.1
2	**9**	14.2	29.1	–1.1
3	**4**	8.2	24.1	9.6
4	**7**	12.3	33.1	8.1
5	**10**	13.7	37.6	9.6
6	**5**	15.9	36.7	12.8
7	**6**	15.7	37.4	12.8
8	**15**	21.6	44.2	16.4
9	**12**	21.4	48.8	14.8
10	**14**	14.2	35.6	15.5
11	**11**	10.1	46.8	21.4
12	**13**	22.1	45.8	29.2

Table S2. Relative Gibbs energy values (kcal mol^{-1}), calculated at the ωB97X-D/def2-TZVPP//ωB97X-D/def2-SVP level of theory in gas-phase, for the NB-endocyclic insertion between different 1,2,5-azadiborolidine derivatives and CO.

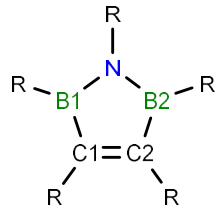


Entry	Reactant	I-1	TS-2C	P-1C
1	**4**	8.2	32.5	14.1
2	**5**	15.9	35.6	17.2
3	**8**	11.2	33.8	19.4
4	**10**	13.7	37.5	23.5

Table S3. Bond lengths (Å), MPP (Å), SDP (Å), and global electrophilicity ω (eV) values for molecules **1**–**15**. MPP and SDP quantities are multiplied by 100.



Molecule	C1-C2	C1-C3	C2-C4	C3-B	C4-B	MPP	SDP	ω
1	1.514	1.343	1.343	1.587	1.587	0.000	0.000	1.519
2	1.526	1.356	1.356	1.589	1.589	0.217	0.591	1.446
3	1.518	1.349	1.349	1.583	1.583	0.416	1.126	2.479



Molecule	C1-C2	C1-B1	C2-B2	N-B1	N-B2	MPP	SDP	ω
4	1.349	1.592	1.592	1.432	1.432	0.000	0.000	1.341
5	1.355	1.591	1.597	1.442	1.437	0.072	0.186	0.843
6	1.355	1.593	1.595	1.441	1.439	0.152	0.389	0.882
7	1.354	1.589	1.592	1.454	1.457	0.416	1.121	0.936
8	1.343	1.592	1.592	1.459	1.459	11.032	28.468	0.882
9	1.355	1.597	1.597	1.459	1.459	11.815	30.497	0.765
10	1.361	1.595	1.595	1.446	1.446	0.234	0.638	1.265
11	1.354	1.585	1.585	1.438	1.438	0.250	0.672	2.137
12	1.423	1.595	1.564	1.432	1.452	0.468	1.259	0.922
13	1.422	1.579	1.579	1.448	1.448	0.018	0.047	1.291
14	1.419	1.574	1.584	1.453	1.455	7.792	21.188	1.029
15	1.415	1.582	1.582	1.437	1.437	0.352	0.956	1.021

Table S4. Bond lengths (Å), total π-backbonding energy ($E_{\pi\text{-BB}}$), and its average ($\overline{E}_{\pi\text{-BB}}$), in kcal mol^{-1}, for the Lewis adduct **I-1** produced by molecules **1**–**15** and CO.

Reactant	B–C(O)	C–O	$E_{\pi\text{-BB}}$	$\overline{E}_{\pi\text{-BB}}$
1	1.550	1.131	29.15	7.29
2	1.568	1.132	27.53	6.88
3	1.591	1.125	22.02	5.51
4	1.605	1.128	17.45	4.36
5	1.630	1.131	15.69	5.23
6	1.632	1.131	14.06	4.69
7	1.612	1.130	16.90	5.63
8	1.593	1.131	27.07	9.02
9	1.591	1.132	24.61	8.20
10	1.634	1.128	15.75	3.94
11	1.654	1.122	12.00	4.00
12	1.637	1.129	18.63	4.66
13	1.738	1.127	6.49	2.16
14	1.657	1.126	12.19	4.06
15	1.633	1.130	17.30	5.77

Table S5. Description of the donor-acceptor NBO stabilizing energies (DASE), which conform the total π-backbonding-like energy ($E_{\pi\text{-BB}}$) in the adduct **I-1** produced by molecules **1**–**15** and CO.

Reactant	Donor NBO (i)	Acceptor NBO (j)	DASE (kcal mol^{-1})
1	σ(C3–B4)	π*(C5–O7)	10.07
	σ(C3–B4)	π*(C5–O7)	4.51
	σ(B4–C6)	π*(C5–O7)	10.05
	σ(B4–C6)	π*(C5–O7)	4.52
2	σ(C1–B4)	π*(C61–O62)	8.46
	σ(C1–B4)	π*(C61–O62)	5.01
	σ(B4–C5)	π*(C61–O62)	12.91
	σ(B4–C5)	π*(C61–O62)	1.15
3	σ(C1–B4)	π*(C61–O62)	5.71
	σ(C1–B4)	π*(C61–O62)	5.68
	σ(B4–C5)	π*(C61–O62)	10.07
	σ(B4–C5)	π*(C61–O62)	0.56
4	σ(N3–B4)	π*(C5–O7)	3.11
	σ(N3–B4)	π*(C5–O7)	0.76
	σ(B4–C6)	π*(C5–O7)	7.80
	σ(B4–C6)	π*(C5–O7)	5.78
5	σ(C1–B3)	π*(C27–O26)	8.79
	σ(C1–B3)	π*(C27–O26)	2.26
	σ(B3–N5)	π*(C27–O26)	4.64
6	σ(C1–B3)	π*(C33–O32)	8.95
	σ(C1–B3)	π*(C33–O32)	0.73
	σ(B3–N5)	π*(C33–O32)	4.38
7	σ(C2–B4)	π*(C47–O48)	6.77
	σ(C2–B4)	π*(C47–O48)	5.40

	σ(B4–N5)	π*(C47–O48)	4.73
8	σ(C2–B4)	π*(C48–O47)	22.51
	σ(C2–B4)	π*(C48–O47)	1.43
	σ(B4–N5)	π*(C48–O47)	3.13
9	σ(C2–B4)	π*(C54–O53)	21.39
	σ(B4–N5)	π*(C54–O53)	2.32
	σ(B4–N5)	π*(C54–O53)	0.90
10	σ(N1–B4)	π*(C61–O62)	3.01
	σ(N1–B4)	π*(C61–O62)	2.96
	σ(B4–C5)	π*(C61–O62)	9.25
	σ(B4–C5)	π*(C61–O62)	0.53
11	σ(N1–B4)	π*(C61–O62)	5.03
	σ(B4–C5)	π*(C61–O62)	4.71
	σ(B4–C5)	π*(C61–O62)	2.26
12	σ(N1–B32)	π*(C65–O66)	3.72
	σ(N1–B32)	π*(C65–O66)	3.33
	σ(B32–C54)	π*(C65–O66)	9.97
	σ(B32–C54)	π*(C65–O66)	1.61
13	σ(N1–B35)	π*(C37–O38)	1.44
	σ(C25–B35)	π*(C37–O38)	3.46
	σ(C25–B35)	π*(C37–O38)	1.59
14	σ(N1–B42)	π*(C44–O45)	3.93
	σ(C14–B42)	π*(C44–O45)	7.13
	σ(C14–B42)	π*(C44–O45)	1.13
15	σ(N1–B3)	π*(C55–O56)	7.07
	σ(B3–C5)	π*(C55–O56)	9.07
	σ(B3–C5)	π*(C55–O56)	1.16

1.7. References

1. E. J. Kantorowski and M. J. Kurth, *Tetrahedron*, 2000, **56**, 4317–4353.
2. B. Biletskyi, P. Colonna, K. Masson, J.-L. Parrain, L. Commeiras and G. Chouraqui, *Chem. Soc. Rev.*, 2021, **50**, 7513–7538.
3. J. R. Donald and W. P. Unsworth, *Chem. Eur. J.*, 2017, **23**, 8780–8799.
4. Y. Shoji, N. Tanaka, K. Mikami, M. Uchiyama and T. Fukushima, *Nat. Chem.*, 2014, **6**, 498–503.
5. H. Braunschweig, T. Dellermann, W. C. Ewing, T. Kramer, C. Schneider and S. Ullrich, *Angew. Chem. Int. Ed.*, 2015, **54**, 10271–10275.
6. M.-A. Légaré, C. Pranckevicius and H. Braunschweig, *Chem. Rev.*, 2019, **119**, 8231–8261.
7. J. Poater, S. Escayola, A. Poater, F. Teixidor, H. Ottosson, C. Viñas and M. Solà, *J. Am. Chem. Soc.*, 2023, **145**, 22527–22538.
8. G. Hernández-Juárez, J. Barroso, A. Vásquez-Espinal, F. Ortíz-Chi, W. Tiznado, F. Murillo and G. Merino, *Phys. Chem. Chem. Phys.*, 2024, **26**, 8089–8093.
9. M. Michel, S. Kar, L. Endres, R. D. Dewhurst, B. Engels and H. Braunschweig, *Nat. Synth.*, 2025, **4**, 869–876.
10. J. Barthel, M. Wühr, R. Buestrich and H. J. Gores, *J. Electrochem. Soc.*, 1995, **142**, 2527–2531.
11. J. Barthel, R. Buestrich, H. J. Gores, M. Schmidt and M. Wühr, *J. Electrochem. Soc.*, 1997, **144**, 3866–3870.
12. K. Xu, S. Zhang, T. R. Jow, W. Xu and C. A. Angell, *Electrochem. Solid-State Lett.*, 2002, **5**, A26–A29.
13. M. Ue, T. Fujii, Z.-B. Zhou, M. Takeda and S. Kinoshita, *Solid State Ion.*, 2006, **177**, 323–331.
14. S. S. Zhang, *Electrochem. Commun.*, 2006, **8**, 1423–1428.
15. J. Scheers, P. Johansson and P. Jacobsson, *J. Electrochem. Soc.*, 2008, **155**, A628–A634.
16. J. Luo, Y. Bi, L. Zhang, X. Zhang and T. L. Liu, *Angew. Chem.*, 2019, **131**, 7041–7045.
17. Z. Huang, S. Wang, R. D. Dewhurst, N. V. Ignat'ev, M. Finze and H. Braunschweig, *Angew. Chem. Int. Ed.*, 2020, **59**, 8800–8816.
18. Q. Wu, M. Esteghamatian, N.-X. Hu, Z. Popovic, G. Enright, Y. Tao, M. D'Iorio and S. Wang, *Chem. Mater.*, 2000, **12**, 79–83.
19. Y.-L. Rao and S. Wang, *Inorg. Chem.*, 2011, **50**, 12263–12274.

20. D. Li, H. Zhang and Y. Wang, *Chem. Soc. Rev.*, 2013, **42**, 8416–8433.
21. H.-B. Cheng, X. Cao, S. Zhang, K. Zhang, Y. Cheng, J. Wang, J. Zhao, L. Zhou, X.-J. Liang and J. Yoon, *Adv. Mater.*, 2023, **35**, 2207546.
22. F. Yang, M. Zhu, J. Zhang and H. Zhou, *Med. Chem. Commun.*, 2018, **9**, 201–211.
23. S. Chatterjee, N. M. Tripathi and A. Bandyopadhyay, *Chem. Commun.*, 2021, **57**, 13629–13640.
24. B. C. Das, M. A. Shareef, S. Das, N. K. Nandwana, Y. Das, M. Saito and L. M. Weiss, *Bioorg. Med. Chem.*, 2022, **63**, 116748.
25. H. Braunschweig, T. Dellermann, R. D. Dewhurst, W. C. Ewing, K. Hammond, J. O. C. Jimenez-Halla, T. Kramer, I. Krummenacher, J. Mies, A. K. Phukan and A. Vargas, *Nat. Chem.*, 2013, **5**, 1025–1028.
26. M. Arrowsmith, J. Böhnke, H. Braunschweig, M. A. Celik, C. Claes, W. C. Ewing, I. Krummenacher, K. Lubitz and C. Schneider, *Angew. Chem. Int. Ed.*, 2016, **55**, 11271–11275.
27. Y. Su, Y. Li, R. Ganguly and R. Kinjo, *Angew. Chem. Int. Ed.*, 2018, **57**, 7846–7849.
28. P. Paetzold, B. Redenz-Stormanns and R. Boese, *Angew. Chem. Int. Ed. Engl.*, 1990, **29**, 900–902.
29. J. Teichmann, H. Stock, H. Pritzkow and W. Siebert, *Eur. J. Inorg. Chem.*, 1998, **1998**, 459–463.
30. A. Fukazawa, J. L. Dutton, C. Fan, L. G. Mercier, A. Y. Houghton, Q. Wu, W. E. Piers and M. Parvez, *Chem. Sci.*, 2012, **3**, 1814–1818.
31. W. Haubold and A. Gemmler, *Chem. Ber.*, 1980, **113**, 3352–3356.
32. W. Siebert, H. Schmidt and R. Full, *Z. Naturforsch. B*, 1980, **35**, 873–881.
33. P. Paetzold, B. Redenz-Stormanns and R. Boese, *Chem. Ber.*, 1991, **124**, 2435–2441.
34. R. Köster, G. Seidel and R. Boese, *Chem. Ber.*, 1994, **127**, 2159–2165.
35. S. Luckert, E. Eversheim, U. Englert, T. Wagner and P. Paetzold, *Z. Anorg. Allg. Chem.*, 2001, **627**, 1815–1823.
36. W. K. Brown, K. K. Klausmeyer and B. M. Lindley, *Chem. Commun.*, 2022, **58**, 867–870.
37. C. Hu, L. Guo, J. Zhang and C. Cui, *Organometallics*, 2021, **40**, 1015–1019.
38. H. Wei, Y. Liu, T. Y. Gopalakrishna, H. Phan, X. Huang, L. Bao, J. Guo, J. Zhou, S. Luo, J. Wu and Z. Zeng, *J. Am. Chem. Soc.*, 2017, **139**, 15760–15767.
39. X.-Y. Wang, A. Narita, X. Feng and K. Müllen, *J. Am. Chem. Soc.*, 2015, **137**, 7668–7671.
40. Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A.

Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

41. J.-D. Chai and M. Head-Gordon, *Phys. Chem. Chem. Phys.*, 2008, **10**, 6615–6620.
42. F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297–3305.
43. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378–6396.
44. L. Goerigk and S. Grimme, *Phys. Chem. Chem. Phys.*, 2011, **13**, 6670–6688.
45. M. Bursch, J.-M. Mewes, A. Hansen and S. Grimme, *Angew. Chem. Int. Ed.*, 2022, **61**, e202205735; *Angew. Chem.*, 2022, **134**, e202205735.
46. R. G. Parr, L. v. Szentpály and S. Liu, *J. Am. Chem. Soc.*, 1999, **121**, 1922–1924.
47. R. G. Pearson, *Inorg. Chem.*, 1988, **27**, 734–740.
48. T. Koopmans, *Physica*, 1934, **1**, 104–113.
49. P. K. Chattaraj and D. R. Roy, *Chem. Rev.*, 2007, **107**, PR46–PR74.
50. A. R. Jupp, T. C. Johnstone and D. W. Stephan, *Dalton Trans.*, 2018, **47**, 7029–7035.
51. R. Pal and P. K. Chattaraj, *J. Comput. Chem.*, 2023, **44**, 278–297.
52. D. I. Martínez-Valencia, L. I. Lugo-Fuentes, G. González-García, J. A. Luján-Montelongo, K. J. Shea, J. E. Báez and J. O. C. Jiménez-Halla, *New J. Chem.*, 2025, **49**, 6936–6945.
53. T. Lu, *J. Mol. Model.*, 2021, **27**, 263.
54. A. Poater, F. Ragone, S. Giudice, C. Costabile, R. Dorta, S. P. Nolan and L. Cavallo, *Organometallics*, 2008, **27**, 2679–2681.
55. A. Poater, B. Cosenza, A. Correa, S. Giudice, F. Ragone, V. Scarano and L. Cavallo, *Eur. J. Inorg. Chem.*, 2009, **2009**, 1759–1766.
56. L. Falivene, Z. Cao, A. Petta, L. Serra, A. Poater, R. Oliva, V. Scarano and L. Cavallo, *Nat. Chem.*, 2019, **11**, 872–879.
57. S. Escayola, N. Bahri-Laleh and A. Poater, *Chem. Soc. Rev.*, 2024, **53**, 853–882.

58. E. D. Glendenning, A. E. Reed, J. E. Carpenter and F. Weinhold, *NBO Version 3.1*, 2001.
59. T. Lu and F. Chen, *J. Comput. Chem.*, 2012, **33**, 580–592.
60. M. Giambiagi, M. S. de Giambiagi and K. C. Mundim, *Struct. Chem.*, 1990, **1**, 423–427.
61. P. Bultinck, R. Ponec and S. Van Damme, *J. Phys. Org. Chem.*, 2005, **18**, 706–718.
62. E. Matito, *Phys. Chem. Chem. Phys.*, 2016, **18**, 11839–11846.
63. T. Lu, *J. Chem. Phys.*, 2024, **161**, 082503.
64. D. Rappoport and F. Furche, *J. Chem. Phys.*, 2010, **133**, 134105.
65. Z. Wang, Y. Zhou, T. B. Marder and Z. Lin, *Org. Biomol. Chem.*, 2017, **15**, 7019–7027.
66. M. J. D. Bosdet and W. E. Piers, *Can. J. Chem.*, 2009, **87**, 8–29.
67. X. Wang, G. Sun, P. Routh, D.-H. Kim, W. Huang and P. Chen, *Chem. Soc. Rev.*, 2014, **43**, 7067–7098.
68. X.-Y. Wang, J.-Y. Wang and J. Pei, *Chem. Eur. J.*, 2015, **21**, 3528–3539.
69. P. B. Pati, E. Jin, Y. Kim, Y. Kim, J. Mun, S. J. Kim, S. J. Kang, W. Choe, G. Lee, H.-J. Shin and Y. S. Park, *Angew. Chem. Int. Ed.*, 2020, **59**, 14891–14895.
70. M. Chen, K. S. Unikela, R. Ramalakshmi, B. Li, C. Darrigan, A. Chrostowska and S.-Y. Liu, *Angew. Chem.*, 2021, **133**, 1580–1584.
71. X. Chen, D. Tan and D.-T. Yang, *J. Mater. Chem. C*, 2022, **10**, 13499–13532.
72. F. Feixas, E. Matito, M. Solà and J. Poater, *J. Phys. Chem. A*, 2008, **112**, 13231–13238.
73. F. Feixas, E. Matito, M. Solà and J. Poater, *Phys. Chem. Chem. Phys.*, 2010, **12**, 7126–7137.
74. F. Feixas, E. Matito, J. Poater and M. Solà, *Chem. Soc. Rev.*, 2015, **44**, 6434–6451.
75. N. C. Baird, *J. Am. Chem. Soc.*, 1972, **94**, 4941–4948.
76. A. Soncini and P. W. Fowler, *Chem. Phys. Lett.*, 2008, **450**, 431–436.
77. F. Feixas, J. Vandenbussche, P. Bultinck, E. Matito and M. Solà, *Phys. Chem. Chem. Phys.*, 2011, **13**, 20690–20703.
78. P. R. von Schleyer and H. Jiao, *Pure Appl. Chem.*, 1996, **68**, 209–218.
79. V. I. Minkin, *Pure Appl. Chem.*, 1999, **71**, 1919–1981.
80. R. Boese, A. H. Maulitz and P. Stellberg, *Chem. Ber.*, 1994, **127**, 1887–1889.
81. M. del R. Merino-García, L. A. Soriano-Agueda, J. de D. Guzmán-Hernández, D. Martínez-Otero, B. L. Rivera, F. Cortés-Guzmán, J. E. Barquera-Lozada and V. Jancik, *Inorg. Chem.*, 2022, **61**, 6785–6798.

82. M. Yáñez, O. Mó, I. Alkorta and J. E. Del Bene, *J. Chem. Theory Comput.*, 2008, **4**, 1869–1876.
83. R. Hoffmann, *Angew. Chem. Int. Ed. Engl.*, 1982, **21**, 711–724.
84. C. G. Wermuth, C. R. Ganellin, P. Lindberg and L. A. Mitscher, *Pure Appl. Chem.*, 1998, **70**, 1129–1143.
85. I. Ghesner, W. E. Piers, M. Parvez and R. McDonald, *Organometallics*, 2004, **23**, 3085–3087.
86. C. Li, D. Xie, Z. Ye, Z. Zhang, F. Wang, CN Pat., 111471064A, 2020.
87. J. H. Barnard, S. Yruegas, K. Huang and C. D. Martin, *Chem. Commun.*, 2016, **52**, 9985–9991.
88. T. Bischof, L. Beßler, I. Krummenacher, L. Erhard, H. Braunschweig and M. Finze, *Chem. Eur. J.*, 2023, **29**, e202300210.
89. D. Loffreda, F. Delbecq, F. Vigné and P. Sautet, *Angew. Chem. Int. Ed.*, 2009, **48**, 8978 –8980
90. R. S. Assary, L. J. Broadbelt and L. A. Curtiss, *J. Mol. Model.*, 2012, **18**, 145–150.
91. L. Zhang, Y.-Q. Su, M.-W. Chang, I. A. W. Filot and E. J. M. Hensen, *J. Phys. Chem. C*, 2019, **123**, 31130–31141.
92. Z. Wang and P. Hu, *Catal. Sci. Technol.*, 2021, **11**, 2604–2615.
93. Y.-L. Cheng, C.-T. Hsieh, Y.-S. Ho, M.-H. Shen, T.-H. Chao and M.-J. Cheng, *Phys. Chem. Chem. Phys.*, 2022, **24**, 2476–2481.
94. M. A. Abdulsattar, *J. Mol. Model.*, 2023, **29**, 304.
95. M. Finze, E. Bernhardt, A. Terheiden, M. Berkei, H. Willner, D. Christen, H. Oberhammer and F. Aubke, *J. Am. Chem. Soc.*, 2002, **124**, 15385–15398.
96. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215–241.
97. R. Krishnan, J. S. Binkley, R. Seeger and J. A. Pople, *J. Chem. Phys.*, 1980, **72**, 650–654.
98. T. Clark, J. Chandrasekhar, G. W. Spitznagel and P. V. R. Schleyer, *J. Comput. Chem.*, 1983, **4**, 294–301.

CHAPTER 2

"If I have seen further, it is by standing

on the shoulders of giants."

Sir Isaac Newton, in a letter

to Robert Hooke (1676)

Unveiling Enhanced Catalytic Efficiency in CO_2-Epoxide Cycloaddition via Atrane Structural Modifications

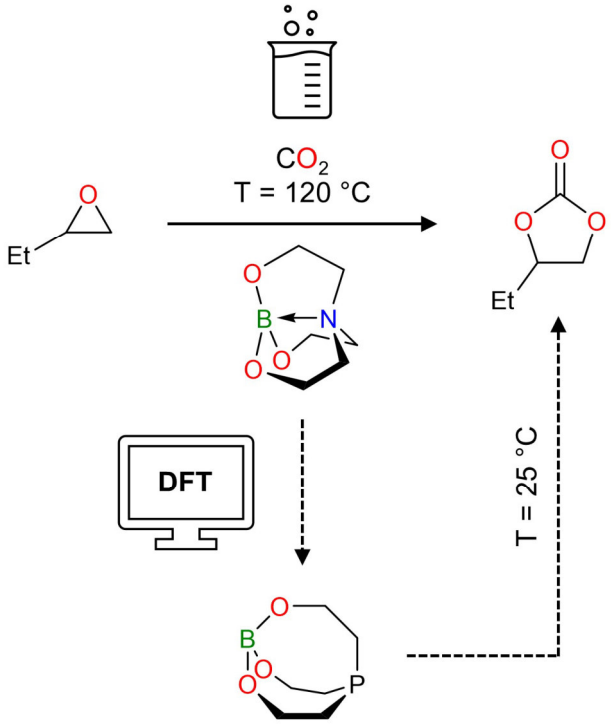
Victor A. Lucas-Rosales,[a,b] Anna Vidal-López,[b] J. Oscar C. Jiménez-Halla,[a*] Albert Poater[b*]

[a.] Departamento de Química, División de Ciencias Naturales y Exactas, Universidad de Guanajuato, Noria Alta S/N 36050, Guanajuato, Guanajuato, México. E-mail: jjimenez@ugto.mx

[b.] Institut de Química Computacional i Catàlisi, Departament de Química, Universitat de Girona, C/ Mª Aurèlia Capmany 69, 17003 Girona, Catalonia, Spain. E-mail: albert.poater@udg.edu

2.1. Abstract

In this study, we have computationally investigated the cycloaddition of CO_2 with 1,2-epoxybutane catalysed by triethanolamine borate (**1**), a green and efficient metal-free bifunctional Lewis's pair catalyst. Employing Density-Functional Theory (DFT), a detailed reaction mechanism is proposed, revising and refining previous mechanistic interpretations. The computed energy profile reveals a high activation barrier ($\Delta G^{\ddagger}$ = 34.9 kcal mol^{-1}) for the ring-opening step, consistent with experimental observations. Employing bromide as a cocatalyst reduces this barrier by 7.5 kcal mol^{-1}, confirming its synergistic role. After elucidating the role of **1**, we explored rational structural modifications to enhance its catalytic performance. Hence, a novel series of modified isoelectronic atranes were designed by substituting heteroatoms in the **1** scaffold. Our results demonstrate that specific structural alterations, such as substituting nitrogen with phosphorus or arsenic, and boron with aluminium, notably reduce the energy barrier associated with the rate-determining epoxide ring-opening step. Among these, the BP-atrane (**3**) displayed a significantly lower barrier ($\Delta G^{\ddagger}$ = 16.0 kcal mol^{-1}) without requiring catalyst pre-activation, suggesting its potential for efficient, low-temperature CO_2 fixation. Our results demonstrate the predictive power of modern computational tools for catalyst design and provide a roadmap for developing next-generation metal-free systems capable of promoting CO_2 conversion under mild conditions.



2.2. Introduction

Excess CO_2, a major greenhouse gas, contributes significantly to global warming and climate change.[1] Converting CO_2 into value-added chemicals is therefore a critical focus in both academic and industrial contexts.[2] Among various strategies, the cycloaddition of CO_2 with epoxides to form cyclic carbonates stands out due to its full atom economy and broad applicability (**Chart 2.1**). Nevertheless, this reaction faces challenges due to the inert nature of CO_2. Over the years, a wide range of catalysts have been developed for this transformation,[3] including both homogeneous and heterogeneous systems,[4] as well as biphasic systems, which have been recently introduced.[5]

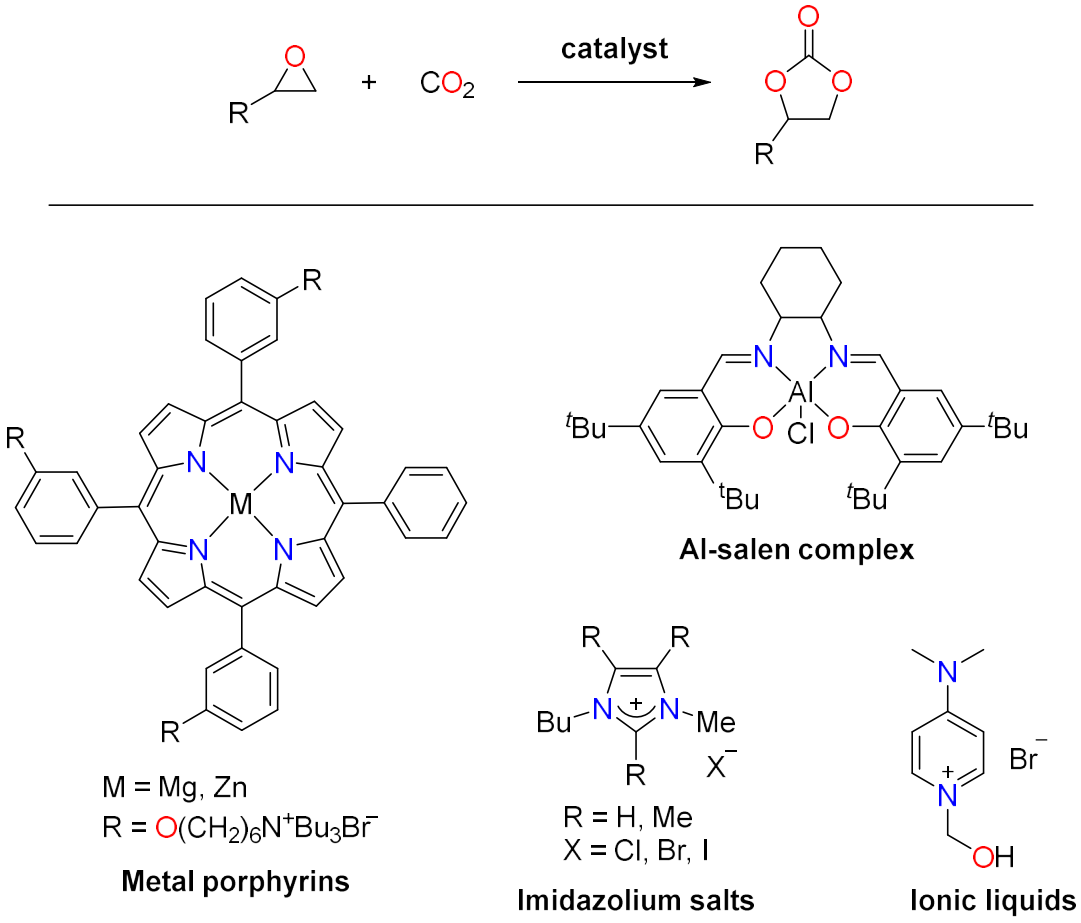


Chart 2.1. Selected catalysts employed in the synthesis of cyclic carbonates.

Homogeneous catalysts (**Chart 2.1**), such as metal porphyrins,[6] salen complexes,[7] imidazolium salts,[8] and ionic liquids (ILs),[9–11] often exhibit high activity under mild

conditions, especially when designed as bifunctional systems that benefit from cooperative catalytic sites.[12–14] For instance, Dai et al. synthesized *N*-heterocyclic carbene precursors with carboxyl groups that showed excellent catalytic performance for CO_2–epoxide coupling.[15] Zhou et al. reported imidazolium-based deep eutectic solvents capable of catalysing the same reaction efficiently without metals, cocatalysts, or solvents.[16]

Despite their high activity, homogeneous catalysts often suffer from drawbacks such as complex synthesis, toxicity, and challenging separation. In contrast, heterogeneous catalysts offer advantages in recyclability and ease of separation from products.[17–19] For example, Nagaraja et al. developed a bifunctional covalent organic framework (COF) that effectively catalysed CO_2 fixation and could be reused multiple times.[20] Similarly, Yang et al. created a porphyrin-based polymer that achieved 99% conversion with a TOF of 12,000 h^{-1}, maintaining performance across several cycles.[21] However, homogeneous systems often require larger catalyst loadings and do not always achieve full conversion of epoxides, posing limitations for industrial applications where catalyst removal and complete conversion are essential.

Boron-based catalysts (**Chart 2.2**), leveraging the Lewis acidity of boron, offer an alternative route. Binary systems combining boranes with Lewis bases have shown promise in CO_2 conversion.[22] Feng et al. used triethylborane with ammonium salts or alkoxides for anionic copolymerization of CO_2 and epoxides.[23] Kerton et al. reported cyclic carbonate formation using triarylboranes with iminium chloride cocatalysts.[24] More recently, Wu et al. developed organoborane catalysts featuring one or two electrophilic boron centres and quaternary ammonium halides, achieving high efficiency in copolymerization reactions.[25]

Triethanolamine borate (**1**), a commercially available and eco-friendly material, can be synthesized directly from a mixture of boric acid and triethanolamine, or employing an aqueous solution.[26,27] It is commonly used as a green rust inhibitor,[28,29] lubricant additive,[30] and flame retardant.[31,32] Structurally, **1** features both a Lewis acid (boron) and a Lewis base (tertiary amine), making it well-suited for catalysing CO_2–epoxide cycloaddition.

It is important to note that **1**, as an atrane, can exists in two conformers, which are crucial for understanding its reactivity. When the nitrogen and boron atoms are oriented towards the geometric centre of the molecule, the structure is referred to as the *endo-endo* conformer. Conversely, when these atoms are oriented away from the centre, the molecule adopts the *exo-exo* conformation. In other atranes, *endo-exo* or *exo-endo* arrangements can be preset, albeit less frequently. Furthermore, while a transannular chemical bond between

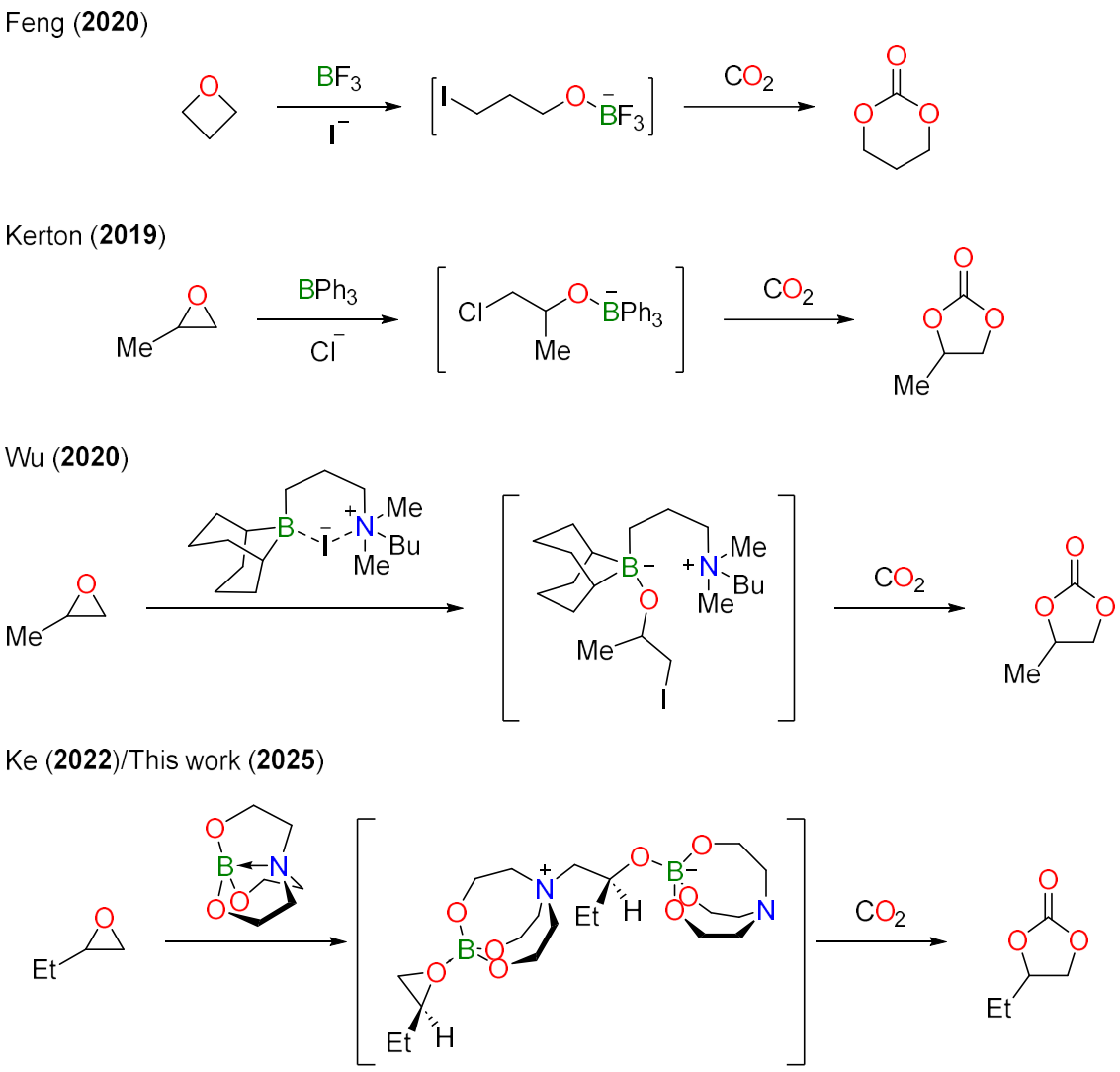
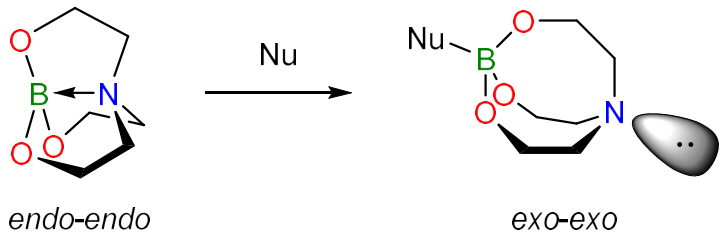


Chart 2.2. Boron-containing catalysts employed in the synthesis of cyclic carbonates from various epoxides and CO_2.

the Lewis acid-base centres may exist in any of these conformations, this is not universally true (e.g., pro- and quasi-atranes)[33]; it depends mainly on the nature of the atoms involved (e.g., triel, tetrel, and pnicogen bonds), as extensively studied via QTAIM analysis by Marín-Luna and coworkers.[34] Phukan and Guha demonstrated that a transannular bond is present in the *endo-endo* conformer of **1** (i.e., N→B bond).[35] Consequently, the conformational landscape for **1** becomes relatively simple: only the *endo-endo* conformer corresponds to a local minimum. However, in the *endo-endo* form, the nitrogen atom lacks a free lone pair of electrons available to react. In contrast, the *exo-exo* conformer restores this reactivity by rendering the lone pair accessible. Therefore, the *exo-exo* conformer is identified as the

catalytically active species. Since this conformer does not exist as a stable structure in solution of **1**, an external nucleophilic agent is required to induce its activation (**Scheme 2.1**).



Scheme 2.1. Activation of catalyst **1** performed by an external nucleophile (Nu) to access the *exo-exo* (*xx*) conformer starting from the e*ndo-endo* (*nn*) one.

In 2022, Ke and coworkers investigated the catalytic performance of **1** as a bifunctional Lewis acid-base catalyst for the cycloaddition of CO_2 with epoxides to form cyclic carbonates under solvent-free conditions (**Chart 2.2**).[36] **1** demonstrated high catalytic activity due to the synergistic effect of its Lewis acidic boron and basic nitrogen centres. Interestingly, a 99% yield of cyclic carbonate was achieved at 120 °C and 1.7 MPa CO_2 with just 1 mol% of **1**. Notably, the reaction was also effective at atmospheric pressure, albeit with longer reaction times. The incorporation of tetrabutylammonium bromide (**TBAB**) as a cocatalyst significantly enhanced activity, enabling quantitative yields even at extremely low catalyst loadings. Remarkably, the system reached turnover frequencies (TOF) as high as 13,333 h^{-1}, setting a benchmark for metal-free catalysts in this reaction. The scope of the catalytic system was further evaluated with a variety of terminal and internal epoxides, yielding the corresponding cyclic carbonates with excellent selectivity (>99%) and high yields. In cases involving internal or sterically hindered epoxides, **TBAB** significantly improved conversions. Mechanistic studies, supported by NMR experiments, suggested that **1** activates the epoxide via coordination and facilitates ring-opening before the CO_2 insertion, either through direct nucleophilic attack by the nitrogen centre or by bromide from **TBAB**. Additionally, the water solubility of **1** and **TBAB** facilitated separation of the catalyst from the product through water washing, rendering the process highly attractive for industrial applications.

Herein, highlighting **1** as a promising, green, and efficient metal-free catalyst for CO_2 fixation, we explore by Density-Functional Theory (DFT) methods not only to elucidate the reaction mechanism, since it is rather known,[15,37–39] but to unveil the role of the catalyst.

Beyond modelling the proposed reaction mechanism and exploring the reactivity profile in detail, modern computational DFT-methods are now sufficiently advanced to predict both the kinetic and thermodynamic performance of catalysts, even those that have not yet been synthesized or tested. This emerging area is known as predictive catalysis.[40–42] In this context and building on the demonstrated success of CO_2 cycloaddition reactions catalysed by **1**, we propose also to explore structural modifications of this atrane scaffold to identify new potential catalysts for the formation of cyclic carbonates under mild conditions.

2.3. Computational Methods

Gaussian 16 software package was employed to perform DFT computations.[43] Solvent-phase geometry optimizations were calculated using the hybrid B3LYP functional[44–47] in conjunction with Grimme D3 dispersion scheme[48,49] and the Pople-type 6-31++G(d,p) basis set.[50–58] In addition to acting as a reagent, 1,2-epoxybutane was considered as implicit solvent (ε = 13.9) based on the SMD continuum model developed by Truhlar et al.[59] Energy minima and transition states were classified according to the number of imaginary vibrational modes (zero and one, respectively) obtained through harmonic frequency calculations. Thermal Gibbs energy corrections were determined by assuming an ideal gas at 298.15 K and 1 atm. Subsequently, the electronic energy was corrected via single-point calculations using the same level of theory, but with an increased triple-z basis set: 6-311++G(d,p).[55–57,60–62] Therefore, Gibbs energies discussed in this study are at the theoretical level (SMD: 1,2-epoxybutane)B3LYP-D3/6-311++G(d,p)//B3LYP-D3/6-31++G(d,p), which follows state-of-the-art protocols for modelling reaction mechanisms[63] and reproduces reliable energies associated with diverse chemical reactions.[64–66] Frontier molecular orbitals and their energies are reported with the same theoretical quality.

Hardness (η) is a reactivity descriptor developed by Parr and Pearson within the conceptual DFT theory, measuring the capacity of a chemical entity to react.[67] Application of vertical ionization potential (I) and electron affinity (A) yields to the operational definition $\eta = ½(I\text{-}A)$. Assuming Koopman's theorem,[68] I and A can be approximated by the negative values of the HOMO and LUMO energies, ε_{HOMO} and ε_{LUMO}, respectively. Hence, the useful equation $\eta = ½(\varepsilon_{LUMO}\text{-}\varepsilon_{HOMO})$ is derived.[69] Although Koopman's theorem has been proven within the Hartree-Fock framework, the latter approximation has demonstrated usefulness in conceptual DFT formalism, describing reactivity trends accurately.[70–72] Moreover, it is acknowledged that the lower the hardness, the more reactive the corresponding compound, and *vice versa*. This is recognized as the Pearson's maximum hardness principle (MHP),[73,74] which is utilized in this work to evaluate the catalytic activity of the different proposed atranes.

2.4. Results and Discussion

2.4.1. Predicting the past: reaction mechanism of the cycloaddition reaction catalysed by triethanolamine borate.

The energy profile corresponding to the cycloaddition reaction between carbon dioxide (CO_2) and 1,2-epoxybutane is presented in **Figure 2.1**. The initial step involves the formation of the Lewis adduct **I-1** between the epoxide and the catalyst. This step requires cleavage of the transannular N–B single bond within atrane **1**, accompanied by the formation of a new O–B single bond between the epoxide oxygen atom and boron. Here, the epoxide acts as the catalyst activator, facilitating the transformation of **1** from its initial *endo-endo* conformation to the active *exo-exo* arrangement. However, the Gibbs energy associated with this activation step is relatively high ($\Delta G_{R\rightarrow I\text{-}1}$ = 19.5 kcal mol^{-1}), primarily due to the weak nucleophilicity of the epoxide responsible for catalyst activation. Interestingly, the transition state **TS-1** involves a high-energy pentacoordinate boron atom, analogous to the transition state characteristic of an S_N2-type reaction.

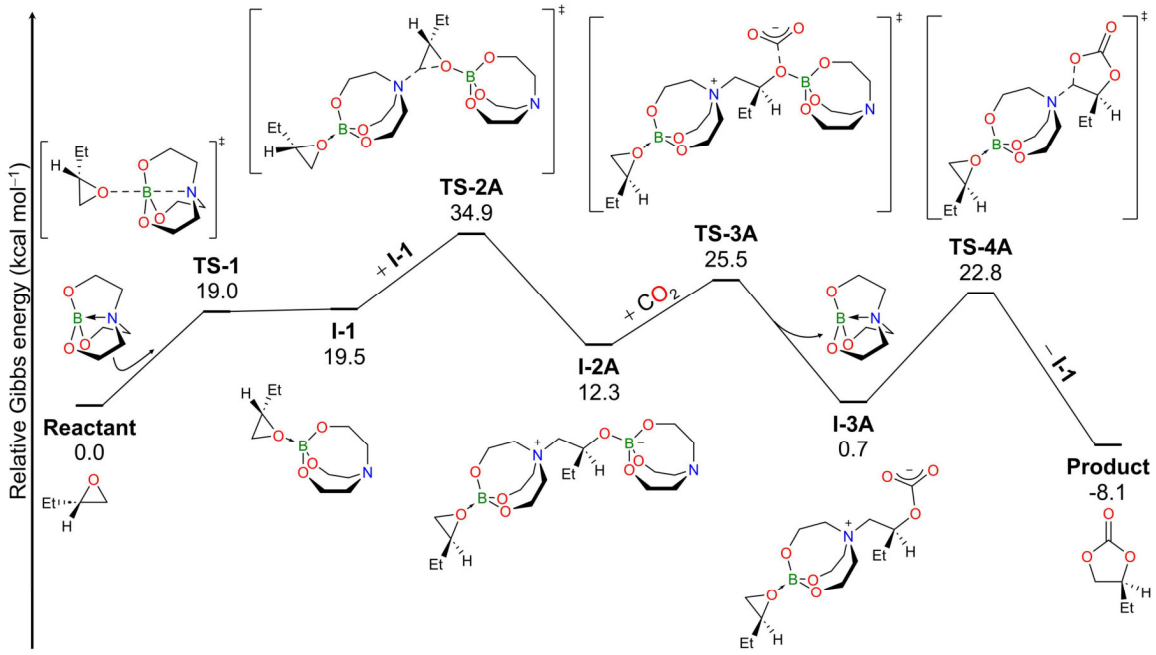


Figure 2.1. Gibbs energy profile for the cycloaddition reaction between 1,2-epoxybutane and CO_2, producing a cyclic carbonate catalysed by **1**. Energy values (kcal mol^{-1}) were calculated at the (SDM: 1,2-epoxybutane)B3LYP-D3/6-311++G(d,p)//B3LYP-D3/6-31++G(d,p) level.

It is noteworthy that **TS-1** is computed to be lower in energy than **I-1**, potentially leading to a misinterpretation of the energy profile. Nevertheless, since the connectivity of **TS-1** along the reaction coordinate in both forward and inverse directions has been successfully verified, this unusual result can be rationalized by considering that the potential energy surface (PES) in this region is relatively flat. Consequently, **TS-1** and **I-1** lie very close in energy, making it difficult to distinguish them clearly with the resolution of the theoretical level employed.

Once the catalyst has been activated, the tertiary amine moiety acts as the basic centre, while the boron atom serves as the Lewis acidic centre. The latter is already fulfilling its acidic function by coordinating the epoxide group. The subsequent reaction step involves two equivalents of **I-1**, where the basic site of the catalyst nucleophilically attacks the epoxide moiety of a second molecule, leading to a ring-opening reaction via **TS-2A**. At this point, two key facts must be emphasized: (1) catalyst activation generates a more effective nucleophile, namely the tertiary amine fragment; and (2) the electrophilicity of the epoxide significantly increases upon coordination to the acidic boron centre of the catalyst. These considerations strongly support the proposed transition state for the ring-opening reaction (**TS-2A**), which is identified as the rate-determining step, consistent with previous literature reports.[75]

The reaction profile then proceeds with the electrophilic addition of CO_2, yielding intermediate **I-3A**. Subsequently, one equivalent of catalyst **1** dissociates. The final ring-closing step occurs through transition state **TS-4A**, producing the targeted cyclic carbonate and regenerating the catalytically active species **I-1**. This regeneration is essential for sustaining the catalytic cycle, despite encountering a high energy barrier for the rate-determining step ($\Delta G^{\ddagger}_{R\rightarrow TS\text{-}2A}$ = 34.9 kcal mol^{-1}). The overall reaction is exergonic, with a Gibbs energy release of –8.1 kcal mol^{-1} ($\Delta G_{R\rightarrow P}$), demonstrating favourable thermodynamics for the chemical process.

2.4.2. After-the-fact explanations: synergistic activity of bromide as cocatalyst.

When bromide is employed as a cocatalyst (**Figure 2.2**), notable differences in the reaction mechanism and its associated thermochemistry emerge. The initial reaction step remains unchanged, involving catalyst activation by the epoxide. Interestingly, despite bromide being a stronger nucleophile, no favourable activation pathway concerning the halide was identified. The main distinction in the energy profile appears during the epoxide ring-opening reaction, which is now facilitated by bromide, rather than a second equivalent of the high-

energy Lewis adduct **I-1**. From this point, the reaction mechanism follows the same previously described pathway: electrophilic addition of CO_2, dissociation of **1**, and ultimately ring closure to yield the cyclic carbonate—completing the overall cycloaddition reaction. In this case, the catalytically active species **I-1** is not regenerated. However, consistent with earlier observations, the rate-determining step remains the epoxide ring-opening reaction, presenting a total energy barrier ($\Delta G^{\ddagger}_{R\rightarrow TS\text{-}2B}$) of 27.4 kcal mol^{-1}, which is 7.5 kcal mol^{-1} lower than the barrier calculated without the cocatalyst ($\Delta G^{\ddagger}_{R\rightarrow TS\text{-}2A}$ = 34.9 kcal mol^{-1}). This kinetic improvement aligns with experimental results that show enhanced reaction yields under identical experimental conditions when employing the cocatalyst.

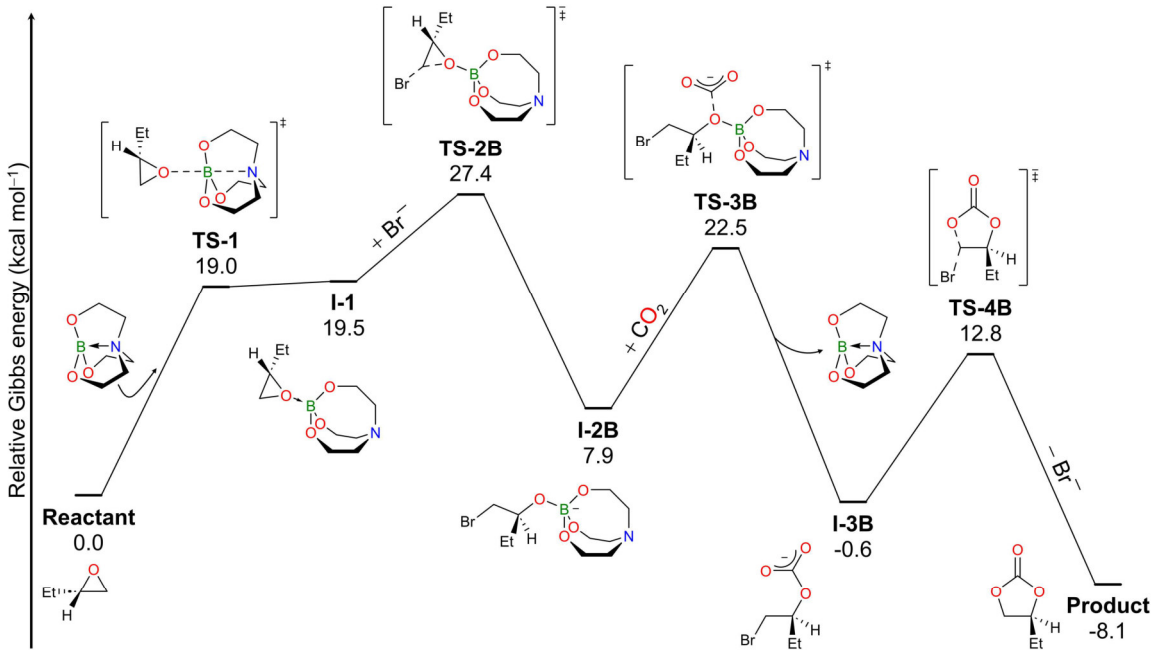
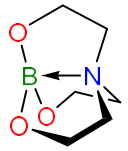


Figure 2.2. Gibbs energy profile for the cycloaddition reaction between 1,2-epoxybutane and CO_2, producing a cyclic carbonate catalysed by **1** and bromide (Br^-)**.** Energy values (kcal mol^{-1}) were calculated at the (SDM: 1,2-epoxybutane)B3LYP-D3/6-311++G(d,p)//B3LYP-D3/6-31++G(d,p) level.

2.4.3. Computational design of new catalysts.

In order to optimize the kinetics of the cycloaddition reaction described above, a new set of atrane-type catalysts, inspired in **1**, was designed (**Chart 2.3**). Composition modifications focused on atom substitutions within the framework of **1** were implemented. Specifically,

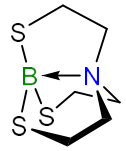
oxygen atoms were replaced by sulphur (equatorial group **E**), and nitrogen atom was substituted by phosphorus (basic centre **Y**). This modification strategy involves replacing first-row p-block elements with second-row analogues from the periodic table.



1

endo-endo

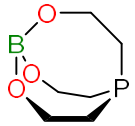
1.690



2

endo-endo

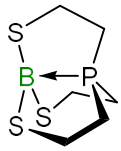
1.686



3

exo-exo

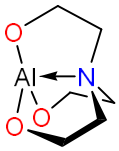
3.156



4

endo-endo

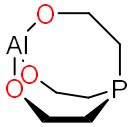
1.953



5

endo-endo

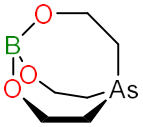
1.974



6

exo-exo

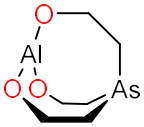
3.246



7

exo-exo

3.220



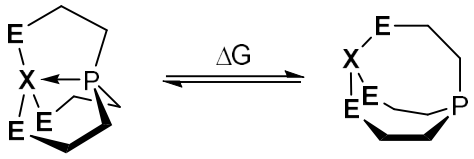
8

endo-exo

2.980

Chart 2.3. Novel atranes proposed herein to study their catalytic activity towards the cycloaddition reaction between 1,2-epoxybutane and CO_2. Each structure is drawn in its lowest-energy conformation. Intramolecular lengths between Lewis's donor (N, P, and As atoms) and acceptor (B and Al atoms) are indicated in Å.

Table 2.1. Exo-exo/endo-endo conformational equilibria for selected atranes.



endo-endo *exo-exo*

Atrane	X	E	ΔG (kcal mol^{-1})
3	B	O	–18.4
4	B	S	19.9
6	Al	O	–2.4

Before exploring potential thermochemical changes in the catalytic cycle, it was essential to investigate the *exo-exo*/*endo-endo* conformational equilibrium for these newly proposed catalysts. For **2**, as with **1**, only the *endo-endo* conformer is identified as a local minimum. However, for atranes **3** and **4**, both *endo-endo* and *exo-exo* conformations are energy minima. Interestingly, catalyst **3** favors the *exo-exo* conformation energetically, whereas **4** exhibits greater stability in the *endo-endo* arrangement, as summarized in **Table 2.1**.

2.4.4. Measuring activity of the equatorial (E) and Lewis's donor (Y) groups.

After identifying the most stable conformer of the newly proposed atranes, the rate-determining step (i.e., the epoxide ring-opening) was recalculated using bromide as a cocatalyst. The resulting energy profiles (**Figure 2.3**) indicate that **2** and **4** are less suitable alternatives in comparison to catalyst **1**, as evidenced by their higher energy barriers ($\Delta G^{\ddagger}_{R\rightarrow TS\text{-}2B}$ = 33.5, 30.5, and 27.4 kcal mol^{-1} for **2**, **4**, and **1**, respectively). Nevertheless, **3** emerges as a particularly promising candidate, significantly reducing the corresponding

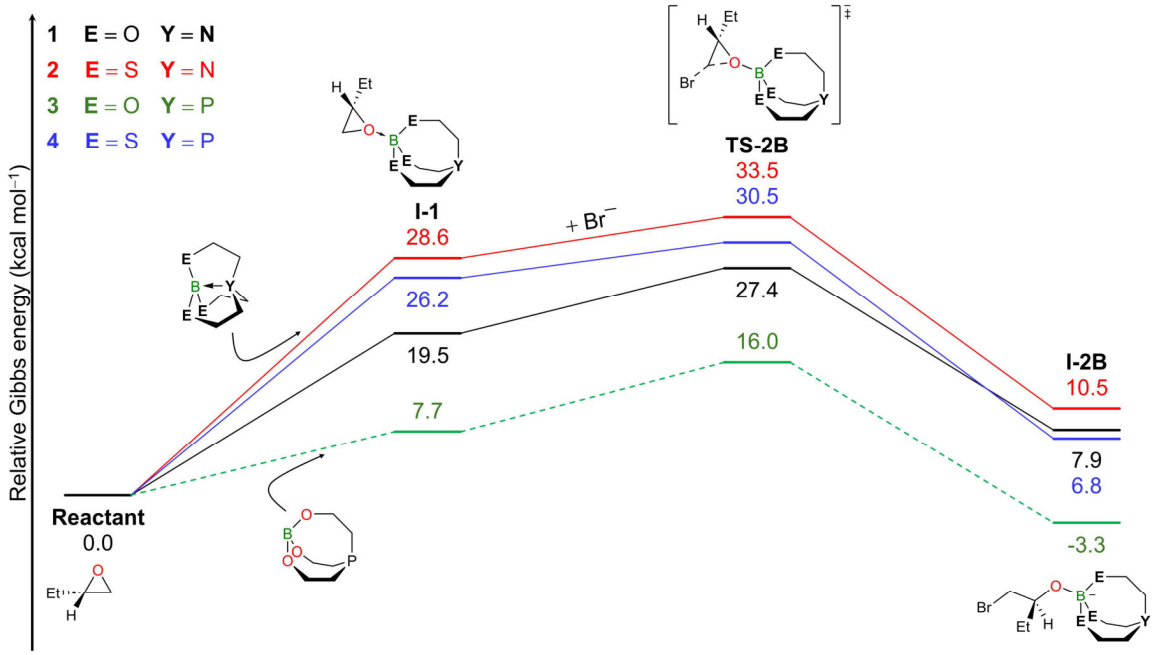


Figure 2.3. Gibbs energy profiles for the ring-opening reaction of 1,2-epoxybutane catalysed by atranes **1**–**4** and bromide (Br^-)**.** Energy values (kcal mol^{-1}) were calculated at the (SDM: 1,2-epoxybutane)B3LYP-D3/6-311++G(d,p)//B3LYP-D3/6-31++G(d,p) level.

energy barrier from 27.4 kcal mol^{-1} (**1**) to 16.0 kcal mol^{-1}. This remarkable outcome provides a practical demonstration of the catalytic activity being regulated by conformational dynamics (i.e., *exo-exo*/*endo-endo* equilibrium). In contrast to **1**, **2** and **4**, the *exo-exo* conformer of **3**, being energetically favorable, is inherently the catalytically active form, thus eliminating the necessity of an external nucleophilic agent to induce catalyst activation. This conclusion is further supported by the substantially lower Gibbs energy for the epoxide coordination step ($\Delta G_{R\rightarrow I\text{-}1}$), decreasing from 19.5 kcal mol^{-1} (**1**) to 7.7 kcal mol^{-1} (**3**). The nearly 12 kcal mol^{-1} difference in Gibbs energy for this step directly translates into a corresponding reduction in the total energy barrier ($\Delta G^{\ddagger}_{R\rightarrow TS\text{-}2B}$) from 27.4 kcal mol^{-1} (**1**) to 16.0 kcal mol^{-1} (**3**), confirming the kinetic advantage of **3**. Hence, rational structural modifications can effectively enhance catalytic performance by stabilizing the active species (i.e., *exo-exo* conformer), leading to a reduction in the Gibbs energy demanded for reaction progression.

2.4.5. Measuring activity of the Lewis's acceptor (X) and donor (Y) centres.

Up to this point, it has become clear that substituting oxygen atoms with sulfur in the original atrane **1** negatively impacts the catalytic performance (e.g., **2** and **4**). On the other hand, replacing the nitrogen atom with phosphorus, while retaining oxygen atoms, effectively reduces the energy barrier associated with the rate-determining step (e.g., **3**). In light of these new insights, oxygen atoms were fixed, and the effects on reaction thermochemistry by substituting the boron atom with aluminium (acidic centre **X**) were examined. Furthermore, the range of the donor atom **Y** was expanded to include N, P, and As, as illustrated in **Chart 2.3**. Firstly, a comprehensive conformational analysis was performed to assess the relative stability of the *endo-endo* and *exo-exo* conformers across these novel atranes. Compound **5**, similar to previous cases, exclusively shows the *endo-endo* conformer as a local minimum. Conversely, **6** exhibits both *endo-endo* and *exo-exo* conformers, with the latter being energetically favoured (**Table 2.1**). Regarding the As-containing atranes, only one local minimum is observed for each compound: the *exo-exo* conformer for **7**, and the less typical *endo-exo* conformer for **8**.

In pursuit of greener catalytic systems,[76–79] investigating the reaction mechanism in the absence of a cocatalyst was compelling, aiming to propose a catalyst capable of facilitating cycloaddition without relying on halogenated additives. Before discussing the thermochemical outcomes under these conditions, it is important to highlight key geometrical features of these newly designed atranes in order to differentiate their reactivity concerning

the ring-opening step. Notably, catalyst **5** is unique in having its basic centre initially deactivated, warranting separate examination according to the mechanism shown in **Figure 2.1**. In this scenario, epoxide plays a crucial role in catalyst activation, as previously argued. However, the activation process is compromised by the presence of Al, which exhibits a hypercoordinated environment in **I-1** (red plot in **Figure 2.4**), displaying a coordination number of five. Such hypercoordination at the Al centre can be attributed to the greater availability of d-type orbitals, contrasting with the bonding scenario observed when a boron atom occupies the same position (black plot in **Figure 2.4**). This phenomenon aligns well with previous findings documented in numerous studies.[80–88] Nevertheless, the enhanced exergonicity of the epoxide coordination step ($\Delta G_{R\rightarrow I\text{-}1}$ = 19.5 and –12.5 kcal mol^{-1} for **1** and **5**, respectively), due to hypercoordination at the Al centre, directly compromises the energy barrier corresponding to the epoxide ring-opening process, which increases from 34.9 kcal mol^{-1} ($\Delta G^{\ddagger}_{R\rightarrow \mathbf{1}\text{-}TS\text{-}2A}$) to 35.2 kcal mol^{-1} ($\Delta G^{\ddagger}_{\mathbf{5}\text{-}I\text{-}1\rightarrow\mathbf{5}\text{-}TS\text{-}2A}$). This is indicative of the catalyst basic centre remaining partially deactivated in intermediate **5-I-1**, reflecting a crucial difference when transitioning from B to Al within atrane skeleton.

