

Supporting Information for

**Quantum Chemical Dissection of The Classic Terpinyl/Pinyl/Bornyl/Camphyl Cation
Conundrum—The Role of Pyrophosphate in Manipulating Pathways to
Monoterpenes**

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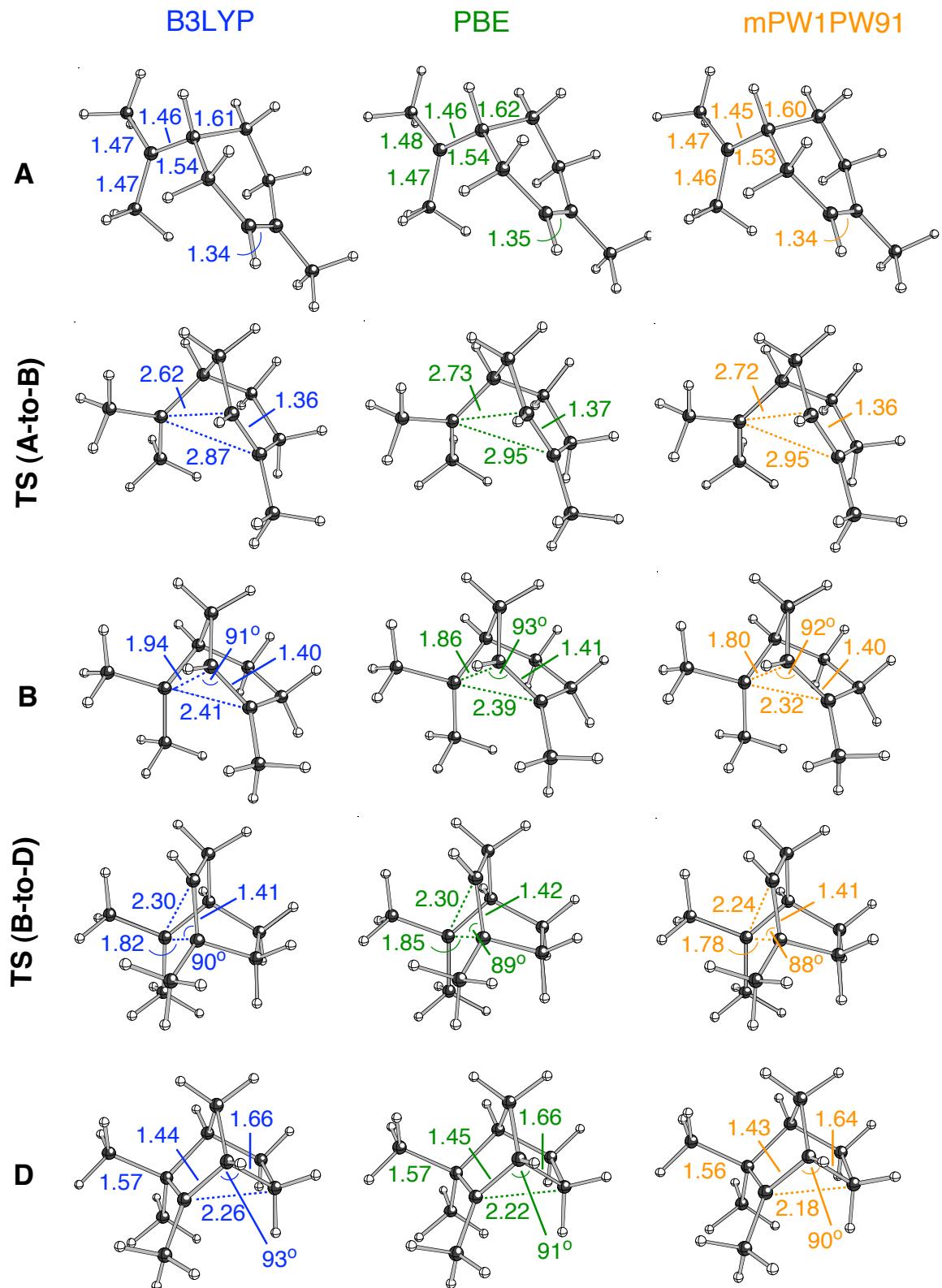
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I. Gaussian03 Full Reference

GAUSSIAN03, Revision D.01

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, 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,
P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

II. Structures involved in the rearrangement of A by different methods



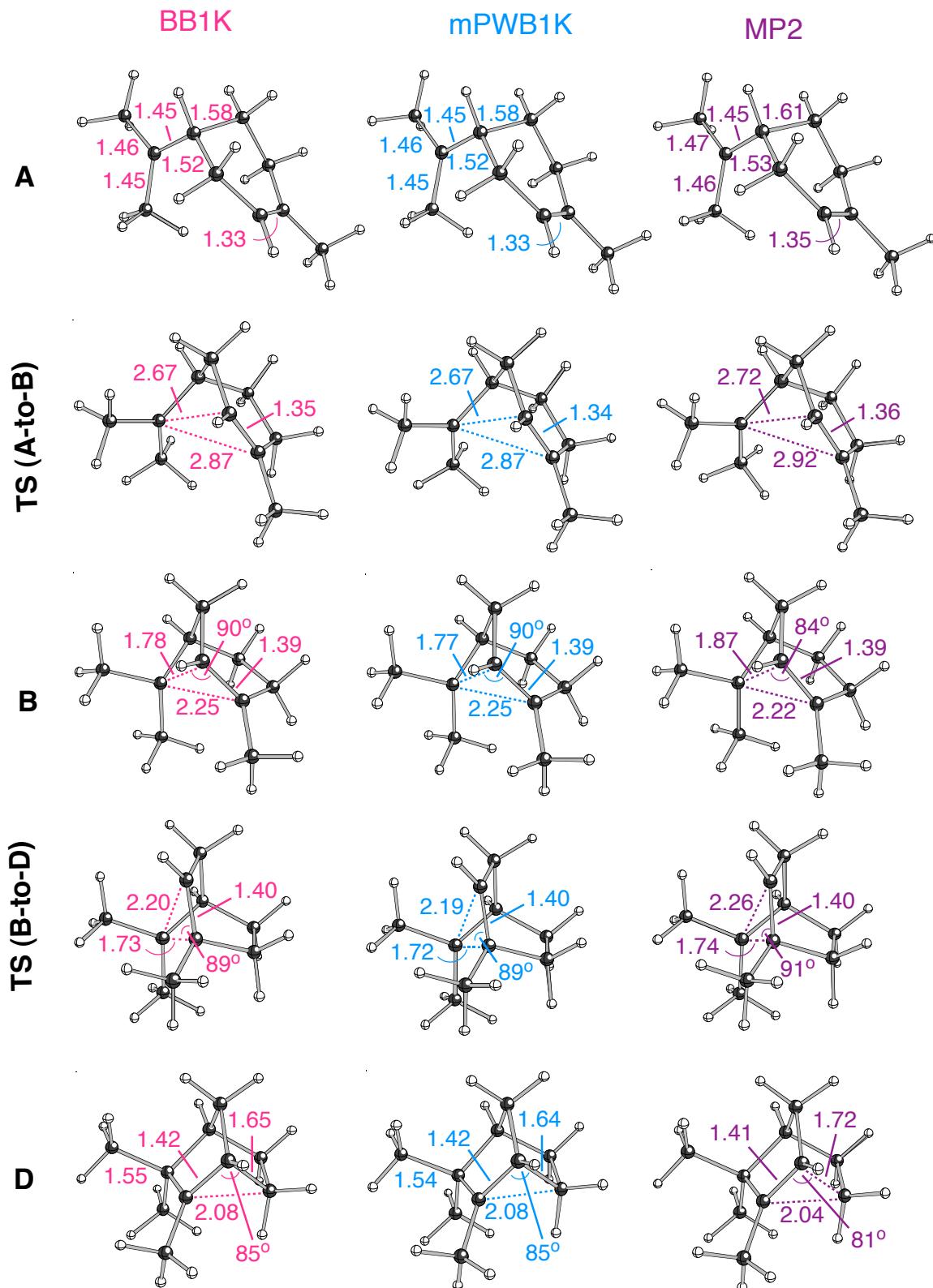


Figure S1. Computed structures of intermediates and transition state structures.

III. Effects of C–H \cdots X interactions

Model of deprotonations. To see if deprotonation at C4, for example, can indeed lead to formal C2–C7 σ -bond formation, we examined proton transfer from **B** to ammonia (a simple model base; Figures S2a-g). In the uncomplexed structure of cation **B**, the C2–C7 distance is 1.94 Å. This distance is decreased to 1.77 Å upon complexation with ammonia (Figure S2b). Thus, it seems that the interaction of a base with a C–H bond (exo hydrogen) of **B** that is antiperiplanar to the C2–C7 bond would promote a change in the **B** structure towards that of the previously proposed pinyl cation intermediate, facilitating facile deprotonation to form α -pinene (**2**).

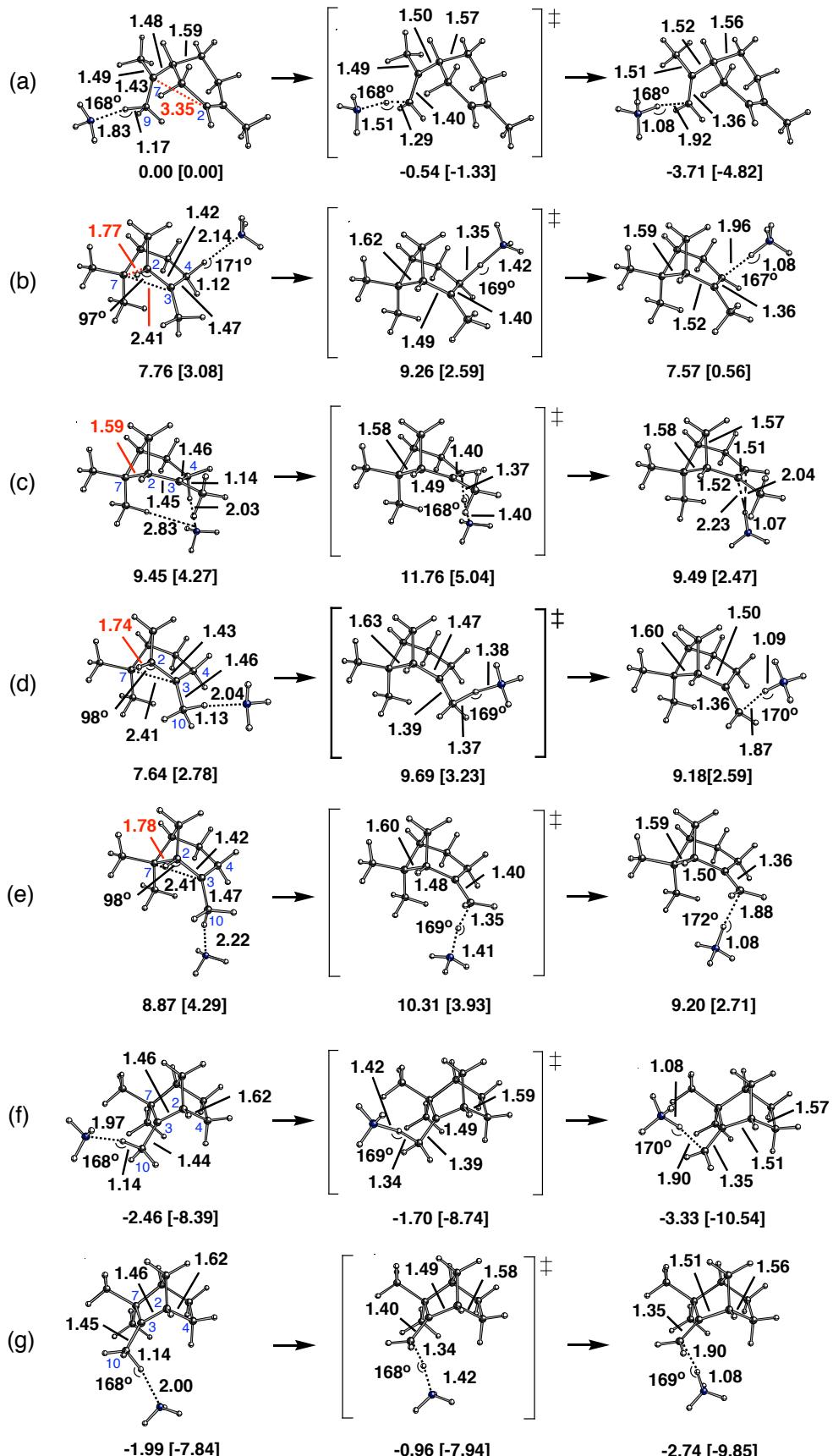


Figure S2. Model of C–H••X interactions and deprotonation to form (a) limonene, (b) and (c) α -pinene (**2**), (d) and (e) β -pinene (**3**), (f) and (g) β -camphene (**6**). Selected distances are shown in Å. Computed relative energies in kcal/mol (relative to the energy of one of complexes in (a)) are from calculations by B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p) and mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p) (in brackets).

A more dramatic change in the **B** structure occurs upon complexation of ammonia with the alternative hydrogen (endo) at C4, which actually led to the pinyl cation intermediate (Figure S2c). Note the C2–C7 distance is considerably decreased (to 1.59 Å) (Figure S2c). It appears that electron donation from the ammonia lone pair to the cationic center C3 of pinyl cation diminishes the ability of that center to participate in hyperconjugation with the C2–C7 bond. For comparison, C10 deprotonations of **B** to form β -pinene are also shown in Figures S2d and S2e. Note that complexation with the hydrogens (endo and exo) at this carbon significantly decreases the C2–C7 distance. We further explored the nature of the cation **B** in the structure where ammonia interacts the hydrogen at C9 that is antiperiplanar to the C2–C7 bond. This specific interaction of ammonia with a C–H bond of **B** brought a change in the **B** structure towards that of the terpinyl cation intermediate (note the C2–C7 distance is apart farther (to 3.35 Å) upon complexation with ammonia). These examples hint that the structure of **B** is susceptible to change by interactions with specifically oriented electron rich groups. In other words, these sorts of structures may adjust to their surroundings in the enzyme. We have observed similar geometric distortions to carbocation structures upon their participation in intermolecular C–H••X interactions for other systems with appropriately oriented C–H and C–C bonds..

Model of pinene formation. If appropriately oriented noncovalent interactions can affect the nature of species involved in the rearrangement and potentially bias their reactivity (Figure S2), under such influence a given rearrangement pathway can be modified. Thus, we examined whether C–H \cdots NH₃ interactions along the reaction pathway from terpinyl cation caused changes to each step of the rearrangement. We were able to locate a transition structure corresponding to the conversion of the terpinyl cation to **B**. The transition structure connected **A** to **B**. In the complex of **A**, ammonia interacts with a hydrogen at C4 of the terpinyl cation (in principle, the pyrophosphate that departed from C3 of LPP may be near to C4 of terpinyl cation). In the transition structure, both the C2–C7 and C3–C7 distances are slightly elongated upon complexation with ammonia at this particular site (Figures S1 and S3). The energy barrier is comparable to that for the uncomplexed conversion (Figure S3). We also located transition structure corresponding to **TS (B-to-D)**. Note a change in the orientation of ammonia which is interacting with a hydrogen at C1 instead of C4. Based on IRC calculations, ammonia migration coincides with the structural changes of **B**. It makes sense that when the reaction progresses, positive charge localizes on C3. The computed energy barrier from **A** is reduced. Thus it appears that electron density transferred from NH₃ to C3 via a C–H in hyperconjugation with that center (Figure S3) provides stabilization to the secondary cation-like transition structure. The energy barrier from **B**, however, is not reduced, since similar C–H \cdots X interactions lower the energy of **B**. Concerted deprotonation/ring closure of **D** will generate α -camphene. While further rearrangement of **B** to **D** is feasible energetically, facile deprotonation of **B** by a juxtaposed base forms α -pinene preferably (Figure S3). If

the departed pyrophosphate from C3 of LPP is nearby after the formation of terpinyll cation, pyrophosphate might play a similar role as ammonia.

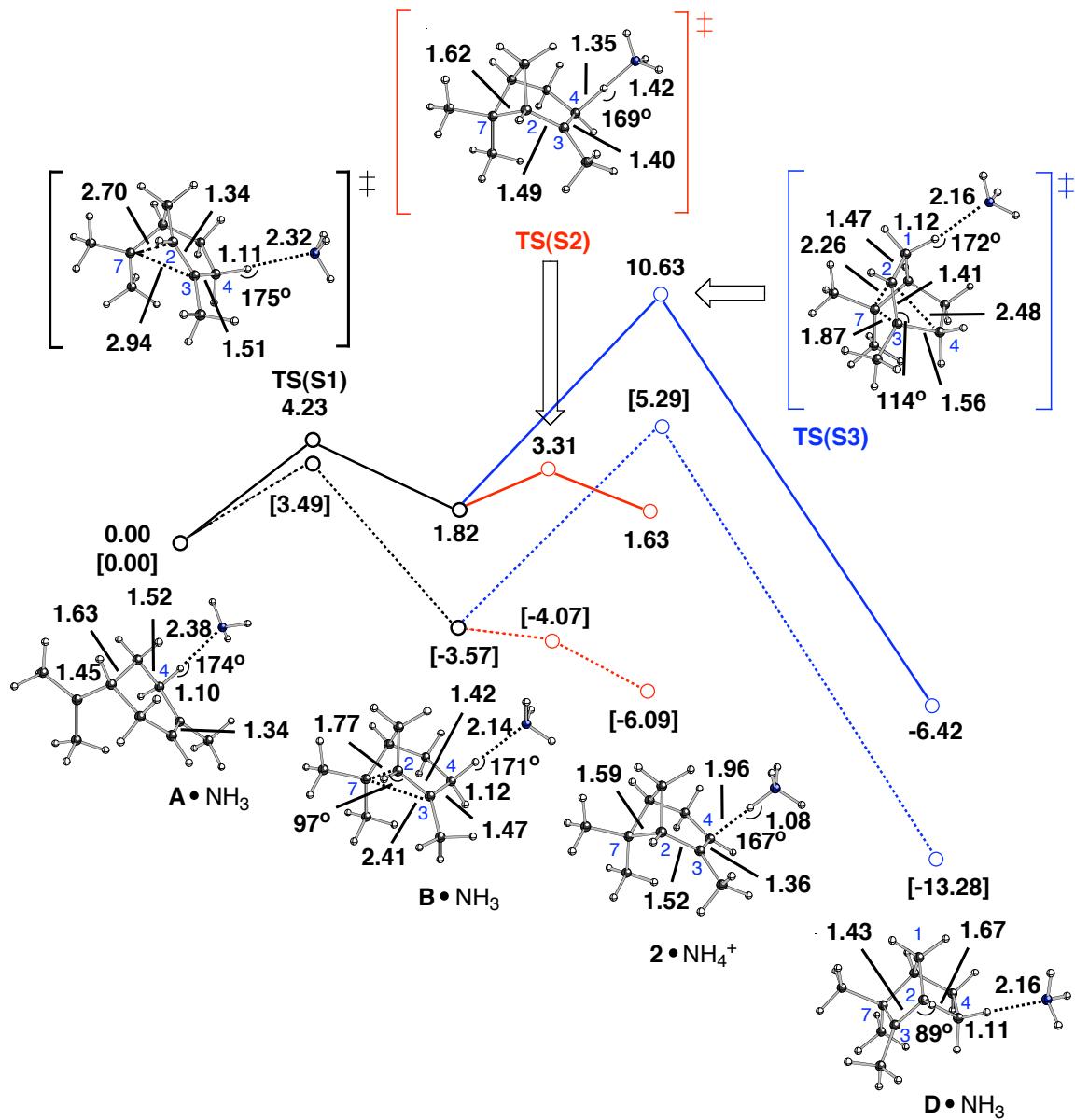


Figure S3. Model of rearrangement of terpinyll cation **A** to the cations that proceed to α -pinene and α -camphene. Computed geometries (selected distances in Å) and relative energies (in kcal/mol and the energy of reference structure **A**•NH₃ is set to 0.00 kcal/mol) of intermediates and transition structures are shown. Solid line pathway: B3LYP/6-

31+G(d,p)//B3LYP/6-31+G(d,p). Dotted line pathway: mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p).

Model of camphene formation. We also examined a potential effect of noncovalent interactions on the structure of **B** relevant to the formation of camphene (Figures S4-5).

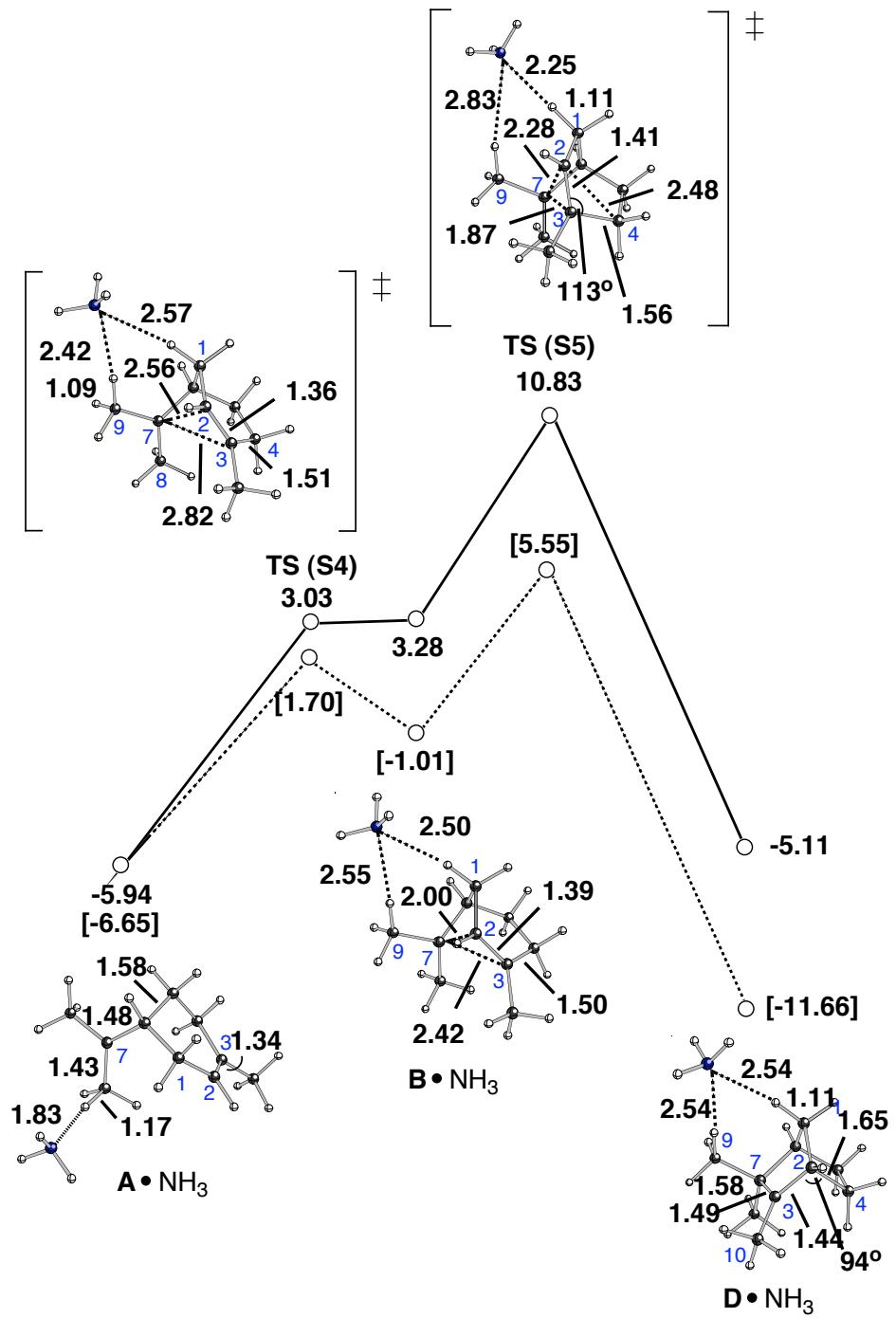


Figure S4. Model of rearrangement of terpinyl cation **A** to the cation that proceeds to camphene. Computed geometries (selected distances in Å) and relative energies (in kcal/mol, relative to that of **A** • NH₃ in Figure S3) of intermediates and transition structures are shown. Solid line pathway: B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p). Dotted line pathway: mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p).

The C2–C7 distance in **B** is elongated slightly farther (to 2.00 Å) upon complexation with ammonia (Figure S4). Electron donation from the ammonia lone pair to the cationic center C7 reduces the intramolecular cation- π interaction in the complex **B**. Thus, it seems that the interaction of an active site base with a C–H bond of **B** would promote a change in the **B** structure towards that of the terpinyl cation (Figure S4). Thus, charge build-up at particular sites in the intermediates and transition structures in the rearrangements can cause alteration in their interaction modes (Figures S4-S5, suggesting that perhaps the intermediates and transition structures may move around to adopt particular intermolecular contacts in the enzyme active site if there is room.

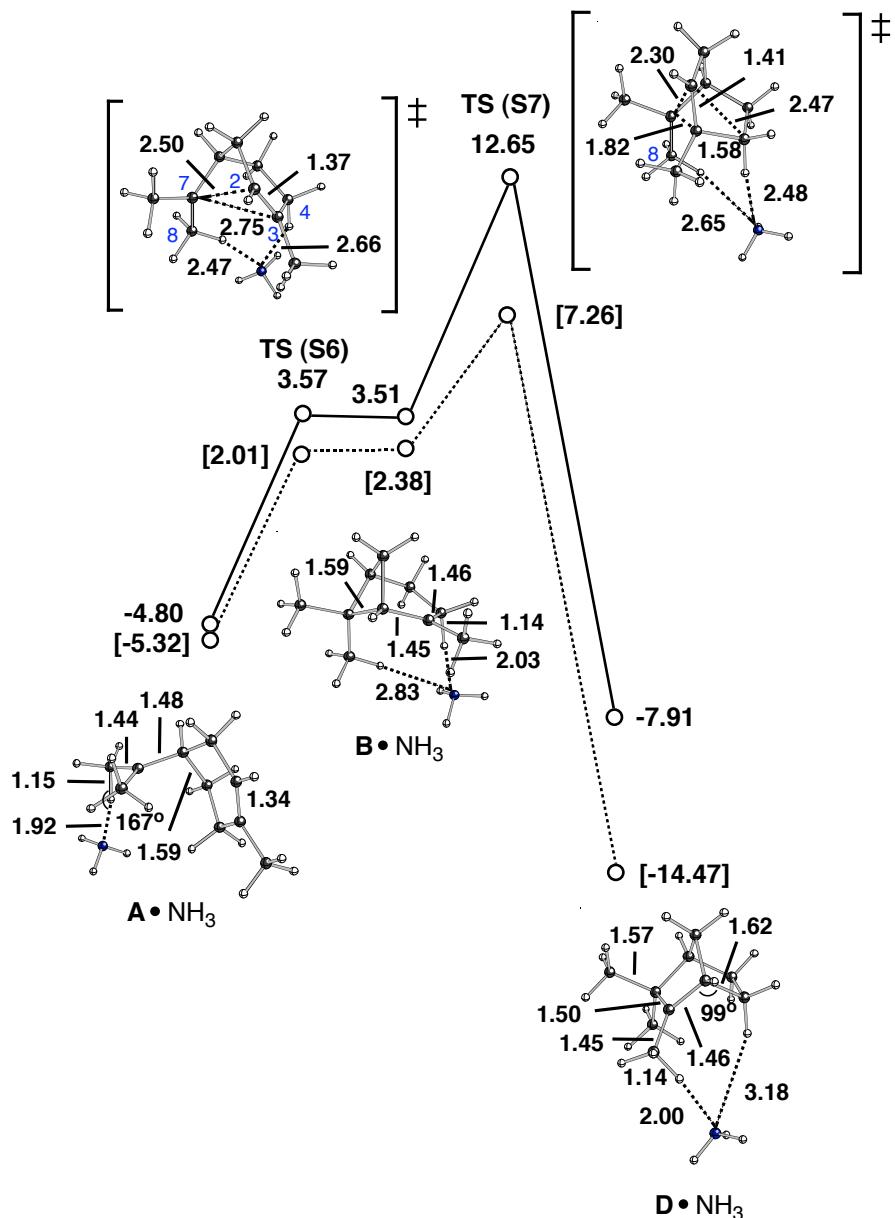


Figure S5. Model of rearrangement of terpinyl cation **A** to the cation that proceeds to β -camphene. Computed geometries (selected distances in Å) and relative energies (in kcal/mol, relative to that of $\mathbf{A} \bullet \text{NH}_3$ in Figure S3) of intermediates and transition structures are shown. Solid line pathway: B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p). Dotted line pathway: mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p).

IV. Water/ammonia as a model nucleophile

We were able to locate transition state structures (**TS(S8)** and **TS(S9)**) that are remarkably similar to **TS1** and **TS2** described in the main paper, respectively (see Figures 3a-b and Figures 5a-b). Based on close similarity between **TS1** and **TS4**, and **TS1** and **TS5**, we initially expected these structures to connect the **B•H₂O** complex and the **D•H₂O** complex to protonated borneol (**9-H⁺**), respectively. IRC calculations (Figure 6b) verified that **TS5** is indeed connected to the **D**•water complex and **9-H⁺**. Note that there is a flat region near transition state structure on the plot. Attack of water on C2 from the righthand side of **D** (as drawn in Scheme 4 and Figure 6b) is a concerted processes coupled with alkyl shifting (migrating C4 from C2 to C3). Note that the alkyl shifting event precedes C–O bond formation. In the water complex of cation **D**, the water molecule interacts with the hydrogen (exo) at C4 via a C-H•••X interaction (at a C-H•••O distance of 2.28 Å). Structures in the flat region resemble the previously proposed bornyl cation. We were unable to locate a secondary cation minimum in the presence of an appropriately oriented water molecule for this system.

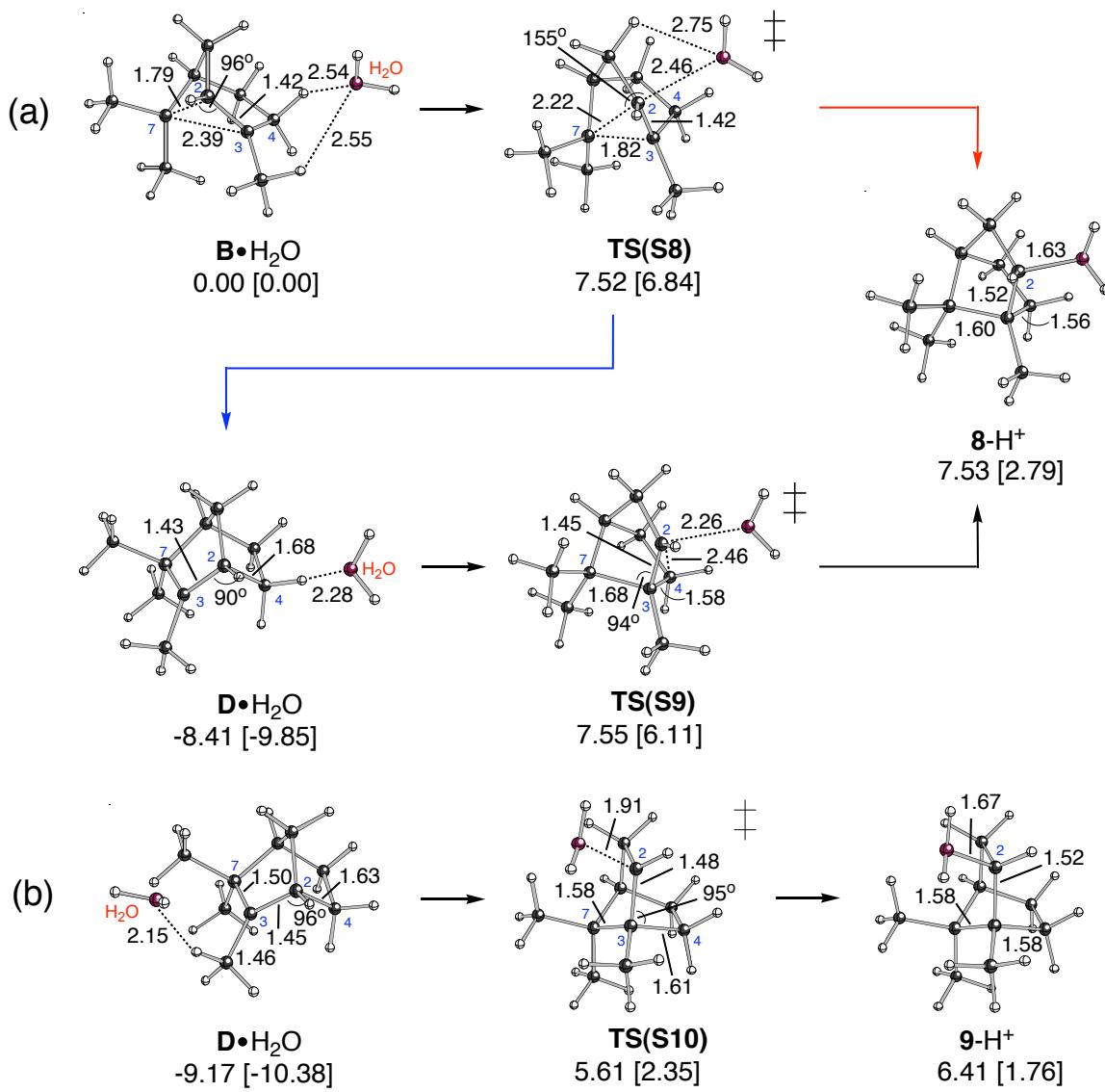


Figure S6. Water-B, water-D complexes, transition state structures, and protonated product alcohols (**8-9**). Selected distances (Å) and energies (kcal/mol; relative to the energy of **B•H₂O** complex in (a)) are shown; B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p) in normal text and mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p) in brackets. **8-H⁺** and **9-H⁺** have higher energy than that of **TS(S8)** and **TS(S10)**, respectively, due to zero point energy corrections.

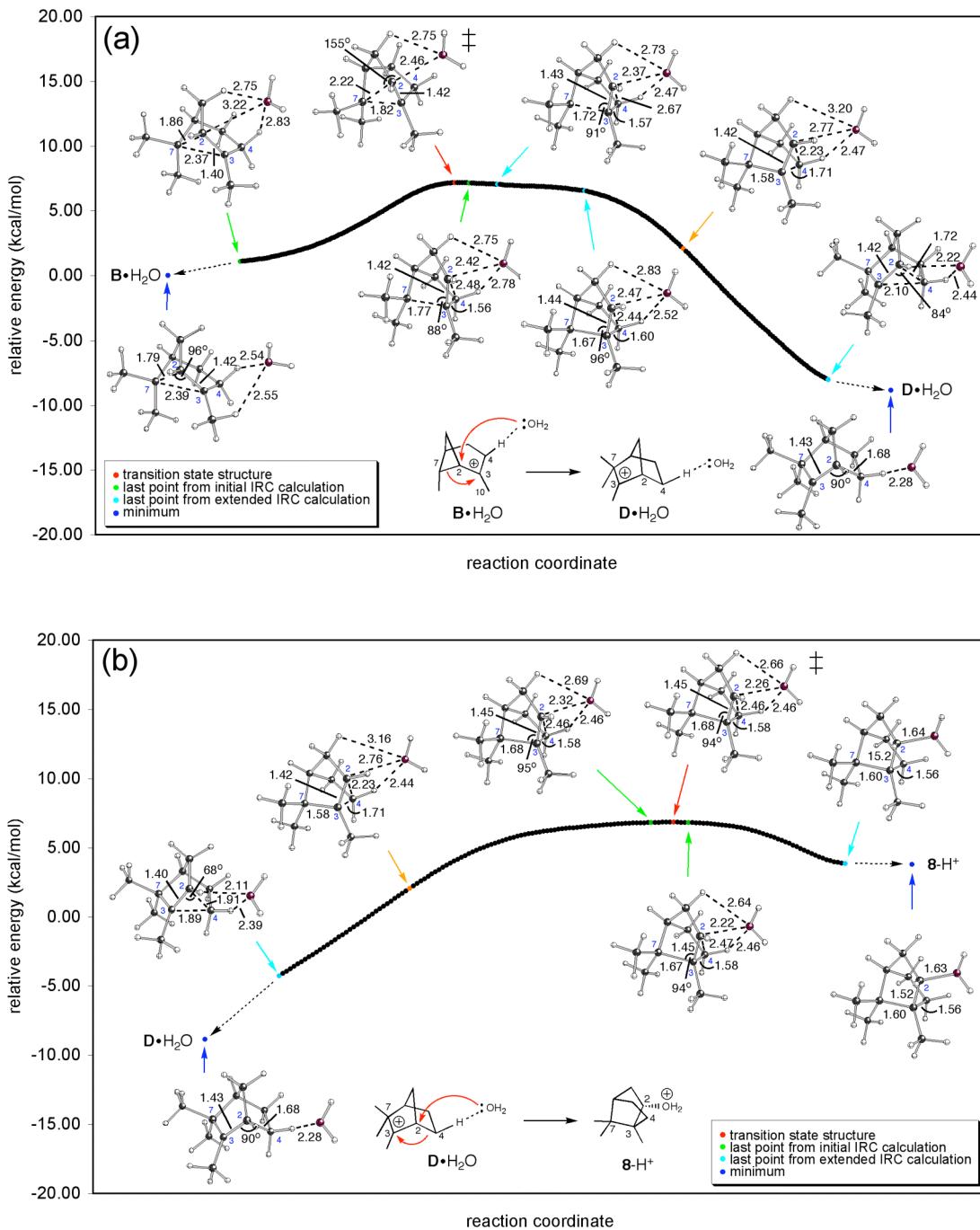


Figure S7. Conversion of **B**•H₂O complex (a) and **D**•H₂O complex (b) to **8**-H⁺ from IRC calculations; B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p). Energies do not include zero point energy corrections (kcal/mol; relative to the energy of **B**•H₂O complex in Figure Xa)). (a) The initial IRC calculation toward **D**•H₂O complex stopped at the point indicated in green at the right (geometry shown). To further verify the connection of **TS(S8)**, IRC calculation was extended using the wavefunction, geometry and force constants from the last point of the previous IRC calculation (i.e., using “rcfc”). This extended IRC calculation stopped

due to a convergence problem. Note that the geometry at the last point from the extended IRC calculation shows close similarity to **TS(S9)**. Two consecutive additional IRC calculations were carried out using the wavefunction and geometry from the last point of the previous IRC calculation, but force constants were recalculated (i.e., using “calcfc”). This led to the structure corresponding to the right end point (in sky-blue) on the plot. (b) IRC calculations toward both directions were extended using the wavefunction, geometry and force constants from the last point of the previous IRC calculation (i.e., using “rcfc”).

We found that the potential energy surface of the reaction via **TS(S8)** is much more complicated than expected; in fact, this reaction pathway appears bifurcate after the transition state structure. IRC calculation from **TS(S8)** towards the water complex with **B** proceeded as expected; the pathway is smoothly downhill (Figure S7a). IRC calculations toward the product complex, however, stopped at a geometry closely resembling **TS(S9)** (righthand side in Figure S7a). To verify the connection of **TS(S8)** to the product complex, it was necessary to extend IRC calculations for this direction. Somewhat cumbersome extensions of IRC calculations were made; the first extension was carried out using the force constants from the previous IRC (i.e., using “rcfc”) and in two additional consecutive extensions, the force constants were recalculated (i.e., using “calcfc”), since the first extended IRC calculation using “rcfc” suffered a convergence problem without showing significant changes in the geometry. The third extension of IRC calculations from recalculation of force constants was sufficient to verify the connection of **TS(S8)** to the product complex that is, somewhat surprisingly, the water and camphyl cation complex (**D**•H₂O complex, Figure S6a) instead of the expected 8-H⁺ (Note that the corresponding **TS1** connects the **B**•NH₃ complex to 7-H⁺; Figure 5a in the main paper). The IRC plot from the combined IRC calculations reveals that the pathway towards the product complex is initially rather flat and then steeply downhill. Note that the plateau region contains structures similar to **TS(S9)**. Full optimizations of the structures in the flat region

of the IRC also led to **TS(S9)**. These observations indicate that **TS(S8)** is directly connected to a second transition state structure, **TS(S9)**, which is consistent with a reaction surface where the pathway bifurcates into two pathways, each leading to a different product (Figures 5a-b and S7a-b). Note that **TS(S9)** itself is connected directly to the **D**•water complex and **8-H⁺** (Figures S6a and S7b).

We also examined attack of water on C2 from the lefthand side of **D** (as drawn in Figure S6b) leading to protonated isoborneol (**9-H⁺**). This reaction, similar to the water addition from the righthand side of **D**, again involves a concerted mechanism in which two reaction events (alkyl shift and water addition) are coupled. Calculations using ammonia instead of water led to a similar result (Figure S8).

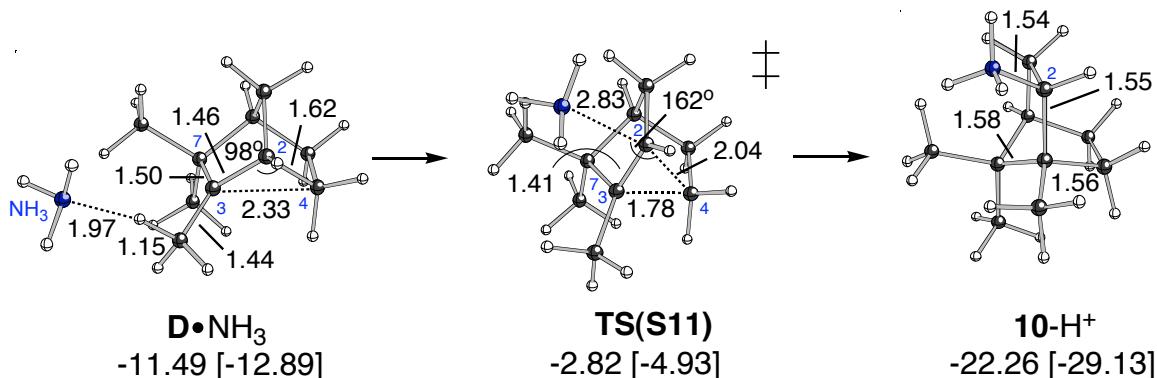


Figure S8. Ammonia-**D** complex, transition state structure and protonated product (**10**). Selected distances (Å) and energies (kcal/mol; relative to the energy of the **B•NH₃** complex in Figure 4 in the main paper) are shown; B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p) in normal text and mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p) in brackets.

V. Model of enzyme-bound pyrophosphate

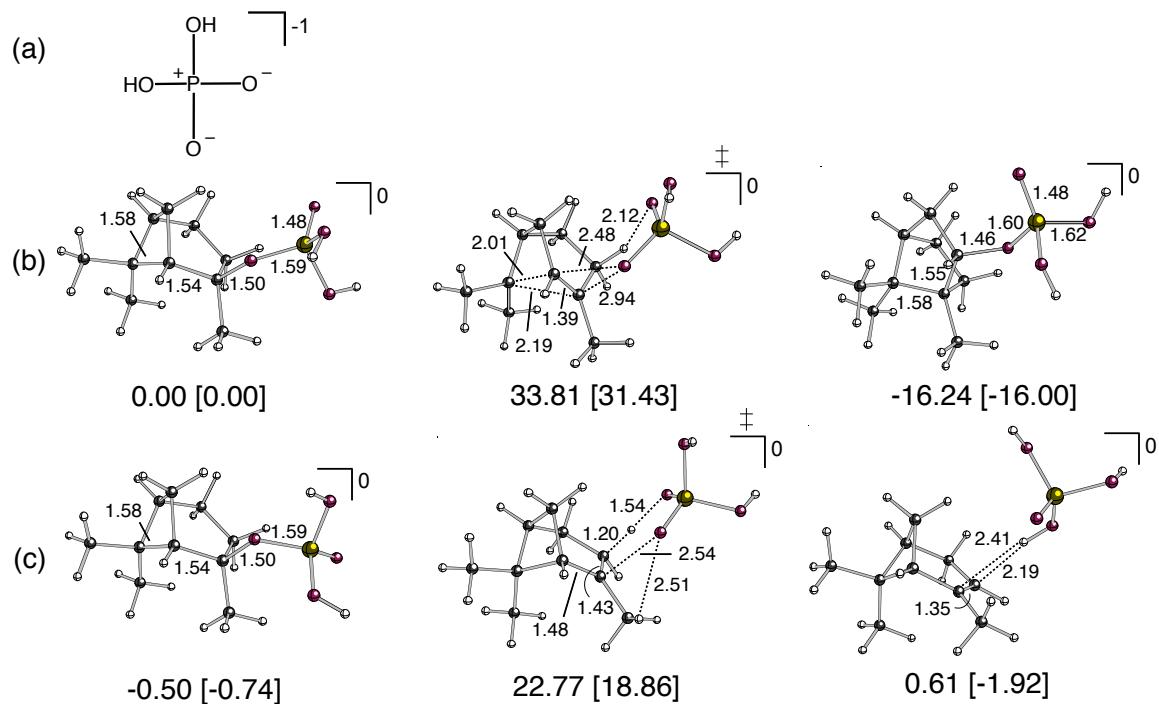


Figure S9. Computed (B3LYP/6-31+G(d,p)) reactant complexes, transition state structures and product complexes (selected distances in Å and energies in kcal/mol; before and after zero-point energy corrections from frequency calculations in normal text and in brackets, respectively); (a) Pyrophosphate model (unsuitable model due to high reactivity; unable to locate a cation complex with this model). (b) Model of BPP formation. (c) Model of α -pinene formation.

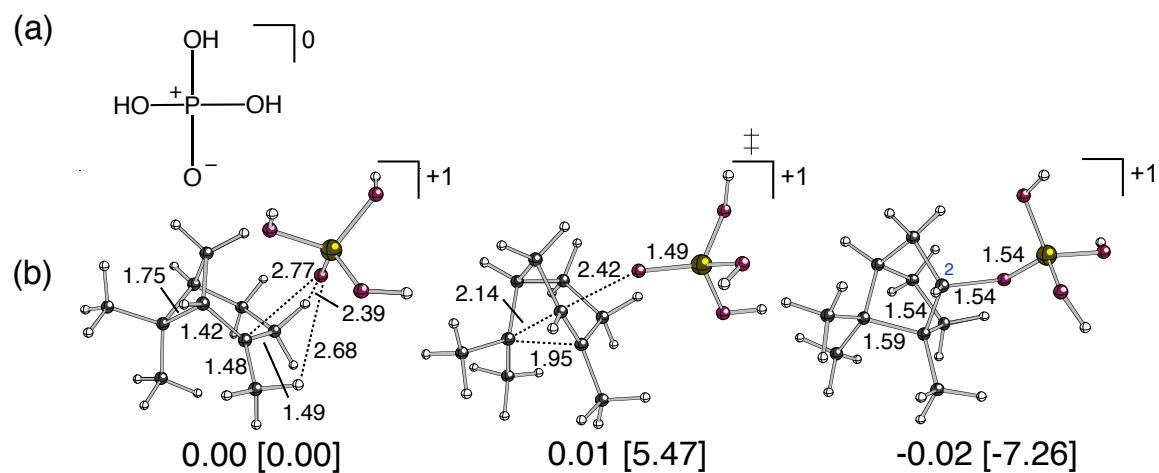


Figure S10. Computed (B3LYP/6-31G(d)) reactant complexes, transition state structures and product complexes (selected distances in Å and energies in kcal/mol; before and after zero-point energy corrections from frequency calculations in normal text and in brackets, respectively); (a) Pyrophosphate model. (b) Model of BPP formation.

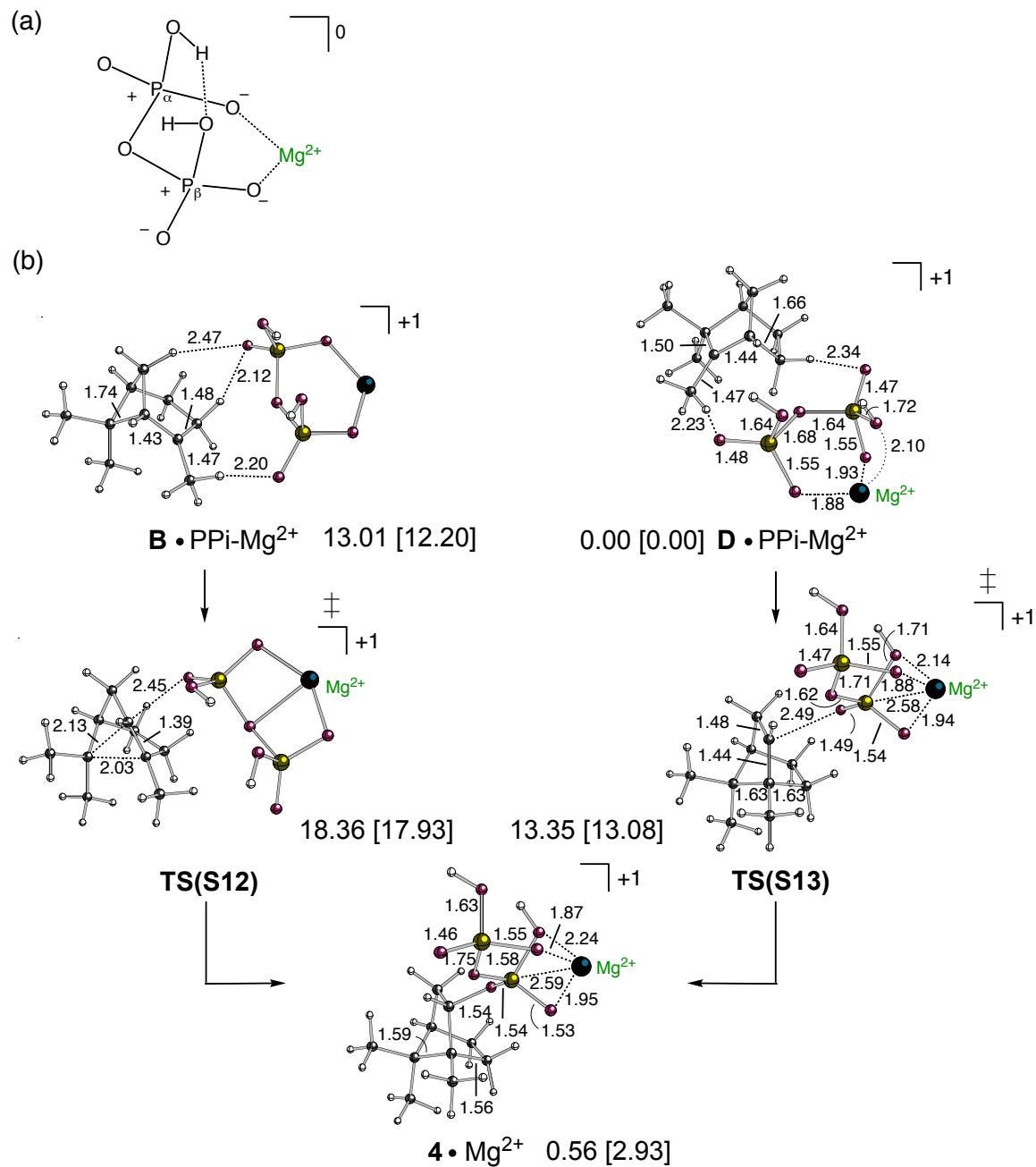


Figure S11. Formation of bornyl diphosphate (BPP) using (a) pyrophosphate model with magnesium ion (B3LYP/6-31G(d)). Computed reactant complexes, transition state structures and product complex (selected distances in Å; energies in kcal/mol: before and after zero-point energy corrections from B3LYP frequency calculation in normal text and in brackets, respectively). In this pyrophosphate model, coordination mode of magnesium ion with pyrophosphate tends to change.