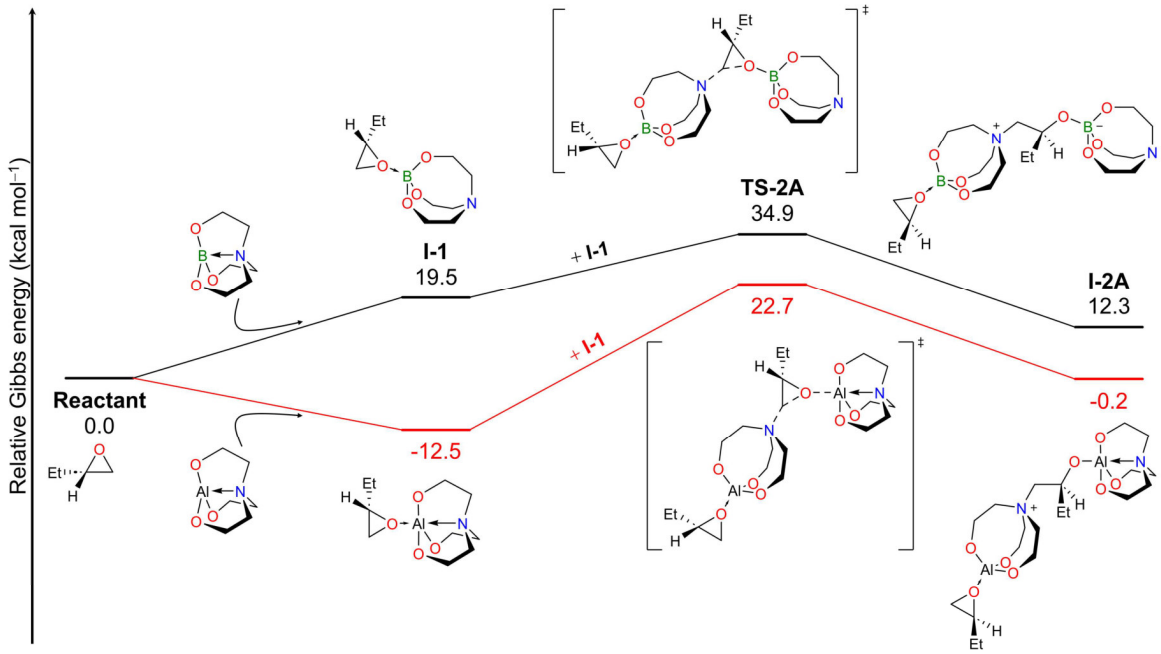


Figure 2.4. Gibbs energy profiles for the ring-opening reaction of 1,2-epoxybutane catalysed by atrane **5** (red) in comparison to **1** (black). Energy values (kcal mol^{-1}) were calculated at the (SDM: 1,2-epoxybutane)B3LYP-D3/6-311++G(d,p)//B3LYP-D3/6-31++G(d,p) level.

A significant improvement in the reaction thermochemistry was observed upon analysing catalysts **3** and **6**–**8** (**Figure 2.5**). In this group of atranes, the basic centre is intrinsically activated due to the conformation of their most stable structures. This structural feature notably reduces the total energy barrier ($\Delta G^{\ddagger}_{R\rightarrow TS\text{-}2C}$) to 27.6 (**7**), and 22.5 kcal mol^{-1} (**3**). Similarly, for catalyst **6** and **8**, the barrier ($\Delta G^{\ddagger}_{I\text{-}1\rightarrow TS\text{-}2C}$) decreased to 16.8 (**8**), and 11.6 kcal mol^{-1} (**6**). It is important to emphasize that when compared to the reaction profile of atrane **1**, which served as the initial reference for this study (**Figure 2.1**), atranes **3**, **6**, **7**, and **8**, enhanced both kinetics and thermodynamics of the epoxide ring-opening reaction. Furthermore, the calculated energy barriers suggest that this reaction is now capable of occurring under mild conditions, thus eliminating demand for the halogenated cocatalyst.

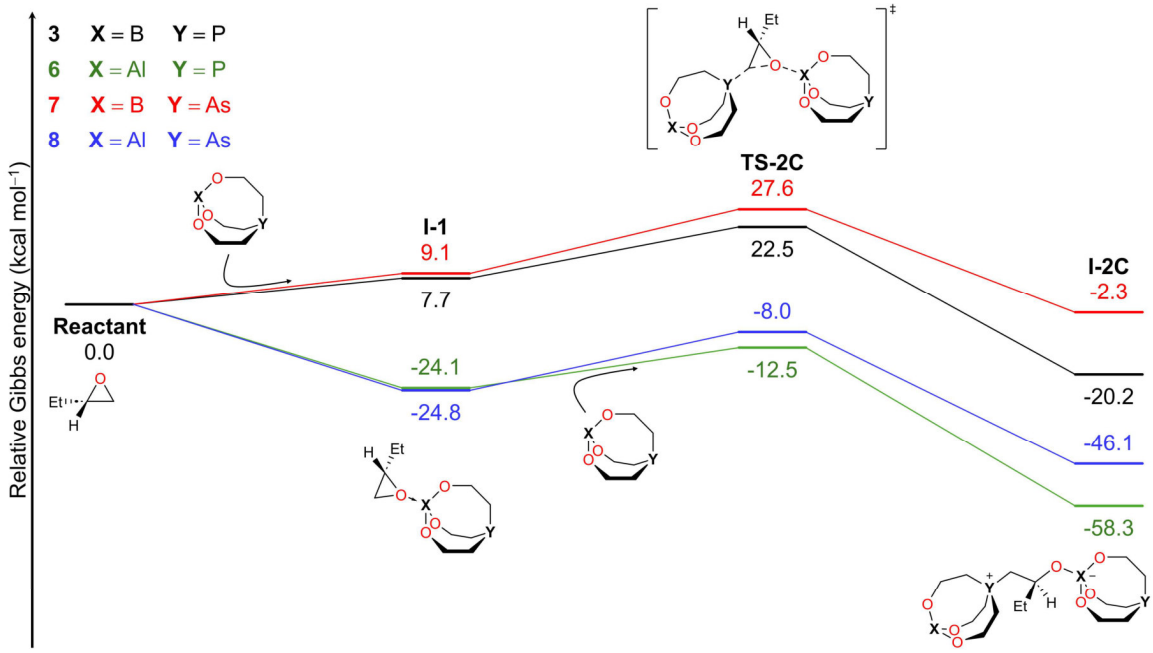


Figure 2.5. Gibbs energy profiles for the ring-opening reaction of 1,2-epoxybutane catalysed by atranes **6**–**8** in comparison to **3**. Energy values (kcal mol^{-1}) were calculated at the (SDM: 1,2-epoxybutane)B3LYP-D3/6-311++G(d,p)//B3LYP-D3/6-31++G(d,p) level.

Interestingly, the ring-opening reaction steps become increasingly exergonic upon substituting B for Al atom (**Figures 2.4**–**2.5**). Moreover, among the Al-containing atranes studied herein, only **5** shows a hypercoordinated Al centre. As discussed previously, this factor plays a pivotal role in the reaction coordinate. In contrast to intermediate **5-I-1**, which has been stated to be partially deactivated, the basic catalytic centre in **6** and **8** is fully

activated from the beginning, as evidenced by the most stable conformer in each case. Then, their catalytic activity is maintained thanks to the absence of hypercoordination at the Al centre in intermediates **6-I-1** and **8-I-1**.

Additionally, the Lewis adduct **I-1** stability, which is formed by epoxide coordination in the catalyst acid centre, is also a fundamental requisite to ensure reliable thermochemistry. The findings of this study demonstrate that epoxide coordination is more exergonic when employing aluminium as the acid centre, rather than boron. Therefore, it is concluded that the improved kinetics and thermodynamics observed in catalysts **6** and **8** can be attributed to two main factors: the presence of aluminium as a better acid centre, promoting epoxide coordination; and the *exo* arrangement of the basic site, facilitating ring-opening reaction. Collectively, these two factors ensure optimal activity through maximizing Lewis's acid-base synergistic effect—a phenomenon inherent in atranes. The absence of hypercoordination when atranes **6** and **8** are utilized, in contrast to **5**, is an intriguing feature that deserves a detailed and rigorous exploration in future research to deepen the understanding of the chemical bonding involved.

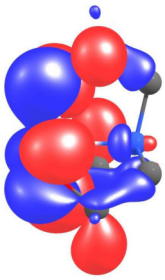
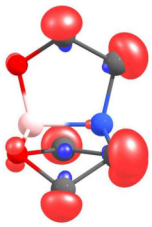
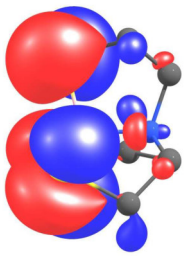
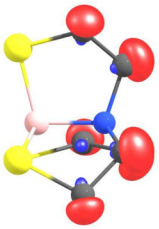
2.4.6. Description of the FMOs to reveal reactivity patterns.

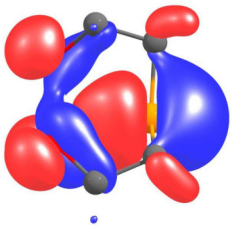
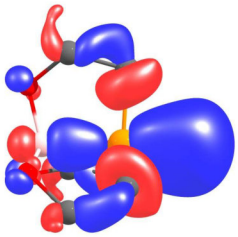
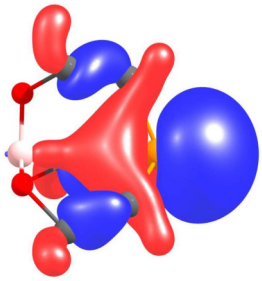
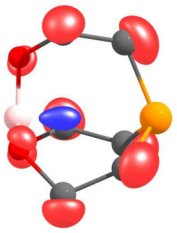
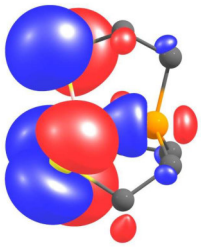
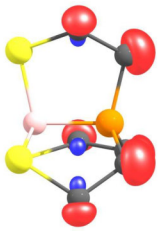
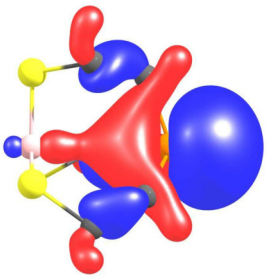
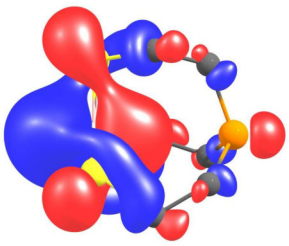
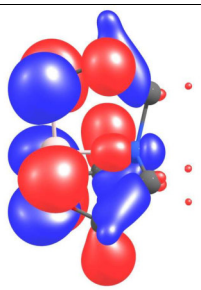
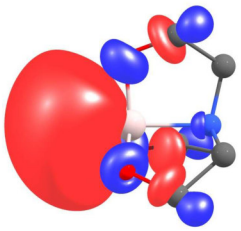
The aforementioned arguments, which are utilized to elucidate the observed reactivity trends, are significantly supported when analysing the frontier molecular orbitals (FMOs) of the involved atranes (**Table 2.2**). For instance, HOMOs of **3**, **6**, **7**, and **8**, whose lowest-energy conformation is the *exo-exo* arrangement, reveal a significant contribution from a p-type orbital centred on the donor atom (e.g., **Y** = P or As), suggesting a superior availability of the corresponding free electron pair in this basic site. In contrast, this phenomenon is not evident in the remaining atranes (**1**, **2**, **4**, and **5**), where *endo-endo* conformation is favoured. Consequently, the hypothesis that the *exo-exo* conformer is the active catalytic species is substantiated. A similar conclusion is reached upon analysis of the LUMOs. A comparison of the B-containing atranes (**1**–**4**, and **7**) with the Al-containing (**5**, **6**, and **8**), in their lowest energy conformation, reveals that Al atom contributes significantly to this orbital, in contrast to the behaviour of the B atom, which participates almost nothing in most cases. This result supports the notion that Al is a superior acid centre in comparison to B, in agreement with the earlier discussed thermochemical results.

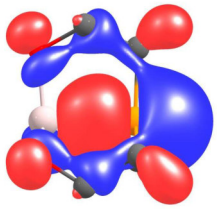
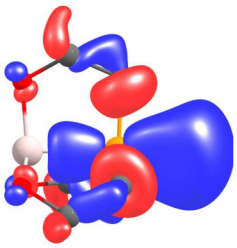
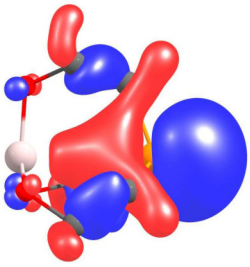
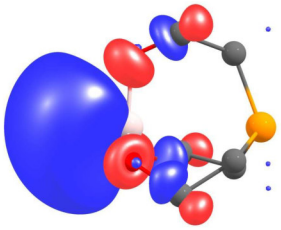
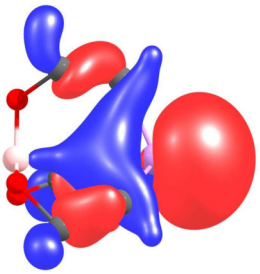
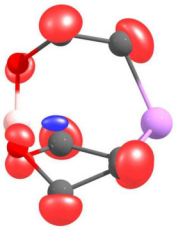
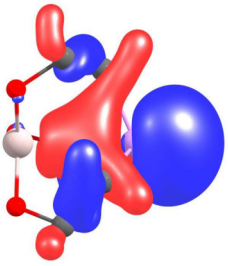
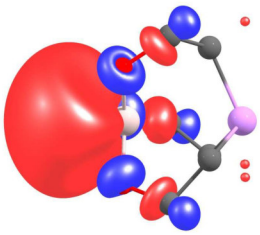
An explanation of the conformational equilibria calculated (**Table 2.1**) is found when analysing FMOs of atranes **3**, **4** and **6** separately. These compounds are unique because of exhibiting a formal *exo-exo*/*endo-endo* equilibrium, in contrast to the rest. Notably, the p-

type orbital centred on the Lewis basic atom displays a more substantial contribution in the HOMOs of $\mathbf{3}_{xx}$, $\mathbf{4}_{xx}$, and $\mathbf{6}_{xx}$ in comparison to their *endo-endo* conformers $\mathbf{3}_{nn}$, $\mathbf{4}_{nn}$, $\mathbf{6}_{nn}$. Moreover, an examination of LUMOs for the conformers of **3** and **4** indicates significant discrepancies (e.g., $\mathbf{3}_{nn}$ *vs.* $\mathbf{4}_{nn}$, or $\mathbf{3}_{xx}$ *vs.* $\mathbf{4}_{xx}$). The case of **6** is worthy to note due to exhibiting a cross similarity: $\mathbf{6}_{nn}$-LUMO is analogous to $\mathbf{3}_{nn}$-LUMO, while $\mathbf{6}_{xx}$-LUMO is comparable to $\mathbf{4}_{xx}$-LUMO. Therefore, the FMOs for the conformers of **6** manifests an intermediate character between those of **3** and **4**. This finding aligns with the Gibbs energy values for conformational equilibrium in each case (**Table 2.1**). It was shown that the most stable arrangement of atrane **3** is *exo-exo* ($\Delta G_{nn\rightarrow xx}$ = –18.4 kcal mol^{-1}), while **4** prefers the *endo-endo* conformation ($\Delta G_{nn\rightarrow xx}$ = 19.9 kcal mol^{-1}). For **6**, a value close to equilibrium was obtained ($\Delta G_{nn\rightarrow xx}$ = –2.4 kcal mol^{-1}), which is an intermediate amount between the Gibbs energy related to **3** and **4**.

Table 2.2. HOMO and LUMO orbitals and their energies (eV), in conjunction with hardness η (eV), for atranes **1**–**8**.

	HOMO	LUMO	η
			
1	–7.215	0.011	3.613
			
2	–5.706	–0.019	2.843

			
3$_{nn}$	–6.515	–0.484	3.015
			
3$_{xx}$	–6.164	–0.115	3.024
			
4$_{nn}$	–5.619	–0.064	2.778
			
4$_{xx}$	–5.992	–1.711	2.140
			
5	–7.225	–0.369	3.428

			
6$_{nn}$	–6.349	–0.461	2.944
			
6$_{xx}$	–6.091	–0.963	2.564
			
7	–6.167	–0.060	3.053
			
8	–6.448	–0.502	2.973

FMOs also illuminate the impact of substituting O atoms (**1** and **3**) with S atoms (**2** and **4**) as equatorial groups **E** in the initial atrane framework. A comparison of HOMOs for **1**–**4** in their *endo-endo* conformation reveals electron delocalization from the O atoms (atranes **1** and **3**$_{nn}$) towards the acid centre B (i.e., n→p partial donation). In the case of S-containing atranes (**2** and **4**$_{nn}$), this donation appears to be negligible because of the presence of more localized orbitals centred on the sulphur atoms. This finding is reasonable,

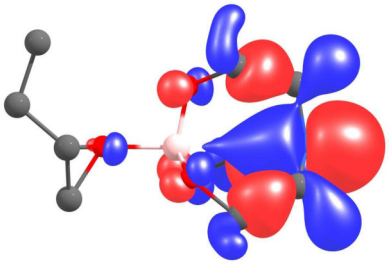
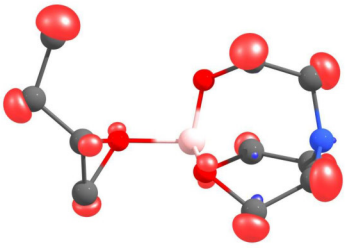
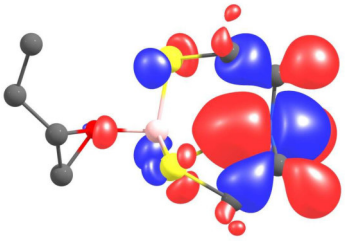
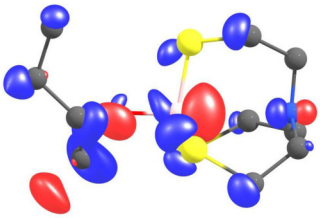
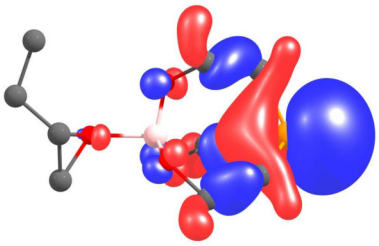
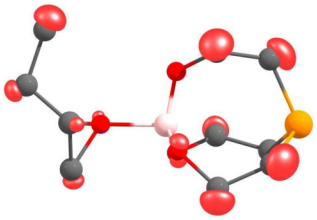
since boron 2p free orbital is anticipated to interact more effectively with oxygen 2p orbitals, while a poorer overlap is expected with the sulphur 3p orbitals. Moreover, the stabilization of the B centre, driven by electron delocalization from neighboring atoms (e.g., **E** = O or S), is reflected in the transannular interaction lengths: 1.690 (**1**), 1.686 (**2**), 1.979 (**3*nn***), and 1.953 Å (**4*nn***). Notably, the transannular length is reduced when S atoms surround the acid B centre (e.g., **1** *vs.* **2**, or **3*nn*** *vs.* **4*nn***). This outcome indicates that S atoms bonded to the B centre electronically destabilize it, favoring a stronger transannular interaction (e.g. N–B or P–B). This phenomenon is consistent with the preceding analysis on the **3*nn*** and **4*nn*** HOMOs. As previously discussed, **3*nn***-HOMO exhibits a greater availability of the free electron pair located in the basic site than the **4*nn***-HOMO.

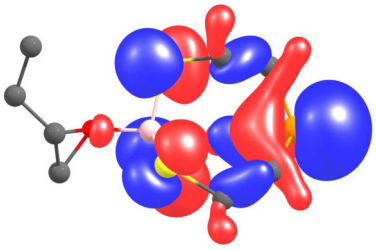
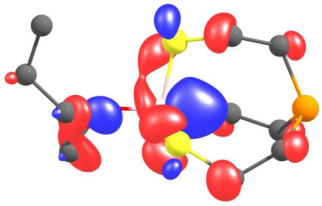
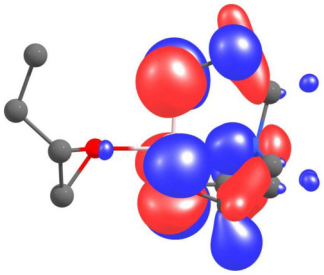
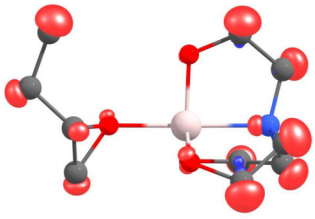
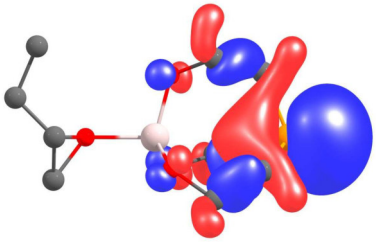
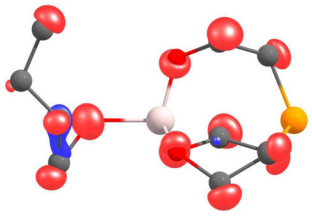
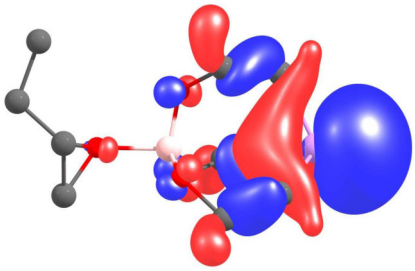
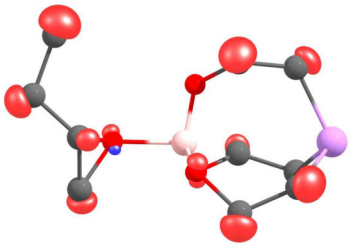
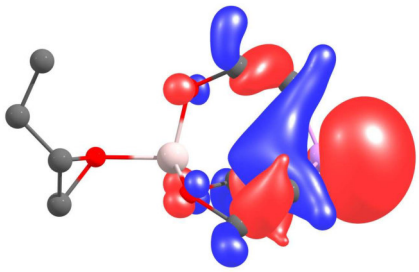
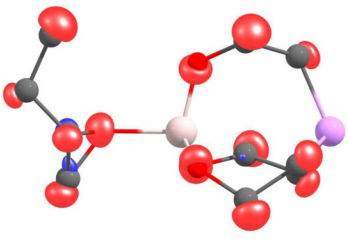
The conclusion regarding the stabilization of the acid centre by neighboring atoms provides a further explanation for the calculated conformational equilibria (**Table 2.1**). However, it is important to highlight that the increased destabilization of the acid centre by surrounding atoms (i.e., **E** groups), constituting the initial atrane, results in a stronger transannular interaction, thus stabilizing the *endo-endo* conformation. Consequently, the catalyst activation process becomes more demanding. This effect is illustrated in **Figure 2.3** (e.g., **1** *vs.* **2**, or **3** *vs.* **4**), even though S-containing atranes are globally softer that O-containing (**Table 2.2**). Hence, the present study emphasizes that catalytic activity of atranes is strongly associated with the stabilization of the transannular bond, which can be modulated by the equatorial functional groups bonded to the acid centre. The ideal scenario is when the **E**-type atoms stabilize the acid centre **X** sufficiently to prevent the formation of the transannular bond **Y**–**E**, thus favoring the *exo-exo* arrangement, which is the catalytically active species.

Regardless of the initial atrane conformer, it is noteworthy that HOMOs of intermediates **I-1** are principally constituted by a p-type orbital centred on the basic atom (**Table 2.3**). Such an orbital description, in conjunction with the *exo-exo* arrangement adopted by the atrane moiety, indicates catalyst activation upon coordination of epoxide, rendering the electronic lone pair accessible to react. Interestingly, catalyst **5** is the only case that deviates from this annotation. In this instance, the electron pair in the basic site remains partially engaged to stabilize the Al centre, which adopts a hypercoordinated environment. This is consistent with the previously stated reactivity, which postulates compromised catalytic activity due to the hypercoordination of the Al atom in **5-I-1**. Additionally, LUMOs are found to be partially located on the epoxide fragment, reinforcing the proposed reaction mechanism.

It is highlighted here that the difference between employing B or Al as acid centre (**X** site); O or S atoms (**E** site); and N, P, or As being the basic centre (**Y** site) is practically negligible in relation to FMOs of **I-1**. Hence, it is suggested that atomic substitutions play a more crucial role in the activation process of the catalyst. However, further computational characterization is required to ensure this conclusion utilizing other types of analysis beyond orbital.

Table 2.3. HOMO and LUMO orbitals and their energies (eV) for the Lewis adduct **I-1**, produced by atranes **1**–**8**.

	HOMO	**LUMO**
		
1	–5.350	–0.002
		
2	–5.318	–0.060
		
3	–5.847	–0.053

			
4	–5.555	–0.227	
			
5	–6.760	–0.004	
			
6	–5.739	–0.122	
			
7	–5.879	–0.011	
			
8	–5.784	–0.080	

2.4.7. Elucidating reactivity trends via statistical analysis.

Performing statistical analysis on the calculated thermochemical data enabled the identification of two significant linear correlations (**Figure 2.6**). The present examination is conducted exclusively on the absence of cocatalyst, as illustrated in **Figures 2.4**–**2.5**. Initially, a strong correlation (R^2 = 0.9362) is identified between the total energy barrier and the reaction energy associated with the ring-opening step ($\Delta G_{R\rightarrow I\text{-}2}$). In a similar manner, total energy barrier and initial hardness (η) of the catalyst are significantly correlated (R^2 = 0.8902). These results offer two key insights: total energy barrier is directly proportional to the exergonicity of the epoxide ring-opening reaction, and to the catalyst's hardness. The first conclusion is a Brønsted-Evans-Polanyi (BEP) relationship,[89–94] while the subsequent one

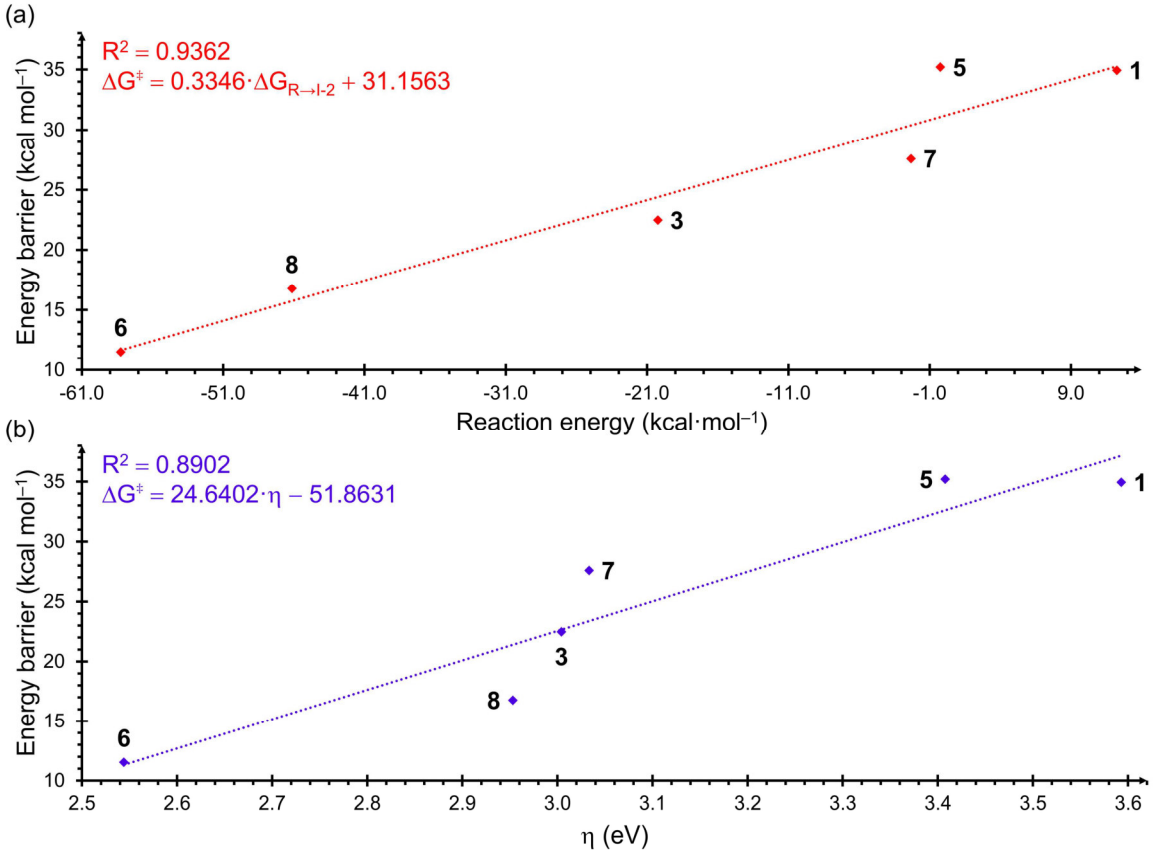


Figure 2.6. Statistical analysis from thermochemistry data regarding the ring-opening reaction between 1,2-epoxybutane and various atranes. Linear correlation of total energy barrier with (a) reaction energy of epoxide ring-opening step, and (b) atrane's hardness (η). All values were calculated at the (SDM: 1,2-epoxybutane)B3LYP-D3/6-311++G(d,p)//B3LYP-D3/6-31++G(d,p) level.

satisfies Pearson's maximum hardness principle.[73,74] It is imperative to emphasize that, in terms of reactivity, catalyst **1** is the lowest-performing candidate. However, it is the only one that has been synthesized, and its catalytic properties have been tested to date. Therefore, experimental characterisation of the catalytic activity of the remaining atranes (**2**–**8**) is strongly recommended.

2.4.8. Pondering the kinetics and thermodynamics of carbonate synthesis.

Finally, it is important to briefly discuss that, although different catalysts alter the thermochemistry and reaction pathways, as systematically categorized in the energy profiles above, the overall Gibbs energy of the reaction ($\Delta G_{R\rightarrow P}$) remains unchanged. Specifically, the formation of the cyclic carbonate through the reaction of 1,2-epoxybutane and CO_2 consistently releases a Gibbs energy of –8.1 kcal mol^{-1}, regardless of the external chemical agents employed. While certain atranes effectively lower the Gibbs energy barrier associated with the rate-determining step, they tend to form highly stable intermediates, such as **I-1** (e.g., intermediates formed by Al-containing atranes) or **I-2C**, potentially impeding the formation of the desired product. For instance, consider the extreme scenario during the ring-opening reaction catalysed by **6**. In this case, the corresponding intermediate **I-2C** exhibits substantial stability, being energetically favoured by –58.3 kcal mol^{-1} relative to the reactants ($\Delta G_{R\rightarrow I\text{-}2C}$, green plot in **Figure 2.5**). Given that the cyclic carbonate product has a Gibbs energy of –8.1 kcal mol^{-1} compared to the initial reactants ($\Delta G_{R\rightarrow P}$ in **Figures 2.1**–**2.2**), the formation of the product starting from intermediate **I-2C** requires overcoming a Gibbs energy change of 50.2 kcal mol^{-1}. This represents a significantly endergonic and thermodynamically unfavorable process.

Following this analysis, our computational results suggest that atrane **3** is particularly promising for cyclic carbonate synthesis, as it lowers the ring-opening barrier to 16.0 kcal mol^{-1} ($\Delta G^{\ddagger}_{R\rightarrow TS\text{-}2B}$, green plot in **Figure 2.3**) while avoiding the formation of overly stable intermediates. This facilitates the formation of cyclic carbonates as an exocyclic process. Although the reaction still needs a halogenated cocatalyst, the relatively low calculated energy barrier implies that mild reaction conditions, such as room temperature, would be necessary to ensure efficient catalysis. Moreover, it is noteworthy that while the other atranes studied herein may not significantly enhance the cycloaddition of 1,2-epoxybutane with CO_2, they remain valuable candidates as potential promoters for the ring-opening of epoxides, a reaction of broad relevance across diverse chemical applications.[95–97]

2.5. Conclusions

This work provides a detailed theoretical investigation into the catalytic performance and mechanistic behaviour of triethanolamine borate (**1**) regarding the cycloaddition reaction of 1,2-epoxybutane and CO_2. Employing a robust computational approach, such as DFT, new insights have been gained into the mechanism initially proposed by Ke and coworkers.[36] The stepwise reaction mechanism has been elucidated involving: (1) catalyst activation, (2) epoxide ring-opening, (3) CO_2 addition, and (4) ring closure, yielding the desired cyclic carbonate. Catalyst **1** acts as a bifunctional Lewis pair with boron centre activating the epoxide and the tertiary amine moiety acting as the nucleophile. However, the rate-determining ring-opening step exhibits a high energy barrier ($\Delta G^{\ddagger}_{R\rightarrow TS\text{-}2A}$ = 34.9 kcal mol^{-1}), limiting catalytic efficiency under mild conditions. This adversity is partially overcome by using bromide as a cocatalyst, which substantially lowers the associated barrier to 27.4 kcal mol^{-1}, in agreement with the improved reactivity observed experimentally.

To optimize catalytic activity, we explored a series of atranes (**Chart 2.3**) through systematic heteroatom substitution. Among these candidates, atrane featuring a boron-phosphorus core (**3**), emerged as a particularly promising system. This novel structure stabilizes the catalytically active *exo-exo* conformation, thus decreasing the ring-opening barrier to 16.0 kcal·mol^{-1}, which is a dramatic improvement in predicted reactivity. While other modified atranes also display favourable kinetics (e.g., **6**–**8**), some suffer from overly stabilized intermediates that may hinder product release. For instance, the Al- and P-containing atrane **6** forms a highly stable intermediate ($\Delta G_{R\rightarrow I\text{-}2C}$ = –58.3 kcal mol^{-1}) rendering the final step endergonic. These findings underscore the importance of balancing energy barrier and Lewis adduct (**I-1**) stability in catalyst design. Additionally, it has been shown that catalyst activity can be sensitively modulated according to the type of Lewis' acid-basic centres as well as by the equatorial groups embedded within the atrane skeleton.

Finally, our results demonstrate how predictive catalysis can guide the development of next-generation, halide- and metal-free systems for CO_2 fixation. The insights gained here provide a foundation for future experimental efforts, particularly those aimed at accessing low-barrier, selective, and recyclable catalytic systems. Atrane **3** emerges as a promising candidate for mild and sustainable CO_2 valorization in industrial and environmental applications, while catalysts **6**–**8** could potentially promote ring-opening reactions.

2.6. References

1. M. Cokoja, C. Bruckmeier, B. Rieger, W. A. Herrmann and F. E. Kühn, *Angew. Chem. Int. Ed Engl.*, 2011, **50**, 8510–8537.
2. Q. Liu, L. Wu, R. Jackstell and M. Beller, *Nat. Commun.*, 2015, **6**, 5933.
3. N. Yadav, F. Seidi, D. Crespy and V. D'Elia, *ChemSusChem*, 2019, **12**, 724–754.
4. W. Natongchai, S. Posada-Pérez, C. Phungpanya, J. A. Luque-Urrutia, M. Solà, V. D'Elia and A. Poater, *J. Org. Chem.*, 2022, **87**, 2873–2886.
5. T. Theerathanagorn, A. Vidal-López, A. Comas-Vives, A. Poater and V. D'Elia, *Green Chem.*, 2023, **25**, 4336-4349.
6. C. Maeda, T. Taniguchi, K. Ogawa and T. Ema, *Angew. Chem. Int. Ed.,* 2015, **54**, 134–138.
7. M.-R. Li, M.-C. Zhang, T.-J. Yue, X.-B. Lu and W.-M. Ren, *RSC Adv.*, 2018, **8**, 39182–39186.
8. F. D. Bobbink, D. Vasilyev, M. Hulla, S. Chamam, F. Menoud, G. Laurenczy, S. Katsyuba and P. J. Dyson, *ACS Catal.*, 2018, **8**, 2589–2594.
9. V. D'Elia, A. A. Ghani, A. Monassier, J. Sofack-Kreutzer, J. D. A. Pelletier, M. Drees, S. V. C. Vummaleti, A. Poater, L. Cavallo, M. Cokoja, J.-M. Basset and F. E. Kühn, *Chem. Eur. J.*, 2014, **20**, 11870–11882.
10. V. D'Elia, H. Dong, A. J. Rossini, C. M. Widdifield, S. V. C. Vummaleti, Y. Minenkov, A. Poater, E. Abou-Hamad, J. D. A. Pelletier, L. Cavallo, L. Emsley and J.-M. Basset, *J. Am. Chem. Soc.*, 2015, **137**, 7728–7739.
11. X. Meng, Z. Ju, S. Zhang, X. Liang, N. von Solms, X. Zhang and X. Zhang, *Green Chem.*, 2019, **21**, 3456–3463.
12. A. Mirabaud, J.-C. Mulatier, A. Martinez, J.-P. Dutasta and V. Dufaud, *ACS Catal.*, 2015, **5**, 6748–6752.
13. Y. Toda, Y. Komiyama, A. Kikuchi and H. Suga, *ACS Catal.*, 2016, **6**, 6906–6910.
14. A. C. S. Gonzalez, A. P. Felgueiras, R. T. Aroso, R. M. B. Carrilho and M. M. Pereira, *J. Organomet. Chem.*, 2021, **950**, 121979.
15. N. Liu, Y.-F. Xie, C. Wang, S.-J. Li, D. Wei, M. Li and B. Dai, *ACS Catal.*, 2018, **8**, 9945–9957.
16. Y. Liu, Z. Cao, Z. Zhou and A. Zhou, *J. CO2 Util.*, 2021, **53**, 101717.
17. C. Yue, W. Wang and F. Li, *ChemSusChem*, 2020, **13**, 5996–6004.
18. R. Das and C. M. Nagaraja, *Green Chem.*, 2021, **23**, 5195–5204.
19. Y.-R. Du, G.-R. Ding, Y.-F. Wang, B.-H. Xu and S.-J. Zhang, *Green Chem.*, 2021, **23**, 2411–2419.

20. R. Das, T. Ezhil, A. S. Palakkal, D. Muthukumar, R. S. Pillai and C. M. Nagaraja, *J. Mater. Chem. A*, 2021, **9**, 23127–23139.
21. L. Liu, S. Jayakumar, J. Chen, L. Tao, H. Li, Q. Yang and C. Li, *ACS Appl. Mater. Interfaces*, 2021, **13**, 29522–29531.
22. C.-J. Zhang, S.-Q. Wu, S. Boopathi, X.-H. Zhang, X. Hong, Y. Gnanou and X.-S. Feng, *ACS Sustainable Chem. Eng.*, 2020, **8**, 13056–13063.
23. D. Zhang, S. K. Boopathi, N. Hadjichristidis, Y. Gnanou and X. Feng, *J. Am. Chem. Soc.*, 2016, **138**, 11117–11120.
24. K. A. Andrea and F. M. Kerton, *ACS Catal.*, 2019, **9**, 1799–1809.
25. Y.-Y. Zhang, G.-W. Yang, R. Xie, L. Yang, B. Li and G.-P. Wu, *Angew. Chem. Int. Ed.*, 2020, **59**, 23291–23298.
26. H. C. Brown and E. A. Fletcher, *J. Am. Chem. Soc.*, 1951, **73**, 2808–2813.
27. A. Sonoda, N. Takagi, K. Ooi and T. Hirotsu, *Bull. Chem. Soc. Jpn.*, 1998, **71**, 161–166.
28. R. Li, J. Li, Y. Wang, J. Chen, Y. Lai and J. Hu, *Chem. Eng. J.*, 2024, **495**, 153193.
29. M. Zhou, L. Zhu, D. Pan, X. Luo, H. Liu, F. Qu, D. Zhao, Z. Xing, S. Jiao, J. Yan and Z. Jiang, *Corros. Sci.*, 2025, **256**, 113186.
30. G. Yang, J. Zhao, L. Cui, S. Song, S. Zhang, L. Yu and P. Zhang, *RSC Adv.*, 2017, **7**, 7944–7953.
31. M. Ocakoğlu, F. Şen and M. V. Kahraman, *Adv. Polym. Technol.*, 2017, **36**, 517–524.
32. Y. Wongnongwa, S. Pithakratanayothin, T. Chaisuwan, R. Tongsri, E. Buarod, T. Yotkaew and R. Krataitong, *Polym. Degrad. Stab.*, 2024, **229**, 110983.
33. J. G. Verkade, *Acc. Chem. Res.*, 1993, **26**, 483–489.
34. M. Marín-Luna, I. Alkorta and J. Elguero, *J. Organomet. Chem.*, 2015, **794**, 206–215.
35. A. K. Phukan and A. K. Guha, *Inorg. Chem.*, 2011, **50**, 1361–1367.
36. Y. Ge, G. Cheng and H. Ke, *J. CO2 Util.*, 2022, **57**, 101873.
37. T. Wang, D. Zheng, J. Zhang, B. Fan, Y. Ma, T. Ren, L. Wang and J. Zhang, *ACS Sustainable Chem. Eng.*, 2018, **6**, 2574–2582.
38. Y. Xie, J. Liang, Y. Fu, M. Huang, X. Xu, H. Wang, S. Tu and J. Li, *J. Mater. Chem. A*, 2018, **6**, 6660–6666.
39. X. Wu, C. Chen, Z. Guo, M. North and A. C. Whitwood, *ACS Catal.*, 2019, **9**, 1895–1906.
40. R. Monreal-Corona, A. Pla-Quintana and A. Poater, *Trends Chem.*, 2023, **5**, P935–946.
41. R. Monreal-Corona, À. Díaz-Jiménez, A. Roglans, A. Poater and A. Pla-Quintana, *Adv. Synth. Catal.*, **365**, 760–766.
42. S. Escayola, N. Bahri-Laleh and A. Poater, *Chem. Soc. Rev.*, 2024, **53**, 853–882.

43. Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
44. S. H. Vosko, L. Wilk and M. Nusair, *Can. J. Phys.*, 1980, **58**, 1200–1211.
45. C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785–789.
46. A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648–5652.
47. P. J. Stephens, F. J. Devlin, C. F. Chabalowski and M. J. Frisch, *J. Phys. Chem.*, 1994, **98**, 11623–11627.
48. S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.
49. S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456–1465.
50. R. Ditchfield, W. J. Hehre and J. A. Pople, *J. Chem. Phys.*, 1971, **54**, 724–728.
51. W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257–2261.
52. P. C. Hariharan and J. A. Pople, *Theoret. Chim. Acta*, 1973, **28**, 213–222.
53. J. D. Dill and J. A. Pople, *J. Chem. Phys.*, 1975, **62**, 2921–2923.
54. M. S. Gordon, J. S. Binkley, J. A. Pople, W. J. Pietro and W. J. Hehre, *J. Am. Chem. Soc.*, 1982, **104**, 2797–2803.
55. M. M. Francl, W. J. Pietro, W. J. Hehre, J. S. Binkley, M. S. Gordon, D. J. DeFrees and J. A. Pople, *J. Chem. Phys.*, 1982, **77**, 3654–3665.
56. T. Clark, J. Chandrasekhar, G. W. Spitznagel and P. V. R. Schleyer, *J. Comput. Chem.*, 1983, **4**, 294–301.
57. G. W. Spitznagel, T. Clark, P. von Ragué Schleyer and W. J. Hehre, *J. Comput. Chem.*, 1987, **8**, 1109–1116.
58. V. A. Rassolov, M. A. Ratner, J. A. Pople, P. C. Redfern and L. A. Curtiss, *J. Comput. Chem.*, 2001, **22**, 976–984.
59. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378–6396.
60. A. D. McLean and G. S. Chandler, *J. Chem. Phys.*, 1980, **72**, 5639–5648.
61. R. Krishnan, J. S. Binkley, R. Seeger and J. A. Pople, *J. Chem. Phys.*, 1980, **72**, 650–654.

62. L. A. Curtiss, M. P. McGrath, J.-P. Blaudeau, N. E. Davis, R. C. Binning Jr and L. Radom, *J. Chem. Phys.*, 1995, **103**, 6104–6113.
63. A. Lledós, *Eur. J. Inorg. Chem.*, 2021, **2021**, 2547–2555.
64. J. Tirado-Rives and W. L. Jorgensen, *J. Chem. Theory Comput.*, 2008, **4**, 297–306.
65. J. Sirirak, N. Lawan, M. W. Van der Kamp, J. N. Harvey and A. J. Mulholland, *PeerJ Phys. Chem.*, 2020, **2**, e8.
66. H. Li, E. Brémond, J. C. Sancho-García and C. Adamo, *RSC Adv.*, 2021, **11**, 26073–26082.
67. R. G. Parr and R. G. Pearson, *J. Am. Chem. Soc.*, 1983, **105**, 7512–7516.
68. T. Koopmans, *Physica*, 1934, **1**, 104–113.
69. R. G. Pearson, *Inorg. Chem.*, 1988, **27**, 734–740.
70. P. Geerlings, F. De Proft and W. Langenaeker, *Chem. Rev.*, 2003, **103**, 1793–1873.
71. B. Saha and P. K. Bhattacharyya, *RSC Adv.*, 2016, **6**, 79768–79780.
72. H. M. Gebremeskel, M. A. Welearegay and T. T. Nadew, *Quantum Engineering*, 2024, **2024**, 5343086.
73. R. G. Pearson, *J. Chem. Educ.*, 1987, **64**, 561–567.
74. W. Grochala, *Phys. Chem. Chem. Phys.*, 2017, **19**, 30964–30983.
75. Y. Ge, G. Cheng, N. Xu, W. Wang and H. Ke, *Catal. Sci. Technol.*, 2019, **9**, 4255–4261.
76. S. Pappuru and D. Chakraborty, *Eur. Polym. J.*, 2019, **121**, 109276.
77. L. Guo, K. J. Lamb and M. North, *Green Chem.*, 2021, **23**, 77–118.
78. A. Mitra, T. Biswas, S. Ghosh, G. Tudu, K. S. Paliwal, S. Ghosh and V. Mahalingam, *Sustainable Energy Fuels*, 2022, **6**, 420–429.
79. P. Lozano and E. García-Verdugo, *Green Chem.*, 2023, **25**, 7041–7057.
80. T. Ooi, D. Uraguchi, N. Kagoshima and K. Maruoka, *J. Am. Chem. Soc.*, 1998, **120**, 5327–5328.
81. K. Maruoka and T. Ooi, *Chem. Eur. J.*, 1999, **5**, 829–833.
82. T. Ooi, J. Morikawa, D. Uraguchi and K. Maruoka, *Tetrahedron Lett.*, 1999, **40**, 2993–2996.
83. R.-C. Yu, C.-H. Hung, J.-H. Huang, H.-Y. Lee and J.-T. Chen, *Inorg. Chem.*, 2002, **41**, 6450–6455.
84. F. A. Vengoechea-Gómez, M.-Á. Velázquez-Carmona, J. Barroso, G. Merino and M.-Á. Muñoz-Hernández, *Inorg. Chim. Acta*, 2018, **482**, 535–541.
85. H. Duan, R. You, S. Xu, Z. Li, K. Qian, T. Cao, W. Huang and X. Bao, *Angew. Chem. Int. Ed.*, 2019, **58**, 12043–12048.
86. H. Fish, S. Hart, K. J. Lamb, M. North, S. C. Z. Quek, A. C. Whitwood, B. Woods and X. Wu, *Dalton Trans.*, 2021, **50**, 587–598.

87. A. J. Kalita, K. Sarmah, F. Yashmin, R. R. Borah, I. Baruah, R. P. Deka and A. K. Guha, *Sci. Rep.*, 2022, **12**, 10041.
88. Z. Zhao, D. Xiao, K. Chen, R. Wang, L. Liang, Z. Liu, I. Hung, Z. Gan and G. Hou, *ACS Cent. Sci.*, 2022, **8**, 795–803.
89. D. Loffreda, F. Delbecq, F. Vigné and P. Sautet, *Angew. Chem. Int. Ed.*, 2009, **48**, 8978–8980.
90. R. S. Assary, L. J. Broadbelt and L. A. Curtiss, *J. Mol. Model.*, 2012, **18**, 145–150.
91. L. Zhang, Y.-Q. Su, M.-W. Chang, I. A. W. Filot and E. J. M. Hensen, *J. Phys. Chem. C*, 2019, **123**, 31130–31141.
92. Z. Wang and P. Hu, *Catal. Sci. Technol.*, 2021, **11**, 2604–2615.
93. Y.-L. Cheng, C.-T. Hsieh, Y.-S. Ho, M.-H. Shen, T.-H. Chao and M.-J. Cheng, *Phys. Chem. Chem. Phys.*, 2022, **24**, 2476–2481.
94. M. A. Abdulsattar, *J. Mol. Model.*, 2023, **29**, 304.
95. N. Deshpande, A. Parulkar, R. Joshi, B. Diep, A. Kulkarni and N. A. Brunelli, *J. Catal.*, 2019, **370**, 46–54.
96. Z. Yan, Z. Ma, J. Deng and G. Luo, *Chem. Eng. Sci.*, 2021, **242**, 116746.
97. F. Vidal, S. Smith and C. K. Williams, *J. Am. Chem. Soc.*, 2023, **145**, 13888–13900.

General Conclusions and Perspectives

The conclusions and perspectives regarding the study of the reactivity of boroles and azadiborolidines towards CO insertion, which was developed in **Chapter 1**, can be summarised as follows.

I. Ring expansion is observed to follow a CO coordination-insertion mechanism. Electron-withdrawing groups have been shown to facilitate CO coordination, whereas electron-donating groups have been demonstrated to control CO insertion.

II. The coordination process has been found to be exergonic in all the boroles that have been analysed. Endocyclic CO insertion is both kinetically and thermodynamically favoured in comparison to the exocyclic process.

III. The computational results obtained in this study provide a rational explanation for the experimental findings previously reported. In the case of pentaphenylborole, the expansion product is unstable, which is the reason why it is not detected experimentally, but its dimer is. The absence of the expansion product from perfluoropentaphenylborole is attributable to a high energy barrier, resulting in the detection of only the corresponding Lewis adduct.

IV. It has been demonstrated that borole and 1,2,5-azadiborolidine are not isolobal, because of the HOMOs and LUMOs inversion. The appropriate categorisation of these boracycles is as isosteres.

V. In both cases, the ground state is singlet and antiaromatic, while the triplet is aromatic, obeying Baird's rule. The triplet is more accessible in the case of borole because it is more aromatic. Antiaromaticity is a significant factor, modulating the electrophilicity of each ring in the singlet state. For instance, it has been demonstrated that borole is more antiaromatic and has a higher global electrophilicity than 1,2,5-azadiborolidine.

VI. The latter discrepancy is especially pronounced in the CO coordination process, which is an endergonic step for all the 1,2,5-azadiborolidine derivatives analysed. From a kinetic perspective, the energy barriers associated with endocyclic insertion are higher than those calculated for borole. Furthermore, the exocyclic insertion is

only competitive in certain examples; NB-endocyclic insertion remains inaccessible, likely attributable to the stability of the B–N–B fragment, which exhibits resemblance to borazine.

VII. The dimerization process of the initial rings is highly sensitive to the size of the substituents; therefore, it is feasible only in the case of 1,2,5-azadiboroline and 1,2,3,4,5-pentamethyl-1,2,5-azadiborolidine.

VIII. CO coordination process can be expressed in terms of a Brønsted-Evans-Polanyi (BEP) equation. The energy barrier for the rate-determining step can be predicted based on the B–C(O) bond length or the π-backbonding energy from the endocyclic σ-MOs to the CO fragment in the corresponding Lewis adduct. In a less pronounced degree, C–O bond length in the coordination compound can also predict the energy barrier related to the insertion process.

IX. The present study demonstrates that the correlation between the global electrophilicity (ω) and the π-backbonding energy is negligible, thus refuting hypotheses proposed in previous studies.

X. The steric environment is virtually identical when exchanging the borole ring for 1,2,5-azadiborolidine. The transition from perproteo to perfluoro derivatives has been shown to result in a substantial enhancement of the $\%V_{Bur}$, which may potentially impact the reaction yield. Similarly, atomic positions 1, 2, and 5 are more sensitive to the size of the substituents than positions 3 and 4. However, no substantial correlations were observed regarding the reaction kinetics or thermodynamics.

XI. It was observed that not all initial heterocycles are completely planar, and no correlations were detected between their degree of planarity and the thermochemistry of the reaction.

XII. It is concluded that the CO_2-induced ring expansion reaction is a process governed by electronic, rather than steric, factors. The selection of substituent groups for subsequent studies must be made with this in mind.

XIII. The final energy profile successfully predicts the formation of a highly substituted and doped tricyclic compound from 1,2,5-tri-*tert*-butyl-1,2,5-azadiborolidine and CO in *n*-pentane solution. THF and DCM can be used interchangeably.

XIV. The computational models developed throughout this work are capable of predicting the formation of this type of polyheterocycles, depending on the substituents used. It is noteworthy that this type of reactivity has never been explored for 1,2,5-azadiborolidine rings. In this sense, for future experimental applications: it is sufficient to optimize the corresponding Lewis adduct to access an approximate energy barrier related to the insertion process. To predict the formation of the expanded ring dimer, it is sufficient to calculate the **TS-3**, which governs the overall kinetics of the reaction, and the **P-2** product, which governs the thermodynamics. It is recommended that this type of calculation be performed using the described methodology, since the reliability of this method has been demonstrated.

On the other hand, the conclusions and perspectives regarding the study of the catalytic activity of atranes towards the CO_2 cycloaddition, which was developed in **Chapter 2**, is summarised as follows.

I. The existing repertoire of reaction mechanisms to produce cyclic carbonates from epoxides and CO_2 was expanded through the utilisation of triethanolamine borate (**1**) as catalysts.

II. It was demonstrated that catalyst **1** exhibited two distinct conformers, each exhibiting divergent reactivity. The *exo-exo* arrangement has been shown to be the catalytically active one, but the *endo-endo* arrangement has been found to be the most stable.

III. Consequently, a nucleophile, in this instance the epoxide, must activate catalyst **1** by transforming it from its *endo-endo* conformer to the *exo-exo* form.

IV. The nucleophilic moiety of the active catalyst is a tertiary amine, which favours the ring-opening of the epoxide, which is also activated by the acid centre of the catalyst (boron atom). This highlights the bifunctional activity of catalyst **1**. The reaction proceeds with an electrophilic addition of CO_2, followed by a ring-closing reaction.

V. It is demonstrated through computational analysis that the presence of halides, such as bromide, has a favourable effect on the reaction by lowering the total energy barrier. The presence of bromide has been shown to facilitate the epoxide ring-opening process, which is the rate-determining step of the reaction.

VI. In terms of predictive catalysis, atomic substitutions were performed on the structure of atrane **1**. The most favourable outcome is the exchange of the N atom for P, which results in a reduction of the total energy barrier to 16.0 kcal mol^{-1}, thereby indicating mild reaction conditions. Further studies are required to elucidate the underlying reason for this remarkable improvement in the reaction kinetics. Such knowledge will facilitate the design of better atranes with potential catalytic applications.

VII. A strong correlation has been demonstrated between the acid centre, the equatorial groups and the donor atom. The findings of this study indicate that the selection of equatorial groups is crucial for the electronic stabilisation of Lewis acids, thereby preventing the formation of transannular bonds between the Lewis' acid and the basic centres (X–Z bonds). This stabilizes the *exo-exo* conformer, which is the catalytically active species, thus avoiding the activation step.

VIII. Similarly, the hypercoordination of acidic centres should be prevented, as this has been demonstrated to compromise the catalytic activity of the atranes in question. However, further evidence is required to understand how to modulate this chemical behaviour.

IX. The epoxide ring-opening reaction was found to be consistent with a Brønsted-Evans-Polanyi (BEP) relationship. Consequently, the kinetics can be predicted by calculating the Gibbs energy release of the ring-opening step. The exergonicity of the process directly correlates with the reduction in the energy barrier. A similar behaviour is observed when considering the hardness (η) of the catalyst in its most stable form, which follows Pearson's maximum hardness principle.

X. It is important to note that certain catalysts have the capacity to overstabilise the intermediate product subsequent to the epoxide ring-opening reaction. This finding suggests that certain atranes could function as catalysts for the formation of cyclic carbonates, while others may offer utility solely in the promotion of epoxide opening.

In this sense, it is inferred that atranes may have different applications in epoxide chemistry.

As demonstrated in this work, boron compounds have the potential to promote ring expansion reactions, and they play a significant role in catalytic processes. The significance of their implementation is such that they have proven capable of reacting with CO and CO_2, two molecules that are of particular interest in the current academic and industrial context. We hope that the results presented here, as well as the established perspectives, will serve as a platform for the development of new generations of boron-based compounds.

Special emphasis is placed on the pivotal role of contemporary computational methods in elucidating experimental findings, which is the classical application nowadays. Nevertheless, it is strongly suggested their utilisation in the pursuit of chemical reactivity prediction, an area that has emerged as a rigorous and effective paradigm. It is highlighted that computational predictive protocols, in combination with experimental work, has the potential to become a highly synergistic combination in the near future.

Acknowledgements

"Soy porque somos."

Ubuntu (concepto africano)

Este proyecto fue realizado con el apoyo de la Secretaría de Ciencia, Humanidades, Tecnología e Innovación (SECIHTI) a través del programa de Becas Nacionales para Estudios de Posgrados 2023-2 (CVU: 1312084). De igual forma, se reconoce al Laboratorio Nacional de Caracterización de Propiedades Fisicoquímicas y de Estructura Molecular (LACAPFEM) UG-UAA-SECIHTI por el tiempo de cálculo proporcionado en el Centro de Supercómputo de Alto Rendimiento "Pípila". Se distingue al Institut de Química Computacional i Catàlisi (IQCC) por suministrar recursos computacionales adicionales mediante el equipo de supercómputo "Beta".

La obtención del Doble Grado de Maestría se realizó siguiendo los lineamientos del Convenio de Colaboración para la Realización de un Programa Interuniversitario de Doble Titulación entre la Universitat de Girona (UdG) y la Universidad de Guanajuato (UG), que involucra a la Maestría en Ciencias Químicas (UG) y al Máster en Catálisis Avanzada y Modelización Molecular (UdG). En este sentido, manifiesto mi más sincero y profundo reconocimiento a todas las autoridades involucradas de la Universidad de Guanajuato y de la Universitat de Girona que hicieron posible la correcta realización del Programa de Doble Titulación. De manera particular, extiendo esta gratitud tanto a los directores de este proyecto, como a los coordinadores de cada programa, cuyo compromiso y profesionalismo, digno de admiración, fueron fundamentales para dar seguimiento a una correspondencia que en ocasiones parecía interminable.

Mi agradecimiento es eterno con el Dr. Óscar Halla, director del presente proyecto y quien me introdujo, con una paciencia incomparable, al *mundo* de la Química Teórica-Computacional; y con el Dr. Albert Poater por recibirme en su grupo de investigación y guiarme en todo momento. A ambos: agradezco su invaluable asesoría académica pero también su dedicación, paciencia, confianza, y motivación constante, que me ayudaron a crecer profesional y personalmente a lo largo de este trabajo de investigación.

Expreso mi admiración y gratitud al Dr. Gabriel Merino y Dr. Miguel Ángel por su activa participación en el desarrollo de este proyecto; a la Dra. Anna Company, Dr. Pedro

Salvador y al Prof. Miquel Solà quienes dedicaron parte de su tiempo a revisar, evaluar y retroalimentar parte de los resultados aquí presentes. Con la misma gratitud, extiendo mi agradecimiento al Dr. Marco Revilla, Dr. Gerardo G., Dr. Oracio S., y al Dr. Crispín C., por el tiempo invertido en la evaluación de este trabajo.

Como al inicio de esta memoria, este trabajo es dedicado a mi madre y a mi padre, por su apoyo y amor incondicional. A mis hermanos, Abel y Luis, por siempre hacerme sentir respaldado a pesar de la distancia. A mi Pao, por todo el amor, cariño, paciencia y soporte aún en los días más complicados; gracias por atreverte a cruzar el Atlántico y acompañarme a descubrir parte de Catalunya. Son mi mayor fuente de inspiración.

A Nancy, Inés, Lázaro y Osbaldo Rosales, por secundarme sin dudarlo. A cada miembro de mi familia; Fercho, Bry, Enrique; Darien, Leo, Cinthya, Toño, Oliver; Juan Pablo y Juan Pablo Jr, gracias por recibirme siempre con una sonrisa y hacer más ligeros los momentos difíciles.

A Gerard, Guillem Pey y Vila, Albert, Roger, Josep María, Pedro, y Miquel, gracias por recibirme con los brazos abiertos y mostrarme la cultura catalana en su estado más natural. *To Francesco, Massimo, Omkar, Johan, Mohammad, Vincent, and Gerardo for all the beer-time shared together in Girona*.

Appendix

Table A.1. Cartesian coordinates of the optimized gas-phase geometries (at the ωB97X-D/def2-SVP level) involved in the reaction mechanisms computed for boracycles **1**–**16** and CO.

1

SCF energy = -180.022907871 a.u.

5	0.000000	0.000000	1.317989
6	0.000000	1.257130	0.348650
6	0.000000	0.756875	-0.898146
1	0.000000	0.000000	2.524289
1	0.000000	2.325486	0.569170
6	0.000000	-0.756875	-0.898146
1	0.000000	1.332208	-1.829309
6	0.000000	-1.257130	0.348650
1	0.000000	-1.332208	-1.829309
1	0.000000	-2.325486	0.569170

1-TS-1

SCF energy = -293.224507034 a.u.

ν = -278.5997 cm^{-1}

6	1.564547	-0.742983	-0.515434
6	1.564008	0.743858	-0.515084
6	0.667528	1.253680	0.354551
5	0.001361	-0.000584	1.098521
6	-1.772579	-0.000333	0.075235
6	0.668273	-1.253909	0.353780
8	-2.658837	0.000100	-0.618869
1	2.236014	-1.323791	-1.155774
1	2.235042	1.325432	-1.155181
1	0.520769	2.324957	0.505752
1	-0.400777	-0.001007	2.240916
1	0.522176	-2.325361	0.504351

1-I-1

SCF energy = -293.247723363 a.u.

6	-1.581818	0.734945	-0.396202
6	-1.581473	-0.735530	-0.396001
6	-0.552456	-1.250000	0.313229
5	0.277169	0.000320	0.921717
6	1.562579	0.000359	0.055435
6	-0.553132	1.250156	0.312939
8	2.459282	-0.000094	-0.634216
1	-2.351827	1.321414	-0.906997
1	-2.351331	-1.322494	-0.906470
1	-0.366353	-2.320166	0.424886
1	0.614615	0.000388	2.093263
1	-0.367407	2.320423	0.424068

1-TS-2

SCF energy = -293.215364495 a.u.

ν = -330.5659 cm^{-1}

6	-0.945418	1.204988	0.028998
6	-1.791125	0.072402	-0.351361
6	-1.262287	-1.140649	-0.099026
5	0.124931	-1.063132	0.617907
6	1.239771	-0.278778	-0.042027
6	0.338374	0.999962	0.404708
8	2.312332	-0.090406	-0.511116
1	-1.361351	2.218400	0.036386
1	-2.761531	0.236803	-0.826659
1	-1.769627	-2.065769	-0.384248
1	0.312053	-1.315420	1.783701
1	0.981248	1.817341	0.742467

1-TS-2B

SCF energy = -293.211742044 a.u.

ν = -464.3576 cm^{-1}

6	0.060957	-1.898152	0.748875
6	0.060957	-0.653576	1.263020
1	0.053513	-0.428845	-2.329572
1	0.053078	-2.826416	-1.327714
1	0.053078	-2.826416	1.327714
1	0.053513	-0.428845	2.329572
1	1.209668	1.514488	0.000000
6	0.060957	-1.898152	-0.748875
5	-0.044729	0.290976	0.000000

6	0.060957	-0.653576	-1.263020
8	-0.340813	2.923454	0.000000
6	0.010720	1.795709	0.000000

1-P-1

SCF energy = -293.241625143 a.u.

6	-0.914518	1.294057	-0.000082
6	-1.785005	0.105934	0.000392
6	-1.338175	-1.175285	0.000028
5	0.182094	-1.420839	-0.000478
6	1.113328	-0.095685	-0.000104
6	0.429667	1.227563	-0.000407
8	2.331156	-0.157247	0.000473
1	-1.410385	2.268577	0.000249
1	-2.861737	0.312075	0.000538
1	-2.081662	-1.977700	-0.000083
1	0.706087	-2.504451	-0.000448
1	1.056196	2.124167	-0.000613

1-P-1B

SCF energy = -293.220049370 a.u.

6	0.068023	-1.857529	0.755341
6	0.068023	-0.611906	1.259769
1	0.068301	-0.386179	-2.326549
1	0.069273	-2.787583	-1.331915
1	0.069273	-2.787583	1.331915
1	0.068301	-0.386179	2.326549
1	1.293342	2.462732	0.000000
6	0.068023	-1.857529	-0.755341
5	0.154799	0.343535	0.000000
6	0.068023	-0.611906	-1.259769
8	-0.730893	2.537960	0.000000
6	0.312018	1.916110	0.000000

2

SCF energy = -1334.137216050 a.u.

6	1.281575	0.298827	-0.028809
6	0.692548	-0.922227	-0.021759
6	-0.828877	-0.808102	-0.032503
5	0.098128	1.358769	-0.031531
6	-1.229960	0.487124	-0.035176
6	-1.707337	-1.999087	-0.032749
6	-2.723163	-2.128653	-0.990088
6	-1.551292	-3.009509	0.926787
6	-3.561744	-3.239890	-0.987671
1	-2.372552	2.330090	-1.648642
6	-2.398250	-4.114827	0.935222
1	-0.762305	-2.926311	1.677096
6	-3.403659	-4.234958	-0.023320
1	-4.345944	-3.327313	-1.742736
1	-2.268862	-4.889584	1.694020
1	-4.064332	-5.104774	-0.019641
6	1.384447	-2.230091	0.008556
6	2.363897	-2.485757	0.978540
6	1.082786	-3.231061	-0.925676
6	3.025292	-3.709979	1.013072
1	2.605743	-1.711558	1.709484
6	1.753383	-4.451317	-0.897178
1	0.317126	-3.050496	-1.683101
6	2.724066	-4.695600	0.073529
1	3.783365	-3.894391	1.777338
1	1.510987	-5.218225	-1.635853
1	3.244142	-5.655672	0.099304
6	-2.630014	0.959213	-0.001046
6	-3.073098	1.931358	-0.911000
6	-3.542555	0.473113	0.948252
6	-4.387882	2.391172	-0.883126
1	-2.852106	-1.344825	-1.739420
6	-4.854800	0.937080	0.980499
1	-3.212125	-0.277048	1.669937
6	-5.284262	1.896261	0.063252
1	-4.712983	3.144258	-1.604465
1	-5.548172	0.547719	1.729525
1	-6.313534	2.260916	0.089582
6	0.219101	2.906334	-0.015923
6	1.293894	3.558229	-0.653292
6	-0.734688	3.706247	0.644875
6	1.403747	4.945961	-0.644491
1	2.054479	2.966348	-1.167800
6	-0.608873	5.092307	0.686085
1	-1.584842	3.233141	1.141745
6	0.456921	5.713727	0.034493
1	2.238481	5.430979	-1.155354
1	-1.349726	5.692280	1.219127
1	0.551174	6.802170	0.056756
6	2.736929	0.555939	-0.039107
6	3.302202	1.445984	0.887287
6	3.586095	-0.061883	-0.970062
6	4.672242	1.697780	0.894142
1	2.654316	1.945795	1.611169

6	4.954833	0.193920	-0.967166
1	3.162211	-0.753018	-1.701984
6	5.504400	1.072576	-0.033452
1	5.090939	2.390473	1.627799
1	5.598050	-0.297417	-1.700779
1	6.578416	1.271354	-0.031427

2-TS-1

SCF energy = -1447.327287090 a.u.

ν = -146.9768 cm^{-1}

5	0.473496	1.233550	0.039364
8	0.015070	0.633126	3.374576
6	0.275478	1.098994	2.380928
6	1.312930	-0.125458	0.013996
6	0.405032	-1.132254	-0.088862
6	-1.011649	-0.606589	-0.121409
6	-1.047041	0.748311	-0.040968
6	2.783699	-0.255978	0.014008
6	3.560592	0.541546	0.869488
6	4.950168	0.450108	0.874483
6	5.597305	-0.431515	0.010165
6	4.841227	-1.215906	-0.861028
6	3.452054	-1.128827	-0.860504
6	0.702609	-2.582606	-0.145542
6	1.514622	-3.173631	0.832121
6	1.805679	-4.534159	0.785431
6	1.292774	-5.324758	-0.242682
6	0.482145	-4.747418	-1.219426
6	0.183535	-3.388041	-1.168268
6	-2.188846	-1.502656	-0.205149
6	-2.351362	-2.558487	0.702746
6	-3.471862	-3.382647	0.638554
6	-4.441043	-3.172048	-0.341628
6	-4.286117	-2.128305	-1.253422
6	-3.170668	-1.297472	-1.183703
6	-2.264621	1.584347	-0.002754
6	-3.286950	1.346394	0.928531
6	-4.426441	2.146521	0.956849
6	-4.568878	3.198460	0.051982
6	-3.559668	3.447515	-0.877261
6	-2.415993	2.652327	-0.900205
6	1.017245	2.675934	-0.229531
6	2.111490	2.868306	-1.090582
6	2.577219	4.147390	-1.394313
6	1.971692	5.263032	-0.819872
6	0.890797	5.096422	0.048034
6	0.414243	3.818952	0.326375
1	-3.053745	-0.475688	-1.893332
1	-5.041019	-1.957640	-2.024107
1	-5.316515	-3.822972	-0.395437
1	-3.586008	-4.196630	1.357683
1	-1.592619	-2.734173	1.468492
1	0.074650	-5.360979	-2.025764
1	1.521386	-6.392096	-0.281465
1	2.439950	-4.978993	1.555266
1	1.923138	-2.551697	1.631631
1	-0.460757	-2.944141	-1.930280
1	-3.183158	0.519497	1.635089
1	-5.209995	1.945176	1.690848
1	-5.464577	3.823345	0.072608
1	-3.661180	4.268488	-1.590707
1	-1.625452	2.856171	-1.625743
1	-0.442831	3.705683	0.995533
1	0.414481	5.968222	0.502356
1	2.342947	6.265677	-1.045122
1	2.608945	2.002194	-1.533729
1	3.423189	4.271584	-2.074085
1	3.064200	1.248855	1.537980
1	5.531835	1.077484	1.553539
1	6.687225	-0.502337	0.009400
1	5.338536	-1.900936	-1.551440
1	2.870948	-1.741684	-1.552129

2-I-1

SCF energy = -1447.347071510 a.u.

6	-1.198565	-0.451059	-0.174883
6	-0.817161	0.848339	-0.020888
6	0.658952	1.008199	-0.079326
5	0.153811	-1.334680	-0.400949
6	1.294886	-0.183046	-0.278607
6	1.310421	2.331883	0.087500
6	2.191371	2.820101	-0.885828
6	1.055423	3.114593	1.221008
6	2.808530	4.058380	-0.726289
1	2.623465	-2.014398	-1.780846
6	1.676460	4.350436	1.383064
1	0.362474	2.749611	1.982140
6	2.554429	4.826205	0.409839
1	3.494885	4.424482	-1.492978
1	1.470662	4.946483	2.274754

1	3.039492	5.796632	0.535844
6	-1.745757	1.985533	0.198293
6	-2.716378	1.916893	1.206196
6	-1.684112	3.135687	-0.600333
6	-3.606749	2.968269	1.407557
1	-2.770840	1.024767	1.833646
6	-2.578448	4.184748	-0.402319
1	-0.926359	3.208274	-1.383558
6	-3.541955	4.104848	0.602578
1	-4.357617	2.898612	2.197551
1	-2.520050	5.072228	-1.036308
1	-4.241942	4.928646	0.758670
6	2.747400	-0.440919	-0.296380
6	3.282927	-1.438538	-1.127139
6	3.630420	0.239942	0.560146
6	4.646408	-1.720014	-1.134790
1	2.397144	2.214078	-1.771152
6	4.992564	-0.045106	0.558191
1	3.241591	0.995405	1.244420
6	5.509836	-1.019976	-0.294620
1	5.033772	-2.496362	-1.798174
1	5.656126	0.499358	1.233702
1	6.579583	-1.239923	-0.295999
6	0.345345	-2.769071	0.285198
6	-0.271911	-3.931525	-0.200931
6	1.105677	-2.876125	1.458683
6	-0.138945	-5.154090	0.455877
1	-0.886314	-3.887142	-1.106238
6	1.237174	-4.093683	2.125148
1	1.607270	-1.991208	1.858637
6	0.616490	-5.237512	1.624639
1	-0.628432	-6.044367	0.054075
1	1.832004	-4.150245	3.039905
1	0.723839	-6.193396	2.142470
6	-2.584062	-0.956588	-0.257785
6	-2.998051	-2.023639	0.554098
6	-3.508025	-0.402073	-1.157512
6	-4.300194	-2.513595	0.474309
1	-2.290043	-2.463155	1.259384
6	-4.806144	-0.897703	-1.241953
1	-3.198776	0.431554	-1.792541
6	-5.207373	-1.954990	-0.424952
1	-4.606976	-3.339023	1.120687
1	-5.510570	-0.454625	-1.949597
1	-6.226063	-2.343686	-0.490622
6	0.036081	-1.380267	-1.964197
8	-0.081143	-1.290800	-3.086836

2-TS-2

SCF energy = -1447.322180740 a.u.

ν = -150.9391 cm^{-1}

6	-1.304130	-0.896391	-0.289562
6	-1.157803	0.451503	-0.188384
6	0.248855	0.898332	-0.355241
5	0.077868	-1.622264	-0.552598
6	1.127387	0.031454	-0.939286
6	0.691190	2.199919	0.207770
6	1.511818	3.059912	-0.532201
6	0.301609	2.577323	1.499551
6	1.937056	4.269689	0.008974
1	2.904764	0.195034	-3.009791
6	0.738980	3.780677	2.045594
1	-0.344122	1.917410	2.082972
6	1.555880	4.630713	1.300660
1	2.573044	4.932575	-0.581298
1	0.437087	4.057522	3.057890
1	1.894662	5.577104	1.727834
6	-2.242243	1.445600	0.015570
6	-3.193715	1.275704	1.029863
6	-2.325201	2.579932	-0.801888
6	-4.209139	2.210196	1.213232
1	-3.133829	0.397350	1.676677
6	-3.341166	3.514894	-0.619577
1	-1.583473	2.730217	-1.589995
6	-4.287133	3.332209	0.388001
1	-4.944222	2.062942	2.007549
1	-3.392402	4.392378	-1.267785
1	-5.082196	4.066756	0.533584
6	2.603664	0.139313	-0.874680
6	3.389826	0.205479	-2.032521
6	3.236759	0.133669	0.377317
6	4.778137	0.287301	-1.936370
1	1.815208	2.776042	-1.541620
6	4.622087	0.213915	0.469408
1	2.628915	0.056391	1.281440
6	5.397351	0.294476	-0.687882
1	5.379069	0.346901	-2.846562
1	5.100278	0.208514	1.451135
1	6.485208	0.360377	-0.614873
6	0.943877	-2.443496	0.466949

6	2.064669	-3.184187	0.059066
6	0.661629	-2.375834	1.841798
6	2.876752	-3.830693	0.987771
1	2.311975	-3.247799	-1.004052
6	1.470513	-3.019873	2.775306
1	-0.202363	-1.798397	2.183835
6	2.581659	-3.748027	2.348259
1	3.747146	-4.397199	0.649660
1	1.237527	-2.951948	3.840453
1	3.218944	-4.252854	3.077995
6	-2.570685	-1.653435	-0.369537
6	-2.659917	-2.924901	0.219451
6	-3.685862	-1.163210	-1.070181
6	-3.838105	-3.665475	0.146391
1	-1.797132	-3.334348	0.749657
6	-4.856797	-1.908533	-1.152187
1	-3.626952	-0.191546	-1.562879
6	-4.941213	-3.158645	-0.537044
1	-3.890362	-4.647423	0.621372
1	-5.711442	-1.511523	-1.704176
1	-5.863931	-3.739614	-0.600151
6	0.616181	-1.215478	-1.906621
8	0.874078	-1.244718	-3.062811

2-TS-2B

SCF energy = -1447.306127670 a.u.

ν = -357.8437 cm^{-1}

6	-1.265257	-0.342388	-0.448340
6	-0.750598	0.873812	-0.127926
6	0.749841	0.874408	-0.127951
5	0.000460	-1.263579	-0.701360
6	1.265453	-0.341416	-0.448273
6	1.526635	2.124917	0.076876
6	2.146062	2.744052	-1.014703
6	1.661321	2.702847	1.344876
6	2.879769	3.915927	-0.843465
1	2.369028	-1.912261	-2.347758
6	2.397470	3.872592	1.517855
1	1.198541	2.219271	2.207859
6	3.006745	4.484169	0.422847
1	3.356384	4.387203	-1.705817
1	2.497472	4.309361	2.513993
1	3.579914	5.404045	0.557252
6	-1.528389	2.123693	0.076979
6	-1.663710	2.701325	1.345048
6	-2.148086	2.742541	-1.014607
6	-2.400760	3.870493	1.518092
1	-1.200707	2.217959	2.208029
6	-2.882707	3.913836	-0.843301
1	-2.052158	2.291944	-2.004885
6	-3.010311	4.481785	0.423079
1	-2.501247	4.307034	2.514281
1	-3.359549	4.384881	-1.705653
1	-3.584191	5.401209	0.557533
6	2.691100	-0.685083	-0.595273
6	3.106124	-1.532945	-1.636078
6	3.665082	-0.213915	0.300766
6	4.445468	-1.886017	-1.784818
1	2.050631	2.293227	-2.004926
6	5.002790	-0.569516	0.153431
1	3.364685	0.431535	1.127306
6	5.400413	-1.405276	-0.890201
1	4.743747	-2.541873	-2.605773
1	5.741780	-0.193208	0.864503
1	6.450666	-1.682074	-1.004669
6	0.001288	-2.850335	0.479374
6	-1.212509	-3.162062	1.106439
6	1.215373	-3.161705	1.106057
6	-1.208895	-3.765970	2.360082
1	-2.159455	-2.931925	0.613800
6	1.212329	-3.765607	2.359706
1	2.162096	-2.931284	0.613123
6	0.001860	-4.063457	2.986739
1	-2.154975	-4.002181	2.851132
1	2.158633	-4.001534	2.850464
1	0.002083	-4.535366	3.971857
6	-2.690635	-0.687096	-0.595514
6	-3.665066	-0.216549	0.300355
6	-3.104922	-1.535273	-1.636358
6	-5.002509	-0.573082	0.152847
1	-3.365223	0.429199	1.126864
6	-4.443999	-1.889280	-1.785270
1	-2.367461	-1.914092	-2.347925
6	-5.399400	-1.409168	-0.890801
1	-5.741866	-0.197236	0.863782
1	-4.741712	-2.545366	-2.606247
1	-6.449446	-1.686692	-1.005412
6	0.000965	-2.665625	-1.220831
8	0.001252	-3.613958	-1.920292

2-P-1

SCF energy = -1447.329487190 a.u.

6	-1.437185	0.044944	-0.315713
6	-0.323861	0.814314	-0.139690
6	1.068011	0.224240	-0.087515
5	-1.171609	-1.492173	-0.325403
6	1.352449	-1.020857	-0.557123
6	2.147227	1.106387	0.445927
6	3.276645	1.419897	-0.317974
6	2.029654	1.647336	1.731722
6	4.264894	2.257694	0.191408
1	2.664234	-2.091181	-2.682898
6	3.021450	2.478178	2.245122
1	1.146699	1.419016	2.333433
6	4.140873	2.789143	1.474335
1	5.138563	2.496723	-0.418727
1	2.914785	2.892313	3.249953
1	4.915212	3.448575	1.872177
6	-0.423629	2.299167	-0.007103
6	-1.246781	2.866143	0.972012
6	0.291993	3.148698	-0.859793
6	-1.353900	4.248619	1.097107
1	-1.813039	2.211536	1.637973
6	0.180679	4.531007	-0.740181
1	0.943096	2.722476	-1.626174
6	-0.640787	5.085733	0.240741
1	-2.000635	4.673716	1.867598
1	0.743961	5.179088	-1.414889
1	-0.724462	6.170193	0.338704
6	2.706299	-1.629846	-0.574890
6	3.243531	-2.146789	-1.761362
6	3.452861	-1.732836	0.607458
6	4.509419	-2.730315	-1.765109
1	3.379536	1.000403	-1.320863
6	4.714302	-2.319495	0.601281
1	3.037572	-1.341668	1.538579
6	5.248788	-2.817255	-0.587086
1	4.919180	-3.123876	-2.698032
1	5.282102	-2.390022	1.531576
1	6.239028	-3.278026	-0.593136
6	-1.949686	-2.615662	0.416015
6	-2.056251	-3.893552	-0.164757
6	-2.500211	-2.422057	1.696645
6	-2.739757	-4.918653	0.484851
1	-1.590414	-4.075326	-1.136349
6	-3.149221	-3.456170	2.364978
1	-2.396600	-1.449808	2.186656
6	-3.284234	-4.702076	1.750528
1	-2.833530	-5.897485	0.009605
1	-3.558238	-3.291388	3.364259
1	-3.806089	-5.511519	2.266521
6	-2.781025	0.626851	-0.599020
6	-3.935008	0.239770	0.096058
6	-2.920185	1.566008	-1.634452
6	-5.174162	0.803829	-0.202631
1	-3.871074	-0.506445	0.886467
6	-4.157584	2.123988	-1.937799
1	-2.039794	1.864118	-2.206714
6	-5.291525	1.751383	-1.216574
1	-6.055682	0.494202	0.363205
1	-4.235526	2.856643	-2.743993
1	-6.262971	2.192652	-1.449386
6	0.203913	-1.866732	-1.044819
8	0.349270	-2.751280	-1.868013

2-P-1B

SCF energy = -1447.328409090 a.u.

6	-0.136423	-1.361299	-0.325871
6	-1.255799	-0.646138	-0.052331
6	-0.997306	0.860121	-0.119198
5	0.998998	-0.273319	-0.507975
6	0.302845	1.133574	-0.400574
6	-2.090592	1.844126	0.038392
6	-2.286364	2.818246	-0.951828
6	-2.943596	1.832594	1.150660
6	-3.305241	3.757948	-0.830582
1	2.206046	1.892474	-2.149907
6	-3.957303	2.779548	1.275216
1	-2.809059	1.081658	1.930675
6	-4.142464	3.743025	0.284910
1	-3.445242	4.508453	-1.611508
1	-4.609694	2.761226	2.150870
1	-4.940703	4.482278	0.380859
6	-2.630761	-1.153288	0.186293
6	-3.025091	-1.645509	1.435708
6	-3.578090	-1.084193	-0.841980
6	-4.333109	-2.075450	1.649456
1	-2.299390	-1.676596	2.252472
6	-4.884446	-1.517821	-0.630252
1	-3.284251	-0.684575	-1.815167

6	-5.265652	-2.014654	0.615499
1	-4.624910	-2.459262	2.629495
1	-5.611424	-1.464571	-1.443378
1	-6.291024	-2.351944	0.781096
6	0.957913	2.453948	-0.475950
6	1.946048	2.686424	-1.445875
6	0.651464	3.488737	0.423009
6	2.589809	3.919209	-1.528867
1	-1.625370	2.833020	-1.821020
6	1.299439	4.717574	0.342898
1	-0.103388	3.322285	1.194383
6	2.268913	4.939811	-0.635735
1	3.350547	4.080456	-2.295937
1	1.047559	5.507614	1.053954
1	2.776099	5.905098	-0.697962
6	3.582583	-0.499025	0.291438
6	3.223270	-0.225147	1.615061
6	4.921876	-0.743189	-0.034144
6	4.196018	-0.195858	2.611466
1	2.175765	-0.027061	1.865084
6	5.892266	-0.715972	0.960237
1	5.173463	-0.951135	-1.076433
6	5.528639	-0.442499	2.282135
1	3.918021	0.019708	3.644961
1	6.938474	-0.906928	0.712224
1	6.293151	-0.420719	3.061981
6	0.010487	-2.823683	-0.473103
6	-0.571183	-3.748565	0.407733
6	0.782046	-3.320861	-1.538204
6	-0.404058	-5.118701	0.220764
1	-1.150172	-3.393831	1.259172
6	0.942658	-4.690438	-1.728132
1	1.257463	-2.620855	-2.228772
6	0.349536	-5.596368	-0.849715
1	-0.863292	-5.818280	0.922913
1	1.540234	-5.051564	-2.568091
1	0.480945	-6.670810	-0.995287
6	2.540143	-0.520159	-0.763710
8	2.804292	-0.693246	-1.948218

3

SCF energy = -3812.297218080 a.u.

6	0.403113	1.253280	0.016549
6	-0.851998	0.760101	0.002586
6	-0.854742	-0.757589	-0.000703
5	1.366482	-0.002672	0.000975
6	0.398646	-1.255236	-0.014301
6	-2.104994	-1.537649	0.027209
6	-2.371875	-2.439990	1.059148
6	-3.058578	-1.398102	-0.982644
6	-3.552409	-3.176444	1.089737
9	2.102003	-2.390757	1.881107
6	-4.245799	-2.121770	-0.970846
9	-2.823015	-0.578087	-1.996625
6	-4.490455	-3.014874	0.071502
9	-3.792231	-4.016922	2.078575
9	-5.129788	-1.980461	-1.940722
9	-5.609661	-3.707950	0.093209
6	-2.099338	1.544812	-0.026182
6	-2.362312	2.447428	-1.058881
6	-3.054075	1.409267	0.983119
6	-3.540128	3.188155	-1.090700
9	-1.497926	2.597887	-2.048139
6	-4.238657	2.137243	0.970099
9	-2.822224	0.588774	1.997563
6	-4.479392	3.030589	-0.072962
9	-3.776317	4.028865	-2.080214
9	-5.123857	1.999630	1.939403
9	-5.596108	3.727635	-0.095813
6	0.750688	-2.681744	-0.023232
6	1.626147	-3.193767	0.937079
6	0.267305	-3.567294	-0.989388
6	2.009909	-4.530013	0.947525
9	-1.508552	-2.594364	2.048726
6	0.633573	-4.910621	-0.997743
9	-0.543195	-3.134953	-1.945484
6	1.509302	-5.391974	-0.027076
9	2.833578	-4.986705	1.873290
9	0.165802	-5.725936	-1.925688
9	1.862764	-6.661864	-0.028530
6	2.921926	-0.005105	0.000254
6	3.656354	0.845410	0.831013
6	3.653105	-0.857696	-0.831229
6	5.046875	0.853202	0.848538
9	3.025136	1.658833	1.668874
6	5.043591	-0.869507	-0.850078
9	3.018775	-1.669201	-1.668584
6	5.739601	-0.009165	-0.001091
9	5.711384	1.657309	1.656748
9	5.704977	-1.675526	-1.658948

9	7.054861	-0.011037	-0.001702
6	0.759998	2.678594	0.025046
6	1.635956	3.187644	-0.936361
6	0.280303	3.565854	0.991440
6	2.023756	4.522717	-0.947619
9	2.108253	2.382942	-1.880730
6	0.650684	4.908059	0.999035
9	-0.530627	3.136174	1.948361
6	1.526818	5.386468	0.027257
9	2.847768	4.976637	-1.874446
9	0.186374	5.725072	1.927232
9	1.884071	6.655302	0.027927

3-TS-1

SCF energy = -3925.491124530 a.u.

ν = -73.4076 cm^{-1}

5	-0.854141	1.071393	-0.032473
8	-0.509415	0.423336	3.761963
6	-0.728577	0.705108	2.693943
6	0.735012	1.107298	-0.072164
6	1.134965	-0.182435	-0.111517
6	-0.035012	-1.132730	-0.131653
6	-1.211157	-0.476160	-0.089350
6	1.641673	2.265239	-0.079321
6	1.518932	3.281657	0.871010
6	2.353510	4.393745	0.879950
6	3.345890	4.512547	-0.090773
6	3.488647	3.521785	-1.059188
6	2.638643	2.419241	-1.048182
6	2.526898	-0.667351	-0.080646
6	3.377704	-0.335911	0.975852
6	4.688803	-0.799629	1.024277
6	5.166599	-1.616212	0.000818
6	4.336133	-1.962960	-1.064107
6	3.030864	-1.484173	-1.093715
6	0.140852	-2.596835	-0.162286
6	0.819869	-3.250659	0.866680
6	0.999935	-4.629213	0.863850
6	0.479834	-5.381187	-0.188852
6	-0.211048	-4.753711	-1.224109
6	-0.375380	-3.371490	-1.202051
6	-2.533030	-1.116558	-0.059925
6	-2.894450	-2.026479	0.935390
6	-4.158936	-2.607645	0.971579
6	-5.096267	-2.272436	-0.003193
6	-4.764655	-1.362652	-1.006211
6	-3.493897	-0.798627	-1.021371
6	-1.845831	2.275208	-0.106538
6	-1.589562	3.376377	-0.929276
6	-2.459484	4.457738	-1.029590
6	-3.635042	4.453600	-0.281103
6	-3.931600	3.373709	0.549144
6	-3.043911	2.304972	0.613996
9	0.583720	3.198196	1.810811
9	2.215061	5.329787	1.801468
9	4.146143	5.559980	-0.093624
9	4.418940	3.638126	-1.989538
9	2.782505	1.518209	-2.010071
9	2.938531	0.413254	1.974931
9	5.475683	-0.481912	2.035278
9	6.405434	-2.061196	0.039226
9	4.794732	-2.727842	-2.037135
9	2.261268	-1.797125	-2.125715
9	1.284609	-2.548868	1.891870
9	1.641063	-5.227370	1.850579
9	0.638520	-6.688555	-0.203295
9	-0.698078	-5.470883	-2.219408
9	-2.034081	-2.337410	1.897776
9	-1.021599	-2.796386	-2.202063
9	-4.477875	-3.462146	1.927092
9	-6.297113	-2.815813	0.022283
9	-5.652567	-1.048091	-1.931681
9	-3.191936	0.062189	-1.984706
9	-0.496960	3.404862	-1.683165
9	-2.187655	5.474332	-1.826185
9	-4.468030	5.468807	-0.360285
9	-5.044494	3.373661	1.259060
9	-3.366437	1.301897	1.422992

3-I-1

SCF energy = -3925.516726070 a.u.

6	-1.189131	-0.496975	-0.316189
6	-0.787114	0.782361	-0.131723
6	0.686910	0.918671	-0.176950
5	0.138655	-1.387980	-0.614167
6	1.294877	-0.268886	-0.417195
6	1.358937	2.217791	0.026448
6	2.214580	2.746769	-0.941084
6	1.154057	2.959730	1.190692
6	2.840793	3.977259	-0.763171

9	2.630340	-1.746237	-2.410108
6	1.763322	4.193976	1.387742
9	0.380400	2.475760	2.150702
6	2.611478	4.701735	0.404906
9	3.640881	4.463324	-1.694446
9	1.557990	4.876395	2.499096
9	3.198958	5.867633	0.581433
6	-1.689235	1.931291	0.092167
6	-2.571251	1.963877	1.173091
6	-1.688063	3.018115	-0.782900
6	-3.421970	3.045745	1.382022
9	-2.601652	0.963622	2.038028
6	-2.525440	4.111899	-0.591757
9	-0.882363	3.009374	-1.836275
6	-3.396496	4.121724	0.496659
9	-4.245480	3.061980	2.413630
9	-2.510014	5.127223	-1.435626
9	-4.197769	5.149871	0.687090
6	2.741868	-0.522368	-0.395524
6	3.357420	-1.283893	-1.392718
6	3.557615	-0.093085	0.659290
6	4.713065	-1.588458	-1.376559
9	2.435275	2.085672	-2.067238
6	4.920054	-0.380129	0.697694
9	3.045531	0.581539	1.675684
6	5.500977	-1.128098	-0.323498
9	5.253523	-2.301683	-2.347158
9	5.660031	0.040825	1.706593
9	6.788749	-1.404956	-0.291120
6	0.312607	-2.842453	0.027252
6	-0.144960	-3.998178	-0.594882
6	0.855527	-2.995456	1.300732
6	-0.066136	-5.257536	-0.009163
9	-0.700409	-3.910553	-1.810019
6	0.957004	-4.236824	1.923440
9	1.279455	-1.932360	1.975515
6	0.492639	-5.372474	1.261976
9	-0.512676	-6.330239	-0.638061
9	1.479109	-4.346243	3.131624
9	0.578514	-6.554301	1.840223
6	-2.591171	-0.940492	-0.379029
6	-3.087023	-1.880790	0.528515
6	-3.477690	-0.441317	-1.337942
6	-4.409730	-2.311036	0.487331
9	-2.298512	-2.365780	1.474334
6	-4.804496	-0.857399	-1.399150
9	-3.053075	0.441010	-2.234170
6	-5.270256	-1.796754	-0.481194
9	-4.855251	-3.193474	1.362148
9	-5.618184	-0.374441	-2.320518
9	-6.524188	-2.198371	-0.528742
6	-0.004943	-1.400973	-2.198578
8	-0.163461	-1.251828	-3.302156

3-TS-2

SCF energy = -3925.472892830 a.u.

ν = -107.6985 cm^{-1}

6	-1.321981	-1.010302	-0.570674
6	-1.130139	0.313669	-0.369332
6	0.278903	0.750941	-0.502622
5	0.036040	-1.780036	-0.845578
6	1.144090	-0.036320	-1.190745
6	0.728023	1.988836	0.177076
6	1.391959	3.006862	-0.513006
6	0.482940	2.177428	1.539887
6	1.798457	4.172536	0.129973
9	2.824583	0.630717	-3.414604
6	0.882710	3.333075	2.201690
9	-0.130090	1.233427	2.234827
6	1.542245	4.334430	1.490282
9	2.417972	5.124771	-0.540991
9	0.648095	3.484270	3.491196
9	1.925662	5.432916	2.104904
6	-2.177904	1.294853	-0.020152
6	-3.061593	1.069532	1.039231
6	-2.295249	2.501573	-0.713732
6	-4.027944	2.008125	1.392001
9	-2.991987	-0.045270	1.746243
6	-3.246627	3.456438	-0.374729
9	-1.486852	2.749313	-1.734302
6	-4.118368	3.204402	0.683783
9	-4.849073	1.775073	2.399063
9	-3.336865	4.587194	-1.049704
9	-5.027743	4.097887	1.013854
6	2.611188	0.114019	-1.123177
6	3.391096	0.397819	-2.250310
6	3.277660	-0.045025	0.098909
6	4.779625	0.480098	-2.168368
9	1.635730	2.890047	-1.805379
6	4.662320	0.028173	0.198508

9	2.589761	-0.267117	1.212656
6	5.415977	0.289369	-0.944199
9	5.494398	0.753099	-3.243043
9	5.260366	-0.140700	1.363885
9	6.727926	0.365908	-0.863548
6	0.901231	-2.597874	0.165477
6	2.035594	-3.303652	-0.251717
6	0.650894	-2.572685	1.543261
6	2.875611	-3.966251	0.636518
9	2.354147	-3.344384	-1.538568
6	1.465655	-3.230923	2.457526
9	-0.361965	-1.877526	2.027683
6	2.581430	-3.929235	1.998548
9	3.939171	-4.620751	0.206830
9	1.206198	-3.185307	3.751085
9	3.364427	-4.549312	2.854434
6	-2.642906	-1.642527	-0.738324
6	-2.955439	-2.856029	-0.114752
6	-3.632760	-1.078529	-1.557241
6	-4.200750	-3.460402	-0.251593
9	-2.053698	-3.468618	0.636060
6	-4.885212	-1.666328	-1.709017
9	-3.391397	0.026896	-2.244397
6	-5.172140	-2.859098	-1.048607
9	-4.464230	-4.596097	0.366244
9	-5.794082	-1.107923	-2.486196
9	-6.353501	-3.422569	-1.187045
6	0.621357	-1.264758	-2.158261
8	0.824688	-1.280843	-3.321932

3-TS-2B

SCF energy = -3925.455214050 a.u.

ν = -379.0200 cm^{-1}

6	1.242466	-0.358982	0.546749
6	0.611215	0.765216	0.145687
6	-0.872848	0.611075	0.103749
5	0.069673	-1.361250	0.927160
6	-1.271365	-0.619998	0.492561
6	-1.755017	1.732020	-0.277870
6	-2.715332	2.243066	0.597206
6	-1.636518	2.324260	-1.536115
6	-3.539911	3.302529	0.228503
9	-2.464780	-1.502658	2.877821
6	-2.444961	3.387009	-1.923668
9	-0.745132	1.855622	-2.397534
6	-3.400914	3.875463	-1.034199
9	-4.440850	3.774193	1.070119
9	-2.320548	3.926910	-3.121864
9	-4.175815	4.879518	-1.389192
6	1.263923	2.065201	-0.119885
6	2.163077	2.245225	-1.171241
6	0.986371	3.162404	0.697943
6	2.771013	3.476340	-1.401788
9	2.445665	1.241514	-1.983718
6	1.578481	4.402673	0.484152
9	0.148581	3.025099	1.714968
6	2.475338	4.556462	-0.572025
9	3.616248	3.628125	-2.404119
9	1.305224	5.424393	1.273652
9	3.045482	5.724290	-0.785643
6	-2.688587	-1.005064	0.590503
6	-3.236071	-1.428699	1.801921
6	-3.544428	-0.930813	-0.511042
6	-4.579479	-1.768321	1.924295
9	-2.849620	1.736179	1.810885
6	-4.892450	-1.261257	-0.413681
9	-3.073118	-0.565548	-1.695947
6	-5.411354	-1.680493	0.809737
9	-5.071420	-2.158529	3.085741
9	-5.678266	-1.189172	-1.473515
9	-6.687275	-1.996422	0.911695
6	0.340648	-3.257228	0.210163
6	1.646387	-3.684817	-0.046192
6	-0.673676	-3.764954	-0.604126
6	1.963138	-4.490993	-1.129331
9	2.621211	-3.327759	0.774652
6	-0.389733	-4.572154	-1.701069
9	-1.941872	-3.489540	-0.358557
6	0.932176	-4.936267	-1.958138
9	3.206180	-4.858080	-1.361964
9	-1.357630	-5.021367	-2.475512
9	1.206596	-5.710405	-2.981341
6	2.707303	-0.382491	0.745930
6	3.574022	-0.914900	-0.207436
6	3.273904	0.213578	1.872946
6	4.954043	-0.883073	-0.043498
9	3.079724	-1.490483	-1.295449
6	4.652940	0.258589	2.062199
9	2.488836	0.755288	2.792787
6	5.494216	-0.288101	1.095618

9	5.751856	-1.404795	-0.957569
9	5.165287	0.825787	3.139520
9	6.801568	-0.248361	1.260815
6	0.118313	-2.603039	1.788757
8	0.098557	-3.304341	2.725468

3-P-1

SCF energy = -3925.498376120 a.u.

6	-1.282272	0.030650	-0.064268
6	-0.042352	0.593288	-0.031713
6	1.224457	-0.194505	-0.010599
5	-1.398298	-1.508940	-0.057234
6	1.259448	-1.547184	-0.037943
6	2.502507	0.567113	0.051113
6	3.409813	0.550545	-1.008724
6	2.833593	1.311586	1.183575
6	4.605709	1.260653	-0.949136
9	2.119537	-3.137947	-2.171191
6	4.018724	2.033723	1.263616
9	2.002578	1.335528	2.214232
6	4.907985	2.004466	0.190067
9	5.449698	1.236764	-1.962885
9	4.309119	2.732278	2.344593
9	6.035772	2.680039	0.253635
6	0.098424	2.076476	-0.001967
6	-0.345484	2.820810	1.091624
6	0.669440	2.762856	-1.073807
6	-0.215857	4.206270	1.124622
9	-0.891697	2.213998	2.130789
6	0.810827	4.145766	-1.062572
9	1.081955	2.089392	-2.135978
6	0.365802	4.867552	0.044421
9	-0.635223	4.893185	2.169716
9	1.351682	4.775059	-2.088023
9	0.492069	6.177233	0.067727
6	2.525113	-2.314802	-0.007425
6	2.889087	-3.105047	-1.098643
6	3.380440	-2.284346	1.094466
6	4.069606	-3.841158	-1.100020
9	3.142116	-0.142026	-2.101681
6	4.568410	-3.008810	1.112767
9	3.069837	-1.553584	2.156131
6	4.909692	-3.791538	0.011212
9	4.402892	-4.574949	-2.144976
9	5.366338	-2.963708	2.164442
9	6.031349	-4.482073	0.018916
6	-2.757496	-2.276725	-0.061840
6	-3.730260	-2.059697	-1.037562
6	-3.054969	-3.200572	0.940388
6	-4.948964	-2.729929	-1.033965
9	-3.486292	-1.209437	-2.031458
6	-4.267025	-3.882006	0.982735
9	-2.186694	-3.406960	1.919774
6	-5.213196	-3.644081	-0.013873
9	-5.846541	-2.515296	-1.978524
9	-4.533266	-4.737118	1.951908
9	-6.363843	-4.283193	0.008885
6	-2.503224	0.874490	-0.081770
6	-3.422280	0.798101	0.965611
6	-2.804013	1.724312	-1.146629
6	-4.599831	1.539274	0.963129
9	-3.173055	0.004501	1.997875
6	-3.971671	2.480474	-1.170342
9	-1.976625	1.811103	-2.178064
6	-4.870801	2.387430	-0.109374
9	-5.450331	1.454192	1.969019
9	-4.234529	3.276594	-2.190232
9	-5.979579	3.098876	-0.122090
6	-0.015716	-2.331448	-0.076084
8	0.011763	-3.543910	-0.140405

3-P-1B

SCF energy = -3925.483605200 a.u.

6	-1.068735	1.329855	0.177905
6	-1.558702	0.070795	0.151223
6	-0.445852	-0.962315	0.248907
5	0.487319	1.179770	0.359400
6	0.758385	-0.377819	0.410773
6	-0.707175	-2.407435	0.138031
6	-0.287049	-3.297477	1.129467
6	-1.376831	-2.932337	-0.969426
6	-0.540312	-4.662673	1.031424
9	2.708467	0.129029	2.330270
6	-1.641800	-4.291855	-1.086936
9	-1.745107	-2.126734	-1.954982
6	-1.219464	-5.158878	-0.079979
9	-0.147684	-5.486534	1.984555
9	-2.270325	-4.765703	-2.146115
9	-1.460422	-6.449119	-0.180876
6	-2.970867	-0.329141	0.034759

6	-3.771119	0.113864	-1.020755
6	-3.551842	-1.170823	0.985388
6	-5.102329	-0.276328	-1.133047
9	-3.265291	0.900021	-1.955562
6	-4.878615	-1.574947	0.892361
9	-2.835575	-1.577291	2.024125
6	-5.655274	-1.123215	-0.173659
9	-5.839710	0.142387	-2.144248
9	-5.407370	-2.365122	1.807694
9	-6.914010	-1.495736	-0.273666
6	2.079525	-1.020948	0.379319
6	3.046309	-0.668741	1.325455
6	2.490249	-1.836586	-0.679956
6	4.371820	-1.068425	1.214938
9	0.344232	-2.850784	2.201384
6	3.809526	-2.268615	-0.802071
9	1.638058	-2.170988	-1.636212
6	4.752780	-1.878736	0.145844
9	5.270528	-0.673858	2.098544
9	4.173389	-3.023723	-1.820659
9	6.007531	-2.260511	0.025525
6	2.919238	2.230447	0.043510
6	4.064505	2.617297	0.746350
6	3.091361	1.507687	-1.138340
6	5.333717	2.248324	0.299087
9	3.976776	3.276976	1.878426
6	4.340818	1.125020	-1.601855
9	2.013991	1.117222	-1.816757
6	5.468571	1.505731	-0.873043
9	6.408182	2.590929	0.981282
9	4.469730	0.399734	-2.697243
9	6.663054	1.144542	-1.286687
6	-1.830287	2.583030	0.149895
6	-1.417576	3.616576	-0.696445
6	-2.947224	2.824223	0.955221
6	-2.083198	4.834444	-0.757666
9	-0.360121	3.432876	-1.478349
6	-3.634138	4.034524	0.909589
9	-3.366230	1.904552	1.813796
6	-3.202426	5.040234	0.047764
9	-1.674315	5.786491	-1.575680
9	-4.685625	4.235552	1.683226
9	-3.848047	6.187912	-0.002418
6	1.538025	2.351054	0.621261
8	1.229050	3.215898	1.414611

4

SCF energy = -183.522590389 a.u.

6	0.000000	0.674684	-1.086918
6	0.000000	-0.674684	-1.086918
1	0.000000	0.000000	2.264398
1	0.000000	2.293894	0.860695
1	0.000000	1.284706	-1.995934
1	0.000000	-1.284706	-1.995934
1	0.000000	-2.293894	0.860695
5	0.000000	1.168018	0.426622
5	0.000000	-1.168018	0.426622
7	0.000000	0.000000	1.254697

4-TS-0

SCF energy = -367.053923595 a.u.

ν = -190.5756 cm^{-1}

6	2.017586	-1.138308	-0.224584
6	2.744340	-0.183527	0.397146
1	0.353071	1.699374	-1.121210
1	0.183305	-0.852215	-1.930387
1	2.259139	-2.206147	-0.191499
1	3.642379	-0.392613	0.987177
1	2.498611	2.327071	0.339965
5	0.820747	-0.437559	-0.996503
5	2.088160	1.221451	0.087513
7	0.874799	0.980249	-0.638367
6	-2.744237	0.183532	-0.397345
6	-2.017736	1.138273	0.224811
1	-0.353119	-1.699369	1.121246
1	-2.498223	-2.327061	-0.340662
1	-3.642171	0.392624	-0.987564
1	-2.259402	2.206086	0.191927
1	-0.183443	0.852120	1.930693
5	-2.087963	-1.221423	-0.087880
5	-0.821025	0.437506	0.996892
7	-0.874721	-0.980186	0.638370

4-I-0

SCF energy = -367.085515274 a.u.

6	-1.966366	1.118287	-0.148597
6	-2.734987	0.072711	0.248497
1	-0.219034	-1.526862	-1.185980
1	-0.178249	1.002764	-1.800185
1	-2.311859	2.157678	-0.064906
1	-3.743907	0.188549	0.655797

1	-2.361610	-2.380602	0.001020
5	-0.529370	0.661499	-0.686528
5	-1.973720	-1.238522	-0.030167
7	-0.595859	-0.918676	-0.464298
6	2.734995	-0.072721	-0.248476
6	1.966359	-1.118290	0.148605
1	0.219045	1.526874	1.185968
1	2.361627	2.380595	-0.001016
1	3.743923	-0.188565	-0.655753
1	2.311852	-2.157683	0.064935
1	0.178227	-1.002746	1.800179
5	1.973722	1.238519	0.030145
5	0.529362	-0.661492	0.686523
7	0.595861	0.918683	0.464285

4-TS-1

SCF energy = -296.706936072 a.u.

ν = -218.5008 cm^{-1}

6	1.538073	0.907262	-0.497854
6	0.678505	1.174002	0.509327
1	0.585926	-2.244703	0.363737
1	2.314389	-1.304642	-1.436824
1	2.092523	1.682082	-1.037743
1	0.454951	2.184115	0.870173
1	-0.278039	-0.436982	2.191733
5	1.606436	-0.663227	-0.696826
5	0.114960	-0.215458	1.071103
7	0.680550	-1.251612	0.206160
8	-2.620426	0.094669	-0.643856
6	-1.812773	0.004984	0.136070

4-I-1

SCF energy = -296.716086672 a.u.

6	-1.613944	0.868314	-0.367205
5	-1.693834	-0.701293	-0.491854
7	-0.599887	-1.241786	0.213842
5	0.211826	-0.144989	0.865372
6	1.581692	-0.036826	0.035758
6	-0.539467	1.208678	0.378079
8	2.502510	0.083169	-0.604067
1	-2.309739	1.615333	-0.764906
1	-2.520468	-1.376611	-1.060393
1	-0.437792	-2.228767	0.356398
1	0.547289	-0.232955	2.037912
1	-0.259811	2.240567	0.619245

4-TS-2

SCF energy = -296.683226195 a.u.

ν = -431.5330 cm^{-1}

6	-0.922066	1.315380	0.005579
5	-1.830066	0.098449	-0.437445
7	-1.219695	-1.106240	-0.073674
5	0.064807	-0.999029	0.639966
6	1.220303	-0.317760	-0.048481
6	0.320975	1.022448	0.436102
8	2.273470	-0.106773	-0.537459
1	-1.257524	2.358446	0.043762
1	-2.899956	0.164486	-0.989528
1	-1.640867	-2.010994	-0.242123
1	0.236246	-1.296102	1.797607
1	1.023237	1.764524	0.833861

4-TS-2B

SCF energy = -296.692249737 a.u.

ν = -588.4131 cm^{-1}

6	-1.952619	0.791144	-0.032317
6	-0.679809	1.241210	0.001893
1	-0.292974	-2.185785	-0.026964
1	-2.882059	-1.554944	-0.115733
1	-2.815626	1.464155	-0.057569
1	-0.389050	2.295415	0.015137
1	1.186819	0.077747	1.223106
5	-1.949499	-0.792576	-0.040787
5	0.249532	-0.040649	0.007893
7	-0.598389	-1.225577	0.029525
8	2.902915	0.057370	-0.113546
6	1.742116	-0.000752	0.001789

4-TS-2C

SCF energy = -296.680634949 a.u.

ν = -336.8007 cm^{-1}

6	1.852578	0.120860	-0.409854
5	0.935804	1.301122	0.006293
7	-0.366758	0.878671	0.483909
5	-0.078674	-1.019831	0.645656
6	-1.200251	-0.274877	-0.089657
6	1.317106	-1.074282	-0.079025
8	-2.260890	-0.116614	-0.583104
1	2.824889	0.204318	-0.903918
1	1.202958	2.477779	0.017881
1	-0.975810	1.557394	0.936940

1	-0.319732	-1.469709	1.736792
1	1.819874	-2.024231	-0.298753

4-P-1

SCF energy = -296.736383652 a.u.

6	-0.875936	1.412611	0.000016
5	-1.845666	0.178293	0.000382
7	-1.292074	-1.142609	-0.000611
5	0.101059	-1.386395	-0.000134
6	1.078480	-0.099955	0.000190
6	0.462203	1.260265	-0.000554
8	2.290161	-0.225923	0.000489
1	-1.283888	2.428784	-0.000289
1	-3.045742	0.310880	0.003304
1	-1.929190	-1.931835	-0.000377
1	0.552641	-2.502153	-0.000181
1	1.163954	2.102960	-0.001242

4-P-1B

SCF energy = -296.718717924 a.u.

6	-2.132157	0.447605	0.000046
6	-1.027380	1.223397	0.000286
1	0.370465	-1.896290	0.000248
1	-2.345705	-2.078430	-0.002780
1	-3.152748	0.843295	-0.000307
1	-1.049456	2.317893	0.000278
1	2.171054	1.639145	-0.001246
5	-1.669559	-1.080705	-0.000509
5	0.230651	0.256299	0.000162
7	-0.237398	-1.087644	0.000922
8	2.621508	-0.321962	0.000019
6	1.807980	0.576602	-0.000511

4-P-1C

SCF energy = -296.712604294 a.u.

6	-1.872755	0.188902	-0.000019
5	-0.863262	1.404465	0.000091
7	0.524720	1.143130	0.000079
5	0.064916	-1.390382	0.000189
6	1.089905	-0.138809	0.000001
6	-1.454105	-1.100851	-0.000140
8	2.295125	-0.275589	-0.000197
1	-2.950555	0.397455	-0.000021
1	-1.235979	2.551139	0.000122
1	1.216048	1.889275	0.000011
1	0.546153	-2.492928	0.000704
1	-2.196251	-1.908011	-0.000250

5

SCF energy = -379.938486609 a.u.

6	1.214638	0.424191	0.003166
6	0.921770	-0.899111	-0.002612
5	-0.163340	1.231044	-0.003682
5	-0.662591	-1.040224	-0.017675
7	-1.241617	0.280565	-0.017817
6	-2.661376	0.555625	-0.016473
1	-3.162968	0.098631	0.852438
1	-2.852915	1.636725	0.023702
1	-3.153709	0.165467	-0.922738
6	-0.289872	2.799186	0.014648
1	0.175164	3.189590	0.936785
1	0.296331	3.229838	-0.815026
1	-1.312544	3.198196	-0.044741
6	2.572056	1.062615	0.003291
1	2.732818	1.632030	-0.928043
1	2.665734	1.790768	0.825942
1	3.394595	0.338459	0.096132
6	1.877124	-2.055454	-0.009881
1	2.929333	-1.755722	0.101825
1	1.640040	-2.766765	0.798564
1	1.790390	-2.623797	-0.951702
6	-1.499121	-2.372176	0.017701
1	-0.959679	-3.228975	-0.412817
1	-1.688588	-2.621964	1.078565
1	-2.484350	-2.289797	-0.466423

5-TS-0

SCF energy = -759.884415687 a.u.

ν = -254.7853 cm^{-1}

6	-1.971353	-1.115365	0.495646
6	-2.741956	-0.095656	0.034751
5	-0.598156	-0.522868	1.031990
5	-1.972744	1.250325	0.287885
7	-0.639894	0.951606	0.787385
6	2.740667	0.095612	-0.024938
6	1.978703	1.122559	-0.482812
5	1.967201	-1.246059	-0.292853
5	0.604016	0.536418	-1.026502
7	0.638113	-0.940373	-0.791650
6	-0.045668	-1.872337	-1.676475

1	0.484392	-1.984723	-2.638221
1	-0.121268	-2.868651	-1.217939
1	-1.065442	-1.530140	-1.894781
6	2.547295	-2.704924	-0.176176
1	2.998639	-2.983567	-1.146162
1	3.348604	-2.776265	0.574629
1	1.784073	-3.465691	0.048137
6	4.112487	0.198785	0.576599
1	4.146088	-0.288224	1.565664
1	4.855213	-0.327057	-0.046735
1	4.455930	1.236636	0.699058
6	2.378753	2.571761	-0.501406
1	2.820173	2.900398	0.453539
1	3.136938	2.754220	-1.281852
1	1.526375	3.230522	-0.723095
6	-0.240766	1.182852	-2.196319
1	-0.330053	2.274840	-2.092308
1	0.288033	0.992897	-3.147288
1	-1.251884	0.760708	-2.303927
6	0.255538	-1.161610	2.199004
1	-0.271466	-0.974927	3.151601
1	0.352127	-2.253076	2.095319
1	1.263508	-0.731254	2.302506
6	-2.389040	-2.557394	0.502434
1	-3.219227	-2.715598	1.212728
1	-2.757261	-2.884929	-0.484408
1	-1.571539	-3.229615	0.801213
6	-4.107991	-0.269225	-0.568509
1	-4.758047	-0.897287	0.063248
1	-4.619950	0.691092	-0.726896
1	-4.045978	-0.772593	-1.549666
6	-2.545875	2.710895	0.160617
1	-3.364402	2.779947	-0.571394
1	-2.966676	3.014436	1.136695
1	-1.779209	3.457141	-0.098531
6	0.032590	1.890525	1.674405
1	0.095496	2.888334	1.217426
1	-0.499202	1.994780	2.636147
1	1.056598	1.561066	1.891627

5-I-0

SCF energy = -759.908335220 a.u.

6	-1.993718	-1.110496	0.305536
6	-2.764995	-0.020563	0.032264
5	-0.483068	-0.713807	0.692438
5	-1.912336	1.249608	0.216004
7	-0.508378	0.888489	0.600800
6	2.764238	0.024591	-0.022122
6	1.999731	1.118067	-0.295944
5	1.909858	-1.243095	-0.223289
5	0.489468	0.723380	-0.692751
7	0.508215	-0.880241	-0.605653
6	-0.002747	-1.661746	-1.737104
1	0.672356	-1.576862	-2.602694
1	-0.095896	-2.725569	-1.474646
1	-0.990751	-1.296362	-2.043812
6	2.398288	-2.736782	-0.156055
1	2.840175	-3.008033	-1.132392
1	3.197587	-2.866283	0.589728
1	1.597920	-3.462308	0.051801
6	4.211549	0.032516	0.391595
1	4.333778	-0.382019	1.406695
1	4.820018	-0.601852	-0.273690
1	4.657366	1.038060	0.389145
6	2.494650	2.537098	-0.230972
1	2.958794	2.767706	0.742108
1	3.265839	2.715100	-0.999412
1	1.689572	3.266133	-0.404457
6	-0.070165	1.360047	-2.062347
1	-0.042368	2.461641	-2.021450
1	0.557347	1.058150	-2.917010
1	-1.107714	1.073913	-2.304166
6	0.085648	-1.349298	2.058868
1	-0.540734	-1.054791	2.916860
1	0.065772	-2.451024	2.014083
1	1.121872	-1.055920	2.297790
6	-2.512063	-2.517695	0.236736
1	-3.311029	-2.670394	0.982933
1	-2.963835	-2.733989	-0.746517
1	-1.731527	-3.267868	0.430313
6	-4.214305	-0.094431	-0.370653
1	-4.811982	-0.665359	0.359714
1	-4.672135	0.900982	-0.466220
1	-4.337511	-0.605620	-1.341347
6	-2.387432	2.746915	0.131038
1	-3.198510	2.876019	-0.601725
1	-2.803085	3.045094	1.110837
1	-1.580095	3.454983	-0.108131
6	-0.006658	1.671609	1.735596
1	0.077755	2.736906	1.476429

1	-0.683362	1.578373	2.599144
1	0.983792	1.314037	2.043421

5-TS-1

SCF energy = -493.119575427 a.u.

ν = -252.4224 cm^{-1}

6	-0.126017	-1.236855	-0.331532
6	-1.324365	-0.655066	-0.073207
5	0.960593	-0.069102	-0.529546
5	-1.128280	0.922556	-0.055590
7	0.251287	1.208415	-0.272692
6	0.877966	2.501677	-0.406173
1	0.160786	3.310746	-0.209774
1	1.713932	2.624966	0.305510
1	1.289604	2.657161	-1.417773
6	2.197459	-0.174686	-1.519399
1	2.709444	-1.147277	-1.453264
1	1.811193	-0.082664	-2.549322
1	2.948893	0.619019	-1.384014
6	0.176561	-2.697639	-0.494482
1	0.424551	-2.921499	-1.546010
1	1.060506	-2.993464	0.095517
1	-0.655849	-3.353836	-0.201153
6	-2.644632	-1.343889	0.118951
1	-2.575614	-2.441339	0.092611
1	-3.099325	-1.056704	1.081761
1	-3.362166	-1.035716	-0.659867
6	-2.289764	1.972457	0.142152
1	-3.068498	1.818129	-0.624372
1	-2.788062	1.795160	1.111043
1	-1.986065	3.028893	0.106793
8	1.650033	-0.268403	2.445534
6	1.682099	-0.266086	1.317452

5-I-1

SCF energy = -493.123261327 a.u.

6	-0.079084	1.232699	-0.242044
6	1.206173	0.843010	-0.044335
5	-1.004623	-0.101657	-0.396791
5	1.278398	-0.739501	-0.006767
7	-0.029082	-1.252739	-0.196495
6	-0.439587	-2.631204	-0.304689
1	0.410299	-3.311377	-0.153716
1	-1.206072	-2.897287	0.445994
1	-0.872107	-2.849690	-1.296047
6	-2.094430	-0.163075	-1.577016
1	-2.784180	0.695929	-1.571305
1	-1.552025	-0.140037	-2.536146
1	-2.703770	-1.080923	-1.564359
6	-0.616523	2.627379	-0.380464
1	-1.070821	2.769216	-1.375165
1	-1.415584	2.829212	0.353518
1	0.152204	3.402330	-0.247809
6	2.409048	1.737203	0.062731
1	2.177021	2.808398	-0.027622
1	2.918688	1.583471	1.028759
1	3.149711	1.487892	-0.714869
6	2.605370	-1.576358	0.188074
1	3.349726	-1.288167	-0.573395
1	3.063446	-1.330087	1.161666
1	2.483065	-2.668560	0.142132
8	-1.906830	0.082160	2.192975
6	-1.659344	-0.018427	1.094047

5-TS-2

SCF energy = -493.096867160 a.u.

ν = -316.2555 cm^{-1}

6	-1.122880	0.553010	-0.016054
6	0.001240	1.308339	-0.100104
5	-0.242978	-1.224229	-0.275597
5	1.384770	0.535801	0.092546
7	1.180305	-0.843311	-0.042261
6	2.144763	-1.907710	0.136393
1	3.152005	-1.498511	0.290506
1	1.898361	-2.534645	1.010782
1	2.180787	-2.569171	-0.745492
6	-0.747360	-1.943141	-1.590896
1	-1.841400	-1.973194	-1.693194
1	-0.317965	-1.462355	-2.483704
1	-0.395950	-2.989444	-1.579097
6	-2.535566	0.973932	-0.312477
1	-3.085452	0.158164	-0.807830
1	-3.076801	1.206394	0.617219
1	-2.574602	1.851628	-0.971209
6	-0.003384	2.768724	-0.454425
1	-1.004985	3.211673	-0.534358
1	0.559312	3.333549	0.306294
1	0.525302	2.933890	-1.408067
6	2.751882	1.273718	0.376947
1	2.942496	2.046199	-0.386821

1	2.692514	1.808403	1.340858
1	3.632179	0.616033	0.415420
8	-1.897369	-0.951048	1.798853
6	-1.168354	-0.891023	0.868775

5-TS-2B

SCF energy = -493.090361988 a.u.

ν = -509.4998 cm^{-1}

6	-0.181182	1.250562	-0.095962
6	-1.457445	0.793305	-0.043703
5	0.740176	-0.039512	-0.107025
5	-1.447544	-0.797969	-0.025393
7	-0.094546	-1.242895	-0.033760
6	0.413135	-2.591806	-0.092200
1	-0.402257	-3.323444	-0.011324
1	0.944021	-2.790220	-1.039524
1	1.120398	-2.797441	0.730215
6	2.005272	0.064884	1.399535
1	2.516614	1.019560	1.580210
1	1.100243	0.010284	2.019601
1	2.664745	-0.779809	1.639843
6	0.301776	2.669499	-0.124947
1	0.891696	2.903144	0.778011
1	0.967875	2.844036	-0.985967
1	-0.516422	3.401228	-0.179852
6	-2.708181	1.624608	-0.010205
1	-2.524347	2.702753	-0.125627
1	-3.405526	1.314444	-0.805518
1	-3.244945	1.477532	0.942176
6	-2.732938	-1.712462	-0.036988
1	-3.445748	-1.384336	0.737676
1	-3.258199	-1.586279	-1.000035
1	-2.547053	-2.787428	0.102574
8	3.291087	0.024818	-0.843501
6	2.194375	-0.021073	-0.451536

5-TS-2C

SCF energy = -493.095120114 a.u.

ν = -197.6925 cm^{-1}

6	-1.256902	-0.782850	0.019177
6	-1.414622	0.563931	0.083443
5	0.239169	-1.269131	-0.179082
5	-0.057314	1.307858	-0.099001
7	1.120980	0.434643	-0.090301
6	2.422769	0.908130	-0.548267
1	2.317164	1.445612	-1.499807
1	2.890265	1.577100	0.190226
1	3.099894	0.055968	-0.704510
6	0.703884	-2.282314	-1.300317
1	0.355923	-3.290030	-1.013064
1	0.241123	-2.048379	-2.271666
1	1.793899	-2.344277	-1.429078
6	-2.329482	-1.826989	0.140903
1	-2.365890	-2.446229	-0.770928
1	-2.103364	-2.516131	0.971664
1	-3.330900	-1.409081	0.310784
6	-2.715714	1.298333	0.271242
1	-3.589756	0.633652	0.314880
1	-2.702572	1.888058	1.203033
1	-2.886266	2.016178	-0.547622
6	0.116018	2.850470	-0.373764
1	0.268416	3.008158	-1.457280
1	-0.771947	3.432889	-0.089235
1	0.996596	3.280558	0.128812
8	2.062211	-0.808205	1.713069
6	1.229647	-0.737801	0.871209

5-P-1

SCF energy = -493.148248881 a.u.

6	1.479408	-0.518860	0.006472
6	1.187440	0.805699	0.033033
5	-1.192649	-0.976392	0.014584
5	-0.305992	1.339432	-0.046807
7	-1.422278	0.427503	0.049007
6	-2.782576	0.957113	0.101333
1	-2.860162	1.776435	0.830358
1	-3.103995	1.347745	-0.877563
1	-3.492913	0.177408	0.400518
6	-2.332703	-2.059882	0.031243
1	-1.911261	-3.065697	-0.098523
1	-2.874238	-2.038675	0.993582
1	-3.086092	-1.883832	-0.754427
6	2.865805	-1.101564	0.034193
1	3.359124	-0.912551	1.001275
1	2.809907	-2.187248	-0.114064
1	3.504396	-0.668984	-0.750548
6	2.288476	1.834108	0.110636
1	3.258686	1.404157	0.390557
1	2.417963	2.340382	-0.861412
1	2.046039	2.623380	0.839085

6	-0.578808	2.892498	-0.187869
1	-0.734497	3.314402	0.823415
1	0.262237	3.445295	-0.628004
1	-1.486146	3.129386	-0.762952
8	0.563740	-2.689709	-0.134774
6	0.344657	-1.491054	-0.051547

5-P-1B

SCF energy = -493.129669291 a.u.

6	-0.293932	1.251503	-0.085194
6	-1.571998	0.804281	-0.009739
5	0.643365	-0.029601	-0.056466
5	-1.531904	-0.789525	0.061163
7	-0.151685	-1.211661	0.013536
6	0.323732	-2.580471	0.037219
1	-0.235905	-3.206540	-0.674293
1	1.383399	-2.627155	-0.248897
1	0.215495	-3.035267	1.035969
6	3.067187	0.415645	1.055442
1	2.856657	1.478584	1.258699
1	2.783889	-0.144162	1.961565
1	4.137741	0.283034	0.846801
6	0.188010	2.669153	-0.170636
1	0.721520	2.956719	0.751746
1	0.909299	2.788775	-0.995474
1	-0.622987	3.396125	-0.320820
6	-2.828140	1.622527	0.013182
1	-2.652525	2.698314	-0.130406
1	-3.530168	1.285486	-0.767182
1	-3.354955	1.494480	0.973984
6	-2.773911	-1.746923	0.135682
1	-3.504724	-1.391765	0.880393
1	-3.298276	-1.708344	-0.836434
1	-2.537165	-2.799653	0.346281
8	2.765334	-0.405513	-1.163467
6	2.240805	-0.043593	-0.124695

5-P-1C

SCF energy = -493.126921835 a.u.

6	1.515034	0.305395	-0.079716
6	0.582866	1.297725	0.021489
5	1.004687	-1.155008	0.028748
5	-0.981633	0.988238	0.017827
7	-1.468232	-0.359335	0.008351
6	-2.894656	-0.662903	-0.023113
1	-3.426545	-0.112904	0.765294
1	-3.339610	-0.393824	-0.993529
1	-3.030381	-1.739106	0.130688
6	1.948854	-2.392698	0.190904
1	2.471172	-2.544543	-0.773320
1	2.744663	-2.218334	0.933575
1	1.407088	-3.318454	0.424543
6	2.997751	0.593660	-0.171972
1	3.395913	0.977321	0.782991
1	3.572121	-0.309249	-0.419526
1	3.223564	1.349013	-0.940529
6	0.983263	2.749964	0.097744
1	2.059319	2.899919	0.250271
1	0.698205	3.277987	-0.828498
1	0.451366	3.261161	0.915646
6	-2.047720	2.158584	0.011707
1	-2.567719	2.184351	0.986809
1	-1.625464	3.157505	-0.155728
1	-2.833688	1.990937	-0.742088
8	-1.003085	-2.590073	-0.096585
6	-0.587553	-1.448393	-0.022919

6

SCF energy = -458.489188614 a.u.