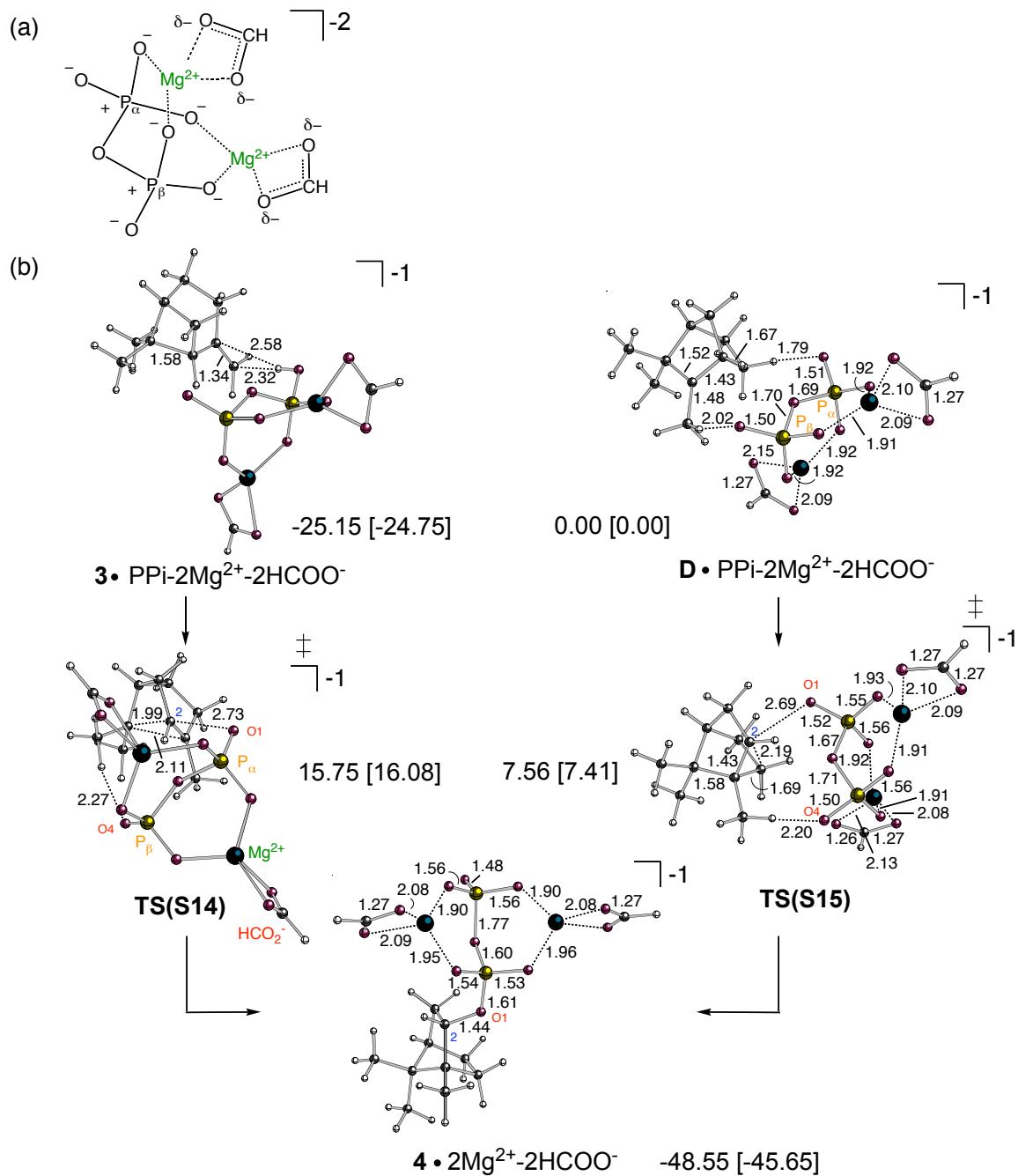
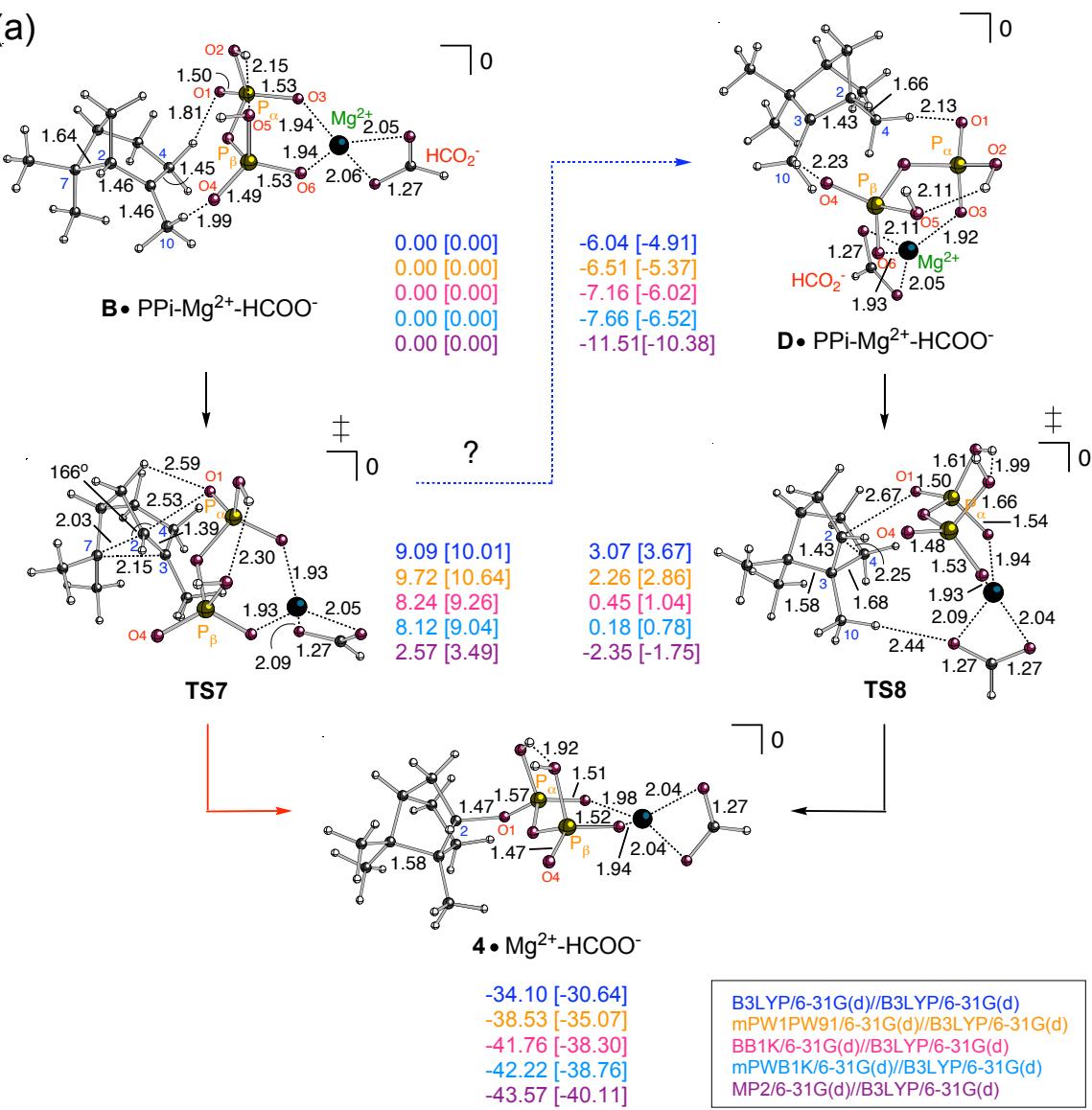


Figure S12. Formation of bornyl diphosphate (BPP) using (a) pyrophosphate model with two magnesium ions and two formate molecules (B3LYP/6-31G(d)). (b) Computed reactant complexes, transition state structures and product complex (selected distances in Å; energies in kcal/mol: before and after zero-point energy corrections from B3LYP frequency calculation in normal text and in brackets, respectively). This model tends to be protonated. The transition state structure **TS(S14)** is connected to BPP and directly to β -pinene (i.e., deprotonated **B**) complex instead of expected **B-PPI** complex.

(a)



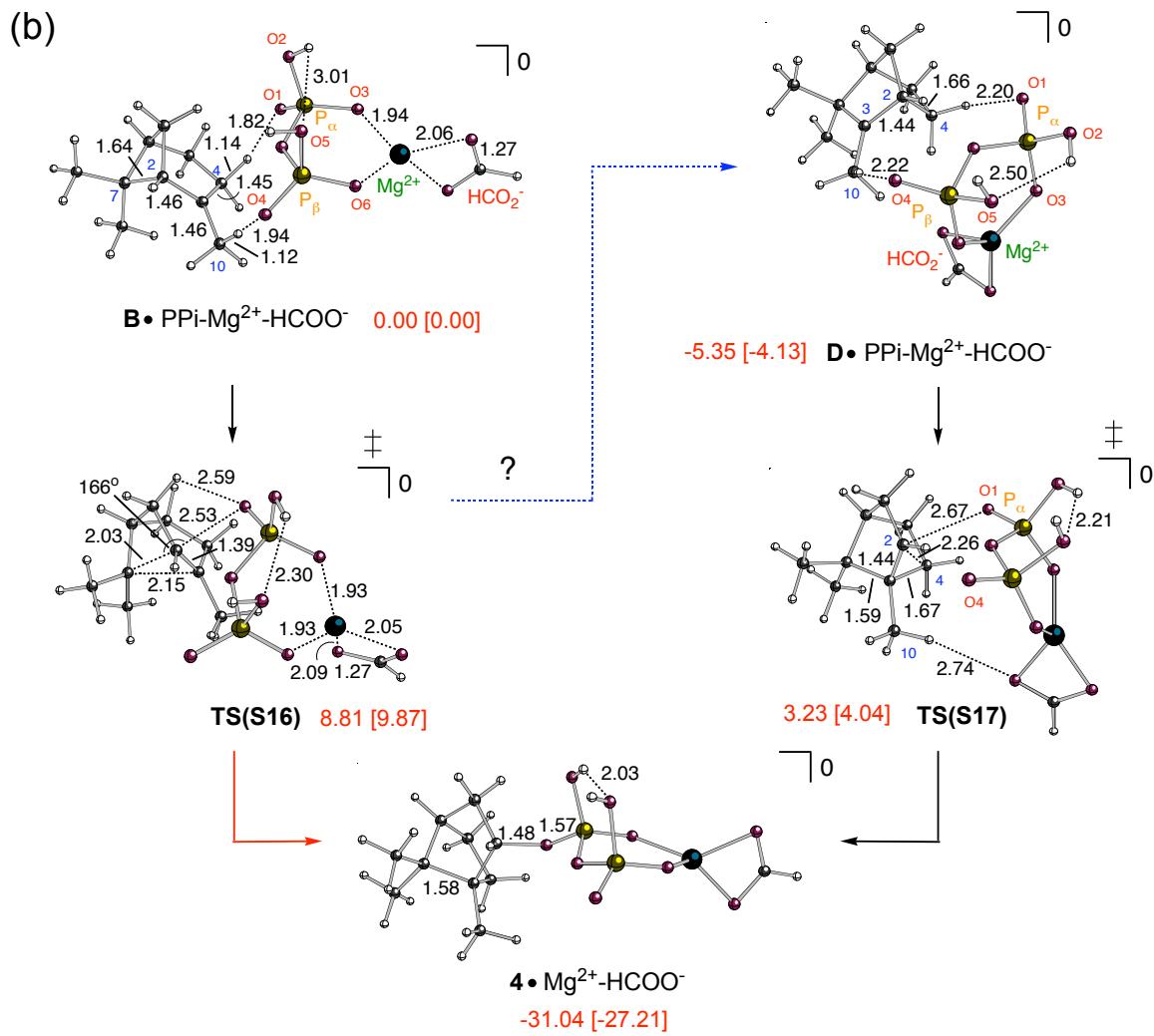


Figure S13. Formation of bornyl diphosphate (BPP). Computed reactant complexes, transition state structures and product complex. Selected distances in Å; (a) B3LYP/6-31G(d), (b) B3LYP/6-31+G(d,p)). Energies in kcal/mol; before and after zero-point energy corrections from frequency calculations by (a) B3LYP/6-31G(d), (b) by B3LYP/6-31+G(d,p) in normal text and in brackets, respectively.

VI. Formation of olefinic monoterpenes

Formation of α -/ β -pinene. We also explored reactions using the pyrophosphate model in differential hydrogen bonding (β -phosphate is a hydrogen bond donor and α -phosphate is an acceptor; Figure S14). Using this model, deprotonation to yield β -pinene is favored slightly energetically.

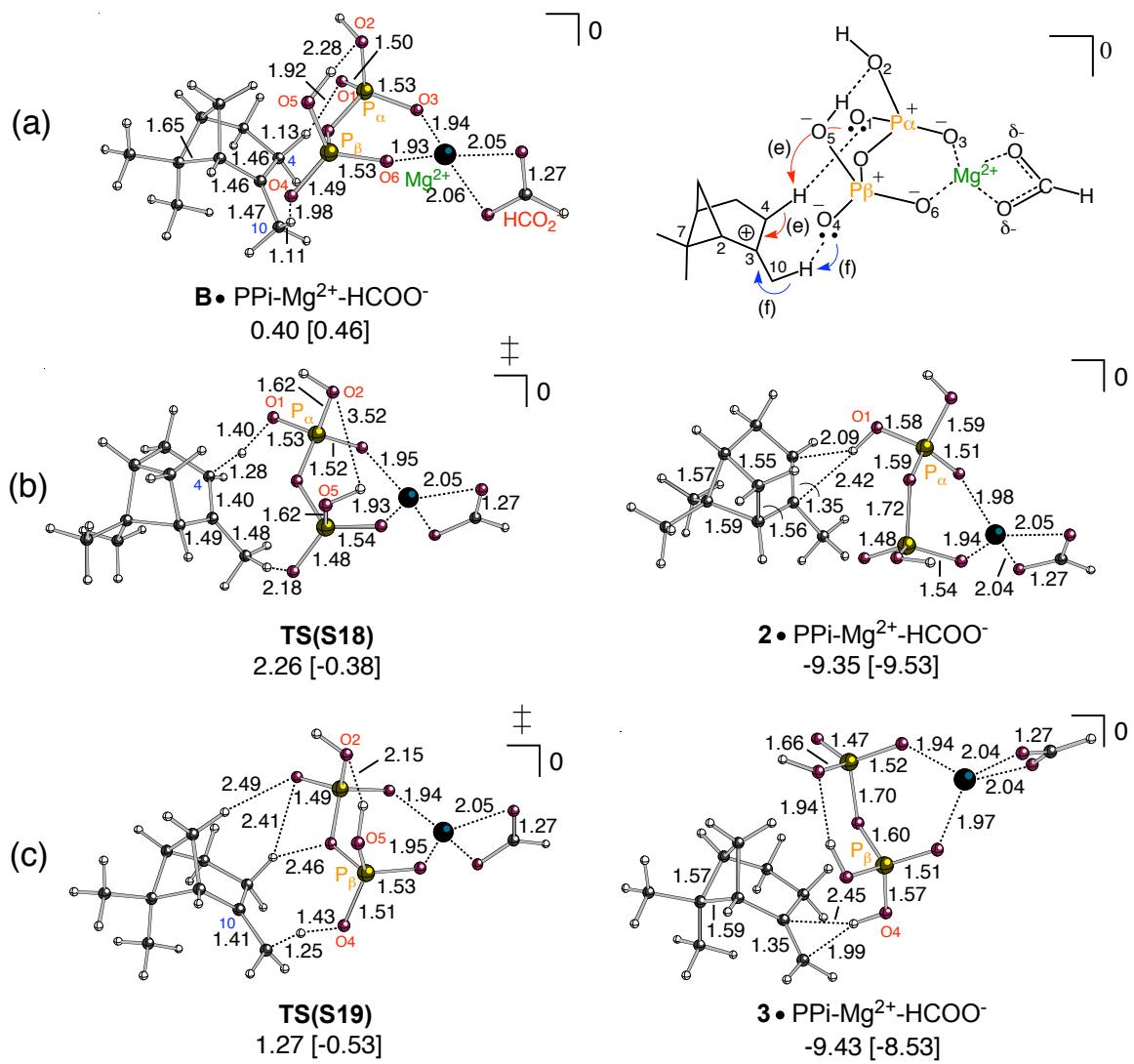


Figure S14. Formation of α -/ β -pinene. Computed (B3LYP/6-31G(d)) geometries (selected distances in Å) and energies (in kcal/mol, relative to the energy of **B**-PPi-Mg²⁺-HCOO⁻ complex in Figure S13a; before and after zero-point energy corrections in normal text and in brackets, respectively.) are shown. (a) **B**-PPi-Mg²⁺-HCOO⁻ complex and schematic picture of the two deprotonation pathways. (b) Transition state structure for deprotonation to form α -pinene and α -pinene complex with PPi-Mg²⁺-HCOO⁻. (c) Transition state structure for deprotonation to form β -pinene and β -pinene complex with PPi-Mg²⁺-HCOO⁻.

Formation of α -/ β -camphene. In the **D**•PPi complex, the pyrophosphate is appropriately positioned for facile deprotonation (Figure S15). The deprotonation reaction via **TS(S20)** is coupled to ring-closure (C3-C4 bond formation) to yield an α -camphene complex with

$\text{PPi-Mg}^{2+}-\text{HCOO}^-$. The energy barrier is estimated to be 3.24-5.74 kcal/mol from the **D**•PPi complex. Note that the **D**•PPi complex is also connected to the BPP complex (Figure S13a). The reaction energy barrier for the former is lower than that for the latter (8.58-9.11 kcal/mol).

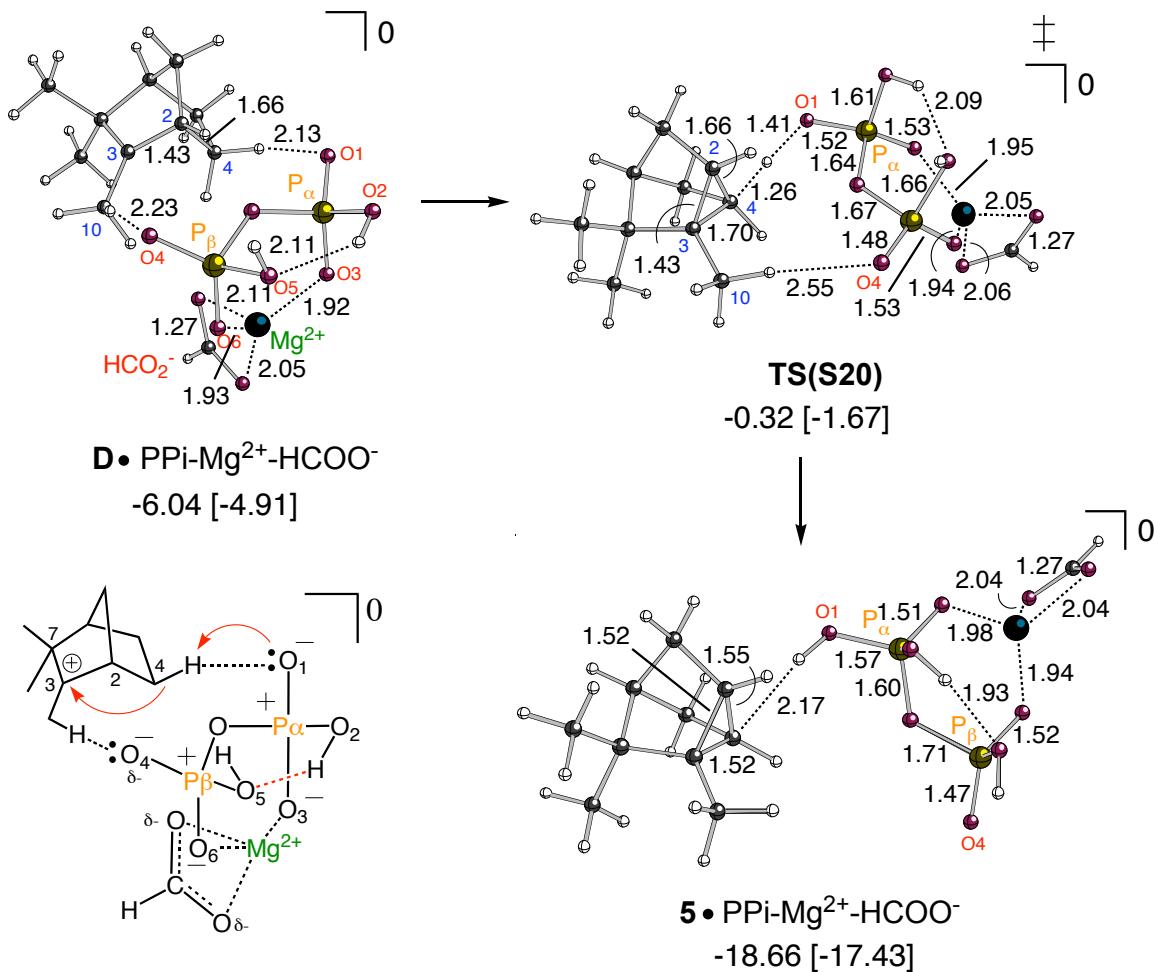


Figure S15. Formation of α -camphene (5). Computed geometries (selected distances in Å) and energies (in kcal/mol; relative to the energy of **B**-PPi-Mg²⁺-HCOO⁻ complex in Figure S13a; B3LYP/6-31G(d)//B3LYP/6-31G(d) are shown; before and after zero-point energy corrections in normal text and in brackets, respectively. The phosphate groups are labeled to distinguish each other and this representation of GPP may be different from literatures elsewhere.

Alternatively, direct deprotonation at C10 of the **D**•**PPi** complex could yield β -camphene. We were unable to locate a transition state structure connecting the **D**•**PPi** complex in Figure S15 directly to β -camphene. Instead we located transition state structure that connects β -camphene to the **D**•**PPi** complex that differs from the **D**•**PPi** complex connected to α -camphene described above (Figure S15). In the **D**•**PPi** complex, α -phosphate interacts with hydrogen (endo) at C4 through C-H \cdots X interaction while β -phosphate interacts with hydrogen at C10 through C-H \cdots X interaction (Figure S16a). These interaction modes position the diphosphate group beneath camphyl cation. This complexation forms an energetically more stable complex than the complexation in the **D**•**PPi** complex in Figure S15 (the pyrophosphate situates in front of camphyl cation). Deprotonation from the **D**•**PPi** complex yielding β -camphene is computed to be exothermic by 15.31-16.22 kcal/mol.

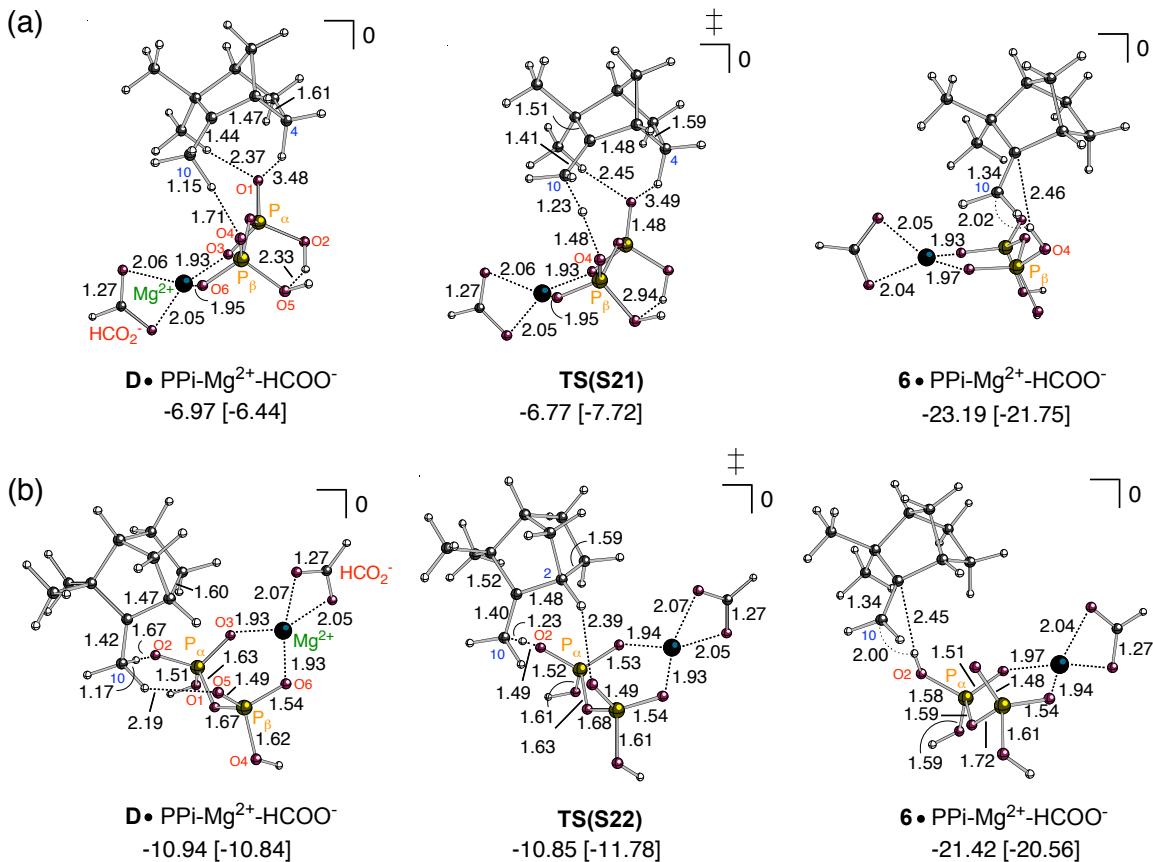


Figure S16. Formation of β -camphene (**6**). Computed reactant complexes, transition state structures and the product complexes (selected distances in Å), and energies (kcal/mol; relative to the energy of the **B**•PPi-Mg²⁺-HCOO⁻ complex in Figure S13a) are shown; B3LYP/6-31G(d)//B3LYP/6-31G(d). Energies before and after zero point energy corrections are shown in normal text and in brackets, respectively.

VII. Rearrangement of A in the presence of pyrophosphate

We located a transition state structure that appears to be a transition state structure connecting **B** and **D** in the presence of pyrophosphate. However, IRC calculations suggest that the transition state structure (**TS(S23)**; Figure S17) is connected to another transition state structure **TS (S24)** which itself is connected to **A** and **B** (pinyll cation: IRC verified). The last geometry from the other direction of the IRC looked like camphyl cation (**D**), but optimization led to camphene. It appears that this complexation

will lead directly to β -camphene via a barrierless deprotonation process. We were unable to locate a camphyl cation complex in this complexation mode. Strong C-H \cdots O interactions in the **A**-PPi complex also suggest facile deprotonation to yield limonene (note that C-H bonds are elongated). In the **B**-PPi complex, a strong C10-H \cdots O (α -phosphate group) interaction suggests facile deprotonation to yield β -pinene.

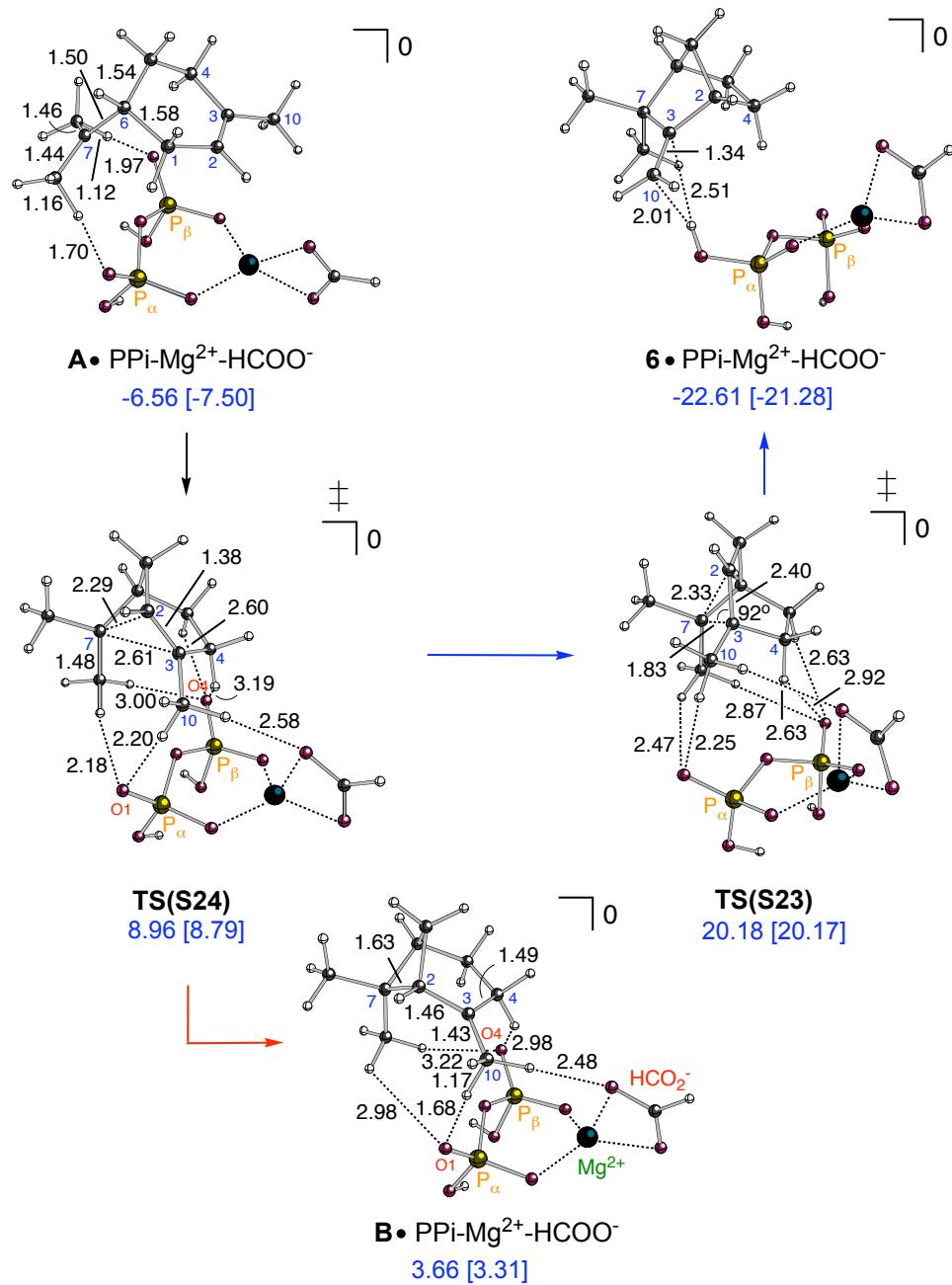


Figure S17. Rearrangement of **A** in the presence of pyrophosphate. Computed reactant complexes, transition state structures and the product complexes (selected distances in Å, and energies (kcal/mol; relative to the energy of the **B**•PPi-Mg²⁺-HCOO⁻ complex in Figure S13a) are shown; B3LYP/6-31G(d)//B3LYP/6-31G(d). Energies before and after zero point energy corrections are shown in normal text and in brackets, respectively. The **A**-PPi complex is located by IRC-independent optimization.

We also located a transition state structure that appears to be a transition state structure connecting **A** and **B** in the presence of pyrophosphate. However, IRC calculations suggest that the transition state structure (**TS(S25)**; Figure S18) is connected to limonene (i.e. deprotonated **A**) and **B**.

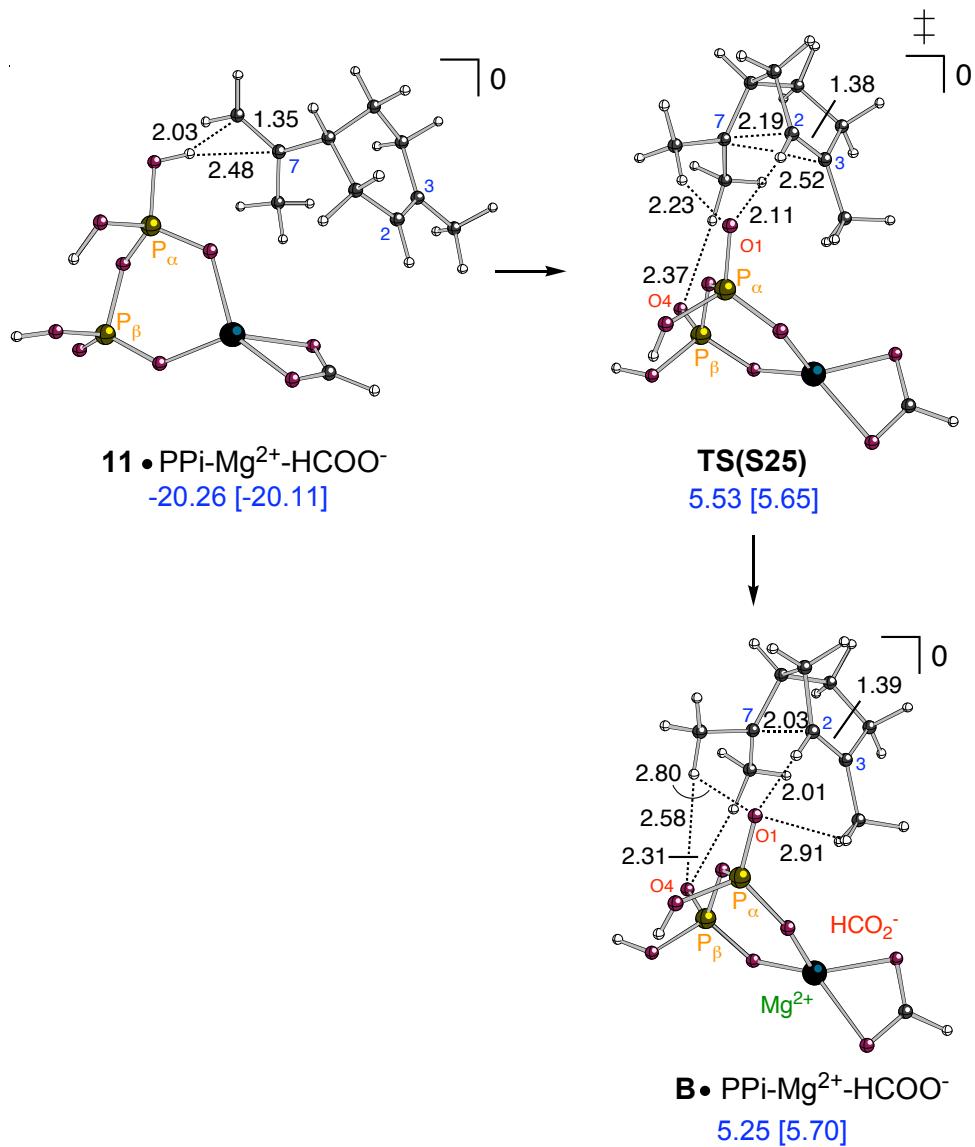


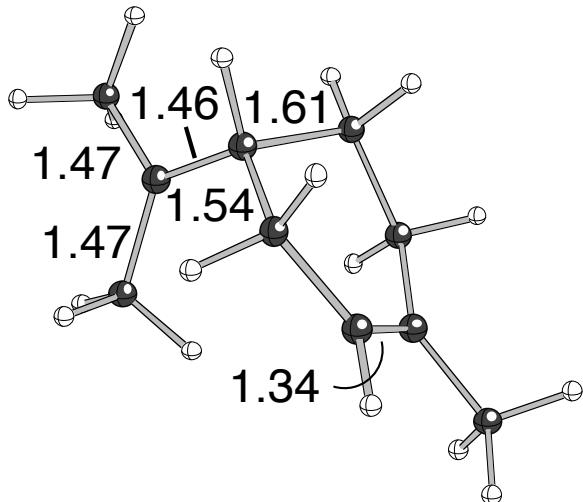
Figure S18. Interconversion of **A** to **B** and formation of limonene (**11**). Selected distances (in Å) and energies (in kcal/mol; relative to the energy of the **B**•PPi-Mg²⁺-HCOO⁻ complex in Figure S13a) are shown; B3LYP/6-31G(d)//B3LYP/6-31G(d). Energies before and after zero point energy corrections are shown in normal text and in brackets, respectively. Proton transfer from **A** to pyrophosphate is observed in the geometry at the last point from IRC calculation toward **A** from **TS(S25)**.

VIII. Coordinates and Energies

Figure 1.

A

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)



HF = -391.0466108 hartrees (-245385.658743108 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.244461 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.751723	-0.190450	0.260721
2	6	3.024128	0.548973	0.358473
3	6	1.346391	-1.035058	1.392358
4	6	0.940972	-0.071839	-0.945254
5	6	0.171786	1.339814	-0.800321
6	6	-0.969478	1.301333	0.213320
7	6	-1.830570	0.058061	0.122569
8	6	-1.411246	-1.033821	-0.536071
9	6	-3.168944	0.128503	0.809394
10	6	-0.089911	-1.175355	-1.254008
11	1	3.047213	1.148586	1.278884
12	1	3.250383	1.165289	-0.511688
13	1	3.829112	-0.192333	0.496355
14	1	1.884704	-0.823613	2.317070
15	1	1.588005	-2.071146	1.086749
16	1	0.260098	-1.042827	1.529763
17	1	1.623794	0.088258	-1.789015
18	1	-0.219246	1.498894	-1.810166
19	1	0.879048	2.146314	-0.591906
20	1	-1.594600	2.186199	0.034934

21	1	-0.596996	1.423591	1.242298
22	1	-2.067511	-1.899295	-0.597904
23	1	-3.057799	0.390954	1.869213
24	1	-3.705919	-0.820977	0.747905
25	1	-3.797510	0.905887	0.357906
26	1	-0.258144	-1.163333	-2.339416
27	1	0.346261	-2.161424	-1.048062

PBE/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.4943175 hartrees (-245035.18423125 kcal/mol)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.9550093 hartrees (-245328.177885843 kcal/mol)

BB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.8157263 hartrees

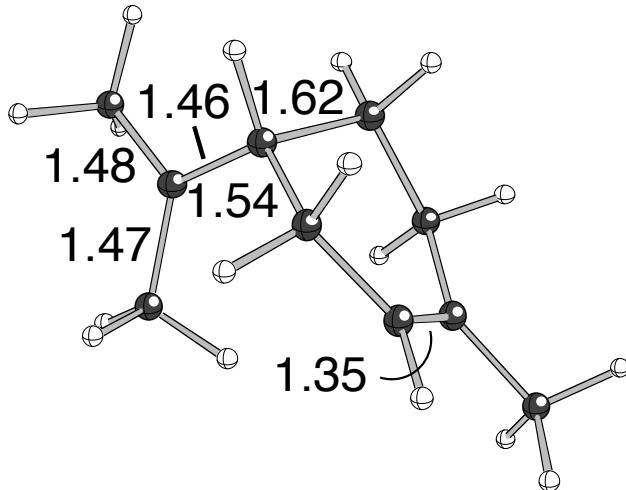
mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.8111513 hartrees (-245233.99744075 kcal/mol)

MP2/6-31+G(d,p)//B3LYP/6-31+G(d,p)

MP2 = -389.7365594 hartrees

PBE/6-31+G(d,p)//PBE/6-31+G(d,p)



HF = -390.4952062 hartrees (-245039.646842562 kcal/mol)

Imaginary Frequencies: none found

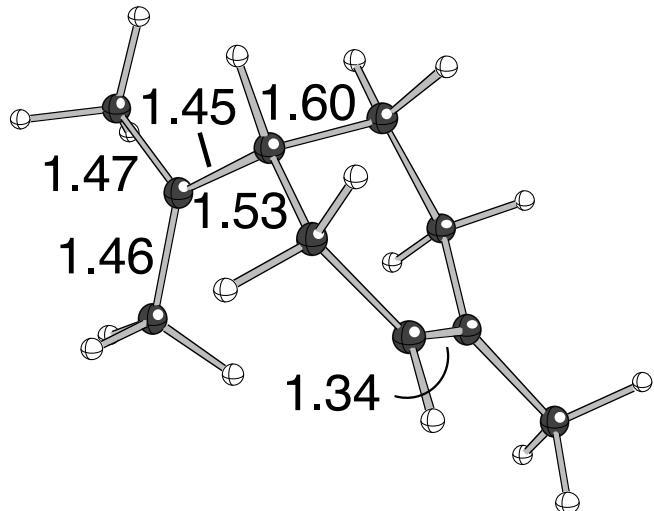
Zero-point correction = 0.237589 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.748638	-0.181305	0.274432
2	6	3.022802	0.558581	0.346090
3	6	1.314466	-0.956373	1.444109
4	6	0.949728	-0.127868	-0.945154
5	6	0.182106	1.296328	-0.866964
6	6	-0.957524	1.311254	0.148448
7	6	-1.826925	0.070128	0.119327
8	6	-1.408388	-1.060584	-0.493387
9	6	-3.164501	0.177501	0.802199
10	6	-0.087304	-1.238620	-1.203490
11	1	3.042298	1.214027	1.237960
12	1	3.270411	1.124798	-0.561686
13	1	3.830528	-0.177851	0.545609
14	1	1.837608	-0.702842	2.376081
15	1	1.546300	-2.019992	1.201009
16	1	0.214853	-0.955950	1.551454
17	1	1.639975	-0.001116	-1.799926
18	1	-0.211721	1.398018	-1.892910
19	1	0.899427	2.115524	-0.703393
20	1	-1.583397	2.195671	-0.078561
21	1	-0.585254	1.490717	1.178076
22	1	-2.075445	-1.930337	-0.514610

23	1	-3.053756	0.494580	1.855205
24	1	-3.709584	-0.777995	0.787470
25	1	-3.795880	0.939994	0.311678
26	1	-0.255894	-1.279126	-2.296950
27	1	0.350944	-2.222371	-0.950158

mPW1PW91/6-31+G(d,p)//mPW1PW91/6-31+G(d,p)



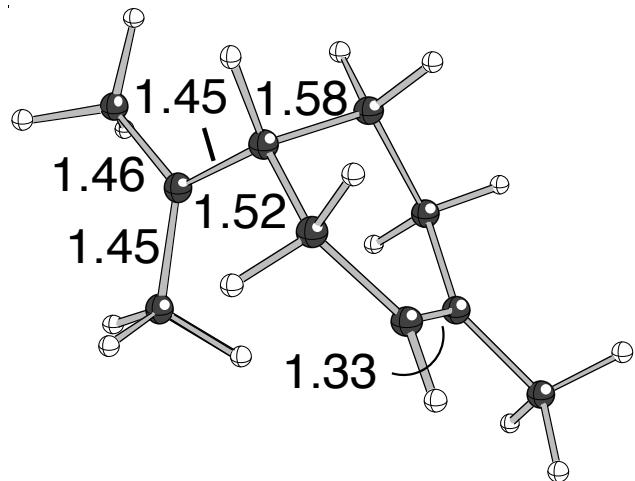
HF = -390.9555321 hartrees (-245328.505948071 kcal/mol)
 Imaginary Frequencies: none found
 Zero-point correction = 0.246358 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.725908	-0.182123	0.274157
2	6	2.979766	0.575177	0.363244
3	6	1.304600	-0.978034	1.423727
4	6	0.938725	-0.127362	-0.947203
5	6	0.187803	1.280180	-0.876261
6	6	-0.936258	1.305336	0.146313
7	6	-1.804240	0.073295	0.121364
8	6	-1.400226	-1.049059	-0.488608
9	6	-3.130784	0.186417	0.809661
10	6	-0.089633	-1.232482	-1.202319
11	1	2.967856	1.224086	1.247890
12	1	3.223879	1.143807	-0.532388

13	1	3.786378	-0.145328	0.568879
14	1	1.821830	-0.733719	2.350417
15	1	1.553210	-2.021503	1.156385
16	1	0.214835	-0.988966	1.530772
17	1	1.635599	-0.018435	-1.786826
18	1	-0.217855	1.385636	-1.886594
19	1	0.898636	2.095073	-0.724291
20	1	-1.555651	2.184822	-0.065103
21	1	-0.553004	1.471751	1.163825
22	1	-2.066012	-1.907934	-0.507160
23	1	-3.010012	0.495242	1.853875
24	1	-3.676401	-0.758040	0.794811
25	1	-3.753650	0.947323	0.327750
26	1	-0.264221	-1.272348	-2.284501
27	1	0.340614	-2.209540	-0.952191

BB1K/6-31+G(d,p)//BB1K/6-31+G(d,p)



HF = -390.8183102 hartrees (-245242.397833602 kcal/mol)

Imaginary Frequencies: none found

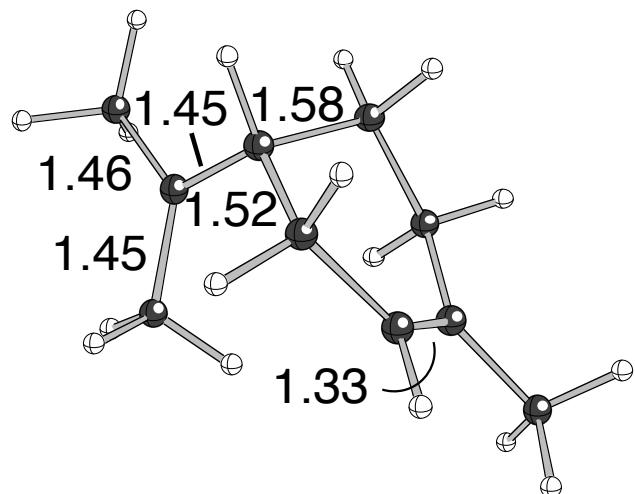
Zero-point correction = 0.250509 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.699203	0.145322	0.302629
2	6	-2.948509	-0.611067	0.292400
3	6	-1.244464	0.734867	1.550692

4	6	-0.939591	0.283572	-0.922110
5	6	-0.206040	-1.112724	-1.057887
6	6	0.887255	-1.299093	-0.031886
7	6	1.777310	-0.099423	0.104337
8	6	1.396679	1.094837	-0.345939
9	6	3.096566	-0.329052	0.762103
10	6	0.091152	1.399085	-1.011997
11	1	-2.938183	-1.370691	1.075879
12	1	-3.196696	-1.043435	-0.669696
13	1	-3.742320	0.081885	0.594322
14	1	-1.774885	0.384281	2.427929
15	1	-1.415599	1.815528	1.440435
16	1	-0.160375	0.656945	1.650306
17	1	-1.645149	0.308905	-1.753572
18	1	0.221979	-1.066742	-2.057886
19	1	-0.920924	-1.931567	-1.047019
20	1	1.488030	-2.158178	-0.331796
21	1	0.477030	-1.571651	0.946513
22	1	2.077197	1.930898	-0.254268
23	1	2.970698	-0.776822	1.748088
24	1	3.654295	0.595179	0.877577
25	1	3.701958	-1.021663	0.178114
26	1	0.261447	1.605044	-2.069840
27	1	-0.325428	2.324135	-0.609144

mPWB1K/6-31+G(d,p)//mPWB1K/6-31+G(d,p)

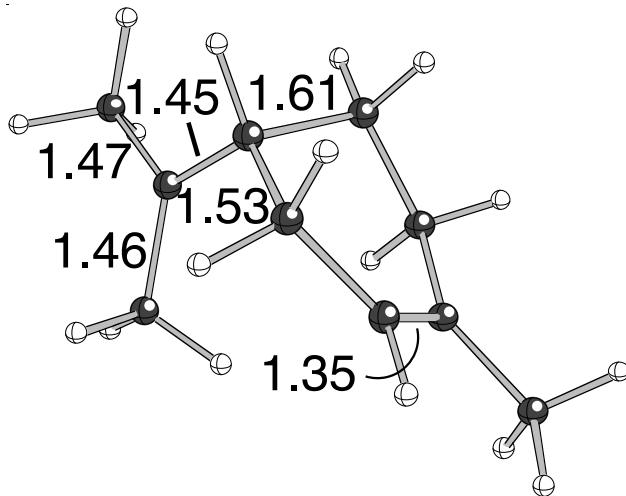


HF = -390.8142227 hartrees (-245239.832886477 kcal/mol)
 Imaginary Frequencies: none found
 Zero-point correction = 0.250995 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.695811	0.138017	0.304699
2	6	-2.942310	-0.620620	0.278091
3	6	-1.239980	0.698257	1.563985
4	6	-0.938558	0.309035	-0.915919
5	6	-0.208662	-1.083383	-1.082573
6	6	0.879622	-1.295510	-0.057939
7	6	1.774515	-0.103927	0.101643
8	6	1.398251	1.100299	-0.321510
9	6	3.092938	-0.352654	0.750790
10	6	0.092439	1.424897	-0.974659
11	1	-2.920692	-1.407325	1.033458
12	1	-3.195102	-1.020916	-0.695979
13	1	-3.736517	0.056294	0.610620
14	1	-1.749068	0.306948	2.436009
15	1	-1.452758	1.774377	1.485533
16	1	-0.153481	0.655393	1.646767
17	1	-1.642941	0.356245	-1.746607
18	1	0.223460	-1.015611	-2.078996
19	1	-0.925074	-1.900140	-1.093106
20	1	1.476549	-2.151647	-0.371236
21	1	0.465257	-1.582009	0.914272
22	1	2.082393	1.930692	-0.213917
23	1	2.966648	-0.818620	1.727542
24	1	3.654863	0.566116	0.882740
25	1	3.693058	-1.036359	0.152228
26	1	0.260414	1.662519	-2.025538
27	1	-0.321673	2.337577	-0.543439

MP2/6-31+G(d,p)//MP2/6-31+G(d,p)



HF = -388.3411913 hartrees (-243687.980952663 kcal/mol)

MP2 = -389.7379658 hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.250185 (Hartree/Particle)

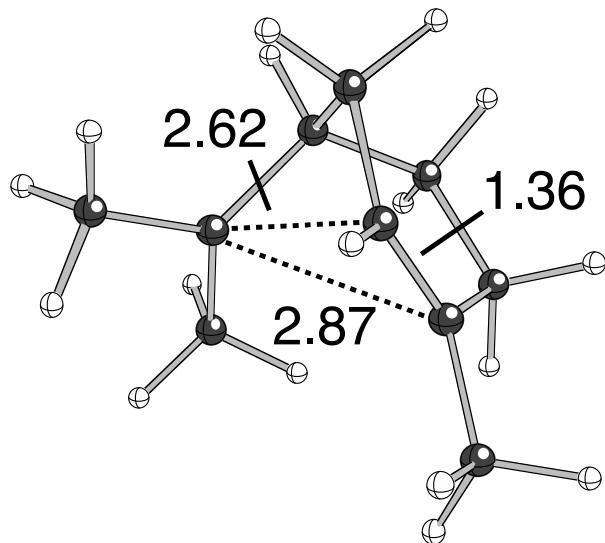
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.695559	0.117687	0.312793
2	6	-2.951962	-0.643660	0.233142
3	6	-1.237153	0.566279	1.628117
4	6	-0.950403	0.398585	-0.892913
5	6	-0.214662	-1.001783	-1.170528
6	6	0.876484	-1.297473	-0.155281
7	6	1.780800	-0.116574	0.093113
8	6	1.405253	1.135228	-0.236800
9	6	3.108817	-0.420011	0.724398
10	6	0.094455	1.515473	-0.873687
11	1	-2.865686	-1.545180	0.848770
12	1	-3.249257	-0.894303	-0.780146
13	1	-3.732514	-0.044844	0.717458
14	1	-1.713414	0.048018	2.455746
15	1	-1.540930	1.626846	1.663221
16	1	-0.149746	0.582249	1.700770
17	1	-1.653366	0.501137	-1.724045
18	1	0.220771	-0.839980	-2.158692
19	1	-0.941023	-1.810622	-1.250818
20	1	1.474075	-2.128073	-0.541959
21	1	0.457529	-1.660994	0.792132
22	1	2.099374	1.952377	-0.068781

23	1	2.975777	-0.957769	1.665960
24	1	3.671690	0.490114	0.924367
25	1	3.705839	-1.058831	0.070736
26	1	0.264165	1.818578	-1.911381
27	1	-0.319699	2.398762	-0.377458

TS (A-to-B)

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)



HF = -391.0395123 hartrees (-245377.29396825 kcal/mol)

Imaginary Frequencies: 1 (-58.7398 1/cm)

Zero-point correction = 0.245035 (Hartree/Particle)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.360507	-0.254380	-0.307845
2	6	-1.279433	-0.429496	-1.773978
3	6	-2.222522	-1.222921	0.408652
4	6	-0.906352	1.028627	0.349037
5	6	0.150238	1.792689	-0.465665
6	6	1.445075	0.943593	-0.644015
7	6	1.469633	-0.335513	0.159583
8	6	0.707190	-0.465813	1.281123
9	6	2.434869	-1.398080	-0.279929

10	6	-0.277066	0.611068	1.691654
11	1	-0.309790	-0.155963	-2.194628
12	1	-1.992018	0.300072	-2.202234
13	1	-1.575524	-1.425555	-2.105031
14	1	-1.990350	-2.253477	0.122047
15	1	-3.245059	-1.043510	0.028949
16	1	-2.243294	-1.118921	1.490623
17	1	-1.807410	1.655895	0.473531
18	1	0.370323	2.715874	0.076186
19	1	-0.240282	2.101707	-1.439693
20	1	2.314473	1.541171	-0.338303
21	1	1.630801	0.710902	-1.699883
22	1	0.833528	-1.340764	1.915077
23	1	2.216926	-1.729524	-1.303283
24	1	2.420839	-2.268429	0.379762
25	1	3.456559	-0.998192	-0.299063
26	1	0.206787	1.462658	2.184750
27	1	-1.013262	0.227410	2.399492

PBE/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.4900341 hartrees (-245032.49639775 kcal/mol)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.9493619 hartrees (-245324.634085869 kcal/mol)

BB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.806342 hartrees (-245230.979605 kcal/mol)

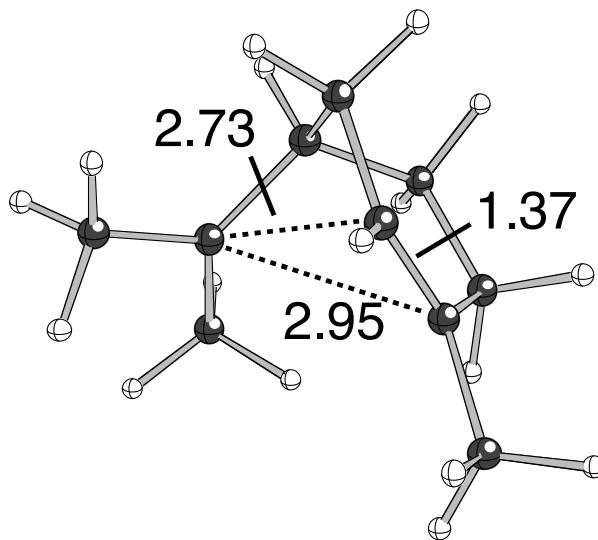
mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.8107804 hartrees (-245233.764701 kcal/mol)

MP2/6-31+G(d,p)//B3LYP/6-31+G(d,p)

MP2 = -389.7318396 hartrees

PBE/6-31+G(d,p)//PBE/6-31+G(d,p)