6	-0.709352	-0.608271	0.158115
6	-0.585831	0.708320	-0.138620
5	0.756486	-1.231437	0.240670
5	0.968742	1.033110	-0.260528
7	1.705205	-0.182070	-0.022813
6	3.146469	-0.294338	-0.021897
1	3.602315	0.277142	0.804389
1	3.459138	-1.342097	0.091213
1	3.584811	0.082805	-0.960482
6	1.150761	-2.719842	0.574705
1	1.680501	-2.756944	1.543135
1	0.286915	-3.396355	0.643286
1	1.850693	-3.130518	-0.172566
6	-1.986997	-1.381724	0.335541
1	-1.876378	-2.076431	1.186146
1	-2.822888	-0.711480	0.593834
6	-1.691134	1.714949	-0.301013
1	-2.663552	1.218110	-0.449395
1	-1.507029	2.305991	-1.215277
6	1.649296	2.420026	-0.561568
1	0.947147	3.181146	-0.931623

1	2.093405	2.809412	0.372821
1	2.480669	2.329484	-1.279813
6	-2.349390	-2.188398	-0.915533
1	-1.541419	-2.886091	-1.186900
1	-3.266616	-2.777272	-0.762594
1	-2.510458	-1.520272	-1.775464
6	-1.782495	2.669061	0.893831
1	-2.014716	2.116515	1.817242
1	-0.828504	3.195214	1.055504
1	-2.564567	3.429065	0.744158

6-TS-0

SCF energy = -916.984795736 a.u.

ν = -248.5139 cm^{-1}

6	-2.111544	-0.719429	0.356053
6	-2.626400	0.497974	0.029625
5	-0.648283	-0.507120	0.947428
5	-1.590458	1.591340	0.483359
7	-0.351694	0.954122	0.897472
6	2.767678	-0.478524	-0.116504
6	2.231523	0.736311	-0.402615
5	1.729171	-1.580408	-0.541252
5	0.765293	0.530021	-0.979838
7	0.491248	-0.941231	-0.952195
6	-0.350080	-1.568629	-1.961804
1	0.130613	-1.551721	-2.955607
1	-0.551902	-2.620120	-1.711923
1	-1.315510	-1.054104	-2.050462
6	1.978927	-3.130869	-0.666429
1	2.156326	-3.381713	-1.727970
1	2.857977	-3.474469	-0.102011
1	1.104695	-3.722607	-0.350086
6	4.128946	-0.738305	0.472208
1	4.628802	-1.537703	-0.101947
1	4.775278	0.149965	0.383763
6	2.926013	2.065295	-0.271230
1	3.606179	2.073723	0.597458
1	2.180673	2.856484	-0.089251
6	0.085781	1.487939	-2.039715
1	0.247715	2.551391	-1.806170
1	0.558632	1.300311	-3.020335
1	-0.994168	1.319480	-2.170821
6	0.028841	-1.460855	2.010015
1	-0.455146	-1.280068	2.986663
1	-0.116751	-2.525872	1.775112
1	1.104457	-1.278330	2.149031
6	-2.715987	-2.099369	0.295351
1	-3.032061	-2.347707	1.326526
1	-1.900028	-2.813901	0.094011
6	-3.988077	0.839044	-0.526839
1	-3.920457	1.794422	-1.073528
1	-4.322855	0.096213	-1.264091
6	-1.840864	3.139689	0.626837
1	-2.724649	3.492469	0.076093
1	-2.004601	3.379213	1.693154
1	-0.968626	3.732640	0.307256
6	0.489338	1.587299	1.904163
1	0.712178	2.628650	1.632725
1	-0.002642	1.598926	2.892308
1	1.445070	1.058998	2.012419
6	-5.043424	0.979810	0.573491
1	-6.020689	1.274053	0.160928
1	-5.173171	0.030484	1.116582
1	-4.743573	1.740513	1.311169
6	-3.865235	-2.389547	-0.664912
1	-4.783209	-1.848491	-0.395636
1	-3.603798	-2.118917	-1.699586
1	-4.104563	-3.463614	-0.654319
6	4.050141	-1.164414	1.940843
1	3.449520	-2.080341	2.057016
1	5.048719	-1.362145	2.359400
1	3.576620	-0.379849	2.552106
6	3.713733	2.416193	-1.537886
1	4.495594	1.666260	-1.732396
1	3.051707	2.438929	-2.417127
1	4.196287	3.401469	-1.449771

6-I-0

SCF energy = -917.008333008 a.u.

6	-2.135604	-0.655582	0.213358
6	-2.650083	0.599661	0.058212
5	-0.571354	-0.623458	0.601095
5	-1.532947	1.625890	0.350933
7	-0.238046	0.939907	0.658865
6	2.748829	-0.552450	-0.093711
6	2.249646	0.701472	-0.276879
5	1.641976	-1.579832	-0.409397
5	0.689957	0.684091	-0.675266
7	0.355575	-0.885407	-0.732920
6	-0.310175	-1.419855	-1.925530

1	0.357056	-1.358728	-2.799102
1	-0.596203	-2.471959	-1.783530
1	-1.216866	-0.845259	-2.152222
6	1.787720	-3.141767	-0.528639
1	2.018445	-3.393544	-1.580040
1	2.616804	-3.533786	0.078593
1	0.866469	-3.684538	-0.266907
6	4.145323	-0.896257	0.362410
1	4.514217	-1.771331	-0.199168
1	4.850005	-0.077934	0.142662
6	3.051618	1.969849	-0.144440
1	3.782934	1.893030	0.678258
1	2.383285	2.809354	0.108286
6	0.260384	1.556558	-1.959535
1	0.510987	2.620047	-1.808783
1	0.801501	1.225215	-2.860930
1	-0.816456	1.509755	-2.193860
6	-0.150862	-1.489705	1.894244
1	-0.712288	-1.159587	2.783752
1	-0.383779	-2.557557	1.749985
1	0.920617	-1.425245	2.146609
6	-2.845838	-1.983565	0.098189
1	-3.319454	-2.180769	1.078330
1	-2.081751	-2.773384	0.006789
6	-4.085351	0.977661	-0.240343
1	-4.136339	2.052202	-0.478532
1	-4.447530	0.461407	-1.143037
6	-1.674833	3.190453	0.447521
1	-2.431328	3.578398	-0.251259
1	-2.024900	3.454606	1.462153
1	-0.730350	3.729237	0.279450
6	0.424491	1.478554	1.851993
1	0.696208	2.534101	1.710240
1	-0.240106	1.407656	2.726841
1	1.339282	0.915743	2.075514
6	-5.033788	0.693799	0.926567
1	-6.063241	1.008922	0.696304
1	-5.058910	-0.379097	1.173042
1	-4.710183	1.228772	1.832955
6	-3.876881	-2.174086	-1.014500
1	-4.806891	-1.619911	-0.829751
1	-3.478426	-1.844759	-1.986533
1	-4.144734	-3.237166	-1.107559
6	4.187814	-1.214533	1.859490
1	3.510140	-2.047552	2.105527
1	5.200343	-1.493779	2.189167
1	3.864774	-0.344625	2.453247
6	3.787760	2.307037	-1.446420
1	4.502251	1.513101	-1.710979
1	3.079368	2.407984	-2.281722
1	4.343168	3.252551	-1.354143

6-TS-1

SCF energy = -571.670696349 a.u.

ν = -251.7392 cm^{-1}

6	0.398542	0.859466	-0.053537
6	1.046664	-0.309897	-0.285421
5	-1.179908	0.593036	-0.203474
5	-0.032403	-1.440955	-0.570483
7	-1.330146	-0.860218	-0.454693
6	-2.602160	-1.497947	-0.697492
1	-3.290629	-1.375925	0.157532
1	-3.110098	-1.078828	-1.582797
1	-2.477301	-2.577261	-0.863238
6	-2.222083	1.663802	-0.741017
1	-3.273742	1.383729	-0.572434
1	-2.060904	2.663856	-0.308725
1	-2.082350	1.756650	-1.831812
6	1.026285	2.205300	0.196282
1	0.383053	2.797466	0.870703
1	1.994139	2.097341	0.713556
6	2.537446	-0.519257	-0.280824
1	3.074912	0.441920	-0.325566
1	2.827475	-1.073831	-1.190302
6	0.262293	-2.953384	-0.920029
1	1.259639	-3.091969	-1.364816
1	0.248621	-3.545946	0.012925
1	-0.481003	-3.406679	-1.594284
6	1.230727	2.990443	-1.103443
1	0.274778	3.139665	-1.627968
1	1.671373	3.980713	-0.911259
1	1.899931	2.443207	-1.784718
6	3.002839	-1.307515	0.946887
1	2.764083	-0.763705	1.874119
1	2.504798	-2.288136	1.001353
1	4.089256	-1.483037	0.924913
8	-1.285588	0.071589	2.809341
6	-1.440344	0.480519	1.768716

6-I-1

SCF energy = -571.674378975 a.u.

6	-0.374832	-0.831716	-0.013200
6	-1.039000	0.331411	-0.234338
5	1.225802	-0.543735	-0.114940
5	0.004863	1.500616	-0.458769
7	1.311057	0.954673	-0.363475
6	2.569574	1.631824	-0.559324
1	3.230644	1.545847	0.322329
1	3.124691	1.218927	-1.419046
1	2.416309	2.704573	-0.743319
6	2.170315	-1.552417	-0.936334
1	3.244170	-1.327430	-0.835693
1	2.021556	-2.606043	-0.651097
1	1.913643	-1.461560	-2.004159
6	-0.985413	-2.194106	0.194274
1	-0.322456	-2.813878	0.823669
1	-1.937169	-2.114231	0.745862
6	-2.536964	0.488389	-0.279399
1	-3.037476	-0.485530	-0.404824
1	-2.811431	1.088494	-1.164144
6	-0.340774	3.019635	-0.738160
1	-1.313521	3.133091	-1.241755
1	-0.423728	3.557593	0.223354
1	0.416275	3.550015	-1.336253
6	-1.226594	-2.923905	-1.131131
1	-0.285533	-3.052217	-1.686118
1	-1.665695	-3.919910	-0.966950
1	-1.911863	-2.348071	-1.771453
6	-3.078929	1.180958	0.974200
1	-2.857759	0.588081	1.875436
1	-2.617853	2.171789	1.109453
1	-4.169080	1.321815	0.916874
8	1.479228	-0.459312	2.622353
6	1.479572	-0.574069	1.497061

6-TS-2

SCF energy = -571.647178019 a.u.

ν = -334.1724 cm^{-1}

6	-0.793594	-0.437543	0.202382
6	-0.477661	0.830705	-0.166442
5	1.038315	-1.224485	-0.034435
5	1.073432	1.200458	-0.191837
7	1.838205	0.027146	-0.150741
6	3.279566	-0.084705	-0.080627
1	3.608722	-0.496136	0.889295
1	3.670302	-0.748168	-0.870285
1	3.753101	0.898489	-0.203779
6	1.090916	-2.389449	-1.104941
1	2.092094	-2.852286	-1.065684
1	0.358276	-3.190527	-0.933077
1	0.953086	-1.989751	-2.121624
6	-2.170021	-1.058541	0.135166
1	-2.237695	-1.880391	0.863951
1	-2.920103	-0.320099	0.461670
6	-1.527217	1.835123	-0.577616
1	-2.434675	1.344033	-0.959244
1	-1.137971	2.451338	-1.404521
6	1.639424	2.675480	-0.253202
1	0.989682	3.343295	-0.840082
1	1.678192	3.097872	0.766652
1	2.655977	2.745997	-0.668738
6	-2.521728	-1.571139	-1.262847
1	-1.806171	-2.336133	-1.596541
1	-3.526363	-2.019599	-1.275095
1	-2.502196	-0.758054	-2.004156
6	-1.898302	2.749421	0.595215
1	-2.326753	2.166637	1.424766
1	-1.014209	3.277336	0.983049
1	-2.636958	3.504714	0.288519
8	-0.213248	-1.690753	2.270453
6	0.222529	-1.346422	1.227555

6-TS-2B

SCF energy = -571.640558031 a.u.

ν = -507.6908 cm^{-1}

6	-0.136242	-0.849712	0.157926
6	-1.267342	-0.145337	-0.097502
5	1.038168	0.212789	0.186191
5	-0.907057	1.395900	-0.259526
7	0.501969	1.545713	-0.107857
6	1.280109	2.760325	-0.108795
1	1.761267	2.940576	0.868248
1	2.079954	2.733386	-0.869450
1	0.648147	3.631148	-0.330956
6	2.450331	-0.295759	-1.093449
1	3.279261	0.396896	-1.292524
1	2.800328	-1.336082	-1.118670
1	1.665925	-0.153584	-1.849046
6	-0.024730	-2.340915	0.349140

1	0.872100	-2.577062	0.946410
1	-0.881355	-2.710511	0.937130
6	-2.659162	-0.716940	-0.174406
1	-2.634117	-1.812222	-0.292906
1	-3.160186	-0.323947	-1.076154
6	-1.929924	2.573740	-0.503802
1	-2.813801	2.236734	-1.067554
1	-2.303306	2.936493	0.470834
1	-1.500338	3.443131	-1.024803
6	0.038590	-3.109904	-0.975106
1	0.896640	-2.789392	-1.585010
1	0.133116	-4.192952	-0.803768
1	-0.869496	-2.935549	-1.571693
6	-3.501200	-0.360143	1.054069
1	-3.045982	-0.766871	1.970201
1	-3.580818	0.730627	1.179914
1	-4.521502	-0.764693	0.971074
8	3.391870	-0.284393	1.312442
6	2.394548	-0.061091	0.752068

6-P-1

SCF energy = -571.699317592 a.u.

6	-0.964595	-0.628423	0.140110
6	-0.765731	0.690827	-0.108438
5	1.729103	-0.920995	0.123198
5	0.693094	1.318861	-0.176700
7	1.865258	0.473067	-0.127432
6	3.189398	1.071133	-0.279639
1	3.470719	1.659926	0.608258
1	3.952856	0.297613	-0.422937
1	3.225665	1.741978	-1.150021
6	2.936662	-1.920158	0.256942
1	3.662544	-1.591008	1.019157
1	2.580269	-2.925845	0.517092
1	3.493586	-1.990857	-0.694004
6	-2.304685	-1.312214	0.230611
1	-2.220087	-2.128015	0.963135
1	-3.069788	-0.616135	0.603293
6	-1.948984	1.621895	-0.281943
1	-2.801404	1.086148	-0.725539
1	-1.693218	2.417641	-0.998786
6	0.891215	2.880329	-0.355707
1	0.010190	3.480965	-0.095220
1	1.750756	3.271124	0.209613
1	1.108687	3.083505	-1.421484
6	-2.745184	-1.903146	-1.112487
1	-2.011223	-2.641020	-1.467659
1	-3.716712	-2.410830	-1.018853
1	-2.840971	-1.121109	-1.881857
6	-2.387455	2.259804	1.040011
1	-2.715490	1.491512	1.756556
1	-1.560358	2.812510	1.511849
1	-3.219757	2.963156	0.886878
8	0.080656	-2.706557	0.510209
6	0.229475	-1.514982	0.283605

6-P-1B

SCF energy = -571.680832361 a.u.

6	-0.208648	-0.883040	0.059083
6	-1.397274	-0.279569	-0.189303
5	0.887154	0.262642	0.127342
5	-1.144423	1.291019	-0.267210
7	0.263943	1.535359	-0.037948
6	0.903215	2.833982	-0.017711
1	1.903368	2.771675	0.435515
1	1.015315	3.257788	-1.030215
1	0.320512	3.553249	0.578179
6	3.485240	0.203208	-0.677772
1	4.491384	0.038123	-0.268195
1	3.287075	-0.518393	-1.487256
1	3.417114	1.207476	-1.126393
6	0.064880	-2.350354	0.230808
1	0.710237	-2.485208	1.115142
1	-0.866645	-2.901305	0.436493
6	-2.740899	-0.941385	-0.319994
1	-2.632336	-2.020058	-0.516003
1	-3.265158	-0.520775	-1.195675
6	-2.193598	2.432888	-0.520039
1	-3.152012	2.065730	-0.914475
1	-2.405567	2.929852	0.444704
1	-1.810466	3.217849	-1.191909
6	0.760879	-2.962882	-0.988003
1	1.717829	-2.458881	-1.197656
1	0.977811	-4.029715	-0.829048
1	0.133611	-2.870776	-1.888000
6	-3.609450	-0.732766	0.924561
1	-3.132199	-1.176069	1.811745
1	-3.760228	0.338728	1.130169
1	-4.601182	-1.194027	0.802591
8	2.754505	-0.242304	1.549831

6	2.444696	0.049476	0.407806

7

SCF energy = -906.251543550 a.u.

6	-1.752601	-0.666499	-0.103957
6	-1.716749	0.678656	0.043807
5	-0.251492	-1.188742	-0.186551
5	-0.188257	1.113736	0.059383
7	0.660485	-0.059586	-0.096759
6	0.110997	-2.726725	-0.214007
1	-0.710974	-3.286605	-0.690312
1	1.018399	-2.952471	-0.790473
6	-2.980296	-1.531186	-0.194147
1	-2.806981	-2.472112	0.355993
1	-3.843133	-1.045773	0.290460
6	-2.898065	1.590837	0.239434
1	-3.799771	1.172357	-0.237024
1	-2.709125	2.557324	-0.256900
6	0.270960	2.624690	0.161869
1	-0.376523	3.138785	0.893229
1	1.303681	2.756153	0.518997
6	-3.335536	-1.866852	-1.646388
1	-2.494873	-2.364885	-2.154931
1	-4.208230	-2.535136	-1.703343
1	-3.566210	-0.951169	-2.212175
6	-3.181674	1.846570	1.723463
1	-3.428606	0.907027	2.241086
1	-2.301556	2.277241	2.226290
1	-4.021766	2.544790	1.858112
6	0.275802	-3.232710	1.230937
1	0.472309	-4.315278	1.265677
1	1.110144	-2.728199	1.744232
1	-0.629977	-3.043434	1.829059
6	0.108112	3.316418	-1.204330
1	0.332739	4.392237	-1.142654
1	0.780224	2.880871	-1.959005
1	-0.918138	3.216112	-1.590980
6	3.239890	-1.656917	-0.397298
1	2.964696	-2.452180	0.310102
1	3.015817	-2.003166	-1.417816
1	4.330886	-1.514860	-0.327758
6	2.931521	0.488330	1.735780
1	2.486228	1.449452	2.034102
1	2.597646	-0.272316	2.459498
1	4.025846	0.581222	1.823256
6	3.113528	1.222331	-1.262543
1	2.889419	2.269130	-1.013043
1	4.209370	1.120664	-1.318343
1	2.707598	1.017766	-2.266038
14	2.430777	-0.005220	-0.009419

7-TS-0

SCF energy = -1812.495506730 a.u.

ν = -263.7278 cm^{-1}

6	1.942052	-0.960812	-0.991292
6	2.775734	-0.193875	-0.240582
5	0.522491	-0.242530	-1.122247
5	2.056445	1.175759	0.022434
7	0.646633	1.115967	-0.436642
6	-2.775768	0.193820	0.240550
6	-1.942118	0.960779	0.991272
5	-2.056444	-1.175808	-0.022443
5	-0.522541	0.242529	1.122244
7	-0.646647	-1.115978	0.436658
14	-0.069030	-2.640072	1.201395
6	-2.862873	-2.475064	-0.495491
6	0.415348	0.576466	2.369712
6	-0.415405	-0.576437	-2.369707
6	2.862912	2.474989	0.495474
14	0.069047	2.640123	-1.201299
6	-1.297252	-3.102882	2.562091
1	-2.243975	-3.488659	2.157338
1	-0.866667	-3.887990	3.204506
1	-1.540139	-2.242397	3.201946
6	-0.008927	-4.047732	-0.059575
1	-0.712258	-4.847610	0.219554
1	-0.270056	-3.715872	-1.073000
1	0.997602	-4.489050	-0.105631
6	1.624506	-2.574548	2.010702
1	2.427576	-2.382536	1.289338
1	1.705614	-1.843004	2.824438
1	1.791514	-3.574512	2.445277
6	-0.092605	0.139515	3.747547
1	-1.152911	0.395798	3.891317
1	-0.000832	-0.944390	3.902702
1	0.473739	0.626676	4.556471
1	1.442230	0.205032	2.226455
1	0.497458	1.673744	2.380309
6	-2.883153	-2.829163	-1.991671
1	-3.094298	-1.960389	-2.630954

1	-1.921348	-3.243678	-2.325163
1	-3.650597	-3.590120	-2.200378
1	-3.905233	-2.308145	-0.171431
1	-2.539323	-3.374140	0.047197
1	-0.497504	-1.673714	-2.380387
1	-1.442288	-0.205014	-2.226440
6	0.092570	-0.139374	-3.747500
1	1.152858	-0.395712	-3.891296
1	-0.473806	-0.626413	-4.556473
1	0.000875	0.944554	-3.902536
6	-1.624484	2.574702	-2.010619
1	-1.791433	3.574696	-2.445153
1	-1.705596	1.843204	-2.824397
1	-2.427589	2.382701	-1.289296
6	0.009008	4.047761	0.059701
1	0.712390	4.847591	-0.219429
1	-0.997494	4.489145	0.105726
1	0.270108	3.715939	1.073148
6	1.297239	3.102956	-2.562020
1	2.244046	3.488559	-2.157303
1	1.539952	2.242515	-3.202004
1	0.866698	3.888196	-3.204304
1	2.539320	3.374099	-0.047132
1	3.905240	2.308083	0.171307
6	2.883329	2.828985	1.991678
1	3.094307	1.960127	2.630900
1	3.650948	3.589760	2.200402
1	1.921627	3.243694	2.325229
6	-2.337396	2.253516	1.662517
1	-1.449086	2.748845	2.079595
1	-2.751417	2.957233	0.917808
6	-4.199027	0.560166	-0.110970
1	-4.885557	0.012623	0.560871
1	-4.370021	1.627587	0.105328
6	4.198996	-0.560273	0.110858
1	4.885507	-0.012792	-0.561054
1	4.369905	-1.627711	-0.105431
6	2.337329	-2.253538	-1.662562
1	1.449010	-2.748919	-2.079564
1	2.751457	-2.957215	-0.917872
6	3.363243	-2.069658	-2.786493
1	3.587431	-3.030875	-3.273026
1	2.987766	-1.381996	-3.558206
1	4.307635	-1.652248	-2.409537
6	4.612553	-0.285884	1.557743
1	5.600131	-0.723568	1.767098
1	4.680880	0.789332	1.767711
1	3.896099	-0.722054	2.270041
6	-4.612457	0.285805	-1.557896
1	-3.896019	0.722120	-2.270122
1	-4.680615	-0.789409	-1.767931
1	-5.600084	0.723360	-1.767286
6	-3.363403	2.069673	2.786367
1	-4.307764	1.652251	2.409347
1	-2.987988	1.382030	3.558129
1	-3.587631	3.030902	3.272856

7-I-0

SCF energy = -1812.508157760 a.u.

6	1.946925	-1.008093	-0.836096
6	2.755867	-0.129125	-0.184439
5	0.417434	-0.484695	-0.923028
5	1.977334	1.191438	0.036315
7	0.520519	1.037940	-0.346708
6	-2.756365	0.128626	0.184890
6	-1.947400	1.008338	0.835475
5	-1.977496	-1.191790	-0.035507
5	-0.417902	0.485146	0.922954
7	-0.520645	-1.037695	0.347018
14	0.009709	-2.463137	1.344068
6	-2.727407	-2.563779	-0.382103
6	0.319948	0.822971	2.325520
6	-0.321595	-0.822137	-2.325082
6	2.727564	2.563110	0.383520
14	-0.008934	2.463397	-1.344216
6	-1.322735	-2.729446	2.666488
1	-1.975420	-3.579691	2.419222
1	-0.859559	-2.942483	3.642285
1	-1.964151	-1.844575	2.794371
6	0.136647	-4.017154	0.273497
1	-0.498455	-4.817320	0.684071
1	-0.178500	-3.845762	-0.763907
1	1.170122	-4.391541	0.248882
6	1.669238	-2.306458	2.206858
1	2.505211	-2.331001	1.497229
1	1.775554	-1.416127	2.837199
1	1.753583	-3.193908	2.857200
6	-0.273499	0.327599	3.644539
1	-1.366958	0.440914	3.668647
1	-0.064962	-0.734693	3.826273

1	0.133079	0.881003	4.505655
1	1.392058	0.561323	2.297960
1	0.308538	1.925684	2.353605
6	-2.720786	-3.089109	-1.826291
1	-2.992777	-2.315790	-2.558562
1	-1.733525	-3.470685	-2.121279
1	-3.435936	-3.918134	-1.938369
1	-3.778767	-2.406621	-0.086090
1	-2.377470	-3.381262	0.263762
1	-0.311980	-1.924874	-2.352580
1	-1.393250	-0.558658	-2.296911
6	0.271671	-0.328748	-3.644928
1	1.364708	-0.445600	-3.670505
1	-0.137798	-0.881041	-4.505392
1	0.066304	0.734165	-3.826633
6	-1.668195	2.307716	-2.207665
1	-1.753690	3.198263	-2.853628
1	-1.772833	1.420438	-2.842582
1	-2.504430	2.327598	-1.498250
6	-0.135555	4.017839	-0.274257
1	0.498275	4.818188	-0.686473
1	-1.169281	4.391435	-0.248335
1	0.181377	3.847437	0.762773
6	1.323908	2.728405	-2.666391
1	1.979838	3.575684	-2.417651
1	1.961977	1.841481	-2.796626
1	0.860823	2.945279	-3.641405
1	2.377916	3.380920	-0.262077
1	3.778937	2.405823	0.087621
6	2.720804	3.087985	1.827867
1	2.993176	2.314566	2.559890
1	3.435633	3.917257	1.940154
1	1.733391	3.469025	2.123045
6	-2.438870	2.316087	1.415005
1	-1.590231	2.921983	1.761806
1	-2.928283	2.910374	0.622137
6	-4.217425	0.358337	-0.135854
1	-4.840869	-0.264196	0.531944
1	-4.496346	1.399915	0.089625
6	4.216833	-0.359453	0.136398
1	4.840547	0.262530	-0.531666
1	4.495168	-1.401261	-0.088748
6	2.438379	-2.315261	-1.416973
1	1.589784	-2.920238	-1.765514
1	2.926612	-2.910917	-0.624406
6	3.424859	-2.159300	-2.580263
1	3.760945	-3.144681	-2.937078
1	2.961442	-1.639902	-3.430212
1	4.314791	-1.584191	-2.288747
6	4.608531	-0.063671	1.585661
1	5.664235	-0.317921	1.764369
1	4.481215	0.997534	1.836753
1	3.998472	-0.648112	2.289742
6	-4.608710	0.062736	-1.585277
1	-3.998673	0.647506	-2.289121
1	-4.480890	-0.998375	-1.836528
1	-5.664470	0.316604	-1.764205
6	-3.423925	2.161216	2.579636
1	-4.313449	1.584435	2.290113
1	-2.958946	1.644072	3.430104
1	-3.760859	3.146883	2.934864

7-TS-1

SCF energy = -1019.433511010 a.u.

ν = -219.1050 cm^{-1}

6	-1.725937	-0.302138	-0.049271
6	-1.521981	1.037519	0.009419
5	-0.290727	-1.003009	-0.265201
5	0.032696	1.311238	-0.075510
7	0.745173	0.060346	-0.109328
6	-0.088493	-2.265374	-1.221852
1	-0.481669	-1.921600	-2.197812
1	0.978207	-2.460176	-1.400738
6	-3.074244	-0.976633	-0.039511
1	-3.006506	-1.952313	0.470621
1	-3.793314	-0.380859	0.546636
6	-2.590189	2.089195	0.162853
1	-3.552984	1.742905	-0.247485
1	-2.314575	2.984689	-0.419079
6	0.652073	2.761126	-0.250901
1	0.106361	3.471146	0.394708
1	1.711383	2.830626	0.040879
6	-3.633165	-1.188445	-1.450077
1	-2.955922	-1.804927	-2.060244
1	-4.612683	-1.689590	-1.421139
1	-3.756217	-0.224440	-1.966707
6	-2.778777	2.492560	1.628599
1	-3.094887	1.629041	2.234431
1	-1.837820	2.869377	2.059617
1	-3.538902	3.281532	1.735459

6	-0.778566	-3.573968	-0.835677
1	-0.645395	-4.350212	-1.604869
1	-0.367477	-3.979501	0.103883
1	-1.861232	-3.447729	-0.686827
6	0.502242	3.207520	-1.716117
1	0.862129	4.236490	-1.870695
1	1.072514	2.551712	-2.392343
1	-0.548439	3.171718	-2.044940
6	3.028382	-1.898499	0.134286
1	2.385433	-2.494163	0.801287
1	3.042616	-2.393293	-0.848014
1	4.052004	-1.940727	0.540245
6	3.044957	0.722517	1.635682
1	2.783391	1.789855	1.680534
1	2.567320	0.226193	2.495982
1	4.135942	0.636801	1.764185
6	3.372363	0.692738	-1.440179
1	3.199444	1.777841	-1.493153
1	4.459818	0.526484	-1.376770
1	3.014548	0.246494	-2.381520
14	2.499472	-0.092164	0.027155
8	-0.243679	-1.546053	2.782731
6	-0.237385	-1.671155	1.661197

7-I-1

SCF energy = -1019.442337200 a.u.

6	-1.545579	1.012135	-0.200122
6	-1.777027	-0.323761	-0.162133
5	0.004946	1.276190	-0.078019
5	-0.350664	-1.078960	0.077975
7	0.708300	0.031706	-0.007696
6	0.638389	2.733218	-0.032029
1	-0.018595	3.377886	0.578296
1	1.621822	2.753952	0.464659
6	-2.608854	2.082496	-0.179664
1	-2.224192	2.992616	-0.668567
1	-3.493916	1.773614	-0.761313
6	-3.118047	-1.005945	-0.116172
1	-3.924534	-0.276674	-0.294985
1	-3.273620	-1.379481	0.912668
6	-0.342566	-2.094473	1.344125
1	-1.094929	-2.891414	1.207625
1	0.626467	-2.610847	1.443707
6	-3.038786	2.430367	1.248480
1	-2.176279	2.756974	1.850379
1	-3.787312	3.237272	1.261481
1	-3.474129	1.551828	1.749542
6	-3.274740	-2.179749	-1.083447
1	-3.120068	-1.864289	-2.127160
1	-2.557000	-2.986357	-0.861257
1	-4.280060	-2.620767	-1.013610
6	0.754425	3.342545	-1.437936
1	1.141391	4.373220	-1.411323
1	1.429790	2.753087	-2.076725
1	-0.223536	3.371058	-1.944511
6	-0.639991	-1.328150	2.635179
1	-0.599443	-1.981066	3.520697
1	0.084101	-0.513121	2.786539
1	-1.637393	-0.863282	2.606816
6	3.438551	0.941810	-0.930530
1	3.120210	0.851743	-1.981196
1	3.354643	1.998402	-0.639962
1	4.504145	0.664570	-0.879263
6	2.891640	-1.963254	-0.385871
1	2.346482	-2.749834	0.156828
1	2.718997	-2.103523	-1.465282
1	3.966442	-2.129895	-0.209193
6	2.952691	0.015948	1.964915
1	2.468166	-0.734660	2.608546
1	4.042896	-0.080238	2.091226
1	2.653639	1.011971	2.327788
14	2.444848	-0.216041	0.170365
6	-0.170537	-1.798837	-1.353146
8	-0.076123	-2.131545	-2.429169

7-TS-2

SCF energy = -1019.415600230 a.u.

ν = -323.8128 cm^{-1}

6	-1.320924	1.104989	-0.158975
6	-1.823398	-0.126226	-0.430554
5	0.265526	1.179854	-0.034519
5	-0.231164	-1.171169	0.070487
7	0.823645	-0.114587	0.080719
6	1.050867	2.558051	-0.065005
1	0.584752	3.244658	0.664668
1	2.098802	2.452504	0.257095
6	-2.189514	2.281262	0.215487
1	-1.718527	3.204977	-0.156901
1	-3.178544	2.221480	-0.265028
6	-3.282172	-0.510309	-0.283257

1	-3.903815	0.326531	-0.641108
1	-3.477946	-0.576660	0.802256
6	-0.618746	-2.060140	1.332066
1	-1.571437	-2.588928	1.168700
1	0.142545	-2.855852	1.418055
6	-2.366044	2.395532	1.733333
1	-1.391670	2.470656	2.240778
1	-2.954930	3.285985	1.999030
1	-2.883159	1.513544	2.140540
6	-3.765731	-1.798268	-0.946835
1	-3.653267	-1.758484	-2.038147
1	-3.212165	-2.680192	-0.590236
1	-4.827944	-1.959719	-0.713148
6	1.000892	3.205132	-1.457849
1	1.486898	4.192791	-1.470895
1	1.506757	2.578056	-2.208112
1	-0.035448	3.343019	-1.804983
6	-0.672039	-1.251894	2.628657
1	-0.913792	-1.880728	3.498900
1	0.290122	-0.755923	2.827160
1	-1.432534	-0.457431	2.567267
6	3.388872	0.286966	-1.428322
1	2.855775	0.053539	-2.363241
1	3.433613	1.380991	-1.325267
1	4.422169	-0.082896	-1.527316
6	2.688978	-2.397921	-0.164824
1	2.318749	-2.939521	0.718731
1	2.128246	-2.753384	-1.043915
1	3.745310	-2.675860	-0.306916
6	3.356818	-0.008617	1.646672
1	2.896769	-0.532290	2.499292
1	4.433364	-0.242986	1.643840
1	3.245784	1.072841	1.818068
14	2.546594	-0.534721	0.036076
6	-0.885643	-1.305159	-1.277719
8	-1.174678	-1.574543	-2.389544

7-TS-2B

SCF energy = -1019.409013450 a.u.

ν = -437.9377 cm^{-1}

6	-1.622435	0.975345	-0.142699
6	-1.751993	-0.368608	-0.269635
5	-0.081946	1.331713	-0.030133
5	-0.278571	-0.951696	-0.238718
7	0.706923	0.125680	-0.098329
6	0.470488	2.813660	0.079273
1	-0.161116	3.364602	0.798607
1	1.496697	2.864354	0.477148
6	-2.757128	1.961089	-0.029721
1	-2.466300	2.916094	-0.496957
1	-3.645090	1.610627	-0.581132
6	-3.024495	-1.158187	-0.394156
1	-3.893715	-0.534109	-0.132987
1	-3.013195	-1.981518	0.342483
6	-0.226071	-2.277422	1.369626
1	-1.019814	-3.039573	1.379492
1	0.733454	-2.789915	1.540509
6	-3.136336	2.220933	1.431474
1	-2.266829	2.573502	2.008320
1	-3.928040	2.981053	1.514909
1	-3.496809	1.298037	1.912049
6	-3.222333	-1.746442	-1.794625
1	-3.266602	-0.946568	-2.549102
1	-2.395684	-2.418026	-2.072931
1	-4.156761	-2.324380	-1.854107
6	0.408278	3.535817	-1.277286
1	0.719355	4.588602	-1.194068
1	1.063098	3.055172	-2.019807
1	-0.610461	3.525712	-1.695181
6	-0.468945	-1.240921	2.460975
1	-0.408742	-1.730697	3.445770
1	0.278728	-0.436562	2.438728
1	-1.459569	-0.775032	2.371782
6	3.237180	1.176710	-1.332511
1	2.802358	1.001066	-2.329016
1	3.093537	2.237550	-1.081461
1	4.321548	0.993128	-1.399994
6	3.021688	-1.726031	-0.473704
1	2.701809	-2.467283	0.274116
1	2.659195	-2.055970	-1.459515
1	4.122987	-1.749936	-0.501826
6	3.086319	0.461453	1.661243
1	2.740829	-0.279548	2.399417
1	4.187335	0.482433	1.695286
1	2.719336	1.449044	1.980439
14	2.470608	0.024290	-0.061164
6	-0.022455	-2.395145	-0.502259
8	0.107938	-3.490659	-0.879760

7-P-1

SCF energy = -1019.455918470 a.u.

6	-1.661656	0.820655	-0.115439
6	-2.186948	-0.414125	-0.306294
5	-0.110487	1.065015	-0.338082
5	0.374974	-1.290857	-0.450555
7	0.846486	0.004019	-0.079517
6	0.333381	2.441348	-0.999862
1	-0.109413	3.304230	-0.474813
1	1.421406	2.595364	-0.988171
6	-2.499059	2.011571	0.287853
1	-2.344172	2.830685	-0.434750
1	-3.572465	1.776020	0.257224
6	-3.637350	-0.800152	-0.182598
1	-3.807781	-1.665391	-0.839339
1	-4.286992	0.013286	-0.538900
6	1.277355	-2.552688	-0.759746
1	0.927790	-2.936483	-1.734514
1	2.339201	-2.291752	-0.891684
6	-2.132726	2.509113	1.689823
1	-1.069350	2.791725	1.754992
1	-2.728674	3.391001	1.968245
1	-2.311031	1.725455	2.441891
6	-4.014674	-1.177072	1.252730
1	-3.391691	-2.009656	1.612763
1	-3.871109	-0.328664	1.939863
1	-5.066858	-1.492464	1.316761
6	-0.142171	2.442772	-2.464569
1	0.131118	3.377284	-2.977339
1	0.311002	1.612307	-3.029058
1	-1.234439	2.326705	-2.541761
6	1.128449	-3.687036	0.267271
1	1.744459	-4.557528	-0.006022
1	1.434750	-3.372677	1.276882
1	0.082788	-4.021235	0.318347
6	3.655064	0.590210	-1.017910
1	3.673832	-0.321699	-1.634790
1	3.326552	1.421975	-1.659202
1	4.686317	0.798782	-0.691300
6	3.151691	-1.023346	1.561687
1	2.414225	-1.274067	2.340104
1	3.403077	-1.944485	1.019017
1	4.065141	-0.673793	2.069512
6	2.469882	1.891468	1.551392
1	1.732721	1.755480	2.359467
1	3.454989	2.030515	2.025015
1	2.222461	2.820028	1.019383
14	2.520363	0.359474	0.458959
6	-1.231215	-1.513595	-0.637560
8	-1.646362	-2.605906	-0.995516

7-P-1B

SCF energy = -1019.451616570 a.u.

6	-1.845202	0.792373	0.061495
6	-1.718105	-0.544550	-0.119304
5	-0.382461	1.420596	0.078000
5	-0.165398	-0.848669	-0.205181
7	0.605210	0.357082	-0.063623
6	-0.095196	2.972019	0.133295
1	-0.786864	3.443445	0.852737
1	0.923005	3.218645	0.471300
6	-3.128665	1.549934	0.266337
1	-3.057225	2.535110	-0.224161
1	-3.974853	1.029094	-0.210590
6	-2.816241	-1.563051	-0.248511
1	-3.759853	-1.180630	0.173393
1	-2.554479	-2.455813	0.347078
6	0.546221	-3.314895	0.696566
1	-0.249600	-4.068855	0.562019
1	1.494976	-3.855226	0.545648
6	-3.432626	1.759040	1.753509
1	-2.609155	2.290176	2.256447
1	-4.351838	2.346726	1.896912
1	-3.561158	0.792191	2.263855
6	-3.033446	-1.986293	-1.705425
1	-3.348015	-1.125607	-2.315297
1	-2.105896	-2.383814	-2.144906
1	-3.809321	-2.762732	-1.782812
6	-0.335790	3.588577	-1.258046
1	-0.195275	4.680041	-1.245375
1	0.356077	3.174511	-2.007254
1	-1.357257	3.391396	-1.618791
6	0.457589	-2.679467	2.079508
1	0.551566	-3.433017	2.873942
1	1.252970	-1.933130	2.232692
1	-0.506775	-2.166047	2.224143
6	2.933256	1.754572	-1.324863
1	2.587439	1.416032	-2.314259
1	2.559831	2.776335	-1.163426
1	4.033812	1.801099	-1.349889

6	3.243485	-1.076532	-0.250951
1	2.998206	-1.816739	0.525504
1	3.014023	-1.520500	-1.230478
1	4.329951	-0.898978	-0.199785
6	2.819742	1.211947	1.716714
1	2.508051	0.497596	2.495274
1	3.908603	1.353939	1.806116
1	2.336400	2.175933	1.935249
14	2.367844	0.561549	0.010706
6	0.391256	-2.327478	-0.451229
8	0.601000	-2.669905	-1.602309

8

SCF energy = -654.823200546 a.u.

6	0.671589	-1.844123	-1.227550
6	-0.671463	-1.844077	-1.227698
5	1.146033	-0.573049	-0.395231
5	-1.145995	-0.573073	-0.395310
7	-0.000003	0.320230	-0.263266
6	-0.000091	1.801962	-0.220028
6	2.600709	-0.592558	0.296299
1	1.283258	-2.659357	-1.628655
1	-1.283032	-2.659323	-1.628919
6	-2.600642	-0.592663	0.296297
6	-0.000104	2.377857	1.201461
1	0.886530	2.057561	1.759990
1	-0.000341	3.478309	1.166246
1	-0.886526	2.057173	1.760096
6	1.224967	2.318105	-0.992315
1	1.190331	3.414982	-1.068445
1	2.169048	2.053006	-0.505248
1	1.235807	1.905370	-2.012868
6	-1.225226	2.317961	-0.992341
1	-1.236103	1.905084	-2.012838
1	-2.169268	2.052861	-0.505210
1	-1.190680	3.414830	-1.068629
6	-2.758926	-2.011295	0.896339
1	-2.706691	-2.799727	0.132687
1	-1.982709	-2.224677	1.649217
1	-3.738164	-2.102154	1.396633
6	-2.871083	0.390349	1.442840
1	-2.119281	0.290391	2.241039
1	-2.885595	1.441248	1.125372
1	-3.856630	0.183419	1.893646
6	-3.664255	-0.420010	-0.806624
1	-3.523891	-1.143850	-1.625072
1	-4.674453	-0.582107	-0.392540
1	-3.645885	0.588219	-1.247928
6	2.871183	0.390507	1.442782
1	2.885645	1.441388	1.125256
1	2.119430	0.290561	2.241023
1	3.856766	0.183627	1.893535
6	3.664226	-0.419916	-0.806746
1	3.645774	0.588271	-1.248126
1	4.674471	-0.581945	-0.392744
1	3.523826	-1.143833	-1.625119
6	2.759115	-2.011140	0.896366
1	2.706875	-2.799619	0.132758
1	3.738382	-2.101933	1.396615
1	1.982944	-2.224529	1.649292

8-TS-0

SCF energy = -1309.571783640 a.u.

ν = -210.7310 cm^{-1}

6	0.726561	-0.187632	2.099112
6	2.021234	0.058272	1.875387
5	0.033016	-0.787319	0.801698
5	2.379243	-0.237641	0.376930
7	1.119519	-0.532446	-0.344048
6	-1.962488	1.031776	-2.043381
6	-0.714809	1.507810	-1.959358
5	-2.348011	0.304982	-0.724358
5	-0.153417	1.453644	-0.478493
7	-1.253974	0.637219	0.337630
6	-1.952125	1.390696	1.494695
6	-3.742221	-0.560567	-0.836150
1	-2.542294	1.071637	-2.970183
1	-0.229421	1.978000	-2.818008
6	0.874855	2.749830	-0.254449
6	-0.404019	-2.377462	1.228809
1	0.287702	-0.115992	3.098298
1	2.706173	0.353798	2.676593
6	4.003062	-0.300908	0.100951
6	1.155264	-1.252278	-1.675108
6	-3.050866	2.292325	0.904789
1	-3.888464	1.716627	0.499120
1	-3.461775	2.935787	1.695936
1	-2.662185	2.943345	0.109072
6	-2.577920	0.432366	2.503212
1	-3.320274	0.976187	3.106465

1	-3.079609	-0.405357	2.027432
1	-1.824683	0.034310	3.188889
6	-1.048761	2.326082	2.295684
1	-0.094717	1.872320	2.566752
1	-0.860254	3.260229	1.763066
1	-1.576780	2.589286	3.223926
6	0.051464	4.010832	-0.638576
1	-0.404670	3.941556	-1.636309
1	-0.756664	4.224673	0.075774
1	0.716528	4.890535	-0.643374
6	1.648096	3.114751	1.031463
1	1.028043	3.559158	1.814641
1	2.173625	2.260570	1.464964
1	2.407125	3.872642	0.778470
6	1.983909	2.621839	-1.329741
1	1.607471	2.503007	-2.351597
1	2.605416	3.531758	-1.324664
1	2.647166	1.772969	-1.125713
6	-4.862618	0.394615	-1.334484
1	-5.223200	1.076843	-0.552443
1	-4.564358	1.005551	-2.197431
1	-5.731457	-0.208039	-1.645804
6	-4.345180	-1.340376	0.340374
1	-4.754065	-0.674245	1.112413
1	-5.186321	-1.955541	-0.020207
1	-3.629230	-2.022581	0.814737
6	-3.548797	-1.576184	-1.998060
1	-2.901091	-2.417260	-1.726475
1	-4.529807	-2.000928	-2.265978
1	-3.132532	-1.117566	-2.905585
6	-1.086014	-3.337946	0.238754
1	-0.471787	-3.592212	-0.630198
1	-1.314716	-4.287844	0.751233
1	-2.039807	-2.943765	-0.129321
6	0.934761	-3.047117	1.652606
1	1.283653	-2.674472	2.624951
1	0.786869	-4.136020	1.748792
1	1.754804	-2.887102	0.944245
6	-1.275191	-2.470193	2.501587
1	-2.327997	-2.226849	2.319741
1	-1.255143	-3.508611	2.874010
1	-0.914649	-1.837046	3.321969
6	-0.247498	-1.616968	-2.201612
1	-0.252498	-2.627343	-2.634175
1	-0.993694	-1.609721	-1.408146
1	-0.586387	-0.930556	-2.981703
6	1.789922	-0.386195	-2.772322
1	2.790889	-0.037588	-2.524809
1	1.857282	-0.974436	-3.700163
1	1.169910	0.487853	-2.987079
6	1.956153	-2.566049	-1.577846
1	2.937968	-2.423763	-1.117979
1	1.424683	-3.325857	-0.995971
1	2.115295	-2.977686	-2.585930
6	4.665080	-0.412296	-1.283780
1	4.513535	0.495989	-1.886472
1	5.755219	-0.517721	-1.150581
1	4.334449	-1.274792	-1.875050
6	4.477278	-1.520921	0.934158
1	4.102379	-1.492762	1.967490
1	4.155315	-2.477945	0.495989
1	5.579818	-1.537867	0.979811
6	4.643208	0.957852	0.739812
1	4.397362	1.079618	1.802204
1	5.741855	0.887351	0.669941
1	4.342997	1.880402	0.221297

8-I-0

SCF energy = -1309.584048050 a.u.

6	-0.679378	-0.254024	-2.120572
6	-1.975419	-0.017990	-1.887020
5	0.157305	-0.695488	-0.833816
5	-2.323845	-0.219366	-0.392044
7	-1.005817	-0.318620	0.399840
6	1.912940	1.197857	1.908786
6	0.595100	1.440372	1.888031
5	2.319898	0.367958	0.676052
5	-0.150566	1.157246	0.490413
7	1.190417	0.535787	-0.406114
6	1.869224	1.394188	-1.508964
6	3.748739	-0.445511	0.849693
1	2.529748	1.427175	2.782883
1	0.118749	1.900160	2.760058
6	-1.069335	2.576993	0.236576
6	0.547285	-2.326769	-1.172383
1	-0.282174	-0.258288	-3.141490
1	-2.679492	0.198137	-2.695800
6	-3.946656	-0.426581	-0.125011
6	-1.082013	-1.114103	1.719664
6	2.826578	2.403046	-0.848419

1	3.677277	1.923814	-0.354235
1	3.245765	3.056946	-1.626130
1	2.314892	3.031013	-0.111210
6	2.666962	0.517987	-2.474255
1	3.356020	1.150399	-3.053138
1	3.256134	-0.238697	-1.960867
1	2.006777	0.014658	-3.187783
6	0.948526	2.245326	-2.384705
1	0.124590	1.684802	-2.826852
1	0.544934	3.102640	-1.848416
1	1.560653	2.639365	-3.209317
6	-0.218471	3.841278	0.515176
1	0.359934	3.773649	1.447259
1	0.493117	4.072745	-0.287697
1	-0.879430	4.719863	0.607182
6	-1.887619	2.871612	-1.041132
1	-1.345989	2.778220	-1.982467
1	-2.763866	2.225784	-1.122009
1	-2.274098	3.904242	-0.984335
6	-2.151409	2.574645	1.347080
1	-1.741253	2.597410	2.364883
1	-2.788229	3.468933	1.242272
1	-2.815941	1.703493	1.278774
6	4.849532	0.583515	1.226542
1	5.200008	1.159745	0.357978
1	4.535979	1.296572	2.000926
1	5.729176	0.043595	1.613462
6	4.373482	-1.326365	-0.245087
1	4.809502	-0.731066	-1.058895
1	5.203997	-1.909037	0.187139
1	3.672673	-2.044508	-0.683607
6	3.594539	-1.341115	2.111646
1	2.976282	-2.229336	1.932734
1	4.589374	-1.703490	2.418346
1	3.162861	-0.801176	2.965714
6	1.232767	-3.233254	-0.132201
1	0.595852	-3.503759	0.715371
1	1.530208	-4.181081	-0.612516
1	2.146752	-2.789287	0.273742
6	-0.753318	-3.049572	-1.616736
1	-1.058189	-2.749119	-2.628685
1	-0.586794	-4.140235	-1.636051
1	-1.617126	-2.860520	-0.970897
6	1.458514	-2.431586	-2.419207
1	2.490678	-2.121035	-2.227496
1	1.500504	-3.485229	-2.744280
1	1.085544	-1.855618	-3.276190
6	0.294586	-1.480377	2.303631
1	0.239869	-2.466161	2.787447
1	1.062217	-1.546682	1.535408
1	0.637375	-0.765945	3.054807
6	-1.806823	-0.338382	2.828748
1	-2.818420	-0.040194	2.562532
1	-1.872153	-0.987123	3.715133
1	-1.256091	0.556226	3.126952
6	-1.819804	-2.446667	1.510983
1	-2.770360	-2.337309	0.989135
1	-1.216361	-3.165887	0.954013
1	-2.036359	-2.892143	2.492517
6	-4.617748	-0.567057	1.254391
1	-4.534678	0.355246	1.848096
1	-5.696330	-0.741542	1.105087
1	-4.245671	-1.401181	1.860657
6	-4.327178	-1.689639	-0.948042
1	-3.974776	-1.633457	-1.987211
1	-3.926656	-2.619641	-0.518557
1	-5.424844	-1.794131	-0.973407
6	-4.700994	0.754717	-0.789397
1	-4.408898	0.929817	-1.832541
1	-5.782004	0.537517	-0.790149
1	-4.563064	1.693536	-0.234270

8-TS-1

SCF energy = -768.006332346 a.u.

ν = -203.5548 cm^{-1}

6	-0.652042	-1.761422	1.247497
6	0.683386	-1.759768	1.123004
5	-1.227533	-0.524363	0.434152
5	1.092761	-0.497053	0.227267
7	-0.120579	0.375268	0.167368
6	-0.191819	1.811809	-0.194060
6	-2.778954	-0.598230	-0.040147
1	-1.206777	-2.563831	1.744948
1	1.335179	-2.552906	1.505349
6	2.201137	-0.747040	-0.938241
6	-0.334897	2.029891	-1.707569
1	-1.199631	1.490350	-2.107856
1	-0.462889	3.099541	-1.934675
1	0.555966	1.678091	-2.243497
6	-1.363949	2.469028	0.552673

1	-1.361465	3.555376	0.378998
1	-2.337652	2.088547	0.235290
1	-1.266328	2.295114	1.635072
6	1.055353	2.563184	0.300284
1	1.109249	2.552842	1.399476
1	1.987702	2.157278	-0.102240
1	0.993790	3.616745	-0.010222
6	1.383030	-1.325685	-2.113160
1	0.787528	-2.198064	-1.799025
1	0.686008	-0.582794	-2.528285
1	2.052149	-1.655520	-2.926071
6	3.030936	0.439288	-1.447431
1	2.422315	1.236531	-1.892544
1	3.639506	0.884901	-0.643025
1	3.732051	0.099882	-2.228871
6	3.203264	-1.821628	-0.476417
1	2.713555	-2.784302	-0.272354
1	3.966367	-2.000672	-1.252404
1	3.739758	-1.518891	0.439385
6	-3.224448	0.192064	-1.280592
1	-3.149606	1.280794	-1.174172
1	-2.641082	-0.098702	-2.168494
1	-4.282325	-0.030084	-1.502567
6	-3.663013	-0.225625	1.168213
1	-3.592855	0.841671	1.425693
1	-4.723274	-0.444376	0.951884
1	-3.385725	-0.801465	2.066032
6	-3.058194	-2.082659	-0.384401
1	-2.955459	-2.746836	0.484292
1	-4.089668	-2.195462	-0.759426
1	-2.379105	-2.453567	-1.169342
8	2.463991	0.451204	2.973121
6	2.229995	0.253525	1.887851

8-I-1

SCF energy = -768.016225631 a.u.

6	-0.592948	-1.790008	1.165108
6	0.742939	-1.693075	1.239387
5	-1.198419	-0.549260	0.385719
5	1.196678	-0.365798	0.409452
7	-0.127028	0.390485	0.187823
6	-0.227309	1.831191	-0.149793
6	-2.764480	-0.631147	-0.051284
1	-1.124697	-2.663793	1.557021
1	1.394239	-2.449776	1.690033
6	2.216253	-0.764338	-0.851904
6	-0.399966	2.051061	-1.661133
1	-1.260783	1.498633	-2.049926
1	-0.547265	3.118875	-1.885824
1	0.488884	1.711392	-2.209664
6	-1.392345	2.465443	0.627269
1	-1.440377	3.547831	0.434406
1	-2.360639	2.038615	0.356230
1	-1.249066	2.313851	1.707973
6	1.019012	2.611808	0.302484
1	1.128232	2.593497	1.398016
1	1.945274	2.251170	-0.158846
1	0.908659	3.667848	0.016414
6	1.328275	-1.374945	-1.945295
1	0.742936	-2.224521	-1.561061
1	0.616284	-0.638919	-2.346083
1	1.944340	-1.742546	-2.783865
6	3.012140	0.404156	-1.451012
1	2.367140	1.184300	-1.875997
1	3.674019	0.880198	-0.707066
1	3.659389	0.044519	-2.269221
6	3.238923	-1.820907	-0.396861
1	2.754937	-2.764647	-0.108728
1	3.948336	-2.050454	-1.209626
1	3.841996	-1.478659	0.462894
6	-3.260651	0.204588	-1.242239
1	-3.191480	1.289162	-1.094616
1	-2.708043	-0.044373	-2.161967
1	-4.323970	-0.018806	-1.436001
6	-3.626647	-0.328845	1.191689
1	-3.560783	0.724861	1.501916
1	-4.689854	-0.547267	0.988568
1	-3.322911	-0.945345	2.053170
6	-3.027564	-2.102704	-0.456379
1	-2.902741	-2.802901	0.380627
1	-4.062844	-2.216338	-0.820736
1	-2.354885	-2.428790	-1.266515
8	2.601191	0.515195	2.558912
6	2.030042	0.249840	1.619392

8-TS-2

SCF energy = -767.997504139 a.u.

ν = -378.0036 cm^{-1}

6	-0.381153	-1.800459	0.968402
6	0.890776	-1.623657	1.369968

5	-1.093991	-0.570714	0.250875
5	1.271231	-0.098848	0.270612
7	-0.116226	0.456696	0.107371
6	-0.294769	1.931205	0.011577
6	-2.649620	-0.743765	-0.158946
1	-0.825478	-2.792980	1.110196
1	1.514093	-2.428523	1.775453
6	2.215786	-0.592875	-0.956404
6	-0.539947	2.354298	-1.442981
1	-1.429811	1.871797	-1.859534
1	-0.676159	3.444451	-1.512368
1	0.317006	2.079864	-2.074530
6	-1.447359	2.375941	0.922161
1	-1.568240	3.468703	0.879517
1	-2.403206	1.925107	0.639626
1	-1.234561	2.094543	1.964527
6	0.958690	2.663324	0.522521
1	1.157038	2.442774	1.580855
1	1.858457	2.414537	-0.054303
1	0.801528	3.747681	0.430546
6	1.335903	-1.234026	-2.037315
1	0.783148	-2.103052	-1.645186
1	0.596898	-0.521072	-2.433321
1	1.952390	-1.587035	-2.881070
6	2.947145	0.620663	-1.559199
1	2.251014	1.374007	-1.955145
1	3.599348	1.112655	-0.820073
1	3.585755	0.297256	-2.398727
6	3.284089	-1.601877	-0.504236
1	2.836951	-2.556123	-0.188602
1	3.978875	-1.824779	-1.330985
1	3.888135	-1.215313	0.333247
6	-3.241334	0.218891	-1.199275
1	-3.266216	1.266428	-0.873777
1	-2.685230	0.173743	-2.148672
1	-4.283816	-0.066574	-1.421113
6	-3.501228	-0.706543	1.125868
1	-3.504601	0.290370	1.592292
1	-4.549506	-0.972253	0.904120
1	-3.133064	-1.421130	1.879595
6	-2.781418	-2.156170	-0.780920
1	-2.574896	-2.960070	-0.060796
1	-3.809687	-2.312211	-1.147970
1	-2.102545	-2.289999	-1.639197
8	2.206581	-0.012506	2.766652
6	1.737957	-0.155255	1.695970

8-TS-2B

SCF energy = -767.990237570 a.u.

ν = -365.0190 cm^{-1}

6	0.766761	-1.799444	-1.237522
6	-0.546493	-1.645331	-1.473636
5	1.327649	-0.554697	-0.412227
5	-0.942511	-0.256515	-0.844177
7	0.260597	0.427532	-0.342815
6	0.345476	1.871550	-0.013957
6	2.839932	-0.658164	0.156213
1	1.320736	-2.684550	-1.567999
1	-1.181933	-2.367156	-1.994391
6	-2.409240	-0.770401	0.681103
6	0.465535	2.093652	1.500572
1	1.319743	1.559906	1.926266
1	0.583794	3.164444	1.726789
1	-0.441712	1.740895	2.012461
6	1.532672	2.488217	-0.769907
1	1.628356	3.560178	-0.540595
1	2.482357	2.006894	-0.518174
1	1.379902	2.379093	-1.854201
6	-0.899005	2.635425	-0.488693
1	-1.068888	2.512899	-1.568147
1	-1.807265	2.337225	0.052547
1	-0.756733	3.708396	-0.295384
6	-1.322359	-1.327599	1.602195
1	-0.748592	-2.140448	1.136890
1	-0.615815	-0.555958	1.933865
1	-1.811983	-1.740144	2.501787
6	-3.172226	0.321927	1.428478
1	-2.505187	1.128007	1.768509
1	-3.980700	0.761666	0.827063
1	-3.635660	-0.113827	2.329980
6	-3.347003	-1.893191	0.248023
1	-2.801834	-2.710585	-0.245606
1	-3.843376	-2.318617	1.137221
1	-4.140368	-1.538802	-0.426549
6	3.322079	0.266248	1.284463
1	3.285779	1.334845	1.038435
1	2.741487	0.111258	2.207014
1	4.373190	0.033550	1.526861
6	3.781069	-0.506833	-1.058623
1	3.773695	0.516964	-1.463911

1	4.820956	-0.741356	-0.771732
1	3.503445	-1.187860	-1.878465
6	2.996536	-2.096543	0.708318
1	2.869864	-2.866066	-0.065131
1	4.004823	-2.229204	1.136237
1	2.268980	-2.305774	1.509635
8	-3.368930	0.557929	-1.471358
6	-2.322982	0.227824	-1.088475

8-TS-2C

SCF energy = -767.981816772 a.u.

ν = -232.9525 cm^{-1}

6	-0.541661	-2.039581	0.741632
6	0.793425	-1.996166	0.858633
5	-1.169673	-0.701908	0.211291
5	1.479585	-0.608920	0.524326
7	-0.169951	0.386657	0.295826
6	-0.299995	1.793052	-0.225063
6	-2.728146	-0.752401	-0.257538
1	-1.094048	-2.951258	0.979787
1	1.375903	-2.851262	1.222996
6	2.769189	-0.601273	-0.440976
6	-0.287762	1.733300	-1.756126
1	-1.011691	1.010746	-2.146032
1	-0.521809	2.719539	-2.184610
1	0.708509	1.433990	-2.112930
6	-1.556517	2.465670	0.344094
1	-1.566065	3.528648	0.059806
1	-2.488903	2.022434	-0.008886
1	-1.536238	2.405336	1.441891
6	0.863800	2.704567	0.216547
1	0.789029	2.986128	1.273704
1	1.845631	2.257779	0.048650
1	0.817204	3.626284	-0.380960
6	2.408426	-1.324845	-1.749287
1	1.996200	-2.328156	-1.563190
1	1.654906	-0.762096	-2.322693
1	3.299508	-1.438931	-2.389912
6	3.438412	0.733895	-0.783820
1	2.813146	1.361120	-1.434463
1	3.694717	1.313284	0.116859
1	4.378479	0.548680	-1.330375
6	3.812781	-1.443319	0.331859
1	3.471296	-2.471468	0.518649
1	4.745309	-1.511492	-0.253170
1	4.065659	-0.987663	1.302783
6	-3.195449	0.032643	-1.496977
1	-3.035932	1.114495	-1.449997
1	-2.698448	-0.336558	-2.408247
1	-4.277978	-0.123267	-1.640276
6	-3.548328	-0.333103	0.986486
1	-3.435369	0.729357	1.238326
1	-4.621092	-0.523317	0.810118
1	-3.256528	-0.914855	1.876193
6	-3.102671	-2.223214	-0.563070
1	-3.056992	-2.864903	0.327180
1	-4.137163	-2.274555	-0.940802
1	-2.446651	-2.664956	-1.329835
8	0.644834	0.905643	2.556090
6	0.842968	0.342327	1.540581

8-P-1

SCF energy = -768.020903219 a.u.

6	-0.959214	-2.030650	0.988910
6	0.233014	-2.479365	1.410850
5	-1.174534	-0.612992	0.287027
5	1.152454	-0.315874	0.171654
7	-0.109456	0.362581	0.417540
6	-0.250770	1.804233	0.783933
6	-2.521886	-0.498305	-0.601911
1	-1.846495	-2.633778	1.215601
1	0.384399	-3.386405	2.006531
6	2.233040	0.022075	-0.979903
6	-0.122811	2.812015	-0.364016
1	-0.839700	2.612700	-1.168201
1	-0.316689	3.824803	0.019895
1	0.885588	2.814405	-0.793551
6	-1.593092	2.007687	1.500429
1	-1.619931	3.006267	1.960069
1	-2.449384	1.937142	0.821341
1	-1.720340	1.263642	2.301975
6	0.849160	2.082395	1.825388
1	0.729977	1.420262	2.695318
1	1.851998	1.919821	1.408802
1	0.796176	3.125138	2.172683
6	1.451616	0.354089	-2.268199
1	0.772166	-0.468698	-2.547238
1	0.842468	1.261040	-2.176991
1	2.149916	0.497995	-3.109744
6	3.217068	1.156774	-0.644244

1	2.729333	2.135948	-0.540686
1	3.762288	0.947229	0.289195
1	3.965386	1.252548	-1.449428
6	3.075303	-1.237825	-1.275761
1	2.441179	-2.108268	-1.512163
1	3.723754	-1.058048	-2.149656
1	3.710161	-1.511269	-0.423158
6	-2.613315	0.705096	-1.549998
1	-2.776646	1.657359	-1.029216
1	-1.701061	0.804134	-2.158011
1	-3.460096	0.576676	-2.244866
6	-3.793781	-0.578318	0.261558
1	-3.915783	0.308871	0.900873
1	-4.688890	-0.647944	-0.379988
1	-3.795331	-1.461332	0.919301
6	-2.470619	-1.752500	-1.512827
1	-2.504774	-2.695228	-0.948152
1	-3.332049	-1.750536	-2.201724
1	-1.557857	-1.768910	-2.131419
8	2.484885	-1.780618	1.624760
6	1.395912	-1.621460	1.098848

8-P-1B

SCF energy = -768.036087896 a.u.

6	1.071614	-2.127294	-0.563918
6	-0.251061	-2.066348	-0.775983
5	1.610568	-0.675802	-0.147939
5	-0.684581	-0.566563	-0.550977
7	0.473284	0.246608	-0.269333
6	0.477149	1.724188	-0.108881
6	3.176011	-0.560883	0.236189
1	1.649168	-3.052482	-0.656477
1	-0.880657	-2.914985	-1.060747
6	-3.221953	-0.402698	0.473733
6	0.760990	2.094620	1.352477
1	1.707117	1.681361	1.710276
1	0.798176	3.187547	1.476580
1	-0.040124	1.705759	1.998638
6	1.507661	2.322093	-1.077952
1	1.587204	3.410635	-0.938974
1	2.505497	1.892955	-0.945172
1	1.197460	2.129431	-2.115886
6	-0.872519	2.350854	-0.480174
1	-1.176590	2.106568	-1.506135
1	-1.675432	2.045401	0.204756
1	-0.784261	3.444023	-0.400118
6	-2.499319	-0.279876	1.818518
1	-1.658954	-0.990384	1.893910
1	-2.099721	0.733328	1.976341
1	-3.188794	-0.499032	2.648173
6	-4.362140	0.611683	0.358177
1	-3.997673	1.640226	0.506524
1	-4.821092	0.557624	-0.638342
1	-5.134858	0.412452	1.116903
6	-3.775608	-1.832064	0.313016
1	-2.976922	-2.586516	0.387038
1	-4.512236	-2.043206	1.104183
1	-4.269869	-1.947931	-0.662662
6	3.760691	0.625575	1.018846
1	3.576536	1.605224	0.562106
1	3.380192	0.655097	2.051077
1	4.855129	0.507315	1.090010
6	3.887258	-0.645646	-1.137828
1	3.739779	0.266668	-1.735961
1	4.973186	-0.774725	-0.990458
1	3.534144	-1.498315	-1.739084
6	3.558635	-1.818991	1.052561
1	3.383926	-2.755995	0.508008
1	4.632198	-1.787910	1.303561
1	3.000958	-1.873399	2.001393
8	-2.642096	0.060588	-1.810474
6	-2.235684	-0.204526	-0.693074

8-P-1C

SCF energy = -768.010192955 a.u.

6	-0.188871	-1.913620	-0.898310
6	1.145717	-1.935839	-0.693984
5	-1.165151	-0.758185	-0.392813
5	1.768822	-0.654709	-0.101913
7	-0.552415	0.547426	-0.192041
6	-1.170123	1.905864	-0.294571
6	-2.610259	-1.269931	0.147940
1	-0.638463	-2.753066	-1.443182
1	1.736346	-2.779678	-1.068328
6	3.322500	-0.351832	-0.017888
6	-2.099154	1.894413	-1.516989
1	-2.868476	1.120189	-1.466553
1	-2.609308	2.864577	-1.608610
1	-1.511596	1.731502	-2.433280
6	-1.890102	2.336540	0.988811

1	-2.288831	3.355883	0.871579
1	-2.728958	1.677494	1.241362
1	-1.179374	2.330483	1.825310
6	-0.079166	2.949380	-0.612833
1	0.549369	3.180710	0.253307
1	0.568861	2.598718	-1.431257
1	-0.568266	3.876945	-0.944431
6	4.154529	-1.306380	-0.886120
1	3.989671	-2.361201	-0.616653
1	3.918134	-1.193692	-1.956602
1	5.231433	-1.101970	-0.761946
6	3.673080	1.100670	-0.383524
1	3.432279	1.318732	-1.437127
1	3.132584	1.817284	0.249192
1	4.754344	1.276708	-0.252456
6	3.657642	-0.600288	1.474916
1	3.426330	-1.633803	1.782431
1	4.738064	-0.445477	1.639320
1	3.105289	0.090663	2.127096
6	-3.907543	-0.486072	-0.100346
1	-3.870446	0.553751	0.241870
1	-4.181001	-0.483548	-1.167223
1	-4.735879	-0.972479	0.441773
6	-2.323640	-1.296145	1.674092
1	-2.201692	-0.287007	2.091685
1	-3.157814	-1.788634	2.201872
1	-1.408502	-1.863834	1.911600
6	-2.901048	-2.721110	-0.287101
1	-2.112125	-3.421032	0.024441
1	-3.838804	-3.070497	0.175491
1	-3.022518	-2.809901	-1.378744
8	1.020988	1.228025	1.322809
6	0.719771	0.457760	0.426492

9

SCF energy = -733.379183541 a.u.

6	-0.677628	1.748115	-0.628890
6	0.677456	1.748167	-0.628729
5	-1.140188	0.306243	-0.121348
5	1.140050	0.306247	-0.121215
7	-0.000044	-0.597759	-0.232546
6	0.000038	-2.009726	-0.687886
6	-2.558346	0.092045	0.622538
6	2.558321	0.092128	0.622490
6	0.000057	-3.055776	0.435816
1	-0.886165	-2.965535	1.072030
1	0.001796	-4.067796	0.002062
1	0.884587	-2.963291	1.074050
6	-1.228033	-2.232453	-1.586948
1	-1.192860	-3.235292	-2.037761
1	-2.169172	-2.156373	-1.030643
1	-1.247556	-1.492205	-2.401722
6	1.228224	-2.232294	-1.586852
1	1.248056	-1.491624	-2.401233
1	2.169291	-2.156750	-1.030358
1	1.192866	-3.234883	-2.038197
6	2.681914	1.257429	1.634419
1	2.694005	2.243343	1.153043
1	1.852866	1.250304	2.360772
1	3.620484	1.160087	2.206344
6	2.715794	-1.195705	1.442593
1	1.891714	-1.320374	2.161659
1	2.761916	-2.099159	0.820441
1	3.655733	-1.161787	2.019502
6	3.721861	0.184696	-0.384342
1	3.698943	1.113840	-0.971402
1	4.688793	0.156601	0.147301
1	3.716395	-0.652729	-1.098428
6	-2.715432	-1.195838	1.442621
1	-2.762115	-2.099181	0.820340
1	-1.890863	-1.320737	2.161078
1	-3.654984	-1.161900	2.020160
6	-3.722153	0.184516	-0.383974
1	-3.716615	-0.652726	-1.098281
1	-4.688949	0.155991	0.147893
1	-3.699663	1.113817	-0.970799
6	-2.681772	1.257317	1.634527
1	-2.693932	2.243253	1.153193
1	-3.620239	1.159946	2.206614
1	-1.852590	1.250154	2.360727
6	-1.484630	2.976810	-0.950105
1	-1.367654	3.754109	-0.174578
1	-1.134898	3.429035	-1.892969
1	-2.558600	2.780732	-1.059628
6	1.484356	2.976982	-0.949737
1	1.134572	3.429366	-1.892497
1	1.367316	3.754109	-0.174042
1	2.558351	2.781031	-1.059279

9-TS-0

SCF energy = -1466.646626280 a.u.

ν = -236.6781 cm^{-1}

6	-1.152801	1.380251	1.513173
6	-2.412478	0.962110	1.241855
5	-0.233549	1.204243	0.207712
5	-2.448999	0.211330	-0.144037
7	-1.059989	0.174102	-0.697554
6	2.334088	-1.739271	-0.848847
6	1.051670	-2.181701	-0.756126
5	2.425457	-0.296501	-0.245136
5	0.243872	-1.333799	0.349884
7	1.220037	-0.116909	0.722874
6	1.893605	-0.159158	2.127352
6	3.728399	0.623844	-0.734864
6	-0.746336	-2.308117	1.296838
6	0.112601	2.794961	-0.336811
6	-3.953007	-0.222140	-0.694421
6	-0.889034	0.064657	-2.206735
6	2.918985	-1.313273	2.185124
1	3.762531	-1.182064	1.500677
1	3.339473	-1.363413	3.200066
1	2.461290	-2.281454	1.958337
6	2.631905	1.144789	2.419515
1	3.157324	1.054353	3.380650
1	3.375652	1.377389	1.662935
1	1.941863	1.989540	2.490299
6	0.971530	-0.387531	3.323711
1	0.116969	0.280508	3.331095
1	0.617478	-1.413250	3.400617
1	1.553710	-0.183336	4.233586
6	0.139465	-3.423783	1.922192
1	0.853017	-3.854089	1.204755
1	0.714411	-3.098194	2.796796
1	-0.508829	-4.246492	2.266879
6	-1.669804	-1.755598	2.412964
1	-1.288104	-0.914674	2.986132
1	-2.624455	-1.429052	1.991998
1	-1.901970	-2.571561	3.118912
6	-1.751830	-3.089942	0.412322
1	-1.294421	-3.881699	-0.184676
1	-2.484250	-3.589852	1.066476
1	-2.319677	-2.430929	-0.253777
6	5.018628	-0.015530	-0.146360
1	5.148930	0.258090	0.911187
1	5.064705	-1.108905	-0.204983
1	5.895687	0.378571	-0.685534
6	3.929406	2.135591	-0.480690
1	4.183696	2.395474	0.553368
1	4.785583	2.471574	-1.088725
1	3.076770	2.746991	-0.774803
6	3.794580	0.520312	-2.288088
1	3.110944	1.241284	-2.756793
1	4.810589	0.778013	-2.629112
1	3.552059	-0.463149	-2.700726
6	0.750431	3.112285	-1.711407
1	0.120234	2.848614	-2.563718
1	0.919842	4.199882	-1.777730
1	1.719090	2.637551	-1.879832
6	-1.261162	3.526085	-0.370913
1	-1.670472	3.699794	0.632330
1	-1.141179	4.513462	-0.848134
1	-2.031800	2.979882	-0.931522
6	0.967761	3.593485	0.672280
1	1.973081	3.182332	0.789229
1	1.083259	4.631130	0.315924
1	0.514907	3.660325	1.664525
6	0.575647	0.276290	-2.639260
1	0.632614	0.883732	-3.552721
1	1.149952	0.799667	-1.876059
1	1.086191	-0.665508	-2.846229
6	-1.321557	-1.320104	-2.753579
1	-1.762368	-1.948157	-1.980027
1	-2.058193	-1.225820	-3.559345
1	-0.470537	-1.864171	-3.174270
6	-1.751180	1.118933	-2.925849
1	-2.813817	0.973498	-2.724066
1	-1.503196	2.140912	-2.636262
1	-1.606569	1.031317	-4.013284
6	-4.245372	-1.033664	-1.973071
1	-3.816022	-2.043711	-1.941298
1	-5.337984	-1.158424	-2.061247
1	-3.914401	-0.552953	-2.900004
6	-4.705020	1.126085	-0.882720
1	-4.569956	1.835186	-0.057216
1	-4.379810	1.643649	-1.796953
1	-5.787523	0.940138	-0.988917
6	-4.675554	-1.054975	0.402049
1	-4.526442	-0.711743	1.428346
1	-5.762190	-1.047409	0.211560

1	-4.354017	-2.104800	0.366950
6	-3.522292	1.294333	2.214898
1	-4.532871	1.156438	1.821311
1	-3.446427	0.679047	3.130020
1	-3.455170	2.344627	2.541543
6	-0.911824	2.152208	2.790227
1	-1.380537	3.150320	2.730028
1	-1.385340	1.654482	3.651453
1	0.140165	2.306940	3.040773
6	0.695129	-3.443814	-1.505669
1	1.192237	-3.469932	-2.486938
1	1.057491	-4.332032	-0.958933
1	-0.368880	-3.582516	-1.688261
6	3.363092	-2.556812	-1.592390
1	4.372080	-2.136684	-1.577693
1	3.421872	-3.570979	-1.164384
1	3.091428	-2.689293	-2.654131

9-I-0

SCF energy = -1466.655803690 a.u.

6	-1.060807	1.605464	1.307187
6	-2.333743	1.212185	1.047396
5	-0.018669	1.158943	0.149376
5	-2.387068	0.219554	-0.152612
7	-0.939735	-0.064131	-0.629225
6	2.231428	-1.860480	-0.538430
6	0.920870	-2.221015	-0.483551
5	2.379849	-0.353457	-0.184513
5	-0.020824	-1.159535	0.335197
7	1.143390	0.050572	0.696236
6	1.786349	0.109883	2.121424
6	3.758547	0.411590	-0.751692
6	-0.939170	-2.062565	1.477178
6	0.303627	2.661911	-0.667722
6	-3.915795	-0.188541	-0.680233
6	-0.826362	-0.291280	-2.155265
6	2.741089	-1.084487	2.336210
1	3.632501	-1.053407	1.704977
1	3.092597	-1.054557	3.377655
1	2.247494	-2.044561	2.167832
6	2.608014	1.386950	2.304458
1	3.133993	1.336383	3.268343
1	3.361538	1.507860	1.529669
1	1.983085	2.283069	2.312267
6	0.827649	0.048919	3.311183
1	-0.015215	0.724024	3.226941
1	0.450561	-0.954625	3.491694
1	1.393295	0.345503	4.206072
6	-0.062991	-3.093645	2.236804
1	0.671550	-3.591378	1.589774
1	0.488062	-2.670606	3.084015
1	-0.708739	-3.882173	2.659496
6	-1.849671	-1.384117	2.535489
1	-1.442690	-0.506495	3.032916
1	-2.800780	-1.071516	2.098105
1	-2.100039	-2.126957	3.312759
6	-1.956694	-2.945500	0.707143
1	-1.506869	-3.813374	0.220239
1	-2.696361	-3.349591	1.418053
1	-2.520037	-2.384252	-0.045547
6	4.984458	-0.197828	-0.009364
1	5.111560	0.261165	0.982614
1	4.950348	-1.281846	0.139273
1	5.900534	0.024911	-0.580768
6	4.064262	1.927816	-0.723991
1	4.200789	2.349198	0.278768
1	5.024141	2.084015	-1.243668
1	3.328173	2.541708	-1.243769
6	3.874745	0.054192	-2.262534
1	3.231511	0.703654	-2.872754
1	4.909407	0.224562	-2.602664
1	3.613996	-0.979265	-2.509504
6	0.952390	2.746631	-2.072212
1	0.300377	2.417737	-2.885581
1	1.197559	3.801191	-2.283589
1	1.883424	2.186961	-2.171546
6	-1.023477	3.460494	-0.808743
1	-1.389200	3.843814	0.151982
1	-0.857070	4.338438	-1.455893
1	-1.851567	2.885299	-1.241401
6	1.203077	3.563913	0.209375
1	2.204476	3.152642	0.345125
1	1.321755	4.546903	-0.277775
1	0.783400	3.763063	1.198678
6	0.618808	-0.182472	-2.678250
1	0.626264	0.281855	-3.673870
1	1.240098	0.440756	-2.039613
1	1.108407	-1.153578	-2.767707
6	-1.345791	-1.679961	-2.595133
1	-1.957117	-2.163655	-1.835328

1	-1.955433	-1.594755	-3.503640
1	-0.523464	-2.356270	-2.836481
6	-1.660937	0.762269	-2.898792
1	-2.723926	0.673412	-2.681044
1	-1.361758	1.782154	-2.665214
1	-1.541183	0.617388	-3.981971
6	-4.254771	-1.159284	-1.831843
1	-3.944246	-2.192825	-1.627112
1	-5.351330	-1.181259	-1.948880
1	-3.844686	-0.868465	-2.804715
6	-4.583167	1.162185	-1.089616
1	-4.260410	2.027193	-0.498035
1	-4.378537	1.408074	-2.141513
1	-5.678741	1.081440	-0.994166
6	-4.715020	-0.795983	0.509844
1	-4.581562	-0.293879	1.470465
1	-5.791836	-0.762949	0.274537
1	-4.454122	-1.851607	0.660016
6	-3.458828	1.765272	1.896503
1	-4.459317	1.615124	1.483322
1	-3.454170	1.309537	2.903184
1	-3.344468	2.850716	2.044644
6	-0.846367	2.570718	2.454530
1	-1.266008	3.560688	2.208026
1	-1.382044	2.238830	3.357719
1	0.197328	2.724516	2.736311
6	0.578102	-3.581598	-1.052097
1	1.070568	-3.733799	-2.025683
1	0.967866	-4.379647	-0.396859
1	-0.482618	-3.769592	-1.203017
6	3.254749	-2.840564	-1.066129
1	4.282377	-2.468711	-1.071423
1	3.246136	-3.764759	-0.464378
1	3.030907	-3.152487	-2.101446

9-TS-1

SCF energy = -846.560045994 a.u.

ν = -174.1927 cm^{-1}

6	-0.612279	1.814428	-0.479518
6	0.727604	1.737630	-0.309152
5	-1.211795	0.365579	-0.184473
5	1.078445	0.208808	0.058316
7	-0.130854	-0.594471	-0.307206
6	-0.232264	-2.035390	-0.645070
6	-2.731809	0.229362	0.384661
6	2.048887	-0.133275	1.325915
6	-0.392559	-2.962546	0.570996
1	-1.243296	-2.671685	1.193177
1	-0.553234	-3.999943	0.239015
1	0.500885	-2.955426	1.206703
6	-1.413759	-2.235078	-1.610103
1	-1.433077	-3.270878	-1.980611
1	-2.380981	-2.038063	-1.139323
1	-1.312109	-1.562725	-2.475461
6	1.006121	-2.490134	-1.436447
1	1.074423	-1.958104	-2.397249
1	1.941992	-2.349207	-0.884668
1	0.920515	-3.562832	-1.664950
6	1.085392	-0.190396	2.530551
1	0.501900	0.741028	2.616851
1	0.369373	-1.019994	2.446114
1	1.645591	-0.317558	3.472564
6	2.865648	-1.432528	1.266978
1	2.249944	-2.334310	1.175874
1	3.577465	-1.424377	0.424323
1	3.461251	-1.545502	2.188980
6	3.061773	0.992349	1.595244
1	2.572459	1.956447	1.788548
1	3.671019	0.751408	2.482943
1	3.762635	1.129570	0.754953
6	-3.109711	-1.038992	1.166389
1	-3.123709	-1.952766	0.559640
1	-2.427346	-1.202844	2.014402
1	-4.123901	-0.925007	1.585874
6	-3.749476	0.427200	-0.757127
1	-3.741803	-0.413532	-1.467217
1	-4.772447	0.504664	-0.349113
1	-3.558671	1.342356	-1.336331
6	-2.904545	1.380829	1.407871
1	-2.822917	2.376492	0.957533
1	-3.899566	1.317241	1.880222
1	-2.154236	1.316370	2.212584
6	-1.303659	3.107911	-0.825202
1	-1.233346	3.844606	-0.006463
1	-0.824686	3.575067	-1.702244
1	-2.367149	2.983735	-1.064524
6	1.634371	2.934315	-0.434361
1	1.353588	3.546770	-1.307007
1	1.556431	3.595802	0.445562
1	2.696072	2.674288	-0.543055

8	2.709069	0.441244	-2.661893
6	2.358114	0.162367	-1.626838

9-I-1

SCF energy = -846.569347361 a.u.

6	0.530991	-1.789260	-0.518654
6	-0.817425	-1.671477	-0.545402
5	1.185122	-0.374564	-0.168144
5	-1.183516	-0.123186	-0.144482
7	0.151557	0.619916	-0.293895
6	0.300825	2.071031	-0.561676
6	2.729403	-0.309348	0.358882
6	-2.051734	0.023683	1.280631
6	0.525115	2.903180	0.712104
1	1.385274	2.546300	1.282819
1	0.699438	3.960175	0.457581
1	-0.350249	2.861535	1.372691
6	1.458276	2.282443	-1.552911
1	1.567385	3.349374	-1.799880
1	2.416029	1.935311	-1.156481
1	1.261033	1.730251	-2.484210
6	-0.938546	2.644055	-1.271746
1	-1.092279	2.170372	-2.253728
1	-1.856901	2.554357	-0.677504
1	-0.786069	3.716802	-1.460003
6	-1.026831	-0.117312	2.414676
1	-0.469466	-1.063734	2.328813
1	-0.292131	0.699742	2.406805
1	-1.532099	-0.113618	3.395660
6	-2.797193	1.358706	1.429032
1	-2.128742	2.227519	1.396158
1	-3.561116	1.492184	0.643201
1	-3.325417	1.398045	2.397184
6	-3.102465	-1.086203	1.444711
1	-2.644981	-2.083156	1.499719
1	-3.670247	-0.935805	2.378460
1	-3.839585	-1.095676	0.623647
6	3.214806	0.939153	1.114709
1	3.222595	1.857856	0.515333
1	2.609736	1.123702	2.015442
1	4.252221	0.779212	1.455631
6	3.699260	-0.567652	-0.812105
1	3.721375	0.277419	-1.517469
1	4.728235	-0.709263	-0.437307
1	3.435271	-1.463480	-1.392601
6	2.869698	-1.454308	1.394469
1	2.725868	-2.451753	0.965554
1	3.877920	-1.436141	1.842469
1	2.144005	-1.337870	2.215849
6	1.177970	-3.126976	-0.787466
1	1.031972	-3.826504	0.053874
1	0.728123	-3.607957	-1.671662
1	2.257211	-3.059881	-0.970215
6	-1.743690	-2.819219	-0.849800
1	-1.465202	-3.301247	-1.802140
1	-1.684421	-3.603865	-0.076813
1	-2.799990	-2.527322	-0.930850
8	-2.858455	-0.007285	-2.270952
6	-2.156141	0.076960	-1.387456

9-TS-2

SCF energy = -846.551026774 a.u.

ν = -314.0731 cm^{-1}

6	0.226442	-1.750863	-0.442841
6	-1.081618	-1.539452	-0.761565
5	1.082640	-0.433830	-0.084212
5	-1.217038	0.267719	-0.071439
7	0.214392	0.696408	-0.190382
6	0.513419	2.088741	-0.635338
6	2.629354	-0.564780	0.399421
6	-2.042878	0.279964	1.324488
6	0.920311	2.985419	0.543262
1	1.827050	2.631164	1.038650
1	1.101497	4.013923	0.195368
1	0.118912	3.020661	1.294111
6	1.600473	2.055817	-1.719629
1	1.827581	3.074488	-2.068429
1	2.534232	1.607779	-1.365558
1	1.249999	1.468667	-2.581846
6	-0.722108	2.733430	-1.291917
1	-1.042987	2.195743	-2.193962
1	-1.577397	2.796462	-0.606560
1	-0.467410	3.760594	-1.590456
6	-1.089985	-0.104489	2.463891
1	-0.661774	-1.108463	2.307328
1	-0.251743	0.603682	2.546658
1	-1.621176	-0.116404	3.430468
6	-2.578776	1.702672	1.571400
1	-1.776307	2.452319	1.615260
1	-3.289251	2.010354	0.787657

1	-3.112689	1.743849	2.536147
6	-3.248288	-0.670996	1.335605
1	-2.938880	-1.725555	1.318876
1	-3.842714	-0.521468	2.252241
1	-3.920792	-0.496907	0.479526
6	3.319118	0.680836	0.979385
1	3.442210	1.499182	0.259426
1	2.777249	1.070166	1.853799
1	4.331712	0.410031	1.323796
6	3.511246	-1.099062	-0.746972
1	3.636840	-0.342172	-1.537209
1	4.518491	-1.354147	-0.374376
1	3.100498	-1.997853	-1.228048
6	2.622080	-1.569315	1.581202
1	2.285230	-2.576249	1.315055
1	3.640951	-1.670303	1.992089
1	1.976476	-1.209544	2.398668
6	0.691324	-3.189592	-0.412132
1	0.373700	-3.684924	0.521729
1	0.254815	-3.766075	-1.241244
1	1.778935	-3.292464	-0.479270
6	-2.070610	-2.653606	-0.993774
1	-1.842262	-3.165721	-1.942836
1	-2.029784	-3.405904	-0.191911
1	-3.101672	-2.287019	-1.072720
8	-2.319779	-0.169416	-2.455231
6	-1.794515	-0.105870	-1.401092

9-TS-2B

SCF energy = -846.546038103 a.u.

ν = -359.9463 cm^{-1}

6	-0.762768	1.781245	-0.625493
6	0.573025	1.697043	-0.830899
5	-1.310641	0.339628	-0.171661
5	0.959776	0.185817	-0.597385
7	-0.247496	-0.626698	-0.405394
6	-0.322902	-2.092752	-0.620663
6	-2.779930	0.205835	0.507005
6	2.295320	0.163875	1.109256
6	-0.372706	-2.882585	0.696204
1	-1.221993	-2.596562	1.321264
1	-0.448023	-3.962008	0.493463
1	0.544035	-2.716859	1.278706
6	-1.542381	-2.406197	-1.501935
1	-1.626457	-3.488797	-1.679723
1	-2.480235	-2.070521	-1.049080
1	-1.439596	-1.902809	-2.475115
6	0.901844	-2.600224	-1.398230
1	1.043245	-2.054643	-2.342600
1	1.827890	-2.539034	-0.808907
1	0.758375	-3.662537	-1.643107
6	1.134264	0.343510	2.087449
1	0.534248	1.238018	1.866334
1	0.462380	-0.523977	2.107940
1	1.553134	0.467866	3.101657
6	3.055269	-1.113828	1.464577
1	2.426111	-2.010957	1.371959
1	3.954268	-1.252872	0.847477
1	3.385830	-1.058278	2.515872
6	3.221999	1.371935	1.186659
1	2.674452	2.316186	1.064893
1	3.704069	1.398108	2.179435
1	4.029515	1.331011	0.440197
6	-3.123153	-1.055555	1.315170
1	-3.140881	-1.977470	0.720930
1	-2.420961	-1.199724	2.150344
1	-4.128063	-0.945504	1.757472
6	-3.856128	0.388477	-0.584164
1	-3.883030	-0.465284	-1.278689
1	-4.856793	0.471796	-0.125499
1	-3.696053	1.292107	-1.189248
6	-2.894715	1.365418	1.527742
1	-2.822240	2.357704	1.069901
1	-3.868465	1.315256	2.044095
1	-2.111370	1.296249	2.300074
6	-1.489719	3.086716	-0.835769
1	-1.336197	3.777253	0.011836
1	-1.109675	3.604565	-1.731201
1	-2.572879	2.968549	-0.964676
6	1.454487	2.834293	-1.262838
1	1.089285	3.271513	-2.207683
1	1.457183	3.652822	-0.523460
1	2.498383	2.531255	-1.425150
8	3.447000	-0.320460	-1.304904
6	2.363411	-0.177054	-0.913653

9-P-1

SCF energy = -846.577758080 a.u.

6	1.562159	-1.463293	-0.330508
6	0.595546	-2.408357	-0.397935

5	1.171102	0.050536	-0.003645
5	-1.132257	-0.361428	0.052816
7	-0.132876	0.533559	-0.465679
6	-0.302529	1.688790	-1.394309
6	2.102062	0.902091	1.018737
6	-2.486779	0.006352	0.855330
6	-0.998585	2.934601	-0.835462
1	-0.495700	3.327105	0.055543
1	-0.991940	3.723305	-1.602548
1	-2.047188	2.735428	-0.585196
6	1.073323	2.084007	-1.951642
1	0.948872	2.792271	-2.783228
1	1.708575	2.568093	-1.201103
1	1.604070	1.201198	-2.343861
6	-1.128423	1.147322	-2.576623
1	-0.616361	0.293222	-3.043421
1	-2.119508	0.807589	-2.246301
1	-1.272865	1.927955	-3.339270
6	-2.208513	1.158836	1.840008
1	-1.428866	0.878598	2.567467
1	-1.881478	2.081011	1.348150
1	-3.119413	1.392390	2.416933
6	-3.656364	0.371644	-0.077344
1	-3.486563	1.307640	-0.629110
1	-3.844289	-0.428343	-0.810251
1	-4.580658	0.507540	0.510238
6	-2.936102	-1.195818	1.714566
1	-2.124861	-1.553093	2.370512
1	-3.773545	-0.893793	2.366162
1	-3.260883	-2.040984	1.096895
6	1.497240	2.240048	1.472305
1	1.560239	3.017378	0.698555
1	0.442687	2.134423	1.761464
1	2.047437	2.622595	2.347867
6	3.553855	1.162394	0.579410
1	3.603553	1.742394	-0.355457
1	4.078879	1.746583	1.354114
1	4.128193	0.240578	0.429381
6	2.111090	-0.010873	2.273616
1	2.594822	-0.981157	2.093038
1	2.652036	0.486960	3.095924
1	1.088455	-0.214130	2.634168
6	2.996566	-1.820455	-0.632814
1	3.599426	-1.874643	0.288673
1	3.081827	-2.792028	-1.136747
1	3.474428	-1.066632	-1.276351
6	0.791188	-3.857906	-0.743052
1	1.071998	-3.988373	-1.800993
1	1.580400	-4.318700	-0.130942
1	-0.148751	-4.402432	-0.585308
8	-1.741368	-2.653940	-0.510294
6	-0.800096	-1.927528	-0.225740

9-P-1B

SCF energy = -846.596833865 a.u.

6	-1.163901	1.721678	-0.865929
6	0.172017	1.713873	-1.089923
5	-1.502475	0.295151	-0.220349
5	0.659691	0.253212	-0.758186
7	-0.457930	-0.638658	-0.630815
6	-0.389817	-2.109147	-0.785837
6	-2.630987	0.130174	0.922024
6	2.742833	0.245495	0.985820
6	0.296270	-2.791266	0.403717
1	-0.227428	-2.585379	1.346346
1	0.325118	-3.881442	0.256670
1	1.336334	-2.447965	0.504098
6	-1.791911	-2.686711	-1.010631
1	-1.713351	-3.750514	-1.277853
1	-2.434196	-2.618128	-0.127011
1	-2.290329	-2.165466	-1.842262
6	0.410395	-2.402364	-2.069248
1	-0.091145	-1.949346	-2.937772
1	1.432698	-2.004750	-2.022695
1	0.473909	-3.488039	-2.237156
6	1.611267	0.331313	2.016680
1	0.875088	1.107122	1.750417
1	1.077224	-0.625122	2.113117
1	2.017608	0.590757	3.006280
6	3.761669	-0.827381	1.383034
1	3.278285	-1.808068	1.515249
1	4.531427	-0.931398	0.606321
1	4.249076	-0.561055	2.333723
6	3.444832	1.611285	0.872259
1	2.736756	2.406889	0.596688
1	3.898990	1.883377	1.838015
1	4.238451	1.576467	0.111614
6	-2.339848	-0.953366	1.973333
1	-2.337315	-1.971609	1.568399
1	-1.364054	-0.785722	2.456094

1	-3.106794	-0.925989	2.765450
6	-3.996630	-0.127219	0.253535
1	-4.035209	-1.097951	-0.261528
1	-4.798477	-0.122233	1.011874
1	-4.242099	0.650799	-0.486743
6	-2.724980	1.457289	1.709084
1	-3.081375	2.291919	1.093586
1	-3.434859	1.346805	2.546062
1	-1.752153	1.746577	2.138767
6	-2.039612	2.920919	-1.094768
1	-1.903851	3.684838	-0.310108
1	-1.780745	3.405537	-2.050215
1	-3.108966	2.668852	-1.128852
6	1.001348	2.879157	-1.546878
1	0.541822	3.373196	-2.418846
1	1.087867	3.649919	-0.761646
1	2.019778	2.577092	-1.830949
8	2.955871	-0.468376	-1.292635
6	2.196118	-0.074422	-0.425550

10

SCF energy = -1337.632011070 a.u.

7	-1.268387	0.003102	-0.000546
5	-0.419411	1.173212	0.008560
6	1.095871	0.676873	0.000360
5	-0.425872	-1.171753	-0.010307
6	1.092183	-0.683692	-0.002055
6	2.293882	1.546353	-0.016781
6	3.315164	1.357392	-0.959960
6	2.422357	2.594352	0.906637
6	4.432600	2.187883	-0.974626
1	1.616581	-2.774452	-1.639110
6	3.546913	3.416510	0.900854
1	1.629026	2.764255	1.638404
6	4.555014	3.217667	-0.041538
1	5.215214	2.028471	-1.719880
1	3.632280	4.221360	1.634351
1	5.433457	3.866849	-0.051562
6	-0.924626	2.652293	0.020684
6	-2.042194	3.057577	0.773138
6	-0.255759	3.630021	-0.737768
6	-2.467992	4.383327	0.774745
1	-2.589801	2.324977	1.370922
6	-0.695404	4.952126	-0.762186
1	0.625033	3.352571	-1.322368
6	-1.799431	5.331684	-0.000086
1	-3.331832	4.677436	1.375207
1	-0.167032	5.690823	-1.368977
1	-2.139779	6.369989	-0.008284
6	2.285680	-1.559329	0.016363
6	2.409943	-2.608304	-0.906509
6	3.306767	-1.375154	0.960707
6	3.530321	-3.436156	-0.898969
1	3.226353	0.548409	-1.688353
6	4.419964	-2.211275	0.977100
1	3.221168	-0.565450	1.688682
6	4.538256	-3.242061	0.044592
1	3.612506	-4.241747	-1.632012
1	5.202457	-2.055572	1.723267
1	5.413268	-3.895826	0.055977
6	-0.939763	-2.647850	-0.023111
6	-2.061100	-3.045463	-0.774103
6	-0.275934	-3.630499	0.733461
6	-2.495510	-4.368381	-0.775854
1	-2.604979	-2.308905	-1.370411
6	-0.724073	-4.949737	0.757688
1	0.607592	-3.359160	1.316805
6	-1.831846	-5.321592	-0.002739
1	-3.362325	-4.656475	-1.374953
1	-0.199524	-5.692295	1.363085
1	-2.179136	-6.357594	0.005464
6	-2.687427	0.007378	0.000547
6	-3.394839	-0.580128	1.053767
6	-3.393109	0.599180	-1.051426
6	-4.787778	-0.579131	1.051249
1	-2.841923	-1.044277	1.872818
6	-4.786029	0.606731	-1.046397
1	-2.838839	1.059971	-1.871449
6	-5.488913	0.015960	0.003059
1	-5.328008	-1.045380	1.878078
1	-5.324880	1.076282	-1.872265
1	-6.580884	0.019399	0.004078

10-TS-0

SCF energy = -2675.260155510 a.u.

ν = -154.2726 cm^{-1}

6	-2.053844	-1.146043	0.489410
6	-2.721025	0.033149	0.592126
5	-0.505800	-0.915147	0.917291
5	-1.728214	1.161454	1.045246

7	-0.418521	0.580465	1.265873	1	-0.306481	3.085485	-2.007155
6	2.702909	0.464163	-0.705715	6	-3.022526	1.905125	-3.646206
6	1.695024	1.335031	-0.989989	1	-3.623923	-0.169573	-3.726270
5	2.113439	-0.977442	-0.573558	1	-2.183758	3.874795	-3.360817
5	0.359055	0.521031	-1.187019	1	-3.853310	2.255199	-4.263268
7	0.614403	-0.931092	-0.762830	6	0.324595	-1.936238	-1.776918
6	3.004582	-2.246195	-0.335688	6	0.736956	-1.693444	-3.095437
6	2.983653	-3.438443	-1.081074	6	-0.267579	-3.157946	-1.470437
6	3.921730	-2.167250	0.730280	6	0.522393	-2.641735	-4.090067
6	3.804605	-4.513479	-0.746026	1	1.220304	-0.746823	-3.348896
1	2.327810	-3.536886	-1.945868	6	-0.488663	-4.104600	-2.468633
6	4.723317	-3.247520	1.085096	1	-0.559721	-3.383085	-0.450884
1	4.009704	-1.242096	1.303874	6	-0.100222	-3.851461	-3.781575
6	4.663498	-4.429127	0.348339	1	0.841770	-2.431383	-5.112644
1	3.769105	-5.425896	-1.345464	1	-0.974080	-5.046071	-2.204764
1	5.406711	-3.161505	1.932333	1	-0.275607	-4.594856	-4.561697
1	5.297411	-5.277277	0.617236	6	0.033035	-1.956046	2.012475
6	4.140512	0.805462	-0.597862	6	0.752195	-3.138496	1.803643
6	4.604619	1.794479	0.279524	6	-0.395164	-1.699663	3.329308
6	5.075252	0.107597	-1.376938	6	1.043841	-4.017724	2.847902
6	5.965969	2.075508	0.374112	1	1.109799	-3.397621	0.809886
1	3.896018	2.332668	0.908861	6	-0.118905	-2.573317	4.376218
6	6.433401	0.400211	-1.293957	1	-0.965098	-0.790954	3.541163
1	1.553445	3.363885	0.826963	6	0.607469	-3.741510	4.139838
6	6.884101	1.383566	-0.413762	1	1.615532	-4.925251	2.640256
1	6.309446	2.843168	1.070953	1	-0.469720	-2.340488	5.384392
1	7.144214	-0.150559	-1.913723	1	0.831318	-4.429091	4.958729
1	7.950806	1.606035	-0.338472	6	-2.740516	-2.427233	0.170998
6	1.939894	2.783714	-1.215070	6	-2.622928	-3.545862	1.011584
6	2.317363	3.238654	-2.484769	6	-3.543833	-2.547705	-0.973390
6	1.820922	3.710044	-0.173355	6	-3.252112	-4.748564	0.693952
6	2.547102	4.592923	-2.712988	1	-2.034969	-3.474835	1.926870
1	2.422080	2.519519	-3.300517	6	-4.164972	-3.750208	-1.295223
6	2.047788	5.066245	-0.403875	1	-4.787850	-1.335618	1.741634
1	4.730508	-0.677200	-2.054247	6	-4.015121	-4.862028	-0.467132
6	2.406044	5.513260	-1.674382	1	-3.145314	-5.602861	1.366451
1	2.838286	4.932049	-3.709627	1	-4.776233	-3.816531	-2.198143
1	1.947103	5.775802	0.420421	1	-4.503649	-5.806724	-0.716239
1	2.583321	6.575744	-1.854079	6	-4.176388	0.233800	0.392561
6	-0.871030	0.992458	-2.041204	6	-4.631016	1.249159	-0.460083
6	-1.841443	0.108232	-2.554387	6	-5.126313	-0.549284	1.063569
6	-1.027652	2.353536	-2.365585	6	-5.993555	1.454549	-0.661921
6	-2.893212	0.548321	-3.347442	1	-3.903928	1.884291	-0.969426
1	-1.772584	-0.954930	-2.337251	6	-6.489150	-0.335763	0.872763
6	-2.090206	2.808659	-3.144831	1	-3.690595	-1.679810	-1.616493

6	-6.928616	0.662443	0.003217
1	-6.325815	2.245349	-1.338520
1	-7.213213	-0.955615	1.406607
1	-7.997639	0.827220	-0.149543
6	-2.207127	2.645027	1.263925
6	-1.573123	3.746580	0.669827
6	-3.355542	2.894910	2.033443
6	-2.060711	5.040729	0.828676
1	-0.668754	3.593653	0.082211
6	-3.837390	4.189961	2.217612
1	-3.889353	2.061017	2.496388
6	-3.195181	5.266924	1.608602
1	-1.547578	5.876555	0.346705
1	-4.728479	4.356755	2.826962
1	-3.579871	6.281044	1.740481
6	0.588400	1.105069	2.117772
6	0.403351	2.273502	2.878845
6	1.815841	0.441336	2.276395
6	1.417081	2.780756	3.687232
1	-0.544585	2.801627	2.849565
6	2.824328	0.942220	3.092797
1	1.977756	-0.517462	1.793804
6	2.644589	2.130989	3.793768
1	1.229987	3.697788	4.250691
1	3.762643	0.389156	3.177989
1	3.435713	2.528686	4.432129

10-I-0

SCF energy = -2675.271435800 a.u.

6	-2.110235	-1.077887	0.365447
6	-2.787415	0.102847	0.434560
5	-0.525034	-0.903282	0.705966
5	-1.808768	1.268930	0.692568
7	-0.404353	0.723664	0.876168
6	2.748208	0.239499	-0.630759
6	1.845299	1.258473	-0.645590
5	2.023054	-1.114025	-0.475722
5	0.323887	0.697937	-0.653289
7	0.505572	-0.923467	-0.589245
6	2.793636	-2.451741	-0.193155
6	2.751098	-3.621640	-0.967754
6	3.639815	-2.447197	0.931280
6	3.480154	-4.753107	-0.603398
1	2.154408	-3.654854	-1.879810
6	4.350100	-3.580691	1.312391
1	3.745032	-1.538109	1.528985
6	4.266737	-4.743184	0.546715
1	3.432013	-5.649513	-1.225904
1	4.980290	-3.553110	2.203841
1	4.828483	-5.634255	0.836417
6	4.225360	0.384215	-0.603901
6	4.855804	1.220138	0.328463
6	5.024153	-0.362776	-1.479645
6	6.244562	1.315096	0.373209
1	4.247433	1.797576	1.027673
6	6.412680	-0.261515	-1.442134
1	1.554630	3.293897	1.205050
6	7.027852	0.578037	-0.514244
1	6.717990	1.971610	1.106787
1	7.018466	-0.848979	-2.135622
1	8.116891	0.655197	-0.479515
6	2.294982	2.673024	-0.728815
6	2.997908	3.093143	-1.868783
6	2.067602	3.601444	0.294269
6	3.432061	4.408191	-1.995994
1	3.194889	2.372603	-2.665569
6	2.513050	4.917403	0.170160
1	4.547225	-1.036237	-2.196134
6	3.188406	5.329072	-0.976417
1	3.968789	4.715467	-2.896220
1	2.328815	5.623718	0.982807
1	3.531273	6.361378	-1.074171
6	-0.619610	1.255443	-1.860646
6	-1.634501	0.491032	-2.465689
6	-0.416446	2.533354	-2.411023
6	-2.403518	0.962053	-3.525134
1	-1.839438	-0.514208	-2.106542
6	-1.187445	3.027463	-3.463138
1	0.364271	3.181842	-2.017212
6	-2.189882	2.244163	-4.027091
1	-3.178492	0.322180	-3.953589
1	-0.995006	4.032750	-3.844678
1	-2.794596	2.625318	-4.853241
6	0.261406	-1.760201	-1.755514
6	0.754915	-1.353155	-3.001794
6	-0.344568	-3.010328	-1.635485
6	0.601196	-2.172072	-4.116474
1	1.238664	-0.381167	-3.102165
6	-0.513069	-3.818055	-2.757185
1	-0.681232	-3.365050	-0.664645

6	-0.043408	-3.403070	-4.001429
1	0.981402	-1.837033	-5.083439
1	-1.009846	-4.783491	-2.645164
1	-0.172725	-4.039618	-4.879013
6	-0.177558	-1.802721	1.994808
6	0.463905	-3.045458	1.927860
6	-0.704303	-1.427829	3.243762
6	0.605155	-3.862997	3.051249
1	0.860973	-3.407844	0.980839
6	-0.570509	-2.232155	4.370630
1	-1.243875	-0.482188	3.341372
6	0.092336	-3.457887	4.279615
1	1.117210	-4.823263	2.955822
1	-0.989423	-1.904373	5.324956
1	0.200237	-4.093480	5.161642
6	-2.813470	-2.356347	0.073529
6	-2.777455	-3.439947	0.963476
6	-3.541828	-2.498831	-1.117359
6	-3.425151	-4.635153	0.653305
1	-2.247664	-3.345908	1.911327
6	-4.175647	-3.696053	-1.432028
1	-4.785075	-1.146625	1.796528
6	-4.115419	-4.774204	-0.549269
1	-3.388421	-5.463628	1.364240
1	-4.724982	-3.785214	-2.371778
1	-4.615908	-5.714369	-0.791501
6	-4.253606	0.239733	0.232030
6	-4.755193	1.100426	-0.754230
6	-5.163228	-0.472777	1.024434
6	-6.127717	1.232943	-0.951144
1	-4.058956	1.672146	-1.371407
6	-6.536084	-0.334888	0.832583
1	-3.610835	-1.657073	-1.808482
6	-7.023712	0.516847	-0.158032
1	-6.498859	1.906809	-1.726737
1	-7.229010	-0.899892	1.460228
1	-8.099998	0.624980	-0.309841
6	-2.221942	2.777724	0.810423
6	-1.398810	3.835920	0.392123
6	-3.449379	3.112626	1.410493
6	-1.779601	5.163775	0.547101
1	-0.429568	3.622131	-0.053413
6	-3.829879	4.442026	1.589945
1	-4.119602	2.324042	1.757800
6	-2.999486	5.471272	1.151386
1	-1.115681	5.960440	0.203855
1	-4.784385	4.672214	2.068266
1	-3.299992	6.513422	1.283232
6	0.378758	1.193073	2.013608
6	-0.075795	2.189852	2.885173
6	1.606945	0.592320	2.320394
6	0.706580	2.624953	3.955593
1	-1.046256	2.653802	2.745839
6	2.390588	1.027729	3.381164
1	1.958954	-0.257907	1.750474
6	1.955465	2.066196	4.200670
1	0.318489	3.413434	4.603719
1	3.344807	0.532341	3.572120
1	2.568885	2.413042	5.034326

10-TS-1

SCF energy = -1450.812738160 a.u.

ν = -225.0755 cm^{-1}

7	1.229386	0.145806	0.098527
5	0.311919	1.234717	-0.044140
6	-1.163201	0.647525	0.015044
5	0.465397	-1.124005	0.222123
6	-1.088477	-0.708620	0.132272
6	-2.405649	1.451729	-0.051557
6	-3.400106	1.318051	0.928793
6	-2.601573	2.386543	-1.078288
6	-4.559579	2.086835	0.877900
1	-1.333931	-3.021766	1.543619
6	-3.766385	3.148939	-1.135360
1	-1.828423	2.515434	-1.839329
6	-4.749031	3.002907	-0.157017
1	-5.322114	1.969487	1.651297
1	-3.903003	3.868398	-1.945857
1	-5.659812	3.604461	-0.198242
6	0.724699	2.733890	-0.240972
6	1.803965	3.102384	-1.063728
6	0.014439	3.761122	0.404654
6	2.151414	4.438895	-1.244652
1	2.382706	2.329616	-1.575940
6	0.373054	5.098637	0.247177
1	-0.837190	3.511554	1.042899
6	1.439170	5.440186	-0.583986
1	2.986059	4.701650	-1.898664
1	-0.188364	5.878653	0.766610
1	1.713575	6.488997	-0.719990

6	-2.211273	-1.672776	0.096047
6	-2.184438	-2.833959	0.884117
6	-3.298909	-1.493720	-0.775165
6	-3.220428	-3.763361	0.833737
1	-3.258186	0.595775	1.736165
6	-4.328328	-2.427898	-0.836526
1	-3.330028	-0.613833	-1.419938
6	-4.298424	-3.563180	-0.026555
1	-3.178735	-4.655214	1.462933
1	-5.160017	-2.269001	-1.526581
1	-5.107344	-4.295462	-0.073389
6	1.038906	-2.527551	-0.234053
6	2.152760	-3.139394	0.361756
6	0.455397	-3.170795	-1.336562
6	2.665034	-4.342464	-0.118200
1	2.644265	-2.660354	1.214493
6	0.968940	-4.369451	-1.831603
1	-0.422017	-2.730082	-1.817482
6	2.074253	-4.959410	-1.221338
1	3.532271	-4.798116	0.365209
1	0.497891	-4.848739	-2.692862
1	2.475579	-5.900980	-1.603584
6	2.642560	0.241515	0.152594
6	3.440466	-0.370898	-0.820644
6	3.257700	0.956343	1.186059
6	4.828076	-0.271001	-0.755048
1	2.960698	-0.925195	-1.628935
6	4.645675	1.060387	1.244626
1	2.633777	1.447109	1.936535
6	5.436632	0.444447	0.276113
1	5.438640	-0.754687	-1.520723
1	5.110860	1.627434	2.053943
1	6.524635	0.524972	0.322967
6	0.536044	-1.167398	2.249631
8	0.486952	-0.799385	3.313709

10-I-1

SCF energy = -1450.817243340 a.u.

7	-1.192084	-0.406413	-0.187641
5	-0.836536	0.961123	-0.020279
6	0.741413	1.076116	-0.092867
5	0.068338	-1.251351	-0.403898
6	1.275281	-0.161400	-0.297681
6	1.507251	2.334722	0.071111
6	2.474508	2.724890	-0.866651
6	1.251567	3.181982	1.158678
6	3.170703	3.921412	-0.716297
1	2.517546	-1.992132	-1.899826
6	1.955322	4.373693	1.315695
1	0.487448	2.900857	1.886928
6	2.916309	4.748760	0.377694
1	3.918109	4.210093	-1.458712
1	1.744711	5.017918	2.172260
1	3.461842	5.687601	0.495595
6	-1.859826	2.131516	0.201545
6	-2.991861	1.978869	1.020709
6	-1.669456	3.376530	-0.422517
6	-3.893575	3.023069	1.212058
1	-3.173218	1.023669	1.519932
6	-2.579430	4.418716	-0.252476
1	-0.790886	3.536606	-1.053307
6	-3.692005	4.244804	0.569691
1	-4.761758	2.881923	1.859935
1	-2.414444	5.374214	-0.755767
1	-4.403103	5.062280	0.711165
6	2.706849	-0.539097	-0.302521
6	3.192175	-1.517485	-1.183057
6	3.607082	0.014068	0.623379
6	4.529293	-1.906472	-1.167459
1	2.680778	2.075728	-1.720871
6	4.941064	-0.381158	0.648709
1	3.250958	0.757881	1.338172
6	5.411189	-1.337908	-0.250985
1	4.880443	-2.664687	-1.870693
1	5.620346	0.060736	1.381109
1	6.458977	-1.645296	-0.230947
6	0.231587	-2.673594	0.312533
6	-0.335763	-3.853568	-0.189986
6	0.909568	-2.748466	1.538418
6	-0.235014	-5.061884	0.498829
1	-0.890275	-3.835773	-1.134511
6	1.008195	-3.949375	2.238429
1	1.372117	-1.849049	1.953767
6	0.437148	-5.111210	1.718609
1	-0.686648	-5.965938	0.083890
1	1.539026	-3.981303	3.192762
1	0.518854	-6.055083	2.262553
6	-2.501790	-0.940557	-0.267442
6	-2.939316	-1.899128	0.655108
6	-3.378430	-0.514620	-1.272878

6	-4.228140	-2.420715	0.567106
1	-2.259480	-2.225468	1.443319
6	-4.668723	-1.032527	-1.352315
1	-3.041871	0.242756	-1.984470
6	-5.098001	-1.990057	-0.434339
1	-4.556310	-3.166853	1.294099
1	-5.343768	-0.683724	-2.136901
1	-6.108362	-2.399385	-0.498494
6	-0.016555	-1.409496	-2.028458
8	-0.113394	-1.334263	-3.149855

10-TS-2

SCF energy = -1450.790194650 a.u.

ν = -290.6384 cm^{-1}

7	-1.285465	-0.875060	-0.251858
5	-1.192996	0.532764	-0.176867
6	0.323803	0.975970	-0.373576
5	0.033321	-1.549440	-0.464616
6	1.138193	0.018751	-0.897581
6	0.847626	2.277485	0.108278
6	1.752796	3.032134	-0.652111
6	0.423431	2.785219	1.345024
6	2.224191	4.256039	-0.185621
1	2.877460	0.043715	-3.025877
6	0.909182	4.000399	1.819810
1	-0.293163	2.218549	1.943872
6	1.808275	4.741371	1.053977
1	2.922356	4.834477	-0.794410
1	0.574907	4.376019	2.789279
1	2.182833	5.699143	1.422027
6	-2.386251	1.517224	0.080765
6	-3.446706	1.185469	0.941571
6	-2.409973	2.782262	-0.529301
6	-4.486750	2.079517	1.183662
1	-3.459233	0.208347	1.431913
6	-3.457774	3.673816	-0.307913
1	-1.590642	3.079287	-1.189721
6	-4.496868	3.324409	0.553535
1	-5.296093	1.803097	1.863263
1	-3.458842	4.648487	-0.800875
1	-5.314248	4.025531	0.738144
6	2.621686	0.025200	-0.882710
6	3.382407	0.028528	-2.058855
6	3.281223	-0.005393	0.355090
6	4.775028	0.018183	-1.995006
1	2.084219	2.655392	-1.621405
6	4.670605	-0.021125	0.414300
1	2.690787	-0.026685	1.273596
6	5.422007	-0.006515	-0.761064
1	5.357057	0.029355	-2.919214
1	5.169796	-0.047936	1.385108
1	6.513226	-0.016827	-0.713895
6	0.839546	-2.347824	0.619834
6	1.898331	-3.204452	0.285683
6	0.560750	-2.135769	1.979344
6	2.656848	-3.827841	1.274562
1	2.139787	-3.381839	-0.765948
6	1.314928	-2.755928	2.972383
1	-0.256455	-1.464195	2.259009
6	2.367145	-3.602785	2.619639
1	3.479208	-4.489832	0.994726
1	1.086903	-2.577447	4.025719
1	2.961590	-4.089165	3.396541
6	-2.463659	-1.650236	-0.427908
6	-2.636805	-2.845055	0.280788
6	-3.454887	-1.243626	-1.329930
6	-3.789742	-3.607742	0.100776
1	-1.867169	-3.171276	0.982318
6	-4.608238	-2.003038	-1.496628
1	-3.315646	-0.322083	-1.897393
6	-4.782187	-3.188770	-0.782607
1	-3.911032	-4.537735	0.660404
1	-5.373835	-1.669018	-2.200130
1	-5.686203	-3.785505	-0.919451
6	0.555094	-1.297707	-1.857201
8	0.807441	-1.337761	-3.006653

10-TS-2B

SCF energy = -1450.781827770 a.u.

ν = -451.0065 cm^{-1}

7	-1.203497	-0.514243	-0.392106
5	-0.911849	0.849781	-0.085175
6	0.658005	1.059865	-0.132567
5	0.094317	-1.195942	-0.602077
6	1.257276	-0.124425	-0.435694
6	1.333931	2.366307	0.044472
6	2.315071	2.811587	-0.854839
6	0.975576	3.208234	1.107477
6	2.930091	4.048864	-0.685098
1	2.525604	-1.452842	-2.432402

6	1.597427	4.442249	1.283449
1	0.199617	2.889717	1.806679
6	2.577543	4.867364	0.388136
1	3.689386	4.377516	-1.398356
1	1.307469	5.079470	2.121956
1	3.060973	5.837716	0.521551
6	-1.965871	1.992154	0.151104
6	-2.699030	2.112152	1.341142
6	-2.137714	2.985512	-0.825311
6	-3.582248	3.171550	1.544808
1	-2.568962	1.372674	2.136941
6	-3.030301	4.038892	-0.635195
1	-1.559665	2.938560	-1.752674
6	-3.755165	4.134764	0.552076
1	-4.137038	3.246260	2.483062
1	-3.153023	4.795505	-1.413670
1	-4.450733	4.962999	0.705787
6	2.708021	-0.379806	-0.564607
6	3.210507	-1.103343	-1.655881
6	3.608979	0.058022	0.418816
6	4.573688	-1.372228	-1.768534
1	2.594800	2.176003	-1.697887
6	4.968485	-0.217269	0.310344
1	3.228791	0.612499	1.279013
6	5.457082	-0.931483	-0.784872
1	4.946130	-1.930866	-2.629949
1	5.654294	0.127847	1.087267
1	6.524760	-1.144656	-0.870405
6	0.349902	-2.698082	0.589842
6	-0.800359	-3.188276	1.222074
6	1.607411	-2.930005	1.162175
6	-0.696528	-3.861927	2.436174
1	-1.782871	-3.043161	0.768786
6	1.706540	-3.602753	2.377150
1	2.513777	-2.583735	0.662560
6	0.555597	-4.063170	3.017084
1	-1.597267	-4.234596	2.928407
1	2.687926	-3.767738	2.826659
1	0.636138	-4.589274	3.970947
6	-2.474832	-1.063713	-0.683169
6	-3.507687	-1.029698	0.260688
6	-2.715203	-1.670803	-1.922789
6	-4.752204	-1.582784	-0.031171
1	-3.321929	-0.580044	1.235496
6	-3.956915	-2.234522	-2.206551
1	-1.923527	-1.689426	-2.674596
6	-4.982736	-2.191412	-1.263809
1	-5.545504	-1.544455	0.718474
1	-4.123970	-2.704418	-3.178202
1	-5.956396	-2.631635	-1.487615
6	0.272672	-2.556867	-1.210405
8	0.427661	-3.519891	-1.851992

10-TS-2C

SCF energy = -1450.785464950 a.u.

ν = -178.3491 cm^{-1}

7	1.329730	-0.172849	0.659982
5	0.593451	1.009584	0.220493
6	-0.960924	0.801815	0.177441
5	-0.122945	-1.504324	0.626083
6	-1.318783	-0.502684	0.335463
6	-1.931167	1.912962	-0.010350
6	-2.902388	2.177637	0.964804
6	-1.887735	2.727334	-1.150045
6	-3.813999	3.217366	0.799549
1	-2.343736	-2.451804	1.893600
6	-2.804463	3.762730	-1.320227
1	-1.125529	2.543947	-1.911001
6	-3.771109	4.011123	-0.346344
1	-4.565047	3.407320	1.569646
1	-2.760298	4.382254	-2.218844
1	-4.488570	4.824004	-0.478496
6	1.326066	2.345611	-0.158339
6	2.421077	2.418844	-1.036746
6	0.867801	3.545945	0.414935
6	3.026879	3.637505	-1.334989
1	2.810494	1.511473	-1.502626
6	1.488536	4.762834	0.141983
1	0.007494	3.531349	1.089105
6	2.566770	4.811784	-0.740320
1	3.868251	3.668594	-2.030894
1	1.119852	5.678114	0.610256
1	3.048191	5.766244	-0.965785
6	-2.695194	-1.051245	0.282099
6	-3.066097	-2.080058	1.161441
6	-3.634977	-0.610463	-0.663063
6	-4.345318	-2.629142	1.122370
1	-2.942985	1.551735	1.859500
6	-4.907685	-1.170989	-0.712795
1	-3.361480	0.174070	-1.370134

6	-5.270782	-2.176072	0.183796
1	-4.617180	-3.420136	1.824412
1	-5.623596	-0.818459	-1.458443
1	-6.271259	-2.612253	0.144687
6	0.177751	-2.828549	-0.153232
6	1.121323	-3.759997	0.313276
6	-0.470704	-3.097843	-1.370675
6	1.414164	-4.912863	-0.411136
1	1.639171	-3.579033	1.259200
6	-0.180122	-4.248107	-2.100695
1	-1.217274	-2.395601	-1.750708
6	0.764109	-5.156428	-1.621119
1	2.151217	-5.624462	-0.032551
1	-0.693131	-4.439692	-3.045766
1	0.991189	-6.060928	-2.190494
6	2.734540	-0.345354	0.456442
6	3.179048	-1.060985	-0.658008
6	3.652627	0.184343	1.364483
6	4.545194	-1.230017	-0.871628
1	2.446337	-1.477335	-1.351941
6	5.017023	0.009126	1.146043
1	3.287820	0.738148	2.229979
6	5.465790	-0.694706	0.028851
1	4.890749	-1.785536	-1.745944
1	5.735072	0.428121	1.854053
1	6.536359	-0.828833	-0.139435
6	0.775648	-1.065706	1.795245
8	1.289981	-1.157773	2.854350

10-P-1

SCF energy = -1450.824403520 a.u.

7	-1.323819	0.100436	0.301943
5	-0.080709	0.811445	0.106898
6	1.306446	0.035438	0.110681
5	-1.349271	-1.326813	0.185487
6	1.365733	-1.321922	0.171509
6	2.552050	0.852918	0.038156
6	3.489897	0.655604	-0.983427
6	2.795526	1.856797	0.983917
6	4.640020	1.437491	-1.053757
1	2.134121	-3.356462	-1.452492
6	3.951678	2.629641	0.923860
1	2.067506	2.037010	1.778214
6	4.877366	2.424501	-0.098053
1	5.359136	1.270421	-1.858694
1	4.125928	3.402632	1.675426
1	5.781708	3.034566	-0.151487
6	-0.083871	2.358817	-0.196436
6	-0.607125	3.327548	0.673323
6	0.491594	2.804850	-1.398026
6	-0.553598	4.684481	0.360787
1	-1.059887	3.024232	1.619578
6	0.522396	4.156944	-1.730238
1	0.935681	2.081351	-2.087685
6	0.004423	5.102354	-0.846159
1	-0.955252	5.419563	1.061964
1	0.967986	4.475457	-2.675217
1	0.041233	6.165438	-1.095061
6	2.627121	-2.107618	0.239562
6	2.878445	-3.125837	-0.688689
6	3.586331	-1.841611	1.224386
6	4.072316	-3.841287	-0.649412
1	3.314988	-0.124201	-1.728017
6	4.774866	-2.564899	1.271334
1	3.399574	-1.052855	1.955958
6	5.024257	-3.562975	0.330298
1	4.257819	-4.625353	-1.386786
1	5.512850	-2.343522	2.045280
1	5.959660	-4.126037	0.362974
6	-2.645228	-2.179834	-0.037099
6	-2.598420	-3.232817	-0.970895
6	-3.867183	-1.958620	0.625237
6	-3.723068	-4.003232	-1.256193
1	-1.663299	-3.456587	-1.486827
6	-4.985893	-2.745928	0.366364
1	-3.951782	-1.162495	1.365786
6	-4.920026	-3.763930	-0.584161
1	-3.660704	-4.802969	-1.997431
1	-5.917866	-2.557875	0.904007
1	-5.801356	-4.373605	-0.797131
6	-2.550392	0.846173	0.334705
6	-3.076380	1.254985	1.559963
6	-3.219344	1.161076	-0.846627
6	-4.268251	1.975698	1.603807
1	-2.545445	0.997817	2.479623
6	-4.410573	1.880391	-0.801147
1	-2.799776	0.835189	-1.800080
6	-4.938684	2.289682	0.422659
1	-4.675581	2.291972	2.566460
1	-4.930129	2.121868	-1.730638

1	-5.873705	2.852484	0.455655
6	0.080189	-2.096324	0.215322
8	0.104690	-3.310698	0.313474

10-P-1B

SCF energy = -1450.829064660 a.u.

7	-0.176145	-1.265530	-0.334767
5	-1.418060	-0.555375	-0.098113
6	-1.100634	1.011130	-0.149326
5	0.850376	-0.286992	-0.531889
6	0.230554	1.163561	-0.392370
6	-2.087880	2.097662	0.034770
6	-2.182472	3.149004	-0.889688
6	-2.965862	2.086470	1.128612
6	-3.124342	4.160213	-0.722057
1	2.189572	1.794485	-2.142495
6	-3.899530	3.105640	1.303004
1	-2.915166	1.268099	1.850456
6	-3.983828	4.144336	0.376874
1	-3.187044	4.967230	-1.455403
1	-4.571339	3.083535	2.163968
1	-4.722216	4.938452	0.507924
6	-2.798447	-1.228534	0.176825
6	-2.914253	-2.395931	0.953857
6	-3.976294	-0.672464	-0.354048
6	-4.154931	-2.978745	1.196511
1	-2.018858	-2.857478	1.377433
6	-5.216997	-1.268434	-0.137555
1	-3.921956	0.242433	-0.949326
6	-5.307733	-2.419654	0.643760
1	-4.223280	-3.879717	1.810182
1	-6.117023	-0.826989	-0.571024
1	-6.280447	-2.883680	0.823361
6	1.015916	2.415887	-0.435323
6	2.018096	2.581352	-1.403741
6	0.821776	3.437609	0.507728
6	2.786688	3.742635	-1.443338
1	-1.506415	3.165971	-1.747474
6	1.598722	4.591730	0.474822
1	0.056007	3.320038	1.277259
6	2.580865	4.750924	-0.503337
1	3.555753	3.855663	-2.210546
1	1.437327	5.373350	1.220649
1	3.188210	5.658449	-0.528709
6	3.456922	-0.601632	0.097632
6	3.218918	-0.075750	1.371979
6	4.731441	-1.075550	-0.233288
6	4.246058	-0.024651	2.311900
1	2.228031	0.313471	1.627209
6	5.754548	-1.031769	0.706868
1	4.890342	-1.478442	-1.235925
6	5.511914	-0.505756	1.978852
1	4.061844	0.395202	3.302730
1	6.748207	-1.407589	0.453408
1	6.317370	-0.469890	2.715853
6	0.013718	-2.670629	-0.416359
6	0.954298	-3.301355	0.403181
6	-0.734812	-3.435489	-1.315604
6	1.144806	-4.679507	0.320845
1	1.536298	-2.706206	1.110760
6	-0.551169	-4.813328	-1.384794
1	-1.463623	-2.940092	-1.959469
6	0.389842	-5.441278	-0.568865
1	1.886056	-5.159418	0.963466
1	-1.144833	-5.400905	-2.088310
1	0.536887	-6.521417	-0.630415
6	2.356615	-0.658031	-0.908382
8	2.564583	-0.966503	-2.071483

10-P-1C

SCF energy = -1450.809124800 a.u.