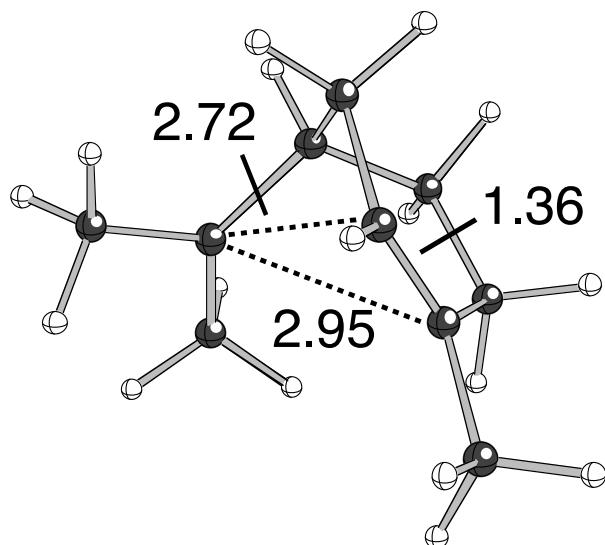
HF = -390.4909261 hartrees (-245036.961037011 kcal/mol)
Imaginary Frequencies: 1 (-54.2816 1/cm)
Zero-point correction = 0.238276 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.411846	-0.094389	-0.363157
2	6	-1.477640	0.605577	-1.662547
3	6	-2.128989	-1.384841	-0.275816
4	6	-0.907453	0.634558	0.856220
5	6	0.101643	1.756593	0.532809
6	6	1.356703	1.186158	-0.182945
7	6	1.510958	-0.310764	-0.073180
8	6	0.832621	-1.024226	0.882560
9	6	2.506424	-0.961775	-0.990024
10	6	-0.218151	-0.392852	1.770532
11	1	-0.472234	0.925405	-1.995793
12	1	-2.020799	1.563806	-1.520172
13	1	-1.963216	0.021302	-2.455214
14	1	-1.912822	-2.023820	-1.149001
15	1	-3.210081	-1.135620	-0.381163
16	1	-2.000178	-1.942804	0.657853
17	1	-1.808711	1.088296	1.332558
18	1	0.379859	2.222146	1.491409
19	1	-0.352058	2.560304	-0.069976

20	1	2.263856	1.651978	0.247932
21	1	1.394923	1.476941	-1.251116
22	1	1.079175	-2.082969	1.027967
23	1	2.238195	-0.796708	-2.049692
24	1	2.589711	-2.044493	-0.815612
25	1	3.507044	-0.512061	-0.856567
26	1	0.219510	0.092858	2.662460
27	1	-0.917788	-1.148794	2.157422

mPW1PW91/6-31+G(d,p)//mPW1PW91/6-31+G(d,p)



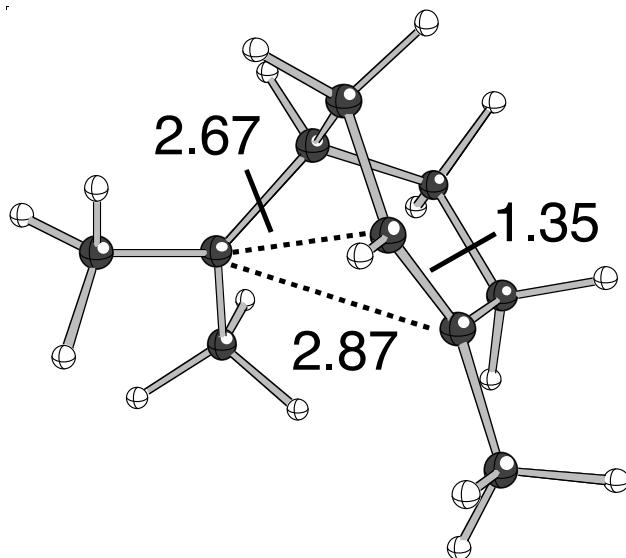
HF = -390.9496361 hartrees (-245324.806149111 kcal/mol)
 Imaginary Frequencies: 1 (-67.6341 1/cm)
 Zero-point correction = 0.246716 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.416946	-0.081672	-0.358084
2	6	-1.482959	0.647838	-1.631307
3	6	-2.118555	-1.371576	-0.307287
4	6	-0.903335	0.601216	0.869396
5	6	0.092865	1.728261	0.574090
6	6	1.348355	1.186862	-0.143044
7	6	1.505634	-0.307235	-0.080574

8	6	0.830857	-1.048546	0.831391
9	6	2.511955	-0.912777	-1.007634
10	6	-0.208550	-0.445115	1.741050
11	1	-0.482243	0.961890	-1.949022
12	1	-2.018718	1.593176	-1.457751
13	1	-1.968537	0.089412	-2.429547
14	1	-1.888956	-1.977775	-1.188305
15	1	-3.188943	-1.121042	-0.414559
16	1	-1.989388	-1.944585	0.605238
17	1	-1.800754	1.027771	1.356132
18	1	0.361991	2.169998	1.535679
19	1	-0.361744	2.534860	-0.006540
20	1	2.242391	1.636188	0.306135
21	1	1.388585	1.508072	-1.191572
22	1	1.063266	-2.105602	0.931760
23	1	2.259188	-0.705736	-2.053413
24	1	2.592267	-1.992730	-0.878315
25	1	3.500843	-0.473753	-0.837431
26	1	0.232473	0.020042	2.629531
27	1	-0.897647	-1.203729	2.114002

BB1K/6-31+G(d,p)//BB1K/6-31+G(d,p)

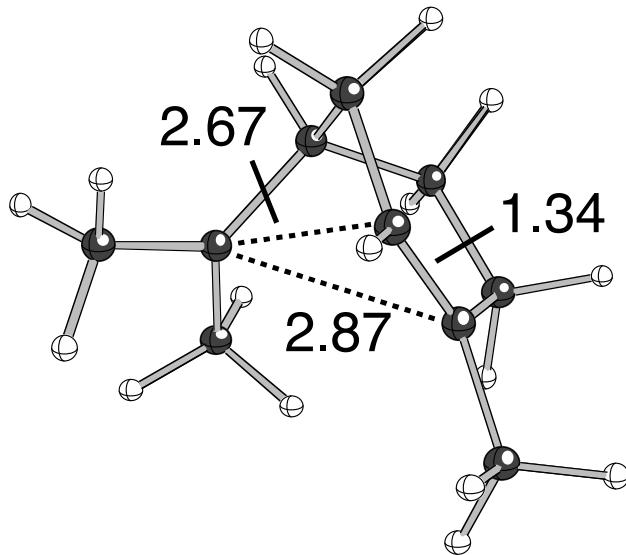


HF = -390.8128608 hartrees (-245238.978280608 kcal/mol)
 Imaginary Frequencies: 1 (-105.9904 1/cm)
 Zero-point correction = 0.250189 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.383870	-0.140272	-0.349046
2	6	-1.428874	0.354080	-1.724205
3	6	-2.036486	-1.423707	-0.094683
4	6	-0.914476	0.750701	0.746907
5	6	0.082745	1.803615	0.275442
6	6	1.327004	1.142702	-0.329110
7	6	1.463987	-0.314058	-0.013425
8	6	0.791833	-0.879520	1.006159
9	6	2.459339	-1.074054	-0.821009
10	6	-0.235358	-0.119118	1.793370
11	1	-0.404399	0.358949	-2.110713
12	1	-1.742570	1.397832	-1.748940
13	1	-2.039513	-0.256126	-2.379841
14	1	-1.841765	-2.130806	-0.898011
15	1	-3.111285	-1.200768	-0.166126
16	1	-1.841460	-1.863998	0.872164
17	1	-1.822767	1.247733	1.119524
18	1	0.346893	2.396312	1.146909
19	1	-0.361094	2.499314	-0.433271
20	1	2.221956	1.647311	0.038184
21	1	1.368389	1.279299	-1.411519
22	1	1.008077	-1.904341	1.277451
23	1	2.208987	-1.043081	-1.881941
24	1	2.527641	-2.112477	-0.512488
25	1	3.447443	-0.624466	-0.725209
26	1	0.209288	0.494285	2.576845
27	1	-0.928888	-0.787184	2.294582

mPWB1K/6-31+G(d,p)//mPWB1K/6-31+G(d,p)



HF = -390.808878 hartrees (-245236.47903378 kcal/mol)

Imaginary Frequencies: 1 (-79.4003 1/cm)

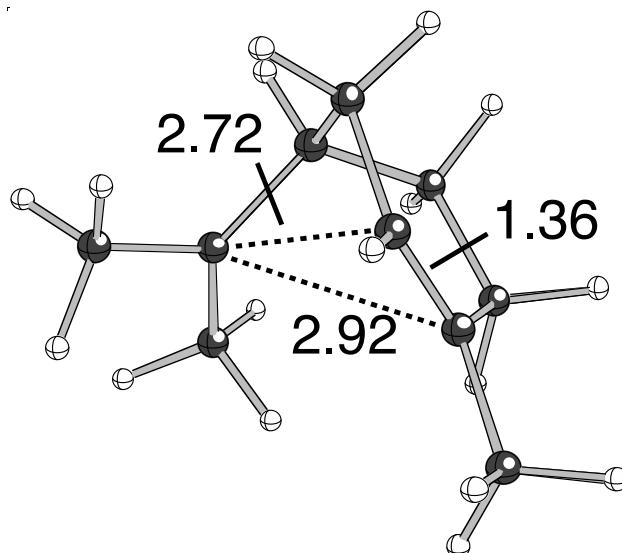
Zero-point correction = 0.251062 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.381510	-0.144632	-0.347799
2	6	-1.422919	0.326892	-1.729583
3	6	-2.029418	-1.425409	-0.075815
4	6	-0.915200	0.762266	0.734494
5	6	0.082206	1.806868	0.249375
6	6	1.323770	1.136474	-0.346478
7	6	1.460593	-0.313757	-0.006645
8	6	0.789687	-0.862421	1.021090
9	6	2.453908	-1.085619	-0.803107
10	6	-0.238029	-0.090276	1.794560
11	1	-0.399188	0.298257	-2.116726
12	1	-1.712864	1.375610	-1.775934
13	1	-2.045947	-0.284425	-2.371582
14	1	-1.838822	-2.140237	-0.872343
15	1	-3.104275	-1.204107	-0.142195
16	1	-1.827319	-1.854507	0.893877
17	1	-1.824224	1.264074	1.096992
18	1	0.347657	2.409295	1.112990
19	1	-0.360141	2.494421	-0.467102
20	1	2.219436	1.646397	0.009619

21	1	1.362220	1.254335	-1.430573
22	1	1.005511	-1.882479	1.307770
23	1	2.200847	-1.071953	-1.863216
24	1	2.523405	-2.118250	-0.478066
25	1	3.441284	-0.634047	-0.717301
26	1	0.205517	0.535342	2.568005
27	1	-0.931628	-0.750041	2.305234

MP2/6-31+G(d,p)//MP2/6-31+G(d,p)



HF = -388.3334978 hartrees (-243683.153204478 kcal/mol)

MP2 = -389.7316363 hartrees

Imaginary Frequencies: 1 (-67.6270 1/cm)

Zero-point correction = 0.250033 (Hartree/Particle)

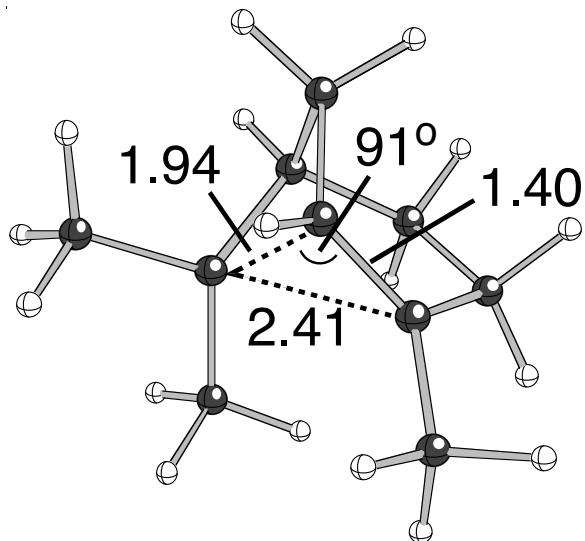
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.409143	-0.094720	-0.355970
2	6	-1.464883	0.540895	-1.679232
3	6	-2.067910	-1.403614	-0.242948
4	6	-0.913947	0.653358	0.831259
5	6	0.086546	1.765768	0.488748
6	6	1.312141	1.183260	-0.242279
7	6	1.485959	-0.302661	-0.056479

8	6	0.825840	-0.987368	0.915126
9	6	2.504893	-0.964022	-0.937793
10	6	-0.224107	-0.330629	1.778286
11	1	-0.499362	0.308760	-2.153331
12	1	-1.536501	1.624541	-1.625420
13	1	-2.240792	0.112870	-2.310506
14	1	-1.948418	-1.988310	-1.154759
15	1	-3.139520	-1.144694	-0.194227
16	1	-1.814726	-1.980245	0.636497
17	1	-1.829241	1.099944	1.264242
18	1	0.382724	2.212054	1.438053
19	1	-0.367979	2.567369	-0.094046
20	1	2.218494	1.679409	0.117118
21	1	1.278144	1.405823	-1.313561
22	1	1.070361	-2.030980	1.086511
23	1	2.245271	-0.842590	-1.992487
24	1	2.594472	-2.027207	-0.721956
25	1	3.482398	-0.498396	-0.797733
26	1	0.206163	0.203158	2.629284
27	1	-0.913828	-1.063111	2.194025

B

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)



HF = -391.0417233 hartrees (-245378.68137075 kcal/mol)

Imaginary Frequencies: none

Zero-point correction = 0.246757 (Hartree/Particle)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.133109	-0.190070	-1.247139
2	6	-1.256796	-0.320257	-0.428683
3	6	-1.641471	0.854667	0.417029
4	6	-0.393133	1.639933	0.952426
5	6	0.860741	1.192069	0.198555
6	6	0.534478	1.182671	-1.314921
7	1	-2.222179	1.516152	-0.244202
8	1	0.068777	-0.966870	-1.981341
9	1	-0.540040	2.713358	0.810886
10	1	-0.287111	1.473605	2.027834
11	1	-0.120277	1.990809	-1.654161
12	1	1.417248	1.168833	-1.952277
13	1	-2.320878	0.557963	1.220281
14	6	-2.057430	-1.570346	-0.370507
15	1	-3.077718	-1.342262	-0.711735
16	1	-1.654613	-2.366893	-0.998644
17	1	-2.163506	-1.922995	0.662507
18	1	1.745856	1.754964	0.514437
19	6	1.042463	-0.339306	0.286676
20	6	0.661059	-1.100146	1.537438
21	1	1.471285	-0.939198	2.262173
22	1	-0.262601	-0.773388	2.013982
23	1	0.609607	-2.177019	1.354411
24	6	2.291064	-0.924877	-0.348298
25	1	3.102296	-0.807073	0.383710
26	1	2.182421	-1.996160	-0.536662
27	1	2.604234	-0.429860	-1.266649

PBE/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.4959599 hartrees (-245036.21483725 kcal/mol)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.9571483 hartrees (-245329.520129733 kcal/mol)

BB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.8213394 hartrees (-245240.3904735 kcal/mol)

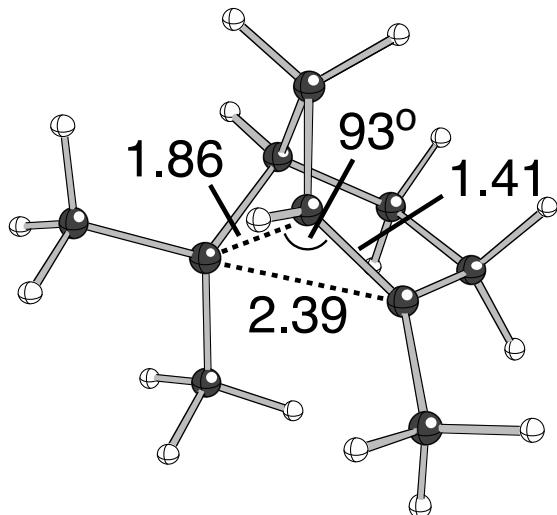
mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.8172081 hartrees (-245237.79808275 kcal/mol)

MP2/6-31+G(d,p)//B3LYP/6-31+G(d,p)

MP2 = -389.7472296 hartrees

PBE/6-31+G(d,p)//PBE/6-31+G(d,p)



HF = -390.497024 hartrees (-245040.78753024 kcal/mol)

Imaginary Frequencies: none found

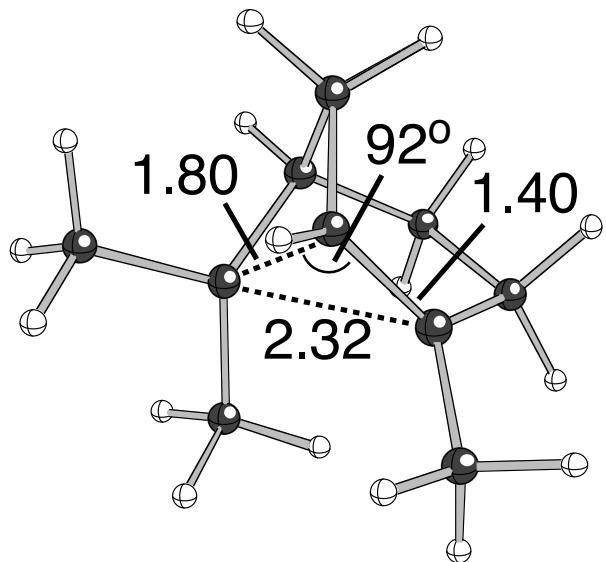
Zero-point correction = 0.240389 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.078554	-0.205044	-1.211215
2	6	-1.254309	-0.320730	-0.435036
3	6	-1.653434	0.865787	0.378668
4	6	-0.411665	1.637356	0.956258

5	6	0.855684	1.198498	0.220437
6	6	0.552677	1.187752	-1.302932
7	1	-2.183428	1.538419	-0.328475
8	1	0.130418	-0.992250	-1.946451
9	1	-0.557109	2.721860	0.836207
10	1	-0.331417	1.441093	2.037700
11	1	-0.121993	1.982336	-1.660785
12	1	1.452409	1.184106	-1.930589
13	1	-2.388387	0.599534	1.154389
14	6	-2.048386	-1.570969	-0.386728
15	1	-3.054217	-1.353031	-0.799735
16	1	-1.608571	-2.391408	-0.971227
17	1	-2.230479	-1.892581	0.654464
18	1	1.742818	1.761098	0.557811
19	6	1.023752	-0.342802	0.274261
20	6	0.622097	-1.120980	1.514827
21	1	1.426550	-0.979537	2.260149
22	1	-0.314140	-0.793546	1.987307
23	1	0.562441	-2.202816	1.314622
24	6	2.309431	-0.905698	-0.318776
25	1	3.097849	-0.783172	0.447747
26	1	2.222766	-1.984293	-0.523160
27	1	2.650729	-0.394833	-1.228560

mPW1PW91/6-31+G(d,p)//mPW1PW91/6-31+G(d,p)



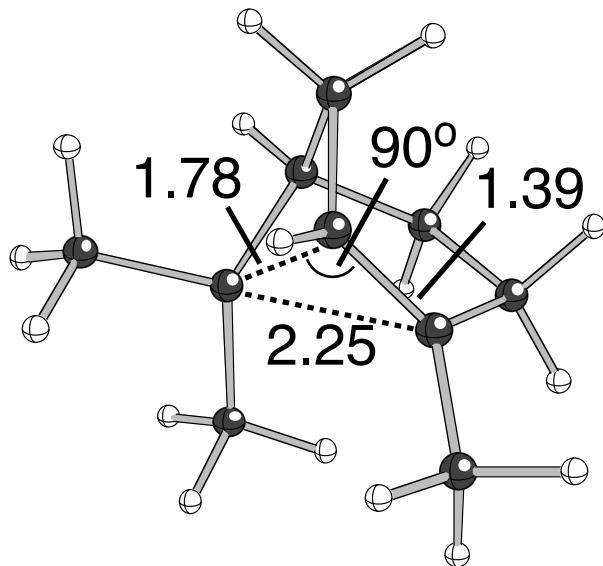
HF = -390.9584897 hartrees (-245330.361871647 kcal/mol)
Imaginary Frequencies: none found

Zero-point correction = 0.249197 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.054020	-0.208741	-1.198011
2	6	-1.226655	-0.314613	-0.433487
3	6	-1.631888	0.869896	0.366413
4	6	-0.404503	1.639186	0.941344
5	6	0.857356	1.189673	0.221438
6	6	0.571088	1.178429	-1.293296
7	1	-2.157730	1.523166	-0.346845
8	1	0.144901	-0.989302	-1.929067
9	1	-0.545644	2.713599	0.810895
10	1	-0.330269	1.455011	2.015559
11	1	-0.093703	1.963552	-1.661194
12	1	1.469063	1.169401	-1.907197
13	1	-2.362605	0.605377	1.133125
14	6	-2.027190	-1.552824	-0.394513
15	1	-2.998607	-1.328284	-0.857924
16	1	-1.572128	-2.377430	-0.942647
17	1	-2.254313	-1.851188	0.633445
18	1	1.741430	1.732345	0.566265
19	6	0.987770	-0.346013	0.266963
20	6	0.577354	-1.112133	1.507241
21	1	1.373033	-0.975999	2.247780
22	1	-0.350211	-0.777785	1.971284
23	1	0.506528	-2.184444	1.310639
24	6	2.278361	-0.920371	-0.291098
25	1	3.045951	-0.802990	0.482357
26	1	2.182432	-1.988833	-0.494273
27	1	2.635831	-0.421138	-1.190159

BB1K/6-31+G(d,p)//BB1K/6-31+G(d,p)



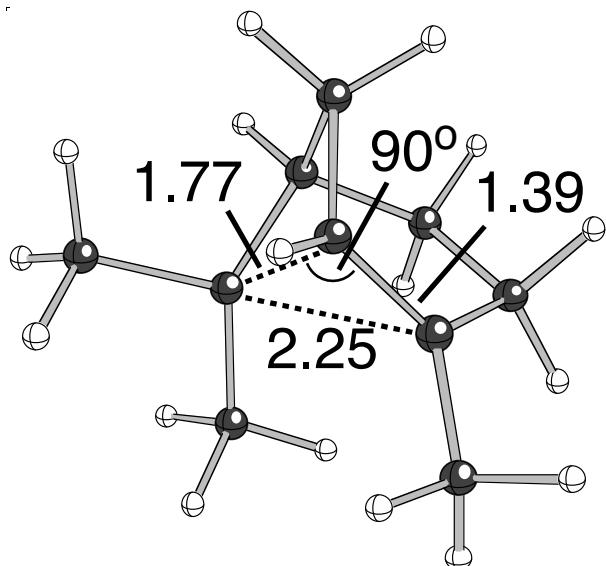
HF = -390.8260343 hartrees (-245247.244783593 kcal/mol)
 Imaginary Frequencies: none found
 Zero-point correction = 0.253571 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.023555	-0.186998	-1.207873
2	6	-1.190365	-0.298736	-0.452559
3	6	-1.608746	0.880356	0.336765
4	6	-0.399078	1.631426	0.941754
5	6	0.860136	1.173477	0.243770
6	6	0.610686	1.187603	-1.267754
7	1	-2.108284	1.533434	-0.386875
8	1	0.185077	-0.960544	-1.935968
9	1	-0.528478	2.703049	0.821256
10	1	-0.344926	1.432502	2.009230
11	1	-0.036774	1.979852	-1.636826
12	1	1.519110	1.179141	-1.857213
13	1	-2.354863	0.615554	1.080812
14	6	-1.979204	-1.538012	-0.417303
15	1	-2.937415	-1.323410	-0.899144
16	1	-1.508437	-2.358172	-0.948519
17	1	-2.216588	-1.826399	0.605361
18	1	1.745402	1.685371	0.613720
19	6	0.944466	-0.355281	0.271669
20	6	0.493188	-1.113868	1.495221

21	1	1.270915	-0.994802	2.249584
22	1	-0.435190	-0.763242	1.935554
23	1	0.405640	-2.178880	1.292842
24	6	2.231723	-0.948933	-0.254924
25	1	2.978122	-0.859213	0.534792
26	1	2.116354	-2.006430	-0.476719
27	1	2.614828	-0.444013	-1.134485

mPWB1K/6-31+G(d,p)//mPWB1K/6-31+G(d,p)



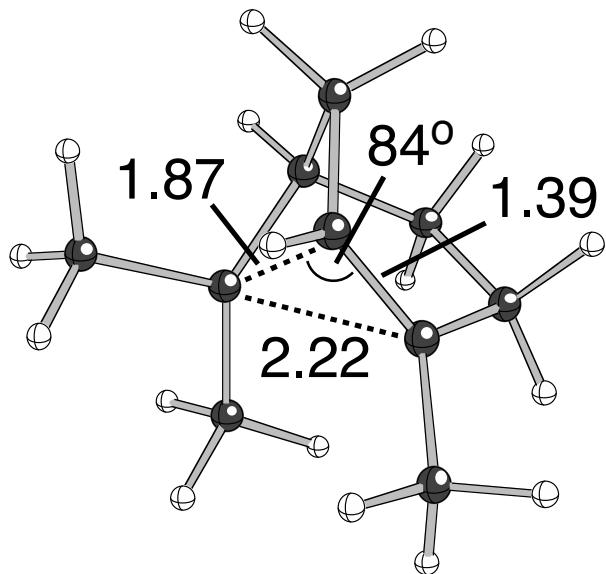
HF = -390.8225224 hartrees (-245245.041031224 kcal/mol)
 Imaginary Frequencies: none found
 Zero-point correction = 0.254100 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.019120	-0.186010	-1.206286
2	6	-1.187146	-0.296155	-0.454124
3	6	-1.606150	0.881579	0.334594
4	6	-0.398099	1.632124	0.939908
5	6	0.860945	1.171459	0.246191
6	6	0.615894	1.187140	-1.264906
7	1	-2.106596	1.533848	-0.388203
8	1	0.189367	-0.959637	-1.933556

9	1	-0.525547	2.702991	0.816386
10	1	-0.346658	1.435778	2.007370
11	1	-0.029271	1.979929	-1.634986
12	1	1.525519	1.177367	-1.851394
13	1	-2.351251	0.615090	1.078182
14	6	-1.974909	-1.534586	-0.420120
15	1	-2.923769	-1.324492	-0.920877
16	1	-1.495210	-2.358043	-0.936964
17	1	-2.229022	-1.813936	0.600192
18	1	1.746080	1.680132	0.618997
19	6	0.939525	-0.356511	0.271477
20	6	0.482546	-1.115703	1.491389
21	1	1.262021	-1.009435	2.244853
22	1	-0.441159	-0.758067	1.934540
23	1	0.383067	-2.178060	1.283413
24	6	2.227498	-0.951194	-0.248794
25	1	2.973901	-0.849959	0.538607
26	1	2.114950	-2.010876	-0.458390
27	1	2.607665	-0.455492	-1.134144

MP2/6-31+G(d,p)//MP2/6-31+G(d,p)



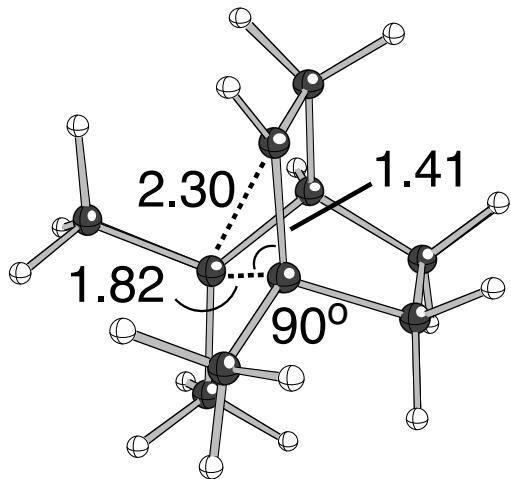
MP2 = -389.7497253 hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.253381 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.042722	-0.126172	-1.285344
2	6	-1.152691	-0.308143	-0.463555
3	6	-1.614780	0.857219	0.351522
4	6	-0.413467	1.651128	0.947585
5	6	0.856102	1.181181	0.256372
6	6	0.627170	1.236023	-1.268144
7	1	-2.166568	1.500716	-0.343745
8	1	0.203239	-0.894551	-2.011883
9	1	-0.550964	2.720664	0.790480
10	1	-0.355546	1.485688	2.023224
11	1	-0.009280	2.052404	-1.613216
12	1	1.543569	1.237596	-1.851411
13	1	-2.322448	0.539748	1.117031
14	6	-1.913047	-1.584123	-0.445041
15	1	-2.881547	-1.391084	-0.917659
16	1	-1.412366	-2.376469	-0.997844
17	1	-2.121249	-1.905655	0.575818
18	1	1.749911	1.673720	0.644973
19	6	0.924243	-0.353832	0.303314
20	6	0.481020	-1.097326	1.546190
21	1	1.279230	-0.952137	2.280601
22	1	-0.442172	-0.741511	1.993970
23	1	0.401765	-2.168223	1.359490
24	6	2.177106	-1.001248	-0.264641
25	1	2.935072	-0.958054	0.522248
26	1	2.003754	-2.051511	-0.498196
27	1	2.571998	-0.499586	-1.143428

TS (B-to-D)

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)



HF = -391.0264352 hartrees (-245369.088088 kcal/mol)

Imaginary Frequencies: 1 (-305.0468 1/cm)

Zero-point correction = 0.246003 (Hartree/Particle)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.301628	0.542172	-1.484538
2	6	-0.328457	0.943489	-0.288547
3	6	0.733687	1.387485	0.789869
4	6	1.661017	0.181051	1.079442
5	6	1.123071	-0.920177	0.148896
6	6	1.369481	-0.471093	-1.305414
7	1	1.272211	2.256994	0.404983
8	1	-0.060729	0.829489	-2.474160
9	1	2.709063	0.404575	0.865712
10	1	1.609878	-0.120992	2.127764
11	1	2.366609	-0.047199	-1.506869
12	1	1.249391	-1.268156	-2.049516
13	1	0.177494	1.721250	1.668490
14	6	-1.601647	1.761232	-0.349023
15	1	-1.368729	2.814323	-0.540074
16	1	-2.278099	1.415753	-1.135725
17	1	-2.133277	1.719136	0.605279
18	1	1.504151	-1.919558	0.372946
19	6	-0.429407	-0.798212	0.234470
20	6	-1.068575	-0.817591	1.615774
21	1	-0.935138	-1.834897	2.009586
22	1	-0.635031	-0.129934	2.339510
23	1	-2.145033	-0.638132	1.558705

24	6	-1.246884	-1.700039	-0.693895
25	1	-1.285492	-2.702878	-0.254603
26	1	-2.279350	-1.346392	-0.768377
27	1	-0.851401	-1.803282	-1.705853

PBE/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.4815315 hartrees (-245027.16101625 kcal/mol)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.9431589 hartrees (-245316.83220975 kcal/mol)

BB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.8078841 hartrees (-245231.94727275 kcal/mol)

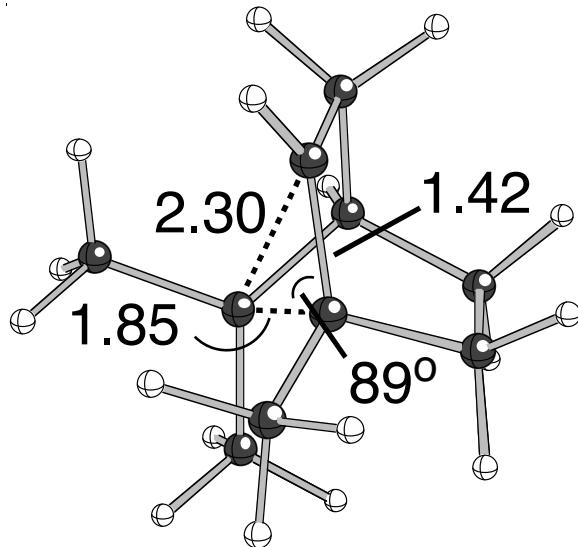
mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.8038945 hartrees (-245229.44379875 kcal/mol)

MP2/6-31+G(d,p)//B3LYP/6-31+G(d,p)

MP2 = -389.7346869 hartrees

PBE/6-31+G(d,p)//PBE/6-31+G(d,p)



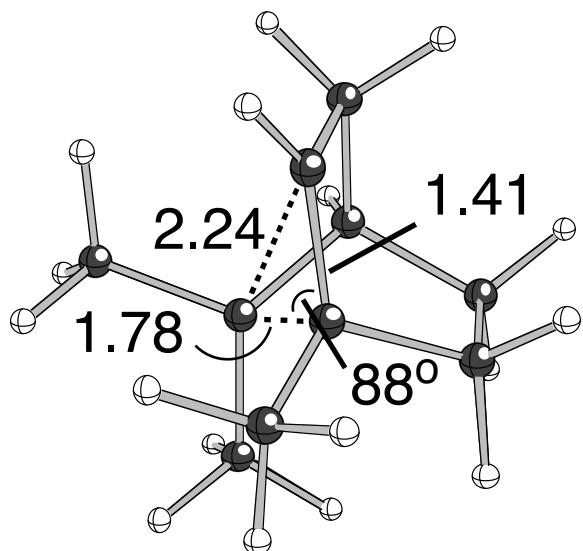
HF = -390.4822689 hartrees (-245031.528557439 kcal/mol)
 Imaginary Frequencies: 1 (-284.5245 1/cm)
 Zero-point correction = 0.239441 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.278646	0.503412	-1.504548
2	6	-0.361844	0.936539	-0.319854
3	6	0.674556	1.441181	0.749499
4	6	1.650342	0.282767	1.077241
5	6	1.164643	-0.869009	0.177483
6	6	1.388800	-0.458080	-1.292083
7	1	1.182783	2.326097	0.335501
8	1	-0.108921	0.731910	-2.509247
9	1	2.697552	0.544031	0.860946
10	1	1.606032	0.005756	2.141624
11	1	2.378025	-0.005509	-1.516785
12	1	1.301758	-1.292452	-2.012483
13	1	0.098439	1.783258	1.623564
14	6	-1.674743	1.683842	-0.394882
15	1	-1.495396	2.751267	-0.608029
16	1	-2.337939	1.287163	-1.179193
17	1	-2.205461	1.636299	0.569049
18	1	1.592417	-1.850496	0.435714
19	6	-0.394372	-0.818489	0.258044
20	6	-1.040095	-0.798803	1.633315

21	1	-0.852306	-1.796968	2.076510
22	1	-0.642534	-0.053829	2.333432
23	1	-2.132874	-0.684513	1.567108
24	6	-1.171635	-1.777405	-0.644148
25	1	-1.192074	-2.768538	-0.158878
26	1	-2.220362	-1.455293	-0.747258
27	1	-0.754924	-1.913910	-1.651988

mPW1PW91/6-31+G(d,p)//mPW1PW91/6-31+G(d,p)



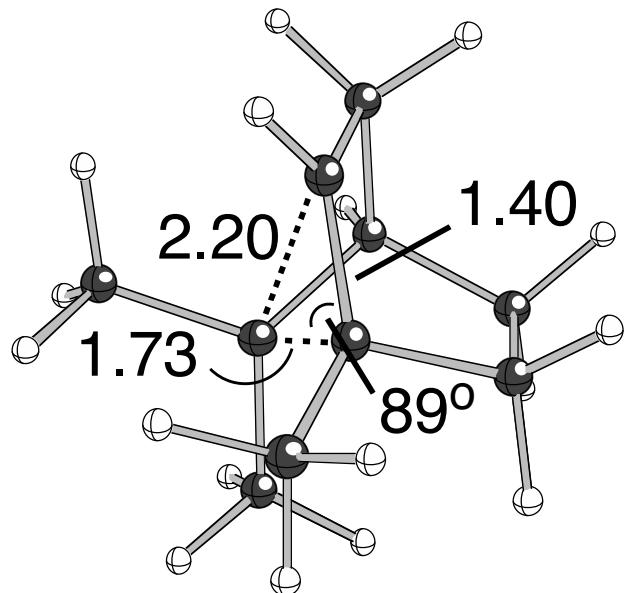
HF = -390.9439431 hartrees (-245321.233734681 kcal/mol)
 Imaginary Frequencies: 1 (-294.1797 1/cm)
 Zero-point correction = 0.248118 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.239677	0.393958	-1.515393
2	6	-0.374848	0.887447	-0.348023
3	6	0.671881	1.479134	0.648537
4	6	1.648308	0.354316	1.042986
5	6	1.168817	-0.838527	0.215626
6	6	1.383328	-0.507473	-1.267532
7	1	1.167929	2.324254	0.166836
8	1	-0.187885	0.528435	-2.510622

9	1	2.685850	0.606839	0.817052
10	1	1.601681	0.139823	2.111893
11	1	2.338753	-0.016042	-1.507216
12	1	1.333103	-1.371623	-1.937961
13	1	0.118994	1.882214	1.498893
14	6	-1.689150	1.617728	-0.452404
15	1	-1.523444	2.652817	-0.763612
16	1	-2.365928	1.152107	-1.171831
17	1	-2.187863	1.651622	0.518081
18	1	1.593717	-1.796145	0.521760
19	6	-0.380451	-0.772615	0.289132
20	6	-1.016608	-0.704274	1.663821
21	1	-0.811261	-1.665724	2.151336
22	1	-0.632535	0.079972	2.312673
23	1	-2.101510	-0.607582	1.595764
24	6	-1.144472	-1.797309	-0.543663
25	1	-1.146019	-2.748353	-0.003865
26	1	-2.188478	-1.497994	-0.661852
27	1	-0.733994	-1.988929	-1.535845

BB1K/6-31+G(d,p)//BB1K/6-31+G(d,p)

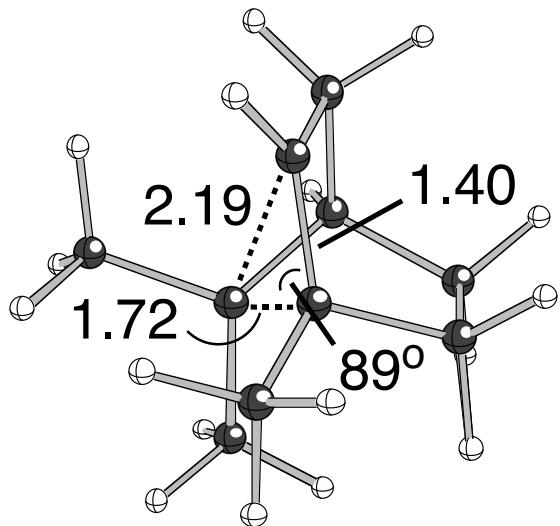


HF = -390.8116715 hartrees (-245238.231982965 kcal/mol)
 Imaginary Frequencies: 1 (-311.9112 1/cm)
 Zero-point correction = 0.251790 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.222537	0.311703	-1.523011
2	6	-0.392270	0.839637	-0.376365
3	6	0.645850	1.507937	0.564963
4	6	1.634086	0.428203	1.017649
5	6	1.177381	-0.800698	0.250339
6	6	1.387769	-0.536066	-1.237264
7	1	1.123041	2.328627	0.036335
8	1	-0.213802	0.385817	-2.515865
9	1	2.663848	0.685556	0.787049
10	1	1.581429	0.264140	2.089949
11	1	2.318866	-0.019270	-1.495863
12	1	1.369049	-1.425707	-1.865705
13	1	0.090769	1.946665	1.389610
14	6	-1.717587	1.532224	-0.502784
15	1	-1.583479	2.539510	-0.891497
16	1	-2.397387	1.001407	-1.164440
17	1	-2.189753	1.625502	0.471562
18	1	1.609845	-1.734167	0.597859
19	6	-0.361685	-0.740862	0.315979
20	6	-0.988751	-0.627873	1.685342
21	1	-0.779233	-1.562525	2.208590
22	1	-0.603760	0.183405	2.291871
23	1	-2.069039	-0.534496	1.616281
24	6	-1.105429	-1.811231	-0.465415
25	1	-1.085688	-2.736475	0.106629
26	1	-2.150236	-1.536260	-0.590909
27	1	-0.695874	-2.029583	-1.448045

mPWB1K/6-31+G(d,p)//mPWB1K/6-31+G(d,p)



HF = -390.8082914 hartrees (-245236.110936414 kcal/mol)

Imaginary Frequencies: 1 (-312.7062 1/cm)

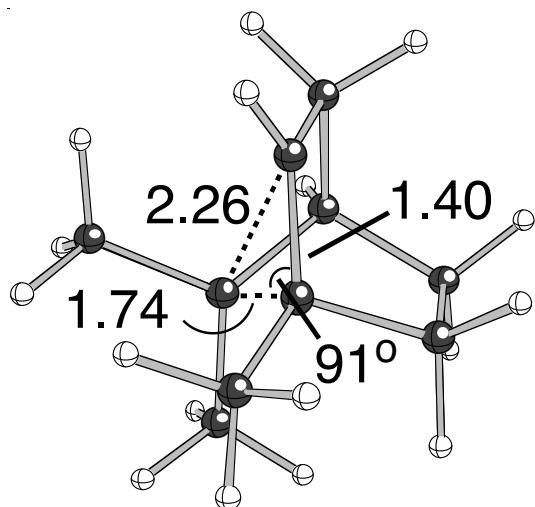
Zero-point correction = 0.252351 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.220730	0.298089	-1.523924
2	6	-0.391615	0.834738	-0.380762
3	6	0.647188	1.510639	0.551644
4	6	1.633275	0.434240	1.013519
5	6	1.176295	-0.798858	0.255553
6	6	1.386785	-0.544915	-1.232815
7	1	1.125164	2.325076	0.015329
8	1	-0.218741	0.361995	-2.515490
9	1	2.663012	0.688689	0.782493
10	1	1.578783	0.278185	2.086313
11	1	2.316011	-0.027134	-1.493741
12	1	1.370350	-1.438245	-1.854837
13	1	0.093949	1.958035	1.372112
14	6	-1.716706	1.524293	-0.510620
15	1	-1.585283	2.526443	-0.911538
16	1	-2.397831	0.984820	-1.163000
17	1	-2.185169	1.628305	0.463796
18	1	1.607152	-1.729893	0.609652
19	6	-0.361348	-0.735492	0.320333
20	6	-0.987036	-0.612427	1.688195
21	1	-0.775454	-1.541354	2.219392

22	1	-0.603203	0.205115	2.286095
23	1	-2.066940	-0.521312	1.618760
24	6	-1.105661	-1.810003	-0.452459
25	1	-1.089863	-2.729856	0.127139
26	1	-2.148772	-1.532917	-0.582681
27	1	-0.694603	-2.037776	-1.431783

MP2/6-31+G(d,p)//MP2/6-31+G(d,p)



MP2 = -389.7356445 hartrees

Imaginary Frequencies: 1 (-358.1132 1/cm)

Zero-point correction = 0.251710 (Hartree/Particle)

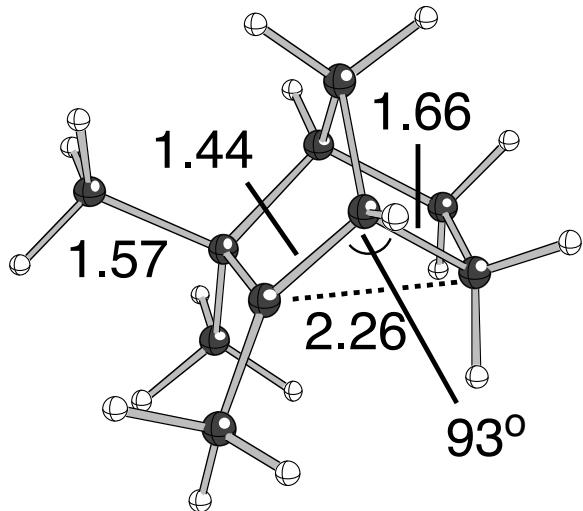
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.282347	0.520586	-1.486632
2	6	-0.379418	0.879906	-0.300674
3	6	0.673490	1.419228	0.745244
4	6	1.642411	0.268023	1.077149
5	6	1.154639	-0.863397	0.169217
6	6	1.393612	-0.432063	-1.282182
7	1	1.170701	2.290962	0.320320
8	1	-0.065056	0.801923	-2.481348
9	1	2.678664	0.530518	0.866428
10	1	1.587454	-0.012149	2.127815

11	1	2.363230	0.044521	-1.486578
12	1	1.315512	-1.243904	-2.011154
13	1	0.095066	1.763526	1.601990
14	6	-1.687113	1.630694	-0.369149
15	1	-1.508621	2.674240	-0.631374
16	1	-2.360020	1.199397	-1.109714
17	1	-2.181818	1.615743	0.601098
18	1	1.557032	-1.846921	0.413303
19	6	-0.388908	-0.772076	0.240475
20	6	-1.021878	-0.805983	1.621423
21	1	-0.818709	-1.799713	2.031923
22	1	-0.633623	-0.072652	2.320859
23	1	-2.103465	-0.694561	1.555312
24	6	-1.164125	-1.727125	-0.664795
25	1	-1.155892	-2.716824	-0.205421
26	1	-2.205754	-1.413859	-0.741550
27	1	-0.765042	-1.827016	-1.672363

D

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)



HF = -391.0562848 hartrees (-245387.818712 kcal/mol)
 Imaginary Frequencies: none
 Zero-point correction = 0.247572 (Hartree/Particle)

Coordinates:

Center	Atomic	Coordinates (Angstroms)
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Number	Number	X	Y	Z
1	6	1.671769	0.752371	0.734037
2	6	-0.394331	0.901117	-0.165922
3	6	0.641012	-1.218334	-0.189499
4	6	1.594459	-0.775427	0.946146
5	1	2.677072	1.143695	0.553470
6	1	1.240025	1.344277	1.545827
7	1	2.575702	-1.236700	0.809354
8	1	1.243726	-1.041941	1.944027
9	6	-0.752377	-0.534768	0.057485
10	6	0.931713	0.975518	-0.729584
11	6	1.202526	-0.400311	-1.369629
12	1	0.679711	-0.531891	-2.318547
13	1	2.268606	-0.567306	-1.539847
14	1	1.242305	1.902572	-1.208943
15	1	0.566594	-2.297031	-0.335723
16	6	-1.767696	-0.910260	-1.084759
17	1	-1.932043	-1.989880	-1.028021
18	1	-2.724353	-0.407854	-0.923437
19	1	-1.415404	-0.672385	-2.089477
20	6	-1.422651	-0.838657	1.411722
21	1	-2.430703	-0.418744	1.460414
22	1	-1.513258	-1.922356	1.530287
23	1	-0.854134	-0.454468	2.261836
24	6	-1.233543	2.061514	0.173085
25	1	-0.669238	2.995677	0.209431
26	1	-1.959658	2.160071	-0.652967
27	1	-1.820235	1.917680	1.083817

PBE/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.5108088 hartrees (-245045.532522 kcal/mol)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.9748913 hartrees (-245336.74429075 kcal/mol)

BB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.8403081 hartrees (-245252.29333275 kcal/mol)

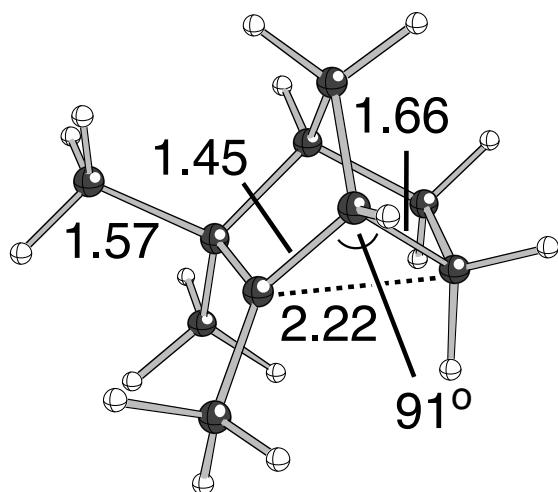
mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -390.8364882 hartrees (-245249.8963455 kcal/mol)

MP2/6-31+G(d,p)//B3LYP/6-31+G(d,p)

MP2 = -389.7641606 hartrees

PBE/6-31+G(d,p)//PBE/6-31+G(d,p)



HF = -390.511713 hartrees (-245050.00502463 kcal/mol)

Imaginary Frequencies: none found

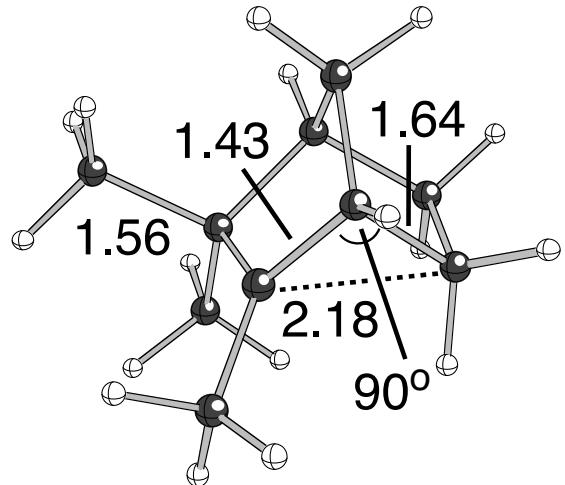
Zero-point correction = 0.241143 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.623528	0.780014	0.739126
2	6	-0.386793	0.896417	-0.187544
3	6	0.649665	-1.226208	-0.155472
4	6	1.581017	-0.741973	0.983277
5	1	2.626959	1.210081	0.579619
6	1	1.148426	1.382869	1.531203
7	1	2.581397	-1.186459	0.863096
8	1	1.222671	-0.999382	1.989869
9	6	-0.748018	-0.537113	0.062204
10	6	0.938646	0.954321	-0.763584

11	6	1.227144	-0.438939	-1.350590
12	1	0.716097	-0.601604	-2.310998
13	1	2.304242	-0.609648	-1.499807
14	1	1.263804	1.875637	-1.262259
15	1	0.579240	-2.317060	-0.272106
16	6	-1.741417	-0.925050	-1.096407
17	1	-1.900865	-2.013479	-1.036055
18	1	-2.710030	-0.423228	-0.951386
19	1	-1.372961	-0.687924	-2.104433
20	6	-1.440642	-0.820805	1.408471
21	1	-2.451967	-0.386339	1.438742
22	1	-1.547565	-1.909498	1.539989
23	1	-0.876200	-0.429294	2.268444
24	6	-1.224964	2.062669	0.140053
25	1	-0.678977	3.015655	0.091769
26	1	-2.014993	2.103383	-0.641093
27	1	-1.758280	1.956291	1.098201

mPW1PW91/6-31+G(d,p)//mPW1PW91/6-31+G(d,p)



HF = -390.9757088 hartrees (-245341.167029088 kcal/mol)

Imaginary Frequencies: none found

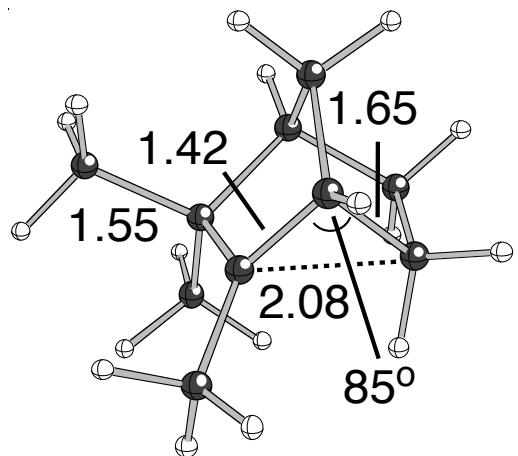
Zero-point correction = 0.249725 (Hartree/Particle)

Coordinates (from last standard orientation):

Center	Atomic Number	Atomic Number	Coordinates (Angstroms)		
			X	Y	Z

1	6	1.593936	0.782293	0.737465
2	6	-0.383158	0.888263	-0.182812
3	6	0.649853	-1.216691	-0.158055
4	6	1.573637	-0.734040	0.972107
5	1	2.584692	1.225107	0.604925
6	1	1.102390	1.362437	1.524201
7	1	2.570956	-1.160209	0.847685
8	1	1.226554	-0.998594	1.970615
9	6	-0.739154	-0.540738	0.058643
10	6	0.930391	0.952662	-0.757076
11	6	1.221435	-0.429633	-1.343266
12	1	0.717877	-0.591536	-2.296992
13	1	2.290256	-0.595231	-1.489050
14	1	1.247213	1.868629	-1.250182
15	1	0.586836	-2.298425	-0.276837
16	6	-1.727444	-0.917741	-1.089120
17	1	-1.882475	-1.998009	-1.043931
18	1	-2.691321	-0.428606	-0.938288
19	1	-1.367273	-0.669697	-2.087790
20	6	-1.420091	-0.826143	1.399464
21	1	-2.425983	-0.402695	1.432619
22	1	-1.517398	-1.906274	1.530975
23	1	-0.860471	-0.434164	2.250609
24	6	-1.224300	2.045153	0.141992
25	1	-0.678866	2.988528	0.114999
26	1	-1.986966	2.090465	-0.651650
27	1	-1.766660	1.927963	1.082040

BB1K/6-31+G(d,p)//BB1K/6-31+G(d,p)



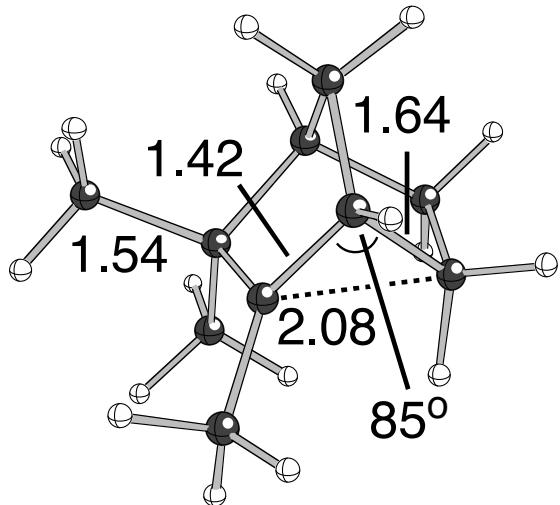
HF = -390.8442066 hartrees (-245258.648083566 kcal/mol)

Imaginary Frequencies: none found
Zero-point correction = 0.253829 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.465734	0.833080	0.759531
2	6	-0.382474	0.868737	-0.201182
3	6	0.688716	-1.199341	-0.140342
4	6	1.572424	-0.668584	0.985239
5	1	2.398395	1.390835	0.711943
6	1	0.860312	1.339386	1.513548
7	1	2.595750	-1.008675	0.854046
8	1	1.250776	-0.962644	1.978496
9	6	-0.707058	-0.562370	0.053762
10	6	0.909346	0.954739	-0.782526
11	6	1.254307	-0.420448	-1.322031
12	1	0.775072	-0.613640	-2.276986
13	1	2.324923	-0.557246	-1.443483
14	1	1.222685	1.868569	-1.268610
15	1	0.660874	-2.279037	-0.241120
16	6	-1.675070	-0.974257	-1.078218
17	1	-1.816685	-2.050494	-1.019119
18	1	-2.643442	-0.499806	-0.943315
19	1	-1.313328	-0.736720	-2.073920
20	6	-1.371275	-0.826384	1.396511
21	1	-2.384655	-0.433285	1.416229
22	1	-1.433932	-1.898401	1.566846
23	1	-0.825219	-0.386439	2.227593
24	6	-1.268313	1.996582	0.096341
25	1	-0.767315	2.956558	0.034275
26	1	-2.036550	1.976249	-0.683986
27	1	-1.785696	1.884274	1.045064

mPWB1K/6-31+G(d,p)//mPWB1K/6-31+G(d,p)



HF = -390.8409388 hartrees (-245256.597506388 kcal/mol)

Imaginary Frequencies: none found

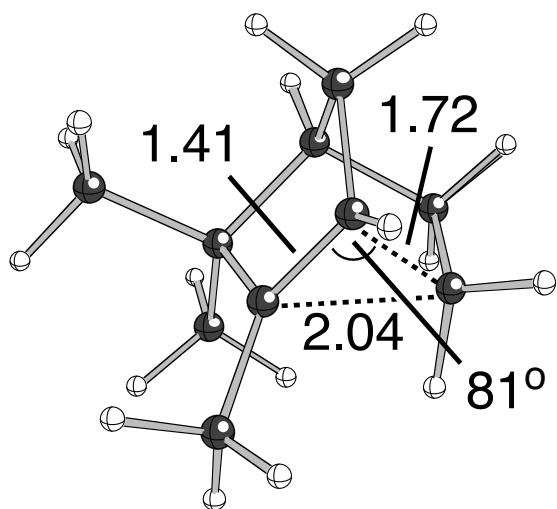
Zero-point correction = 0.254444 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.457650	0.836202	0.759633
2	6	-0.382110	0.867034	-0.202583
3	6	0.690725	-1.197856	-0.138315
4	6	1.571005	-0.663648	0.986457
5	1	2.386486	1.399380	0.716690
6	1	0.846444	1.338674	1.510937
7	1	2.595286	-0.999072	0.855987
8	1	1.250153	-0.958175	1.979202
9	6	-0.704672	-0.563414	0.053435
10	6	0.908030	0.954217	-0.783770
11	6	1.255895	-0.420330	-1.319629
12	1	0.778288	-0.615838	-2.274249
13	1	2.326289	-0.555577	-1.439310
14	1	1.220758	1.867526	-1.269826
15	1	0.664817	-2.277193	-0.237357
16	6	-1.670388	-0.977023	-1.077041
17	1	-1.813445	-2.052335	-1.015301
18	1	-2.637966	-0.501393	-0.945005
19	1	-1.306930	-0.742771	-2.072291
20	6	-1.368265	-0.825169	1.395178
21	1	-2.381750	-0.433804	1.413204

22	1	-1.429260	-1.896307	1.567925
23	1	-0.823808	-0.382565	2.225221
24	6	-1.270700	1.991805	0.093130
25	1	-0.773239	2.952732	0.028244
26	1	-2.039497	1.966335	-0.685570
27	1	-1.785650	1.879482	1.042527

MP2/6-31+G(d,p)//MP2/6-31+G(d,p)



MP2 = -389.7670177 hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.253399 (Hartree/Particle)

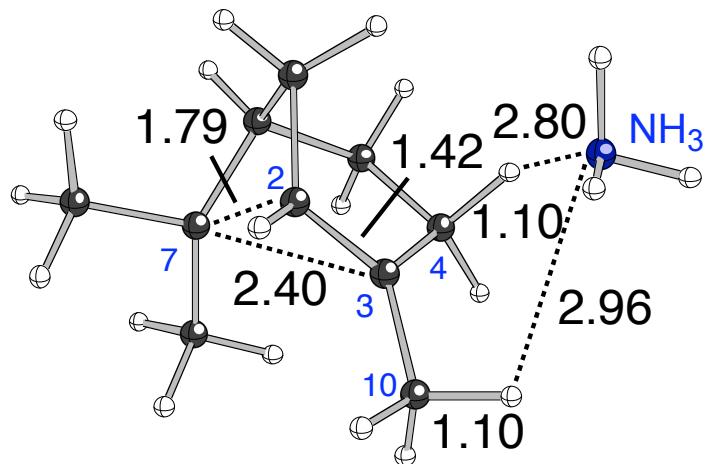
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.421649	0.846798	0.788182
2	6	-0.352180	0.875745	-0.211975
3	6	0.686659	-1.216350	-0.106649
4	6	1.557046	-0.655746	1.029133
5	1	2.333912	1.434912	0.676020
6	1	0.808551	1.368682	1.526642
7	1	2.592157	-0.975076	0.913383
8	1	1.222614	-0.940249	2.023917
9	6	-0.712513	-0.558835	0.051875
10	6	0.906884	0.929144	-0.848542

11	6	1.279149	-0.471283	-1.310679
12	1	0.810252	-0.702589	-2.266195
13	1	2.355553	-0.606658	-1.410966
14	1	1.259834	1.836885	-1.325526
15	1	0.654647	-2.302484	-0.178976
16	6	-1.672692	-0.985000	-1.089409
17	1	-1.824717	-2.061963	-1.015201
18	1	-2.639817	-0.497583	-0.969397
19	1	-1.294913	-0.759396	-2.084960
20	6	-1.400852	-0.812923	1.393617
21	1	-2.412326	-0.407195	1.393088
22	1	-1.475180	-1.888029	1.560453
23	1	-0.862987	-0.376823	2.234784
24	6	-1.228668	2.035815	0.070303
25	1	-0.705281	2.983951	-0.031874
26	1	-2.021274	2.004928	-0.685453
27	1	-1.707931	1.964499	1.045131

Figure 4.