7	-1.274255	-1.285758	-0.286065
5	-1.193478	0.111971	0.037277
6	0.205452	0.871279	-0.070650
5	1.289633	-1.362141	-0.194947
6	1.376639	0.198357	-0.282055
6	0.175052	2.360996	0.014490
6	0.559742	3.140964	-1.083455
6	-0.260939	3.005818	1.178312
6	0.509239	4.531304	-1.018544
1	3.182136	-0.310035	-2.201096
6	-0.295095	4.396001	1.250004
1	-0.581396	2.409637	2.035811
6	0.085401	5.163475	0.149757
1	0.808051	5.124716	-1.885542
1	-0.633004	4.882330	2.167549
1	0.048402	6.253768	0.202420
6	-2.520157	0.875142	0.408147
6	-3.349287	0.412347	1.443102
6	-2.927757	2.022566	-0.291550

6	-4.528703	1.074347	1.776416
1	-3.073088	-0.489703	1.995832
6	-4.119941	2.672874	0.018003
1	-2.303119	2.420890	-1.094876
6	-4.920166	2.204117	1.058775
1	-5.152144	0.699535	2.591278
1	-4.420025	3.557056	-0.548862
1	-5.850885	2.718084	1.310055
6	2.695237	0.870421	-0.459231
6	3.522295	0.472998	-1.518131
6	3.163516	1.859855	0.417745
6	4.769584	1.062345	-1.713159
1	0.905705	2.648488	-1.995116
6	4.416308	2.437690	0.233689
1	2.540754	2.176095	1.256352
6	5.221682	2.046298	-0.836040
1	5.394698	0.743875	-2.550176
1	4.765236	3.202210	0.931268
1	6.201954	2.505106	-0.982234
6	2.418548	-2.281101	0.360793
6	2.423849	-3.670664	0.112805
6	3.458676	-1.759318	1.159991
6	3.429246	-4.490407	0.617825
1	1.628008	-4.099328	-0.498101
6	4.449549	-2.580593	1.687601
1	3.494072	-0.691005	1.378402
6	4.440927	-3.947864	1.409593
1	3.419151	-5.560742	0.400207
1	5.237534	-2.152558	2.310985
1	5.225404	-4.593018	1.812828
6	-2.530976	-1.954468	-0.478106
6	-2.890564	-3.005887	0.365053
6	-3.398655	-1.546541	-1.489252
6	-4.122435	-3.634680	0.205894
1	-2.199481	-3.325045	1.147760
6	-4.634027	-2.171079	-1.641298
1	-3.106523	-0.727448	-2.148743
6	-4.999876	-3.215076	-0.793641
1	-4.400679	-4.454883	0.871089
1	-5.314667	-1.838827	-2.427772
1	-5.968541	-3.704658	-0.913448
6	-0.116149	-2.016345	-0.627823
8	-0.205728	-3.071802	-1.220676

11

SCF energy = -3815.796727690 a.u.

6	-0.669225	-1.106840	-0.004726
6	0.684638	-1.098040	-0.001229
5	1.162574	0.413520	0.008641
5	-1.166951	0.398132	-0.012850
7	-0.007780	1.249636	-0.003194
6	2.634149	0.942562	0.014840
6	3.097810	1.845804	0.969104
6	3.547109	0.499456	-0.940312
6	4.413483	2.298347	0.984103
9	-1.099049	2.704321	2.082281
6	4.869434	0.931710	-0.960850
9	3.149284	-0.349761	-1.881881
6	5.298474	1.837009	0.009608
9	4.829698	3.148023	1.904323
9	5.711291	0.503711	-1.882702
9	6.545945	2.257418	0.006850
6	1.567484	-2.275341	-0.020640
6	1.460001	-3.270005	-0.995367
6	2.572915	-2.416005	0.938267
6	2.321707	-4.363344	-1.018089
9	0.540230	-3.177681	-1.944218
6	3.445437	-3.498514	0.936467
9	2.694403	-1.505347	1.896220
6	3.315684	-4.477016	-0.048073
9	2.206519	-5.287194	-1.954375
9	4.381509	-3.611115	1.860749
9	4.134128	-5.509616	-0.061588
6	-0.017277	2.655148	-0.002861
6	-0.581270	3.363996	1.058017
6	0.537051	3.372398	-1.063165
6	-0.603746	4.755385	1.061842
9	2.277130	2.278010	1.920825
6	0.540041	4.764004	-1.066238
9	1.064538	2.720517	-2.087470
6	-0.036742	5.455411	-0.001985
9	-1.142980	5.412707	2.071572
9	1.070082	5.429383	-2.075581
9	-0.045926	6.773675	-0.001511
6	-2.645552	0.907288	-0.016048
6	-3.549508	0.452786	0.942353
6	-3.123965	1.804243	-0.968956
6	-4.877460	0.867188	0.966602
9	-3.137431	-0.389463	1.884007

6	-4.445612	2.239143	-0.980078
9	-2.311606	2.247481	-1.922722
6	-5.321427	1.766257	-0.002898
9	-5.710703	0.428483	1.891249
9	-4.875956	3.083084	-1.899086
9	-6.574335	2.170160	0.003509
6	-1.536812	-2.295379	0.016515
6	-2.539780	-2.450935	-0.942604
6	-1.418015	-3.285443	0.994429
6	-3.398891	-3.544116	-0.938364
9	-2.671767	-1.544113	-1.902805
6	-2.266130	-4.389248	1.019684
9	-0.500562	-3.178575	1.943942
6	-3.257786	-4.518034	0.049153
9	-4.332832	-3.670801	-1.862992
9	-2.140582	-5.308729	1.958958
9	-4.063358	-5.560684	0.064936

11-TS-0

SCF energy = -7631.530941780 a.u.

ν = -101.8812 cm^{-1}

6	-2.487695	-0.891933	0.240780
6	-2.988620	0.358044	0.428684
5	-0.990563	-0.888765	0.743199
5	-1.820089	1.398712	0.543390
7	-0.517757	0.600892	0.857248
6	2.895181	0.003608	-0.202205
6	2.108771	1.105962	-0.175096
5	2.095041	-1.248944	-0.640739
5	0.575412	0.680078	-0.611834
7	0.695272	-0.873270	-0.911330
6	2.826108	-2.650611	-0.861072
6	3.131196	-3.254027	-2.081337
6	3.351654	-3.292962	0.264290
6	3.859969	-4.438277	-2.182784
9	2.775290	-2.696724	-3.232917
6	4.076437	-4.476988	0.209194
9	3.154372	-2.772806	1.472594
6	4.328153	-5.058845	-1.030352
9	4.116042	-4.962884	-3.367580
9	4.522148	-5.046385	1.314116
9	5.014780	-6.179894	-1.110692
6	4.354583	-0.014608	0.044649
6	4.916602	0.313513	1.278294
6	5.229280	-0.392890	-0.976383
6	6.289585	0.256192	1.499344
9	4.142348	0.693692	2.285673
6	6.605205	-0.460103	-0.782198
9	2.209825	2.773339	2.296398
6	7.136785	-0.130846	0.463309
9	6.790653	0.569390	2.680057
9	7.406149	-0.820111	-1.767861
9	8.438557	-0.186050	0.660750
6	2.828478	2.402275	0.038395
6	3.637119	2.852828	-1.013975
6	2.883697	3.141690	1.215423
6	4.424271	3.991873	-0.922612
9	3.633108	2.196731	-2.166628
6	3.664299	4.291736	1.335500
9	4.748346	-0.691865	-2.175100
6	4.443253	4.717055	0.267586
9	5.154838	4.387784	-1.949726
9	3.680486	4.959138	2.476167
9	5.189396	5.798876	0.374663
6	-0.203609	1.554642	-1.777781
6	-1.282403	1.084315	-2.540569
6	0.156821	2.864674	-2.122865
6	-1.911897	1.788538	-3.565614
9	-1.839752	-0.094025	-2.291052
6	-0.456169	3.619947	-3.115454
9	1.069293	3.534683	-1.427571
6	-1.499898	3.079114	-3.857512
9	-2.919139	1.244007	-4.217724
9	-0.087836	4.874021	-3.313465
9	-2.101830	3.790553	-4.784419
6	0.337036	-1.438335	-2.180880
6	0.817237	-0.882736	-3.373325
6	-0.422984	-2.598062	-2.296351
6	0.467751	-1.387102	-4.618786
9	1.664175	0.137586	-3.328495
6	-0.758630	-3.142783	-3.531291
9	-0.938179	-3.170999	-1.218772
6	-0.307022	-2.540983	-4.699774
9	0.930873	-0.821071	-5.717849
9	-1.520327	-4.219107	-3.586722
9	-0.624364	-3.046899	-5.874307
6	-0.681304	-1.973633	1.878532
6	0.046556	-3.157354	1.771669
6	-1.251194	-1.746138	3.138026
6	0.246710	-4.030466	2.837516

9	0.641555	-3.495860	0.640791
6	-1.089898	-2.599157	4.224048
9	-1.982008	-0.653746	3.352677
6	-0.332230	-3.756532	4.071823
9	0.980454	-5.114883	2.672659
9	-1.648530	-2.316038	5.385759
9	-0.159686	-4.576434	5.086017
6	-3.387493	-2.077073	0.087806
6	-4.068951	-2.583145	1.200152
6	-3.671376	-2.684608	-1.137537
6	-4.917817	-3.683227	1.122882
9	-3.932272	-2.008591	2.387597
6	-4.515436	-3.786657	-1.243379
9	-4.236451	1.315219	2.748673
6	-5.145072	-4.288740	-0.109022
9	-5.523788	-4.132411	2.206605
9	-4.740233	-4.335022	-2.421369
9	-5.952069	-5.325000	-0.200155
6	-4.449528	0.602412	0.516730
6	-5.318306	0.322174	-0.540647
6	-5.013299	1.048505	1.711467
6	-6.693918	0.478783	-0.418805
9	-4.833951	-0.072686	-1.706006
6	-6.388780	1.214196	1.858603
9	-3.157991	-2.218691	-2.259839
6	-7.231032	0.922057	0.789453
9	-7.491213	0.216651	-1.437576
9	-6.893303	1.631734	3.004461
9	-8.533354	1.072151	0.914785
6	-1.928998	2.919408	0.114752
6	-1.028706	3.916313	0.509767
6	-2.915261	3.352932	-0.781878
6	-1.098582	5.237545	0.089716
9	-0.005489	3.609444	1.294711
6	-3.020506	4.666024	-1.232360
9	-3.772702	2.494783	-1.320349
6	-2.105269	5.617417	-0.794615
9	-0.201481	6.114781	0.491398
9	-3.951019	4.993855	-2.107602
9	-2.177938	6.855284	-1.224995
6	0.060346	0.863015	2.171445
6	-0.595683	1.706545	3.067436
6	1.143699	0.164780	2.709867
6	-0.151482	1.971225	4.351693
9	-1.750863	2.255581	2.694273
6	1.605836	0.385646	4.005436
9	1.755843	-0.793159	2.040313
6	0.967324	1.299078	4.832430
9	-0.816019	2.807604	5.123067
9	2.631602	-0.308455	4.452853
9	1.400881	1.513997	6.054718

11-I-0

SCF energy = -7631.540517780 a.u.

6	-2.316298	-0.952385	0.100348
6	-2.919313	0.240422	0.349085
5	-0.730255	-0.933450	0.503149
5	-1.861886	1.358856	0.542349
7	-0.499407	0.674757	0.865541
6	2.830399	0.052260	-0.251031
6	2.062111	1.165822	-0.194439
5	2.005318	-1.226897	-0.461437
5	0.485448	0.797646	-0.472753
7	0.519675	-0.854850	-0.679446
6	2.773731	-2.624663	-0.591964
6	3.106069	-3.275119	-1.782639
6	3.371630	-3.168394	0.551993
6	3.925861	-4.402415	-1.837001
9	2.691517	-2.826614	-2.961856
6	4.189674	-4.290448	0.542066
9	3.151649	-2.616352	1.739329
6	4.467358	-4.919798	-0.668087
9	4.195924	-4.966177	-2.999878
9	4.697115	-4.758839	1.666584
9	5.240477	-5.984108	-0.703651
6	4.301736	0.023770	-0.080804
6	4.917322	0.380868	1.119393
6	5.124843	-0.408764	-1.121696
6	6.296971	0.301442	1.287362
9	4.190245	0.807342	2.142405
6	6.505471	-0.500944	-0.979256
9	2.150051	2.889378	2.186999
6	7.092819	-0.139478	0.232050
9	6.851912	0.643373	2.434797
9	7.258198	-0.915452	-1.980961
9	8.399586	-0.216667	0.379254
6	2.796177	2.458698	-0.047104
6	3.590364	2.885768	-1.117319
6	2.830976	3.238456	1.105493
6	4.355169	4.043937	-1.062901

9	3.600006	2.191703	-2.247643
6	3.592001	4.402602	1.188375
9	4.586977	-0.747497	-2.285078
6	4.360630	4.806951	0.102800
9	5.077180	4.419465	-2.102998
9	3.598046	5.109220	2.303983
9	5.086749	5.904385	0.173897
6	-0.269505	1.645444	-1.688141
6	-1.273630	1.168199	-2.543990
6	0.038308	2.991687	-1.935320
6	-1.884747	1.910307	-3.555241
9	-1.768381	-0.056253	-2.423270
6	-0.555401	3.778464	-2.913544
9	0.866064	3.663607	-1.139412
6	-1.528867	3.235783	-3.744310
9	-2.821647	1.358429	-4.299058
9	-0.239499	5.057950	-3.014525
9	-2.116226	3.973359	-4.659846
6	0.357711	-1.409315	-2.017939
6	0.902208	-0.793218	-3.155761
6	-0.262547	-2.640430	-2.221176
6	0.712132	-1.310184	-4.431350
9	1.645323	0.298476	-3.062821
6	-0.438337	-3.187467	-3.485889
9	-0.790442	-3.295871	-1.203373
6	0.054563	-2.523293	-4.601713
9	1.220782	-0.680812	-5.472512
9	-1.085267	-4.327527	-3.616976
9	-0.107338	-3.029276	-5.804375
6	-0.584040	-1.963050	1.768724
6	0.083919	-3.187467	1.778295
6	-1.241580	-1.680135	2.975308
6	0.183550	-4.020310	2.889515
9	0.710115	-3.632563	0.695774
6	-1.179977	-2.482911	4.110166
9	-1.994235	-0.589819	3.104355
6	-0.455706	-3.668399	4.071169
9	0.877347	-5.142240	2.812822
9	-1.818716	-2.128900	5.210406
9	-0.380772	-4.444268	5.132288
6	-3.181616	-2.165278	-0.100069
6	-3.883341	-2.708115	0.983575
6	-3.445447	-2.750797	-1.340447
6	-4.719824	-3.814725	0.864657
9	-3.793365	-2.162929	2.188986
6	-4.276026	-3.856779	-1.491186
9	-4.274497	1.031021	2.680213
6	-4.922442	-4.393565	-0.383234
9	-5.341458	-4.292411	1.927546
9	-4.469868	-4.377279	-2.688417
9	-5.717509	-5.435300	-0.513937
6	-4.397730	0.375357	0.422084
6	-5.233547	0.087292	-0.659809
6	-5.011061	0.738936	1.620590
6	-6.618389	0.139516	-0.555011
9	-4.710578	-0.218347	-1.836739
6	-6.397003	0.802886	1.751557
9	-2.912639	-2.262596	-2.447665
6	-7.202884	0.495102	0.659742
9	-7.380864	-0.133755	-1.598595
9	-6.944558	1.143110	2.904107
9	-8.515141	0.550092	0.769034
6	-2.084237	2.892730	0.187296
6	-1.273272	3.942293	0.638552
6	-3.084935	3.286245	-0.712091
6	-1.447993	5.271195	0.276531
9	-0.229123	3.690315	1.417694
6	-3.292556	4.605720	-1.106502
9	-3.856570	2.389909	-1.313794
6	-2.469169	5.608557	-0.607980
9	-0.630713	6.200282	0.730891
9	-4.233310	4.894343	-1.985471
9	-2.637222	6.855857	-0.983551
6	0.021292	0.932590	2.200721
6	-0.685778	1.727320	3.105680
6	1.129541	0.286282	2.748905
6	-0.253555	2.007115	4.391464
9	-1.871844	2.211408	2.752185
6	1.590754	0.530666	4.040357
9	1.789520	-0.641157	2.076936
6	0.901665	1.399925	4.872616
9	-0.967753	2.796548	5.168761
9	2.658658	-0.105882	4.476982
9	1.322515	1.636352	6.095915

11-TS-1

SCF energy = -3928.983545160 a.u.

ν = -138.8291 cm^{-1}

7	1.160817	0.424438	0.135117
5	-0.007957	1.228524	0.017435

6	-1.267654	0.277585	0.069737
5	0.757732	-0.977013	0.299526
6	-0.839332	-1.002992	0.192541
6	-2.669130	0.722716	-0.007464
6	-3.610229	0.365902	0.960450
6	-3.095084	1.551161	-1.047553
6	-4.926649	0.814496	0.899015
9	-0.739246	-3.125429	2.086180
6	-4.403617	2.014036	-1.130342
9	-2.240577	1.893577	-2.003215
6	-5.322873	1.640039	-0.151202
9	-5.797539	0.467927	1.829653
9	-4.782798	2.789235	-2.129855
9	-6.567643	2.068339	-0.218794
6	-0.009197	2.790740	-0.111992
6	0.682929	3.462179	-1.116634
6	-0.746067	3.566230	0.780144
6	0.651044	4.848065	-1.240477
9	1.381215	2.771337	-2.011742
6	-0.800927	4.953796	0.691973
9	-1.413145	2.972530	1.766416
6	-0.095756	5.592553	-0.327758
9	1.311439	5.459601	-2.206431
9	-1.500691	5.664502	1.557185
9	-0.134653	6.905278	-0.428770
6	-1.703677	-2.198123	0.139445
6	-1.606924	-3.223328	1.082164
6	-2.627636	-2.380693	-0.896844
6	-2.398134	-4.365824	1.027540
9	-3.256424	-0.402122	1.982318
6	-3.431205	-3.514431	-0.975308
9	-2.736614	-1.483149	-1.863822
6	-3.319285	-4.509487	-0.006888
9	-2.284533	-5.305074	1.948715
9	-4.287923	-3.656792	-1.969626
9	-4.076387	-5.585555	-0.074322
6	1.736755	-2.179544	-0.009694
6	2.926774	-2.423614	0.675839
6	1.472687	-3.006765	-1.101726
6	3.794966	-3.455859	0.333067
9	3.274052	-1.657673	1.711162
6	2.316538	-4.047270	-1.479753
9	0.393521	-2.797063	-1.849056
6	3.484784	-4.270188	-0.754748
9	4.905694	-3.660645	1.016986
9	2.029982	-4.806864	-2.520372
9	4.298528	-5.246717	-1.098382
6	2.486867	0.886460	0.143958
6	3.357054	0.599962	-0.909007
6	2.971024	1.633816	1.217799
6	4.678887	1.035101	-0.887497
9	2.921571	-0.088179	-1.950852
6	4.284687	2.090826	1.249092
9	2.163562	1.909074	2.234109
6	5.142206	1.781841	0.194597
9	5.491300	0.753433	-1.889090
9	4.725110	2.796841	2.274154
9	6.391778	2.201396	0.218071
6	0.791765	-0.972062	2.567239
8	0.683210	-0.779102	3.669440

11-I-1

SCF energy = -3928.992805540 a.u.

7	-1.230527	0.126228	-0.307168
5	-0.292727	1.163116	-0.104021
6	1.151047	0.544184	-0.155112
5	-0.499410	-1.185611	-0.603120
6	1.058666	-0.791645	-0.374188
6	2.400981	1.304498	0.022922
6	3.427502	1.261239	-0.922494
6	2.579179	2.135623	1.130484
6	4.587951	2.016376	-0.777205
9	1.498614	-2.787613	-2.332696
6	3.728475	2.900324	1.298496
9	1.641184	2.188283	2.066622
6	4.737533	2.837118	0.338625
9	5.541415	1.963736	-1.690203
9	3.875457	3.671380	2.360524
9	5.833652	3.554603	0.487233
6	-0.665237	2.677472	0.090338
6	-1.517366	3.122242	1.097343
6	-0.123433	3.643447	-0.753957
6	-1.825194	4.468812	1.269462
9	-2.048470	2.248282	1.946431
6	-0.406776	4.999048	-0.616328
9	0.686360	3.269701	-1.742288
6	-1.265402	5.407637	0.403469
9	-2.633819	4.863351	2.236351
9	0.117370	5.891855	-1.436619
9	-1.549317	6.686254	0.549646

6	2.181187	-1.747335	-0.328230
6	2.352058	-2.726988	-1.307770
6	3.092206	-1.757956	0.735437
6	3.384307	-3.656511	-1.271161
9	3.306467	0.502025	-2.004286
6	4.137510	-2.675972	0.797200
9	2.967020	-0.906781	1.739305
6	4.287742	-3.625181	-0.210959
9	3.514161	-4.556053	-2.228679
9	4.979108	-2.658939	1.813690
9	5.274053	-4.496743	-0.158485
6	-1.099320	-2.538699	0.012674
6	-2.134305	-3.236190	-0.602301
6	-0.688179	-3.010662	1.257537
6	-2.735058	-4.358370	-0.041469
9	-2.592975	-2.815938	-1.789231
6	-1.258289	-4.131958	1.854834
9	0.259657	-2.373331	1.934192
6	-2.286106	-4.807401	1.198825
9	-3.713799	-4.990635	-0.663323
9	-0.843515	-4.553781	3.035004
9	-2.836404	-5.868204	1.753628
6	-2.626690	0.266838	-0.341985
6	-3.427474	-0.212067	0.698701
6	-3.256332	0.892582	-1.420232
6	-4.812528	-0.078751	0.660432
9	-2.869085	-0.781444	1.751791
6	-4.638457	1.045798	-1.469477
9	-2.518337	1.350938	-2.423974
6	-5.418393	0.549692	-0.426480
9	-5.554229	-0.536305	1.651900
9	-5.211198	1.641737	-2.499171
9	-6.729495	0.680076	-0.464822
6	-0.592897	-1.218753	-2.254016
8	-0.617996	-1.055020	-3.363440

11-TS-2

SCF energy = -3928.945734820 a.u.

ν = -287.7607 cm^{-1}

7	-1.262765	-0.973555	-0.406503
5	-1.161709	0.417783	-0.242323
6	0.336741	0.884433	-0.435614
5	0.037167	-1.651265	-0.703658
6	1.150057	0.015306	-1.084741
6	0.843135	2.138168	0.160879
6	1.570351	3.079614	-0.572359
6	0.563030	2.433587	1.497661
6	2.011761	4.266665	0.005167
9	2.814541	0.510715	-3.394124
6	0.996546	3.610875	2.097297
9	-0.123495	1.566280	2.227404
6	1.726890	4.529150	1.344051
9	2.692472	5.144460	-0.707322
9	0.729875	3.859163	3.365362
9	2.145128	5.648069	1.897692
6	-2.361457	1.383356	0.053727
6	-3.324652	1.107061	1.024063
6	-2.486010	2.590257	-0.634104
6	-4.371030	1.981963	1.302646
9	-3.251777	-0.012249	1.733196
6	-3.517822	3.489780	-0.385195
9	-1.601155	2.904430	-1.575150
6	-4.464242	3.176816	0.590027
9	-5.266313	1.695489	2.229934
9	-3.612755	4.621676	-1.058254
9	-5.449255	4.014098	0.840245
6	2.627753	0.099475	-1.077439
6	3.393445	0.307820	-2.229924
6	3.312705	-0.019093	0.139131
6	4.785705	0.345604	-2.177305
9	1.834190	2.871820	-1.851043
6	4.700654	0.008708	0.209821
9	2.638517	-0.154941	1.273724
6	5.439600	0.192560	-0.957366
9	5.486837	0.545607	-3.276602
9	5.315770	-0.121518	1.370860
9	6.754487	0.228723	-0.904337
6	0.863409	-2.541968	0.282305
6	1.771920	-3.497346	-0.182619
6	0.768439	-2.384810	1.669535
6	2.539265	-4.279116	0.675159
9	1.926261	-3.685986	-1.486859
6	1.518663	-3.150135	2.554769
9	-0.024300	-1.461756	2.183677
6	2.406031	-4.100635	2.051215
9	3.383943	-5.177942	0.203250
9	1.413779	-2.975259	3.858850
9	3.125198	-4.828340	2.878502
6	-2.469216	-1.659389	-0.652749
6	-2.891381	-2.716407	0.157037

6	-3.284310	-1.287363	-1.727528
6	-4.092667	-3.376323	-0.088153
9	-2.153030	-3.100714	1.182695
6	-4.493998	-1.927654	-1.977303
9	-2.900934	-0.303940	-2.527465
6	-4.895709	-2.979835	-1.155697
9	-4.476959	-4.369101	0.691643
9	-5.251004	-1.556086	-2.992331
9	-6.035483	-3.598457	-1.387931
6	0.557193	-1.260295	-2.072110
8	0.755802	-1.270104	-3.228851

11-TS-2B

SCF energy = -3928.936473730 a.u.

ν = -461.6499 cm^{-1}

7	1.239622	-0.349729	0.467226
5	0.587433	0.838398	0.031914
6	-0.961197	0.593314	-0.004545
5	0.184565	-1.323162	0.797357
6	-1.227769	-0.650466	0.460555
6	-1.943251	1.628152	-0.374680
6	-2.938965	2.081532	0.492407
6	-1.852073	2.234929	-1.628861
6	-3.824748	3.089043	0.118392
9	-2.116223	-1.591160	2.954315
6	-2.722043	3.244460	-2.024557
9	-0.912956	1.835399	-2.477592
6	-3.716511	3.668441	-1.144204
9	-4.758030	3.503899	0.955697
9	-2.619595	3.794526	-3.220648
9	-4.552118	4.621752	-1.505037
6	1.292022	2.227192	-0.181892
6	2.255597	2.457995	-1.159479
6	0.921060	3.311161	0.611530
6	2.836982	3.708625	-1.348775
9	2.630026	1.468545	-1.961776
6	1.480940	4.575885	0.455895
9	0.009187	3.142205	1.564930
6	2.445832	4.768943	-0.532104
9	3.745315	3.899658	-2.287810
9	1.114454	5.581979	1.228348
9	2.988574	5.958011	-0.695934
6	-2.595507	-1.155118	0.691981
6	-2.990190	-1.594908	1.955223
6	-3.562761	-1.145746	-0.316612
6	-4.289812	-2.018005	2.216685
9	-3.045647	1.575435	1.711655
6	-4.868177	-1.563292	-0.081037
9	-3.241063	-0.764414	-1.543914
6	-5.233147	-1.997895	1.192428
9	-4.634467	-2.420083	3.426053
9	-5.759504	-1.557918	-1.055644
9	-6.468485	-2.394085	1.424583
6	0.503314	-3.105124	-0.124238
6	1.810626	-3.551993	-0.326343
6	-0.460323	-3.555057	-1.025672
6	2.183554	-4.316197	-1.422392
9	2.748242	-3.256410	0.568053
6	-0.123674	-4.319321	-2.140578
9	-1.739466	-3.260237	-0.866880
6	1.201853	-4.702410	-2.335157
9	3.433563	-4.698649	-1.590257
9	-1.051585	-4.704711	-2.995280
9	1.526527	-5.435441	-3.375469
6	2.607462	-0.358055	0.810046
6	3.585890	-0.727353	-0.113076
6	3.017273	0.074243	2.071948
6	4.937136	-0.677616	0.212025
9	3.228486	-1.171930	-1.305879
6	4.364934	0.129993	2.416076
9	2.104418	0.447572	2.955161
6	5.326068	-0.242744	1.478235
9	5.850131	-1.044606	-0.667687
9	4.735356	0.544128	3.613659
9	6.605121	-0.193081	1.792646
6	0.299120	-2.586803	1.626924
8	0.315399	-3.400795	2.452317

11-P-1

SCF energy = -3928.996077950 a.u.

7	-1.304736	-0.026852	-0.015370
5	-0.032683	0.647277	0.013871
6	1.312626	-0.175831	0.036120
5	-1.362600	-1.449875	-0.015200
6	1.322902	-1.528286	0.016998
6	2.586400	0.587462	0.060310
6	3.507137	0.520789	-0.986121
6	2.884313	1.426035	1.134891
6	4.681267	1.268883	-0.969068
9	2.070634	-3.242797	-2.067019

6	4.047711	2.186062	1.173983
9	2.038419	1.504691	2.153642
6	4.951948	2.100374	0.116112
9	5.535287	1.197511	-1.972875
9	4.305729	2.970387	2.203713
9	6.061411	2.809771	0.140798
6	0.019786	2.224783	-0.002624
6	-0.489144	2.996073	1.038333
6	0.614188	2.901311	-1.064521
6	-0.413355	4.385396	1.038624
9	-1.051744	2.397194	2.083093
6	0.708294	4.288913	-1.103798
9	1.103934	2.207333	-2.087159
6	0.188356	5.029557	-0.042376
9	-0.898671	5.092368	2.041515
9	1.272544	4.904084	-2.125660
9	0.266186	6.343580	-0.060352
6	2.560848	-2.340744	0.047064
6	2.870164	-3.188981	-1.016971
6	3.448773	-2.284342	1.121692
6	4.027110	-3.960794	-1.017108
9	3.264293	-0.246409	-2.036327
6	4.613504	-3.046058	1.141316
9	3.190683	-1.499411	2.158105
6	4.899632	-3.887377	0.067747
9	4.308813	-4.750067	-2.036561
9	5.441213	-2.980251	2.168545
9	5.999358	-4.612281	0.076825
6	-2.719128	-2.237370	-0.044139
6	-3.618730	-2.145245	-1.102640
6	-3.060781	-3.073668	1.016094
6	-4.816890	-2.852054	-1.121845
9	-3.326068	-1.372117	-2.146372
6	-4.251877	-3.792892	1.035645
9	-2.249680	-3.168287	2.060280
6	-5.129470	-3.678328	-0.042301
9	-5.650191	-2.751561	-2.141375
9	-4.561050	-4.569027	2.056975
9	-6.260944	-4.352057	-0.040801
6	-2.508062	0.730607	-0.046949
6	-3.374051	0.732436	1.045472
6	-2.847135	1.479154	-1.172923
6	-4.557816	1.463476	1.018563
9	-3.071435	0.027308	2.121457
6	-4.018693	2.228422	-1.209953
9	-2.041317	1.483560	-2.221139
6	-4.876794	2.215541	-0.111176
9	-5.371612	1.455238	2.056643
9	-4.324555	2.937859	-2.279144
9	-5.991713	2.915803	-0.140815
6	0.021349	-2.275341	0.004734
8	0.008446	-3.488576	0.008149

11-P-1B

SCF energy = -3928.975384930 a.u.

7	0.845731	0.547480	0.372201
5	-0.419387	1.187175	0.135604
6	-1.534546	0.057846	0.141715
5	0.589431	-0.836912	0.673992
6	-0.948045	-1.123368	0.453670
6	-2.959560	0.273844	-0.153776
6	-3.975386	-0.142972	0.709346
6	-3.334971	0.948952	-1.317251
6	-5.316228	0.102674	0.425463
9	-0.916245	-2.832115	2.676697
6	-4.666450	1.206646	-1.622518
9	-2.398422	1.344289	-2.171646
6	-5.660661	0.777870	-0.743998
9	-6.260278	-0.292515	1.259421
9	-4.993996	1.838999	-2.734293
9	-6.927530	1.012052	-1.020028
6	-0.628034	2.726340	-0.033459
6	0.123522	3.487744	-0.927939
6	-1.612943	3.392626	0.696314
6	-0.085758	4.852301	-1.100648
9	1.053131	2.901890	-1.674340
6	-1.848848	4.756511	0.554062
9	-2.346195	2.720975	1.576519
6	-1.077888	5.485005	-0.351596
9	0.634433	5.546376	-1.961505
9	-2.780921	5.362672	1.264618
9	-1.287578	6.775530	-0.500283
6	-1.614767	-2.436871	0.470409
6	-1.557580	-3.255151	1.600377
6	-2.316110	-2.912894	-0.641010
6	-2.173580	-4.502305	1.634345
9	-3.677822	-0.762601	1.840736
6	-2.937840	-4.158133	-0.630890
9	-2.383926	-2.188338	-1.748665
6	-2.868594	-4.951720	0.512655

9	-2.114152	-5.253670	2.717874
9	-3.587495	-4.592128	-1.695966
9	-3.457111	-6.130698	0.531614
6	2.845241	-2.175314	0.226636
6	4.206866	-1.962185	0.457158
6	2.458230	-2.663008	-1.020588
6	5.148527	-2.213832	-0.537285
9	4.626361	-1.429040	1.588475
6	3.380784	-2.956313	-2.015847
9	1.162650	-2.817597	-1.281578
6	4.734396	-2.732092	-1.764053
9	6.426844	-1.969734	-0.325274
9	2.993987	-3.430638	-3.184007
9	5.623443	-2.991432	-2.697418
6	2.106521	1.154324	0.541547
6	3.111367	0.984810	-0.411680
6	2.404754	1.872394	1.699378
6	4.393780	1.478783	-0.202402
9	2.852920	0.318999	-1.526566
6	3.675614	2.401363	1.910916
9	1.467937	2.041817	2.616630
6	4.674837	2.192291	0.961692
9	5.342122	1.265311	-1.096735
9	3.942689	3.078293	3.010946
9	5.884786	2.670948	1.164036
6	1.804469	-1.721235	1.213681
8	1.950782	-1.842758	2.409589

12

SCF energy = -1319.307318250 a.u.

7	-0.587234	-0.263282	-0.045202
6	-3.206322	0.246129	-0.049721
6	-3.819608	-0.410615	-1.136495
6	-5.165944	-0.767444	-1.053757
1	-5.637591	-1.270715	-1.903785
6	-5.927901	-0.496128	0.087280
6	-5.305608	0.146801	1.157806
1	-5.882964	0.360388	2.062606
6	-3.959711	0.523066	1.105583
6	-3.020818	-0.730119	-2.377461
1	-2.234331	-1.471737	-2.162793
1	-2.520619	0.167223	-2.775219
1	-3.658311	-1.138468	-3.173720
6	-7.384238	-0.878950	0.141515
1	-7.800621	-0.743812	1.149601
1	-7.531707	-1.930225	-0.149050
1	-7.979622	-0.262932	-0.551181
6	-3.309521	1.185620	2.296333
1	-4.042612	1.415734	3.081754
1	-2.809481	2.124552	2.012436
1	-2.540305	0.531812	2.738623
6	1.107629	-1.760930	0.177073
6	1.693375	-3.004670	0.365810
1	2.779945	-3.108525	0.402893
6	0.848095	-4.111882	0.507357
1	1.286207	-5.101251	0.654503
6	-0.540035	-3.970599	0.466648
1	-1.175520	-4.850946	0.581717
6	-1.132098	-2.715389	0.285346
1	-2.216811	-2.592284	0.262957
6	-0.298724	-1.614247	0.140378
5	-1.692139	0.643354	-0.125330
5	0.672737	0.454899	-0.120944
6	3.124295	-0.300100	0.035302
6	3.718141	0.222990	1.195893
6	5.099048	0.421030	1.200959
1	5.570813	0.830350	2.099217
6	5.893187	0.106696	0.093609
6	5.269498	-0.408664	-1.043572
1	5.873085	-0.650470	-1.923251
6	3.887860	-0.615619	-1.097668
6	2.873302	0.567917	2.393277
1	2.192145	1.404787	2.171110
1	2.245441	-0.284159	2.694973
1	3.498953	0.857692	3.248060
6	7.384947	0.313140	0.143275
1	7.846297	0.172164	-0.843984
1	7.634633	1.325614	0.494772
1	7.856757	-0.399011	0.838796
6	3.225464	-1.139991	-2.343000
1	3.956282	-1.274515	-3.151565
1	2.731822	-2.107170	-2.161174
1	2.445625	-0.446494	-2.693289
6	-1.038783	2.087887	-0.297476
6	-1.636353	3.335925	-0.440858
1	-2.726750	3.427712	-0.450613
6	-0.834100	4.478335	-0.570258
1	-1.299159	5.460774	-0.682036
6	0.554901	4.370104	-0.558348
1	1.167693	5.269175	-0.658877

6	1.170624	3.118046	-0.420134
1	2.261685	3.042060	-0.414932
6	0.380341	1.981707	-0.292230
7	1.715858	-0.497986	0.010633

12-TS-1

SCF energy = -1432.481435990 a.u.

ν = -217.6670 cm^{-1}

7	-0.500886	-0.262051	0.429511
6	-3.125884	0.127950	-0.110459
6	-3.194233	-0.696810	-1.264099
6	-4.428545	-1.170603	-1.711475
1	-4.458163	-1.807172	-2.601495
6	-5.625046	-0.846973	-1.070249
6	-5.556238	0.008113	0.025648
1	-6.483176	0.307867	0.524330
6	-4.339125	0.510557	0.502684
6	-1.969180	-1.058848	-2.075402
1	-1.354352	-1.821274	-1.574110
1	-1.326213	-0.184805	-2.256168
1	-2.264480	-1.462920	-3.053417
6	-6.940865	-1.369952	-1.584411
1	-7.758677	-1.169780	-0.877967
1	-6.896718	-2.455939	-1.756753
1	-7.203384	-0.897893	-2.544646
6	-4.404079	1.461889	1.676434
1	-5.410307	1.894729	1.767629
1	-3.696641	2.297309	1.578557
1	-4.191931	0.952261	2.631573
6	1.231380	-1.723627	0.569699
6	1.853515	-2.940068	0.816976
1	2.934398	-3.045118	0.700516
6	1.054329	-4.018191	1.214686
1	1.522022	-4.985047	1.411568
6	-0.327423	-3.876846	1.361724
1	-0.927518	-4.735576	1.669826
6	-0.956330	-2.650806	1.119988
1	-2.036693	-2.532279	1.226205
6	-0.168808	-1.575241	0.725190
5	-1.679791	0.621691	0.333165
5	0.708990	0.437621	0.086027
6	3.165646	-0.301263	-0.103907
6	3.949700	0.404520	0.823477
6	5.300251	0.603939	0.534795
1	5.917760	1.156298	1.249386
6	5.883297	0.114848	-0.638135
6	5.074357	-0.579543	-1.539244
1	5.510474	-0.958440	-2.468175
6	3.714564	-0.793762	-1.297592
6	3.333703	0.938931	2.089204
1	2.619161	1.749132	1.872567
1	2.775112	0.153488	2.620271
1	4.101772	1.336605	2.766022
6	7.350837	0.324867	-0.907655
1	7.603270	0.106391	-1.954665
1	7.651245	1.361449	-0.693809
1	7.965841	-0.331515	-0.271267
6	2.848138	-1.510504	-2.297729
1	3.398786	-1.712239	-3.226198
1	2.482215	-2.470019	-1.900173
1	1.957363	-0.912778	-2.545155
6	-1.036411	2.044529	-0.086951
6	-1.654823	3.263675	-0.356511
1	-2.741254	3.364591	-0.275865
6	-0.883245	4.363719	-0.747543
1	-1.366965	5.321387	-0.954628
6	0.500290	4.245336	-0.883578
1	1.089693	5.111578	-1.193861
6	1.132869	3.022588	-0.637763
1	2.215129	2.929123	-0.765610
6	0.372178	1.924852	-0.239057
7	1.783854	-0.494981	0.164099
6	-1.630311	0.923302	2.374470
8	-1.112700	1.052472	3.368125

12-I-1

SCF energy = -1432.487855540 a.u.

7	0.484792	-0.327772	-0.721595
6	3.062141	0.113981	0.019002
6	2.930638	-0.242009	1.384861
6	4.054423	-0.635616	2.114131
1	3.929395	-0.903988	3.167834
6	5.328974	-0.688219	1.548522
6	5.456066	-0.308661	0.215389
1	6.446890	-0.318617	-0.248924
6	4.353357	0.092140	-0.548733
6	1.603407	-0.198348	2.105476
1	0.930008	-0.997561	1.761100
1	1.086012	0.758780	1.946094
1	1.746800	-0.326836	3.186891

6	6.515184	-1.141018	2.358871
1	7.461812	-0.944876	1.835878
1	6.462268	-2.222977	2.560257
1	6.551713	-0.630454	3.333052
6	4.615825	0.497380	-1.982041
1	5.694559	0.551006	-2.183391
1	4.203729	1.492008	-2.216849
1	4.199663	-0.227448	-2.701869
6	-1.223622	-1.788416	-0.410375
6	-1.829486	-3.033495	-0.297697
1	-2.894972	-3.113773	-0.070899
6	-1.033739	-4.170632	-0.474938
1	-1.489191	-5.159365	-0.389126
6	0.332295	-4.060396	-0.747804
1	0.931169	-4.965157	-0.870751
6	0.946814	-2.809233	-0.857906
1	2.017800	-2.716175	-1.050090
6	0.161025	-1.672894	-0.694625
5	1.726597	0.546890	-0.767417
5	-0.698362	0.424035	-0.424300
6	-3.124141	-0.265590	0.105604
6	-4.125412	-0.345182	-0.874852
6	-5.446761	-0.102034	-0.494847
1	-6.233470	-0.162625	-1.252624
6	-5.787132	0.223266	0.820932
6	-4.765678	0.296427	1.770742
1	-5.013703	0.542107	2.807570
6	-3.430812	0.053959	1.437334
6	-3.767699	-0.666525	-2.300822
1	-3.036110	0.057256	-2.691951
1	-3.304151	-1.661501	-2.385802
1	-4.655535	-0.644175	-2.947025
6	-7.216404	0.520323	1.195024
1	-7.404165	0.320623	2.259572
1	-7.455384	1.580418	1.010814
1	-7.919914	-0.082820	0.603242
6	-2.339151	0.135907	2.470727
1	-2.757662	0.270887	3.477062
1	-1.721562	-0.775079	2.468981
1	-1.661473	0.980245	2.267296
6	1.063973	2.028357	-0.477330
6	1.701047	3.262116	-0.355156
1	2.784854	3.342475	-0.483062
6	0.951000	4.398417	-0.038865
1	1.447677	5.365687	0.069415
6	-0.429549	4.305301	0.150818
1	-1.002276	5.201542	0.401097
6	-1.077590	3.074161	0.029631
1	-2.157330	3.004111	0.189701
6	-0.339511	1.932752	-0.289726
7	-1.770107	-0.504348	-0.253310
6	1.823831	0.674894	-2.396796
8	1.611086	0.808728	-3.497234

12-TS-2

SCF energy = -1432.462840440 a.u.

ν = -410.0795 cm^{-1}

7	0.501774	-0.415528	-0.872517
6	3.046894	0.018959	-0.050746
6	2.917500	-0.086003	1.356263
6	4.038523	-0.386994	2.129108
1	3.928591	-0.461681	3.215369
6	5.294966	-0.604553	1.556982
6	5.407171	-0.518524	0.171018
1	6.378946	-0.700027	-0.297688
6	4.309013	-0.211965	-0.640202
6	1.590959	0.109126	2.047709
1	0.880042	-0.683908	1.770298
1	1.129236	1.070211	1.777507
1	1.710273	0.085413	3.139330
6	6.480081	-0.943002	2.422423
1	7.408606	-0.994104	1.836979
1	6.339131	-1.916624	2.917733
1	6.618096	-0.191834	3.215223
6	4.516023	-0.160087	-2.136652
1	5.485318	-0.597732	-2.411611
1	4.501609	0.872323	-2.519204
1	3.734507	-0.712055	-2.679638
6	-1.192789	-1.868877	-0.436515
6	-1.792328	-3.108138	-0.247071
1	-2.856056	-3.179189	-0.009628
6	-0.990580	-4.247916	-0.360571
1	-1.437991	-5.233101	-0.213748
6	0.372952	-4.144220	-0.651855
1	0.977668	-5.050427	-0.725786
6	0.977460	-2.899661	-0.847211
1	2.043883	-2.813880	-1.064817
6	0.185315	-1.760344	-0.743263
5	1.782548	0.321562	-0.946237
5	-0.679296	0.336860	-0.594063

6	-3.086149	-0.326509	0.037074
6	-4.098548	-0.353587	-0.933981
6	-5.409185	-0.089780	-0.532034
1	-6.205454	-0.109848	-1.281789
6	-5.727372	0.200872	0.797635
6	-4.695528	0.214110	1.739088
1	-4.927370	0.428111	2.786564
6	-3.370528	-0.049767	1.382754
6	-3.761180	-0.653049	-2.369468
1	-3.053782	0.089615	-2.769609
1	-3.276834	-1.636699	-2.468844
1	-4.661367	-0.645675	-2.998581
6	-7.145643	0.518255	1.195785
1	-7.318205	0.323374	2.263669
1	-7.373737	1.580757	1.012124
1	-7.866993	-0.076845	0.617393
6	-2.266038	-0.041806	2.405294
1	-2.666078	0.100618	3.418030
1	-1.701771	-0.986767	2.384301
1	-1.543321	0.765331	2.206436
6	0.961427	2.146333	-0.710401
6	1.509898	3.391792	-0.409056
1	2.558947	3.604615	-0.632205
6	0.703554	4.370114	0.170904
1	1.128246	5.343421	0.426344
6	-0.646921	4.110817	0.417842
1	-1.274674	4.887836	0.859935
6	-1.194536	2.862845	0.119182
1	-2.246564	2.658639	0.338106
6	-0.393465	1.858520	-0.433827
7	-1.741946	-0.581899	-0.348613
6	1.845117	1.328259	-2.067984
8	2.054459	1.977335	-3.016515

12-TS-2B

SCF energy = -1432.444294590 a.u.

ν = -452.5655 cm^{-1}

7	-0.357633	0.733883	-0.651626
6	-3.204261	0.336535	-0.045404
6	-4.333015	-0.477021	-0.309302
6	-5.204494	-0.798790	0.729922
1	-6.069751	-1.433513	0.515969
6	-5.017074	-0.312049	2.023755
6	-3.950194	0.557569	2.243574
1	-3.812143	0.986395	3.240377
6	-3.045249	0.910223	1.236775
6	-4.739605	-0.912265	-1.701197
1	-5.256805	-1.881373	-1.671386
1	-3.911983	-0.994240	-2.416198
1	-5.439837	-0.171064	-2.118834
6	-5.936908	-0.713154	3.144705
1	-5.981033	0.058525	3.925948
1	-5.581626	-1.643141	3.617411
1	-6.957982	-0.897533	2.781461
6	-1.951225	1.877366	1.602335
1	-0.986899	1.365610	1.732749
1	-2.196290	2.385094	2.544656
1	-1.802151	2.646521	0.835297
6	1.630622	1.796367	-0.348564
6	2.516205	2.865506	-0.321624
1	3.560520	2.710265	-0.041985
6	2.034593	4.129609	-0.677403
1	2.714046	4.984320	-0.666716
6	0.703370	4.307686	-1.056619
1	0.350123	5.300850	-1.341412
6	-0.189775	3.231106	-1.084949
1	-1.224952	3.382313	-1.396490
6	0.274290	1.969897	-0.723020
5	-1.600769	0.051076	-1.073506
5	0.639102	-0.245043	-0.317775
6	3.149591	-0.079667	0.241563
6	3.910848	-0.698787	-0.763010
6	5.164466	-1.210052	-0.423245
1	5.763542	-1.696935	-1.198568
6	5.675293	-1.110239	0.874054
6	4.891879	-0.487570	1.848017
1	5.272566	-0.406438	2.870414
6	3.627965	0.031213	1.555617
6	3.372979	-0.813721	-2.164091
1	2.534805	-1.527225	-2.208874
1	2.990496	0.153021	-2.524343
1	4.149978	-1.160623	-2.858485
6	7.048311	-1.638767	1.199627
1	7.179391	-1.784886	2.281003
1	7.236449	-2.600239	0.699669
1	7.827457	-0.936148	0.862496
6	2.782769	0.680830	2.618092
1	3.272598	0.629834	3.599684
1	2.588584	1.739400	2.384820
1	1.801328	0.188003	2.694613

6	-1.249225	-1.529398	-1.038917
6	-1.961299	-2.687890	-1.352598
1	-2.970485	-2.641952	-1.757982
6	-1.388509	-3.948074	-1.156145
1	-1.959810	-4.842390	-1.416921
6	-0.103090	-4.077226	-0.633604
1	0.330404	-5.068570	-0.482887
6	0.625881	-2.933127	-0.308201
1	1.636503	-3.022222	0.100778
6	0.064045	-1.672557	-0.509380
7	1.866408	0.439409	-0.080155
6	-2.632666	0.934443	-1.725974
8	-3.276155	1.720895	-2.294514

12-P-1

SCF energy = -1432.525164230 a.u.

7	0.677255	-0.033066	-0.210901
6	3.279827	0.280494	0.037120
6	3.715157	-0.247937	1.268192
6	5.009629	-0.754745	1.379816
1	5.343209	-1.161693	2.339679
6	5.890900	-0.757998	0.293894
6	5.446330	-0.225619	-0.917023
1	6.123832	-0.214120	-1.776297
6	4.158183	0.298801	-1.059100
6	2.776817	-0.290719	2.450226
1	1.972528	-1.027349	2.287412
1	2.298269	0.686552	2.623238
1	3.302263	-0.570369	3.373698
6	7.278992	-1.325958	0.439936
1	7.866738	-1.194915	-0.479245
1	7.243502	-2.403208	0.666859
1	7.822349	-0.837343	1.263374
6	3.707384	0.877609	-2.377247
1	4.468640	0.750456	-3.159262
1	3.506595	1.954667	-2.268342
1	2.781181	0.397263	-2.733402
6	-0.777246	-1.797942	-0.240737
6	-1.183832	-3.125299	-0.298402
1	-2.243967	-3.382611	-0.254232
6	-0.193620	-4.104166	-0.414436
1	-0.482608	-5.156148	-0.462666
6	1.157039	-3.755394	-0.473847
1	1.913841	-4.536366	-0.568617
6	1.562714	-2.418363	-0.415034
1	2.618065	-2.151190	-0.465419
6	0.582250	-1.440211	-0.290904
5	1.810907	0.812252	-0.102325
5	-0.685895	0.484914	-0.116222
6	-2.977966	-0.705309	-0.035257
6	-3.748003	-0.680434	-1.206548
6	-5.137585	-0.750866	-1.084856
1	-5.748247	-0.734340	-1.992332
6	-5.763816	-0.845108	0.160666
6	-4.963532	-0.869805	1.306510
1	-5.437259	-0.948367	2.289313
6	-3.571201	-0.801434	1.231926
6	-3.080488	-0.556463	-2.549086
1	-2.567668	0.413927	-2.642843
1	-2.318631	-1.338051	-2.691295
1	-3.812828	-0.634121	-3.363595
6	-7.265824	-0.892118	0.269504
1	-7.587083	-1.487963	1.135878
1	-7.681464	0.120863	0.395298
1	-7.721449	-1.325280	-0.632134
6	-2.714341	-0.804561	2.468733
1	-3.317707	-0.977651	3.369710
1	-1.938467	-1.583426	2.416621
1	-2.195693	0.160280	2.586319
6	0.087488	2.911803	0.009081
6	-0.132340	4.288477	0.103959
1	0.734803	4.952259	0.098958
6	-1.428389	4.784169	0.203529
1	-1.599292	5.860016	0.283999
6	-2.509975	3.901883	0.202376
1	-3.528868	4.287924	0.280947
6	-2.295912	2.528336	0.101588
1	-3.155060	1.853644	0.098566
6	-0.996381	2.007375	0.005367
7	-1.559532	-0.638579	-0.132902
6	1.502674	2.409400	-0.092463
8	2.425221	3.201870	-0.173214

12-P-1B

SCF energy = -1432.499318140 a.u.

7	-0.042740	0.679233	-0.532660
6	-3.906619	0.333404	-0.173145
6	-5.183644	0.238933	-0.776436
6	-6.275292	-0.105247	0.022652
1	-7.260304	-0.194991	-0.444876

6	-6.153334	-0.330617	1.395299
6	-4.890268	-0.202017	1.973967
1	-4.777569	-0.353393	3.051283
6	-3.762935	0.115358	1.215127
6	-5.414555	0.484949	-2.245652
1	-6.439339	0.200741	-2.522598
1	-4.710844	-0.080882	-2.872399
1	-5.258120	1.542442	-2.496657
6	-7.351466	-0.722540	2.218294
1	-7.183183	-0.542455	3.289159
1	-7.572528	-1.794636	2.091255
1	-8.248481	-0.165303	1.911114
6	-2.431511	0.245642	1.917537
1	-1.756106	-0.587195	1.663266
1	-2.568291	0.223635	3.006874
1	-1.915993	1.184656	1.668459
6	1.869091	1.835478	-0.116611
6	2.670546	2.954286	0.062094
1	3.738915	2.846158	0.260777
6	2.064972	4.213111	-0.025793
1	2.673277	5.109480	0.111312
6	0.700711	4.340589	-0.292842
1	0.255020	5.334545	-0.365945
6	-0.106110	3.212836	-0.482215
1	-1.167065	3.305028	-0.718967
6	0.486842	1.961690	-0.386173
5	-1.269443	-0.018209	-0.717524
5	1.042514	-0.272476	-0.353073
6	3.546249	0.007842	0.144338
6	4.324253	-0.404406	-0.949788
6	5.618915	-0.863099	-0.704945
1	6.233431	-1.187428	-1.550084
6	6.151109	-0.914203	0.587159
6	5.348572	-0.498501	1.651161
1	5.745744	-0.540778	2.669486
6	4.044066	-0.037127	1.454340
6	3.759166	-0.358765	-2.344324
1	2.952244	-1.098447	-2.469606
1	3.325765	0.627776	-2.566305
1	4.533707	-0.574673	-3.092195
6	7.561193	-1.394275	0.814063
1	7.764310	-1.557917	1.881485
1	7.751394	-2.338727	0.282593
1	8.291701	-0.657693	0.443263
6	3.180027	0.384908	2.611992
1	3.691741	0.220304	3.569525
1	2.912596	1.450931	2.543925
1	2.234626	-0.179017	2.622927
6	-0.915008	-1.567248	-0.710989
6	-1.726631	-2.688516	-0.852311
1	-2.803030	-2.578279	-1.013048
6	-1.155563	-3.966730	-0.781035
1	-1.786621	-4.851589	-0.892636
6	0.212437	-4.118648	-0.566380
1	0.643277	-5.121200	-0.510603
6	1.039824	-2.996582	-0.415323
1	2.111209	-3.126746	-0.239396
6	0.481518	-1.726067	-0.487532
7	2.220395	0.468710	-0.086486
6	-2.697442	0.638411	-0.998514
8	-2.756887	1.308300	-2.021557

13

SCF energy = -798.709429699 a.u.

7	-0.083932	-0.000002	-0.000410
6	-0.146063	2.523483	-0.000086
1	-0.640567	3.499638	-0.000338
6	1.220000	2.507811	0.000115
6	1.971630	1.241468	0.000147
6	3.373003	1.205973	0.000436
1	3.939739	2.138030	0.000670
6	4.066249	0.000010	0.000548
1	5.157684	0.000012	0.000881
6	3.373009	-1.205948	0.000264
1	3.939702	-2.138038	0.000364
6	1.971646	-1.241423	-0.000171
6	1.220072	-2.507772	-0.000381
6	-0.145994	-2.523494	-0.000344
1	-0.640475	-3.499660	-0.000295
6	1.280929	0.000013	-0.000144
6	2.006068	-3.793183	-0.000234
1	2.656305	-3.864681	-0.886282
1	1.332947	-4.659976	-0.000821
1	2.655020	-3.864961	0.886761
6	2.005869	3.793293	0.000104
1	2.654757	3.865318	0.887126
1	1.332659	4.660019	-0.000662
1	2.656149	3.864706	-0.885917
6	-2.400870	0.710910	-0.000344
6	-3.606852	1.405321	-0.000342

1	-3.620836	2.499050	-0.000389
6	-4.815573	0.696667	0.000129
1	-5.765174	1.237429	0.000234
6	-4.815564	-0.696757	0.000429
1	-5.765153	-1.237538	0.000717
6	-3.606835	-1.405400	0.000397
1	-3.620820	-2.499129	0.000467
6	-2.400859	-0.710983	-0.000033
5	-0.898378	1.197074	0.000017
5	-0.898343	-1.197103	-0.000536

13-TS-1

SCF energy = -911.878591879 a.u.

ν = -96.4940 cm^{-1}

7	0.020695	0.176721	-0.033606
6	-0.185058	-2.333819	-0.500764
1	-0.743396	-3.229151	-0.794955
6	1.168418	-2.373670	-0.568312
6	1.997765	-1.186527	-0.234211
6	3.390407	-1.244606	-0.198778
1	3.897635	-2.201724	-0.329086
6	4.163836	-0.093801	-0.017075
1	5.251950	-0.172201	0.018644
6	3.553649	1.145446	0.081933
1	4.176720	2.035056	0.184266
6	2.151766	1.275285	0.044648
6	1.483874	2.581339	0.080910
6	0.123672	2.683622	-0.016455
1	-0.307603	3.689799	-0.016510
6	1.381813	0.087079	-0.054747
6	2.345421	3.813341	0.194379
1	2.942266	3.800775	1.120289
1	1.727793	4.720886	0.200988
1	3.052830	3.888838	-0.646514
6	1.887086	-3.611830	-1.039154
1	2.527148	-3.398255	-1.909483
1	1.170357	-4.393861	-1.321680
1	2.539356	-4.020417	-0.250340
6	-2.348129	-0.398611	-0.202935
6	-3.598705	-1.000346	-0.334106
1	-3.699732	-2.090247	-0.321380
6	-4.737575	-0.205182	-0.496064
1	-5.717798	-0.673833	-0.613893
6	-4.628842	1.186266	-0.511298
1	-5.526309	1.797014	-0.636412
6	-3.380358	1.797919	-0.370797
1	-3.307098	2.889214	-0.387424
6	-2.232630	1.017492	-0.217231
5	-0.877977	-1.017380	0.029497
5	-0.708493	1.405443	-0.091326
6	-1.014900	-1.470535	1.746866
8	-1.165711	-1.979054	2.740877

13-I-1

SCF energy = -911.878599227 a.u.

7	0.019168	0.173117	-0.021085
6	-0.185520	-2.339690	-0.490804
1	-0.744303	-3.233154	-0.789706
6	1.167089	-2.376349	-0.564271
6	1.996839	-1.189036	-0.227596
6	3.389125	-1.245900	-0.195778
1	3.896836	-2.202722	-0.326492
6	4.162416	-0.093695	-0.018572
1	5.250663	-0.171400	0.014817
6	3.551871	1.145225	0.076928
1	4.174402	2.035833	0.173811
6	2.149376	1.273863	0.042588
6	1.480345	2.579161	0.071871
6	0.119930	2.679269	-0.026127
1	-0.312365	3.685008	-0.033624
6	1.380324	0.084553	-0.047984
6	2.340724	3.812758	0.177074
1	2.939534	3.805737	1.101785
1	1.722088	4.719652	0.180175
1	3.046338	3.884644	-0.665659
6	1.886156	-3.608893	-1.049261
1	2.519530	-3.386681	-1.922374
1	1.169867	-4.391055	-1.332603
1	2.545219	-4.021452	-0.268181
6	-2.350494	-0.406663	-0.189635
6	-3.600817	-1.009738	-0.318743
1	-3.702127	-2.099415	-0.294556
6	-4.738525	-0.216300	-0.494931
1	-5.718209	-0.686059	-0.612785
6	-4.629367	1.175052	-0.524543
1	-5.526062	1.784516	-0.660883
6	-3.381720	1.787843	-0.384073
1	-3.308138	2.878887	-0.411648
6	-2.234346	1.009191	-0.216901
5	-0.879865	-1.025883	0.056005

5	-0.711134	1.399721	-0.090669
6	-1.005375	-1.454062	1.735871
8	-1.140080	-1.915360	2.754769

13-TS-2

SCF energy = -911.844231440 a.u.

ν = -473.4275 cm^{-1}

7	0.125918	0.070375	0.254550
6	-0.043704	-2.457715	-0.210475
1	-0.602915	-3.378925	-0.393509
6	1.296756	-2.463171	-0.393766
6	2.116656	-1.246845	-0.154812
6	3.504763	-1.271608	-0.265203
1	4.015612	-2.216719	-0.453111
6	4.268814	-0.104659	-0.159503
1	5.356134	-0.158881	-0.236917
6	3.643396	1.117396	0.000963
1	4.250433	2.022732	0.038203
6	2.240233	1.214159	0.101457
6	1.559606	2.508998	0.170023
6	0.195102	2.580862	0.137248
1	-0.262100	3.575372	0.131005
6	1.489833	0.009929	0.092498
6	2.400016	3.758827	0.217340
1	3.073155	3.756522	1.088921
1	1.764737	4.651823	0.279854
1	3.030657	3.852683	-0.680813
6	2.008590	-3.707683	-0.857610
1	2.567402	-3.526415	-1.789225
1	1.291394	-4.518365	-1.040693
1	2.732164	-4.060905	-0.105659
6	-2.460368	-0.405616	0.060023
6	-3.707933	-0.908747	-0.308047
1	-3.956342	-1.959250	-0.132606
6	-4.645175	-0.051983	-0.881491
1	-5.615245	-0.438522	-1.202048
6	-4.347410	1.304651	-1.034512
1	-5.092878	1.975581	-1.467851
6	-3.104762	1.806458	-0.645895
1	-2.882352	2.867656	-0.786619
6	-2.131663	0.957091	-0.109220
5	-0.651040	-1.179286	0.416297
5	-0.607204	1.288757	0.133336
6	-1.730009	-1.230124	1.469849
8	-2.447063	-1.493210	2.355982

13-TS-2B

SCF energy = -911.844582013 a.u.

ν = -423.4404 cm^{-1}

7	-0.022524	0.225723	0.094513
6	-0.151490	-2.476508	-0.263543
1	-0.701461	-3.322161	-0.688819
6	1.157373	-2.281868	-0.595308
6	1.958670	-1.118775	-0.165694
6	3.358116	-1.170281	-0.158583
1	3.865442	-2.124181	-0.310948
6	4.121636	-0.024080	0.037922
1	5.210131	-0.092854	0.069609
6	3.497871	1.214289	0.142602
1	4.116666	2.108246	0.232475
6	2.101430	1.338722	0.118364
6	1.429817	2.645577	0.119031
6	0.074053	2.735933	-0.015407
1	-0.364662	3.737779	-0.056515
6	1.331718	0.142670	0.052547
6	2.284948	3.881902	0.225073
1	2.871609	3.882979	1.157398
1	1.662476	4.785871	0.215336
1	2.999525	3.952401	-0.610205
6	1.835415	-3.275464	-1.502494
1	2.350213	-2.771727	-2.333498
1	1.115705	-3.997135	-1.908347
1	2.594827	-3.844174	-0.941805
6	-2.413367	-0.334553	0.017362
6	-3.667094	-0.936537	-0.045512
1	-3.780770	-2.013950	0.104287
6	-4.793928	-0.152105	-0.308586
1	-5.778525	-0.621140	-0.376795
6	-4.672008	1.228049	-0.480191
1	-5.562832	1.828853	-0.678556
6	-3.419413	1.840514	-0.396193
1	-3.334979	2.923605	-0.522732
6	-2.280796	1.068249	-0.158176
5	-0.968692	-0.874104	0.366207
5	-0.758326	1.454352	-0.048789
6	-0.638312	-2.039965	1.257985
8	-0.644806	-2.828542	2.139155

13-P-1

SCF energy = -911.920411550 a.u.