B-NH₃



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6210039 hartrees (-280886.656157289 kcal/mol)
 Imaginary Frequencies: none found
 Zero-point correction = 0.283377 (Hartree/Particle)

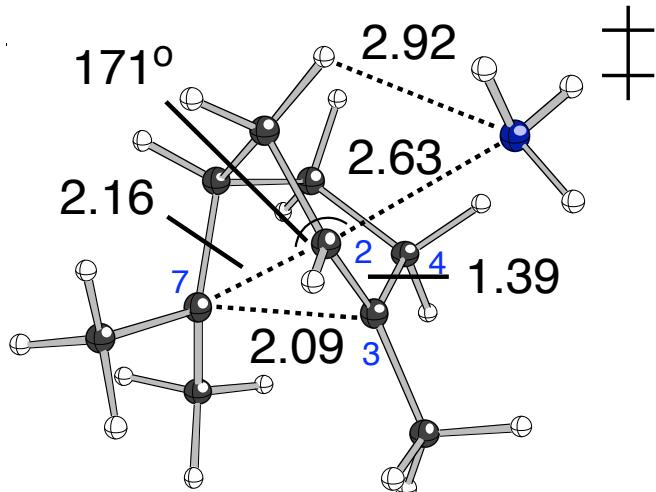
mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5200115 hartrees (-280818.80721625 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.123746	-0.185820	-0.901072
2	6	0.757777	0.669091	0.031131
3	6	0.854116	0.192836	1.437998
4	6	-0.369663	-0.690269	1.861879
5	6	-1.131130	-1.156621	0.618239
6	6	-0.092952	-1.631841	-0.430486
7	1	1.766098	-0.424240	1.432259
8	1	0.227418	0.068998	-1.954402
9	1	-0.017351	-1.556841	2.427123
10	1	-1.019886	-0.117060	2.528579
11	1	0.798766	-2.128989	-0.039993
12	1	-0.521301	-2.247883	-1.219722
13	1	1.041141	1.017076	2.131117
14	6	1.236144	2.020169	-0.334657
15	1	2.316589	2.046253	-0.137339
16	1	1.063752	2.269863	-1.382674
17	1	0.792155	2.782193	0.317541
18	1	-1.949017	-1.837649	0.873062
19	6	-1.535554	0.047666	-0.272614
20	6	-1.978969	1.360342	0.359729
21	1	-3.005680	1.224137	0.720714
22	1	-1.381685	1.686494	1.212404
23	1	-2.004015	2.168450	-0.377616
24	6	-2.443176	-0.283363	-1.455527
25	1	-3.463198	-0.399124	-1.067736
26	1	-2.460299	0.534249	-2.181532
27	1	-2.180474	-1.205815	-1.973841
28	7	3.641027	-0.554930	-0.641117
29	1	3.881626	-0.200588	-1.565721
30	1	4.408234	-0.278225	-0.029812
31	1	3.697903	-1.569923	-0.712317

TS1



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6156328 hartrees (-280878.809582 kcal/mol)
 Imaginary Frequencies: 1 (-154.6595 1/cm)
 Zero-point correction = 0.284314 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

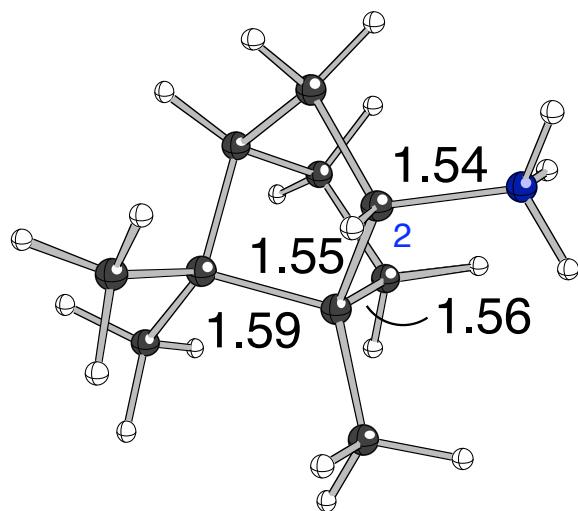
HF = -447.5143657 hartrees (-280815.26447675 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.851275	-0.261504	-0.584266
2	6	0.363370	0.886513	0.034906
3	6	0.176750	0.842412	1.544777
4	6	-0.610740	-0.441017	1.954835
5	6	-0.808104	-1.251818	0.669684
6	6	0.592582	-1.585831	0.096804
7	1	1.177122	0.845318	1.993957
8	1	1.172096	-0.212643	-1.618432
9	1	-0.065084	-1.029431	2.696705
10	1	-1.571059	-0.177535	2.405360
11	1	1.330800	-1.823586	0.867514
12	1	0.589320	-2.406068	-0.623205
13	1	-0.315700	1.754307	1.891742
14	6	0.438470	2.224936	-0.642730

15	1	1.313584	2.769440	-0.266770
16	1	0.535501	2.139642	-1.728260
17	1	-0.436038	2.839658	-0.409490
18	1	-1.469439	-2.112921	0.812198
19	6	-1.303741	-0.279429	-0.423728
20	6	-2.388762	0.727322	-0.100545
21	1	-3.317312	0.149904	0.020070
22	1	-2.239524	1.292874	0.817515
23	1	-2.551376	1.423439	-0.927270
24	6	-1.511627	-0.835505	-1.825760
25	1	-2.531598	-1.239142	-1.867738
26	1	-1.455792	-0.045602	-2.580446
27	1	-0.830574	-1.639460	-2.104420
28	7	3.471213	-0.266695	-0.375707
29	1	3.883807	0.512056	-0.886110
30	1	3.829353	-0.212593	0.576038
31	1	3.856575	-1.117266	-0.782868

7-H⁺



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6656385 hartrees (-280910.18815875 kcal/mol)

Imaginary Frequencies: none

Zero-point correction = 0.292080 (Hartree/Particle)

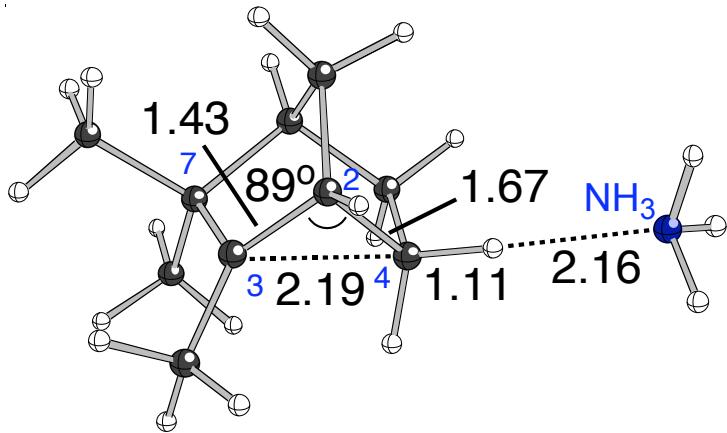
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.575421 hartrees (-280853.5766775 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.205368	0.226948	0.713227
2	6	-0.168177	0.661472	-0.355584
3	6	-0.355529	-0.246502	-1.607201
4	6	0.128159	-1.656781	-1.143877
5	6	0.524943	-1.411450	0.329616
6	6	-0.788016	-1.209919	1.127606
7	1	-1.381228	-0.247714	-2.003756
8	1	-1.218483	0.923637	1.553731
9	1	-0.645025	-2.426716	-1.235183
10	1	0.977235	-1.998833	-1.738999
11	1	-1.541772	-1.962275	0.863226
12	1	-0.642814	-1.273271	2.208251
13	1	0.247958	0.141429	-2.430808
14	6	-0.166811	2.158430	-0.648750
15	1	-1.097645	2.488662	-1.130680
16	1	-0.030739	2.754059	0.260136
17	1	0.639469	2.416352	-1.340967
18	1	1.170866	-2.182649	0.755207
19	6	1.132097	0.028963	0.297143
20	6	2.389645	0.159652	-0.582034
21	1	3.198742	-0.441132	-0.154225
22	1	2.254009	-0.166474	-1.614185
23	1	2.738371	1.197044	-0.604980
24	6	1.504890	0.587967	1.686553
25	1	2.361501	0.034410	2.083580
26	1	1.808761	1.637222	1.614113
27	1	0.715446	0.525817	2.440238
28	7	-2.649192	0.275124	0.195567
29	1	-2.903140	1.223021	-0.103091
30	1	-2.770020	-0.345651	-0.611481
31	1	-3.312157	-0.015483	0.920706

D-NH₃



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.637174 hartrees (-280892.326685 kcal/mol)

Imaginary Frequencies: none

Zero-point correction = 0.284368 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

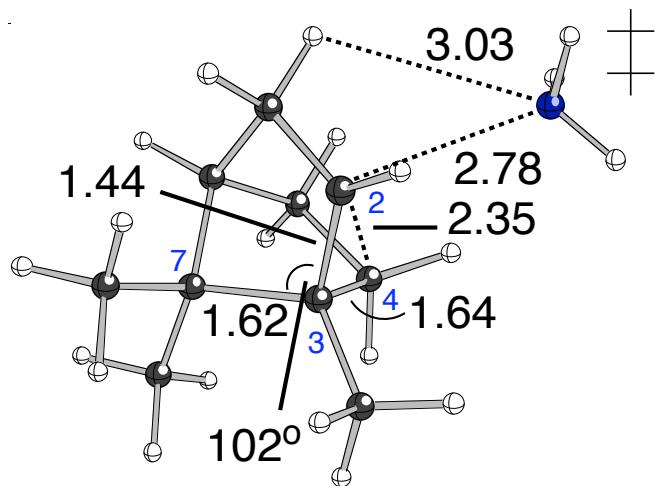
HF = -447.5387705 hartrees (-280830.57848875 kcal/mol)

Coordinates:

Center	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.582138	0.495031	-0.857920
2	6	-0.625720	0.931048	-0.227463
3	6	1.216870	0.157920	0.652467
4	6	0.661508	-1.243337	0.967508
5	6	-0.427614	-1.413502	-0.117674
6	6	0.339525	-0.933157	-1.367189
7	1	2.299571	0.212617	0.426514
8	1	1.197797	1.208389	-1.401483
9	1	1.438385	-2.002253	0.840652
10	1	0.282577	-1.327270	1.986971
11	1	1.273366	-1.475639	-1.530134
12	1	-0.233581	-0.948715	-2.296485
13	1	1.008558	0.912022	1.417447
14	6	-0.975056	2.335225	0.071823
15	1	-0.130801	3.016099	-0.050687
16	1	-1.742433	2.626710	-0.663560
17	1	-1.431803	2.457742	1.057460

18	1	-0.877504	-2.405961	-0.175588
19	6	-1.478886	-0.267142	0.095842
20	6	-2.154843	-0.229809	1.478943
21	1	-2.638224	-1.192203	1.671474
22	1	-1.450509	-0.039764	2.292276
23	1	-2.931314	0.539118	1.518982
24	6	-2.602002	-0.323066	-0.995648
25	1	-3.145945	-1.262962	-0.866139
26	1	-3.309364	0.499025	-0.859826
27	1	-2.226988	-0.287361	-2.019947
28	7	4.424175	0.239782	0.051654
29	1	4.862136	-0.400471	0.711516
30	1	4.760757	-0.024343	-0.872316
31	1	4.810574	1.161483	0.247160

TS2



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6171034 hartrees (-280884.208554534 kcal/mol)
 Imaginary Frequencies: 1 (-168.7577 1/cm)
 Zero-point correction = 0.283470 (Hartree/Particle)

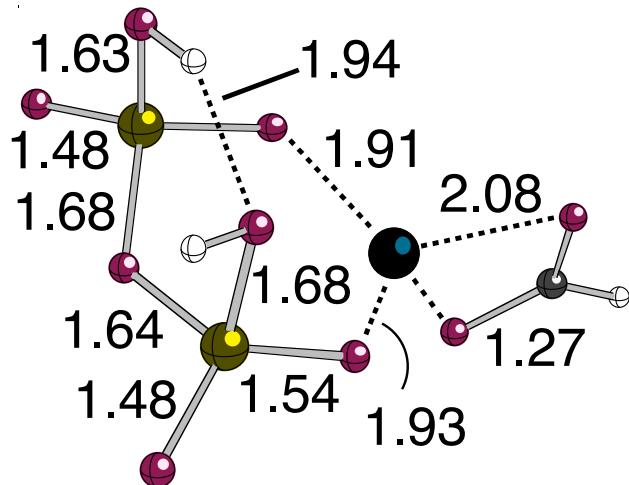
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5181043 hartrees (-280822.085629293 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.883507	0.283079	0.897266
2	6	0.028877	0.798000	-0.093457
3	6	-0.546250	0.026607	-1.415877
4	6	-0.166114	-1.457356	-1.224139
5	6	0.523995	-1.453154	0.162453
6	6	-0.591809	-1.135623	1.179759
7	1	-1.611076	0.210651	-1.544548
8	1	-1.038285	-2.116255	-1.238527
9	1	0.510665	-1.802974	-2.008152
10	1	-1.484142	-1.770933	1.158473
11	1	-0.233853	-1.180993	2.221970
12	6	0.161005	2.302890	-0.258339
13	1	-0.806539	2.762489	-0.483596
14	1	0.553405	2.769575	0.649983
15	1	0.839743	2.543477	-1.080593
16	1	1.094404	-2.353493	0.396735
17	6	1.335779	-0.119974	0.164484
18	6	2.386743	0.001758	-0.948695
19	1	3.187291	-0.720943	-0.757317
20	1	2.012246	-0.188791	-1.954712
21	1	2.843844	0.995521	-0.942300
22	6	2.040442	0.213138	1.494830
23	1	2.833661	-0.516503	1.684972
24	1	2.515009	1.197228	1.438462
25	1	1.385651	0.222037	2.370362
26	1	-0.013255	0.512755	-2.237054
27	1	-1.613628	0.869689	1.442180
28	7	-3.556004	0.183551	0.132795
29	1	-4.095654	0.076011	0.991046
30	1	-3.891917	1.037043	-0.311397
31	1	-3.830500	-0.586640	-0.475257

Figure 6b.



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1600.2071299 hartrees (-1004145.97608355 kcal/mol)

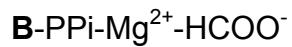
Imaginary Frequencies: none found

Zero-point correction = 0.078753 (Hartree/Particle)

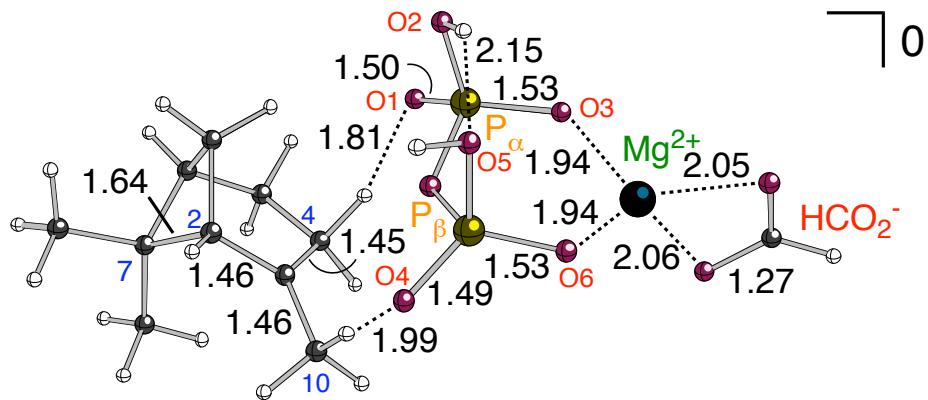
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-1.983583	1.436410	1.273288
2	15	-1.140037	1.516191	-0.117335
3	8	-1.648976	2.582504	-1.007164
4	8	-1.471754	0.012834	-0.782878
5	8	0.367309	1.476700	0.239700
6	15	-1.105332	-1.474107	-0.206336
7	8	-1.841959	-2.525947	-0.948850
8	8	-1.684607	-1.374068	1.361793
9	8	0.421370	-1.536686	-0.030970
10	1	-1.888907	0.536953	1.650480
11	1	-2.556503	-1.801530	1.357593
12	12	1.570752	0.006639	0.050689
13	8	3.350716	-0.084382	1.128611
14	6	3.941205	-0.002612	0.010760
15	1	5.045322	-0.007961	-0.007759
16	8	3.314530	0.084797	-1.085788

Figure 7.



B3LYP/6-31G(d)//B3LYP/6-31G(d)



HF = -1991.3515597 hartrees (-1249593.01722735 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.327366 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3.131560	0.651625	-0.095325
2	6	2.244161	-0.049588	-1.020989
3	6	2.021668	-1.461788	-0.766381
4	6	3.169400	-2.166759	0.017967
5	6	4.071127	-1.123525	0.689284
6	6	3.153737	-0.032682	1.302881
7	1	1.137757	-1.451830	-0.049101
8	1	3.094634	1.739585	-0.184931
9	1	2.726387	-2.818636	0.776106
10	1	3.743596	-2.799546	-0.668893
11	1	2.191594	-0.360253	1.701900
12	1	3.658135	0.600605	2.032858
13	1	4.827120	-1.592991	1.327313
14	6	4.588619	-0.065744	-0.337128
15	6	4.987200	-0.505630	-1.748532
16	1	5.939508	-1.047894	-1.703826
17	1	4.260944	-1.164485	-2.232929
18	1	5.139206	0.363230	-2.400114
19	6	5.692903	0.839866	0.221696
20	1	6.634437	0.277778	0.255902

21	1	5.848624	1.708580	-0.427941
22	1	5.488647	1.204476	1.230927
23	1	1.675588	-2.003790	-1.651064
24	8	-2.408623	-1.058412	1.066902
25	15	-0.974026	-0.652682	1.418022
26	8	-0.962432	0.177111	2.805175
27	8	-0.516385	0.499238	0.307213
28	8	0.116464	-1.678401	1.421851
29	15	-1.382409	1.810486	-0.202041
30	8	-1.739336	2.543891	1.231115
31	8	-2.713233	1.291108	-0.739329
32	8	-0.465584	2.644634	-1.031128
33	6	1.647653	0.669363	-2.149251
34	1	1.180323	0.017142	-2.889411
35	1	0.886892	1.380409	-1.746510
36	1	2.395333	1.322245	-2.620248
37	12	-3.583867	-0.391472	-0.319276
38	8	-4.315977	-1.607337	-1.808864
39	8	-5.616285	-0.647249	-0.289222
40	6	-5.460824	-1.391017	-1.306492
41	1	-6.344536	-1.860681	-1.765145
42	1	-1.482269	0.998891	2.708160
43	1	-1.161079	3.316369	1.342472

mPW1PW91/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.0671216 hartrees (-1249394.618804 kcal/mol)

MP2/6-31G(d)//B3LYP/6-31G(d)

MP2 = -1986.6628535 hartrees

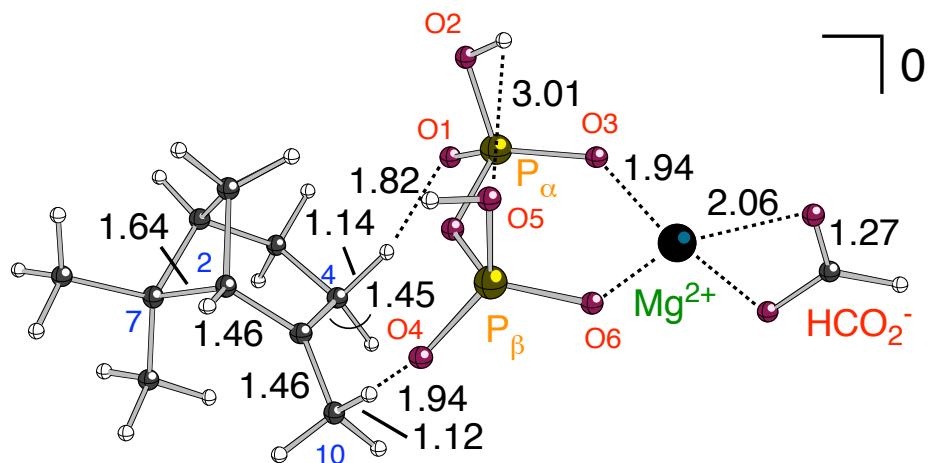
BB1K/6-31G(d)//B3LYP/6-31G(d)

HF = -1990.9173679 hartrees (-1249300.64835725 kcal/mol)

mPWB1K/6-31G(d)//B3LYP/6-31G(d)

HF = -1990.9195774 hartrees (-1249302.0348185 kcal/mol)

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)



HF = -1991.4362977 hartrees (-1249646.19116973 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.324850 (Hartree/Particle)

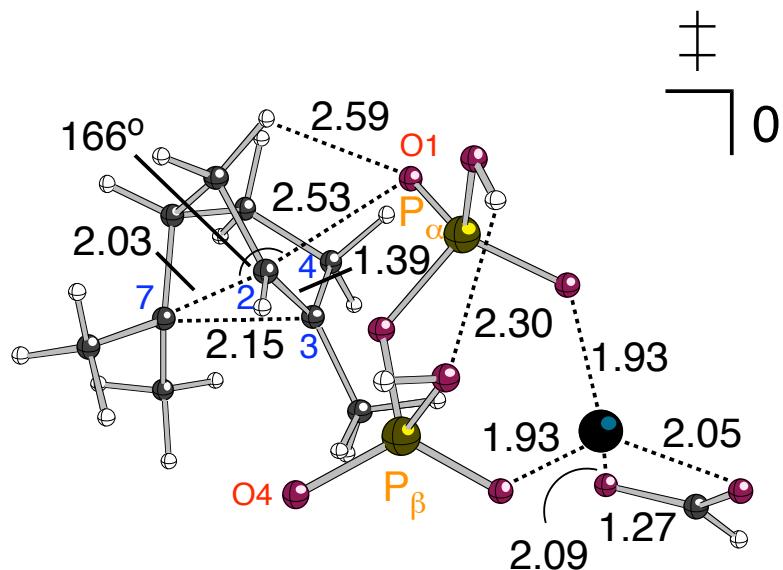
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3.142967	0.660648	0.128762
2	6	2.339483	0.284686	-1.033450
3	6	2.165262	-1.138060	-1.276577
4	6	3.294304	-2.036825	-0.687192
5	6	4.109805	-1.254748	0.350311
6	6	3.113471	-0.446074	1.223466
7	1	1.231186	-1.383758	-0.677551
8	1	3.061521	1.715443	0.398412
9	1	2.840421	-2.914395	-0.219090
10	1	3.935998	-2.392274	-1.501434
11	1	2.145487	-0.904741	1.429608
12	1	3.546901	-0.078359	2.152757
13	1	4.846922	-1.892395	0.848965
14	6	4.640719	0.094964	-0.232572
15	6	5.139494	0.155866	-1.678915
16	1	6.107026	-0.354473	-1.749802
17	1	4.469929	-0.315572	-2.402471
18	1	5.295472	1.194006	-1.993554
19	6	5.672522	0.783813	0.669488
20	1	6.631140	0.258788	0.580860
21	1	5.831813	1.821194	0.356161

22	1	5.394835	0.787790	1.725157
23	1	1.905550	-1.359396	-2.315322
24	8	-2.461423	-1.331564	0.605715
25	15	-0.990511	-1.175679	1.003757
26	8	-0.904143	-1.116728	2.622742
27	8	-0.499110	0.332977	0.528895
28	8	0.056647	-2.119761	0.498531
29	15	-1.329708	1.754786	0.354947
30	8	-1.742705	2.130287	1.890603
31	8	-2.643512	1.432309	-0.351722
32	8	-0.352901	2.735129	-0.215904
33	6	1.766634	1.317147	-1.892868
34	1	1.385017	0.942320	-2.843392
35	1	0.940497	1.811307	-1.320258
36	1	2.483506	2.134300	-2.044416
37	12	-3.675162	-0.207947	-0.412461
38	8	-4.671545	-0.831832	-2.107174
39	8	-5.722851	-0.317492	-0.226349
40	6	-5.742890	-0.705461	-1.436214
41	1	-6.706987	-0.936380	-1.912074
42	1	-1.666193	-0.661102	3.010305
43	1	-1.093082	2.734117	2.277964

TS3

B3LYP/6-31G(d)//B3LYP/6-31G(d)



mPW1PW91/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.0516359 hartrees (-1249384.90152725 kcal/mol)

MP2/6-31G(d)//B3LYP/6-31G(d)

MP2 = -1986.6587636 hartrees

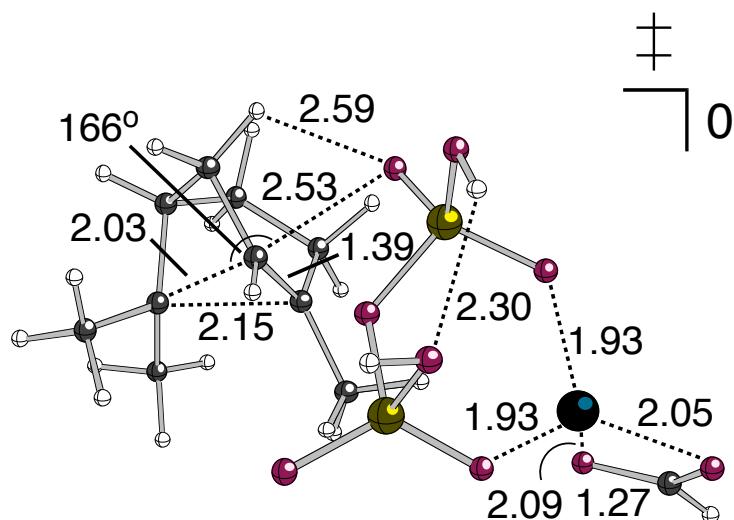
BB1K/6-31G(d)//B3LYP/6-31G(d)

HF = -1990.9042403 hartrees (-1249292.41078825 kcal/mol)

mPWB1K/6-31G(d)//B3LYP/6-31G(d)

HF = -1990.9066409 hartrees (-1249293.91716475 kcal/mol)

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)



HF = -1991.4222588 hartrees (-1249637.38161959 kcal/mol)

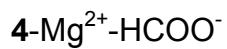
Imaginary Frequencies: 1 (-159.4485 1/cm)

Zero-point correction = 0.326538 (Hartree/Particle)

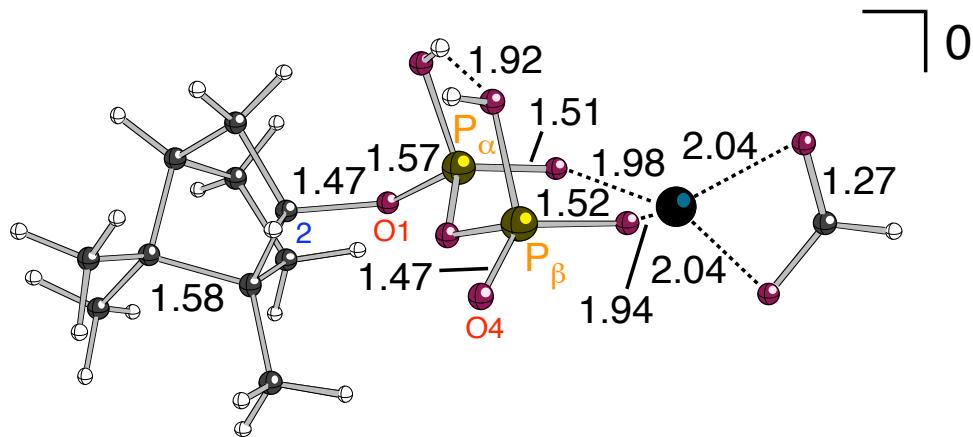
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	6	-2.119377	-0.409333	0.243080
2	6	-2.127786	0.957823	-0.009944
3	6	-2.942617	1.835868	0.910658
4	6	-4.356315	1.221139	1.160112
5	6	-4.352302	-0.184413	0.551966
6	6	-3.170612	-0.965880	1.176331
7	1	-2.374393	1.881923	1.848361
8	1	-4.576813	1.166185	2.229512
9	1	-5.130617	1.845711	0.704481
10	1	-2.959289	-0.736888	2.223108
11	1	-3.252081	-2.048765	1.076354
12	6	-1.166830	1.585755	-0.966730
13	1	-0.388563	2.106575	-0.393180
14	1	-0.675847	0.851821	-1.609084
15	1	-1.656058	2.348738	-1.581234
16	1	-5.335600	-0.665435	0.605649
17	6	-3.783208	-0.095655	-0.882272
18	6	-4.216440	1.031554	-1.804286
19	1	-5.249040	0.810811	-2.110479
20	1	-4.214591	2.023878	-1.354478
21	1	-3.609037	1.057130	-2.713103
22	6	-3.683268	-1.393686	-1.677714
23	1	-4.651358	-1.555105	-2.171013
24	1	-2.926405	-1.321280	-2.463964
25	1	-3.466112	-2.272760	-1.071572
26	1	-3.000068	2.856376	0.522425
27	8	1.610188	-2.089963	2.307597
28	15	0.983816	-0.802737	1.554297
29	8	-0.386024	-0.504843	2.079494
30	8	0.795327	-1.334301	-0.007620
31	8	2.032439	0.320149	1.511204
32	15	1.946390	-1.616938	-1.172164
33	8	1.284795	-2.245652	-2.344845
34	8	2.940165	-2.669386	-0.377948
35	8	2.750500	-0.317423	-1.295641
36	1	-1.401999	-1.038988	-0.271870
37	1	2.398879	-2.414452	1.839192
38	1	2.799485	-3.563365	-0.722384
39	12	2.865483	1.138040	-0.030660
40	8	4.249707	2.648210	0.003516
41	6	3.324170	3.439491	-0.360876
42	1	3.557235	4.504820	-0.504405
43	8	2.140513	3.026425	-0.561800



B3LYP/6-31G(d)//B3LYP/6-31G(d)



HF = -1991.4058988 hartrees (-1249627.11555599 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.332877 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.029260	0.156133	-0.201141
2	6	-3.019264	-0.502135	0.790046
3	6	-3.171008	-1.989480	0.360024
4	6	-3.972980	-1.921698	-0.976313
5	6	-4.166575	-0.401889	-1.182681
6	6	-2.783105	0.181481	-1.555689
7	1	-2.197394	-2.471126	0.245841
8	1	-3.429854	-2.373606	-1.812928
9	1	-4.931923	-2.443650	-0.900723
10	1	-2.263925	-0.423212	-2.304331
11	1	-2.846774	1.199648	-1.950169
12	6	-2.647896	-0.301224	2.253389
13	1	-1.677525	-0.759622	2.476127
14	1	-2.578196	0.762149	2.511569
15	1	-3.389535	-0.762102	2.915270
16	1	-4.958088	-0.142164	-1.892951
17	6	-4.374674	0.124615	0.273969
18	6	-5.625367	-0.437949	0.973473

19	1	-6.529225	-0.083579	0.463065
20	1	-5.667610	-1.528851	0.995589
21	1	-5.679703	-0.084641	2.009897
22	6	-4.465869	1.660534	0.381719
23	1	-5.399630	2.010833	-0.074118
24	1	-4.481119	1.975019	1.431872
25	1	-3.649511	2.198400	-0.107585
26	1	-3.710922	-2.546948	1.131570
27	8	0.452423	0.669366	-2.051319
28	15	0.609292	-0.043075	-0.630899
29	8	-0.790761	-0.642401	-0.262644
30	8	0.912369	1.135404	0.409606
31	8	1.661180	-1.125948	-0.593403
32	15	2.355905	2.043417	0.411498
33	8	2.233441	3.143832	1.381291
34	8	2.280956	2.579635	-1.157029
35	8	3.458643	0.991573	0.428455
36	1	-1.736881	1.150258	0.142829
37	1	1.075945	1.431514	-2.115482
38	1	2.133571	3.540814	-1.150263
39	12	3.494214	-0.917498	0.113165
40	8	5.054095	-1.946335	-0.706797
41	6	5.107655	-2.580646	0.392668
42	1	5.867612	-3.364793	0.523396
43	8	4.304182	-2.330871	1.344061

mPW1PW91/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.1285225 hartrees (-1249433.14786875 kcal/mol)

MP2/6-31G(d)//B3LYP/6-31G(d)

MP2 = -1986.7322916 hartrees

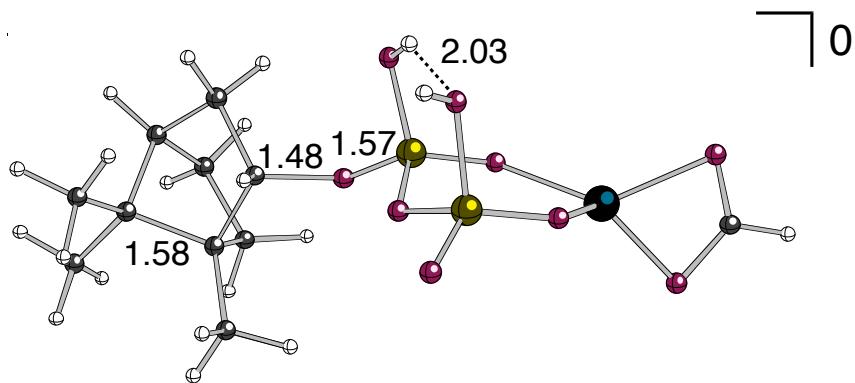
BB1K/6-31G(d)//B3LYP/6-31G(d)

HF = -1990.9839127 hartrees (-1249342.40521925 kcal/mol)

mPWB1K/6-31G(d)//B3LYP/6-31G(d)

HF = -1990.986865 hartrees (-1249344.2577875 kcal/mol)

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)



HF = -1991.4857587 hartrees (-1249677.22844184 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.330947 (Hartree/Particle)

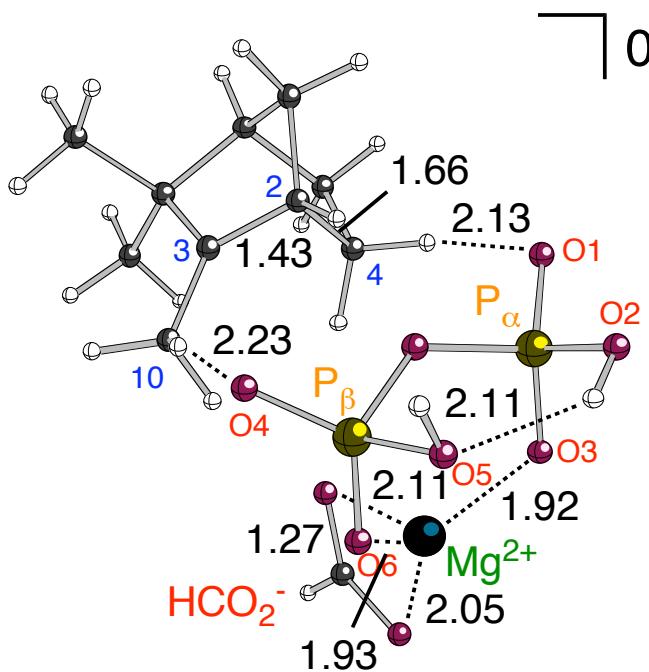
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.051685	0.096607	-0.330624
2	6	-2.990959	-0.394978	0.796117
3	6	-3.143592	-1.934527	0.625727
4	6	-4.010000	-2.095860	-0.661671
5	6	-4.219776	-0.632443	-1.115626
6	6	-2.854213	-0.122128	-1.638569
7	1	-2.169888	-2.422886	0.546337
8	1	-3.507436	-2.688129	-1.432920
9	1	-4.961921	-2.591379	-0.449160
10	1	-2.357777	-0.853043	-2.282610
11	1	-2.938713	0.807419	-2.207859
12	6	-2.562502	0.041703	2.191761
13	1	-1.594342	-0.397445	2.455382
14	1	-2.461718	1.130182	2.267440
15	1	-3.287115	-0.285727	2.944708
16	1	-5.040965	-0.495030	-1.826011
17	6	-4.372493	0.133253	0.238705
18	6	-5.587548	-0.306818	1.075664
19	1	-6.513495	-0.065060	0.540906
20	1	-5.607357	-1.374272	1.300969
21	1	-5.613496	0.232261	2.029120

22	6	-4.476252	1.664646	0.085505
23	1	-5.438398	1.926178	-0.369478
24	1	-4.437637	2.154741	1.064613
25	1	-3.697642	2.112925	-0.535741
26	1	-3.638235	-2.357818	1.504751
27	8	0.471607	0.581467	-2.110091
28	15	0.606089	-0.072211	-0.656187
29	8	-0.795085	-0.681905	-0.315191
30	8	0.858841	1.152525	0.343319
31	8	1.680476	-1.128696	-0.555745
32	15	2.302608	2.060195	0.396175
33	8	2.140505	3.173475	1.350796
34	8	2.301928	2.578068	-1.177036
35	8	3.399551	1.005058	0.475395
36	1	-1.771432	1.139697	-0.172556
37	1	1.090326	1.333391	-2.219449
38	1	2.155370	3.535855	-1.204710
39	12	3.517164	-0.903281	0.149070
40	8	5.114270	-1.880747	-0.681116
41	6	5.194532	-2.526356	0.411513
42	1	5.980099	-3.284606	0.534736
43	8	4.380692	-2.308774	1.363651

D-PPi-Mg²⁺-HCOO⁻

B3LYP/6-31G(d)//B3LYP/6-31G(d)



HF = -1991.3611901 hartrees (-1249599.06039965 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.329174 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.822100	-1.099921	-0.188398
2	6	2.335687	-0.123049	0.728230
3	6	1.746661	-0.012369	-1.442125
4	6	3.194190	0.034605	-1.971338
5	6	3.970221	-0.730837	-0.874068
6	6	3.029134	-1.932039	-0.656064
7	1	1.001801	-0.518834	-2.074154
8	1	3.278874	-0.495379	-2.924921
9	1	3.552103	1.054512	-2.129832
10	1	2.805715	-2.478392	-1.575954
11	1	3.360680	-2.649524	0.099095
12	6	1.549165	0.629857	1.714513
13	1	0.973525	1.410250	1.183981
14	1	0.796928	-0.009032	2.203145
15	1	2.183054	1.139411	2.445066
16	1	5.011384	-0.960632	-1.114165
17	6	3.810835	0.058559	0.472005

18	6	4.267420	1.528955	0.442267
19	1	5.315891	1.577887	0.128351
20	1	3.676345	2.137766	-0.246363
21	1	4.197710	1.986166	1.434297
22	6	4.562020	-0.662103	1.636070
23	1	5.635319	-0.623163	1.422807
24	1	4.383910	-0.149670	2.586059
25	1	4.276447	-1.709305	1.757109
26	1	1.331015	0.960374	-1.168133
27	8	-3.124059	-2.161441	-1.280221
28	15	-1.899019	-1.114777	-1.381724
29	8	-0.812714	-1.613738	-2.264948
30	8	-1.304194	-1.114147	0.189149
31	8	-2.451426	0.312441	-1.588828
32	15	-2.026322	-0.669226	1.605506
33	8	-1.113985	-1.045386	2.719569
34	8	-3.402360	-1.572797	1.584265
35	8	-2.496297	0.778734	1.413001
36	1	0.848578	-1.544261	-0.002699
37	1	-3.643295	-2.003538	-0.466901
38	1	-3.260875	-2.374848	2.114366
39	12	-2.151262	1.670124	-0.264778
40	8	-2.164825	3.701096	-0.500800
41	6	-0.901474	3.684198	-0.421551
42	1	-0.350741	4.635356	-0.485344
43	8	-0.254497	2.600024	-0.271492

mPW1PW91/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.0774889 hartrees (-1249401.12428475 kcal/mol)

MP2/6-31G(d)//B3LYP/6-31G(d)

MP2 = -1986.6812031 hartrees

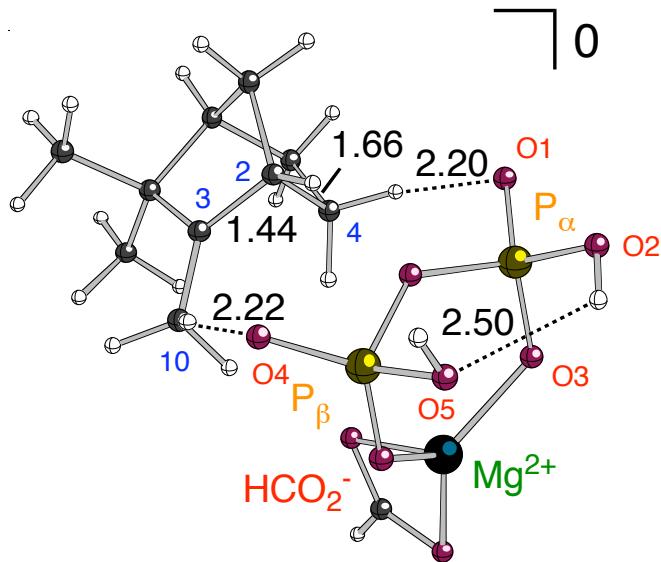
BB1K/6-31G(d)//B3LYP/6-31G(d)

HF = -1990.9287735 hartrees (-1249307.80537125 kcal/mol)

mPWB1K/6-31G(d)//B3LYP/6-31G(d)

HF = -1990.9317837 hartrees (-1249309.69427175 kcal/mol)

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)



HF = -1991.4448277 hartrees (-1249651.54383003 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.326796 (Hartree/Particle)

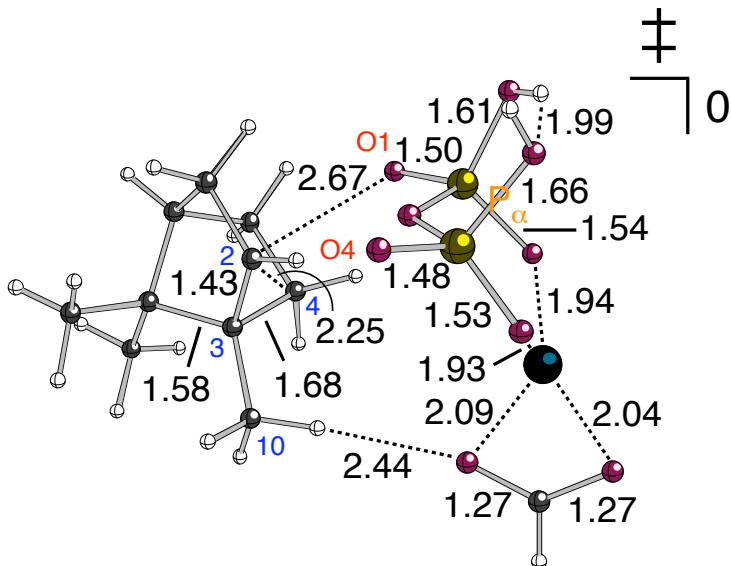
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.812569	-1.060202	-0.243470
2	6	2.353078	-0.134897	0.713399
3	6	1.739211	0.072805	-1.453124
4	6	3.186367	0.133695	-1.985350
5	6	3.960523	-0.694831	-0.932021
6	6	3.002573	-1.890564	-0.759438
7	1	0.998379	-0.402648	-2.110285
8	1	3.262124	-0.347006	-2.964768
9	1	3.552800	1.156678	-2.092730
10	1	2.760184	-2.389633	-1.700444
11	1	3.329092	-2.646523	-0.041905
12	6	1.587497	0.582961	1.739456
13	1	0.977688	1.357098	1.242592
14	1	0.862360	-0.084893	2.231614
15	1	2.229728	1.091079	2.461283
16	1	4.995405	-0.928584	-1.193143

17	6	3.827783	0.031893	0.452495
18	6	4.314559	1.492752	0.491397
19	1	5.361100	1.534040	0.172172
20	1	3.732622	2.146293	-0.161822
21	1	4.261672	1.900999	1.504705
22	6	4.571640	-0.761768	1.575332
23	1	5.642374	-0.739271	1.350495
24	1	4.415961	-0.289139	2.548672
25	1	4.260702	-1.805018	1.651151
26	1	1.329552	1.035167	-1.138780
27	8	-3.206498	-2.105086	-1.441290
28	15	-1.939809	-1.097926	-1.408223
29	8	-0.862231	-1.558274	-2.325509
30	8	-1.366116	-1.263349	0.153585
31	8	-2.451455	0.355631	-1.500001
32	15	-1.968222	-0.775282	1.612704
33	8	-1.001502	-1.209807	2.663972
34	8	-3.399417	-1.567513	1.693784
35	8	-2.338956	0.706759	1.462096
36	1	0.838003	-1.504544	-0.061374
37	1	-3.851980	-1.898308	-0.746197
38	1	-3.297146	-2.393904	2.188040
39	12	-2.140544	1.712354	-0.172943
40	8	-2.242328	3.744159	-0.374957
41	6	-0.974580	3.786268	-0.348929
42	1	-0.470489	4.760299	-0.430291
43	8	-0.277803	2.728606	-0.231601

TS4

B3LYP/6-31G(d)//B3LYP/6-31G(d)



HF = -1991.3466727 hartrees (-1249589.95058598 kcal/mol)
 Imaginary Frequencies: 1 (-123.8208 1/cm)
 Zero-point correction = 0.328320 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.806468	-0.623013	0.408999
2	6	2.619169	0.556909	0.422738
3	6	2.552670	0.696772	-1.246730
4	6	3.514781	-0.384968	-1.768831
5	6	3.916748	-1.131314	-0.473112
6	6	2.606676	-1.796663	0.007841
7	1	1.540475	0.607861	-1.638595
8	1	3.011166	-1.046815	-2.476904
9	1	4.382728	0.051777	-2.269843
10	1	2.064534	-2.412683	-0.714749
11	1	2.755723	-2.412313	0.909798
12	6	2.155210	1.805674	1.150566
13	1	1.145953	2.106119	0.850185
14	1	2.151746	1.642150	2.233648
15	1	2.828850	2.642458	0.939047
16	1	4.760120	-1.818293	-0.572533
17	6	4.100082	0.014180	0.569704
18	6	5.177910	1.047292	0.205503
19	1	6.162515	0.565547	0.209015
20	1	5.042573	1.508976	-0.774743

21	1	5.208110	1.850561	0.949431
22	6	4.397275	-0.470054	2.003612
23	1	5.378464	-0.956772	2.039695
24	1	4.429925	0.379370	2.694368
25	1	3.661627	-1.176973	2.397931
26	1	2.904169	1.725845	-1.369114
27	8	-2.076902	-2.253270	-1.872831
28	15	-1.212670	-1.015817	-1.316699
29	8	0.234145	-1.163996	-1.683391
30	8	-1.296314	-1.197496	0.334872
31	8	-1.913229	0.314564	-1.635216
32	15	-2.654342	-1.090516	1.303354
33	8	-2.341917	-1.642880	2.639206
34	8	-3.691241	-2.070086	0.459466
35	8	-3.186321	0.332451	1.099556
36	1	0.748231	-0.673043	0.655074
37	1	-2.906530	-2.330648	-1.354690
38	1	-3.802627	-2.892733	0.964653
39	12	-2.510889	1.529188	-0.251922
40	8	-3.058465	3.472832	-0.555090
41	6	-1.919864	3.806280	-0.103784
42	1	-1.663419	4.875529	-0.046301
43	8	-1.073660	2.943164	0.280782

mPW1PW91/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.0635132 hartrees (-1249392.354533 kcal/mol)

MP2/6-31G(d)//B3LYP/6-31G(d)

MP2 = -1986.6665918 hartrees

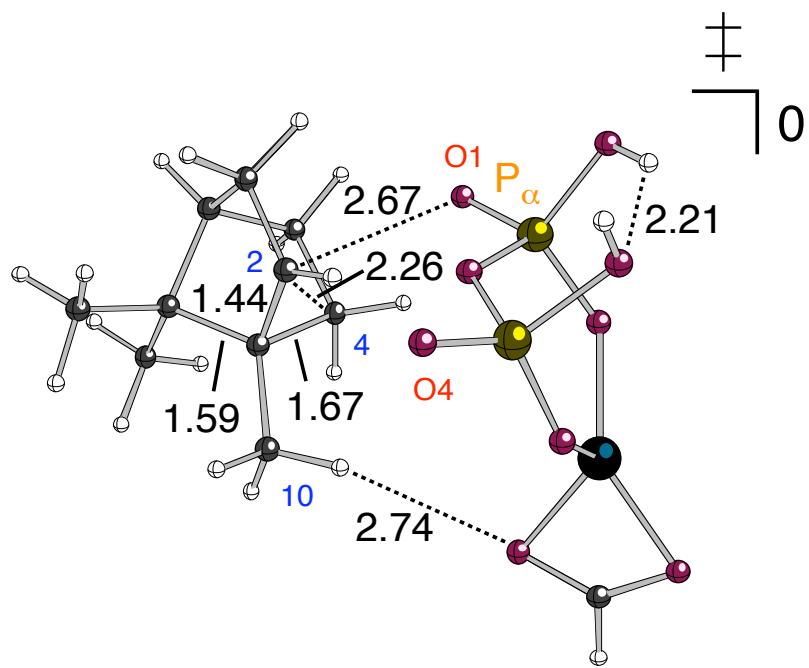
BB1K/6-31G(d)//B3LYP/6-31G(d)

HF = -1990.9166569 hartrees (-1249300.20220475 kcal/mol)

mPWB1K/6-31G(d)//B3LYP/6-31G(d)

HF = -1990.9192895 hartrees (-1249301.85416125 kcal/mol)

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)



HF = -1991.4311452 hartrees (-1249642.95792445 kcal/mol)

Imaginary Frequencies: 1 (-117.9793 1/cm)

Zero-point correction = 0.326130 (Hartree/Particle)

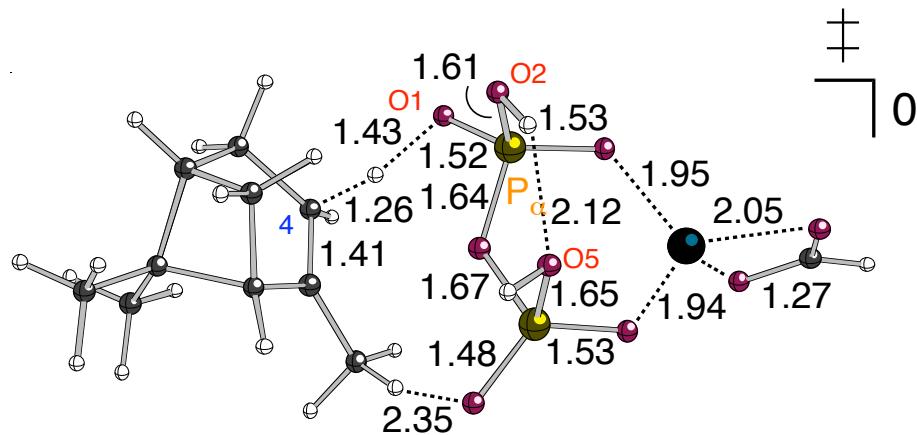
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.905971	-0.775067	0.313794
2	6	2.549736	0.495967	0.484160
3	6	2.450606	0.863485	-1.143118
4	6	3.542321	0.005515	-1.807421
5	6	4.052729	-0.859495	-0.627801
6	6	2.847764	-1.755427	-0.257141
7	1	1.454667	0.697043	-1.550736
8	1	3.128709	-0.609588	-2.609484
9	1	4.339961	0.620712	-2.231058
10	1	2.382114	-2.328757	-1.064384
11	1	3.088848	-2.473044	0.543507
12	6	1.925362	1.552702	1.378213
13	1	0.891465	1.764447	1.091285
14	1	1.928612	1.230811	2.424105
15	1	2.481812	2.491785	1.309197

16	1	4.978855	-1.406481	-0.816797
17	6	4.092875	0.140655	0.569464
18	6	5.020140	1.348550	0.362727
19	1	6.056743	1.002003	0.287070
20	1	4.804046	1.933092	-0.532935
21	1	4.967698	2.025904	1.221008
22	6	4.467907	-0.498360	1.922235
23	1	5.507537	-0.842153	1.897989
24	1	4.387686	0.238699	2.727484
25	1	3.843793	-1.350587	2.203322
26	1	2.657749	1.937078	-1.118877
27	8	-2.034388	-2.236769	-2.002560
28	15	-1.164751	-1.046696	-1.349220
29	8	0.274541	-1.162182	-1.760382
30	8	-1.206719	-1.366080	0.277915
31	8	-1.880616	0.297248	-1.552839
32	15	-2.503625	-1.225821	1.323168
33	8	-2.143156	-1.847003	2.621060
34	8	-3.638440	-2.106965	0.506205
35	8	-2.963359	0.231489	1.210448
36	1	0.873363	-1.005545	0.567432
37	1	-2.900420	-2.313146	-1.562980
38	1	-3.774650	-2.950185	0.962960
39	12	-2.550533	1.499486	-0.185728
40	8	-3.401438	3.334607	-0.495206
41	6	-2.308505	3.854297	-0.105893
42	1	-2.218850	4.950051	-0.075314
43	8	-1.322567	3.136263	0.246782

Figure 10.