7	0.200056	-0.124340	0.000081

6	0.760071	-2.614796	-0.000258
1	0.441679	-3.660823	-0.000303
6	2.085965	-2.317609	-0.000060
6	2.513730	-0.915185	-0.000029
6	3.882110	-0.602279	-0.000198
1	4.614970	-1.409036	-0.000313
6	4.331621	0.708423	-0.000258
1	5.401291	0.924237	-0.000422
6	3.406911	1.743289	-0.000114
1	3.769347	2.771324	-0.000151
6	2.027693	1.498414	0.000041
6	1.082635	2.619979	0.000174
6	-0.253041	2.380205	0.000198
1	-0.914422	3.251429	0.000276
6	1.566965	0.150706	0.000036
6	1.620667	4.026260	0.000208
1	2.244652	4.218353	0.886979
1	0.798680	4.753246	0.000495
1	2.244165	4.218508	-0.886881
6	3.127673	-3.404347	0.000045
1	3.776952	-3.340863	-0.887239
1	2.647817	-4.390987	0.000554
1	3.777522	-3.340214	0.886849
6	-2.814989	-0.703772	-0.000017
6	-4.183838	-0.983722	-0.000218
1	-4.497275	-2.029900	-0.000269
6	-5.105632	0.056858	-0.000315
1	-6.177250	-0.155158	-0.000455
6	-4.652707	1.377660	-0.000215
1	-5.371861	2.200007	-0.000233
6	-3.286613	1.651171	-0.000068
1	-2.963938	2.694440	-0.000061
6	-2.332406	0.620272	0.000015
5	-0.257357	-1.493048	0.000001
5	-0.789027	0.949458	0.000116
6	-1.831984	-1.826425	0.000299
8	-2.203724	-2.988356	0.000554

13-P-1B

SCF energy = -911.873481827 a.u.

7	0.074603	0.170767	0.072587
6	-0.588465	-2.964287	0.102622
1	-0.493490	-4.027153	0.351759
6	-1.736278	-2.328404	0.427587
6	-2.148817	-0.934908	0.074538
6	-3.527175	-0.761162	-0.129073
1	-4.180333	-1.631934	-0.104493
6	-4.105410	0.475786	-0.370147
1	-5.179222	0.557737	-0.544656
6	-3.306832	1.603474	-0.342944
1	-3.770600	2.579959	-0.476410
6	-1.921659	1.512528	-0.143204
6	-1.137408	2.756969	-0.044666
6	0.199224	2.724870	0.200082
1	0.732341	3.675265	0.294057
6	-1.314788	0.222921	-0.009085
6	-1.851858	4.075889	-0.190033
1	-2.339419	4.164561	-1.173270
1	-1.141689	4.906089	-0.088656
1	-2.632810	4.199799	0.576348
6	-2.772473	-3.152626	1.165898
1	-3.260256	-2.567694	1.959086
1	-2.303482	-4.033963	1.621281
1	-3.562405	-3.518931	0.491470
6	2.455354	-0.419688	-0.038401
6	3.676505	-1.078826	-0.158987
1	3.707028	-2.141150	-0.412388
6	4.857784	-0.354387	0.038440
1	5.825097	-0.855131	-0.046887
6	4.811505	1.008524	0.335359
1	5.744380	1.558111	0.483473
6	3.584829	1.677271	0.434219
1	3.565309	2.749453	0.648966
6	2.405250	0.961441	0.251655
5	0.984552	-0.919120	-0.208711
5	0.892395	1.378570	0.228198
6	0.580374	-2.402727	-0.591231
8	1.303080	-3.105448	-1.282624

14

SCF energy = -915.329721086 a.u.

7	0.336272	-1.011571	0.024666
6	-0.714707	-3.270850	-1.055225
1	0.233055	-3.485685	-1.570425
1	-1.546128	-3.427169	-1.759102
1	-0.831983	-4.029678	-0.260540
6	-2.441251	2.610290	1.133441
1	-3.193918	2.868237	1.892718
1	-2.493357	3.390121	0.355691
1	-1.451678	2.668167	1.605216

6	-5.874176	-0.810873	-0.191190
1	-6.129107	-0.975920	-1.250028
1	-6.546114	-0.034146	0.199588
1	-6.089246	-1.748882	0.343399
6	-1.711789	0.338559	0.186615
6	-2.077469	-0.965061	-0.236842
6	-3.407658	-1.334001	-0.372806
1	-3.672846	-2.339760	-0.715882
6	-4.426108	-0.423263	-0.045752
6	-4.054752	0.832663	0.431077
1	-4.842383	1.531878	0.730484
6	-2.713478	1.242031	0.559536
6	0.937380	1.467737	-0.069513
6	0.606146	2.808410	-0.341431
1	-0.442678	3.102006	-0.357286
6	1.575436	3.759551	-0.620609
1	1.293806	4.793064	-0.832333
6	2.918139	3.374160	-0.644289
1	3.694770	4.107834	-0.872378
6	3.272939	2.055078	-0.402631
1	4.326695	1.783941	-0.468540
6	2.301003	1.079743	-0.112826
6	2.678794	-0.331552	0.122105
6	4.018377	-0.710032	0.321985
1	4.796037	0.053730	0.327325
6	4.388746	-2.028098	0.538565
1	5.438887	-2.281475	0.694691
6	3.404607	-3.016698	0.580202
1	3.672409	-4.057619	0.773483
6	2.073568	-2.673985	0.401555
1	1.306960	-3.442219	0.484947
6	1.689747	-1.344287	0.157635
5	-0.129677	0.361725	0.119189
5	-0.777934	-1.832238	-0.425451

14-TS-1

SCF energy = -1028.510523730 a.u.

ν = -231.9448 cm^{-1}

7	0.390630	-1.039884	-0.127015
6	-0.532341	-3.207505	-1.434137
1	0.452217	-3.359303	-1.901589
1	-1.310595	-3.328856	-2.203204
1	-0.678811	-4.028478	-0.709505
6	-2.522026	2.386920	1.257339
1	-3.207255	2.475894	2.114149
1	-2.714107	3.252922	0.603096
1	-1.494122	2.484732	1.633794
6	-5.796824	-0.885562	-0.714799
1	-5.949312	-1.015697	-1.797536
1	-6.506297	-0.123592	-0.363072
1	-6.059371	-1.840716	-0.233860
6	-1.705722	0.236852	0.134388
6	-2.000848	-1.006051	-0.480115
6	-3.315149	-1.358988	-0.763931
1	-3.536662	-2.314382	-1.251545
6	-4.370933	-0.503168	-0.413323
6	-4.064190	0.694116	0.234866
1	-4.885059	1.353019	0.537323
6	-2.745700	1.086890	0.523293
6	0.857999	1.480186	-0.212524
6	0.428625	2.769172	-0.553250
1	-0.630235	3.017923	-0.469028
6	1.317146	3.732728	-1.020170
1	0.960454	4.731804	-1.280220
6	2.663881	3.404128	-1.170724
1	3.371756	4.145096	-1.549352
6	3.108335	2.122804	-0.863862
1	4.157805	1.877924	-1.035101
6	2.222716	1.147448	-0.378486
6	2.689024	-0.231291	-0.078941
6	4.047264	-0.521572	0.121643
1	4.772907	0.293348	0.120533
6	4.499253	-1.817275	0.337775
1	5.563132	-2.005651	0.493511
6	3.581576	-2.866865	0.369646
1	3.918119	-3.890212	0.549353
6	2.227822	-2.607470	0.201588
1	1.504420	-3.419728	0.273030
6	1.762948	-1.302990	-0.023632
5	-0.111305	0.317427	0.231016
5	-0.669027	-1.820842	-0.700656
6	0.035272	0.173522	2.191779
8	-0.111313	-0.133245	3.265000

14-I-1

SCF energy = -1028.512952060 a.u.

7	0.423857	-1.069734	-0.047271
6	-0.434249	-3.218122	-1.411982
1	0.558225	-3.336421	-1.872833
1	-1.200263	-3.344348	-2.192607

1	-0.566388	-4.056482	-0.705060
6	-2.585454	2.244989	1.435600
1	-3.111154	2.165010	2.400440
1	-2.999291	3.123871	0.916748
1	-1.528569	2.460542	1.646811
6	-5.744553	-0.956568	-0.824132
1	-5.846346	-1.070017	-1.914596
1	-6.472320	-0.202349	-0.493723
1	-6.026308	-1.919678	-0.370585
6	-1.707556	0.161268	0.237401
6	-1.957685	-1.060096	-0.436014
6	-3.259070	-1.409713	-0.783329
1	-3.452379	-2.348596	-1.313188
6	-4.335888	-0.574937	-0.448601
6	-4.068915	0.601387	0.254230
1	-4.907156	1.246128	0.539320
6	-2.768593	0.987013	0.619920
6	0.788383	1.472701	-0.173381
6	0.289116	2.719361	-0.563241
1	-0.772983	2.935248	-0.432585
6	1.113759	3.682492	-1.140245
1	0.703614	4.649658	-1.439284
6	2.460610	3.393532	-1.350415
1	3.116531	4.133713	-1.814318
6	2.970099	2.148331	-0.995076
1	4.015660	1.925303	-1.215213
6	2.152119	1.176648	-0.398822
6	2.685902	-0.171656	-0.063479
6	4.057874	-0.397047	0.115916
1	4.746009	0.449945	0.089784
6	4.570445	-1.670367	0.337727
1	5.644013	-1.811019	0.476441
6	3.701710	-2.759245	0.392766
1	4.088317	-3.765024	0.571218
6	2.333228	-2.562008	0.250947
1	1.646308	-3.404264	0.339806
6	1.807825	-1.281504	0.028639
5	-0.104736	0.279704	0.411224
5	-0.609061	-1.846899	-0.654509
6	0.045942	0.223885	2.060887
8	0.034521	0.123853	3.182356

14-TS-2

SCF energy = -1028.476750560 a.u.

ν = -411.1991 cm^{-1}

7	0.619951	-1.058206	0.258722
6	-0.137216	-3.325968	-0.930410
1	0.849149	-3.406899	-1.411499
1	-0.907109	-3.567406	-1.678299
1	-0.186982	-4.117393	-0.162025
6	-3.072484	2.076660	1.433850
1	-3.447200	1.816060	2.435839
1	-3.776157	2.789184	0.981453
1	-2.111877	2.586151	1.582991
6	-5.294873	-1.213787	-1.646725
1	-5.040664	-1.421999	-2.697054
1	-6.079425	-0.445166	-1.631226
1	-5.718144	-2.138730	-1.224720
6	-1.812857	0.015590	0.570841
6	-1.784250	-1.196307	-0.159668
6	-2.926437	-1.580904	-0.859326
1	-2.919662	-2.513551	-1.431370
6	-4.077983	-0.784123	-0.872298
6	-4.065703	0.413338	-0.153123
1	-4.959196	1.045305	-0.162440
6	-2.957753	0.831360	0.592357
6	0.828936	1.498689	0.007522
6	0.232068	2.728663	-0.284851
1	-0.805525	2.906638	0.002522
6	0.925529	3.724032	-0.967021
1	0.441594	4.677569	-1.188412
6	2.235488	3.485770	-1.378517
1	2.786632	4.251315	-1.929176
6	2.841395	2.263345	-1.106343
1	3.855305	2.087171	-1.469375
6	2.160532	1.257030	-0.405592
6	2.809975	-0.049057	-0.102348
6	4.203043	-0.198464	-0.114313
1	4.832380	0.671157	-0.310607
6	4.812352	-1.423555	0.135679
1	5.900923	-1.504217	0.120319
6	4.026251	-2.536622	0.425232
1	4.491002	-3.501001	0.640593
6	2.641959	-2.412415	0.469215
1	2.022355	-3.267471	0.740493
6	2.023590	-1.186455	0.202180
5	0.148915	0.278504	0.717122
5	-0.377752	-1.918540	-0.263916
6	-0.743231	0.269835	1.923840
8	-1.204105	0.340124	3.004228

14-TS-2B

SCF energy = -1028.480700240 a.u.

ν = -468.4369 cm^{-1}

7	0.408893	-1.135596	0.260265
6	-0.315483	-3.290750	-1.160404
1	0.709814	-3.386946	-1.548742
1	-1.023696	-3.435089	-1.990641
1	-0.477699	-4.130381	-0.461350
6	-2.761039	2.133417	1.526273
1	-3.563680	2.206827	2.275068
1	-2.861385	3.009510	0.864485
1	-1.805749	2.222082	2.060405
6	-5.712689	-1.169305	-0.861208
1	-5.747158	-1.302978	-1.953609
1	-6.472873	-0.424567	-0.587428
1	-6.002356	-2.130044	-0.407536
6	-1.770605	0.037809	0.441954
6	-1.954897	-1.179568	-0.261501
6	-3.223234	-1.562655	-0.681767
1	-3.363304	-2.506436	-1.219382
6	-4.336684	-0.753215	-0.409381
6	-4.134906	0.429528	0.302713
1	-5.002263	1.056509	0.535029
6	-2.867864	0.846278	0.747036
6	0.817340	1.535117	0.024855
6	0.235876	2.718906	-0.440060
1	-0.701712	3.066654	-0.003005
6	0.850129	3.450743	-1.448348
1	0.393749	4.371569	-1.816619
6	2.054056	2.994085	-1.989892
1	2.539884	3.557709	-2.789434
6	2.633919	1.815380	-1.533278
1	3.554639	1.453837	-1.995586
6	2.031656	1.063434	-0.513542
6	2.632434	-0.213623	-0.059695
6	4.022985	-0.386700	-0.020288
1	4.671448	0.462864	-0.245930
6	4.589068	-1.610924	0.314003
1	5.674539	-1.721160	0.346649
6	3.760549	-2.692068	0.617306
1	4.194496	-3.658006	0.884237
6	2.379412	-2.538045	0.603527
1	1.726228	-3.370049	0.870220
6	1.800131	-1.306784	0.274410
5	-0.224710	0.097478	0.774842
5	-0.578527	-1.931885	-0.412941
6	0.490776	1.042466	1.697982
8	0.923179	1.699771	2.565954

14-P-1

SCF energy = -1028.536388520 a.u.

7	0.439566	-0.736315	0.124810
6	-0.672097	-2.672721	-1.312753
1	0.347399	-2.949344	-1.612752
1	-1.283416	-2.547621	-2.220608
1	-1.101187	-3.534978	-0.773829
6	-3.733964	2.701021	0.864981
1	-3.249102	2.878844	1.834515
1	-4.806524	2.924313	0.954201
1	-3.275462	3.417480	0.169361
6	-5.816096	-1.658560	-0.501522
1	-5.767589	-2.184023	-1.466915
1	-6.725630	-1.042170	-0.491714
1	-5.922040	-2.425542	0.282302
6	-2.264383	0.702313	0.188840
6	-2.145179	-0.635583	-0.254284
6	-3.309096	-1.374043	-0.484834
1	-3.237642	-2.407370	-0.834585
6	-4.579952	-0.830773	-0.271927
6	-4.663240	0.490466	0.166482
1	-5.651211	0.933026	0.325802
6	-3.533560	1.282272	0.403962
6	1.754645	1.447599	-0.058355
6	1.814861	2.841364	-0.263484
1	0.903909	3.425675	-0.133255
6	3.001465	3.464525	-0.617811
1	3.030878	4.544507	-0.776677
6	4.158894	2.697622	-0.782109
1	5.094807	3.176445	-1.079553
6	4.130012	1.326939	-0.569900
1	5.048354	0.757004	-0.714461
6	2.939099	0.683161	-0.190745
6	2.899880	-0.760799	0.114244
6	4.077928	-1.505528	0.307195
1	5.044595	-1.012170	0.204669
6	4.052332	-2.845710	0.658379
1	4.987950	-3.388336	0.805526
6	2.824829	-3.480988	0.855900
1	2.784832	-4.526811	1.167113
6	1.648939	-2.770255	0.678337

1	0.691130	-3.253553	0.872095
6	1.664864	-1.424125	0.280377
5	0.420534	0.697773	0.165543
5	-0.749858	-1.351926	-0.444379
6	-0.993686	1.451945	0.395013
8	-0.985421	2.607343	0.796669

14-P-1B

SCF energy = -1028.514578510 a.u.

7	0.103544	1.078589	-0.180888
6	-0.794192	3.184593	1.246826
1	0.239063	3.409176	1.548371
1	-1.446790	3.220461	2.132945
1	-1.129261	4.004580	0.586144
6	-2.677056	-2.479533	-1.302686
1	-3.600911	-2.956029	-1.659457
1	-2.190469	-3.180805	-0.604804
1	-1.991605	-2.348649	-2.150530
6	-6.013162	0.600086	0.902615
1	-6.071724	0.751257	1.991752
1	-6.693843	-0.220377	0.636823
1	-6.389679	1.519470	0.427608
6	-1.966170	-0.225540	-0.355093
6	-2.278546	0.977839	0.323549
6	-3.575436	1.242218	0.737160
1	-3.814264	2.171536	1.264935
6	-4.598559	0.313504	0.473019
6	-4.271722	-0.867585	-0.194862
1	-5.067059	-1.591028	-0.400068
6	-2.963899	-1.170318	-0.615903
6	1.581081	-1.719463	-0.163839
6	1.651268	-3.067337	0.205867
1	1.012855	-3.782278	-0.318225
6	2.503663	-3.482240	1.222357
1	2.544191	-4.534200	1.512058
6	3.300842	-2.539542	1.870312
1	3.963943	-2.846436	2.682021
6	3.263127	-1.203767	1.481137
1	3.905252	-0.479733	1.987245
6	2.412875	-0.763034	0.455548
6	2.535657	0.644844	-0.027370
6	3.833769	1.153239	-0.205503
1	4.681737	0.493799	-0.009731
6	4.069169	2.449971	-0.644316
1	5.093123	2.804695	-0.775730
6	2.988179	3.278946	-0.934388
1	3.148808	4.296138	-1.297269
6	1.695507	2.795748	-0.781223
1	0.843697	3.429407	-1.033262
6	1.447378	1.494421	-0.324408
5	-0.426261	-0.176966	-0.643899
5	-0.958255	1.823750	0.486288
6	0.538852	-1.332753	-1.172740
8	0.383121	-1.956351	-2.205363

15

SCF energy = -1034.357346850 a.u.

7	-0.001590	-0.650779	0.094071
1	-0.003548	-1.660226	0.157808
5	-1.188915	0.156458	0.029389
5	1.188179	0.152510	0.028637
6	-0.705646	1.659571	-0.073421
6	-1.404714	2.858447	-0.156781
1	-2.498905	2.865412	-0.161078
6	-0.691219	4.063211	-0.236216
1	-1.228697	5.012406	-0.302118
6	0.702740	4.061221	-0.233013
1	1.243259	5.008834	-0.296744
6	1.412335	2.854379	-0.150803
1	2.506579	2.857870	-0.150913
6	0.709421	1.657650	-0.069415
6	-2.659425	-0.389864	0.051165
6	-3.298035	-0.673772	1.273629
6	-4.612110	-1.144479	1.271226
1	-5.102409	-1.362550	2.225245
6	-5.317862	-1.341066	0.080449
6	-4.672547	-1.053562	-1.123552
1	-5.207201	-1.202733	-2.066794
6	-3.357941	-0.579472	-1.154854
6	-2.564844	-0.451568	2.574817
1	-2.295422	0.610044	2.699064
1	-1.625935	-1.026289	2.610374
1	-3.173335	-0.746062	3.441082
6	-6.746264	-1.820799	0.104003
1	-6.899158	-2.586542	0.878926
1	-7.043962	-2.250074	-0.863183
1	-7.436387	-0.990278	0.324908
6	-2.679037	-0.293063	-2.472873
1	-2.206400	0.702194	-2.471745
1	-3.388118	-0.329363	-3.311490

1	-1.882894	-1.027565	-2.676744
6	2.657382	-0.397801	0.028673
6	3.227922	-0.877807	-1.165497
6	4.547117	-1.335885	-1.163872
1	4.987197	-1.699510	-2.097773
6	5.320841	-1.335730	-0.000187
6	4.743075	-0.851995	1.175904
1	5.336280	-0.834560	2.095667
6	3.427452	-0.382770	1.206285
6	2.414971	-0.887615	-2.438497
1	3.030075	-1.145724	-3.311739
1	1.956771	0.096624	-2.627885
1	1.593039	-1.618970	-2.380645
6	6.731615	-1.865242	-0.009587
1	6.744310	-2.950212	0.185040
1	7.347260	-1.385413	0.764819
1	7.216727	-1.701617	-0.982795
6	2.826007	0.127008	2.494002
1	2.034593	-0.549332	2.856032
1	2.364115	1.117660	2.355454
1	3.579596	0.212616	3.289095

15-TS-1

SCF energy = -1147.531935870 a.u.

ν = -221.2495 cm^{-1}

7	0.073233	-0.405428	0.719679
1	0.060768	-1.357298	1.062417
5	-1.156421	0.367427	0.450943
5	1.225577	0.203593	0.151229
6	-0.628066	1.712485	-0.265202
6	-1.286810	2.866890	-0.687396
1	-2.369025	2.970396	-0.557992
6	-0.556580	3.894120	-1.292313
1	-1.067153	4.798754	-1.631947
6	0.823737	3.772836	-1.471364
1	1.379184	4.583703	-1.948996
6	1.491654	2.623391	-1.040780
1	2.572564	2.527657	-1.181149
6	0.769944	1.597056	-0.430470
6	-2.551409	-0.360802	0.196956
6	-3.327121	-0.958576	1.216090
6	-4.536942	-1.587561	0.902892
1	-5.122892	-2.039701	1.709303
6	-5.006469	-1.676384	-0.405927
6	-4.203575	-1.145898	-1.415533
1	-4.522066	-1.249997	-2.457547
6	-2.993353	-0.503782	-1.141819
6	-2.900698	-0.974010	2.667965
1	-3.176082	-0.041957	3.189314
1	-1.816852	-1.116579	2.787793
1	-3.397137	-1.793549	3.206640
6	-6.328230	-2.325538	-0.721768
1	-6.611739	-3.059833	0.045743
1	-6.301931	-2.838216	-1.694328
1	-7.130918	-1.571741	-0.770283
6	-2.170918	-0.023012	-2.316762
1	-2.260440	1.063675	-2.462112
1	-2.500453	-0.513016	-3.243608
1	-1.100165	-0.235696	-2.186065
6	2.653925	-0.447562	0.071258
6	3.032069	-1.158497	-1.084379
6	4.308399	-1.717717	-1.164467
1	4.594977	-2.267183	-2.066935
6	5.230947	-1.588693	-0.121922
6	4.845893	-0.874216	1.014097
1	5.558414	-0.754369	1.836306
6	3.574216	-0.303871	1.124185
6	2.052547	-1.314675	-2.222987
1	2.509591	-1.813203	-3.088952
1	1.672523	-0.335598	-2.557464
1	1.177319	-1.909769	-1.915888
6	6.593715	-2.224188	-0.222007
1	6.530780	-3.313386	-0.066205
1	7.284722	-1.820934	0.531894
1	7.040097	-2.062559	-1.214636
6	3.186980	0.474740	2.359029
1	2.307969	0.029248	2.851405
1	2.921066	1.514215	2.105682
1	4.002841	0.507365	3.094354
6	-1.291821	1.421289	2.195029
8	-0.973322	2.126939	3.015025

15-I-1

SCF energy = -1147.537005030 a.u.

7	0.086868	-0.319508	0.819384
1	0.097684	-1.155770	1.389182
5	-1.186718	0.482483	0.574210
5	1.207603	0.169900	0.113909
6	-0.652408	1.633990	-0.463503
6	-1.326995	2.686739	-1.082405

1	-2.392751	2.853475	-0.897361
6	-0.634748	3.514330	-1.969765
1	-1.157575	4.332148	-2.472115
6	0.724039	3.304142	-2.222826
1	1.251936	3.961299	-2.918088
6	1.405534	2.262782	-1.589925
1	2.469759	2.100157	-1.785470
6	0.723040	1.426186	-0.704104
6	-2.583348	-0.281994	0.325326
6	-3.566118	-0.480398	1.321522
6	-4.745227	-1.172602	1.024206
1	-5.491387	-1.312975	1.812509
6	-4.992013	-1.699729	-0.241450
6	-4.003361	-1.535313	-1.210897
1	-4.157086	-1.967265	-2.204727
6	-2.815063	-0.846555	-0.953313
6	-3.398543	0.016198	2.740916
1	-3.514819	1.109855	2.819072
1	-2.418116	-0.253944	3.164686
1	-4.158258	-0.423759	3.401628
6	-6.282845	-2.409883	-0.554454
1	-6.712020	-2.880753	0.341742
1	-6.139401	-3.189579	-1.316577
1	-7.032514	-1.702503	-0.945467
6	-1.801025	-0.750425	-2.068373
1	-1.749214	0.266604	-2.484670
1	-2.057880	-1.437082	-2.886818
1	-0.790035	-1.001773	-1.720340
6	2.660935	-0.433488	0.154313
6	3.083600	-1.366122	-0.811814
6	4.390882	-1.855923	-0.775343
1	4.711680	-2.578666	-1.532378
6	5.301941	-1.440003	0.199755
6	4.873236	-0.507600	1.146532
1	5.576043	-0.160958	1.910691
6	3.570624	-0.001195	1.136523
6	2.120326	-1.832689	-1.876537
1	2.616511	-2.459870	-2.630112
1	1.658907	-0.977497	-2.396435
1	1.298874	-2.421558	-1.437508
6	6.699791	-2.002031	0.237050
1	6.709144	-3.001190	0.702267
1	7.376338	-1.360630	0.819626
1	7.117986	-2.109817	-0.774822
6	3.135881	1.008465	2.172085
1	2.361526	0.590301	2.835120
1	2.703834	1.904848	1.698131
1	3.975276	1.333153	2.802765
6	-1.155969	1.514484	1.839547
8	-0.907492	2.301275	2.611347

15-TS-2

SCF energy = -1147.511919850 a.u.

ν = -398.3885 cm^{-1}

7	0.148909	-0.429173	0.925098
1	0.249234	-1.261669	1.493115
5	-1.177512	0.243280	0.867361
5	1.220012	0.127680	0.211919
6	-0.608940	1.779483	-0.266663
6	-1.297048	2.730575	-1.022421
1	-2.300334	3.051174	-0.729182
6	-0.685809	3.275297	-2.148727
1	-1.221602	4.004624	-2.760326
6	0.616118	2.897183	-2.492175
1	1.092896	3.339724	-3.369856
6	1.302100	1.954435	-1.727084
1	2.317142	1.653047	-2.002347
6	0.690020	1.364884	-0.616216
6	-2.547530	-0.424297	0.442360
6	-3.600678	-0.498282	1.383335
6	-4.804031	-1.114354	1.030129
1	-5.606367	-1.175827	1.771604
6	-5.006369	-1.658517	-0.238625
6	-3.957952	-1.586859	-1.157592
1	-4.092839	-2.020326	-2.153325
6	-2.737248	-0.986220	-0.841168
6	-3.453586	0.056162	2.781993
1	-3.416853	1.156338	2.785937
1	-2.528793	-0.293468	3.265602
1	-4.296363	-0.250072	3.416655
6	-6.324391	-2.285014	-0.610706
1	-6.805028	-2.756236	0.258757
1	-6.202265	-3.048737	-1.392092
1	-7.021513	-1.524372	-0.998736
6	-1.652929	-0.944634	-1.887896
1	-1.458254	0.086532	-2.221245
1	-1.929783	-1.538596	-2.769630
1	-0.705146	-1.335877	-1.494128
6	2.702425	-0.401611	0.222348
6	3.147613	-1.356447	-0.711608

6	4.478265	-1.780038	-0.687226
1	4.816299	-2.519795	-1.419908
6	5.389442	-1.279651	0.246851
6	4.937535	-0.326998	1.162223
1	5.638820	0.084214	1.895071
6	3.612872	0.118115	1.161644
6	2.186751	-1.925365	-1.727823
1	2.705495	-2.532354	-2.482749
1	1.639473	-1.126786	-2.254069
1	1.432701	-2.567326	-1.244479
6	6.812833	-1.773632	0.273742
1	6.875613	-2.764051	0.753170
1	7.465677	-1.092251	0.837414
1	7.222375	-1.877370	-0.742116
6	3.154891	1.153643	2.160541
1	2.387154	0.744592	2.836373
1	2.704963	2.024008	1.655692
1	3.986386	1.517877	2.779556
6	-1.198150	1.659876	1.383795
8	-1.392647	2.660749	1.966871

15-TS-2B

SCF energy = -1147.501676800 a.u.

ν = -457.2357 cm^{-1}

7	0.142660	0.282942	1.336673
1	0.288507	-0.470819	1.989037
5	-1.136977	0.974659	1.089287
5	1.104567	0.646772	0.365272
6	-0.792969	2.136433	0.041837
6	-1.441082	3.304709	-0.353112
1	-2.424568	3.567064	0.044619
6	-0.825528	4.168552	-1.264372
1	-1.336213	5.084802	-1.570722
6	0.437517	3.874837	-1.779113
1	0.903552	4.555294	-2.495867
6	1.115094	2.730167	-1.352031
1	2.123268	2.516987	-1.720290
6	0.515054	1.873017	-0.429564
6	-2.463046	-0.315383	0.570717
6	-2.250058	-1.623162	1.060471
6	-2.690203	-2.715772	0.309625
1	-2.505436	-3.725302	0.689634
6	-3.370215	-2.554704	-0.895887
6	-3.664426	-1.253891	-1.308416
1	-4.247486	-1.105052	-2.222297
6	-3.252755	-0.132074	-0.587090
6	-1.593890	-1.935792	2.387271
1	-2.180019	-2.701433	2.915355
1	-1.518477	-1.074212	3.063410
1	-0.584051	-2.352727	2.243034
6	-3.836085	-3.739564	-1.698184
1	-3.315493	-4.660037	-1.400099
1	-3.667744	-3.581119	-2.773346
1	-4.916216	-3.904511	-1.556598
6	-3.696736	1.218777	-1.079981
1	-3.902344	1.908852	-0.251527
1	-4.619046	1.121592	-1.668807
1	-2.932100	1.684762	-1.717535
6	2.473480	-0.097328	0.155460
6	2.489381	-1.305802	-0.570005
6	3.700142	-1.971232	-0.774430
1	3.706466	-2.905750	-1.344712
6	4.905136	-1.470023	-0.273946
6	4.874662	-0.269970	0.439437
1	5.809034	0.141960	0.833833
6	3.679529	0.420700	0.659797
6	1.204998	-1.864404	-1.137869
1	1.380617	-2.791650	-1.700895
1	0.723965	-1.142401	-1.817512
1	0.468787	-2.082836	-0.348136
6	6.197001	-2.219035	-0.477885
1	6.332800	-2.987696	0.300727
1	7.064672	-1.545364	-0.430479
1	6.215572	-2.732205	-1.450511
6	3.675895	1.705183	1.453224
1	3.175154	1.566990	2.425097
1	3.130140	2.502210	0.924048
1	4.695513	2.064780	1.650497
6	-2.388841	0.986388	1.927644
8	-3.339720	1.157039	2.577368

15-P-1

SCF energy = -1147.568525120 a.u.

7	-0.166959	-0.316316	0.221321
1	-0.233593	-1.319762	0.363970
5	-1.375413	0.413763	0.082052
5	1.144949	0.243089	0.082106
6	0.137752	2.617699	-0.249619
6	0.267140	3.991990	-0.463899
1	-0.640628	4.596613	-0.518744

6	1.530847	4.559345	-0.603910
1	1.633012	5.633521	-0.774383
6	2.668456	3.753935	-0.527938
1	3.659859	4.198881	-0.639791
6	2.539097	2.382815	-0.310464
1	3.432988	1.755257	-0.250974
6	1.277003	1.789025	-0.167068
6	-2.769990	-0.306824	0.064498
6	-3.687082	-0.145694	1.123524
6	-4.908528	-0.817792	1.084306
1	-5.611072	-0.694357	1.914514
6	-5.263047	-1.638169	0.009044
6	-4.351418	-1.781135	-1.036596
1	-4.612746	-2.414316	-1.890160
6	-3.111750	-1.134308	-1.022217
6	-3.354708	0.751747	2.290478
1	-3.328668	1.802268	1.963213
1	-2.368851	0.513289	2.721876
1	-4.098458	0.661233	3.094068
6	-6.604124	-2.323898	-0.020417
1	-6.823589	-2.811276	0.941410
1	-6.650645	-3.087989	-0.808887
1	-7.410619	-1.597409	-0.209675
6	-2.157688	-1.336901	-2.178423
1	-1.693182	-0.392202	-2.501521
1	-2.672255	-1.766631	-3.048877
1	-1.339939	-2.025262	-1.909720
6	2.409529	-0.695292	0.150734
6	2.893039	-1.310012	-1.021001
6	4.022295	-2.127137	-0.954745
1	4.396004	-2.597552	-1.869705
6	4.691182	-2.355401	0.251973
6	4.202714	-1.736987	1.403789
1	4.715742	-1.898865	2.356714
6	3.075593	-0.909967	1.369889
6	2.191026	-1.076389	-2.337500
1	2.725945	-1.545842	-3.174387
1	2.101720	0.000270	-2.555219
1	1.168284	-1.486541	-2.323676
6	5.901232	-3.252400	0.296754
1	5.621811	-4.302764	0.117062
1	6.404264	-3.202603	1.272516
1	6.632167	-2.973405	-0.477191
6	2.586887	-0.230042	2.626350
1	1.520785	-0.438252	2.809429
1	2.691900	0.864444	2.547255
1	3.148816	-0.556941	3.512032
6	-1.232672	2.021387	-0.105215
8	-2.220592	2.734821	-0.133144

15-P-1B

SCF energy = -1147.544980770 a.u.

7	0.303209	-0.090319	0.747626
1	0.205698	-1.016414	1.140679
5	-0.720807	0.905613	0.707346
5	1.516494	0.393209	0.136507
6	-0.112261	2.187459	0.020369
6	-0.628949	3.451983	-0.239169
1	-1.651799	3.708411	0.049802
6	0.184476	4.406918	-0.865990
1	-0.210565	5.404327	-1.073101
6	1.495704	4.096949	-1.221362
1	2.115972	4.853156	-1.708624
6	2.024491	2.826300	-0.952062
1	3.058236	2.591461	-1.222725
6	1.223700	1.875421	-0.329888
6	-3.167971	-0.215759	0.615714
6	-3.132085	-1.579913	0.932454
6	-4.028599	-2.444409	0.293814
1	-4.009455	-3.508489	0.549134
6	-4.945116	-1.986168	-0.650190
6	-4.954559	-0.619621	-0.952373
1	-5.668085	-0.241000	-1.690573
6	-4.084810	0.276193	-0.334157
6	-2.159420	-2.143449	1.941323
1	-2.649807	-2.893296	2.578550
1	-1.748002	-1.372301	2.607403
1	-1.321984	-2.655195	1.437826
6	-5.926144	-2.921707	-1.306956
1	-5.636770	-3.972995	-1.170330
1	-6.006296	-2.725616	-2.386432
1	-6.932480	-2.794577	-0.876414
6	-4.124185	1.745669	-0.672033
1	-4.357013	2.346702	0.219227
1	-4.881710	1.956281	-1.438803
1	-3.151746	2.093926	-1.055275
6	2.839984	-0.435805	-0.000291
6	2.982501	-1.393844	-1.022737
6	4.174067	-2.113026	-1.130974
1	4.280184	-2.851047	-1.932369

6	5.235390	-1.911160	-0.243856
6	5.081877	-0.953901	0.760857
1	5.904006	-0.776245	1.461041
6	3.903673	-0.214254	0.894304
6	1.858656	-1.622707	-2.005572
1	2.130783	-2.366210	-2.767104
1	1.591822	-0.689366	-2.527481
1	0.946929	-1.977935	-1.499815
6	6.498400	-2.724955	-0.358018
1	6.378566	-3.703975	0.134078
1	7.350440	-2.218541	0.117317
1	6.757143	-2.917531	-1.409529
6	3.762517	0.803677	2.000635
1	3.012356	0.483203	2.741563
1	3.431003	1.778351	1.608945
1	4.711091	0.957980	2.533095
6	-2.209613	0.754887	1.266418
8	-2.562469	1.472049	2.185714

16

SCF energy = -1149.912118920 a.u.

9	0.000000	2.470925	-0.065771
9	-1.120285	1.356010	-1.533100
9	-1.881578	1.576307	0.478007
9	2.305911	0.841341	0.478007
9	1.734482	0.292190	-1.533100
9	2.139884	-1.235463	-0.065771
9	-0.614197	-1.648200	-1.533100
9	-0.424333	-2.417648	0.478007
9	-2.139884	-1.235463	-0.065771
8	0.000000	0.000000	2.898510
6	-0.762583	1.384087	-0.252107
6	1.579946	-0.031627	-0.252107
6	-0.817362	-1.352460	-0.252107
6	0.000000	0.000000	1.779821
5	0.000000	0.000000	0.186853

CO

SCF energy = -113.185369295 a.u.

8	0.000000	0.000000	0.483491
6	0.000000	0.000000	-0.644655

Table A.2. Cartesian coordinates of the optimized gas-phase geometries (at the B3LYP-D3/6-31++G(d,p) level) implicated in the studied cycloaddition reaction of 1,2-epoxybutane and CO_2, catalysed by atranes **1**–**8**.

1,2-epoxybutane

SCF energy = -232.455391869 a.u.

8	1.103525	0.915818	-0.235755
1	1.828880	-0.963774	-0.975628
1	2.595439	-0.385729	0.599427
6	0.390789	-0.131144	0.485635
1	0.313671	0.076700	1.554399
6	-0.863223	-0.657505	-0.164538
1	-1.098867	-1.625011	0.298438
1	-0.661706	-0.846382	-1.225612
6	-2.047994	0.301792	-0.006419
1	-2.265830	0.486965	1.052026
1	-1.837273	1.266304	-0.481455
1	-2.950606	-0.111696	-0.468509
6	1.728442	-0.383797	-0.059186

CO_2

SCF energy = -188.586479494 a.u.

6	0.000000	0.000000	0.000000
8	0.000000	0.000000	1.169483
8	0.000000	0.000000	-1.169483

Bromide

SCF energy = -2571.88184219 a.u.

35	0.000000	0.000000	0.000000

1

SCF energy = -541.328761822 a.u.

5	0.001186	-0.000031	-0.884328
6	1.343814	-0.563206	1.144506
6	2.182739	-0.285561	-0.107652
6	-0.185193	1.445494	1.143513
6	-0.843858	2.032158	-0.109696
6	-1.161771	-0.882058	1.142993
6	-1.339178	-1.746592	-0.109898
1	2.530373	0.757099	-0.124810
1	-0.976427	-1.448278	2.058724
1	-2.345118	-2.170643	-0.169734
1	-0.610352	-2.569292	-0.125923
1	3.053576	-0.944112	-0.165643
1	1.231965	-1.640215	1.285040
1	1.740139	-0.118110	2.059960
1	-1.920425	1.810615	-0.127717
1	-0.709618	3.115586	-0.168218
1	-0.769323	1.567566	2.058610
1	0.803483	1.886541	1.284775
1	-2.037559	-0.245105	1.282234
7	-0.000769	-0.000213	0.805711
8	1.304595	-0.545274	-1.206961
8	-0.178577	1.401082	-1.208108
8	-1.122341	-0.855985	-1.208459

2

SCF energy = -1510.19076077 a.u.

5	0.000503	0.000543	-0.673638
6	-1.365138	0.446775	1.495324
6	-2.409489	0.017477	0.477180
6	0.295531	-1.400912	1.497308
6	1.189697	-2.092252	0.481362
6	1.066342	0.959300	1.495870
6	1.219212	2.076518	0.477741
1	-2.544629	-1.068153	0.467951
1	0.786029	1.316752	2.491254
1	2.107286	2.672957	0.697351
1	0.346662	2.735938	0.463887
1	-3.369846	0.490906	0.693560
1	-1.353262	1.535363	1.571876
1	-1.535957	0.027641	2.491411
1	2.197919	-1.668430	0.470930
1	1.259222	-3.160235	0.700000
1	0.742281	-1.336739	2.494057
1	-0.652888	-1.934535	1.571537
1	2.002100	0.402837	1.572196
7	-0.001676	0.002208	1.012500
16	-1.765601	0.598081	-1.146815
16	0.364211	-1.829722	-1.142668
16	1.404350	1.227022	-1.145145

3_{nn}

SCF energy = -827.890636980 a.u.

5	-0.000255	-0.000310	-0.969318
6	-1.231161	-1.355156	1.110154
6	-1.187885	-1.978781	-0.318720
6	1.791120	-0.390410	1.107748
6	2.307545	-0.038377	-0.321122
6	-0.556050	1.746179	1.108752
6	-1.121787	2.016142	-0.319627
1	-0.346112	-2.682902	-0.380094
1	-1.287016	1.944181	1.895996
1	-1.145333	3.093068	-0.514420
1	-2.150984	1.634577	-0.376716
1	-2.111284	-2.534415	-0.510955
1	-2.198862	-0.879046	1.298658
1	-1.036720	-2.088686	1.896064
1	2.493842	1.043286	-0.380114
1	3.250706	-0.558655	-0.516270
1	2.329575	0.144396	1.893566
1	1.861257	-1.466584	1.295694
1	0.340555	2.346679	1.295488
15	0.001019	0.000680	1.009713
8	-1.058716	-0.955133	-1.307645
8	1.355323	-0.438105	-1.309244
8	-0.299649	1.392973	-1.308001

3_{xx}

SCF energy = -827.921081219 a.u.

5	-1.448980	-0.006065	0.005155
6	0.990284	-0.422986	-1.699373
6	-0.417277	-0.003206	-2.133366
6	0.988969	1.686767	0.475074
6	-0.414321	1.849441	1.066815
6	1.003841	-1.252167	1.214395
6	-0.398566	-1.850516	1.069619
1	-0.511994	1.086994	-2.160819
1	1.717119	-2.085341	1.206395
1	-0.600521	-2.523666	1.907800
1	-0.489464	-2.419665	0.138975
1	-0.626319	-0.393875	-3.133458
1	1.088654	-1.513360	-1.775791
1	1.695908	0.002025	-2.423530
1	-0.499501	1.330742	2.027010
1	-0.625132	2.910686	1.227606
1	1.699411	2.103812	1.199175
1	1.077629	2.297868	-0.432074
1	1.099425	-0.772830	2.196916
15	1.706698	0.007054	-0.005406
8	-1.414662	-0.563512	-1.253228
8	-1.417829	1.362427	0.150984
8	-1.404805	-0.816772	1.117009

4_{nn}

SCF energy = -1796.78650553 a.u.

5	0.000802	0.000271	-0.835402
6	-1.140388	1.371830	1.539139
6	-2.041035	1.570192	0.300669
6	-0.619721	-1.672117	1.539252
6	-0.341369	-2.552456	0.301619
6	1.756922	0.299825	1.540641
6	2.380964	0.980759	0.303297
1	-2.781559	0.766983	0.236580
1	1.862427	0.909022	2.443534
1	3.472059	0.968350	0.371609
1	2.056986	2.024133	0.239762
1	-2.576616	2.520982	0.367746
1	-0.524679	2.259437	1.715769
1	-1.721033	1.157780	2.441711
1	0.724010	-2.794305	0.238932
1	-0.898371	-3.490746	0.368930
1	-0.144989	-2.068116	2.442210
1	-1.696274	-1.581625	1.715395
1	2.216911	-0.677450	1.717447
15	-0.000633	0.000361	1.117738
16	-1.025915	1.590723	-1.250909
16	-0.863121	-1.684108	-1.251487
16	1.891810	0.094047	-1.249878

4_{xx}

SCF energy = -1796.75528408 a.u.

5	1.374921	-0.000441	-0.001646
6	-1.455577	1.622506	-0.730973
6	-0.132805	1.819721	-1.484431
6	-1.456944	-1.444799	-1.036908
6	-0.133700	-2.195438	-0.832988
6	-1.452998	-0.176427	1.772489
6	-0.129005	0.376081	2.318019
1	0.002384	1.074415	-2.269840
1	-2.247543	0.298545	2.363013
1	-0.125427	0.285290	3.408945

1	0.007136	1.428635	2.064679
1	-0.130695	2.809953	-1.951227
1	-1.531172	2.341957	0.094318
1	-2.251608	1.895271	-1.436484
1	0.003775	-2.502672	0.204961
1	-0.132405	-3.094887	-1.456934
1	-2.252646	-2.192356	-0.919805
1	-1.533669	-1.089131	-2.072308
1	-1.529264	-1.250858	1.982630
15	-2.074014	0.000712	0.002354
16	1.344441	1.792295	-0.368287
16	1.342094	-1.214816	-1.370573
16	1.346147	-0.578885	1.734467

5

SCF energy = -758.939525983 a.u.

13	0.001765	0.000880	-1.065538
6	0.361179	-1.413211	1.239132
6	1.239108	-1.973417	0.102214
6	1.038457	1.020610	1.241916
6	1.088246	2.059943	0.103936
6	-1.407611	0.389656	1.237821
6	-2.328920	-0.087354	0.097187
1	2.264613	-1.586115	0.187877
1	-1.713582	-0.020443	2.206612
1	-3.298447	0.415138	0.188226
1	-2.504585	-1.169741	0.178212
1	1.286602	-3.064387	0.193642
1	-0.567798	-1.986119	1.294658
1	0.865352	-1.473171	2.209991
1	0.237834	2.752229	0.184317
1	2.007345	2.648955	0.199361
1	0.834819	1.488296	2.211480
1	1.998885	0.502476	1.301526
1	-1.439863	1.480454	1.297282
7	-0.001993	-0.000639	0.908460
8	0.686901	-1.621610	-1.179122
8	1.068018	1.403844	-1.176448
8	-1.745285	0.221277	-1.181134

6*nn*

SCF energy = -1045.49796393 a.u.

13	0.000065	0.000214	-1.161011
6	-0.398829	1.808825	1.211499
6	-1.098963	2.219464	-0.118530
6	-1.366149	-1.251068	1.211622
6	-1.372964	-2.061133	-0.119444
6	1.766309	-0.558485	1.210982
6	2.471833	-0.158961	-0.119522
1	-2.146402	1.885999	-0.085025
1	2.319391	-0.178391	2.074867
1	3.422779	-0.703888	-0.169893
1	2.708393	0.914561	-0.086665
1	-1.104097	3.315452	-0.168703
1	0.578145	2.298998	1.295251
1	-1.003494	2.098000	2.076054
1	-0.560068	-2.801158	-0.087898
1	-2.319381	-2.613882	-0.169301
1	-1.312691	-1.920412	2.075221
1	-2.279675	-0.651305	1.296930
1	1.702865	-1.649535	1.295793
15	-0.000046	-0.000157	1.147944
8	-0.456033	1.714009	-1.296615
8	-1.257956	-1.250639	-1.297174
8	1.712320	-0.461708	-1.297747

6*xx*

SCF energy = -1045.50128751 a.u.

13	1.453032	-0.050978	-0.210957
6	-0.909262	1.492059	1.172400
6	0.350851	2.208835	0.675412
6	-1.358587	0.202608	-1.595322
6	-0.174194	-0.490978	-2.276834
6	-1.055243	-1.579548	0.904372
6	0.336393	-1.735604	1.526784
1	0.201354	2.584355	-0.346492
1	-1.781312	-1.880967	1.668765
1	0.414443	-2.747004	1.943280
1	0.466439	-1.027794	2.357422
1	0.527903	3.077528	1.320772
1	-0.742230	1.123378	2.192375
1	-1.698716	2.249560	1.244081
1	-0.197134	-1.571774	-2.079141
1	-0.274050	-0.354280	-3.360262
1	-2.268125	-0.172360	-2.079598
1	-1.321047	1.279676	-1.802041
1	-1.167564	-2.289811	0.075574
15	-1.756801	0.061434	0.255741
8	1.526446	1.381608	0.738706
8	1.095881	0.063409	-1.890042

8	1.398035	-1.584209	0.567676

7

SCF energy = -2720.36372506 a.u.

5	1.728128	-0.001587	0.001111
6	-0.681098	-1.626170	-0.839571
6	0.719221	-2.110414	-0.475497
6	-0.681440	0.085966	1.827312
6	0.719242	0.642386	2.065202
6	-0.677029	1.540926	-0.988268
6	0.723866	1.467204	-1.588107
1	0.792809	-2.360401	0.588126
1	-1.383779	1.759709	-1.796312
1	0.978656	2.416463	-2.069835
1	0.797637	0.671610	-2.336990
1	0.972531	-3.003234	-1.055789
1	-0.734474	-1.440306	-1.919537
1	-1.389484	-2.433607	-0.623791
1	0.794182	1.688368	1.748844
1	0.972088	0.586518	3.128668
1	-1.389591	0.675787	2.419833
1	-0.735202	-0.943175	2.204223
1	-0.730591	2.382447	-0.286305
33	-1.491508	0.001339	-0.001251
8	1.703441	-1.109805	-0.815296
8	1.702380	-0.153990	1.369160
8	1.706399	1.259319	-0.550344

8

SCF energy = -2937.95337086 a.u.

13	1.510556	-0.004970	-0.010424
6	-0.639735	-1.577942	0.977419
6	0.374056	-1.280077	2.079655
6	-0.630339	1.636344	0.884888
6	0.373157	2.441523	0.062560
6	-0.654425	-0.050778	-1.850659
6	0.343756	-1.166663	-2.149319
1	-0.076113	-0.640191	2.850439
1	-1.526818	-0.178642	-2.498816
1	0.619513	-1.121400	-3.210831
1	-0.116669	-2.148145	-1.973830
1	0.658088	-2.223229	2.564113
1	-0.220744	-2.277785	0.247377
1	-1.505856	-2.075425	1.424511
1	-0.088252	2.787793	-0.871976
1	0.663379	3.333808	0.632200
1	-1.494164	2.272155	1.101898
1	-0.199380	1.355008	1.850911
1	-0.224844	0.925984	-2.094743
33	-1.468891	0.004987	0.010035
8	1.564827	-0.644243	1.594979
8	1.561334	1.704826	-0.258593
8	1.542492	-1.076126	-1.366906

1-TS-1

SCF energy = -773.770941820 a.u.

ν = -108.3655 cm^{-1}

5	-0.184016	-0.207682	0.221798
6	-3.024675	-0.409836	0.946466
6	-1.834544	-0.608843	1.901204
6	-2.328149	1.774253	-0.095039
6	-0.823759	2.036747	-0.285168
6	-2.549474	-0.288309	-1.522426
6	-1.352593	-1.253901	-1.582320
1	-1.588413	0.333004	2.405745
1	-3.450863	-0.859437	-1.792196
1	-1.178544	-1.573161	-2.615056
1	-1.550171	-2.144380	-0.973907
1	-2.085737	-1.352805	2.664081
1	-3.378136	-1.389355	0.608648
1	-3.841205	0.048564	1.524967
1	-0.544864	1.909669	-1.337974
1	-0.581177	3.061575	0.013870
1	-2.869001	2.411178	-0.811566
1	-2.621575	2.096477	0.909186
1	-2.419268	0.487849	-2.283505
7	-2.728007	0.380813	-0.240876
8	-0.690310	-1.090373	1.181541
8	-0.051737	1.148655	0.535270
8	-0.162424	-0.600419	-1.120859
8	1.903264	-0.672026	0.643773
1	3.140481	-2.418422	0.608420
1	1.737707	-2.408553	-0.597533
6	2.848750	-0.497739	-0.458221
1	2.359110	-0.112630	-1.352153
6	4.161438	0.143267	-0.095442
1	4.872447	-0.072550	-0.903711
1	4.551039	-0.328044	0.814340
6	4.025033	1.657460	0.098018
1	3.654955	2.137998	-0.815061

1	3.321134	1.884742	0.905829
1	4.990387	2.108335	0.350307
6	2.462553	-1.842104	-0.017638

1-I-1

SCF energy = -773.773404434 a.u.

5	0.076166	-0.263454	0.226831
6	-2.955843	-0.473968	0.914718
6	-1.733461	-0.695669	1.818295
6	-2.273553	1.766339	0.035680
6	-0.768945	1.996732	-0.171963
6	-2.500297	-0.175929	-1.526447
6	-1.299270	-1.130514	-1.607896
1	-1.488295	0.234662	2.345628
1	-3.374712	-0.750128	-1.870572
1	-1.163199	-1.429217	-2.654480
1	-1.504258	-2.037129	-1.025275
1	-1.991930	-1.448658	2.572605
1	-3.295818	-1.439736	0.525697
1	-3.757057	-0.095499	1.568719
1	-0.523724	1.902094	-1.237141
1	-0.530394	3.022088	0.135463
1	-2.787243	2.492021	-0.614321
1	-2.537621	2.023707	1.066916
1	-2.358009	0.641768	-2.241106
7	-2.793314	0.425058	-0.226517
8	-0.587296	-1.171439	1.115382
8	0.053317	1.120211	0.595549
8	-0.079415	-0.536443	-1.171570
8	1.690523	-0.637520	0.554361
1	2.896931	-2.389206	0.705215
1	1.622440	-2.419032	-0.641279
6	2.749490	-0.525161	-0.486404
1	2.333373	-0.175264	-1.427685
6	4.011202	0.136466	-0.013806
1	4.799973	-0.137595	-0.726355
1	4.294000	-0.279595	0.959463
6	3.869177	1.659943	0.063562
1	3.605189	2.079804	-0.913605
1	3.085765	1.941936	0.774442
1	4.807959	2.119331	0.388462
6	2.305161	-1.843732	-0.023922

2-I-1

SCF energy = -1742.62065203 a.u.

5	-0.283874	-0.266577	-0.150820
6	3.104318	-0.491123	-0.864409
6	2.037099	-0.832659	-1.910854
6	2.475711	1.821315	-0.172636
6	1.063718	2.356941	0.096902
6	2.726941	0.027365	1.544728
6	1.672754	-1.008914	1.954775
1	1.716251	0.071827	-2.435252
1	3.719891	-0.400087	1.776046
1	1.789610	-1.262826	3.013872
1	1.787041	-1.923748	1.367184
1	2.447905	-1.529261	-2.649779
1	3.439246	-1.413479	-0.379027
1	3.977506	-0.077258	-1.401576
1	0.821382	2.266834	1.159513
1	1.010802	3.416616	-0.176047
1	3.183610	2.449852	0.398558
1	2.714610	1.958174	-1.232134
1	2.613478	0.919986	2.168212
7	2.633313	0.420662	0.155703
16	0.547059	-1.649957	-1.209444
16	-0.255679	1.514957	-0.868933
16	-0.053645	-0.406832	1.759850
8	-1.863966	-0.629530	-0.454456
1	-3.043504	-2.373500	-0.798897
1	-1.924527	-2.460147	0.678345
6	-3.037562	-0.563128	0.482757
1	-2.733968	-0.252921	1.479784
6	-4.248809	0.106074	-0.095111
1	-5.105159	-0.255710	0.489601
1	-4.391763	-0.239523	-1.124674
6	-4.168602	1.633762	-0.032227
1	-4.051899	1.978211	1.001495
1	-3.313964	2.002386	-0.607736
1	-5.080510	2.081675	-0.439091
6	-2.539217	-1.860185	0.014051

3-I-1

SCF energy = -1060.38630888 a.u.

5	-0.279937	-0.295809	-0.242114
6	2.777367	-0.734147	-1.184491
6	1.444029	-0.756837	-1.937937
6	2.024658	1.955102	-0.123820
6	0.524742	1.990200	0.185115
6	2.275576	-0.373494	1.737187

6	1.047614	-1.276533	1.589998
1	1.230189	0.233641	-2.356504
1	3.068921	-0.977638	2.195760
1	0.806204	-1.696234	2.574360
1	1.271811	-2.113227	0.918180
1	1.533371	-1.458662	-2.776002
1	3.007265	-1.737619	-0.803432
1	3.558673	-0.499103	-1.918708
1	0.356085	1.806929	1.252744
1	0.150222	2.995881	-0.041302
1	2.488529	2.773463	0.441733
1	2.190995	2.184130	-1.184423
1	2.058577	0.436218	2.445949
15	3.081022	0.444672	0.248016
8	0.346041	-1.205264	-1.147258
8	-0.246704	1.084928	-0.599578
8	-0.115377	-0.584096	1.146494
8	-1.925543	-0.643784	-0.549416
1	-3.181022	-2.364597	-0.650878
1	-1.881712	-2.408491	0.671183
6	-2.959584	-0.486685	0.507240
1	-2.516441	-0.134460	1.435483
6	-4.212104	0.202974	0.049632
1	-4.992208	-0.029936	0.785914
1	-4.530570	-0.224581	-0.907504
6	-4.024314	1.719273	-0.065464
1	-3.721990	2.151499	0.895098
1	-3.250964	1.960576	-0.801899
1	-4.956148	2.201639	-0.376852
6	-2.560110	-1.823975	0.057456

4-I-1

SCF energy = -2029.22438320 a.u.

5	-0.557293	-0.302582	-0.162548
6	3.002593	-0.832925	-1.122015
6	1.726522	-0.904287	-1.969608
6	2.343576	2.008521	-0.309976
6	0.890041	2.273983	0.103186
6	2.600562	-0.158166	1.801749
6	1.425927	-1.140376	1.892383
1	1.429847	0.085706	-2.325086
1	3.457864	-0.661012	2.268854
1	1.433314	-1.593141	2.889692
1	1.523382	-1.947334	1.162369
1	1.935649	-1.520250	-2.850898
1	3.196957	-1.797265	-0.636042
1	3.832033	-0.684239	-1.826176
1	0.727628	2.025223	1.154839
1	0.692967	3.345099	-0.014807
1	2.938254	2.826842	0.117282
1	2.458250	2.097751	-1.397599
1	2.408083	0.729373	2.417506
15	3.316052	0.478684	0.185289
16	0.256037	-1.698512	-1.204529
16	-0.431914	1.464908	-0.885963
16	-0.259108	-0.422189	1.732789
8	-2.122579	-0.609703	-0.438237
1	-3.372430	-2.312851	-0.733560
1	-2.237154	-2.417818	0.730361
6	-3.281708	-0.484294	0.517767
1	-2.949948	-0.167376	1.503553
6	-4.473145	0.221169	-0.056308
1	-5.333015	-0.095534	0.549095
1	-4.646009	-0.139100	-1.076106
6	-4.332048	1.745312	-0.025300
1	-4.183154	2.104875	0.999031
1	-3.474762	2.068821	-0.623459
1	-5.233268	2.220204	-0.425090
6	-2.838720	-1.806440	0.064589

5-I-1

SCF energy = -991.434009708 a.u.

13	0.146937	-0.189047	-0.173180
6	2.916487	-0.796861	-0.457921
6	2.113735	-1.329721	-1.654658
6	2.312642	1.621502	-0.537017
6	0.978243	2.377668	-0.449951
6	2.270987	0.398039	1.633228
6	1.299557	-0.620009	2.249843
1	2.231091	-0.657080	-2.518975
1	3.305442	0.232068	1.960625
1	1.174376	-0.392812	3.316985
1	1.722385	-1.634832	2.181644
1	2.519021	-2.307023	-1.948965
1	3.009848	-1.588820	0.289919
1	3.926222	-0.478045	-0.747258
1	0.858016	2.818805	0.552201
1	0.991141	3.207775	-1.168725
1	3.144016	2.199974	-0.113736
1	2.538472	1.416184	-1.586680

1	1.974350	1.405351	1.937433
7	2.150788	0.317959	0.155259
8	0.740329	-1.448875	-1.307041
8	-0.101193	1.496973	-0.732271
8	0.046434	-0.563887	1.582052
8	-1.721013	-0.659620	-0.526923
1	-2.922363	-2.394265	-0.835933
1	-1.733527	-2.509591	0.577469
6	-2.838637	-0.594903	0.451380
1	-2.485309	-0.291155	1.434238
6	-4.076138	0.082349	-0.062160
1	-4.903279	-0.228896	0.589167
1	-4.296899	-0.289821	-1.068796
6	-3.942914	1.608548	-0.061942
1	-3.738463	1.984538	0.946924
1	-3.123022	1.927803	-0.713145
1	-4.865994	2.076688	-0.418116
6	-2.368578	-1.890224	-0.048849

6-I-1

SCF energy = -1278.01615041 a.u.

13	-0.340986	-0.311459	-0.258875
6	2.927385	-0.967826	-0.973745
6	1.724022	-1.077556	-1.919203
6	2.218850	1.934538	-0.398503
6	0.744527	2.217973	-0.082320
6	2.320470	-0.086724	1.870372
6	1.157592	-1.085741	1.930749
1	1.599628	-0.134793	-2.472289
1	3.136935	-0.517052	2.464306
1	1.018819	-1.365296	2.984918
1	1.431215	-2.004714	1.391154
1	1.959064	-1.853110	-2.661875
1	3.025005	-1.896583	-0.396758
1	3.821430	-0.909621	-1.607596
1	0.585449	2.188243	1.005925
1	0.530539	3.246313	-0.406515
1	2.792682	2.791580	-0.023365
1	2.363552	1.925749	-1.486614
1	2.032612	0.842266	2.379426
15	3.163602	0.439095	0.264242
8	0.507644	-1.448021	-1.277791
8	-0.172251	1.355844	-0.747336
8	-0.081058	-0.573020	1.451976
8	-2.164572	-0.687384	-0.516297
1	-3.539197	-2.310908	-0.668826
1	-2.294293	-2.477077	0.691563
6	-3.229597	-0.477582	0.528296
1	-2.791535	-0.161782	1.473156
6	-4.411225	0.301101	0.035752
1	-5.222405	0.125424	0.754252
1	-4.734481	-0.106217	-0.928248
6	-4.107144	1.798732	-0.073032
1	-3.796253	2.207886	0.894658
1	-3.302047	1.981349	-0.791994
1	-4.993821	2.347048	-0.405313
6	-2.905250	-1.829500	0.069527

7-I-1

SCF energy = -2952.82819253 a.u.

5	0.666697	-0.350848	0.251667
6	-2.345392	-0.901671	1.327976
6	-0.987968	-0.830273	2.022248
6	-1.646921	1.919293	0.200561
6	-0.171363	1.931490	-0.189410
6	-1.894129	-0.526515	-1.738610
6	-0.661335	-1.406277	-1.549395
1	-0.800533	0.183086	2.396278
1	-2.675840	-1.132628	-2.211881
1	-0.398206	-1.861604	-2.512707
1	-0.872877	-2.219645	-0.845354
1	-0.996140	-1.505640	2.887080
1	-2.514870	-1.916305	0.945203
1	-3.121487	-0.718853	2.080767
1	-0.055487	1.715827	-1.258116
1	0.234674	2.934863	-0.009092
1	-2.141153	2.750584	-0.316379
1	-1.750755	2.115264	1.275433
1	-1.665902	0.288427	-2.437445
33	-2.789246	0.329767	-0.175489
8	0.092167	-1.256314	1.191449
8	0.622590	1.034208	0.584906
8	0.486476	-0.672648	-1.125603
8	2.342535	-0.653249	0.529116
1	3.681960	-2.311753	0.569196
1	2.361778	-2.389971	-0.730557
6	3.345466	-0.420724	-0.539552
1	2.868884	-0.071167	-1.452413
6	4.569784	0.321655	-0.087071
1	5.349282	0.146021	-0.839658

1	4.924193	-0.109946	0.855559
6	4.306436	1.823587	0.065727
1	3.972469	2.261434	-0.881806
1	3.528925	2.008517	0.813923
1	5.215954	2.345692	0.379187
6	3.021526	-1.786605	-0.114699

8-I-1

SCF energy = -3170.46044798 a.u.