TS5



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.3509132 hartrees (-1249592.61154213 kcal/mol)

Imaginary Frequencies: 1 (-351.8309 1/cm)

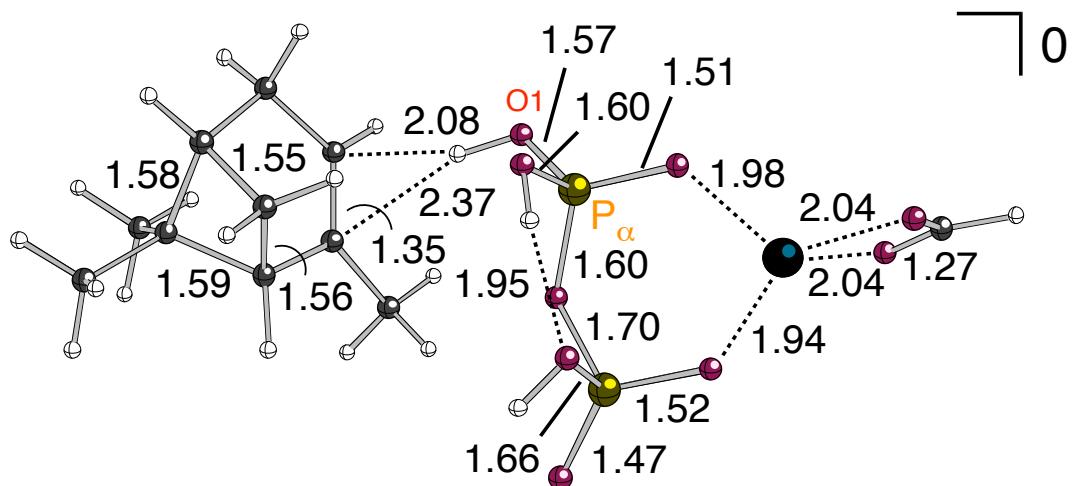
Zero-point correction = 0.324205 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.976210	0.689062	0.246808
2	6	-2.192310	-0.221870	1.117028
3	6	-2.200120	-1.590790	0.789004
4	6	-3.322839	-2.072607	-0.155043
5	6	-4.040773	-0.866573	-0.781893
6	6	-2.961019	0.157584	-1.219910
7	1	-1.150397	-1.665324	0.104050
8	1	-2.777613	1.745318	0.441468
9	1	-2.900358	-2.707517	-0.941418
10	1	-4.026473	-2.693980	0.413225
11	1	-2.014613	-0.231841	-1.598313
12	1	-3.335732	0.912016	-1.911852
13	1	-4.792920	-1.180822	-1.513335
14	6	-4.500086	0.166406	0.305543
15	6	-5.066030	-0.340105	1.635533
16	1	-6.058548	-0.777584	1.471974
17	1	-4.448865	-1.103445	2.117563
18	1	-5.189602	0.488062	2.344180
19	6	-5.456437	1.231824	-0.248994
20	1	-6.447116	0.788078	-0.407315
21	1	-5.572393	2.055204	0.465463

22	1	-5.131348	1.659484	-1.200530
23	1	-1.917140	-2.269842	1.598867
24	8	2.402591	-1.253791	-0.790343
25	15	0.927579	-0.985382	-1.068557
26	8	0.708575	-0.505895	-2.592130
27	8	0.460608	0.316598	-0.188000
28	8	-0.077284	-2.075085	-0.750301
29	15	1.246005	1.781986	-0.054682
30	8	1.403896	2.170594	-1.652748
31	8	2.656893	1.459928	0.430534
32	8	0.335532	2.712718	0.656464
33	6	-1.472753	0.332900	2.288443
34	1	-0.877406	-0.417316	2.814334
35	1	-0.847223	1.182142	1.983235
36	1	-2.224975	0.737539	2.984002
37	12	3.643544	-0.203379	0.283358
38	8	4.648636	-1.023019	1.873958
39	8	5.672056	-0.311637	0.039123
40	6	5.704896	-0.834086	1.196186
41	1	6.675520	-1.130535	1.621811
42	1	1.126021	0.368984	-2.729357
43	1	0.794966	2.899105	-1.858461

2-PPI-Mg²⁺-HCOO⁻



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.3700621 hartrees (-1249604.62766837 kcal/mol)

Imaginary Frequencies: none found

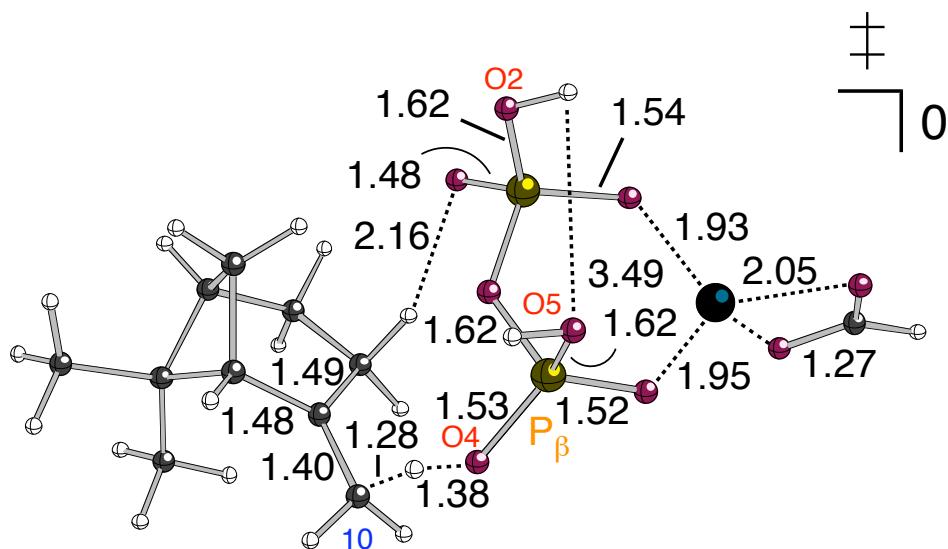
Zero-point correction = 0.328298 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-3.455668	0.635266	0.226984
2	6	-2.778764	-0.413077	1.095946
3	6	-2.940700	-1.700027	0.719898
4	6	-3.824001	-2.035960	-0.468675
5	6	-4.374562	-0.744560	-1.105617
6	6	-3.203155	0.262701	-1.265514
7	1	-0.939925	-1.566014	0.162869
8	1	-3.246661	1.656646	0.561418
9	1	-3.267292	-2.615905	-1.219254
10	1	-4.646587	-2.687251	-0.138611
11	1	-2.219427	-0.143382	-1.520849
12	1	-3.433436	1.078936	-1.952589
13	1	-4.999445	-0.962569	-1.979412
14	6	-4.967577	0.225462	-0.016372
15	6	-5.784968	-0.357602	1.139238
16	1	-6.738749	-0.752154	0.766146
17	1	-5.273683	-1.164230	1.669546
18	1	-6.022951	0.423842	1.872246
19	6	-5.782205	1.370855	-0.638862
20	1	-6.748961	0.995346	-0.997000
21	1	-5.987512	2.144872	0.110928
22	1	-5.285411	1.855011	-1.484152
23	1	-2.544767	-2.516516	1.324919
24	8	2.415122	-1.342109	-0.500734
25	15	1.003765	-0.808703	-0.528061
26	8	0.494335	-0.389087	-1.982701
27	8	0.827115	0.497500	0.380896
28	8	-0.007500	-1.880967	0.010873
29	15	1.762791	1.910297	0.205107
30	8	1.446201	2.189585	-1.398612
31	8	3.202764	1.414484	0.257732
32	8	1.203800	2.958602	1.075235
33	6	-2.044460	0.029986	2.329908
34	1	-1.591077	-0.812198	2.862855
35	1	-1.257930	0.756090	2.090979
36	1	-2.738214	0.533475	3.017268
37	12	4.014032	-0.334383	0.074456
38	8	5.364119	-1.168700	1.358039
39	8	5.838890	-0.707182	-0.758044
40	6	6.175642	-1.157894	0.381131

41	1	7.193823	-1.548009	0.524447
42	1	0.762945	0.539605	-2.175507
43	1	0.922276	3.005190	-1.475283

TS6



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.3475912 hartrees (-1249590.52695391 kcal/mol)

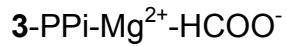
Imaginary Frequencies: 1 (-656.2043 1/cm)

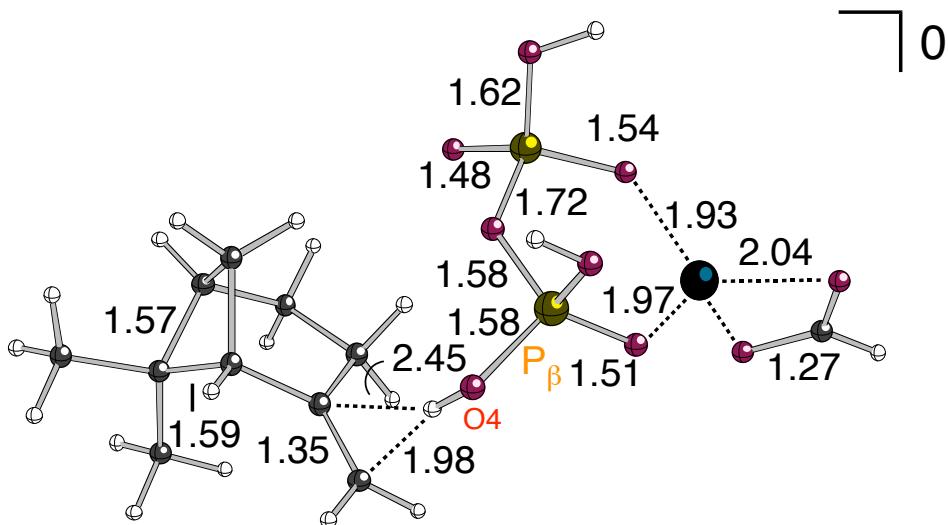
Zero-point correction = 0.323458 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3.312214	0.612625	0.220450
2	6	2.343077	0.549260	-0.894113
3	6	1.921117	-0.825351	-1.291222
4	6	2.990027	-1.917359	-0.979695
5	6	3.975410	-1.423826	0.088122
6	6	3.174506	-0.627840	1.153931
7	1	1.045485	-1.057239	-0.658106
8	1	3.414922	1.615824	0.644191
9	1	2.471358	-2.808993	-0.615426
10	1	3.523033	-2.198141	-1.895292

11	1	2.165236	-0.976938	1.382330
12	1	3.724810	-0.477679	2.083569
13	1	4.640159	-2.226888	0.424642
14	6	4.658468	-0.082561	-0.341837
15	6	5.050175	0.134471	-1.806213
16	1	5.912830	-0.495329	-2.056322
17	1	4.254243	-0.103264	-2.517520
18	1	5.345743	1.176638	-1.978153
19	6	5.854957	0.292466	0.542817
20	1	6.710338	-0.346643	0.290797
21	1	6.155756	1.332379	0.368607
22	1	5.658202	0.174103	1.611319
23	1	1.574998	-0.851105	-2.329349
24	8	-2.531165	-1.271897	0.780427
25	15	-1.101710	-1.117218	1.319186
26	8	-1.221555	-0.952432	2.927260
27	8	-0.569513	0.402111	0.844316
28	8	-0.010831	-2.050201	0.940783
29	15	-1.345570	1.743514	0.373186
30	8	-1.956463	2.403199	1.717074
31	8	-2.534126	1.382655	-0.502551
32	8	-0.255462	2.648344	-0.189614
33	6	1.839638	1.707533	-1.501736
34	1	1.411765	1.601094	-2.500060
35	1	0.813582	2.028775	-0.803143
36	1	2.415703	2.623784	-1.350340
37	12	-3.532775	-0.285790	-0.543074
38	8	-4.212981	-1.062030	-2.315571
39	8	-5.571360	-0.391806	-0.695096
40	6	-5.380322	-0.886197	-1.849188
41	1	-6.250310	-1.169535	-2.460653
42	1	-2.139297	-0.758786	3.178321
43	1	-1.274026	2.890095	2.207765





B3LYP/6-31G(d)//B3LYP/6-31G(d)

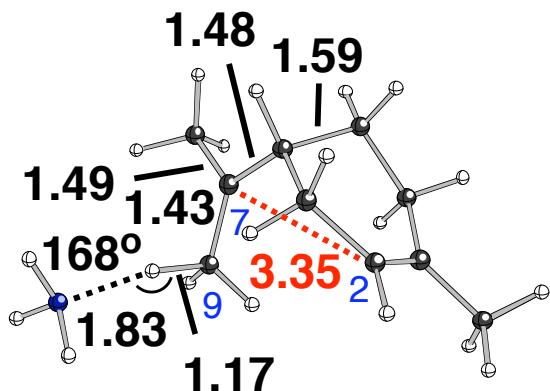
HF = -1991.3625284 hartrees (-1249599.90019628 kcal/mol)
 Imaginary Frequencies: none found
 Zero-point correction = 0.327650 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3.404983	-0.093590	0.725949
2	6	2.370100	0.996854	0.650632
3	6	1.892867	1.299063	-0.761577
4	6	2.936495	0.928062	-1.856475
5	6	3.930458	-0.124957	-1.341575
6	6	3.171480	-1.123088	-0.423212
7	1	1.003621	0.686142	-0.949498
8	1	3.556492	-0.454611	1.749793
9	1	2.399353	0.528949	-2.723207
10	1	3.477651	1.819009	-2.196261
11	1	2.141017	-1.367142	-0.694017
12	1	3.720255	-2.051373	-0.253553
13	1	4.542371	-0.529759	-2.156390
14	6	4.693146	0.383507	-0.068015
15	6	5.107283	1.854591	0.022823
16	1	5.902641	2.071281	-0.701773
17	1	4.286358	2.551004	-0.165671
18	1	5.502435	2.081372	1.021200
19	6	5.914839	-0.484968	0.268399

20	1	6.728599	-0.279911	-0.438597
21	1	6.286353	-0.256248	1.275225
22	1	5.706524	-1.557843	0.226953
23	1	1.575360	2.344357	-0.844692
24	8	-2.638485	-0.656066	-1.315281
25	15	-1.308946	-1.423927	-1.287883
26	8	-1.686319	-2.997545	-1.276489
27	8	-0.718448	-1.255487	0.315278
28	8	-0.171163	-1.086592	-2.164032
29	15	-1.365688	-0.683756	1.641853
30	8	-2.083180	-1.874056	2.428378
31	8	-2.378153	0.408242	1.400500
32	8	-0.140839	-0.298437	2.556754
33	6	1.922527	1.656272	1.738345
34	1	1.250239	2.508409	1.654134
35	1	0.546859	0.290393	2.125674
36	1	2.315317	1.441060	2.731174
37	12	-3.397345	0.756349	-0.245692
38	8	-3.805643	2.677684	-0.804437
39	8	-5.382244	1.231090	-0.222639
40	6	-5.026830	2.387745	-0.610402
41	1	-5.795211	3.155585	-0.781910
42	1	-2.650083	-3.111133	-1.313986
43	1	-1.476811	-2.598115	2.660551

Figure S2a



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6332889 hartrees (-280889.88878475 kcal/mol)

Imaginary Frequencies: none

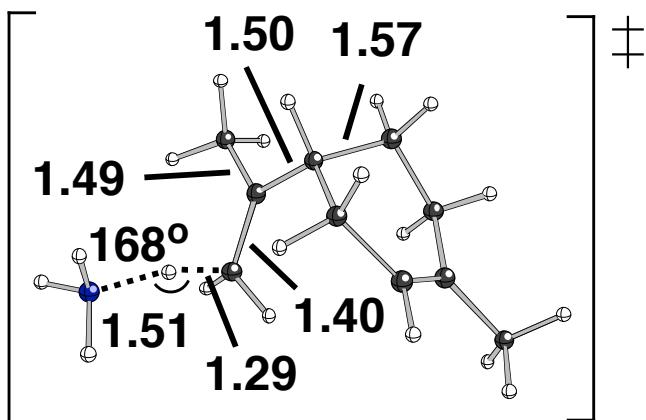
Zero-point correction = 0.281248 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5250814 hartrees (-280821.9885785 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.137717	0.863669	-0.218474
2	6	-1.798582	2.163302	-0.502231
3	6	-1.422196	-0.249319	-1.069021
4	6	-0.237496	0.773226	0.952699
5	6	1.082522	1.585326	0.621885
6	6	1.960016	0.875766	-0.412664
7	6	2.114375	-0.610187	-0.159962
8	6	1.292794	-1.263957	0.676667
9	6	3.235613	-1.294737	-0.896243
10	6	0.149003	-0.636459	1.439498
11	1	-1.292912	2.616852	-1.369234
12	1	-1.757607	2.867778	0.329550
13	1	-2.835595	2.009717	-0.821959
14	1	-0.654713	-1.024926	-1.083051
15	1	-1.803168	0.016557	-2.058158
16	1	-2.339754	-0.762151	-0.549355
17	1	-0.725856	1.336395	1.760338
18	1	1.611576	1.652619	1.577886
19	1	0.845642	2.607345	0.313263
20	1	2.950189	1.349053	-0.402355
21	1	1.579586	1.037152	-1.433722
22	1	1.452573	-2.325789	0.854171
23	1	3.148410	-1.141481	-1.979640
24	1	3.249951	-2.370536	-0.704572
25	1	4.207496	-0.881823	-0.598858
26	1	0.414729	-0.555236	2.502632
27	1	-0.726192	-1.298403	1.416832
28	7	-3.787408	-1.770067	-0.058889
29	1	-3.522133	-2.753559	-0.050485
30	1	-4.181906	-1.557918	0.855928
31	1	-4.538449	-1.670956	-0.739906



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6325782 hartrees (-280893.919146282 kcal/mol)

Imaginary Frequencies: 1 (-428.6889 1/cm)

Zero-point correction = 0.279676 (Hartree/Particle)

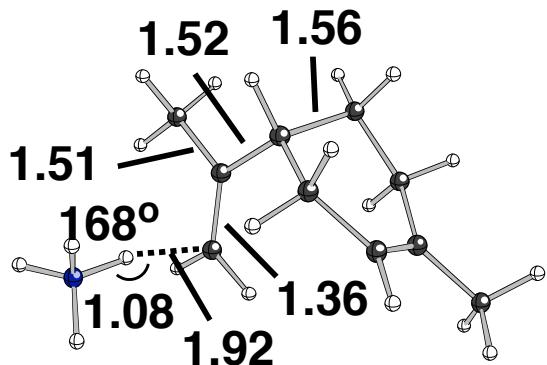
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5256327 hartrees (-280826.809775577 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.177917	0.776255	-0.239488
2	6	-1.846326	2.080633	-0.526521
3	6	-1.437772	-0.323477	-1.065857
4	6	-0.278630	0.711559	0.954953
5	6	1.004964	1.576168	0.684059
6	6	1.914622	0.941610	-0.373551
7	6	2.126694	-0.544853	-0.169590
8	6	1.327708	-1.257001	0.641147
9	6	3.277212	-1.161183	-0.920721
10	6	0.159522	-0.691817	1.416706
11	1	-1.173320	2.668869	-1.168440
12	1	-2.027878	2.671957	0.374260
13	1	-2.773878	1.951803	-1.090454
14	1	-0.716012	-1.140254	-1.046624
15	1	-1.867236	-0.105314	-2.046214
16	1	-2.453425	-0.864561	-0.490095

17	1	-0.818123	1.215925	1.769009
18	1	1.532915	1.628431	1.642015
19	1	0.738013	2.601987	0.413947
20	1	2.885539	1.452334	-0.351391
21	1	1.523240	1.118015	-1.388044
22	1	1.529364	-2.316651	0.787843
23	1	3.187241	-0.978414	-1.999356
24	1	3.335282	-2.240956	-0.761541
25	1	4.230418	-0.717821	-0.607003
26	1	0.422284	-0.624561	2.481621
27	1	-0.687615	-1.390145	1.380878
28	7	-3.642999	-1.695132	-0.059629
29	1	-3.510638	-2.661311	-0.358043
30	1	-3.770018	-1.695794	0.952089
31	1	-4.505622	-1.354978	-0.483869



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6430434 hartrees (-280900.486163934 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.285085 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

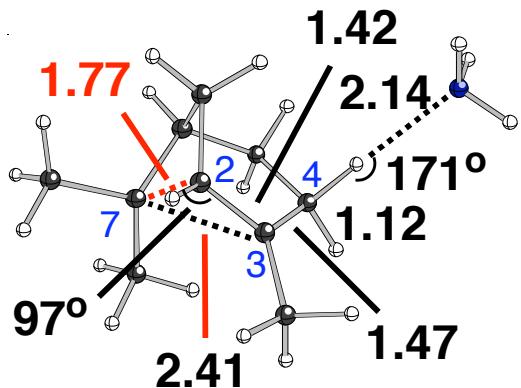
HF = -447.5366006 hartrees (-280833.692242506 kcal/mol)

Coordinates (from last standard orientation):

Center	Atomic	Coordinates (Angstroms)
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Number	Number	X	Y	Z
1	6	-1.230796	0.751382	-0.304123
2	6	-2.091522	1.984471	-0.429209
3	6	-1.261616	-0.213974	-1.255230
4	6	-0.324411	0.706002	0.916681
5	6	0.938538	1.588885	0.690375
6	6	1.888570	0.991172	-0.353700
7	6	2.150566	-0.485109	-0.144078
8	6	1.344935	-1.228225	0.631485
9	6	3.350695	-1.059361	-0.849499
10	6	0.135762	-0.698071	1.367410
11	1	-1.464706	2.882363	-0.472785
12	1	-2.736266	2.110366	0.449774
13	1	-2.712018	1.969692	-1.328911
14	1	-0.563273	-1.047682	-1.234304
15	1	-1.833905	-0.067263	-2.170548
16	1	-2.673210	-1.148396	-0.358514
17	1	-0.888504	1.163560	1.740598
18	1	1.456094	1.659692	1.654117
19	1	0.656571	2.609805	0.413869
20	1	2.840531	1.536048	-0.325092
21	1	1.496892	1.146478	-1.370595
22	1	1.579074	-2.280652	0.786594
23	1	3.295758	-0.876717	-1.930592
24	1	3.442784	-2.136968	-0.688990
25	1	4.274183	-0.581575	-0.499249
26	1	0.356294	-0.657789	2.443631
27	1	-0.693374	-1.419569	1.280279
28	7	-3.449772	-1.822925	-0.032109
29	1	-3.340734	-2.722607	-0.509241
30	1	-3.378107	-1.968306	0.978936
31	1	-4.370012	-1.433039	-0.254897

Figure S2b



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6226497 hartrees (-280883.21268675 kcal/mol)

Imaginary Frequencies: none

Zero-point correction = 0.282983 (Hartree/Particle)

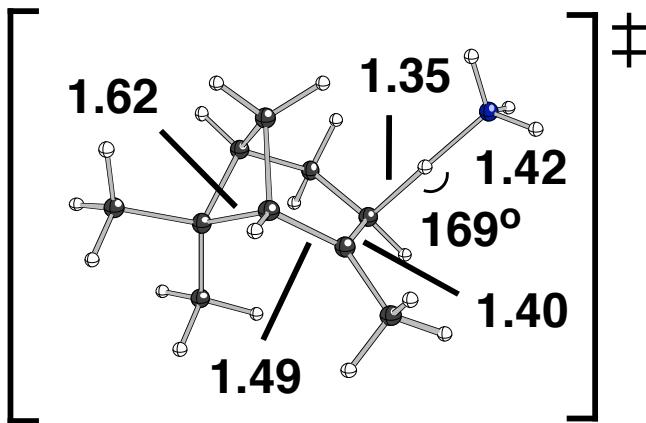
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.521906 hartrees (-280819.996015 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.375510	0.174626	-1.120775
2	6	0.393632	1.030808	-0.285074
3	6	1.156676	0.410623	0.810588
4	6	0.466570	-0.874216	1.383819
5	6	-0.616357	-1.364818	0.419089
6	6	-0.028709	-1.321603	-1.014056
7	1	2.129485	0.106964	0.340354
8	1	-0.767944	0.608930	-2.039550
9	1	1.214878	-1.657983	1.528393
10	1	0.043096	-0.648694	2.367167
11	1	1.033142	-1.562328	-1.108851
12	1	-0.591030	-1.910739	-1.736460
13	1	1.419456	1.137114	1.585031
14	6	0.405890	2.500195	-0.476581
15	1	1.436756	2.796439	-0.724520
16	1	-0.251564	2.835794	-1.280084
17	1	0.167054	3.022230	0.457507

18	1	-1.072468	-2.299134	0.760556
19	6	-1.620953	-0.231843	0.070927
20	6	-2.050789	0.769391	1.135858
21	1	-2.764940	0.266698	1.799180
22	1	-1.241372	1.145804	1.763213
23	1	-2.572939	1.622700	0.691893
24	6	-2.836515	-0.664677	-0.747085
25	1	-3.539117	-1.157992	-0.063609
26	1	-3.350672	0.199366	-1.177503
27	1	-2.607501	-1.368261	-1.547932
28	7	4.084563	-0.540120	-0.246711
29	1	4.725173	0.249920	-0.192380
30	1	4.428315	-1.231626	0.417394
31	1	4.206647	-0.945269	-1.173078



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6178322 hartrees (-280880.1897055 kcal/mol)

Imaginary Frequencies: 1 (-873.1894 1/cm)

Zero-point correction = 0.280547 (Hartree/Particle)

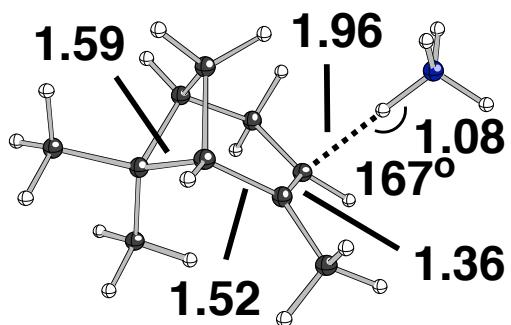
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5202598 hartrees (-280818.9630245 kcal/mol)

Coordinates:

Center	Atomic	Coordinates (Angstroms)
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Number	Number	X	Y	Z
1	6	-0.463225	0.413379	-0.969840
2	6	0.624724	0.996860	-0.142659
3	6	1.195094	0.185337	0.839698
4	6	0.436653	-1.098158	1.223670
5	6	-0.712491	-1.351708	0.231259
6	6	-0.180324	-1.102690	-1.204931
7	1	2.306713	-0.213780	0.180745
8	1	-0.759863	1.044165	-1.811042
9	1	1.109393	-1.965446	1.243686
10	1	0.052558	-0.989542	2.244663
11	1	0.852975	-1.387786	-1.425545
12	1	-0.822222	-1.510191	-1.983827
13	1	1.732137	0.705976	1.638899
14	6	1.055970	2.401681	-0.377350
15	1	1.322706	2.558742	-1.429874
16	1	0.199357	3.064377	-0.188681
17	1	1.880170	2.712431	0.268462
18	1	-1.224385	-2.294949	0.442449
19	6	-1.613250	-0.078305	0.053537
20	6	-1.944199	0.784041	1.274495
21	1	-2.632725	0.239445	1.930031
22	1	-1.075674	1.063194	1.876490
23	1	-2.452188	1.705804	0.970063
24	6	-2.917053	-0.370189	-0.704287
25	1	-3.611910	-0.897124	-0.041155
26	1	-3.398899	0.563419	-1.012723
27	1	-2.782618	-0.987652	-1.594635
28	7	3.544805	-0.767330	-0.234584
29	1	4.054716	-1.134257	0.569449
30	1	3.416830	-1.530129	-0.899475
31	1	4.127897	-0.056879	-0.677440



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6259329 hartrees (-280885.27289475 kcal/mol)

Imaginary Frequencies: none

Zero-point correction = 0.285955 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

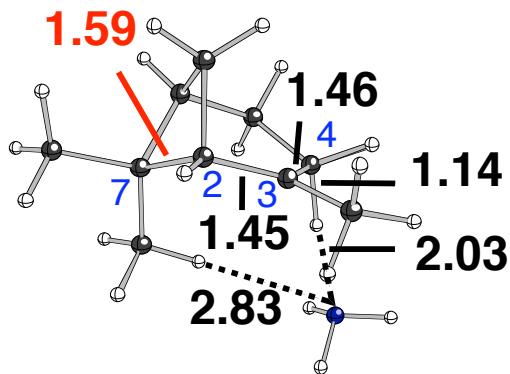
HF = -447.5288985 hartrees (-280824.38380875 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.344577	0.317143	-0.941044
2	6	0.743295	0.891176	-0.053415
3	6	1.033399	0.198994	1.077574
4	6	0.193369	-1.012653	1.452412
5	6	-0.856299	-1.296764	0.359012
6	6	-0.156323	-1.228324	-1.024860
7	1	2.575284	-0.368329	0.012080
8	1	-0.480651	0.885347	-1.865827
9	1	0.815652	-1.905486	1.617333
10	1	-0.292451	-0.817938	2.417852
11	1	0.870276	-1.614289	-1.090150
12	1	-0.736542	-1.682750	-1.826514
13	1	1.717320	0.614041	1.821081
14	6	1.361159	2.211196	-0.417674
15	1	1.782033	2.200451	-1.431848
16	1	0.585371	2.987316	-0.427369
17	1	2.132826	2.525028	0.292454
18	1	-1.454551	-2.181242	0.598229
19	6	-1.629923	0.012780	-0.051164
20	6	-2.043274	1.006314	1.037597
21	1	-2.825176	0.563988	1.665271
22	1	-1.226285	1.311465	1.694958
23	1	-2.465389	1.912322	0.588180
24	6	-2.864087	-0.284731	-0.919032
25	1	-3.663332	-0.705169	-0.298862
26	1	-3.245729	0.640154	-1.364832
27	1	-2.675948	-0.989541	-1.732127
28	7	3.507459	-0.785819	-0.344472
29	1	4.277986	-0.139899	-0.151412
30	1	3.687677	-1.675121	0.129617

31 1 3.448987 -0.950403 -1.353249

Figure S2c



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6196931 hartrees (-280881.35742025 kcal/mol)

Imaginary Frequencies: none

Zero-point correction = 0.282711 (Hartree/Particle)

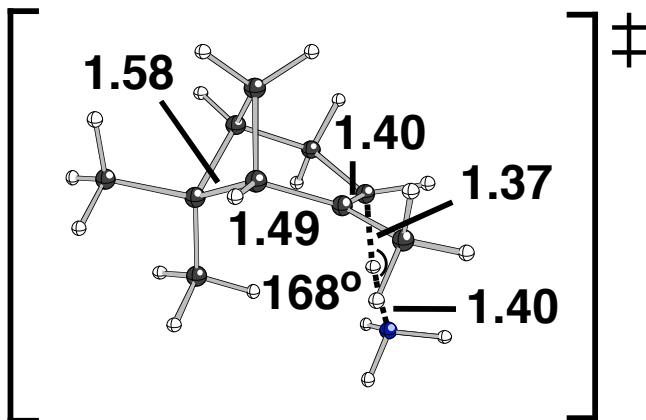
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5197345 hartrees (-280818.63339875 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.870898	0.838334	-0.618662
2	6	-0.498512	1.200518	-0.306134
3	6	-1.174748	0.537563	0.799866
4	6	-0.262119	-0.314923	1.719925
5	6	1.183608	-0.304015	1.199830
6	6	1.555788	1.143955	0.820118
7	1	-1.806391	1.259594	1.335022
8	1	1.281148	1.325988	-1.505083
9	1	-0.288969	0.101193	2.732502
10	1	-0.640703	-1.338649	1.791739
11	1	1.149749	1.964394	1.417653
12	1	2.615731	1.322379	0.643781

13	1	-1.964973	-0.108650	0.299141
14	6	-1.174666	2.274644	-1.068218
15	1	-2.178642	2.498899	-0.706131
16	1	-0.560759	3.186053	-1.033090
17	1	-1.209642	1.995164	-2.130536
18	1	1.859487	-0.837682	1.873737
19	6	1.246888	-0.675783	-0.321608
20	6	0.316960	-1.757634	-0.877600
21	1	0.626979	-2.737609	-0.498751
22	1	-0.734070	-1.621901	-0.616819
23	1	0.390524	-1.794459	-1.970019
24	6	2.678984	-0.968811	-0.795316
25	1	2.984239	-1.953558	-0.426192
26	1	2.727244	-0.994488	-1.888830
27	1	3.420171	-0.247347	-0.443989
28	7	-3.519621	-1.320669	-0.198475
29	1	-3.477108	-2.215123	0.286835
30	1	-4.381908	-0.870098	0.103325
31	1	-3.633253	-1.532508	-1.188176



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

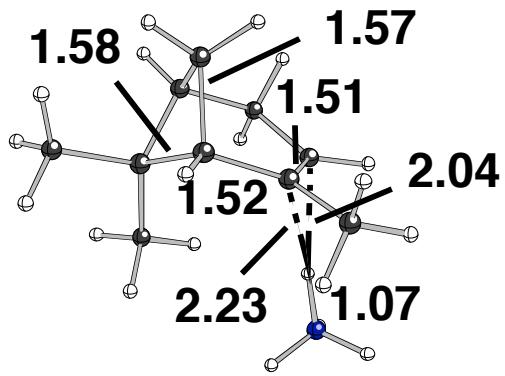
HF = -447.6139601 hartrees (-280877.75996275 kcal/mol)
 Imaginary Frequencies: 1 (-991.3226 1/cm)
 Zero-point correction = 0.280655 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5164618 hartrees (-280816.5797795 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.742293	0.923880	-0.564117
2	6	-0.708645	1.085722	-0.273400
3	6	-1.253765	0.377872	0.798412
4	6	-0.273664	-0.383705	1.709462
5	6	1.172716	-0.214657	1.202759
6	6	1.402880	1.273361	0.837823
7	1	-2.109292	0.863368	1.282348
8	1	1.067841	1.461801	-1.457790
9	1	-0.354172	0.016542	2.726955
10	1	-0.531840	-1.447960	1.780952
11	1	0.910987	2.035889	1.447911
12	1	2.450765	1.541058	0.712856
13	1	-2.086311	-0.510337	0.173787
14	6	-1.498690	2.060818	-1.076743
15	1	-2.538615	2.144025	-0.752729
16	1	-1.030447	3.051607	-1.000901
17	1	-1.460134	1.798374	-2.141852
18	1	1.887789	-0.694198	1.877714
19	6	1.288113	-0.543308	-0.328470
20	6	0.514307	-1.726627	-0.914107
21	1	0.964054	-2.668876	-0.582527
22	1	-0.536447	-1.749782	-0.623708
23	1	0.561782	-1.711435	-2.008935
24	6	2.748828	-0.664032	-0.796036
25	1	3.173118	-1.606559	-0.433663
26	1	2.801728	-0.675476	-1.890043
27	1	3.394834	0.141453	-0.441852
28	7	-3.059900	-1.440373	-0.196895
29	1	-2.940632	-2.315254	0.314198
30	1	-3.989441	-1.077184	0.016569
31	1	-3.022508	-1.650393	-1.194523



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6231209 hartrees (-280883.50836475 kcal/mol)

Imaginary Frequencies: none

Zero-point correction = 0.286198 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

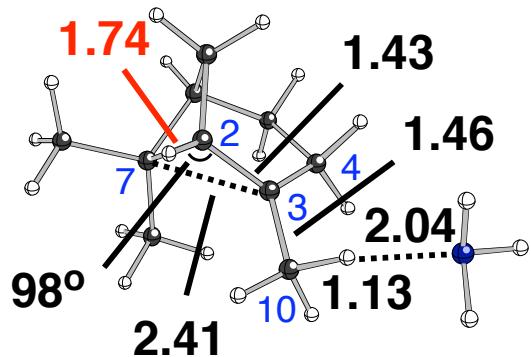
HF = -447.5261001 hartrees (-280822.62781275 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.580364	-0.670750	-0.856433
2	6	0.828147	-0.918028	-0.343591
3	6	1.031229	-0.744232	0.985120
4	6	-0.134755	-0.343837	1.874485
5	6	-1.437256	-0.256131	1.049646
6	6	-1.511879	-1.488373	0.104844
7	1	1.961368	-1.071018	1.456340
8	1	-0.666840	-0.817750	-1.937322
9	1	-0.248959	-1.100804	2.662031
10	1	0.062006	0.599706	2.403824
11	1	-1.119269	-2.438291	0.477612
12	1	-2.506899	-1.651599	-0.306579
13	1	2.239761	0.708873	0.228037
14	6	1.847677	-1.488358	-1.292115
15	1	2.805133	-1.703601	-0.804338
16	1	1.478085	-2.433636	-1.708471
17	1	2.015234	-0.832143	-2.157367
18	1	-2.298314	-0.035869	1.688182

19	6	-1.237060	0.626181	-0.237103
20	6	-0.428716	1.924744	-0.130280
21	1	-1.055901	2.730645	0.265183
22	1	0.427504	1.845002	0.545415
23	1	-0.082012	2.247387	-1.121699
24	6	-2.562698	0.969032	-0.940403
25	1	-3.139070	1.678188	-0.336086
26	1	-2.369316	1.440804	-1.910866
27	1	-3.196880	0.099542	-1.120508
28	7	3.007863	1.436219	0.055474
29	1	3.214433	1.929708	0.928522
30	1	3.858052	0.978121	-0.284136
31	1	2.680887	2.111706	-0.641113

Figure S2d



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6232654 hartrees (-280883.5990385 kcal/mol)

Imaginary Frequencies: none

Zero-point correction = 0.283401 (Hartree/Particle)

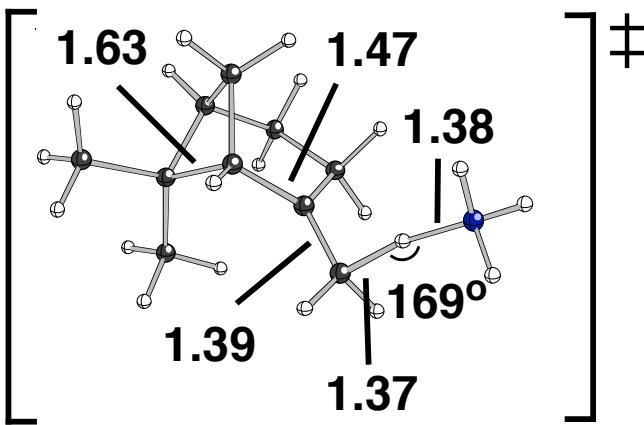
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.52281 hartrees (-280820.563275 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	6	-0.136170	-0.434588	0.873102
2	6	0.760719	-0.040371	-0.167936
3	6	0.617727	1.351888	-0.680388
4	6	-0.860294	1.869223	-0.626213
5	6	-1.688886	0.999081	0.323884
6	6	-0.841757	0.732310	1.595012
7	1	1.230194	1.958737	0.007948
8	1	0.107659	-1.363703	1.388440
9	1	-0.870622	2.907277	-0.284009
10	1	-1.283089	1.861059	-1.634960
11	1	-0.195710	1.546118	1.936305
12	1	-1.426392	0.375778	2.441270
13	1	1.071798	1.466470	-1.667782
14	6	1.767133	-0.941281	-0.711555
15	1	2.749213	-0.628290	-0.241480
16	1	1.611935	-1.987124	-0.436833
17	1	1.917086	-0.820803	-1.788627
18	1	-2.702292	1.390810	0.452486
19	6	-1.597107	-0.504155	-0.065703
20	6	-1.560616	-0.918069	-1.533974
21	1	-2.571093	-0.808565	-1.944761
22	1	-0.891723	-0.325972	-2.161677
23	1	-1.283722	-1.971678	-1.639599
24	6	-2.550639	-1.425871	0.696480
25	1	-3.550984	-1.308755	0.261827
26	1	-2.262217	-2.474437	0.578740
27	1	-2.626016	-1.204999	1.761820
28	7	4.641227	-0.283320	0.442915
29	1	4.738698	-0.228137	1.455003
30	1	5.201844	-1.077898	0.140019
31	1	5.086189	0.548353	0.059215



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6178312 hartrees (-280880.189078 kcal/mol)

Imaginary Frequencies: 1 (-947.2638 1/cm)

Zero-point correction = 0.281229 (Hartree/Particle)

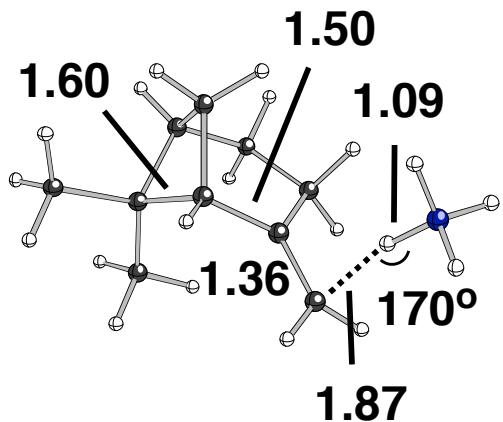
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5199103 hartrees (-280818.74371325 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.078051	-0.652836	-0.569339
2	6	-0.848345	0.030956	0.351641
3	6	-0.639183	1.515466	0.488488
4	6	0.829464	1.960109	0.204908
5	6	1.572587	0.896120	-0.614779
6	6	0.598475	0.314182	-1.674265
7	1	-1.294638	1.974844	-0.268165
8	1	-0.231923	-1.669753	-0.825428
9	1	0.818426	2.909128	-0.339316
10	1	1.348754	2.145195	1.149900
11	1	-0.124707	0.997772	-2.129537
12	1	1.102661	-0.234085	-2.468847
13	1	-1.004096	1.874248	1.455367
14	6	-1.871008	-0.636988	1.021208
15	1	-2.943434	-0.498846	0.181437
16	1	-1.817018	-1.727061	1.051424

17	1	-2.280083	-0.170474	1.919292
18	1	2.548651	1.258435	-0.950569
19	6	1.551098	-0.494021	0.105763
20	6	1.675475	-0.563053	1.629389
21	1	2.701226	-0.316188	1.924793
22	1	1.009408	0.116699	2.166961
23	1	1.470475	-1.578086	1.986863
24	6	2.521659	-1.508723	-0.513666
25	1	3.543978	-1.259256	-0.208006
26	1	2.306728	-2.520358	-0.153982
27	1	2.500953	-1.526416	-1.605169
28	7	-4.150786	-0.492813	-0.494993
29	1	-4.025005	-0.705488	-1.484998
30	1	-4.768719	-1.199997	-0.095332
31	1	-4.615769	0.412106	-0.417819



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6236452 hartrees (-280883.837363 kcal/mol)
 Imaginary Frequencies: none
 Zero-point correction = 0.286233 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

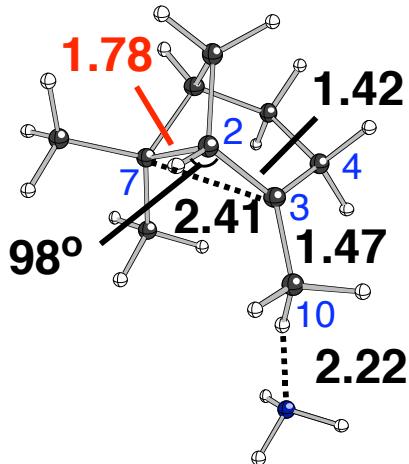
HF = -447.525938 hartrees (-280822.526095 kcal/mol)

Coordinates:

Center	Atomic	Coordinates (Angstroms)
--------	--------	-------------------------

Number	Number	X	Y	Z
1	6	0.051610	-0.770087	-0.301712
2	6	-0.854907	0.099605	0.515699
3	6	-0.665434	1.592450	0.290926
4	6	0.760785	1.960179	-0.219366
5	6	1.445734	0.749893	-0.873665
6	6	0.385036	-0.072730	-1.657591
7	1	-1.391092	1.901879	-0.474820
8	1	-0.251569	-1.823178	-0.292837
9	1	0.682391	2.777932	-0.943063
10	1	1.372964	2.333186	0.607099
11	1	-0.414431	0.482932	-2.161118
12	1	0.823898	-0.767066	-2.373369
13	1	-0.928337	2.151347	1.194355
14	6	-1.760257	-0.399949	1.395288
15	1	-3.112485	-0.493471	0.102515
16	1	-1.796856	-1.469381	1.601335
17	1	-2.284952	0.252661	2.092003
18	1	2.361912	1.043382	-1.395366
19	6	1.555626	-0.452711	0.129361
20	6	1.849103	-0.178603	1.606365
21	1	2.880887	0.170798	1.725098
22	1	1.193980	0.569501	2.059213
23	1	1.747250	-1.098907	2.192629
24	6	2.515239	-1.546424	-0.364883
25	1	3.550853	-1.210217	-0.243263
26	1	2.393861	-2.461135	0.225839
27	1	2.377529	-1.806893	-1.417040
28	7	-4.004654	-0.630702	-0.504611
29	1	-3.740208	-0.908847	-1.453778
30	1	-4.590480	-1.361688	-0.091125
31	1	-4.537735	0.242345	-0.544573

Figure S2e



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6213078 hartrees (-280882.3706445 kcal/mol)
 Imaginary Frequencies: none
 Zero-point correction = 0.283406 (Hartree/Particle)

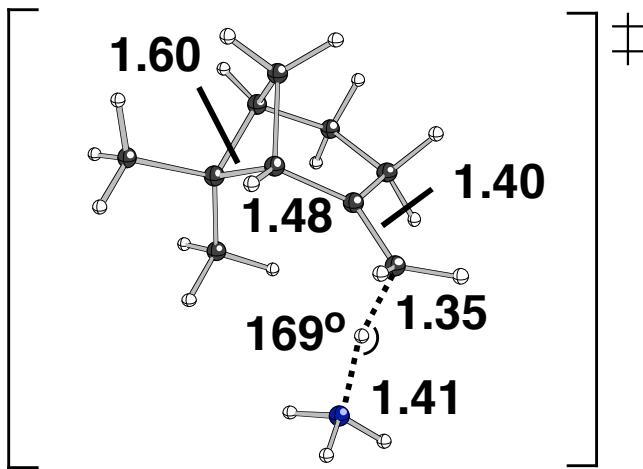
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5204003 hartrees (-280819.05118825 kcal/mol)

Coordinates:

Center	Atomic	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.865512	-0.268759	1.173404
2	6	-0.367174	-0.845670	0.767190
3	6	-0.345594	-1.690003	-0.461487
4	6	0.712924	-1.205759	-1.511165
5	6	1.722558	-0.264575	-0.847072
6	6	2.121017	-0.876854	0.518924
7	1	-0.057941	-2.692859	-0.103639
8	1	0.894322	0.172600	2.168631
9	1	1.234383	-2.070354	-1.929702
10	1	0.199875	-0.710499	-2.340402
11	1	2.194190	-1.967121	0.562324
12	1	3.030029	-0.451694	0.940722
13	1	-1.347099	-1.797218	-0.886221
14	6	-1.636452	-0.588289	1.459625
15	1	-2.112789	-1.554018	1.686414

16	1	-1.520646	-0.014172	2.380024
17	1	-2.360556	-0.095427	0.773762
18	1	2.523732	0.021595	-1.535427
19	6	1.008713	0.918523	-0.139400
20	6	-0.227025	1.557538	-0.758137
21	1	0.107129	2.181690	-1.596093
22	1	-0.964934	0.855394	-1.147640
23	1	-0.729161	2.218052	-0.044924
24	6	1.932176	2.006536	0.405356
25	1	2.240179	2.633670	-0.440975
26	1	1.406857	2.650637	1.116041
27	1	2.837147	1.627882	0.881048
28	7	-4.124981	0.617934	-0.373963
29	1	-4.805591	-0.138878	-0.413174
30	1	-4.535570	1.339475	0.216309
31	1	-4.078617	1.009573	-1.312761



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6168673 hartrees (-280879.58423075 kcal/mol)

Imaginary Frequencies: 1 (-896.9959 1/cm)

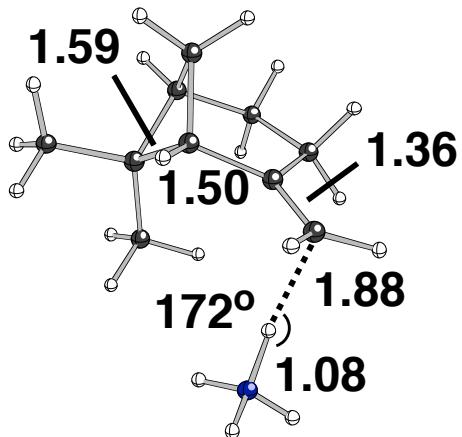
Zero-point correction = 0.281255 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5188296 hartrees (-280818.065574 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.352432	-0.013998	-1.079742
2	6	0.685246	-0.895768	-0.507287
3	6	0.254186	-1.762257	0.645825
4	6	-1.089421	-1.350117	1.310480
5	6	-1.859566	-0.361706	0.422222
6	6	-1.714281	-0.801368	-1.057928
7	1	0.162827	-2.768995	0.209285
8	1	-0.035980	0.483973	-1.999876
9	1	-1.697879	-2.244047	1.477477
10	1	-0.906287	-0.912945	2.297135
11	1	-1.678596	-1.871765	-1.276868
12	1	-2.434118	-0.333062	-1.727628
13	1	1.071254	-1.858278	1.370532
14	6	1.994106	-0.933917	-0.988809
15	1	2.154770	-0.579639	-2.008715
16	1	2.648484	0.033083	-0.314147
17	1	2.606016	-1.791868	-0.700943
18	1	-2.864785	-0.173691	0.810235
19	6	-0.989010	0.893503	0.079475
20	6	-0.058885	1.477688	1.146988
21	1	-0.649863	1.931053	1.950158
22	1	0.602165	0.740109	1.612944
23	1	0.557520	2.276629	0.716184
24	6	-1.811976	2.039476	-0.527010
25	1	-2.394377	2.527184	0.262548
26	1	-1.157291	2.796402	-0.972652
27	1	-2.515201	1.713004	-1.295843
28	7	3.548424	0.957279	0.250330
29	1	3.056448	1.653126	0.810639
30	1	4.227701	0.486163	0.848204
31	1	4.060427	1.443396	-0.486257



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6239681 hartrees (-280884.03998275 kcal/mol)

Imaginary Frequencies: none

Zero-point correction = 0.286591 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

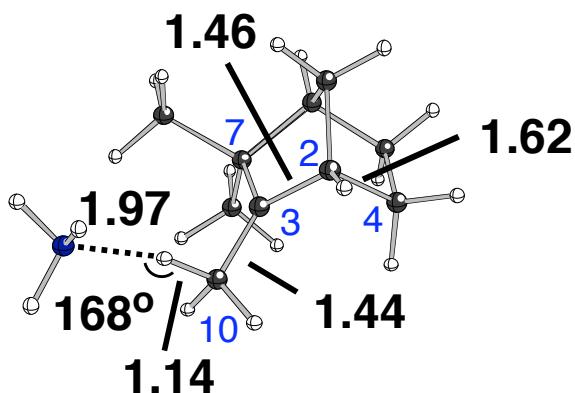
HF = -447.5261063 hartrees (-280822.63170325 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.366010	-0.062526	-1.079869
2	6	0.675466	-0.982998	-0.517261
3	6	0.226616	-1.796490	0.690016
4	6	-1.065921	-1.269059	1.380170
5	6	-1.825859	-0.290430	0.471010
6	6	-1.747421	-0.795973	-0.996224
7	1	0.044480	-2.810673	0.312772
8	1	-0.060214	0.380618	-2.033479
9	1	-1.714466	-2.117286	1.620878
10	1	-0.827661	-0.788853	2.335700
11	1	-1.754305	-1.875933	-1.166227
12	1	-2.485233	-0.337668	-1.654102
13	1	1.048466	-1.907440	1.406387
14	6	1.899056	-1.144217	-1.081116
15	1	2.119598	-0.704389	-2.053104
16	1	2.791015	0.238783	-0.172552

17	1	2.577934	-1.920807	-0.728586
18	1	-2.809325	-0.043960	0.883239
19	6	-0.919403	0.914069	0.040455
20	6	0.058197	1.506761	1.062633
21	1	-0.486862	2.009458	1.868855
22	1	0.704247	0.758032	1.534868
23	1	0.679286	2.278417	0.581759
24	6	-1.726970	2.069554	-0.571518
25	1	-2.268634	2.607767	0.214317
26	1	-1.065227	2.787368	-1.070744
27	1	-2.463496	1.737027	-1.305774
28	7	3.415046	1.008009	0.261997
29	1	2.806083	1.686204	0.730694
30	1	4.059649	0.597338	0.942780
31	1	3.952834	1.477785	-0.471429

Figure S2f



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6402675 hartrees (-280894.26785625 kcal/mol)
 Imaginary Frequencies: none
 Zero-point correction = 0.284312 (Hartree/Particle)

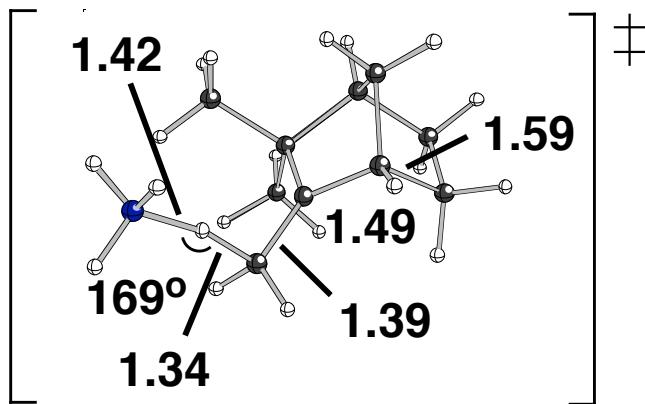
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5415142 hartrees (-280832.3001605 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	6	0.370142	-1.432798	0.204796
2	6	-0.326044	-0.298641	-0.396310
3	6	1.667160	-1.452671	-0.765306
4	6	2.536507	-0.283371	-0.235827
5	6	1.600663	0.386608	0.798428
6	6	1.007027	-0.856875	1.492387
7	1	2.115887	-2.438713	-0.616173
8	1	-0.157121	-2.386490	0.222845
9	1	3.432249	-0.659918	0.264562
10	1	2.868022	0.388318	-1.029257
11	1	1.767917	-1.526404	1.900996
12	1	0.277208	-0.646705	2.276265
13	1	1.410603	-1.371971	-1.825137
14	6	-1.466952	-0.396449	-1.272187
15	1	-1.533679	-1.357925	-1.789209
16	1	-2.378963	-0.394924	-0.580842
17	1	-1.597789	0.447975	-1.951414
18	1	2.084618	1.120647	1.445397
19	6	0.350117	0.967944	0.047318
20	6	0.656165	1.952082	-1.101965
21	1	1.287155	2.759473	-0.718253
22	1	1.181300	1.481579	-1.936231
23	1	-0.259141	2.405725	-1.491022
24	6	-0.616301	1.684747	1.051286
25	1	-0.092758	2.562061	1.441536
26	1	-1.519288	2.023007	0.537428
27	1	-0.911812	1.060927	1.896548
28	7	-4.156955	-0.500290	0.261726
29	1	-4.380603	0.240878	0.923272
30	1	-4.849895	-0.445747	-0.482932
31	1	-4.316126	-1.383217	0.743820



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6368558 hartrees (-280892.1270145 kcal/mol)

Imaginary Frequencies: 1 (-833.6668 1/cm)

Zero-point correction = 0.282110 (Hartree/Particle)

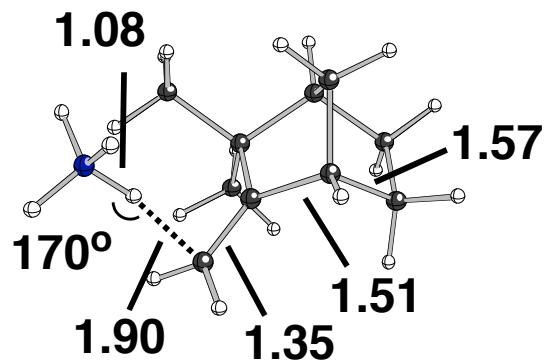
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5398697 hartrees (-280831.26823675 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.377965	-1.445314	0.094694
2	6	-0.384083	-0.297666	-0.462866
3	6	1.725814	-1.431489	-0.742243
4	6	2.507149	-0.222317	-0.149458
5	6	1.486805	0.392179	0.837839
6	6	0.880521	-0.889194	1.451629
7	1	2.230621	-2.385330	-0.565793
8	1	-0.134290	-2.408985	0.068847
9	1	3.391177	-0.559997	0.397973
10	1	2.853441	0.475629	-0.913703
11	1	1.627494	-1.543541	1.908930
12	1	0.084273	-0.717334	2.180034
13	1	1.547026	-1.352537	-1.818147
14	6	-1.502390	-0.389081	-1.284995
15	1	-1.659406	-1.339789	-1.799439
16	1	-2.519313	-0.469213	-0.416862
17	1	-1.787092	0.492463	-1.861276

18	1	1.916594	1.109087	1.541006
19	6	0.263213	0.981940	0.049014
20	6	0.623845	1.957166	-1.092860
21	1	1.250481	2.762567	-0.696990
22	1	1.168490	1.474767	-1.907371
23	1	-0.274099	2.415791	-1.517345
24	6	-0.707141	1.716490	1.016911
25	1	-0.205235	2.606287	1.408076
26	1	-1.604870	2.049760	0.486290
27	1	-1.010090	1.104599	1.870441
28	7	-3.754953	-0.585955	0.281362
29	1	-3.899758	0.200340	0.914678
30	1	-4.529226	-0.602755	-0.383012
31	1	-3.791735	-1.446406	0.828143



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6445546 hartrees (-280896.9580115 kcal/mol)

Imaginary Frequencies: none

Zero-point correction = 0.287209 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

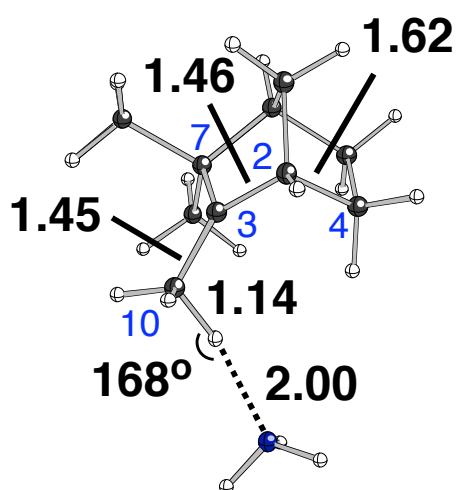
HF = -447.547846 hartrees (-280836.273365 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.409551	-1.452947	0.064491
2	6	0.360965	-0.277852	0.617406

3	6	-1.841633	-1.367208	0.693615
4	6	-2.489597	-0.161599	-0.057626
5	6	-1.333453	0.355423	-0.947644
6	6	-0.697990	-0.985898	-1.383384
7	1	-2.375424	-2.302062	0.499044
8	1	0.070390	-2.424912	0.207132
9	1	-3.317369	-0.494539	-0.690292
10	1	-2.892038	0.595973	0.617186
11	1	-1.400516	-1.643037	-1.903893
12	1	0.195870	-0.882849	-2.007473
13	1	-1.804231	-1.231524	1.777910
14	6	1.327469	-0.327662	1.561560
15	1	1.560949	-1.263337	2.068931
16	1	2.690064	-0.549684	0.255482
17	1	1.734212	0.580203	2.004928
18	1	-1.657157	1.020690	-1.752314
19	6	-0.196698	0.986625	-0.066341
20	6	-0.678021	2.035655	0.956603
21	1	-1.235171	2.830851	0.450045
22	1	-1.323304	1.604922	1.725124
23	1	0.172012	2.501239	1.465964
24	6	0.868288	1.658919	-0.967656
25	1	0.438993	2.536400	-1.461443
26	1	1.718432	2.011754	-0.370050
27	1	1.234345	0.994897	-1.759334
28	7	3.587590	-0.657131	-0.338346
29	1	3.605080	0.075317	-1.053816
30	1	4.413013	-0.566123	0.260799
31	1	3.600045	-1.574993	-0.791651

Figure S2g



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6396485 hartrees (-280893.87943375 kcal/mol)

Imaginary Frequencies: none

Zero-point correction = 0.284440 (Hartree/Particle)

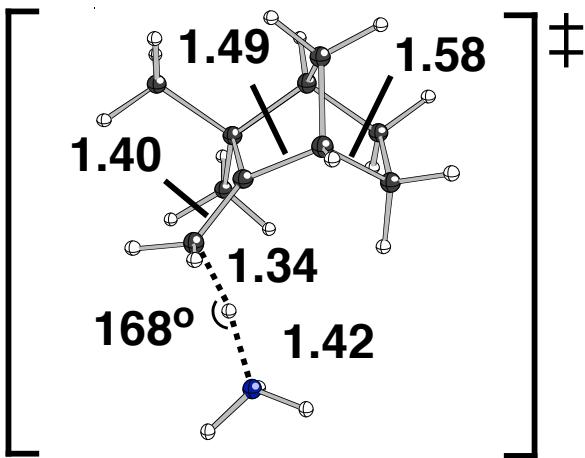
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5407623 hartrees (-280831.82834325 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.338435	-1.014593	-1.144382
2	6	0.163882	0.297741	-0.739707
3	6	0.117869	-1.879003	0.143446
4	6	-0.911809	-1.484020	1.234252
5	6	-1.715604	-0.354970	0.544291
6	6	-1.863266	-0.937720	-0.876305
7	1	0.038282	-2.922284	-0.174240
8	1	0.034481	-1.420233	-2.084492
9	1	-1.574164	-2.321261	1.468255
10	1	-0.439451	-1.175036	2.168010
11	1	-2.321239	-1.929850	-0.890675
12	1	-2.395172	-0.303889	-1.587680
13	1	1.158562	-1.701952	0.426294
14	6	1.408060	0.889515	-1.175392
15	1	1.657174	0.640102	-2.211042
16	1	1.475489	1.962388	-0.982709
17	1	-2.639368	-0.074100	1.053326
18	6	-0.762703	0.865743	0.292252
19	6	-0.053964	1.446087	1.532971
20	1	-0.809140	1.765809	2.257213
21	1	0.598391	0.719831	2.022384
22	1	0.547498	2.321741	1.274617
23	6	-1.536777	2.038158	-0.411798
24	1	-2.310755	2.379154	0.281860
25	1	-0.862931	2.873430	-0.615861
26	1	-2.020951	1.750949	-1.346206
27	1	2.238948	0.416947	-0.557672
28	7	3.952143	-0.193918	0.271380

29	1	4.658794	0.434412	-0.107804
30	1	4.014792	-0.122113	1.285292
31	1	4.242235	-1.138253	0.023694



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6357515 hartrees (-280891.43406625 kcal/mol)
 Imaginary Frequencies: 1 (-840.4048 1/cm)
 Zero-point correction = 0.282176 (Hartree/Particle)

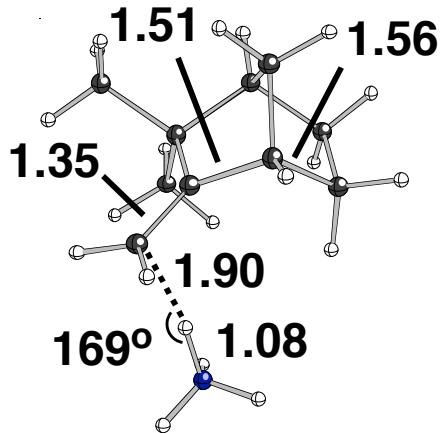
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5386632 hartrees (-280830.511158 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.371828	-1.083282	-1.072437
2	6	0.306796	0.200205	-0.742373
3	6	-0.228986	-1.970579	0.227624
4	6	-1.231903	-1.322670	1.228901
5	6	-1.735596	-0.084345	0.450585
6	6	-1.868644	-0.678983	-0.969288
7	1	-0.504345	-2.995694	-0.035020
8	1	-0.025752	-1.573606	-1.983765
9	1	-2.068293	-1.996791	1.431393
10	1	-0.779240	-1.083294	2.193296

11	1	-2.524528	-1.552709	-1.014322
12	1	-2.184485	0.028232	-1.738744
13	1	0.798714	-2.002011	0.603662
14	6	1.553808	0.606239	-1.207217
15	1	1.895262	0.159304	-2.143388
16	1	1.819710	1.657325	-1.081711
17	1	-2.634772	0.372911	0.868802
18	6	-0.571527	0.947666	0.251026
19	6	0.185953	1.356332	1.531881
20	1	-0.517199	1.787324	2.251068
21	1	0.680818	0.511731	2.018937
22	1	0.939942	2.119175	1.314229
23	6	-1.102917	2.246737	-0.423601
24	1	-1.788438	2.743138	0.269937
25	1	-0.282705	2.935892	-0.643225
26	1	-1.642909	2.058521	-1.353503
27	1	2.444908	0.046589	-0.381498
28	7	3.587005	-0.418135	0.324994
29	1	3.705942	-1.425944	0.221484
30	1	4.423198	0.036275	-0.043313
31	1	3.524196	-0.203337	1.320110



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6436494 hartrees (-280896.3899985 kcal/mol)
 Imaginary Frequencies: none
 Zero-point correction = 0.287235 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

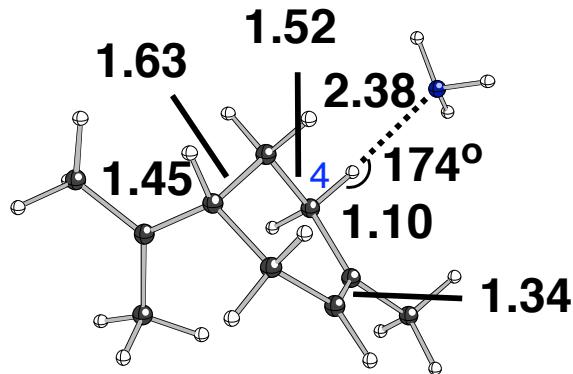
HF = -447.5467638 hartrees (-280835.5942845 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.436722	-1.077047	-1.092544
2	6	0.292075	0.218182	-0.821832
3	6	-0.260226	-2.000960	0.155085
4	6	-1.164377	-1.328322	1.237142
5	6	-1.669954	-0.054437	0.519079
6	6	-1.905374	-0.614730	-0.903408
7	1	-0.598438	-3.012676	-0.086712
8	1	-0.176962	-1.550597	-2.041944
9	1	-2.013654	-1.971733	1.483624
10	1	-0.642561	-1.130187	2.176382
11	1	-2.610163	-1.451224	-0.924270
12	1	-2.225710	0.125633	-1.639720
13	1	0.788738	-2.088509	0.467920
14	6	1.398683	0.661960	-1.458779
15	1	1.793928	0.127929	-2.322166
16	1	1.782023	1.668130	-1.291970
17	1	-2.532586	0.410366	1.002608
18	6	-0.499380	0.961153	0.274357
19	6	0.355367	1.272720	1.520167
20	1	-0.268169	1.690488	2.317305
21	1	0.846059	0.382993	1.931585
22	1	1.121591	2.020775	1.285608
23	6	-1.050422	2.303088	-0.267260
24	1	-1.655569	2.790646	0.504071
25	1	-0.235876	2.983099	-0.535761
26	1	-1.675921	2.171296	-1.152762
27	1	2.616670	-0.129405	-0.236029
28	7	3.453199	-0.475861	0.352285
29	1	4.322234	-0.071206	-0.007984
30	1	3.322857	-0.187442	1.326147
31	1	3.511092	-1.496994	0.306031

Figure S3

A-NH₃



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.622977 hartrees (-280883.4180675 kcal/mol)

Imaginary Frequencies: none

Zero-point correction = 0.280409 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

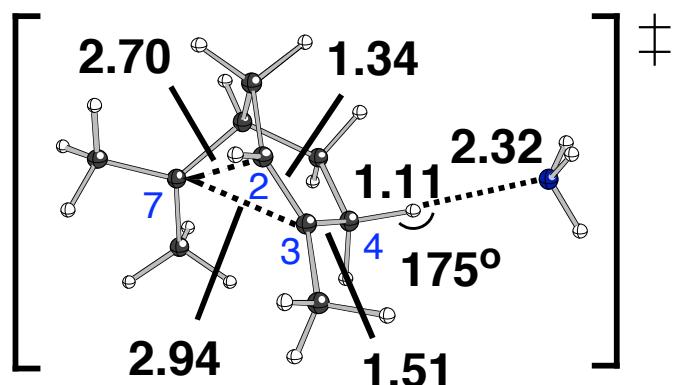
HF = -447.5136424 hartrees (-280814.810606 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.151475	-0.470530	-0.226992
2	6	2.896971	-1.732574	-0.405146
3	6	2.282918	0.566758	-1.261499
4	6	1.317154	-0.287673	0.946936
5	6	-0.062172	-1.068047	0.583626
6	6	-0.950430	-0.320279	-0.400928
7	6	-1.045553	1.166414	-0.136303
8	6	-0.176716	1.795154	0.671576
9	6	-2.170395	1.888479	-0.830351
10	6	0.972704	1.143967	1.403673
11	1	2.679000	-2.170492	-1.388540
12	1	2.732554	-2.461922	0.388235
13	1	3.969756	-1.481120	-0.447055
14	1	2.699441	0.201174	-2.200864
15	1	2.983531	1.314633	-0.844831
16	1	1.350012	1.120653	-1.404485
17	1	1.742872	-0.881153	1.764281
18	1	-0.545963	-1.130768	1.563620
19	1	0.149019	-2.089099	0.256729

20	1	-1.953469	-0.772113	-0.323964
21	1	-0.633942	-0.493701	-1.441773
22	1	-0.296572	2.861125	0.854063
23	1	-2.125886	1.738279	-1.916736
24	1	-2.146313	2.963107	-0.633497
25	1	-3.140450	1.498298	-0.500340
26	1	0.743935	1.089376	2.476701
27	1	1.867091	1.777487	1.337970
28	7	-4.031649	-1.869578	0.030691
29	1	-3.989458	-2.874731	0.186085
30	1	-4.570193	-1.480330	0.801936
31	1	-4.589152	-1.731673	-0.809932

TS(S1)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6167605 hartrees (-280879.51721375 kcal/mol)
 Imaginary Frequencies: 1 (-64.9756 1/cm)
 Zero-point correction = 0.280929 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

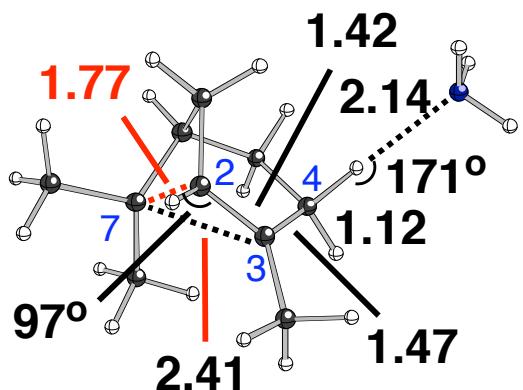
HF = -447.5086041 hartrees (-280811.64907275 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.950616	-0.333550	-0.268626

2	6	1.998688	-0.283083	-1.744252
3	6	3.121585	0.226930	0.440538
4	6	0.928424	-1.189402	0.432123
5	6	-0.344415	-1.442073	-0.398174
6	6	-1.090213	-0.115606	-0.713677
7	6	-0.605072	1.071828	0.074166
8	6	0.093760	0.915216	1.232370
9	6	-1.014285	2.428600	-0.425717
10	6	0.527723	-0.451237	1.721732
11	1	1.042829	0.037769	-2.171944
12	1	2.127204	-1.318374	-2.104316
13	1	2.810897	0.333371	-2.130045
14	1	3.389623	1.212504	0.045905
15	1	3.970361	-0.427931	0.169606
16	1	3.044708	0.252350	1.524409
17	1	1.432541	-2.153453	0.634946
18	1	-0.984560	-2.102450	0.192930
19	1	-0.122933	-1.986229	-1.321499
20	1	-2.163707	-0.252007	-0.492121
21	1	-1.054515	0.123966	-1.785443
22	1	0.312247	1.786332	1.846435
23	1	-0.634109	2.606425	-1.439785
24	1	-0.661299	3.233001	0.223718
25	1	-2.107414	2.492482	-0.491846
26	1	-0.273967	-0.985695	2.245915
27	1	1.353180	-0.373923	2.431777
28	7	-4.374992	-0.725469	0.034750
29	1	-4.594828	-1.716476	0.111453
30	1	-4.714570	-0.286942	0.888397
31	1	-4.947599	-0.362167	-0.724651

B-NH₃



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6226497 hartrees (-280883.21268675 kcal/mol)

Imaginary Frequencies: none

Zero-point correction = 0.282983 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

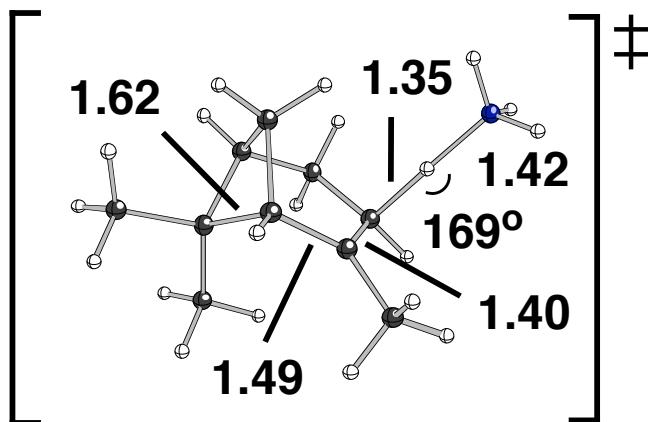
HF = -447.521906 hartrees (-280819.996015 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.375510	0.174626	-1.120775
2	6	0.393632	1.030808	-0.285074
3	6	1.156676	0.410623	0.810588
4	6	0.4666570	-0.874216	1.383819
5	6	-0.616357	-1.364818	0.419089
6	6	-0.028709	-1.321603	-1.014056
7	1	2.129485	0.106964	0.340354
8	1	-0.767944	0.608930	-2.039550
9	1	1.214878	-1.657983	1.528393
10	1	0.043096	-0.648694	2.367167
11	1	1.033142	-1.562328	-1.108851
12	1	-0.591030	-1.910739	-1.736460
13	1	1.419456	1.137114	1.585031
14	6	0.405890	2.500195	-0.476581
15	1	1.436756	2.796439	-0.724520
16	1	-0.251564	2.835794	-1.280084
17	1	0.167054	3.022230	0.457507
18	1	-1.072468	-2.299134	0.760556
19	6	-1.620953	-0.231843	0.070927
20	6	-2.050789	0.769391	1.135858
21	1	-2.764940	0.266698	1.799180
22	1	-1.241372	1.145804	1.763213
23	1	-2.572939	1.622700	0.691893
24	6	-2.836515	-0.664677	-0.747085
25	1	-3.539117	-1.157992	-0.063609
26	1	-3.350672	0.199366	-1.177503
27	1	-2.607501	-1.368261	-1.547932
28	7	4.084563	-0.540120	-0.246711
29	1	4.725173	0.249920	-0.192380

30	1	4.428315	-1.231626	0.417394
31	1	4.206647	-0.945269	-1.173078

TS(S2)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6178322 hartrees (-280880.1897055 kcal/mol)
 Imaginary Frequencies: 1 (-873.1894 1/cm)
 Zero-point correction = 0.280547 (Hartree/Particle)

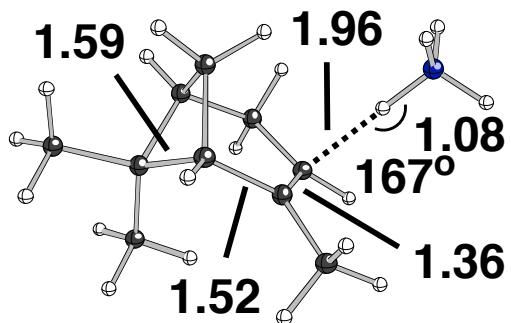
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5202598 hartrees (-280818.9630245 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.463225	0.413379	-0.969840
2	6	0.624724	0.996860	-0.142659
3	6	1.195094	0.185337	0.839698
4	6	0.436653	-1.098158	1.223670
5	6	-0.712491	-1.351708	0.231259
6	6	-0.180324	-1.102690	-1.204931
7	1	2.306713	-0.213780	0.180745
8	1	-0.759863	1.044165	-1.811042
9	1	1.109393	-1.965446	1.243686

10	1	0.052558	-0.989542	2.244663
11	1	0.852975	-1.387786	-1.425545
12	1	-0.822222	-1.510191	-1.983827
13	1	1.732137	0.705976	1.638899
14	6	1.055970	2.401681	-0.377350
15	1	1.322706	2.558742	-1.429874
16	1	0.199357	3.064377	-0.188681
17	1	1.880170	2.712431	0.268462
18	1	-1.224385	-2.294949	0.442449
19	6	-1.613250	-0.078305	0.053537
20	6	-1.944199	0.784041	1.274495
21	1	-2.632725	0.239445	1.930031
22	1	-1.075674	1.063194	1.876490
23	1	-2.452188	1.705804	0.970063
24	6	-2.917053	-0.370189	-0.704287
25	1	-3.611910	-0.897124	-0.041155
26	1	-3.398899	0.563419	-1.012723
27	1	-2.782618	-0.987652	-1.594635
28	7	3.544805	-0.767330	-0.234584
29	1	4.054716	-1.134257	0.569449
30	1	3.416830	-1.530129	-0.899475
31	1	4.127897	-0.056879	-0.677440



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6259329 hartrees (-280885.27289475 kcal/mol)
 Imaginary Frequencies: none
 Zero-point correction = 0.285955 (Hartree/Particle)

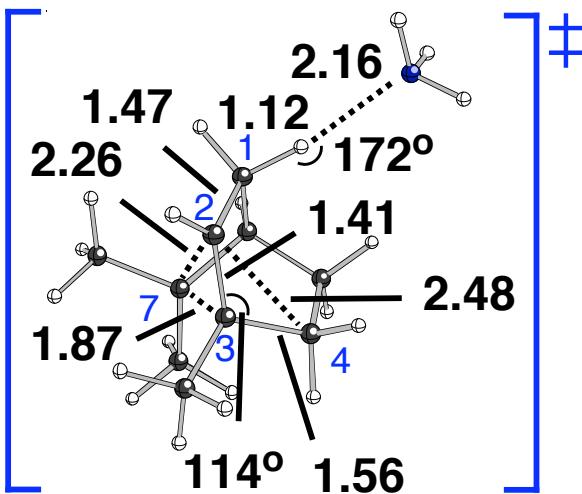
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5288985 hartrees (-280824.38380875 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.344577	0.317143	-0.941044
2	6	0.743295	0.891176	-0.053415
3	6	1.033399	0.198994	1.077574
4	6	0.193369	-1.012653	1.452412
5	6	-0.856299	-1.296764	0.359012
6	6	-0.156323	-1.228324	-1.024860
7	1	2.575284	-0.368329	0.012080
8	1	-0.480651	0.885347	-1.865827
9	1	0.815652	-1.905486	1.617333
10	1	-0.292451	-0.817938	2.417852
11	1	0.870276	-1.614289	-1.090150
12	1	-0.736542	-1.682750	-1.826514
13	1	1.717320	0.614041	1.821081
14	6	1.361159	2.211196	-0.417674
15	1	1.782033	2.200451	-1.431848
16	1	0.585371	2.987316	-0.427369
17	1	2.132826	2.525028	0.292454
18	1	-1.454551	-2.181242	0.598229
19	6	-1.629923	0.012780	-0.051164
20	6	-2.043274	1.006314	1.037597
21	1	-2.825176	0.563988	1.665271
22	1	-1.226285	1.311465	1.694958
23	1	-2.465389	1.912322	0.588180
24	6	-2.864087	-0.284731	-0.919032
25	1	-3.663332	-0.705169	-0.298862
26	1	-3.245729	0.640154	-1.364832
27	1	-2.675948	-0.989541	-1.732127
28	7	3.507459	-0.785819	-0.344472
29	1	4.277986	-0.139899	-0.151412
30	1	3.687677	-1.675121	0.129617
31	1	3.448987	-0.950403	-1.353249

TS(S3)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.608249 hartrees (-280874.1762475 kcal/mol)
 Imaginary Frequencies: 1 (-269.1714 1/cm)
 Zero-point correction = 0.282619 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

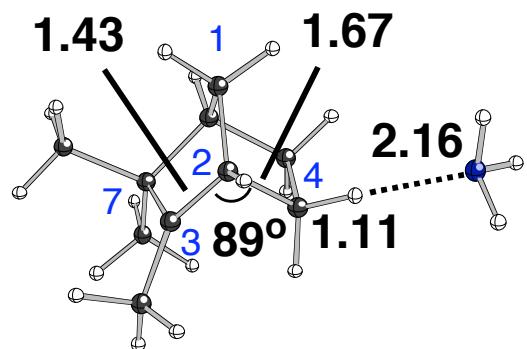
HF = -447.5074278 hartrees (-280810.9109445 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.267505	0.388307	-1.260598
2	6	-0.629705	0.992989	-0.356287
3	6	0.012465	1.337963	1.020095
4	6	0.599355	0.037278	1.630305
5	6	0.304191	-1.035322	0.570558
6	6	1.107779	-0.687193	-0.702976
7	1	0.777830	2.101041	0.853032
8	1	0.216419	0.584255	-2.333559
9	1	1.672674	0.118116	1.814806
10	1	0.125957	-0.203012	2.585252
11	1	2.157684	-0.351385	-0.514598
12	1	1.201765	-1.510777	-1.419157
13	1	-0.752761	1.794610	1.651795

14	6	-1.688135	1.942893	-0.871987
15	1	-1.272317	2.951511	-0.973213
16	1	-2.078896	1.638955	-1.847176
17	1	-2.524606	2.012600	-0.170999
18	1	0.453837	-2.057884	0.928073
19	6	-1.151880	-0.747433	0.084671
20	6	-2.247171	-0.596990	1.127919
21	1	-2.388997	-1.590817	1.576252
22	1	-2.024186	0.095990	1.937278
23	1	-3.199445	-0.315115	0.671565
24	6	-1.680884	-1.605689	-1.064994
25	1	-2.025403	-2.558372	-0.646772
26	1	-2.548300	-1.134931	-1.537113
27	1	-0.950512	-1.836409	-1.841666
28	7	4.264195	0.000511	-0.189241
29	1	4.660061	-0.702423	0.432370
30	1	4.741365	-0.106215	-1.082792
31	1	4.547353	0.905864	0.181075

D-NH₃



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.637174 hartrees (-280892.326685 kcal/mol)

Imaginary Frequencies: none

Zero-point correction = 0.284368 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

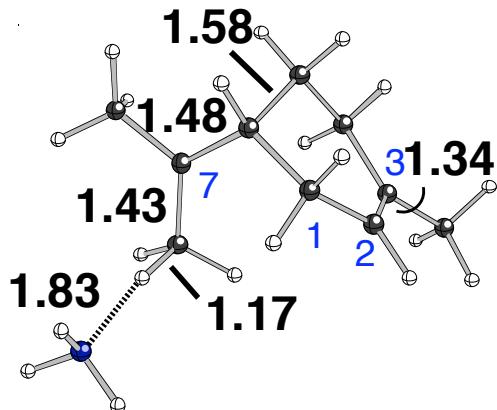
HF = -447.5387705 hartrees (-280830.57848875 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.582138	0.495031	-0.857920
2	6	-0.625720	0.931048	-0.227463
3	6	1.216870	0.157920	0.652467
4	6	0.661508	-1.243337	0.967508
5	6	-0.427614	-1.413502	-0.117674
6	6	0.339525	-0.933157	-1.367189
7	1	2.299571	0.212617	0.426514
8	1	1.197797	1.208389	-1.401483
9	1	1.438385	-2.002253	0.840652
10	1	0.282577	-1.327270	1.986971
11	1	1.273366	-1.475639	-1.530134
12	1	-0.233581	-0.948715	-2.296485
13	1	1.008558	0.912022	1.417447
14	6	-0.975056	2.335225	0.071823
15	1	-0.130801	3.016099	-0.050687
16	1	-1.742433	2.626710	-0.663560
17	1	-1.431803	2.457742	1.057460
18	1	-0.877504	-2.405961	-0.175588
19	6	-1.478886	-0.267142	0.095842
20	6	-2.154843	-0.229809	1.478943
21	1	-2.638224	-1.192203	1.671474
22	1	-1.450509	-0.039764	2.292276
23	1	-2.931314	0.539118	1.518982
24	6	-2.602002	-0.323066	-0.995648
25	1	-3.145945	-1.262962	-0.866139
26	1	-3.309364	0.499025	-0.859826
27	1	-2.226988	-0.287361	-2.019947
28	7	4.424175	0.239782	0.051654
29	1	4.862136	-0.400471	0.711516
30	1	4.760757	-0.024343	-0.872316
31	1	4.810574	1.161483	0.247160

Figure S4.

A-NH₃



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6332889 hartrees (-280889.88878475 kcal/mol)

Imaginary Frequencies: none

Zero-point correction = 0.281248 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

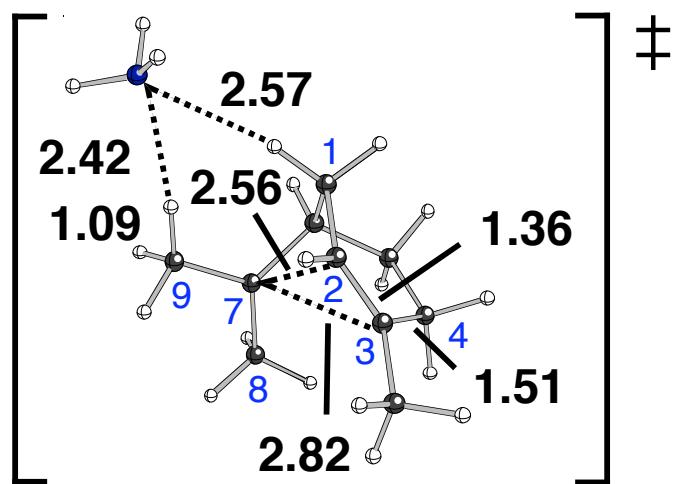
HF = -447.5250814 hartrees (-280821.9885785 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.137717	0.863669	-0.218474
2	6	-1.798582	2.163302	-0.502231
3	6	-1.422196	-0.249319	-1.069021
4	6	-0.237496	0.773226	0.952699
5	6	1.082522	1.585326	0.621885
6	6	1.960016	0.875766	-0.412664
7	6	2.114375	-0.610187	-0.159962
8	6	1.292794	-1.263957	0.676667
9	6	3.235613	-1.294737	-0.896243
10	6	0.149003	-0.636459	1.439498
11	1	-1.292912	2.616852	-1.369234
12	1	-1.757607	2.867778	0.329550
13	1	-2.835595	2.009717	-0.821959
14	1	-0.654713	-1.024926	-1.083051
15	1	-1.803168	0.016557	-2.058158
16	1	-2.339754	-0.762151	-0.549355

17	1	-0.725856	1.336395	1.760338
18	1	1.611576	1.652619	1.577886
19	1	0.845642	2.607345	0.313263
20	1	2.950189	1.349053	-0.402355
21	1	1.579586	1.037152	-1.433722
22	1	1.452573	-2.325789	0.854171
23	1	3.148410	-1.141481	-1.979640
24	1	3.249951	-2.370536	-0.704572
25	1	4.207496	-0.881823	-0.598858
26	1	0.414729	-0.555236	2.502632
27	1	-0.726192	-1.298403	1.416832
28	7	-3.787408	-1.770067	-0.058889
29	1	-3.522133	-2.753559	-0.050485
30	1	-4.181906	-1.557918	0.855928
31	1	-4.538449	-1.670956	-0.739906

TS(S4)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6193456 hartrees (-280881.139364 kcal/mol)
 Imaginary Frequencies: 1 (-59.2103 1/cm)
 Zero-point correction = 0.281610 (Hartree/Particle)

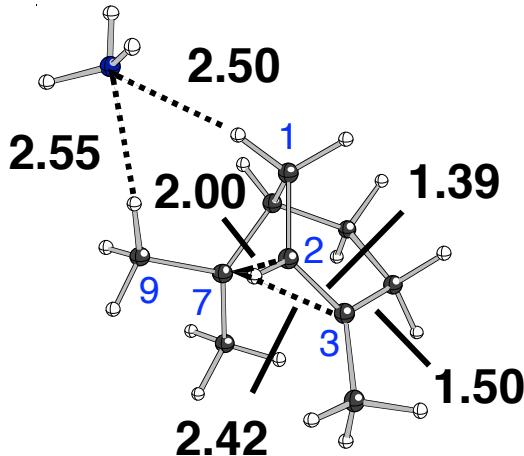
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5121406 hartrees (-280813.8682265 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.239845	1.205177	-0.362807
2	6	0.794762	2.070373	-0.975190
3	6	-1.537162	1.139227	-1.073058
4	6	-0.126088	0.745166	1.074218
5	6	1.319363	0.716954	1.593896
6	6	2.192563	-0.278918	0.768655
7	6	1.423392	-1.075015	-0.260017
8	6	0.092906	-1.316207	-0.089586
9	6	2.204259	-1.652171	-1.404433
10	6	-0.674810	-0.695849	1.061138
11	1	1.817769	1.745902	-0.780902
12	1	0.697508	3.048250	-0.467921
13	1	0.637528	2.231708	-2.042443
14	1	-1.397979	0.986631	-2.147725
15	1	-1.957042	2.159123	-0.979885
16	1	-2.271379	0.441879	-0.664088
17	1	-0.734600	1.433271	1.686231
18	1	1.283615	0.413788	2.643299
19	1	1.769173	1.714452	1.583875
20	1	2.667284	-0.996947	1.451018
21	1	3.030007	0.234204	0.280663
22	1	-0.422327	-1.987210	-0.773619
23	1	2.692074	-0.860741	-1.987985
24	1	1.578356	-2.245721	-2.074584
25	1	3.010311	-2.294553	-1.027774
26	1	-0.490159	-1.201976	2.016555
27	1	-1.750283	-0.731387	0.878462
28	7	-4.177012	-0.878982	0.031615
29	1	-4.180565	-1.897454	0.013991
30	1	-4.641243	-0.609037	0.897249
31	1	-4.794997	-0.583739	-0.722608

B-NH₃



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6206168 hartrees (-280881.937042 kcal/mol)
 Imaginary Frequencies: none
 Zero-point correction = 0.283276 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

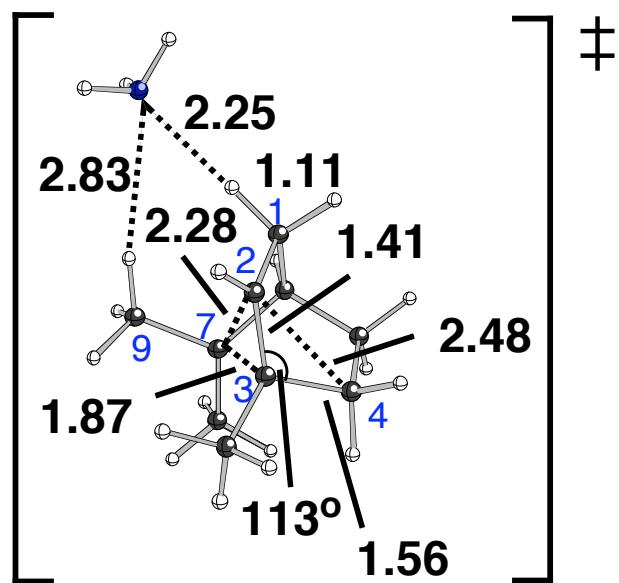
HF = -447.5181217 hartrees (-280817.62136675 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.019303	-0.542228	0.917535
2	6	-1.368432	-0.559470	0.839238
3	6	-1.994326	-1.115748	-0.406631
4	6	-1.170092	-0.772271	-1.695905
5	6	0.198036	-0.215253	-1.298499
6	6	0.817059	-1.149457	-0.231521
7	1	-2.011135	-2.207467	-0.271459
8	1	0.490458	-0.278644	1.861813
9	1	-1.032656	-1.671044	-2.302074
10	1	-1.725613	-0.058754	-2.310854
11	1	0.624431	-2.214952	-0.394295
12	1	1.888243	-0.998648	-0.087314
13	1	-3.039611	-0.806240	-0.491505
14	6	-2.237135	-0.066123	1.942745
15	1	-2.857773	-0.899866	2.299649
16	1	-1.668968	0.327240	2.787851

17	1	-2.940625	0.694383	1.582265
18	1	0.815562	0.004435	-2.177185
19	6	0.050214	0.993608	-0.355372
20	6	-1.095842	1.965476	-0.498515
21	1	-0.835507	2.625936	-1.338391
22	1	-2.060745	1.517737	-0.733778
23	1	-1.197732	2.602795	0.383955
24	6	1.320136	1.686690	0.091181
25	1	1.578578	2.393748	-0.711523
26	1	1.154729	2.282307	0.993252
27	1	2.176040	1.025798	0.237760
28	7	4.225647	-0.549814	0.469238
29	1	4.462727	-1.540488	0.476120
30	1	4.572221	-0.171688	1.349253
31	1	4.794333	-0.129242	-0.263748

TS(S5)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6079144 hartrees (-280873.966286 kcal/mol)
 Imaginary Frequencies: 1 (-307.1820 1/cm)
 Zero-point correction = 0.282603 (Hartree/Particle)

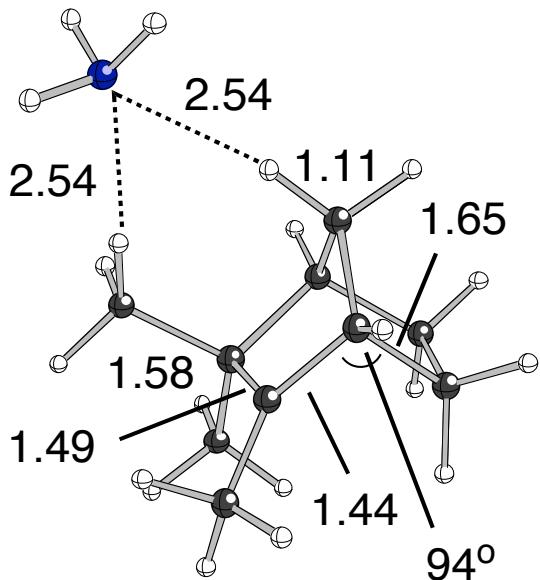
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5069992 hartrees (-280810.641998 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.272554	0.300153	1.296368
2	6	1.030618	-0.077097	0.922952
3	6	1.871861	1.114729	0.363864
4	6	1.117494	1.730048	-0.843238
5	6	-0.155960	0.876878	-0.959662
6	6	-1.016433	1.103867	0.299974
7	1	2.021580	1.832871	1.174857
8	1	-0.769117	-0.114832	2.176075
9	1	0.870748	2.782247	-0.681474
10	1	1.718155	1.682480	-1.754618
11	1	-1.125774	2.153999	0.614373
12	1	-2.049865	0.718652	0.222718
13	1	2.859827	0.733370	0.096436
14	6	1.779033	-1.114188	1.730462
15	1	2.273852	-0.641475	2.586161
16	1	1.119586	-1.898708	2.112037
17	1	2.562828	-1.583336	1.129343
18	1	-0.699631	1.020492	-1.897588
19	6	0.305036	-0.592569	-0.725474
20	6	1.471266	-1.122961	-1.542894
21	1	1.109521	-1.209019	-2.577525
22	1	2.354922	-0.487805	-1.560246
23	1	1.761049	-2.127205	-1.223150
24	6	-0.784799	-1.661589	-0.656290
25	1	-1.041822	-1.948441	-1.682718
26	1	-0.413011	-2.563688	-0.161132
27	1	-1.706031	-1.343468	-0.165833
28	7	-4.175685	-0.019994	0.231796
29	1	-4.687871	0.775007	0.610492
30	1	-4.484199	-0.833596	0.761215
31	1	-4.518322	-0.151220	-0.718367

D-NH₃



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6349893 hartrees (-280890.95578575 kcal/mol)

Imaginary Frequencies: none

Zero-point correction = 0.284276 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5360889 hartrees (-280828.89578475 kcal/mol)

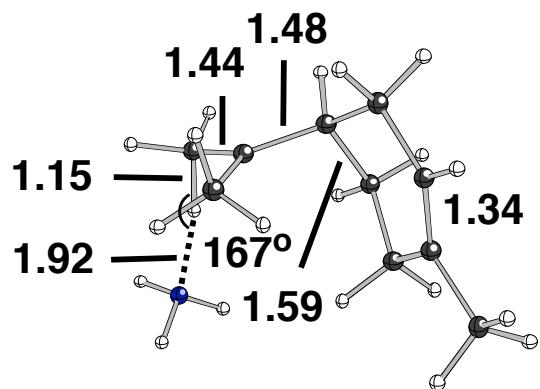
Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.080174	-1.008285	1.012173
2	6	-0.323653	0.410011	0.898624
3	6	-1.656154	-1.410758	0.729369
4	6	-1.779148	-1.315187	-0.807613
5	6	-0.441073	-0.645714	-1.204375
6	6	0.551780	-1.435586	-0.327776
7	1	-1.725339	-2.424058	1.135015
8	1	0.280177	-1.395840	1.963889
9	1	-1.841952	-2.310977	-1.253876
10	1	-2.663088	-0.758898	-1.123371
11	1	0.487180	-2.516298	-0.477826

12	1	1.596729	-1.125150	-0.400875
13	1	-2.377418	-0.798012	1.277652
14	6	-0.504600	1.329979	2.033428
15	1	-0.692212	0.809511	2.974665
16	1	0.456835	1.860513	2.144980
17	1	-1.260351	2.097527	1.848739
18	1	-0.236258	-0.624030	-2.275977
19	6	-0.400038	0.779268	-0.546669
20	6	-1.549442	1.732191	-0.925694
21	1	-1.579140	1.839043	-2.014030
22	1	-2.526716	1.369379	-0.597955
23	1	-1.397938	2.729103	-0.503472
24	6	0.967231	1.495715	-0.865341
25	1	1.016147	1.613496	-1.951918
26	1	0.978829	2.489940	-0.411281
27	1	1.850560	0.943303	-0.535379
28	7	3.975276	-0.326402	0.018697
29	1	4.264107	-1.222353	0.407865
30	1	4.428510	0.386261	0.588127
31	1	4.406035	-0.267448	-0.902609

Figure S5.