13	-0.698179	-0.348298	-0.244420
6	2.490531	-1.340438	-0.874205
6	1.308840	-1.446592	-1.836392
6	1.893003	1.789452	-0.787357
6	0.464095	2.185482	-0.420830
6	1.884435	0.096217	1.912960
6	0.746154	-0.909347	2.078028
1	1.279591	-0.572923	-2.504798
1	2.682640	-0.177305	2.612896
1	0.560599	-1.043919	3.153796
1	1.045157	-1.892865	1.684772
1	1.464943	-2.327361	-2.476373
1	2.450207	-2.164642	-0.150942
1	3.412340	-1.479515	-1.451230
1	0.375329	2.330751	0.666469
1	0.247340	3.158169	-0.886203
1	2.538743	2.661554	-0.630980
1	1.947245	1.550505	-1.856829
1	1.539278	1.093804	2.212177
33	2.860271	0.323953	0.177209
8	0.058320	-1.614845	-1.176786
8	-0.515483	1.263691	-0.883543
8	-0.476455	-0.486373	1.483778
8	-2.538288	-0.675219	-0.481945
1	-3.960968	-2.256408	-0.624465
1	-2.727026	-2.447053	0.741861
6	-3.597601	-0.419914	0.554106
1	-3.152728	-0.108581	1.497160
6	-4.751288	0.390788	0.046583
1	-5.574472	0.246589	0.758368
1	-5.078016	-0.013673	-0.917456
6	-4.399501	1.877413	-0.071369
1	-4.093581	2.286526	0.897958
1	-3.575980	2.028257	-0.776827
1	-5.262872	2.449179	-0.424947
6	-3.314524	-1.786680	0.110664

1-TS-2A

SCF energy = -1547.54675700 a.u.

ν = -463.9370 cm^{-1}

5	3.837168	0.315452	-0.296040
6	6.488546	-1.358675	-0.811891
6	5.885285	-0.180173	-1.590557
6	6.445119	-0.255838	1.426634
6	5.263241	0.689052	1.693737
6	5.079525	-2.306069	1.016481
6	3.728543	-2.082438	0.320439
1	6.326570	0.758729	-1.232131
1	5.346499	-3.359284	0.835190
1	2.998120	-2.767675	0.770972
1	3.815943	-2.345026	-0.741890
1	6.166935	-0.294753	-2.645478
1	6.168077	-2.299078	-1.273543
1	7.578595	-1.291438	-0.956083
1	4.520539	0.174688	2.317272
1	5.640459	1.544880	2.268832
1	6.819391	-0.560119	2.417063
1	7.253231	0.304321	0.943839
1	4.949665	-2.195893	2.098723
7	6.197798	-1.450837	0.619169
8	4.466628	-0.103829	-1.534516
8	4.643715	1.203844	0.522949
8	3.219526	-0.764290	0.457586
8	2.671838	1.252290	-0.814265
1	0.739830	1.011524	-1.936950
1	1.194254	-0.448780	-0.853713
6	1.537919	1.517933	0.058917
1	1.672463	1.070543	1.043458
6	1.137568	2.973041	0.108808
1	0.160665	3.027444	0.604344
1	1.006606	3.346074	-0.913328
6	2.161181	3.822956	0.867323
1	2.287569	3.461580	1.894234
1	3.138978	3.787971	0.377536
1	1.837565	4.867758	0.912076
6	1.045824	0.612833	-0.979713
5	-4.127982	-0.590747	-0.177965
6	-1.279148	-1.135289	-1.388399
6	-2.663590	-1.594150	-1.864148
6	-1.864321	1.297647	-1.246359

6	-3.291786	1.623938	-0.790425
6	-1.215787	0.031943	0.831276
6	-2.331505	-0.799583	1.475248
1	-3.052052	-0.890092	-2.609448
1	-0.271304	-0.421827	1.159814
1	-2.215439	-0.721774	2.562567
1	-2.212924	-1.854628	1.201770
1	-2.536828	-2.564564	-2.357653
1	-0.825438	-1.911953	-0.764826
1	-0.660930	-1.044718	-2.293321
1	-3.285282	1.912455	0.267542
1	-3.630773	2.490881	-1.369177
1	-1.266703	2.192414	-1.035185
1	-1.847287	1.149786	-2.330464
1	-1.237867	1.052925	1.223899
7	-1.194436	0.131414	-0.639567
8	-3.610756	-1.768618	-0.815580
8	-4.230734	0.575772	-1.005654
8	-3.643988	-0.354121	1.152698
8	-5.728603	-0.994510	0.001990
1	-6.863547	-2.645119	0.730901
1	-5.330290	-2.253191	1.697095
6	-6.544400	-0.491286	1.146214
1	-5.950191	0.148432	1.793599
6	-7.904056	0.008832	0.756031
1	-8.506064	0.035249	1.673568
1	-8.373947	-0.713854	0.080204
6	-7.846244	1.399484	0.115894
1	-7.393571	2.127642	0.798258
1	-7.249895	1.380803	-0.802002
1	-8.852039	1.749563	-0.136241
6	-6.153593	-1.902781	1.082792

5-TS-2A

SCF energy = -1982.83457641 a.u.

ν = -488.2533 cm^{-1}

13	-4.108861	0.153162	0.161026
6	-6.015200	-1.944628	0.762029
6	-5.730494	-1.080892	1.998424
6	-6.805723	-0.206951	-0.829347
6	-6.166510	1.059229	-1.415782
6	-5.163720	-1.918218	-1.571744
6	-3.662373	-2.116354	-1.322618
1	-6.554310	-0.365964	2.156250
1	-5.690661	-2.873759	-1.698499
1	-3.188491	-2.462127	-2.251994
1	-3.506767	-2.905964	-0.569365
1	-5.694306	-1.728476	2.885583
1	-5.338513	-2.803596	0.763786
1	-7.046616	-2.322702	0.750702
1	-5.831877	0.869405	-2.448816
1	-6.926377	1.851539	-1.466261
1	-7.509156	-0.677542	-1.529859
1	-7.355770	0.060050	0.077041
1	-5.298224	-1.332613	-2.485177
7	-5.718457	-1.135856	-0.443003
8	-4.501629	-0.391805	1.837443
8	-5.074134	1.470407	-0.610549
8	-3.077113	-0.900100	-0.890050
8	-2.717250	1.302146	0.735460
1	-0.787409	0.982938	1.911768
1	-1.198018	-0.404309	0.725035
6	-1.557030	1.611597	-0.058947
1	-1.638277	1.234092	-1.080579
6	-1.168010	3.073665	-0.015877
1	-0.183422	3.177073	-0.487817
1	-1.066984	3.387400	1.029708
6	-2.193849	3.948367	-0.743017
1	-2.287086	3.651326	-1.794099
1	-3.182168	3.858863	-0.281926
1	-1.896208	5.001515	-0.713546
6	-1.028643	0.645285	0.912963
13	4.253179	-0.563852	0.196126
6	1.183087	-1.106398	1.360289
6	2.494707	-1.610572	1.978799
6	1.773769	1.359361	1.284006
6	3.171912	1.831095	0.863602
6	1.170066	0.120713	-0.862507
6	2.212660	-0.742394	-1.586442
1	2.850257	-0.883868	2.722911
1	0.199932	-0.277951	-1.185706
1	1.969841	-0.676084	-2.656196
1	2.078685	-1.793285	-1.292614
1	2.238660	-2.528728	2.525304
1	0.780874	-1.868634	0.686381
1	0.483495	-1.020751	2.204089
1	3.157794	2.101793	-0.201984
1	3.361853	2.755837	1.425896
1	1.118086	2.219921	1.115077
1	1.764518	1.158192	2.359161

1	1.231128	1.152131	-1.221335
7	1.170266	0.177509	0.619745
8	3.526937	-1.911716	1.044485
8	4.227910	0.914106	1.131518
8	3.567625	-0.343356	-1.402506
8	6.053730	-0.995544	-0.048009
1	7.336364	-2.612307	-0.585737
1	5.861698	-2.399054	-1.685246
6	6.926822	-0.523625	-1.184180
1	6.347269	0.038157	-1.914395
6	8.219967	0.083506	-0.732493
1	8.880681	0.096955	-1.609066
1	8.681922	-0.570387	0.015051
6	8.028896	1.500701	-0.182990
1	7.581103	2.157713	-0.936776
1	7.372721	1.493646	0.693346
1	8.990851	1.929365	0.113706
6	6.610582	-1.946075	-1.041887

1-TS-2B

SCF energy = -3345.66505873 a.u.

ν = -395.8527 cm^{-1}

5	-1.012313	0.233532	0.414013
6	-3.926412	-0.913032	0.958317
6	-2.990747	-0.095826	1.861752
6	-3.829359	0.632420	-0.999378
6	-2.486871	1.341965	-1.236839
6	-2.960305	-1.700121	-1.203848
6	-1.534094	-1.928113	-0.680461
1	-3.228366	0.971412	1.762162
1	-3.451106	-2.686292	-1.196438
1	-1.031185	-2.627551	-1.361440
1	-1.578028	-2.405088	0.307297
1	-3.193252	-0.382846	2.902060
1	-3.795605	-1.979229	1.173343
1	-4.951327	-0.651635	1.266765
1	-1.945993	0.837048	-2.047675
1	-2.703600	2.364991	-1.571869
1	-4.354443	0.646409	-1.967853
1	-4.433823	1.227174	-0.305787
1	-2.912831	-1.379797	-2.250462
7	-3.801388	-0.739217	-0.489384
8	-1.607396	-0.311321	1.621538
8	-1.658894	1.437536	-0.085884
8	-0.746115	-0.749978	-0.620970
8	0.382400	0.760319	0.932385
1	2.287621	-0.121786	1.743238
1	1.427821	-1.205101	0.481676
6	1.487794	0.930360	-0.016430
1	1.182121	0.721543	-1.040949
6	2.251414	2.216583	0.157229
1	3.216172	2.075844	-0.343980
1	2.461618	2.362201	1.223549
6	1.504923	3.422279	-0.418371
1	1.312356	3.288873	-1.489286
1	0.540188	3.562735	0.080231
1	2.090980	4.338498	-0.291478
6	1.786099	-0.236647	0.793705
35	4.227353	-1.030349	-0.165374

2-TS-2B

SCF energy = -4314.51727914 a.u.

ν = -345.0941 cm^{-1}

5	-0.704338	0.222403	0.294879
6	-3.860387	-1.277985	0.912641
6	-2.943239	-0.769339	2.031642
6	-4.107690	0.741405	-0.536755
6	-2.996722	1.727923	-0.921919
6	-3.286466	-1.408926	-1.511858
6	-1.838919	-1.916857	-1.481819
1	-3.118976	0.296921	2.202443
1	-3.941036	-2.294784	-1.616185
1	-1.641654	-2.517855	-2.376695
1	-1.678772	-2.549335	-0.604319
1	-3.171350	-1.303373	2.961245
1	-3.698805	-2.352427	0.776178
1	-4.902900	-1.155351	1.262595
1	-2.541760	1.426218	-1.869752
1	-3.427703	2.726916	-1.055254
1	-4.884380	0.804158	-1.322456
1	-4.576220	1.074530	0.395269
1	-3.435221	-0.800870	-2.410348
7	-3.658826	-0.621201	-0.359037
16	-1.148004	-1.011046	1.730813
16	-1.655952	1.913814	0.322035
16	-0.573468	-0.586354	-1.472975
8	0.712916	0.671449	0.745367
1	2.529473	-0.292160	1.587869
1	1.769597	-1.236464	0.162082
6	1.884650	0.939813	-0.121528

1	1.648052	0.843769	-1.180140
6	2.636428	2.187605	0.251359
1	3.651035	2.056659	-0.143451
1	2.721774	2.233145	1.343330
6	1.989734	3.459685	-0.299913
1	1.937154	3.429052	-1.394491
1	0.970012	3.577753	0.080550
1	2.569748	4.342999	-0.013480
6	2.082938	-0.302817	0.605352
35	4.666540	-1.022581	-0.130007

3-TS-2B

SCF energy = -3632.27763397 a.u.

ν = -401.6873 cm^{-1}

5	-0.795373	0.357318	0.434634
6	-3.668391	-0.978640	1.326493
6	-2.662969	-0.060812	2.030524
6	-3.722558	1.002727	-0.896750
6	-2.314667	1.568872	-1.121188
6	-2.620227	-1.740180	-1.352670
6	-1.223585	-1.810937	-0.726345
1	-2.953276	0.987356	1.886822
1	-2.983829	-2.770383	-1.462287
1	-0.602492	-2.467027	-1.351012
1	-1.283503	-2.268749	0.268769
1	-2.713849	-0.269143	3.107561
1	-3.395985	-2.029082	1.492862
1	-4.638760	-0.831740	1.818700
1	-1.826809	1.030712	-1.942904
1	-2.420935	2.616587	-1.432373
1	-4.293836	1.194806	-1.814601
1	-4.227940	1.565299	-0.100722
1	-2.551218	-1.329837	-2.368718
15	-4.018617	-0.812414	-0.510886
8	-1.312709	-0.257431	1.641308
8	-1.483660	1.570711	0.031204
8	-0.563002	-0.560225	-0.661173
8	0.621619	0.883236	0.913501
1	2.491426	-0.068335	1.739146
1	1.571880	-1.139670	0.511967
6	1.729374	0.978749	-0.039973
1	1.413218	0.761439	-1.059229
6	2.547909	2.234834	0.103908
1	3.500401	2.049332	-0.406172
1	2.775665	2.390830	1.165128
6	1.840135	3.457986	-0.484416
1	1.634692	3.315543	-1.551830
1	0.884678	3.638742	0.019401
1	2.458127	4.355327	-0.375693
6	1.982614	-0.182889	0.793428
35	4.342705	-1.149742	-0.167185

4-TS-2B

SCF energy = -4601.12217103 a.u.

ν = -328.9967 cm^{-1}

5	-0.457291	0.304549	0.324341
6	-3.723050	-1.346977	1.253441
6	-2.677994	-0.630178	2.118200
6	-4.045595	1.143812	-0.432427
6	-2.746692	1.841501	-0.859800
6	-3.114165	-1.450630	-1.702045
6	-1.660626	-1.839133	-1.402200
1	-2.843271	0.450594	2.118919
1	-3.626120	-2.374670	-2.002882
1	-1.328911	-2.539658	-2.176384
1	-1.577315	-2.350527	-0.440054
1	-2.798873	-0.977754	3.150293
1	-3.449439	-2.399891	1.110043
1	-4.653335	-1.359760	1.837030
1	-2.327461	1.374816	-1.754969
1	-2.989894	2.878813	-1.115840
1	-4.823491	1.487325	-1.127480
1	-4.362013	1.491823	0.558994
1	-3.163920	-0.788422	-2.575578
15	-4.282296	-0.720581	-0.425834
16	-0.905971	-0.931275	1.745934
16	-1.401719	1.989462	0.384220
16	-0.412523	-0.492935	-1.442724
8	0.972039	0.726455	0.737139
1	2.766995	-0.275493	1.568324
1	1.954314	-1.221156	0.173330
6	2.138674	0.943193	-0.157198
1	1.879385	0.832987	-1.208887
6	2.929351	2.175994	0.179539
1	3.929179	2.016763	-0.241705
1	3.045931	2.233573	1.267910
6	2.295002	3.454396	-0.371713
1	2.209520	3.409499	-1.463664
1	1.289827	3.600239	0.037033
1	2.902027	4.328558	-0.115110

6	2.299285	-0.288890	0.595844
35	4.859135	-1.125883	-0.144553

3-TS-2C

SCF energy = -1888.30402651 a.u.

ν = -451.6666 cm^{-1}

5	2.616142	0.460182	-0.487008
6	5.542668	-0.854430	-1.176592
6	4.785668	0.372400	-1.696724
6	5.154956	0.217128	1.578636
6	3.761034	0.844621	1.689987
6	3.837717	-2.333966	0.763925
6	2.640161	-2.008937	-0.134738
1	5.081297	1.261214	-1.126219
1	4.110008	-3.381096	0.577687
1	1.857909	-2.755584	0.057838
1	2.928619	-2.101767	-1.188944
1	5.086457	0.537289	-2.739585
1	5.269921	-1.739700	-1.765746
1	6.609400	-0.677975	-1.366959
1	3.063339	0.121947	2.130205
1	3.828304	1.697410	2.378323
1	5.494727	0.003913	2.600678
1	5.862048	0.950212	1.168956
1	3.538309	-2.278182	1.818688
15	5.447031	-1.375401	0.625470
8	3.371385	0.235154	-1.698550
8	3.244681	1.349705	0.467317
8	2.062372	-0.737164	0.112987
8	1.380721	1.323159	-1.020841
1	-0.489340	0.989971	-2.244198
1	0.062972	-0.510020	-1.271413
6	0.192414	1.405873	-0.187096
1	0.329030	0.897039	0.767001
6	-0.382449	2.795790	-0.060962
1	-1.388014	2.693488	0.364876
1	-0.495759	3.228216	-1.061881
6	0.480444	3.697545	0.825246
1	0.587003	3.273724	1.830306
1	1.483432	3.815551	0.403812
1	0.030677	4.690884	0.921472
6	-0.156960	0.546397	-1.315543
5	-5.417291	-0.661873	0.742251
6	-3.536455	-1.670748	-1.382705
6	-5.048095	-1.891306	-1.259577
6	-3.907756	1.313116	-0.949713
6	-5.050856	1.577741	0.035299
6	-2.451725	-0.359514	1.130137
6	-3.452547	-1.131519	1.995086
1	-5.602875	-1.127573	-1.813415
1	-1.479044	-0.858711	1.216104
1	-3.132472	-1.101852	3.040135
1	-3.518222	-2.177886	1.681450
1	-5.307948	-2.872747	-1.665653
1	-2.999714	-2.500138	-0.906177
1	-3.279964	-1.701265	-2.448412
1	-4.664459	1.815265	1.031372
1	-5.647864	2.423720	-0.316113
1	-3.277999	2.209790	-0.981294
1	-4.313134	1.177957	-1.959926
1	-2.319047	0.652766	1.530501
15	-2.717004	-0.119286	-0.713389
8	-5.453123	-1.892220	0.124851
8	-5.937912	0.442163	0.104914
8	-4.755818	-0.514327	1.940710

6-TS-2C

SCF energy = -2323.51978814 a.u.

ν = -425.3230 cm^{-1}

13	2.782738	0.500134	-0.480167
6	5.697921	-1.159514	-1.258767
6	5.062981	0.043410	-1.970177
6	5.708325	0.388129	1.353484
6	4.403927	1.129799	1.675798
6	4.172280	-2.217980	1.145203
6	2.864711	-2.149365	0.345114
1	5.469786	0.975721	-1.551488
1	4.456429	-3.276973	1.197046
1	2.188829	-2.913156	0.757534
1	3.059036	-2.430195	-0.701046
1	5.377912	0.003926	-3.023077
1	5.254100	-2.087567	-1.642304
1	6.753596	-1.182242	-1.558516
1	3.759930	0.488062	2.295779
1	4.667368	2.002942	2.290612
1	6.259142	0.290027	2.297957
1	6.332950	1.012645	0.701462
1	3.985120	-1.903240	2.180267
15	5.762699	-1.349029	0.618374
8	3.640046	0.058051	-1.943709
8	3.698498	1.599268	0.534549

8	2.199098	-0.896200	0.414486
8	1.266097	1.409500	-1.010714
1	-0.555950	1.000982	-2.253138
1	0.040068	-0.488361	-1.292131
6	0.062983	1.419443	-0.174493
1	0.215493	0.899587	0.772253
6	-0.565462	2.781096	-0.027457
1	-1.555621	2.636173	0.421118
1	-0.716010	3.215670	-1.022106
6	0.287004	3.703237	0.848467
1	0.427507	3.275390	1.847555
1	1.276379	3.858366	0.406639
1	-0.193068	4.680083	0.961772
6	-0.199930	0.565106	-1.329701
13	-5.589560	-0.553503	0.786574
6	-3.676147	-1.733760	-1.474594
6	-5.204486	-1.826410	-1.554550
6	-3.860462	1.312526	-1.063708
6	-4.801572	1.880848	0.003936
6	-2.459510	-0.472621	1.059543
6	-3.336123	-1.339494	1.968654
1	-5.609708	-0.984197	-2.131700
1	-1.451353	-0.904247	1.075098
1	-2.835808	-1.426287	2.940179
1	-3.432044	-2.352951	1.556137
1	-5.460776	-2.746329	-2.093057
1	-3.282672	-2.585821	-0.907166
1	-3.288273	-1.830070	-2.495631
1	-4.257370	2.061692	0.941093
1	-5.175468	2.848169	-0.350984
1	-3.136765	2.095571	-1.314723
1	-4.428744	1.109323	-1.979506
1	-2.371404	0.534657	1.484066
15	-2.790166	-0.218808	-0.782971
8	-5.827098	-1.896150	-0.262094
8	-5.943740	1.038954	0.239717
8	-4.634221	-0.765012	2.202161

7-TS-2C

SCF energy = -5673.20261223 a.u.

ν = -469.0892 cm^{-1}

5	2.362623	0.736069	-0.458810
6	5.135137	-0.723851	-1.498791
6	4.359020	0.511986	-1.947687
6	5.140968	0.654251	1.295729
6	3.764110	1.271286	1.534200
6	3.614907	-2.031487	0.875264
6	2.361930	-1.713481	0.064349
1	4.757288	1.410355	-1.460194
1	3.825773	-3.103474	0.775700
1	1.565681	-2.406128	0.371595
1	2.543630	-1.877929	-1.004685
1	4.502190	0.638444	-3.029462
1	4.709485	-1.622188	-1.964036
1	6.161515	-0.636392	-1.875362
1	3.132138	0.577140	2.101230
1	3.891110	2.174049	2.146865
1	5.636392	0.551490	2.269113
1	5.760873	1.341849	0.706093
1	3.427074	-1.846479	1.940440
33	5.334586	-1.133617	0.439241
8	2.955931	0.416603	-1.737812
8	3.101264	1.685368	0.345066
8	1.870093	-0.401694	0.289384
8	1.072116	1.577536	-0.908384
1	-0.711207	1.083384	-2.209256
1	-0.006470	-0.378045	-1.277916
6	-0.140580	1.493378	-0.115456
1	0.017732	0.969273	0.825320
6	-0.862160	2.811048	0.031877
1	-1.845760	2.608341	0.470689
1	-1.031579	3.239738	-0.962580
6	-0.083549	3.788486	0.915771
1	0.073503	3.373171	1.917930
1	0.899511	4.007435	0.487336
1	-0.628790	4.731815	1.021799
6	-0.357377	0.642355	-1.286856
5	-5.480760	-0.575556	0.956128
6	-3.856821	-1.931639	-1.253937
6	-5.361209	-1.962385	-0.994366
6	-4.056852	1.222044	-1.023789
6	-5.034588	1.603095	0.081447
6	-2.494895	-0.428869	1.219882
6	-3.490661	-1.112094	2.150359
1	-5.876787	-1.171460	-1.548653
1	-1.526208	-0.933498	1.313491
1	-3.131199	-1.056619	3.182049
1	-3.632278	-2.165632	1.888806
1	-5.774196	-2.927000	-1.303953
1	-3.370170	-2.774635	-0.750558

1	-3.686733	-2.055573	-2.329220
1	-4.506433	1.839122	1.011678
1	-5.621595	2.477189	-0.215295
1	-3.421094	2.086259	-1.239549
1	-4.610370	0.990439	-1.940713
1	-2.344307	0.604554	1.552137
33	-2.803906	-0.308202	-0.748445
8	-5.633097	-1.832780	0.416807
8	-5.976119	0.528716	0.298834
8	-4.755783	-0.415779	2.115895

8-TS-2C

SCF energy = -6108.42841309 a.u.

ν = -434.8968 cm^{-1}

13	-2.410288	1.191370	0.330278
6	-4.333481	-1.386432	1.635468
6	-4.150559	0.025776	2.187844
6	-5.318674	0.050091	-1.058736
6	-4.391851	1.149466	-1.582566
6	-2.859116	-1.976854	-1.089671
6	-1.606318	-1.371684	-0.465359
1	-4.947569	0.687210	1.816007
1	-2.750566	-3.068562	-1.088602
1	-0.735578	-1.835679	-0.952102
1	-1.551388	-1.633288	0.603133
1	-4.258808	-0.012910	3.282105
1	-3.469676	-2.003188	1.914783
1	-5.205077	-1.836697	2.124982
1	-3.653340	0.718347	-2.275120
1	-5.002337	1.853793	-2.166693
1	-5.954001	-0.271951	-1.892840
1	-5.994022	0.468506	-0.301688
1	-2.931343	-1.668675	-2.140499
33	-4.670917	-1.697792	-0.312406
8	-2.869239	0.575607	1.905052
8	-3.740870	1.897893	-0.558056
8	-1.518537	0.030131	-0.644914
8	-1.108391	2.454904	0.737444
1	0.592386	1.990197	2.210723
1	-0.030656	0.521354	1.242718
6	0.200081	2.383611	0.076011
1	0.155776	1.855871	-0.875856
6	0.937294	3.695124	0.013445
1	1.994376	3.453958	-0.157546
1	0.870327	4.189768	0.989134
6	0.410198	4.602492	-1.099782
1	0.491816	4.112862	-2.076834
1	-0.642566	4.855327	-0.934604
1	0.979821	5.536123	-1.139632
6	0.288480	1.551900	1.267510
13	4.691531	-1.400284	-0.771991
6	3.202634	-1.439406	1.730190
6	4.704862	-1.623404	1.943665
6	4.259133	1.267328	0.303517
6	4.766885	1.300804	-1.136130
6	1.985400	-0.518711	-1.129793
6	2.127779	-2.016066	-1.386175
1	5.115021	-0.763953	2.490203
1	0.924794	-0.254800	-1.143921
1	1.659021	-2.251690	-2.350031
1	1.592277	-2.582187	-0.613078
1	4.858355	-2.512202	2.569006
1	2.748732	-2.332142	1.287771
1	2.726331	-1.292680	2.704755
1	3.990103	1.710657	-1.795825
1	5.629909	1.976611	-1.187531
1	3.974293	2.283024	0.596625
1	5.048180	0.942668	0.988925
1	2.474995	0.062006	-1.917190
33	2.591716	0.177251	0.669722
8	5.447904	-1.788865	0.730506
8	5.162863	0.018351	-1.636745
8	3.491445	-2.459042	-1.422921

1-I-2A

SCF energy = -1547.59169425 a.u.

5	-3.692960	0.463828	0.263068
6	-6.644771	-0.876403	0.254348
6	-6.165674	0.536109	0.622607
6	-5.566714	-0.934850	-1.991156
6	-4.218258	-0.205709	-2.101505
6	-4.854020	-2.540186	-0.225262
6	-3.845006	-1.990734	0.795301
1	-6.254495	1.186345	-0.258165
1	-5.349318	-3.393565	0.265678
1	-3.147445	-2.806770	1.036501
1	-4.376050	-1.735757	1.722815
1	-6.854853	0.925999	1.385228
1	-6.697029	-1.488982	1.161420
1	-7.679318	-0.759489	-0.106974

1	-3.407680	-0.946399	-2.061801
1	-4.181992	0.262148	-3.096286
1	-5.584950	-1.663804	-2.817598
1	-6.378669	-0.224409	-2.182693
1	-4.312532	-2.946096	-1.087345
7	-5.876466	-1.628326	-0.739726
8	-4.854923	0.607701	1.153746
8	-3.999552	0.810904	-1.142371
8	-3.080531	-0.888450	0.347272
8	-2.716602	1.469313	0.772609
1	-0.523073	1.285271	2.148034
1	-1.066843	-0.227073	1.389022
6	-1.428516	1.476848	0.179754
1	-1.457027	0.916370	-0.761892
6	-1.011432	2.916828	-0.139861
1	-0.022438	2.906972	-0.613629
1	-0.919568	3.478576	0.799486
6	-1.997496	3.620360	-1.076941
1	-2.089815	3.079321	-2.025571
1	-2.993107	3.679544	-0.630110
1	-1.658680	4.638295	-1.299148
6	-0.558751	0.719396	1.214910
5	3.988320	-0.528868	0.287849
6	1.222780	-0.800132	1.876283
6	2.673587	-1.062385	2.275152
6	1.771578	1.579655	1.176822
6	3.102911	1.737798	0.449855
6	0.930633	-0.127777	-0.565158
6	2.012116	-1.102832	-1.022754
1	3.097988	-0.187935	2.778551
1	-0.016801	-0.648443	-0.713597
1	1.763036	-1.316402	-2.068201
1	1.936707	-2.044663	-0.470611
1	2.610648	-1.865367	3.018076
1	0.756458	-1.692754	1.456859
1	0.697614	-0.540525	2.798084
1	2.945436	1.751342	-0.633633
1	3.461011	2.731751	0.739450
1	1.169330	2.439638	0.897567
1	1.904631	1.606490	2.259194
1	0.929648	0.775006	-1.176486
7	0.910195	0.341274	0.892981
8	3.532295	-1.507003	1.239964
8	4.113819	0.807336	0.800126
8	3.339164	-0.609725	-0.993507
8	5.530738	-0.958229	0.056776
1	6.616153	-2.759007	-0.292341
1	4.983687	-2.642422	-1.164169
6	6.214395	-0.811161	-1.270237
1	5.541298	-0.374546	-2.003243
6	7.594550	-0.232613	-1.179212
1	8.102496	-0.486532	-2.118676
1	8.141516	-0.728408	-0.370083
6	7.572150	1.285792	-0.977874
1	7.043388	1.783093	-1.798682
1	7.067022	1.546807	-0.042271
1	8.590876	1.683461	-0.939355
6	5.860034	-2.140887	-0.766354

5-I-2A

SCF energy = -1982.87707773 a.u.

13	-2.993669	-0.315472	0.273455
6	-4.720835	-2.731733	0.057402
6	-5.379178	-1.483123	-0.543248
6	-2.634429	-2.847384	-1.277893
6	-1.485180	-1.855649	-1.495070
6	-2.546085	-3.122872	1.179470
6	-2.675025	-2.148656	2.356127
1	-5.282398	-1.502934	-1.642268
1	-2.920468	-4.126185	1.432370
1	-1.963419	-2.442268	3.142293
1	-3.683662	-2.224347	2.796538
1	-6.455871	-1.505368	-0.319362
1	-5.027530	-2.823037	1.103167
1	-5.028238	-3.648907	-0.466793
1	-0.619145	-2.139367	-0.871893
1	-1.153846	-1.911711	-2.542504
1	-2.295060	-3.892163	-1.337002
1	-3.384625	-2.691287	-2.058243
1	-1.489034	-3.213845	0.913082
7	-3.257525	-2.544727	0.024403
8	-4.786916	-0.312441	-0.015233
8	-1.915354	-0.548758	-1.179322
8	-2.416705	-0.829257	1.922602
8	-2.698887	1.462665	0.544517
1	-0.604706	3.895290	-0.444369
1	-0.990044	3.322222	1.194731
6	-2.136475	2.365885	-0.369540
1	-1.928509	1.868211	-1.327321
6	-3.113336	3.524199	-0.673277

1	-2.630743	4.232857	-1.358934
1	-3.317743	4.064196	0.261603
6	-4.423930	3.032947	-1.290375
1	-4.236023	2.504377	-2.233230
1	-4.940162	2.340354	-0.620980
1	-5.095052	3.872863	-1.502427
6	-0.838076	3.015620	0.157539
13	3.452758	0.418568	0.162571
6	1.480607	3.116173	0.882994
6	2.979975	3.056918	0.576657
6	0.829294	1.988263	-1.336215
6	1.605688	0.753404	-1.791377
6	0.180447	0.892948	0.928453
6	1.263111	0.163882	1.718943
1	3.149132	3.215954	-0.495707
1	-0.575912	1.180509	1.655226
1	0.688536	-0.560955	2.310402
1	1.745429	0.842325	2.433553
1	3.378624	3.941910	1.090948
1	1.292312	2.976265	1.948430
1	1.175760	4.129842	0.615276
1	1.110758	-0.155843	-1.428760
1	1.488199	0.759114	-2.883106
1	-0.128805	1.928441	-1.848457
1	1.326610	2.904086	-1.659157
1	-0.294222	0.226839	0.211760
7	0.481505	2.192287	0.152231
8	3.684122	1.916393	1.040309
8	2.994455	0.741729	-1.493211
8	2.233532	-0.549429	0.961888
8	5.036088	-0.545248	0.134636
1	6.823487	-0.960167	1.219100
1	5.278342	-1.003261	2.238033
6	5.137641	-2.049521	0.292324
1	4.171279	-2.474537	0.556717
6	5.890085	-2.712861	-0.818842
1	6.160079	-3.713490	-0.456954
1	6.822187	-2.166934	-0.999187
6	5.050627	-2.812275	-2.096826
1	4.126464	-3.372538	-1.917137
1	4.778573	-1.816491	-2.461962
1	5.611397	-3.323758	-2.884722
6	5.758299	-1.161938	1.276587

1-I-2B

SCF energy = -3345.70317730 a.u.

5	-0.895244	0.431532	0.484751
6	-4.109890	0.036457	0.574739
6	-3.209655	1.193685	1.038075
6	-3.204960	-0.105004	-1.743723
6	-1.706365	0.202281	-1.884908
6	-2.928903	-2.022443	-0.178554
6	-1.761437	-1.905387	0.813336
1	-3.138196	1.936386	0.232113
1	-3.636960	-2.740220	0.266943
1	-1.334718	-2.912178	0.934596
1	-2.153055	-1.600249	1.793795
1	-3.717712	1.679876	1.883479
1	-4.311766	-0.626937	1.423355
1	-5.072753	0.497631	0.300475
1	-1.152114	-0.742746	-1.966133
1	-1.569935	0.740460	-2.834624
1	-3.478088	-0.707979	-2.624999
1	-3.773628	0.829199	-1.814398
1	-2.568860	-2.475077	-1.109433
7	-3.652219	-0.800692	-0.535626
8	-1.915983	0.818235	1.475672
8	-1.163335	1.004416	-0.855115
8	-0.717302	-1.041103	0.411732
8	0.364724	1.046734	0.986763
1	2.763563	-0.028612	1.861083
1	1.620056	-1.185618	1.098437
6	1.545774	0.802044	0.238433
1	1.287843	0.484945	-0.781939
6	2.388315	2.077362	0.174882
1	3.368021	1.834703	-0.253419
1	2.563336	2.414938	1.205676
6	1.729090	3.191034	-0.639448
1	1.583283	2.879193	-1.680605
1	0.748187	3.450940	-0.229867
1	2.347237	4.095958	-0.641269
6	2.284845	-0.342435	0.931989
35	3.741780	-1.079121	-0.223970

2-I-2B

SCF energy = -4314.56143622 a.u.

5	-0.561625	0.413224	0.443806
6	-4.189611	-0.006993	0.582299
6	-3.422509	1.209874	1.119047
6	-3.423289	-0.092304	-1.798140

6	-1.982520	0.148168	-2.269082
6	-3.139981	-2.088689	-0.322758
6	-1.985249	-2.305588	0.663374
1	-3.259680	1.928280	0.310122
1	-3.987508	-2.701789	0.041231
1	-1.805206	-3.382781	0.764887
1	-2.265200	-1.918009	1.647446
1	-4.031301	1.700617	1.888163
1	-4.360436	-0.714632	1.400904
1	-5.187143	0.358066	0.269140
1	-1.443427	-0.803421	-2.304693
1	-2.004895	0.560171	-3.285544
1	-3.916548	-0.709903	-2.573884
1	-3.958814	0.862971	-1.773465
1	-2.860330	-2.493922	-1.301188
7	-3.545436	-0.714029	-0.500060
16	-1.799116	0.859741	1.903012
16	-0.996401	1.321372	-1.259888
16	-0.373530	-1.560891	0.197177
8	0.702603	0.973956	0.915461
1	3.165491	0.012903	1.838870
1	2.045186	-1.189104	1.131108
6	1.925155	0.780360	0.206783
1	1.717039	0.474175	-0.826590
6	2.724996	2.085452	0.212576
1	3.724085	1.879292	-0.189689
1	2.858340	2.386721	1.260760
6	2.072750	3.219189	-0.577758
1	1.970142	2.952508	-1.635431
1	1.072572	3.444225	-0.195593
1	2.675328	4.132517	-0.514765
6	2.686571	-0.337076	0.922968
35	4.141844	-1.063896	-0.224993

3-I-2B

SCF energy = -3632.31532314 a.u.

5	-0.680584	0.504039	0.509839
6	-3.997906	0.328003	0.919702
6	-2.935014	1.407381	1.166504
6	-3.013363	0.157959	-1.885267
6	-1.486194	0.305915	-1.880584
6	-2.668512	-2.151032	-0.046091
6	-1.527778	-1.840913	0.932174
1	-2.864448	2.058519	0.285938
1	-3.275167	-2.949468	0.402235
1	-1.029874	-2.793408	1.168211
1	-1.946217	-1.455856	1.871358
1	-3.287710	2.029569	2.001842
1	-4.090888	-0.313786	1.805842
1	-4.962490	0.842578	0.813754
1	-1.023112	-0.688870	-1.896308
1	-1.200801	0.809366	-2.816306
1	-3.292032	-0.324441	-2.831956
1	-3.484745	1.149676	-1.897834
1	-2.259458	-2.565249	-0.977263
15	-3.896712	-0.827330	-0.555444
8	-1.658651	0.917480	1.528729
8	-0.967017	1.082034	-0.820777
8	-0.536348	-0.968528	0.432689
8	0.608711	1.092829	0.980251
1	2.965686	-0.042636	1.845595
1	1.791115	-1.176388	1.092838
6	1.769020	0.803531	0.217229
1	1.486437	0.479654	-0.794856
6	2.647846	2.052294	0.123133
1	3.614836	1.774998	-0.312857
1	2.845055	2.400743	1.146229
6	2.010432	3.171050	-0.701704
1	1.848174	2.847682	-1.736962
1	1.039651	3.461258	-0.287954
1	2.651318	4.059756	-0.722022
6	2.479399	-0.353507	0.919534
35	3.916775	-1.142530	-0.226628

4-I-2B

SCF energy = -4601.16759876 a.u.

5	-0.320754	0.496524	0.482500
6	-4.139176	0.283329	0.947305
6	-3.135472	1.420569	1.191088
6	-3.309496	0.163626	-1.959624
6	-1.792852	0.187046	-2.198645
6	-2.968289	-2.255477	-0.195166
6	-1.823969	-2.168481	0.824517
1	-2.940918	1.972517	0.267418
1	-3.656089	-3.029241	0.172117
1	-1.586161	-3.189304	1.145199
1	-2.137359	-1.614843	1.713792
1	-3.593344	2.121425	1.898624
1	-4.176854	-0.391832	1.811698
1	-5.132677	0.749284	0.895312

1	-1.361652	-0.808829	-2.064116
1	-1.623696	0.474851	-3.242956
1	-3.766016	-0.265100	-2.862365
1	-3.705458	1.184449	-1.885375
1	-2.600926	-2.622004	-1.161994
15	-4.112747	-0.816436	-0.575055
16	-1.514332	1.004902	1.947584
16	-0.783708	1.369553	-1.224113
16	-0.214518	-1.479838	0.272689
8	0.970021	1.027267	0.907741
1	3.415425	0.017072	1.805368
1	2.245054	-1.173689	1.162416
6	2.164934	0.764835	0.172493
1	1.916200	0.425192	-0.841313
6	3.005551	2.041185	0.100827
1	3.983349	1.786336	-0.324877
1	3.183871	2.378813	1.131069
6	2.363692	3.163837	-0.713526
1	2.210468	2.856487	-1.753890
1	1.387372	3.441182	-0.305095
1	2.999895	4.056238	-0.712152
6	2.907468	-0.349623	0.912002
35	4.315455	-1.161205	-0.237819

3-I-2C

SCF energy = -1888.37697967 a.u.

5	2.387956	0.666999	-0.480153
6	5.552708	-0.374563	-0.813475
6	4.833487	0.970747	-0.978528
6	4.415395	-0.498605	1.932312
6	2.985077	0.056467	1.902374
6	3.561036	-2.470657	-0.122198
6	2.598251	-1.780318	-1.096662
1	4.890992	1.533426	-0.038178
1	3.954578	-3.361821	-0.629481
1	1.875934	-2.537491	-1.437642
1	3.153549	-1.445146	-1.982407
1	5.384093	1.547051	-1.735840
1	5.512672	-0.938730	-1.754685
1	6.613685	-0.153755	-0.635545
1	2.274443	-0.775586	1.812373
1	2.798730	0.537040	2.874231
1	4.507006	-1.112193	2.838653
1	5.133076	0.324322	2.047561
1	3.008879	-2.836796	0.753653
15	5.070582	-1.577298	0.543623
8	3.492882	0.883204	-1.423662
8	2.739632	1.031091	0.908733
8	1.852124	-0.715968	-0.543275
8	1.325479	1.613717	-0.934218
1	-1.098170	1.215383	-2.090955
1	-0.311218	-0.227398	-1.425436
6	0.078745	1.540322	-0.271620
1	0.208940	1.037146	0.696336
6	-0.459810	2.950985	-0.008629
1	-1.439769	2.877439	0.479703
1	-0.617523	3.450236	-0.973941
6	0.469507	3.786102	0.875018
1	0.612341	3.309194	1.851798
1	1.454611	3.897512	0.413796
1	0.053861	4.785619	1.043709
6	-0.856814	0.683121	-1.163592
5	-5.064509	-0.967381	0.588874
6	-2.827341	-1.450817	-1.414311
6	-4.283615	-1.929245	-1.451798
6	-3.739331	1.372841	-0.793263
6	-5.007826	1.358616	0.068340
6	-2.196745	-0.253183	1.320373
6	-3.163871	-1.224830	2.009278
1	-4.914947	-1.227042	-2.002834
1	-1.180143	-0.652835	1.403913
1	-2.953005	-1.224140	3.080204
1	-3.037644	-2.240741	1.626131
1	-4.320574	-2.899622	-1.950289
1	-2.176106	-2.218577	-0.982179
1	-2.486075	-1.262389	-2.438891
1	-4.777190	1.578765	1.114215
1	-5.693543	2.119827	-0.308302
1	-3.249197	2.345236	-0.687397
1	-3.995289	1.248469	-1.851795
1	-2.212049	0.724903	1.813093
15	-2.442144	0.093634	-0.477011
8	-4.792574	-2.118564	-0.115220
8	-5.683940	0.088687	-0.040576
8	-4.530086	-0.792459	1.844710

6-I-2C

SCF energy = -2323.59843136 a.u.

13	2.596670	0.641646	-0.457878
6	5.801671	-0.650325	-1.136453

6	5.178890	0.703792	-1.507666
6	5.216480	-0.113244	1.784997
6	3.813742	0.449864	2.056644
6	3.971258	-2.500071	0.409551
6	2.815915	-2.145998	-0.538598
1	5.411590	1.437502	-0.720775
1	4.321904	-3.500925	0.124580
1	2.147858	-3.021445	-0.571892
1	3.212409	-2.014844	-1.557318
1	5.685682	1.050887	-2.421509
1	5.528478	-1.398610	-1.892301
1	6.890616	-0.529804	-1.209932
1	3.123702	-0.382580	2.264440
1	3.879354	1.042554	2.982841
1	5.585301	-0.524707	2.733984
1	5.896924	0.708960	1.526779
1	3.588987	-2.593610	1.434800
15	5.553129	-1.483597	0.536073
8	3.786077	0.663756	-1.767094
8	3.304162	1.286733	1.035212
8	2.049660	-1.021680	-0.144881
8	1.210011	1.635978	-0.952216
1	-1.109479	1.099902	-2.101624
1	-0.381711	-0.318840	-1.330911
6	-0.017694	1.510742	-0.257429
1	0.138370	1.001071	0.707356
6	-0.605045	2.892717	0.045334
1	-1.553818	2.772152	0.583744
1	-0.830756	3.395805	-0.904338
6	0.336712	3.751644	0.892772
1	0.567874	3.254858	1.842634
1	1.282025	3.929891	0.373138
1	-0.117879	4.721979	1.119933
6	-0.922257	0.613335	-1.137636
13	-5.494776	-0.918854	0.603640
6	-2.950344	-1.452306	-1.453758
6	-4.416350	-1.828587	-1.713267
6	-3.772071	1.430463	-0.886390
6	-4.976605	1.666404	0.035465
6	-2.345970	-0.254741	1.304889
6	-3.226718	-1.304047	1.997146
1	-4.927335	-1.021917	-2.253522
1	-1.304807	-0.586146	1.391612
1	-2.852016	-1.411017	3.019950
1	-3.120660	-2.276569	1.500868
1	-4.412429	-2.709784	-2.362646
1	-2.427462	-2.265824	-0.939334
1	-2.459129	-1.304677	-2.423139
1	-4.643603	1.821292	1.069292
1	-5.463658	2.587612	-0.299056
1	-3.178411	2.348699	-0.918753
1	-4.112215	1.227880	-1.908138
1	-2.429028	0.713006	1.810835
15	-2.554391	0.085449	-0.502486
8	-5.126458	-2.172568	-0.514096
8	-5.948333	0.610311	-0.038164
8	-4.606622	-0.914365	2.075748

7-I-2C

SCF energy = -5673.27563230 a.u.

5	1.721876	1.285508	-0.175032
6	4.744813	-0.245566	-0.342593
6	4.240232	1.126053	0.105703
6	2.742198	-1.270860	1.764554
6	1.452390	-0.466915	1.632187
6	2.258648	-1.877099	-1.241638
6	1.801143	-0.573879	-1.896921
1	4.054029	1.124566	1.187483
1	2.618030	-2.549460	-2.030879
1	1.135681	-0.834377	-2.734529
1	2.664060	-0.050600	-2.327701
1	5.041242	1.857319	-0.079920
1	4.880965	-0.257272	-1.431407
1	5.735021	-0.412132	0.099490
1	0.780364	-0.982412	0.935973
1	0.962139	-0.461842	2.616971
1	2.497176	-2.196672	2.301041
1	3.467894	-0.734259	2.387824
1	1.406361	-2.387948	-0.775795
33	3.692957	-1.870447	0.126354
8	3.100581	1.582650	-0.596941
8	1.611663	0.887830	1.247374
8	1.072512	0.282735	-1.043122
8	1.029796	2.593813	-0.357052
1	-2.130021	2.687469	-1.303389
1	-0.730969	1.820736	-1.958276
6	-0.330336	2.784408	-0.043056
1	-0.525835	2.439277	0.981671
6	-0.633005	4.290566	-0.067172
1	-1.695907	4.428509	0.170375

1	-0.481899	4.660589	-1.090544
6	0.227437	5.089146	0.912803
1	0.086387	4.730743	1.940178
1	1.289270	4.993231	0.668786
1	-0.033496	6.152912	0.886737
6	-1.273174	2.059519	-1.043278
5	-3.629273	-2.087943	0.572278
6	-1.524918	-1.169412	-1.436501
6	-2.520036	-2.319574	-1.534461
6	-4.038407	0.693562	-0.658552
6	-4.972777	-0.127136	0.228723
6	-1.805013	0.170279	1.518163
6	-1.912109	-1.263924	2.028247
1	-3.452946	-2.027029	-2.024181
1	-0.818271	0.573457	1.738872
1	-1.700557	-1.277298	3.099454
1	-1.199631	-1.918893	1.519468
1	-2.063321	-3.129585	-2.108271
1	-0.616287	-1.512657	-0.942473
1	-1.258488	-0.796180	-2.428967
1	-4.837445	0.120610	1.285957
1	-6.008429	0.083286	-0.048315
1	-4.192759	1.760816	-0.470117
1	-4.231290	0.496605	-1.717777
1	-2.546273	0.808574	2.008253
33	-2.098699	0.405706	-0.404028
8	-2.782429	-2.836953	-0.210950
8	-4.760766	-1.538104	0.013151
8	-3.260216	-1.754028	1.855512

8-I-2C

SCF energy = -6108.50081800 a.u.

13	-2.142446	1.383622	0.108571
6	-3.542348	-1.460077	1.717134
6	-3.365424	-0.032857	2.231642
6	-5.207164	-0.158524	-0.667922
6	-4.514748	1.038005	-1.325783
6	-2.608125	-1.846035	-1.291721
6	-1.318974	-1.132603	-0.894795
1	-4.274435	0.554176	2.029563
1	-2.386050	-2.915071	-1.400934
1	-0.517241	-1.520157	-1.541948
1	-1.050445	-1.412372	0.135810
1	-3.258321	-0.075298	3.327497
1	-2.596156	-2.007413	1.816109
1	-4.264541	-1.975649	2.361809
1	-3.889153	0.689600	-2.162398
1	-5.298855	1.674763	-1.764900
1	-5.958944	-0.540020	-1.369900
1	-5.754907	0.175438	0.222441
1	-2.937501	-1.492107	-2.277167
33	-4.219624	-1.817814	-0.125459
8	-2.219509	0.613969	1.708160
8	-3.759758	1.838532	-0.429856
8	-1.370485	0.270892	-1.040652
8	-1.064755	2.801432	0.225996
1	1.258933	1.994210	1.956401
1	0.024904	0.880275	1.388459
6	0.328178	2.595251	0.048485
1	0.506109	2.230768	-0.972943
6	1.099082	3.908394	0.197994
1	2.171142	3.688170	0.106976
1	0.936633	4.295318	1.213170
6	0.698190	4.958065	-0.838633
1	0.832267	4.573264	-1.857410
1	-0.351885	5.244099	-0.725073
1	1.308362	5.862497	-0.738253
6	0.832612	1.534703	1.058425
13	4.441902	-1.884756	-0.515273
6	1.826007	-1.350013	1.393847
6	3.000463	-2.256335	1.752043
6	3.935558	1.116910	0.804188
6	5.126026	0.708341	-0.061215
6	1.953534	0.046228	-1.552963
6	2.304662	-1.341622	-2.084999
1	3.763389	-1.704789	2.316419
1	0.897398	0.259942	-1.737904
1	1.981679	-1.393581	-3.129992
1	1.760692	-2.115633	-1.528781
1	2.620164	-3.054314	2.398988
1	1.089874	-1.900550	0.799733
1	1.328365	-0.999224	2.304434
1	4.923781	0.916581	-1.119608
1	5.987023	1.314569	0.240053
1	3.757829	2.193235	0.711723
1	4.121057	0.884805	1.857433
1	2.555294	0.815206	-2.046017
33	2.179311	0.311641	0.383127
8	3.573478	-2.874632	0.589074
8	5.477787	-0.672776	0.126921

8	3.721463	-1.588575	-2.047652

1-TS-3A

SCF energy = -1736.17764842 a.u.

ν = -140.7833 cm^{-1}

5	-3.060826	0.266287	0.181447
6	-5.084796	2.721005	0.201263
6	-5.242970	1.287493	0.728674
6	-2.940508	3.207601	1.380189
6	-1.964237	2.032011	1.531000
6	-3.008447	3.165587	-1.114728
6	-2.917878	1.780024	-1.773866
1	-4.973663	1.254091	1.792259
1	-3.481169	3.824178	-1.860484
1	-2.302382	1.878387	-2.678084
1	-3.918047	1.458228	-2.089566
1	-6.302012	1.010270	0.648034
1	-5.501557	2.780770	-0.810048
1	-5.715420	3.356948	0.842339
1	-1.175642	2.124636	0.774061
1	-1.485111	2.113474	2.515487
1	-2.330234	4.120389	1.471845
1	-3.638639	3.210313	2.224042
1	-1.997372	3.554479	-0.950102
7	-3.732396	3.278611	0.152172
8	-4.492779	0.325392	0.003897
8	-2.570258	0.749729	1.458218
8	-2.321038	0.778435	-0.961952
8	-2.788731	-1.304258	0.254535
1	-0.431346	-2.885463	-1.058468
1	-1.074347	-1.294495	-1.501531
6	-1.475599	-1.840608	0.551710
1	-1.068309	-1.163812	1.304963
6	-1.650984	-3.228867	1.176375
1	-0.656134	-3.655514	1.341544
1	-2.142346	-3.889315	0.450722
6	-2.429502	-3.199360	2.491414
1	-1.922932	-2.566460	3.229543
1	-3.438029	-2.805583	2.343365
1	-2.514743	-4.207161	2.910825
6	-0.585454	-1.861770	-0.714735
5	3.827075	0.028684	-0.514135
6	1.348911	-1.279805	-2.036961
6	2.852100	-1.316625	-2.295134
6	1.641855	-2.148305	0.352592
6	2.862431	-1.564204	1.063349
6	0.665246	0.179130	-0.052447
6	1.702417	1.231534	-0.425613
1	3.294761	-2.213160	-1.849261
1	-0.289105	0.524581	-0.450770
1	1.312690	2.160362	0.005686
1	1.744519	1.369974	-1.510267
1	2.937838	-1.418331	-3.382708
1	0.876463	-0.433873	-2.537731
1	0.948341	-2.197905	-2.470672
1	2.559486	-0.732032	1.706972
1	3.209479	-2.371754	1.717345
1	0.963567	-2.438983	1.153469
1	1.895192	-3.041130	-0.221371
1	0.579846	0.097615	1.030345
7	0.830104	-1.251830	-0.586622
8	3.575010	-0.158507	-1.918308
8	3.951521	-1.189255	0.239825
8	3.001503	1.029689	0.105593
8	5.338674	0.603707	-0.501256
1	6.452485	2.110740	-1.516726
1	4.705508	2.571358	-1.098425
6	5.810957	1.578434	0.536309
1	5.015932	1.803912	1.242049
6	7.158844	1.251350	1.105579
1	7.526993	2.168748	1.582949
1	7.847696	1.011684	0.288478
6	7.094719	0.108573	2.123580
1	6.418885	0.355730	2.949873
1	6.732425	-0.811284	1.653375
1	8.086090	-0.088696	2.542733
6	5.603700	2.016909	-0.846527
6	-3.767244	-2.272258	-0.757608
8	-4.667118	-2.735535	-0.092589
8	-3.315061	-2.273812	-1.885212

1-TS-3B

SCF energy = -3534.28862844 a.u.

ν = -193.3396 cm^{-1}

5	0.991184	0.308427	0.053678
6	4.157533	0.145202	-0.238459
6	3.240966	1.334721	0.089145
6	3.254890	-1.400845	1.502407
6	1.752940	-1.273052	1.799453
6	3.009386	-1.964930	-0.915293

6	1.831153	-1.295067	-1.638185
1	3.159585	1.445235	1.178375
1	3.732477	-2.242702	-1.698735
1	1.406227	-2.027873	-2.337676
1	2.198926	-0.448902	-2.232725
1	3.720380	2.243363	-0.298696
1	4.369235	0.139537	-1.313352
1	5.112906	0.348781	0.271149
1	1.210093	-2.076763	1.285710
1	1.610745	-1.416416	2.879160
1	3.545288	-2.412336	1.828977
1	3.808009	-0.695853	2.132899
1	2.666907	-2.899878	-0.457947
7	3.698854	-1.197126	0.122871
8	1.949554	1.252739	-0.492467
8	1.194844	-0.013196	1.459466
8	0.787130	-0.868920	-0.778430
8	-0.348639	1.131920	0.050627
1	-2.836629	0.537143	-1.319812
1	-1.514663	-0.665981	-1.383853
6	-1.564193	0.466500	0.468184
1	-1.238566	-0.321581	1.153865
6	-2.466720	1.454268	1.203568
1	-3.398697	0.932417	1.449174
1	-2.731789	2.268255	0.516815
6	-1.828267	2.016781	2.473826
1	-1.575688	1.211028	3.172972
1	-0.908318	2.560862	2.241114
1	-2.512536	2.704872	2.981571
6	-2.239994	-0.170786	-0.745689
35	-3.499215	-1.592827	-0.167788
6	-0.505627	2.333866	-1.225082
8	-0.465331	3.419326	-0.695761
8	-0.624017	1.768570	-2.286952

1-I-3A

SCF energy = -1194.87025231 a.u.

8	3.599264	-0.164197	1.143153
1	2.478494	0.926475	-1.857561
1	2.781363	-0.715053	-1.266412
6	3.221348	0.836709	0.170509
1	2.610577	1.512540	0.775496
6	4.408101	1.652980	-0.366672
1	3.980148	2.521585	-0.882711
1	4.955571	1.069362	-1.111370
6	5.355170	2.118426	0.740078
1	4.819181	2.690443	1.506855
1	5.839160	1.268959	1.231970
1	6.140301	2.759251	0.325720
6	2.397747	0.265832	-0.993081
5	-2.329921	-0.273133	-0.389977
6	0.409313	-0.720590	-1.977511
6	-1.042688	-0.604689	-2.438019
6	0.286480	1.514595	-0.751446
6	-1.030883	1.758312	-0.022029
6	0.701136	-0.663010	0.558956
6	-0.561378	-1.492803	0.769507
1	-1.268321	0.422670	-2.741529
1	1.537840	-1.359616	0.608936
1	-0.410085	-1.977200	1.740436
1	-0.633046	-2.284901	0.017867
1	-1.090638	-1.226307	-3.339026
1	0.678536	-1.755689	-1.761946
1	1.019089	-0.376545	-2.815756
1	-0.933097	1.497413	1.036557
1	-1.182624	2.841804	-0.078571
1	1.022206	2.151626	-0.260415
1	0.224776	1.819534	-1.797089
1	0.822072	0.071066	1.354709
7	0.880239	0.098562	-0.762548
8	-2.022770	-1.086825	-1.536783
8	-2.172130	1.141405	-0.591009
8	-1.770989	-0.759420	0.842548
8	-3.934522	-0.428042	-0.266131
1	-5.370053	-2.003532	-0.278521
1	-3.788298	-2.387987	0.609886
6	-4.634783	-0.398110	1.060310
1	-3.921831	-0.253360	1.867702
6	-5.867695	0.454746	1.076148
1	-6.449295	0.145441	1.954267
1	-6.472802	0.232017	0.190623
6	-5.536698	1.948426	1.154242
1	-4.946612	2.174065	2.049500
1	-4.959391	2.264956	0.279610
1	-6.454064	2.543761	1.192695
6	-4.528566	-1.653033	0.311005
6	4.462450	-1.222043	0.810197
8	4.704881	-1.966216	1.794697
8	4.874324	-1.320646	-0.371146

1-I-3B

SCF energy = -2992.97605131 a.u.

8	-1.592650	-0.206112	-0.863040
1	0.417329	-0.913120	1.193442
1	0.453279	-1.653736	-0.431543
6	-0.336636	0.369437	-0.420716
1	0.089425	0.733654	-1.361085
6	-0.519723	1.554114	0.529362
1	0.477464	1.970736	0.716582
1	-0.902882	1.192126	1.487630
6	-1.442596	2.634673	-0.036794
1	-1.073318	3.008711	-0.999421
1	-2.453661	2.244579	-0.193032
1	-1.511742	3.483778	0.651451
6	0.569820	-0.729812	0.133526
35	2.487071	-0.236792	-0.042837
6	-2.446247	-0.859581	0.041475
8	-3.521101	-1.232001	-0.497823
8	-2.072636	-1.010886	1.230132

1-TS-4A

SCF energy = -1194.83088154 a.u.

ν = -486.1236 cm^{-1}

8	4.508515	0.168568	1.079764
1	2.736412	-0.456417	-1.577231
1	2.733139	-1.490848	-0.025538
6	3.386076	0.640793	0.288046
1	2.646281	0.952590	1.027150
6	3.815193	1.834004	-0.571196
1	2.990078	2.087289	-1.245032
1	4.653228	1.522234	-1.204229
6	4.199996	3.051374	0.270679
1	3.355509	3.387944	0.883874
1	5.034178	2.821113	0.940834
1	4.503822	3.884141	-0.371561
6	2.882534	-0.539265	-0.510555
5	-2.405548	-0.489634	-0.160922
6	0.386313	-1.620292	-1.088541
6	-1.006385	-1.746953	-1.712765
6	0.329263	0.892631	-0.953306
6	-1.046521	1.489029	-0.625011
6	0.476560	-0.475572	1.149028
6	-0.844186	-1.085261	1.631563
1	-1.150245	-0.962257	-2.464048
1	1.274618	-1.086317	1.589014
1	-0.819910	-1.058442	2.726797
1	-0.910074	-2.135356	1.326225
1	-1.026136	-2.711095	-2.233090
1	0.583892	-2.474315	-0.435022
1	1.088058	-1.686213	-1.928912
1	-1.085478	1.761786	0.435979
1	-1.128858	2.414459	-1.206201
1	1.048617	1.652835	-0.635834
1	0.442819	0.762456	-2.032893
1	0.575127	0.534280	1.554277
7	0.718081	-0.392297	-0.316023
8	-2.081342	-1.742783	-0.783181
8	-2.160126	0.674767	-0.963821
8	-2.001158	-0.374236	1.213209
8	-4.047472	-0.540687	-0.141615
1	-5.578863	-1.885764	0.482436
1	-4.100801	-1.799681	1.599706
6	-4.845884	0.161812	0.908652
1	-4.194064	0.680936	1.606695
6	-6.019063	0.926965	0.371500
1	-6.691141	1.109349	1.220028
1	-6.561720	0.299237	-0.343776
6	-5.599180	2.252615	-0.271227
1	-5.070474	2.887977	0.448125
1	-4.932778	2.078555	-1.122091
1	-6.475789	2.801233	-0.629302
6	-4.764645	-1.301764	0.900415
6	5.302819	-0.700793	0.350104
8	6.397173	-1.023984	0.829612
8	4.777458	-1.083320	-0.758209

1-TS-4B

SCF energy = -2992.95254950 a.u.

ν = -459.2208 cm^{-1}

8	-1.815021	0.091948	-0.811920
1	0.382198	-0.886278	1.348402
1	0.248344	-1.731976	-0.297566
6	-0.480809	0.405820	-0.311778
1	0.081603	0.679295	-1.204481
6	-0.541297	1.575441	0.666396
1	0.478789	1.735361	1.032091
1	-1.156250	1.278141	1.525207
6	-1.085569	2.856709	0.033488
1	-0.461453	3.173488	-0.810652
1	-2.106166	2.714523	-0.335959

1	-1.103260	3.671891	0.764444
6	0.106849	-0.849913	0.307586
35	2.511864	-0.281888	-0.095829
6	-2.459289	-0.866320	-0.062321
8	-3.661320	-1.071421	-0.294616
8	-1.713455	-1.457874	0.798074

1,2-butylene carbonate

SCF energy = -421.083873783 a.u.

8	-0.220177	-0.677706	0.633299
1	-0.076500	2.258136	-0.658634
1	-0.809288	2.155392	0.976860
6	0.611819	0.530014	0.528125
1	1.016254	0.707677	1.526117
6	1.716645	0.307491	-0.492036
1	2.262105	1.255766	-0.576618
1	1.254461	0.113763	-1.468653
6	2.673097	-0.822950	-0.109478
1	3.145149	-0.625840	0.860108
1	2.147201	-1.780483	-0.041824
1	3.466097	-0.925931	-0.856869
6	-0.425848	1.587728	0.126629
6	-1.380405	-0.483767	-0.015185
8	-2.205022	-1.352052	-0.218708
8	-1.521967	0.796062	-0.413193