A-NH₃



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6316297 hartrees (-280888.84763675 kcal/mol)

Imaginary Frequencies: none

Zero-point correction = 0.281411 (Hartree/Particle)

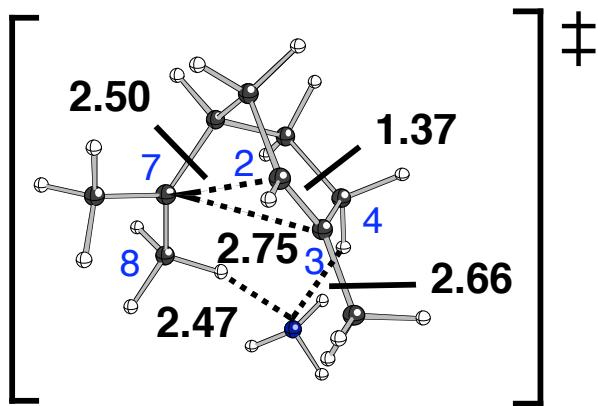
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.5231265 hartrees (-280820.76187875 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.089150	-1.097494	0.259574
2	6	2.489971	-0.984596	-0.066901
3	6	0.696321	-1.113488	1.681296
4	6	0.080525	-1.154378	-0.822982
5	6	-0.062690	0.292310	-1.456939
6	6	-0.796186	1.272814	-0.539086
7	6	-2.037307	0.688626	0.104382
8	6	-2.248701	-0.636705	0.129597
9	6	-3.002672	1.677269	0.703500
10	6	-1.322745	-1.679190	-0.450408
11	1	2.755082	0.131409	0.040592
12	1	2.752867	-1.275360	-1.085117
13	1	3.140564	-1.447802	0.682527
14	1	1.484902	-0.754831	2.345509
15	1	0.518479	-2.175382	1.931494
16	1	-0.257473	-0.609140	1.858117
17	1	0.517566	-1.771892	-1.617915
18	1	-0.643194	0.133020	-2.371162
19	1	0.916145	0.675903	-1.757130
20	1	-1.079179	2.149646	-1.135904
21	1	-0.125351	1.664929	0.242119
22	1	-3.163075	-1.018831	0.579238
23	1	-2.507744	2.310778	1.451066
24	1	-3.846639	1.178394	1.186109
25	1	-3.399306	2.351263	-0.065863
26	1	-1.765514	-2.095636	-1.365594
27	1	-1.241048	-2.532957	0.234077
28	7	3.603191	1.852043	0.154137
29	1	3.307476	2.519209	-0.556138
30	1	3.498096	2.312470	1.056503
31	1	4.601016	1.699505	0.016311

TS(S6)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6186855 hartrees (-280880.72515125 kcal/mol)

Imaginary Frequencies: 1 (-62.6056 1/cm)

Zero-point correction = 0.281804 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

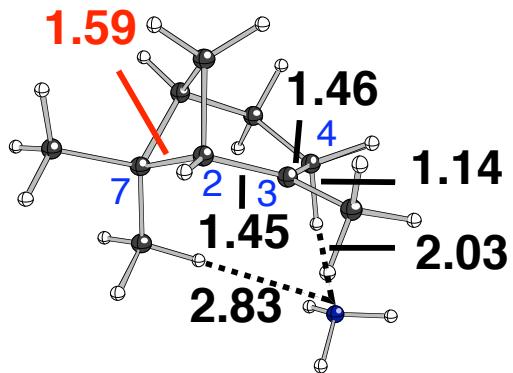
HF = -447.5118359 hartrees (-280813.67702725 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.811459	-1.187882	-0.286411
2	6	-0.525483	-1.718821	-0.626244
3	6	1.919845	-1.637533	-1.170953
4	6	1.100956	-0.616416	1.090070
5	6	-0.149114	-0.023601	1.756571
6	6	-0.747002	1.125315	0.886994
7	6	0.075052	1.463800	-0.332818
8	6	1.421225	1.235148	-0.343893
9	6	-0.631042	2.126841	-1.478133
10	6	2.093354	0.530291	0.818650
11	1	-1.381614	-1.094166	-0.347123
12	1	-0.631102	-2.622946	0.004276
13	1	-0.602049	-2.033260	-1.668529
14	1	1.672223	-1.498971	-2.227153
15	1	1.988976	-2.729834	-1.024613
16	1	2.894765	-1.209924	-0.949140
17	1	1.515691	-1.426459	1.713125

18	1	0.146117	0.348138	2.741141
19	1	-0.909134	-0.790440	1.932562
20	1	-0.824517	2.039874	1.490864
21	1	-1.770138	0.884329	0.579806
22	1	2.019143	1.586992	-1.181836
23	1	-1.439757	1.489531	-1.856918
24	1	0.045677	2.367197	-2.301255
25	1	-1.105366	3.056949	-1.140217
26	1	2.219219	1.174779	1.696289
27	1	3.088650	0.174629	0.548283
28	7	-3.796391	-0.740155	0.008227
29	1	-4.187020	-0.552048	0.930084
30	1	-4.258445	-0.095605	-0.631076
31	1	-4.122075	-1.670538	-0.249149

B-NH₃



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6196931 hartrees (-280881.35742025 kcal/mol)
 Imaginary Frequencies: none
 Zero-point correction = 0.282711 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

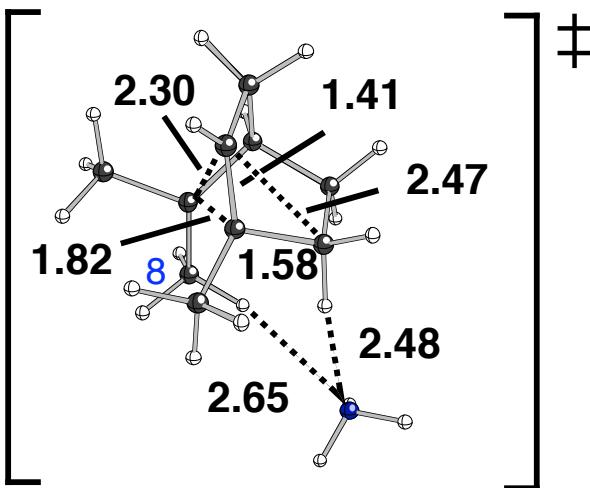
HF = -447.5197345 hartrees (-280818.63339875 kcal/mol)

Coordinates:

Center	Atomic Number	Coordinates (Angstroms)		
Number	Number	X	Y	Z

1	6	0.870898	0.838334	-0.618662
2	6	-0.498512	1.200518	-0.306134
3	6	-1.174748	0.537563	0.799866
4	6	-0.262119	-0.314923	1.719925
5	6	1.183608	-0.304015	1.199830
6	6	1.555788	1.143955	0.820118
7	1	-1.806391	1.259594	1.335022
8	1	1.281148	1.325988	-1.505083
9	1	-0.288969	0.101193	2.732502
10	1	-0.640703	-1.338649	1.791739
11	1	1.149749	1.964394	1.417653
12	1	2.615731	1.322379	0.643781
13	1	-1.964973	-0.108650	0.299141
14	6	-1.174666	2.274644	-1.068218
15	1	-2.178642	2.498899	-0.706131
16	1	-0.560759	3.186053	-1.033090
17	1	-1.209642	1.995164	-2.130536
18	1	1.859487	-0.837682	1.873737
19	6	1.246888	-0.675783	-0.321608
20	6	0.316960	-1.757634	-0.877600
21	1	0.626979	-2.737609	-0.498751
22	1	-0.734070	-1.621901	-0.616819
23	1	0.390524	-1.794459	-1.970019
24	6	2.678984	-0.968811	-0.795316
25	1	2.984239	-1.953558	-0.426192
26	1	2.727244	-0.994488	-1.888830
27	1	3.420171	-0.247347	-0.443989
28	7	-3.519621	-1.320669	-0.198475
29	1	-3.477108	-2.215123	0.286835
30	1	-4.381908	-0.870098	0.103325
31	1	-3.633253	-1.532508	-1.188176

TS(S7)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.604964 hartrees (-280872.11491 kcal/mol)

Imaginary Frequencies: 1 (-318.1136 1/cm)

Zero-point correction = 0.282560 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

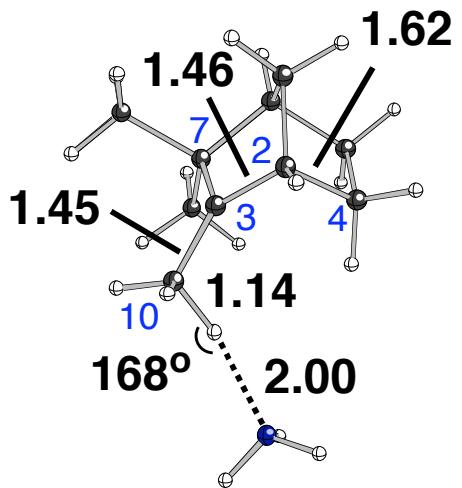
HF = -447.5042161 hartrees (-280808.89560275 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.631683	0.248921	1.170201
2	6	-0.329595	-0.262190	1.011008
3	6	0.728738	0.897725	0.847287
4	6	0.344792	1.726938	-0.403173
5	6	-0.928239	1.036476	-0.919127
6	6	-2.035116	1.234447	0.136382
7	1	0.729236	1.488431	1.767339
8	1	-2.345202	-0.149803	1.894940
9	1	0.158151	2.777822	-0.167503
10	1	1.144396	1.702097	-1.147057
11	1	-2.108872	2.250867	0.555005
12	1	-3.045301	1.002871	-0.222076
13	1	1.714839	0.435208	0.743953
14	6	0.113019	-1.459532	1.825233

15	1	0.395461	-1.147482	2.836535
16	1	-0.672583	-2.215615	1.911040
17	1	0.994026	-1.924581	1.375593
18	1	-1.223708	1.334950	-1.928299
19	6	-0.647958	-0.489535	-0.768421
20	6	0.634856	-1.039910	-1.376090
21	1	0.541782	-0.910579	-2.464273
22	1	1.553694	-0.549158	-1.056173
23	1	0.727771	-2.113310	-1.190561
24	6	-1.801955	-1.436568	-1.105420
25	1	-1.848609	-1.545881	-2.194639
26	1	-1.618320	-2.433552	-0.694576
27	1	-2.786571	-1.106983	-0.768509
28	7	3.983533	0.040290	-0.166920
29	1	4.313390	0.250559	-1.107317
30	1	4.446688	0.706197	0.449198
31	1	4.363842	-0.874725	0.068538

D-NH₃



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6396485 hartrees (-280893.87943375 kcal/mol)
 Imaginary Frequencies: none
 Zero-point correction = 0.284440 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

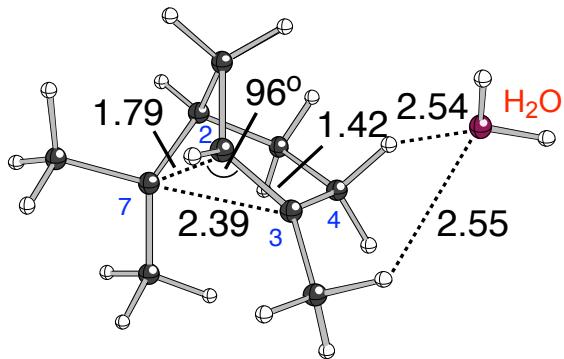
HF = -447.5407623 hartrees (-280831.82834325 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.338435	-1.014593	-1.144382
2	6	0.163882	0.297741	-0.739707
3	6	0.117869	-1.879003	0.143446
4	6	-0.911809	-1.484020	1.234252
5	6	-1.715604	-0.354970	0.544291
6	6	-1.863266	-0.937720	-0.876305
7	1	0.038282	-2.922284	-0.174240
8	1	0.034481	-1.420233	-2.084492
9	1	-1.574164	-2.321261	1.468255
10	1	-0.439451	-1.175036	2.168010
11	1	-2.321239	-1.929850	-0.890675
12	1	-2.395172	-0.303889	-1.587680
13	1	1.158562	-1.701952	0.426294
14	6	1.408060	0.889515	-1.175392
15	1	1.657174	0.640102	-2.211042
16	1	1.475489	1.962388	-0.982709
17	1	-2.639368	-0.074100	1.053326
18	6	-0.762703	0.865743	0.292252
19	6	-0.053964	1.446087	1.532971
20	1	-0.809140	1.765809	2.257213
21	1	0.598391	0.719831	2.022384
22	1	0.547498	2.321741	1.274617
23	6	-1.536777	2.038158	-0.411798
24	1	-2.310755	2.379154	0.281860
25	1	-0.862931	2.873430	-0.615861
26	1	-2.020951	1.750949	-1.346206
27	1	2.238948	0.416947	-0.557672
28	7	3.952143	-0.193918	0.271380
29	1	4.658794	0.434412	-0.107804
30	1	4.014792	-0.122113	1.285292
31	1	4.242235	-1.138253	0.023694

Figure S6a.

B-H₂O



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -467.4888629 hartrees (-293353.936358379 kcal/mol)
 Imaginary Frequencies: none found
 Zero-point correction = 0.270331 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -467.3829983 hartrees (-293282.83143325 kcal/mol)

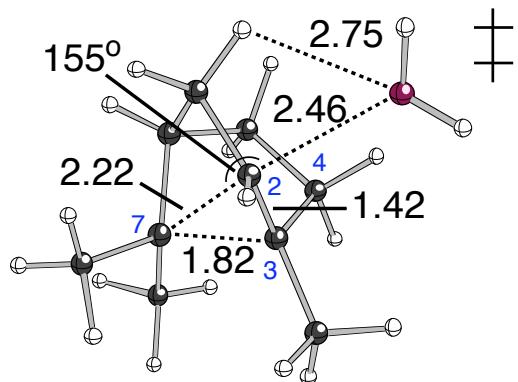
Comments:

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.016912	0.061216	-0.997494
2	6	0.755585	0.594835	0.062632
3	6	0.965728	-0.268906	1.254829
4	6	-0.256317	-1.205289	1.545490
5	6	-1.169485	-1.266389	0.318792
6	6	-0.276099	-1.452628	-0.934245
7	1	1.841278	-0.877561	0.972892
8	1	0.099607	-2.208846	1.791882
9	1	-0.798152	-0.834499	2.420179
10	1	0.614801	-2.073295	-0.805508
11	1	-0.820603	-1.798874	-1.811357
12	6	1.325221	1.955552	0.005511
13	1	2.402606	1.806023	-0.180979
14	1	0.923681	2.556086	-0.813212
15	1	1.240908	2.484719	0.959543
16	1	-2.000257	-1.963888	0.463082

17	6	-1.584388	0.156621	-0.142257
18	6	-1.871362	1.249283	0.879701
19	1	-2.858503	1.047472	1.313034
20	1	-1.162951	1.304892	1.707703
21	1	-1.926179	2.232930	0.403662
22	6	-2.628838	0.207858	-1.255092
23	1	-3.608469	0.022458	-0.796393
24	1	-2.667189	1.198173	-1.717512
25	1	-2.484673	-0.538026	-2.037238
26	1	1.267353	0.316029	2.127408
27	8	3.740635	-0.316917	-0.610191
28	1	-0.003989	0.606025	-1.940656
29	1	4.562923	-0.341500	-0.101385
30	1	3.993932	-0.595896	-1.500817

TS(S8)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -467.4774341 hartrees (-293346.764672091 kcal/mol)
 Imaginary Frequencies: 1 (-119.2049 1/cm)
 Zero-point correction = 0.270880 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

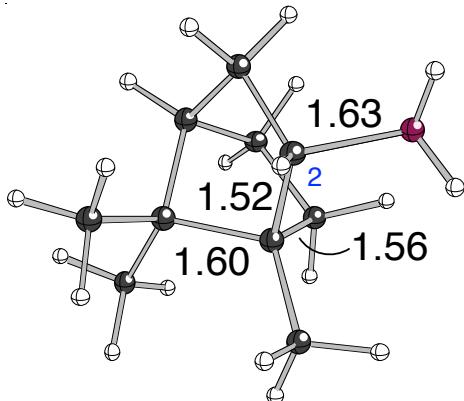
HF = -467.3726516 hartrees (-293276.338879 kcal/mol)

Comments:

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.878109	0.094061	0.813007
2	6	-0.240776	0.748583	-0.268818
3	6	-0.374321	-0.012365	-1.614665
4	6	0.269897	-1.416581	-1.439581
5	6	0.676147	-1.452556	0.040986
6	6	-0.618015	-1.377722	0.891332
7	1	-1.437167	-0.074212	-1.862578
8	1	-0.426929	-2.223148	-1.680784
9	1	1.137434	-1.541777	-2.091756
10	1	-1.448848	-1.960668	0.476119
11	1	-0.494608	-1.694651	1.930317
12	6	-0.255555	2.261167	-0.328385
13	1	-1.192902	2.609693	-0.775482
14	1	-0.162670	2.717468	0.661481
15	1	0.555343	2.635368	-0.958731
16	1	1.333143	-2.286407	0.301139
17	6	1.278705	-0.043829	0.330592
18	6	2.393314	0.452414	-0.586188
19	1	3.255821	-0.206923	-0.418768
20	1	2.160081	0.425169	-1.649369
21	1	2.705540	1.465547	-0.320959
22	6	1.689381	0.239489	1.781906
23	1	2.676053	-0.204714	1.951822
24	1	1.790490	1.315078	1.955181
25	1	1.017686	-0.166068	2.540679
26	1	0.106811	0.573087	-2.401190
27	8	-3.281933	0.082261	0.277523
28	1	-1.258579	0.653302	1.664504
29	1	-3.790798	0.872032	0.045612
30	1	-3.914445	-0.522234	0.691467

8-H⁺



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -467.4828208 hartrees (-293350.144880208 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.276287 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -467.3845017 hartrees (-293283.77481675 kcal/mol)

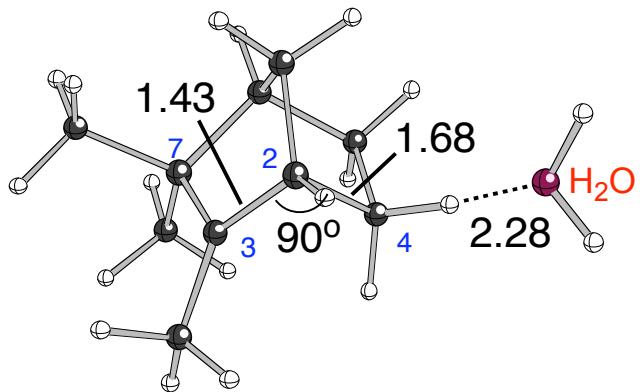
Comments:

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.141988	0.208873	0.751548
2	6	-0.175084	0.678139	-0.327897
3	6	-0.399977	-0.195400	-1.600534
4	6	0.101605	-1.616947	-1.200270
5	6	0.525347	-1.427724	0.272259
6	6	-0.773778	-1.237633	1.100462
7	1	-1.442575	-0.195388	-1.931353
8	1	-0.674085	-2.380866	-1.306361
9	1	0.942422	-1.933854	-1.820621
10	1	-1.553677	-1.950319	0.811329
11	1	-0.619893	-1.341250	2.177018
12	6	-0.172330	2.184482	-0.568624
13	1	-1.109667	2.532186	-1.024849

14	1	-0.019127	2.749922	0.356555
15	1	0.622573	2.460278	-1.266517
16	1	1.168443	-2.218399	0.664788
17	6	1.142401	0.010172	0.286853
18	6	2.376166	0.180123	-0.616133
19	1	3.188714	-0.448848	-0.237503
20	1	2.210359	-0.092121	-1.658916
21	1	2.733180	1.214476	-0.593139
22	6	1.541154	0.518436	1.689012
23	1	2.410214	-0.042901	2.045686
24	1	1.834530	1.572271	1.649924
25	1	0.768265	0.421637	2.456843
26	1	0.178388	0.226745	-2.425180
27	8	-2.659234	0.211853	0.150898
28	1	-1.267944	0.894798	1.589192
29	1	-2.910058	1.078273	-0.224002
30	1	-3.327297	-0.056578	0.809863

D-H₂O



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -467.5029729 hartrees (-293362.790524479 kcal/mol)
 Imaginary Frequencies: none found
 Zero-point correction = 0.271032 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

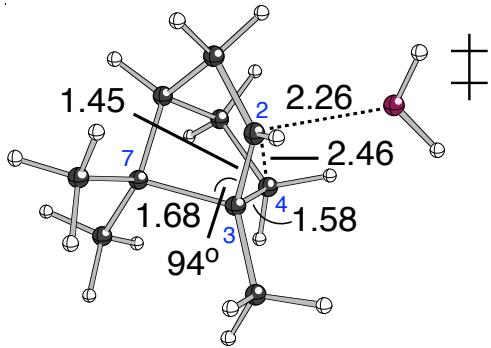
HF = -467.3993998 hartrees (-293293.1233745 kcal/mol)

Comments:

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.817519	0.388141	0.543840
2	6	0.429414	0.933601	0.100788
3	6	-1.116809	-0.182992	-1.005163
4	6	-0.336476	-1.509749	-1.054048
5	6	0.540858	-1.418289	0.217234
6	6	-0.502197	-0.939983	1.248344
7	1	-2.208741	-0.255799	-0.956854
8	1	-1.016501	-2.362324	-0.979330
9	1	0.236116	-1.625345	-1.975380
10	1	-1.377718	-1.589919	1.306976
11	1	-0.118634	-0.789490	2.259514
12	6	0.655376	2.340082	-0.285833
13	1	-0.272753	2.905980	-0.383071
14	1	1.234936	2.795548	0.533926
15	1	1.269110	2.439765	-1.185237
16	1	1.092448	-2.326005	0.467269
17	6	1.464340	-0.157185	0.062122
18	6	2.376290	-0.146465	-1.178874
19	1	2.991627	-1.051028	-1.181754
20	1	1.817054	-0.119211	-2.117191
21	1	3.055509	0.710359	-1.165369
22	6	2.362145	0.038152	1.332863
23	1	3.026901	-0.827132	1.405266
24	1	2.979276	0.934128	1.229750
25	1	1.800208	0.112825	2.265374
26	1	-0.871114	0.518659	-1.807269
27	8	-4.117751	0.340266	0.141552
28	1	-1.620479	1.042354	0.874327
29	1	-4.741164	0.942728	-0.286306
30	1	-4.666608	-0.250109	0.675303

TS(S9)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -467.4779602 hartrees (-293347.094805102 kcal/mol)

Imaginary Frequencies: 1 (-95.4823 1/cm)

Zero-point correction = 0.271466 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -467.374397 hartrees (-293277.4341175 kcal/mol)

Comments:

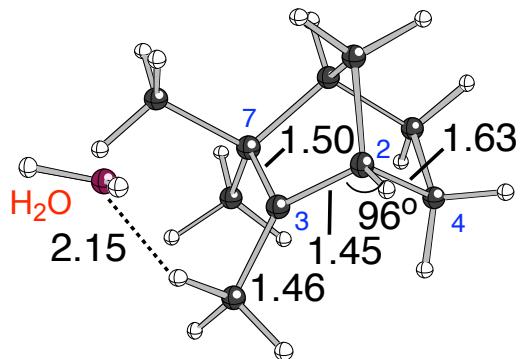
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.940821	0.201476	0.871203
2	6	-0.149000	0.744544	-0.215056
3	6	-0.477861	-0.059560	-1.533141
4	6	0.016419	-1.511219	-1.291070
5	6	0.560166	-1.456250	0.151190
6	6	-0.651189	-1.246409	1.089739
7	1	-1.545201	-0.005887	-1.749098
8	1	-0.788634	-2.244096	-1.389866
9	1	0.794586	-1.796439	-2.001974
10	1	-1.515843	-1.880111	0.856656
11	1	-0.432683	-1.415993	2.150520
12	6	-0.102466	2.256951	-0.363667
13	1	-1.058186	2.644268	-0.732873
14	1	0.120441	2.756676	0.583972
15	1	0.661481	2.549457	-1.088507

16	1	1.188218	-2.304339	0.432096
17	6	1.250244	-0.056662	0.239562
18	6	2.374797	0.197372	-0.770127
19	1	3.206823	-0.472797	-0.522485
20	1	2.104773	0.013950	-1.809548
21	1	2.751974	1.220691	-0.689414
22	6	1.782440	0.334299	1.630602
23	1	2.678923	-0.252835	1.853123
24	1	2.076500	1.388040	1.647016
25	1	1.081784	0.177637	2.455042
26	1	0.049846	0.434802	-2.351675
27	8	-3.090438	0.152649	0.160292
28	1	-1.385162	0.825114	1.642159
29	1	-3.502473	0.960714	-0.181551
30	1	-3.740040	-0.247300	0.758654

Figure S6b.

D-H₂O



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -467.5045514 hartrees (-293363.781049014 kcal/mol)
 Imaginary Frequencies: none found
 Zero-point correction = 0.271407 (Hartree/Particle)

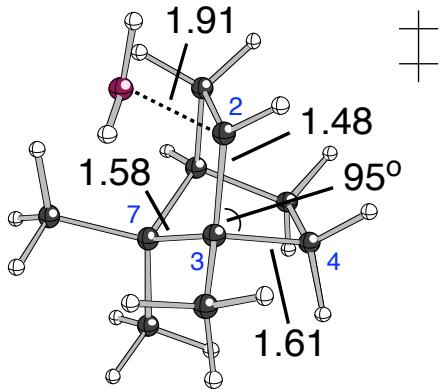
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -467.4006202 hartrees (-293293.8891755 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.198327	-1.419121	0.087130
2	6	0.308455	-0.165428	0.614867
3	6	-1.656914	-1.348177	0.815757
4	6	-2.455974	-0.358512	-0.066714
5	6	-1.365130	0.195608	-1.014065
6	6	-0.608858	-1.100827	-1.368668
7	1	-2.022219	-2.378364	0.780619
8	1	-3.219347	-0.883497	-0.646466
9	1	-2.963883	0.410027	0.517652
10	1	-1.255203	-1.876633	-1.786153
11	1	0.249922	-0.972611	-2.029462
12	1	-1.602963	-1.063386	1.870310
13	6	1.256729	-0.048032	1.717956
14	1	1.212405	-0.897927	2.404963
15	1	2.244921	-0.126297	1.212046
16	1	1.215617	0.903179	2.250149
17	1	-1.740346	0.785954	-1.851774
18	6	-0.304880	0.966243	-0.149120
19	6	-0.854453	2.109002	0.730020
20	1	-1.401371	2.811957	0.094599
21	1	-1.536807	1.756539	1.506916
22	1	-0.046533	2.663332	1.214306
23	6	0.832970	1.556670	-1.058608
24	1	0.365368	2.286089	-1.725760
25	1	1.575734	2.072471	-0.445794
26	1	1.346364	0.807907	-1.662372
27	8	3.639262	-0.608330	-0.356514
28	1	4.300276	0.033986	-0.649874
29	1	4.092484	-1.462367	-0.384199
30	1	0.349776	-2.328279	0.331089

TS(S10)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -467.4833179 hartrees (-293350.456815429 kcal/mol)

Imaginary Frequencies: 1 (-183.2524 1/cm)

Zero-point correction = 0.273722 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

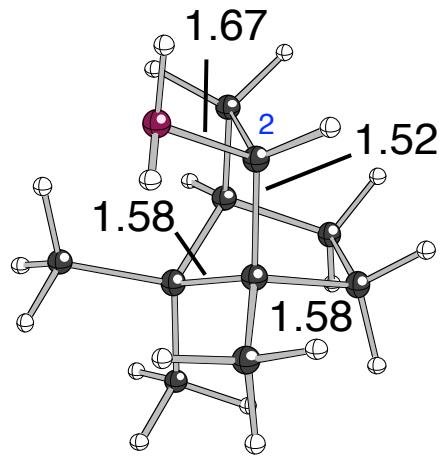
HF = -467.3826422 hartrees (-293282.6079805 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.084745	-0.869794	0.269136
2	6	0.138515	0.150437	0.783183
3	6	-0.927513	-0.914237	1.358913
4	6	-1.678428	-1.446362	0.110627
5	6	-0.894303	-0.780202	-1.038841
6	6	0.521786	-1.432453	-1.010212
7	1	-0.463194	-1.701747	1.961794
8	1	-1.658369	-2.537439	0.044310
9	1	-2.727072	-1.143517	0.113118
10	1	0.516518	-2.526828	-1.007945
11	1	1.121289	-1.112582	-1.867486
12	1	-1.567047	-0.346858	2.040250
13	6	0.632052	1.138929	1.828955
14	1	1.144296	0.636776	2.657179
15	1	1.311130	1.883585	1.396909
16	1	-0.208531	1.693717	2.253250
17	1	-1.367517	-0.838838	-2.020991

18	6	-0.618243	0.661087	-0.505447
19	6	-1.891050	1.466731	-0.179627
20	1	-2.475685	1.614074	-1.093070
21	1	-2.546784	0.998843	0.556159
22	1	-1.628545	2.460249	0.197394
23	6	0.232341	1.532086	-1.450744
24	1	-0.360936	1.801900	-2.329877
25	1	0.515450	2.469865	-0.960603
26	1	1.146181	1.055134	-1.806107
27	8	2.700400	-0.002655	-0.263372
28	1	2.976906	0.691757	0.358822
29	1	3.444954	-0.621364	-0.359398
30	1	1.624350	-1.492825	0.977613

9-H⁺



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -467.4841045 hartrees (-293350.950414795 kcal/mol)
 Imaginary Frequencies: none found
 Zero-point correction = 0.275784 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

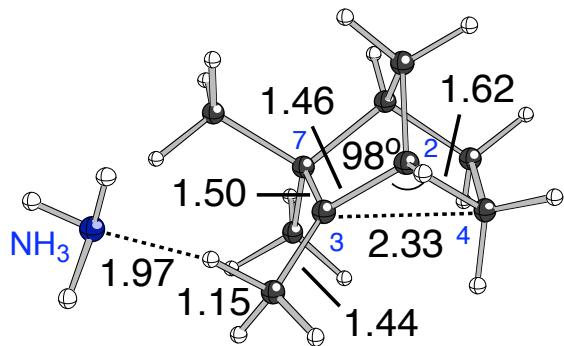
HF = -467.3856524 hartrees (-293284.496881 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.188085	-0.802369	0.220569
2	6	0.161160	0.170341	0.775585
3	6	-0.841848	-0.864166	1.424564
4	6	-1.580775	-1.506346	0.212875
5	6	-0.874828	-0.844080	-0.990465
6	6	0.568490	-1.427614	-1.026599
7	1	-0.329343	-1.597353	2.056769
8	1	-1.487443	-2.595723	0.194100
9	1	-2.648292	-1.278850	0.227260
10	1	0.597170	-2.520008	-0.985227
11	1	1.103914	-1.119764	-1.928819
12	1	-1.518669	-0.314347	2.083000
13	6	0.675495	1.223063	1.750988
14	1	1.216584	0.773549	2.592270
15	1	1.322864	1.969752	1.270578
16	1	-0.161437	1.784808	2.174090
17	1	-1.395520	-0.951259	-1.944472
18	6	-0.642746	0.622619	-0.508189
19	6	-1.938775	1.386647	-0.170120
20	1	-2.547008	1.496723	-1.073412
21	1	-2.561232	0.907206	0.586086
22	1	-1.706762	2.396086	0.184697
23	6	0.133632	1.502247	-1.509841
24	1	-0.506436	1.721905	-2.369901
25	1	0.396967	2.466320	-1.060563
26	1	1.049512	1.056011	-1.899930
27	8	2.542117	0.039099	-0.262616
28	1	2.781985	0.729588	0.385393
29	1	3.313894	-0.536735	-0.418292
30	1	1.654976	-1.462760	0.951099

Figure S8.

D-NH₃



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6402706 hartrees (-280898.746204206 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.284333 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

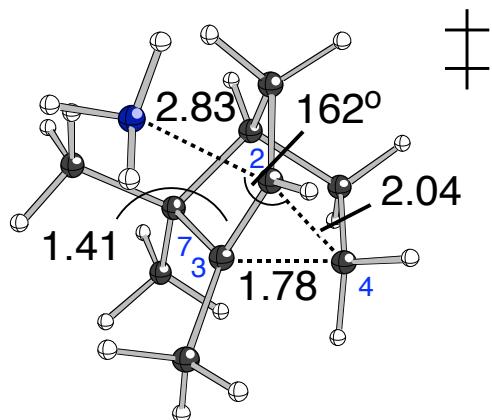
HF = -447.541517 hartrees (-280832.3019175 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.367353	-1.432847	0.201609
2	6	-0.326250	-0.296657	-0.398743
3	6	1.666132	-1.452885	-0.765999
4	6	2.535976	-0.285493	-0.233091
5	6	1.599168	0.383899	0.800699
6	6	1.002642	-0.860034	1.491369
7	1	2.113396	-2.439676	-0.617474
8	1	3.430445	-0.663928	0.268150
9	1	2.869615	0.387125	-1.024839
10	1	1.761917	-1.531272	1.900183
11	1	0.271758	-0.650162	2.274332
12	1	1.411726	-1.370330	-1.826205
13	6	-1.465868	-0.391288	-1.276617
14	1	-1.533235	-1.351767	-1.795384
15	1	-2.378674	-0.389891	-0.586341
16	1	-1.594443	0.454573	-1.954495
17	1	2.082940	1.116119	1.449863
18	6	0.350726	0.968210	0.048388

19	6	0.660089	1.954054	-1.098539
20	1	1.291400	2.759943	-0.712212
21	1	1.186123	1.484427	-1.932731
22	1	-0.253934	2.409553	-1.488455
23	6	-0.616713	1.684376	1.051877
24	1	-0.092428	2.559750	1.445481
25	1	-1.517802	2.025598	0.536690
26	1	-0.915747	1.059199	1.894879
27	1	-0.161353	-2.385796	0.217023
28	7	-4.153748	-0.501412	0.262179
29	1	-4.229065	-1.199486	0.999903
30	1	-4.488140	0.377557	0.652875
31	1	-4.817798	-0.769676	-0.462212

TS(S11)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6259705 hartrees (-280889.772748455 kcal/mol)
 Imaginary Frequencies: 1 (-132.2823 1/cm)
 Zero-point correction = 0.283856 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

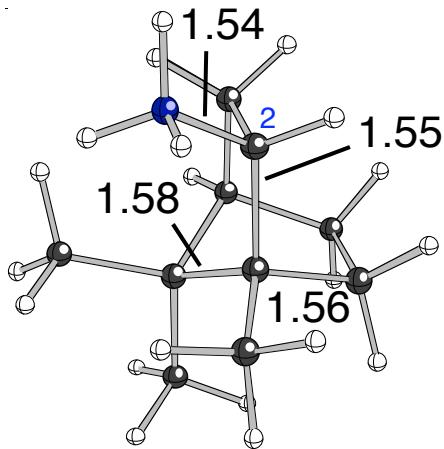
HF = -447.5283477 hartrees (-280824.03818175 kcal/mol)

Coordinates (from last standard orientation):

Center	Atomic	Coordinates (Angstroms)
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Number	Number	X	Y	Z
1	6	0.848174	-0.910750	0.317748
2	6	0.087619	0.193250	0.754943
3	6	-0.960936	-1.170475	1.226726
4	6	-1.795741	-1.448749	-0.026149
5	6	-0.993663	-0.685103	-1.102292
6	6	0.400136	-1.360414	-1.036474
7	1	-0.488273	-2.039393	1.692586
8	1	-1.853642	-2.517627	-0.244614
9	1	-2.814818	-1.074623	0.080588
10	1	0.392921	-2.447279	-1.158030
11	1	1.100586	-0.952904	-1.773025
12	1	-1.448372	-0.615662	2.031087
13	6	0.491885	1.067564	1.913608
14	1	0.980461	0.494570	2.706529
15	1	1.203320	1.820078	1.558546
16	1	-0.367025	1.592298	2.339103
17	1	-1.444690	-0.667207	-2.095482
18	6	-0.727542	0.717061	-0.464742
19	6	-1.997541	1.495055	-0.078829
20	1	-2.615695	1.656186	-0.967436
21	1	-2.617384	0.993572	0.667959
22	1	-1.739534	2.481184	0.318433
23	6	0.144626	1.632874	-1.350549
24	1	-0.408138	1.902833	-2.255418
25	1	0.381822	2.562601	-0.824854
26	1	1.088059	1.175176	-1.655265
27	1	1.605562	-1.395258	0.920602
28	7	3.493377	-0.043931	-0.207871
29	1	4.013835	-0.780060	-0.683229
30	1	3.595043	0.791106	-0.782429
31	1	4.000218	0.146051	0.655503

10-H⁺



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -447.6653684 hartrees (-280914.495324684 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.292274 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

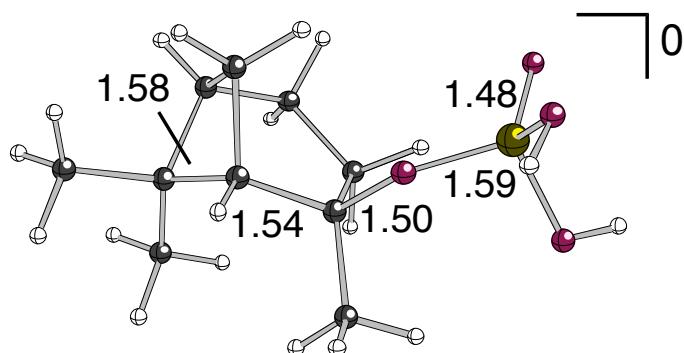
HF = -447.5753254 hartrees (-280853.5166885 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.261985	-0.742659	0.216882
2	6	0.145312	0.173381	0.785862
3	6	-0.835186	-0.857303	1.435181
4	6	-1.526929	-1.549773	0.220263
5	6	-0.836733	-0.878309	-0.988551
6	6	0.619908	-1.413666	-1.027977
7	1	-0.304771	-1.562295	2.084086
8	1	-1.388462	-2.634536	0.217611
9	1	-2.603858	-1.368401	0.215004
10	1	0.665177	-2.503857	-0.964854
11	1	1.134068	-1.130914	-1.953270
12	1	-1.553000	-0.335597	2.072170
13	6	0.611596	1.262630	1.747361
14	1	1.154956	0.840666	2.602205
15	1	1.249616	2.019910	1.272647

16	1	-0.247686	1.800939	2.156291
17	1	-1.362442	-1.006470	-1.937897
18	6	-0.653410	0.596655	-0.511837
19	6	-1.970240	1.333958	-0.194707
20	1	-2.588056	1.397953	-1.096291
21	1	-2.570938	0.858443	0.580742
22	1	-1.766704	2.359888	0.130028
23	6	0.101708	1.495888	-1.518625
24	1	-0.589568	1.842468	-2.292669
25	1	0.497497	2.399232	-1.038185
26	1	0.908918	1.002512	-2.074385
27	1	1.622429	-1.456556	0.961453
28	7	2.533472	0.039093	-0.164223
29	1	3.232228	-0.580693	-0.585897
30	1	2.312673	0.777824	-0.840737
31	1	2.955545	0.481020	0.658396

Figure S9b.



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -1034.8736401 hartrees (-649383.20916275 kcal/mol)

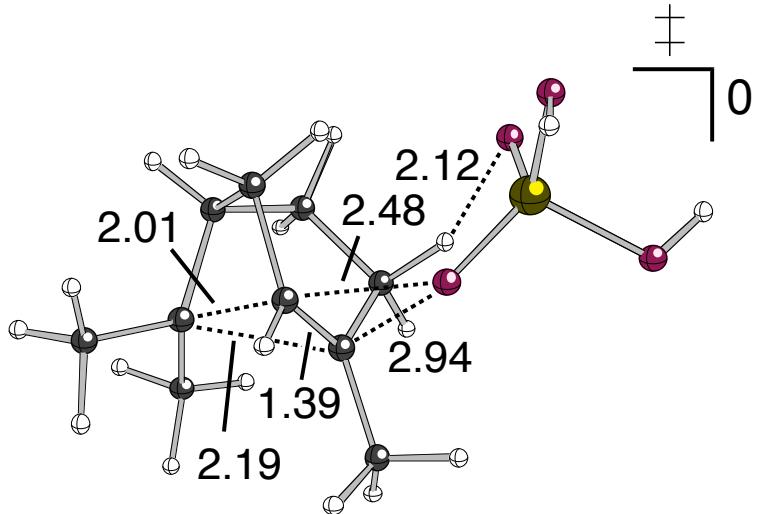
Imaginary Frequencies: none

Zero-point correction = 0.289079 (Hartree/Particle)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.243682	-0.020302	-0.915755
2	6	-0.129721	0.639603	-0.085627

3	6	-0.268794	0.281935	1.425376
4	6	-1.306231	-0.836213	1.763566
5	6	-2.181606	-1.226336	0.562532
6	6	-1.238385	-1.547662	-0.623917
7	1	0.705733	0.002130	1.829200
8	1	-1.177279	0.311457	-1.958402
9	1	-0.780079	-1.733716	2.107724
10	1	-1.932470	-0.502015	2.599412
11	1	-0.273974	-2.000367	-0.383020
12	1	-1.709310	-2.130671	-1.416408
13	6	-0.021010	2.146748	-0.320522
14	1	0.811245	2.567572	0.249908
15	1	0.148504	2.350293	-1.382276
16	1	-0.941873	2.649353	-0.016337
17	1	-2.939315	-1.966405	0.847185
18	6	-2.669797	0.030140	-0.234747
19	6	-3.173197	1.253887	0.542387
20	1	-4.139211	1.016494	1.005005
21	1	-2.509109	1.586381	1.341272
22	1	-3.340320	2.103963	-0.130262
23	6	-3.759137	-0.324373	-1.265999
24	1	-4.703918	-0.548093	-0.756254
25	1	-3.938543	0.523577	-1.938208
26	1	-3.506322	-1.187866	-1.885903
27	8	3.371545	-0.665297	-1.358557
28	15	2.535603	-0.228573	-0.050429
29	8	2.681775	-1.199764	1.057145
30	8	1.110263	0.061550	-0.696690
31	8	3.061257	1.266950	0.337109
32	1	3.165783	-0.126946	-2.136880
33	1	3.726502	1.219021	1.039914
34	1	-0.549444	1.202361	1.944952



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -1034.819757 hartrees (-649349.3975175 kcal/mol)

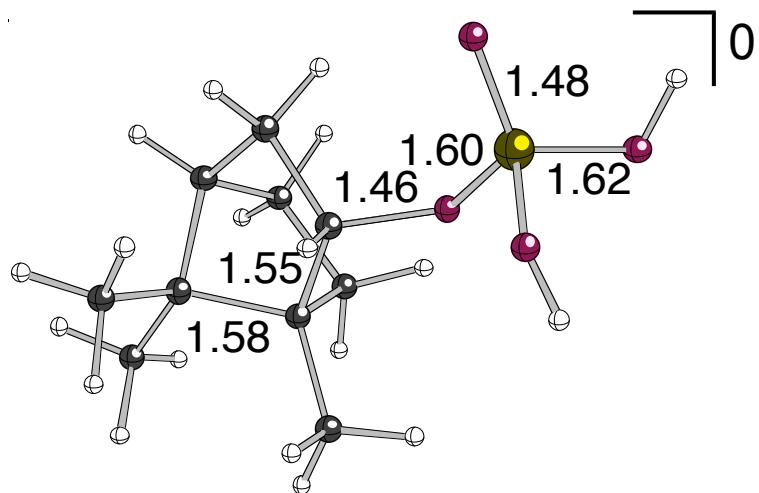
Imaginary Frequencies: 1 (-227.0734 1/cm)

Zero-point correction = 0.285278 (Hartree/Particle)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.723571	-0.281636	-0.794303
2	6	-0.882405	0.934282	-0.136169
3	6	-0.801887	0.948134	1.362958
4	6	-1.588054	-0.251213	1.981280
5	6	-2.008833	-1.171329	0.832876
6	6	-0.732840	-1.546655	0.037618
7	1	0.272253	0.817815	1.584198
8	1	-0.602017	-0.287446	-1.869951
9	1	-0.953322	-0.797835	2.682958
10	1	-2.460862	0.106971	2.537178
11	1	0.171847	-1.647169	0.644088
12	1	-0.847211	-2.432810	-0.588210
13	6	-0.869863	2.218799	-0.895242
14	1	0.146811	2.624645	-0.808957
15	1	-1.069748	2.076455	-1.959882
16	1	-1.563636	2.952939	-0.473575
17	1	-2.630554	-2.006101	1.177812
18	6	-2.665688	-0.319962	-0.275060
19	6	-3.637751	0.790772	0.088247

20	1	-4.576828	0.313169	0.403538
21	1	-3.311444	1.436626	0.903152
22	1	-3.870100	1.415113	-0.779855
23	6	-3.183205	-1.066146	-1.500299
24	1	-4.186156	-1.447709	-1.262918
25	1	-3.289769	-0.395834	-2.358957
26	1	-2.567061	-1.915411	-1.796486
27	8	3.683460	-1.318342	-0.342480
28	15	2.609125	-0.099262	-0.055983
29	8	2.050976	-0.314147	1.330636
30	8	1.685676	0.041739	-1.253543
31	8	3.568025	1.248840	-0.066113
32	1	3.922661	-1.325243	-1.279943
33	1	4.066276	1.293602	0.762277
34	1	-1.128531	1.912152	1.763834



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -1034.8995149 hartrees (-649399.44559975 kcal/mol)

Imaginary Frequencies: none

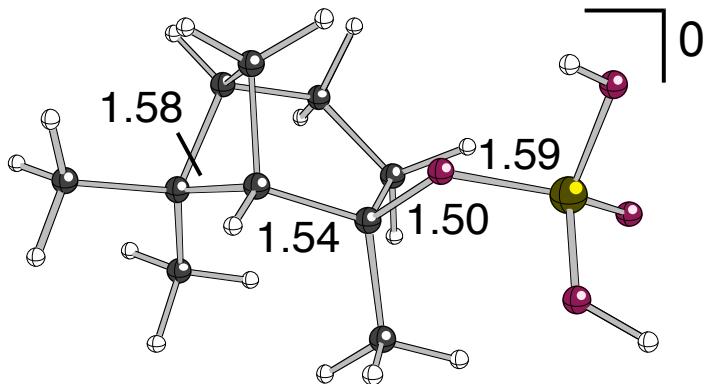
Zero-point correction = 0.289453 (Hartree/Particle)

Coordinates:

Center	Atomic Number	Atomic Number	Coordinates (Angstroms)		
			X	Y	Z

1	6	-0.009466	0.088644	0.336129
2	6	1.190948	0.545160	-0.530162
3	6	1.361831	-0.509814	-1.661435
4	6	1.918746	-1.769519	-0.927904
5	6	1.955016	-1.314480	0.549914
6	6	0.486348	-1.210300	1.028238
7	1	0.412001	-0.700047	-2.165860
8	1	-0.271530	0.866026	1.059410
9	1	1.278631	-2.647430	-1.061240
10	1	2.914744	-2.041500	-1.290570
11	1	-0.115147	-2.067743	0.715791
12	1	0.396598	-1.136766	2.115023
13	6	1.081771	1.981245	-1.027713
14	1	0.216190	2.094769	-1.690655
15	1	0.965598	2.691091	-0.200328
16	1	1.969597	2.271646	-1.599780
17	1	2.586899	-1.934063	1.194416
18	6	2.384884	0.184149	0.438359
19	6	3.776789	0.394159	-0.185840
20	1	4.545597	-0.043215	0.461992
21	1	3.889413	-0.051222	-1.175878
22	1	4.000745	1.463002	-0.277769
23	6	2.388165	0.937331	1.784851
24	1	3.202848	0.563373	2.415801
25	1	2.566005	2.007893	1.630363
26	1	1.466105	0.836792	2.360674
27	8	-2.909427	1.540681	0.392969
28	15	-2.650424	-0.038817	0.137573
29	8	-2.943586	-0.839175	1.345335
30	8	-1.184765	-0.125709	-0.507123
31	8	-3.521972	-0.387986	-1.180639
32	1	-2.812989	2.078223	-0.407136
33	1	-4.245728	-0.991987	-0.959441
34	1	2.058591	-0.138525	-2.419360

Figure S9c.



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -1034.8744354 hartrees (-649394.056957854 kcal/mol)

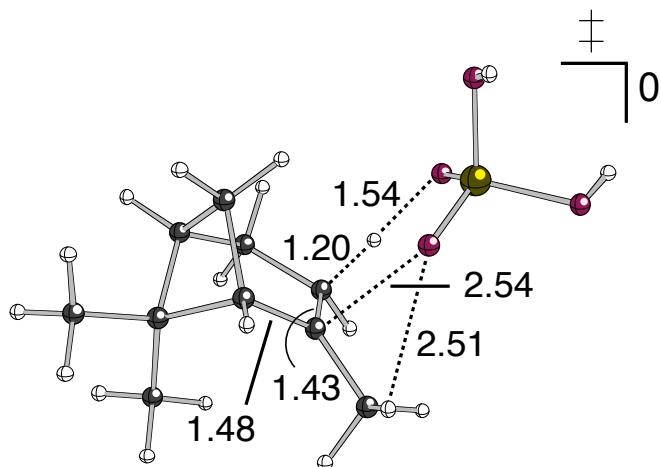
Imaginary Frequencies: none found

Zero-point correction = 0.288698 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.213871	0.006809	-0.881194
2	6	-0.104650	0.439708	0.091519
3	6	-0.400227	-0.046950	1.542719
4	6	-1.594471	-1.043651	1.689914
5	6	-2.407153	-1.205248	0.395210
6	6	-1.417498	-1.530262	-0.751934
7	1	0.514813	-0.479184	1.951476
8	1	-1.021815	0.424292	-1.876337
9	1	-1.220493	-2.032166	1.981718
10	1	-2.245598	-0.708762	2.505970
11	1	-0.535899	-2.122537	-0.496114
12	1	-1.891217	-1.968529	-1.631294
13	1	-0.591433	0.839120	2.154783
14	6	0.190534	1.938207	0.019931
15	1	-0.706534	2.508938	0.267748
16	1	0.973655	2.217520	0.731541
17	1	0.513363	2.217451	-0.986587
18	1	-3.269673	-1.865622	0.547206
19	6	-2.674324	0.174511	-0.297150
20	6	-3.082351	1.369548	0.575213
21	1	-4.101844	1.213254	0.949102
22	1	-2.441987	1.528153	1.443452
23	1	-3.093483	2.297171	-0.009723

24	6	-3.713983	0.064625	-1.429059
25	1	-4.715961	-0.084489	-1.009235
26	1	-3.736072	0.988862	-2.019098
27	1	-3.518756	-0.760939	-2.117313
28	8	3.277547	-1.457702	-0.543150
29	15	2.613379	-0.080697	-0.023967
30	8	2.967279	0.226930	1.379801
31	8	1.088935	-0.294455	-0.435988
32	8	3.103122	1.047552	-1.094123
33	1	3.011434	-1.693210	-1.444182
34	1	3.889737	1.508738	-0.766937



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -1034.837348 hartrees (-649370.78424348 kcal/mol)

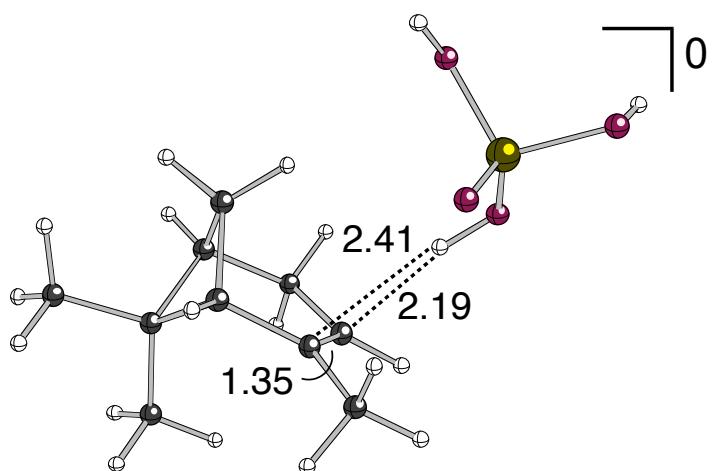
Imaginary Frequencies: 1 (-203.7999 1/cm)

Zero-point correction = 0.282843 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.306167	-0.053933	-0.903344
2	6	-0.604918	0.980225	-0.111755
3	6	-0.439051	0.727884	1.284886
4	6	-1.352300	-0.368230	1.891907
5	6	-2.061602	-1.155073	0.779055
6	6	-1.013171	-1.466804	-0.321717

7	1	0.689264	0.319360	1.312185
8	1	-1.242533	0.111397	-1.980092
9	1	-0.756416	-1.052809	2.504620
10	1	-2.084659	0.102077	2.559630
11	1	0.012916	-1.655962	-0.006894
12	1	-1.324551	-2.249671	-1.012919
13	1	-0.340978	1.638463	1.884539
14	6	-0.303253	2.304989	-0.711200
15	1	-1.253931	2.859457	-0.769279
16	1	0.388438	2.883212	-0.095010
17	1	0.099470	2.198074	-1.718889
18	1	-2.660945	-1.977589	1.184466
19	6	-2.773209	-0.202239	-0.239959
20	6	-3.507326	1.038915	0.276990
21	1	-4.423575	0.733585	0.796435
22	1	-2.923537	1.641396	0.976909
23	1	-3.808157	1.687371	-0.554769
24	6	-3.712412	-0.948303	-1.199720
25	1	-4.624041	-1.243091	-0.666106
26	1	-4.009829	-0.298379	-2.030617
27	1	-3.271606	-1.852615	-1.624747
28	8	3.211029	-1.633994	-0.418471
29	15	2.605780	-0.147251	-0.085808
30	8	2.129980	-0.205534	1.364847
31	8	1.613874	0.286848	-1.138970
32	8	3.914552	0.831925	-0.199421
33	1	3.423205	-1.713426	-1.359740
34	1	4.509748	0.699369	0.552655



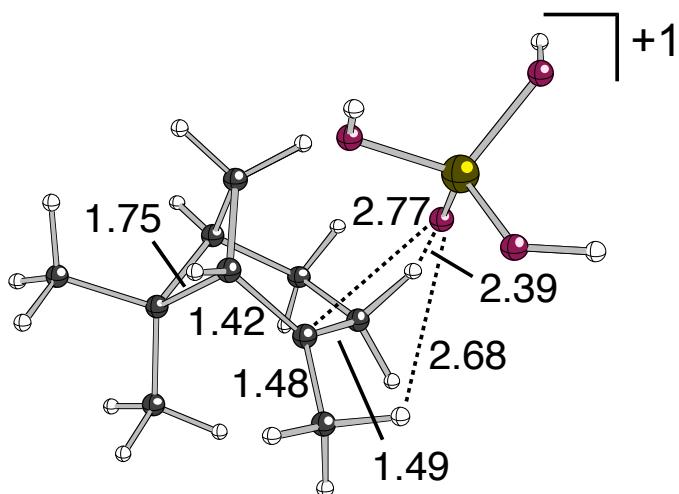
B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -1034.8726715 hartrees (-649392.950092965 kcal/mol)
 Imaginary Frequencies: none found
 Zero-point correction = 0.285043 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.575630	-0.059115	-0.864469
2	6	-0.875719	1.082567	-0.141533
3	6	-0.896807	1.039900	1.207112
4	6	-1.656580	-0.066023	1.917304
5	6	-2.267747	-1.041118	0.890436
6	6	-1.177502	-1.393055	-0.160293
7	1	1.219323	0.539766	0.924601
8	1	-1.480617	0.012980	-1.952539
9	1	-0.997073	-0.615706	2.604419
10	1	-2.442487	0.375985	2.547385
11	1	-0.146703	-1.481770	0.193876
12	1	-1.422110	-2.276712	-0.751210
13	1	-0.462437	1.842872	1.802632
14	6	-0.255358	2.183461	-0.954401
15	1	-1.012656	2.648225	-1.599586
16	1	0.178690	2.962724	-0.320214
17	1	0.532611	1.792737	-1.610091
18	1	-2.803883	-1.860558	1.383508
19	6	-3.024130	-0.269861	-0.255305
20	6	-3.876993	0.949756	0.104821
21	1	-4.758885	0.636464	0.677598
22	1	-3.339260	1.693806	0.695382
23	1	-4.239632	1.444952	-0.804444
24	6	-3.881163	-1.208970	-1.121014
25	1	-4.777958	-1.518162	-0.570204
26	1	-4.213958	-0.692200	-2.029214
27	1	-3.357034	-2.115916	-1.431615
28	8	2.800528	-1.739809	0.049095
29	15	3.007846	-0.140453	-0.173441
30	8	2.191396	0.466072	1.062272
31	8	2.698095	0.318156	-1.544720
32	8	4.524041	0.166244	0.270198
33	1	2.909696	-2.220701	-0.784690
34	1	4.709983	-0.052532	1.195317

Figure S10b.



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1035.1680653 hartrees (-649578.312656403 kcal/mol)

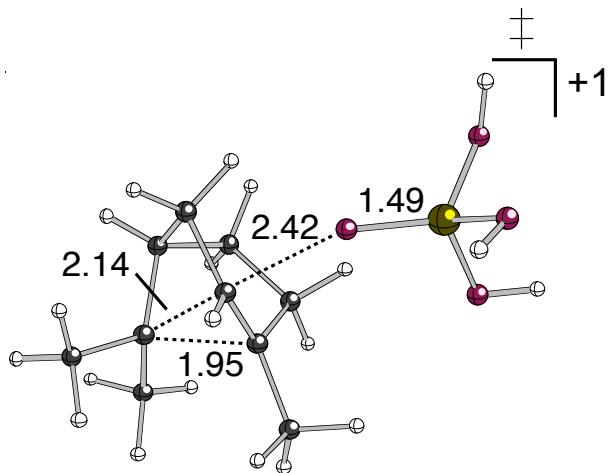
Imaginary Frequencies: none found

Zero-point correction = 0.298015 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.085027	0.532232	-0.368063
2	6	0.891856	-0.876260	-0.353198
3	6	1.200964	-1.595743	0.910210
4	6	2.353386	-0.919521	1.726934
5	6	2.587174	0.506420	1.220134
6	6	1.204235	1.178054	1.022751
7	1	0.254537	-1.519606	1.469361
8	1	0.660079	1.069048	-1.215259
9	1	2.085751	-0.897558	2.787040
10	1	3.263237	-1.521105	1.639120
11	1	0.413445	0.901535	1.724438
12	1	1.252935	2.263983	0.951954
13	6	0.485503	-1.629029	-1.559381
14	1	-0.494669	-2.074083	-1.333776
15	1	0.384282	-0.999443	-2.445776
16	1	1.168491	-2.464467	-1.755314
17	1	3.335701	1.034106	1.819392
18	6	2.832440	0.521206	-0.314546

19	6	3.645009	-0.589215	-0.974591
20	1	4.704757	-0.412257	-0.753025
21	1	3.409281	-1.597710	-0.627098
22	1	3.536894	-0.565644	-2.064203
23	6	3.264826	1.871480	-0.888979
24	1	4.328272	2.012565	-0.656523
25	1	3.161923	1.886577	-1.978525
26	1	2.719709	2.722881	-0.477874
27	8	-4.057201	0.382867	1.156030
28	15	-2.941334	0.117989	0.026518
29	8	-1.716478	-0.565497	0.513025
30	8	-2.569996	1.511591	-0.670081
31	8	-3.817917	-0.588148	-1.115228
32	1	-3.681534	0.432442	2.051554
33	1	-4.437590	-1.255674	-0.773521
34	1	1.372715	-2.661678	0.735838
35	1	-3.327988	1.952008	-1.093175



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1035.1596687 hartrees (-649573.043705937 kcal/mol)

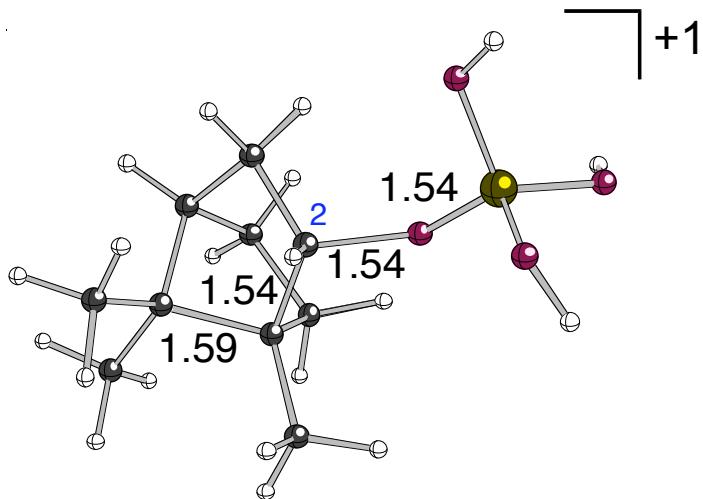
Imaginary Frequencies: 1 (-161.0501 1/cm)

Zero-point correction = 0.298332 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	6	0.740949	-0.052797	0.876266
2	6	1.083676	0.708887	-0.246134
3	6	1.022407	-0.006583	-1.597805
4	6	1.865593	-1.314370	-1.527721
5	6	2.331391	-1.415772	-0.071511
6	6	1.073040	-1.520564	0.827324
7	1	-0.032767	-0.214589	-1.804489
8	1	0.505952	0.444661	1.811437
9	1	1.279890	-2.193394	-1.810127
10	1	2.717972	-1.266667	-2.211008
11	1	0.261356	-2.111999	0.393525
12	1	1.270043	-1.913484	1.826927
13	6	0.919096	2.205648	-0.224279
14	1	-0.090990	2.451611	-0.573586
15	1	1.039986	2.622286	0.780408
16	1	1.627452	2.695810	-0.898984
17	1	3.079654	-2.198083	0.088875
18	6	2.810368	0.003234	0.337327
19	6	3.759484	0.758675	-0.582873
20	1	4.723421	0.231325	-0.538415
21	1	3.454811	0.797070	-1.628235
22	1	3.933254	1.778099	-0.227021
23	6	3.274437	0.190747	1.783567
24	1	4.330721	-0.101788	1.834476
25	1	3.222694	1.242560	2.082897
26	1	2.735450	-0.407986	2.519654
27	8	-4.167112	0.444369	0.946216
28	15	-2.862051	-0.020117	0.131891
29	8	-3.444211	-1.226259	-0.745796
30	8	-1.664335	-0.258158	0.978356
31	8	-2.543952	1.067221	-1.002801
32	1	-3.951902	0.872641	1.792744
33	1	-3.270428	1.198247	-1.637755
34	1	1.366352	0.663753	-2.389907
35	1	-3.997930	-1.848331	-0.242553



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1035.183369 hartrees (-649587.91588119 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.301754 (Hartree/Particle)

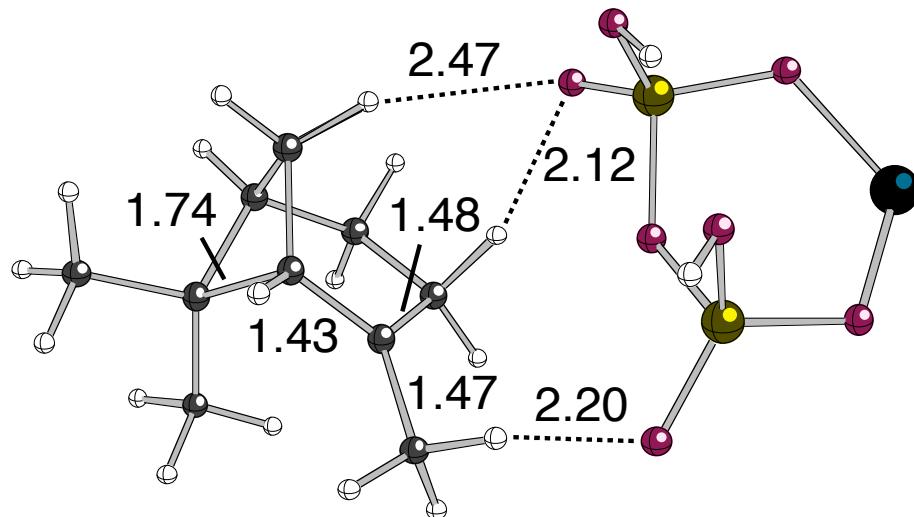
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.077146	0.104769	0.382488
2	6	1.219388	0.522957	-0.555930
3	6	1.383323	-0.599755	-1.622466
4	6	1.979867	-1.805177	-0.832995
5	6	2.035881	-1.269379	0.613985
6	6	0.573250	-1.159164	1.115248
7	1	0.432652	-0.837353	-2.107908
8	1	-0.230041	0.915042	1.045354
9	1	1.363128	-2.706683	-0.909452
10	1	2.974853	-2.071485	-1.198645
11	1	-0.022461	-2.038025	0.850101
12	1	0.499900	-1.032270	2.198559
13	6	1.080637	1.928425	-1.126834
14	1	0.209166	2.004510	-1.789218
15	1	0.972791	2.682788	-0.338369
16	1	1.958825	2.193507	-1.723700
17	1	2.679163	-1.845220	1.284459
18	6	2.439080	0.228262	0.417199
19	6	3.811511	0.431165	-0.249234
20	1	4.599026	0.037260	0.403139

21	1	3.913434	-0.059122	-1.219029
22	1	4.016223	1.497689	-0.393946
23	6	2.452583	1.057371	1.718308
24	1	3.296525	0.747368	2.344116
25	1	2.590608	2.122060	1.498843
26	1	1.552933	0.961644	2.333419
27	8	-3.109719	1.500308	0.241006
28	15	-2.633182	0.014982	0.017147
29	8	-2.804726	-0.670989	1.421983
30	8	-1.182990	-0.196390	-0.447706
31	8	-3.586892	-0.555847	-1.101307
32	1	-3.298767	2.032350	-0.554998
33	1	-3.291225	-1.364182	-1.561304
34	1	2.054550	-0.255834	-2.413846
35	1	-3.614935	-0.462281	1.924816

Figure S11b.

B-PPI-Mg²⁺



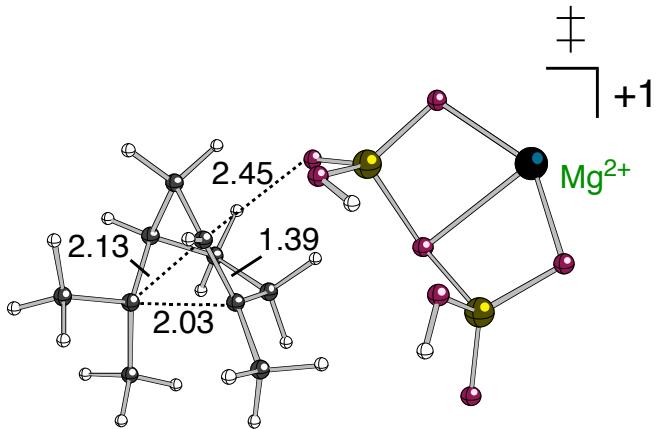
B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1801.8728329 hartrees (-1130693.22137308 kcal/mol)
 Imaginary Frequencies: none found
 Zero-point correction = 0.303537 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.535203	0.353793	0.817341
2	6	1.920227	0.783632	-0.397777
3	6	1.763224	-0.231556	-1.460047
4	6	2.919381	-1.291821	-1.463445
5	6	3.661714	-1.258290	-0.125391
6	6	2.602529	-1.176355	1.004514
7	1	0.835875	-0.771783	-1.180682
8	1	2.453638	1.035994	1.664331
9	1	2.489313	-2.283734	-1.624567
10	1	3.597951	-1.086339	-2.297481
11	1	1.666969	-1.716299	0.837311
12	1	2.996714	-1.432637	1.987473
13	1	4.423698	-2.041783	-0.063649
14	6	4.154582	0.177940	0.207842
15	6	4.684190	1.088770	-0.896894
16	1	5.692932	0.750100	-1.163858
17	1	4.090404	1.088066	-1.813998
18	1	4.774353	2.122976	-0.547581
19	6	5.072908	0.279168	1.426755
20	1	6.073135	-0.059043	1.126817
21	1	5.164720	1.315953	1.765907
22	1	4.754974	-0.335177	2.270753
23	1	1.593431	0.223254	-2.439660
24	8	-3.074146	-1.892831	-0.400906
25	15	-1.682825	-1.500369	0.213394
26	8	-1.796992	-1.528064	1.810150
27	8	-1.547292	0.131884	-0.137804
28	8	-0.471980	-2.180118	-0.296122
29	15	-2.487020	1.446313	0.169402
30	8	-2.967491	1.116425	1.702679
31	8	-3.762094	1.221980	-0.709967
32	8	-1.700595	2.689100	0.031638
33	6	1.495585	2.181012	-0.594631
34	1	1.659982	2.527006	-1.619885
35	1	0.399822	2.226710	-0.422759
36	1	1.949707	2.865478	0.127460
37	12	-4.095553	-0.549766	-1.158246
38	1	-2.365867	-0.813759	2.160827
39	1	-2.849994	1.888271	2.283323

TS(S12)



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1801.8643027 hartrees (-1130687.86858728 kcal/mol)

Imaginary Frequencies: 1 (-168.0223 1/cm)

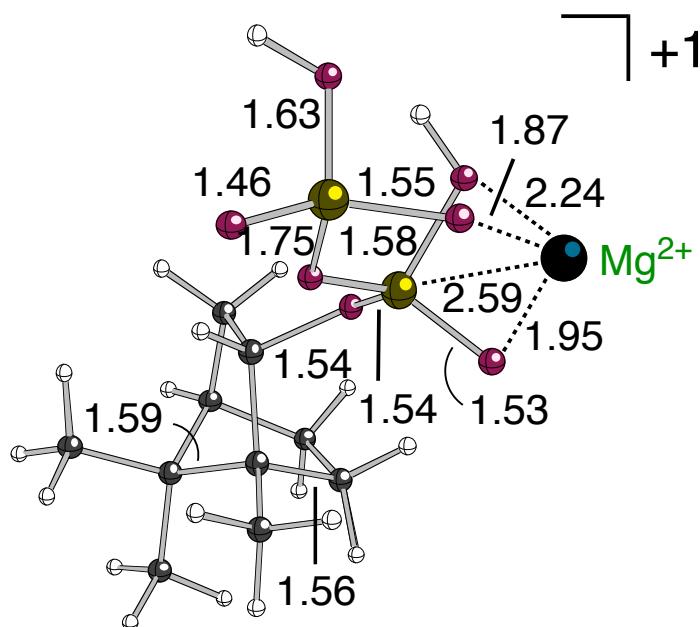
Zero-point correction = 0.304143 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.044982	-0.513146	0.552882
2	6	2.078102	0.588722	-0.299797
3	6	2.402018	0.311800	-1.762750
4	6	3.699494	-0.546455	-1.867461
5	6	4.080027	-0.908508	-0.428522
6	6	2.902732	-1.699446	0.192206
7	1	1.541005	-0.229271	-2.171546
8	1	3.537378	-1.450668	-2.460198
9	1	4.499293	0.016649	-2.356762
10	1	2.395816	-2.375401	-0.501400
11	1	3.174077	-2.274102	1.079975
12	6	1.368842	1.865895	0.055823
13	1	0.369594	1.870086	-0.398291
14	1	1.245780	1.982995	1.137150
15	1	1.899683	2.739169	-0.336553
16	1	5.058974	-1.393651	-0.356210
17	6	3.969335	0.386780	0.412979
18	6	4.567612	1.679323	-0.116052
19	1	5.660053	1.561742	-0.062828
20	1	4.314955	1.915955	-1.149233

21	1	4.304881	2.531345	0.517323
22	6	4.249237	0.276450	1.909849
23	1	5.333694	0.374722	2.050503
24	1	3.782929	1.098090	2.462983
25	1	3.944540	-0.668447	2.361735
26	1	2.480813	1.249754	-2.318966
27	8	-1.459049	-1.001744	1.930371
28	15	-1.396996	-1.336024	0.369896
29	8	-0.020363	-1.685619	-0.062437
30	8	-1.884708	0.098903	-0.389051
31	8	-2.584582	-2.252031	-0.072738
32	15	-3.018414	1.322018	-0.080841
33	8	-2.504711	2.648705	-0.453632
34	8	-3.233714	1.112807	1.531063
35	8	-4.256087	0.664763	-0.766782
36	1	1.592766	-0.418184	1.535732
37	1	-2.219227	-0.429777	2.170140
38	1	-3.190127	1.966608	1.997056
39	12	-3.677024	-1.099357	-1.097145

4-Mg²⁺



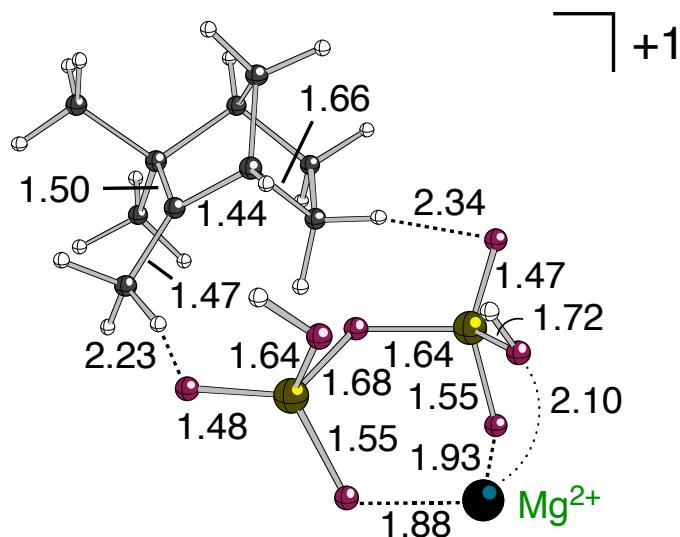
B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1801.8926718 hartrees (-1130705.67048122 kcal/mol)
Imaginary Frequencies: none found

Zero-point correction = 0.308596 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.456324	0.216992	0.620677
2	6	2.334638	-0.000233	-0.623655
3	6	2.807374	-1.483266	-0.610022
4	6	3.817410	-1.559722	0.575593
5	6	3.775342	-0.127091	1.151172
6	6	2.394693	0.047681	1.832082
7	1	1.966632	-2.172935	-0.494993
8	1	3.530595	-2.305644	1.323815
9	1	4.821358	-1.823894	0.232679
10	1	2.113553	-0.820864	2.434823
11	1	2.347136	0.925918	2.481740
12	6	1.702177	0.453536	-1.933980
13	1	0.846872	-0.177037	-2.211028
14	1	1.354202	1.491855	-1.886392
15	1	2.421317	0.378108	-2.755896
16	1	4.614775	0.120756	1.806391
17	6	3.637023	0.761062	-0.127290
18	6	4.820221	0.645726	-1.104751
19	1	5.737737	0.989138	-0.613260
20	1	5.001974	-0.367900	-1.467186
21	1	4.663185	1.287154	-1.978991
22	6	3.446097	2.264358	0.160827
23	1	4.384597	2.690477	0.532115
24	1	3.188299	2.805909	-0.756221
25	1	2.678204	2.494843	0.905019
26	1	3.278565	-1.727556	-1.565986
27	8	-2.173592	-1.432907	1.183353
28	15	-1.068753	-0.776662	0.119293
29	8	0.338420	-0.830577	0.730751
30	8	-1.555242	0.713722	-0.067681
31	8	-1.385252	-1.687137	-1.069322
32	15	-3.243684	1.183786	-0.080194
33	8	-3.344710	2.549271	-0.594847
34	8	-3.507800	0.986608	1.520394
35	8	-3.953540	-0.036842	-0.713885
36	1	0.917065	1.163675	0.602401
37	1	-2.513347	-0.794130	1.853401
38	1	-3.564358	1.843578	1.981269
39	12	-3.299656	-1.793305	-0.713684

D-PPi-Mg²⁺**B3LYP/6-31G(d)//B3LYP/6-31G(d)**

HF = -1801.8935592 hartrees (-1130706.22733359 kcal/mol)

Imaginary Frequencies: none found

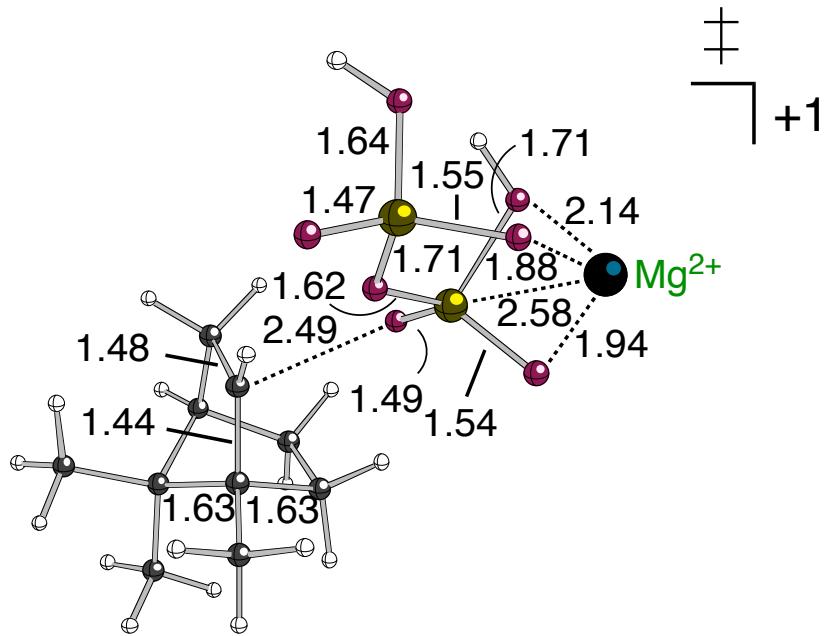
Zero-point correction = 0.304818 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.938862	-0.177522	0.777630
2	6	2.636268	0.743364	-0.078058
3	6	1.753329	-1.277783	-0.452192
4	6	3.110018	-2.009757	-0.490810
5	6	3.982814	-1.129506	0.433384
6	6	3.010817	-0.902870	1.609430
7	1	0.906256	-1.868442	-0.084397
8	1	3.017939	-3.015906	-0.072242
9	1	3.505180	-2.109938	-1.503366
10	1	2.631889	-1.833752	2.038961
11	1	3.401227	-0.284010	2.420788
12	6	2.037649	1.915297	-0.736422
13	1	0.943728	1.935658	-0.694551
14	1	2.380229	2.788398	-0.151451
15	1	2.413248	2.068847	-1.752750

16	1	4.961140	-1.545349	0.682263
17	6	4.066568	0.299230	-0.211023
18	6	4.634137	0.354860	-1.641636
19	1	5.622987	-0.114660	-1.654741
20	1	4.004781	-0.167475	-2.367237
21	1	4.755568	1.387597	-1.981862
22	6	4.913017	1.266234	0.686669
23	1	5.937630	0.882769	0.713229
24	1	4.934404	2.269961	0.253100
25	1	4.552943	1.342745	1.714804
26	1	1.448804	-0.834021	-1.404597
27	8	-3.580424	-1.082659	0.851880
28	15	-2.092278	-1.431133	0.054226
29	8	-1.227549	-2.446073	0.677870
30	8	-1.403279	0.054929	0.154193
31	8	-2.740166	-1.563953	-1.343945
32	15	-2.146427	1.559914	0.132359
33	8	-1.101167	2.578959	-0.098808
34	8	-2.781578	1.580976	1.638854
35	8	-3.383878	1.422394	-0.790774
36	1	0.975737	0.112233	1.189674
37	1	-3.485588	-0.581660	1.687351
38	1	-2.316784	2.219324	2.205767
39	12	-4.147275	-0.285823	-1.011126

TS(S13)



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1801.8722815 hartrees (-1130692.87536406 kcal/mol)

Imaginary Frequencies: 1 (-87.9138 1/cm)

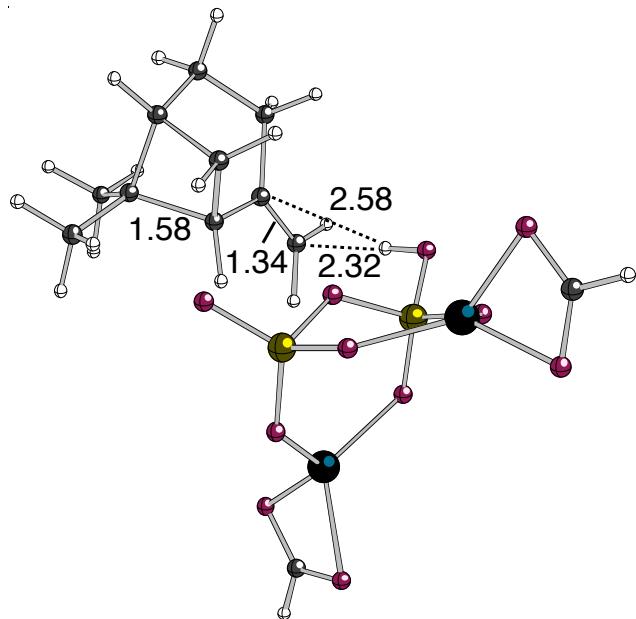
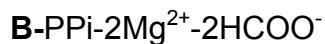
Zero-point correction = 0.304392 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.775009	0.490645	-0.412858
2	6	-2.656120	0.186953	0.689510
3	6	-2.770367	-1.431063	0.582650
4	6	-3.584036	-1.701993	-0.702516
5	6	-3.831299	-0.278915	-1.256826
6	6	-2.451835	0.247286	-1.702401
7	1	-1.783763	-1.890165	0.587013
8	1	-3.030369	-2.321260	-1.413170
9	1	-4.523436	-2.216060	-0.485143
10	1	-1.853601	-0.411052	-2.344660
11	1	-2.506307	1.207818	-2.238979
12	6	-2.289561	0.698268	2.073086
13	1	-1.324226	0.295756	2.398477
14	1	-2.222635	1.790699	2.093452
15	1	-3.039996	0.390931	2.807093
16	1	-4.600875	-0.212616	-2.028597
17	6	-4.088931	0.573923	0.024811
18	6	-5.281987	0.124798	0.879645
19	1	-6.206024	0.317038	0.321918
20	1	-5.277420	-0.932696	1.147377
21	1	-5.338144	0.707535	1.804741
22	6	-4.245567	2.087772	-0.215598
23	1	-5.180441	2.283334	-0.751492
24	1	-4.302509	2.622383	0.738239
25	1	-3.434943	2.543567	-0.792267
26	1	-3.293735	-1.716239	1.499285
27	8	2.688601	-1.468005	-1.099197
28	15	1.375802	-1.000787	-0.116243
29	8	0.023384	-1.213695	-0.698784
30	8	1.678789	0.582426	0.042004
31	8	1.860033	-1.755616	1.140599
32	15	3.212343	1.331920	0.053217
33	8	3.065157	2.730514	0.473009
34	8	3.582801	1.120907	-1.533962
35	8	4.146326	0.323888	0.772950

36	1	-0.804695	0.970013	-0.326049
37	1	2.925787	-0.800343	-1.782312
38	1	3.540785	1.966445	-2.013665
39	12	3.743492	-1.509289	0.766180

Figure S12b.



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -2379.7242496 hartrees (-1493300.7638665 kcal/mol)

Imaginary Frequencies: none found

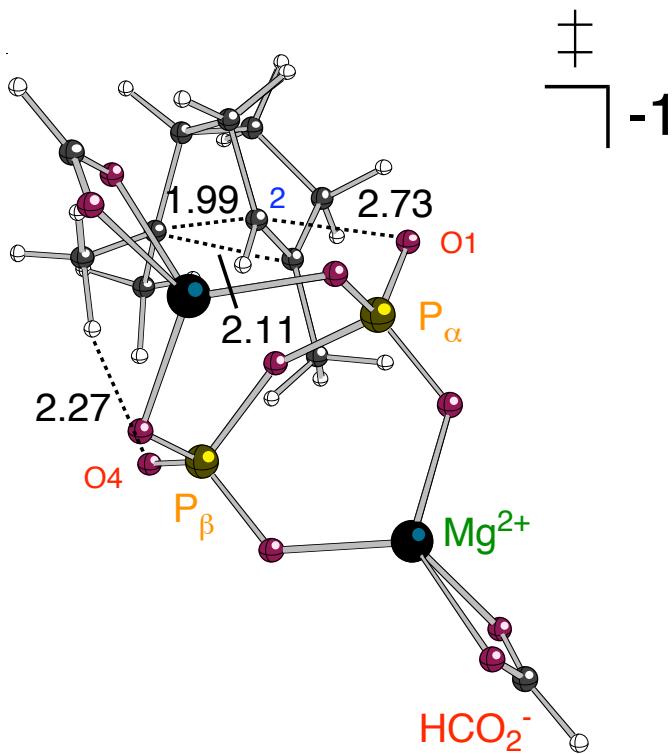
Zero-point correction = 0.332068 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.767998	-0.313250	0.051928
2	6	3.171652	-0.395437	-1.394067
3	6	3.857043	-1.707645	-1.768568
4	6	4.517026	-2.428319	-0.554540
5	6	3.884513	-1.979158	0.775790
6	6	2.367082	-1.733405	0.556967
7	1	3.085219	-2.368611	-2.183479

8	1	4.391676	-3.512452	-0.672180
9	1	5.598737	-2.243368	-0.538979
10	1	1.843154	-2.382316	-0.151768
11	1	1.772396	-1.671473	1.467454
12	6	2.928749	0.577370	-2.286930
13	1	0.789497	-0.309495	-2.365992
14	1	2.426152	1.498980	-1.999698
15	1	3.255247	0.501312	-3.322857
16	1	4.202471	-2.624759	1.605211
17	6	4.042484	-0.432443	0.979535
18	6	5.339634	0.252909	0.540455
19	1	6.172174	-0.040950	1.194752
20	1	5.626925	0.025728	-0.490377
21	1	5.235077	1.343016	0.612433
22	6	3.713081	0.005190	2.416148
23	1	4.470255	-0.377652	3.115001
24	1	3.721312	1.100389	2.486909
25	1	2.727923	-0.328447	2.752695
26	1	4.580062	-1.547121	-2.577073
27	8	-2.457192	-0.736748	-1.502419
28	15	-1.111147	-0.024812	-1.358999
29	8	-0.117717	-0.673709	-2.447157
30	8	-0.428659	-0.396696	0.040914
31	8	-1.139405	1.503881	-1.517997
32	15	-1.056105	-0.010201	1.625524
33	8	-0.037137	-0.540065	2.575178
34	8	-1.221964	1.536017	1.546620
35	1	2.088182	0.517246	0.253926
36	12	-1.069860	2.680404	0.036423
37	8	-1.944781	4.557792	-0.086358
38	6	-0.766993	5.022585	-0.140385
39	1	-0.631022	6.114668	-0.224614
40	8	0.258382	4.280747	-0.101462
41	12	-3.366077	-1.428516	0.085029
42	8	-5.438313	-1.577867	0.000147
43	8	-2.448841	-0.702395	1.590672
44	8	-4.121052	-3.365776	0.001089
45	6	-5.269715	-2.832859	-0.030323
46	1	-6.157300	-3.486828	-0.086539

TS(S14)



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -2379.6590693 hartrees (-1493259.86257644 kcal/mol)

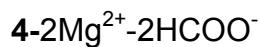
Imaginary Frequencies: 1 (-110.3787 1/cm)

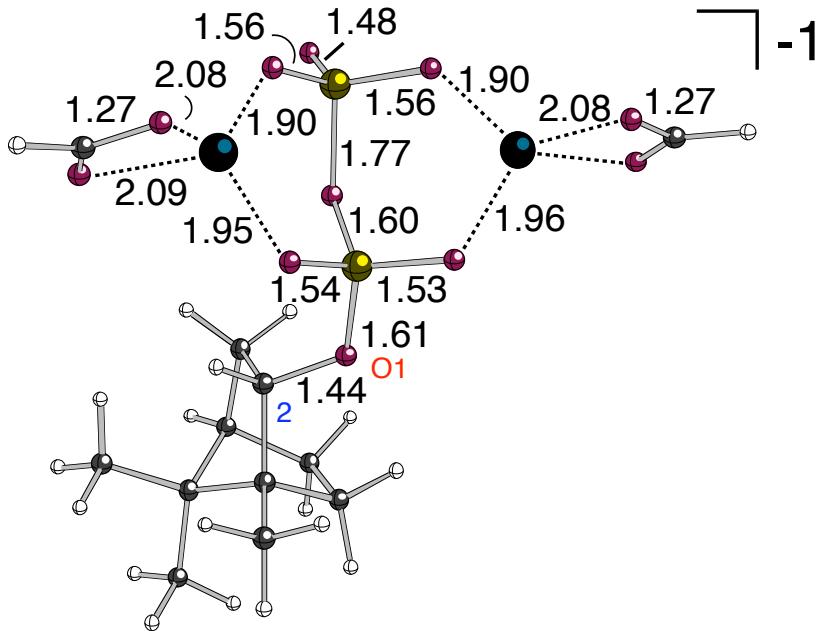
Zero-point correction = 0.331886 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.158470	-0.563966	-0.599697
2	6	-2.190325	-1.938520	-0.405911
3	6	-3.282633	-2.719726	-1.106872
4	6	-4.661146	-2.004212	-0.934690
5	6	-4.386320	-0.635943	-0.303756
6	6	-3.369246	0.106674	-1.206948
7	1	-3.002110	-2.760503	-2.167225
8	1	-5.165860	-1.882534	-1.898863
9	1	-5.322837	-2.602550	-0.298804
10	1	-3.483346	-0.084648	-2.279331
11	1	-3.322317	1.184562	-1.046785
12	6	-1.036222	-2.639541	0.237050
13	1	-0.282551	-2.796731	-0.546865

14	1	-0.565504	-2.019271	1.008638
15	1	-1.327606	-3.612628	0.646503
16	1	-5.310062	-0.096776	-0.059942
17	6	-3.436365	-0.841820	0.902147
18	6	-3.664770	-1.997018	1.868801
19	1	-4.519632	-1.721074	2.503713
20	1	-3.893824	-2.957628	1.403932
21	1	-2.797423	-2.118373	2.524078
22	6	-2.993463	0.384381	1.695596
23	1	-3.729630	0.536628	2.499479
24	1	-2.009939	0.214061	2.158845
25	1	-2.930212	1.300009	1.105447
26	1	-3.311763	-3.753400	-0.748689
27	8	1.161311	1.816503	-1.741271
28	15	1.051395	0.268984	-1.568100
29	8	-0.046587	-0.431242	-2.333126
30	8	0.520740	0.183037	0.045587
31	8	2.444705	-0.416961	-1.581745
32	15	1.171833	0.455701	1.591801
33	8	0.186189	-0.209592	2.518996
34	8	2.598054	-0.160427	1.545058
35	1	-1.297961	-0.018416	-0.236342
36	12	3.465377	-0.850103	-0.016707
37	8	5.550760	-0.905366	-0.116281
38	6	5.451794	-2.164501	-0.026515
39	1	6.377684	-2.768556	-0.033833
40	8	4.339788	-2.759561	0.070794
41	12	0.480862	2.615918	-0.100613
42	8	-0.129301	4.611999	-0.204292
43	8	1.215079	2.016878	1.598556
44	8	-1.634464	2.979141	-0.144816
45	6	-1.326337	4.205375	-0.201153
46	1	-2.137584	4.955400	-0.249618





B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -2379.7615372 hartrees (-1493324.16220837 kcal/mol)

Imaginary Frequencies: none found

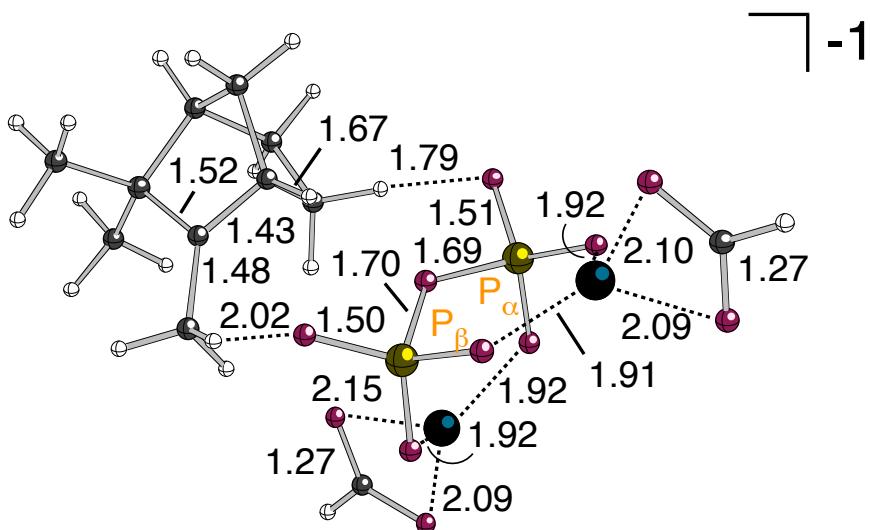
Zero-point correction = 0.335979 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.130970	-0.214131	-0.100350
2	6	3.407932	-0.779398	-0.778912
3	6	3.428202	-2.307829	-0.492671
4	6	3.769155	-2.405937	1.026380
5	6	3.857786	-0.921617	1.451689
6	6	2.417389	-0.358550	1.422278
7	1	2.463644	-2.757313	-0.737693
8	1	2.997701	-2.937297	1.593197
9	1	4.714279	-2.934148	1.196931
10	1	1.692313	-1.031377	1.886332
11	1	2.330016	0.603188	1.936324
12	6	3.520920	-0.417863	-2.254030
13	1	2.662131	-0.812735	-2.808317
14	1	3.535664	0.668696	-2.403166
15	1	4.431190	-0.835385	-2.702465
16	1	4.379868	-0.760167	2.401827

17	6	4.516925	-0.245877	0.206614
18	6	5.934496	-0.757351	-0.110931
19	1	6.619332	-0.500695	0.707821
20	1	5.989824	-1.838364	-0.259031
21	1	6.323620	-0.280984	-1.019523
22	6	4.616780	1.289513	0.307108
23	1	5.361064	1.567962	1.064280
24	1	4.948053	1.719626	-0.646296
25	1	3.680508	1.781075	0.579441
26	1	4.183568	-2.803798	-1.112799
27	8	-1.441254	-1.276160	-1.148342
28	15	-0.493654	-0.268655	-0.495682
29	8	0.969296	-0.949226	-0.538767
30	8	-0.810425	-0.111334	1.061099
31	8	-0.426165	1.119726	-1.153719
32	15	-2.315768	0.529665	1.727799
33	8	-2.140870	0.462845	3.200020
34	8	-3.370551	-0.408264	1.070945
35	8	-2.379716	1.938372	1.064947
36	1	1.983787	0.829210	-0.391469
37	12	-1.292566	2.656131	-0.313027
38	8	-1.851231	4.247921	-1.523807
39	6	-0.869846	4.876055	-1.025971
40	1	-0.676232	5.909592	-1.362022
41	8	-0.103605	4.362760	-0.158280
42	12	-3.159428	-1.692554	-0.311936
43	8	-3.705638	-3.697061	-0.181679
44	8	-4.711718	-2.280988	-1.565196
45	6	-4.572231	-3.437622	-1.068232
46	1	-5.230905	-4.250247	-1.421169

D-PPi-2Mg²⁺-2HCOO⁻



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -2379.6841657 hartrees (-1493275.61081841 kcal/mol)

Imaginary Frequencies: none found

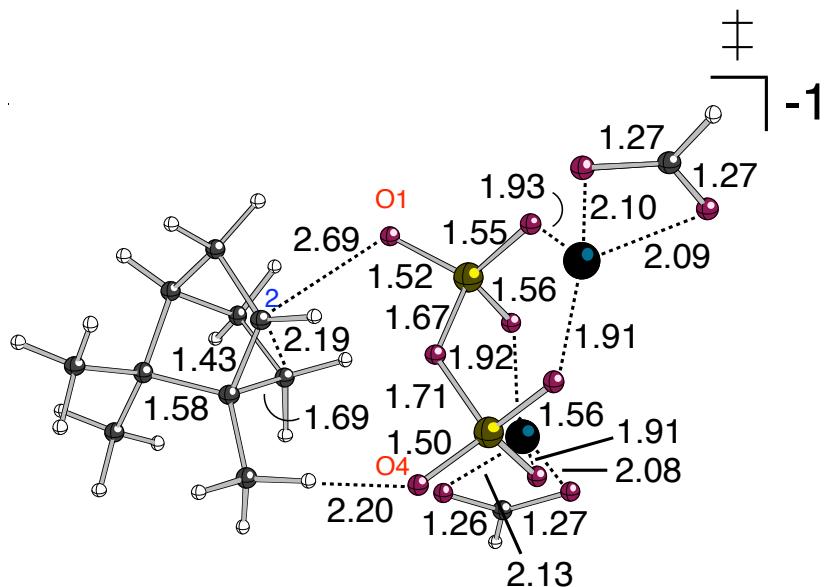
Zero-point correction = 0.331353 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.988362	-1.504687	-0.006012
2	6	-2.934558	-0.740997	-0.747480
3	6	-2.213035	-0.424534	1.251920
4	6	-3.452831	-0.962078	1.985339
5	6	-4.017379	-1.968171	0.958581
6	6	-2.725123	-2.718452	0.569565
7	1	-1.218956	-0.559629	1.765190
8	1	-3.161547	-1.481132	2.904585
9	1	-4.160317	-0.175619	2.260542
10	1	-2.200809	-3.139208	1.431716
11	1	-2.858112	-3.510494	-0.173779
12	6	-2.611467	0.288083	-1.756419
13	1	-1.668188	0.028817	-2.271471
14	1	-3.451411	0.432012	-2.445597
15	1	-2.427943	1.257440	-1.266587
16	1	-4.853393	-2.581929	1.308012
17	6	-4.339381	-1.161937	-0.346331
18	6	-5.313193	0.016974	-0.170273
19	1	-6.263024	-0.340565	0.245237

20	1	-4.917758	0.790294	0.492770
21	1	-5.529248	0.490029	-1.134163
22	6	-4.895144	-2.090359	-1.461383
23	1	-5.877554	-2.467124	-1.154047
24	1	-5.023050	-1.536404	-2.397022
25	1	-4.250326	-2.948130	-1.666766
26	1	-2.262062	0.630330	0.974332
27	8	2.805720	-0.379872	1.514057
28	15	1.341211	0.129228	1.555265
29	8	0.415836	-0.614327	2.496375
30	8	0.697494	-0.173703	0.026041
31	8	1.279530	1.688949	1.647134
32	15	1.229302	0.182500	-1.545517
33	8	0.257264	-0.543804	-2.439707
34	8	2.704644	-0.299223	-1.599304
35	8	1.141288	1.744896	-1.576385
36	1	-0.949701	-1.524187	-0.323048
37	12	0.507187	2.482450	0.078054
38	8	-0.142490	4.467009	0.113847
39	6	-1.330605	4.039537	0.135188
40	1	-2.156685	4.773560	0.151053
41	8	-1.614088	2.803996	0.139783
42	12	3.759771	-0.819809	-0.089338
43	8	4.875684	-2.594394	-0.163945
44	8	5.839059	-0.591870	-0.146112
45	6	5.902844	-1.855549	-0.177358
46	1	6.898762	-2.333915	-0.218066

TS(S15)



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -2379.672123 hartrees (-1493268.05390373 kcal/mol)

Imaginary Frequencies: 1 (-158.9527 1/cm)

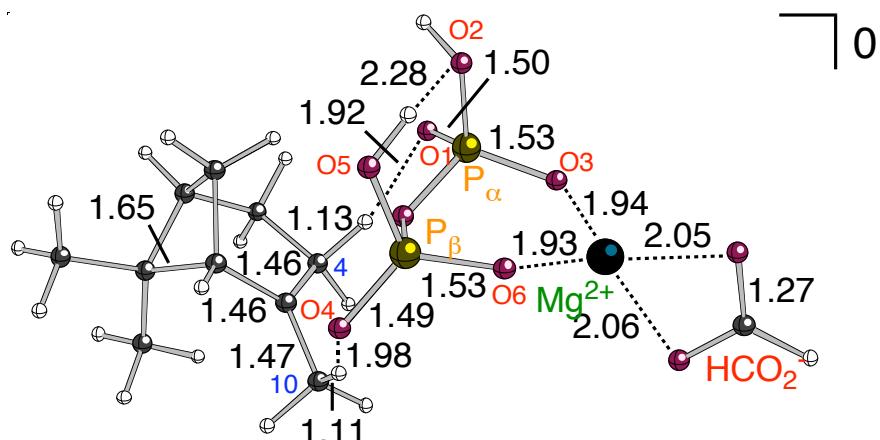
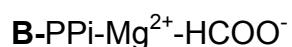
Zero-point correction = 0.331114 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.905457	-1.589506	-0.012159
2	6	2.863248	-0.762098	0.655892
3	6	2.700526	0.370230	-0.584793
4	6	3.529723	-0.203193	-1.746182
5	6	3.908197	-1.609674	-1.222103
6	6	2.550234	-2.347088	-1.110251
7	1	1.668273	0.569804	-0.857102
8	1	2.923709	-0.260063	-2.653179
9	1	4.414291	0.405107	-1.956614
10	1	1.912514	-2.347082	-1.996566
11	1	2.672282	-3.388962	-0.774904
12	6	2.576934	-0.212944	2.041355
13	1	1.508877	-0.002441	2.195062
14	1	2.868741	-0.953119	2.796908
15	1	3.154624	0.699318	2.225631
16	1	4.664656	-2.139984	-1.807634
17	6	4.269555	-1.357166	0.273587
18	6	5.434704	-0.380008	0.497733
19	1	6.363791	-0.806762	0.099678
20	1	5.287677	0.593915	0.026151
21	1	5.585819	-0.206340	1.569027
22	6	4.587353	-2.639714	1.068338
23	1	5.504092	-3.104939	0.685805
24	1	4.755595	-2.403254	2.124687
25	1	3.791304	-3.388697	1.030116
26	1	3.106870	1.258749	-0.093186
27	8	-2.353153	-0.729216	-1.519594
28	15	-0.947629	-0.098798	-1.337981
29	8	0.209501	-0.860796	-1.965840
30	8	-0.602979	-0.199329	0.297103
31	8	-0.951846	1.429462	-1.643695
32	15	-1.442908	0.378814	1.666521
33	8	-0.597048	-0.067271	2.821725
34	8	-2.856693	-0.260375	1.535828
35	8	-1.516870	1.919188	1.411107

36	1	0.845147	-1.592390	0.232218
37	12	-0.739343	2.649425	-0.170786
38	8	-0.625617	4.692222	-0.529051
39	6	0.625607	4.601874	-0.346920
40	1	1.236285	5.518890	-0.437681
41	8	1.200670	3.511807	-0.067431
42	12	-3.543612	-1.080199	-0.046934
43	8	-4.442266	-2.975299	0.050260
44	8	-5.601742	-1.135752	-0.409060
45	6	-5.527510	-2.385996	-0.225360
46	1	-6.450868	-2.988114	-0.309505

Figure S14a.



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.3509167 hartrees (-1249592.61373842 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.327456 (Hartree/Particle)

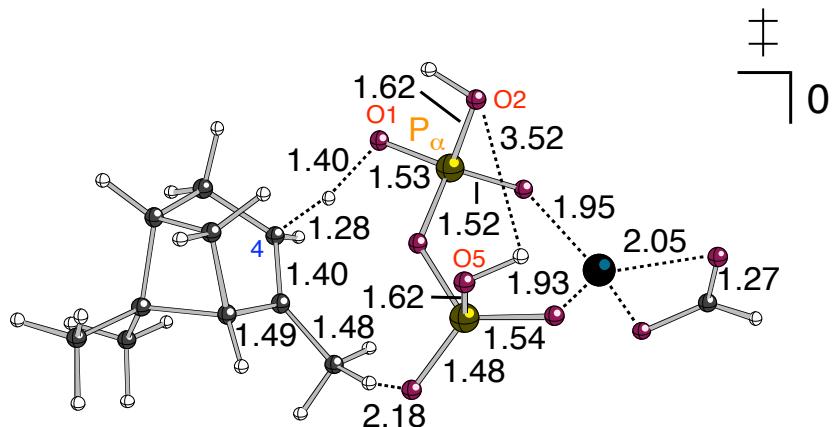
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.786222	-0.668185	0.145159
2	6	-2.080600	-0.318213	-1.080091
3	6	-2.137675	1.079701	-1.504177

4	6	-3.396588	1.846750	-0.992847
5	6	-4.059562	1.078443	0.157528
6	6	-2.930966	0.561256	1.086272
7	1	-1.244633	1.541816	-0.995863
8	1	-2.515914	-1.647287	0.543483
9	1	-3.091012	2.838978	-0.648176
10	1	-4.096506	1.990323	-1.823954
11	1	-2.046412	1.191850	1.189131
12	1	-3.278562	0.251689	2.071743
13	1	-4.886562	1.644916	0.598586
14	6	-4.365717	-0.400934	-0.237880
15	6	-4.868023	-0.722851	-1.647482
16	1	-5.911784	-0.399361	-1.742248
17	1	-4.302826	-0.234680	-2.446551
18	1	-4.846148	-1.803414	-1.832806
19	6	-5.251871	-1.134338	0.776275
20	1	-6.286683	-0.787030	0.663879
21	1	-5.241043	-2.214225	0.591960
22	1	-4.956474	-0.967016	1.814381
23	1	-1.953737	1.191220	-2.577203
24	8	2.395632	1.511121	-0.166936
25	15	1.049961	1.540696	0.551405
26	8	1.400369	1.679231	2.152360
27	8	0.403614	0.031305	0.458399
28	8	-0.034709	2.491989	0.151365
29	15	1.062187	-1.410346	1.004943
30	8	0.925420	-1.258405	2.610065
31	8	2.547227	-1.360030	0.622532
32	8	0.172667	-2.491014	0.497321
33	6	-1.397737	-1.359734	-1.850550
34	1	-0.965482	-1.006547	-2.788171
35	1	-0.635954	-1.817485	-1.181690
36	1	-2.097855	-2.187657	-2.039066
37	12	3.539272	-0.046404	-0.390922
38	8	4.386684	-0.461924	-2.219040
39	8	5.585304	0.043626	-0.421933
40	6	5.504173	-0.269687	-1.649775
41	1	6.429803	-0.377411	-2.235854
42	1	0.722879	2.226883	2.581422
43	1	1.418476	-0.474403	2.915186

Figure S14b.

TS(S18)



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.3479577 hartrees (-1249590.75693633 kcal/mol)

Imaginary Frequencies: 1 (-564.9440 1/cm)

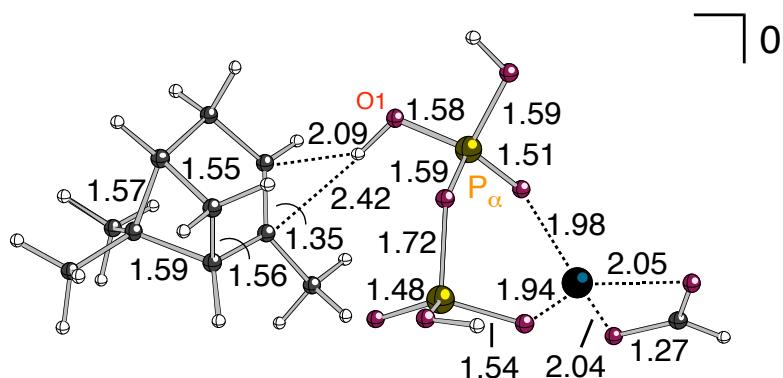
Zero-point correction = 0.323151 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.864995	0.629311	-0.479572
2	6	2.056800	-0.498775	-1.009855
3	6	2.168047	-1.735399	-0.354490
4	6	3.389399	-1.927885	0.568416
5	6	4.092805	-0.579665	0.801491
6	6	2.998484	0.486424	1.067647
7	1	1.162966	-1.648749	0.430957
8	1	2.584935	1.594350	-0.905817
9	1	3.073005	-2.356698	1.526186
10	1	4.074094	-2.651952	0.108452
11	1	2.103111	0.170192	1.604449
12	1	3.379233	1.404784	1.514643
13	1	4.920524	-0.675028	1.512787
14	6	4.401471	0.158001	-0.548006
15	6	4.883616	-0.650690	-1.755774
16	1	5.909917	-0.998079	-1.584109
17	1	4.271878	-1.531371	-1.970202
18	1	4.899525	-0.026559	-2.657748
19	6	5.342502	1.357861	-0.365831
20	1	6.365583	1.000727	-0.193860
21	1	5.355187	1.978139	-1.269645

22	1	5.072215	2.001893	0.474780
23	1	1.842630	-2.608894	-0.927077
24	8	-2.246661	-1.349130	0.613486
25	15	-1.003474	-0.887387	1.356620
26	8	-1.489635	-0.496326	2.848790
27	8	-0.426913	0.471537	0.692407
28	8	0.204226	-1.816286	1.436363
29	15	-1.165256	1.851677	0.073873
30	8	-1.192411	2.825917	1.369288
31	8	-2.624227	1.464713	-0.215553
32	8	-0.254842	2.350286	-0.984565
33	6	1.187500	-0.275474	-2.188776
34	1	0.601119	-1.157174	-2.460541
35	1	0.542642	0.598213	-2.011957
36	1	1.831672	-0.003696	-3.039571
37	12	-3.481893	-0.252333	-0.417714
38	8	-4.268287	-0.965172	-2.174261
39	8	-5.513518	-0.495185	-0.399732
40	6	-5.397216	-0.899664	-1.598092
41	1	-6.299848	-1.201141	-2.150726
42	1	-0.737368	-0.440323	3.460548
43	1	-2.071637	2.807907	1.780903

2-PPi-Mg²⁺-HCOO⁻



B3LYP/6-31G(d)//B3LYP/6-31G(d)

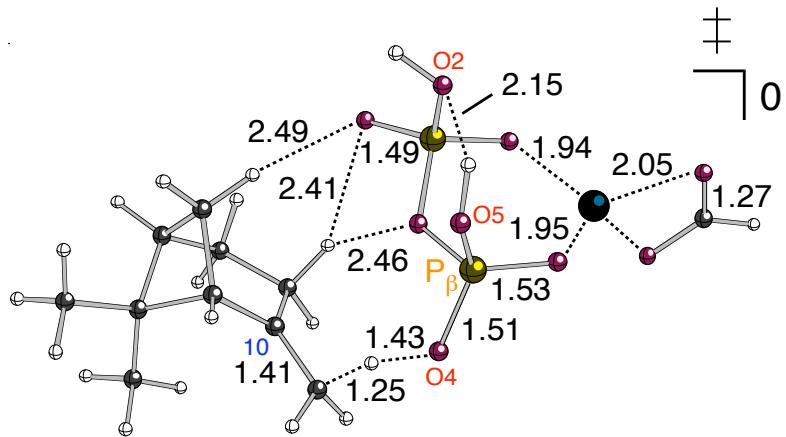
HF = -1991.366463 hartrees (-1249602.36919713 kcal/mol)
 Imaginary Frequencies: none found
 Zero-point correction = 0.327089 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3.061286	0.042827	-0.947032
2	6	2.338895	-1.219327	-0.504951
3	6	2.583301	-1.644137	0.752400
4	6	3.595084	-0.909224	1.615370
5	6	4.160354	0.307548	0.855068
6	6	2.975527	1.077838	0.211005
7	1	0.747398	-0.773032	1.258682
8	1	2.773839	0.359391	-1.952817
9	1	3.137516	-0.578248	2.559816
10	1	4.402561	-1.599703	1.900843
11	1	2.032762	1.122166	0.762798
12	1	3.239163	2.088714	-0.103479
13	1	4.879487	0.864122	1.468173
14	6	4.604301	-0.085255	-0.602807
15	6	5.322558	-1.418828	-0.827178
16	1	6.308904	-1.403491	-0.345406
17	1	4.771161	-2.276533	-0.434803
18	1	5.488523	-1.590620	-1.898558
19	6	5.435626	1.019290	-1.275572
20	1	6.453355	1.032456	-0.864817
21	1	5.517951	0.831538	-2.353372
22	1	5.016096	2.020782	-1.147807
23	1	2.158018	-2.577271	1.123318
24	8	-2.274752	-0.874246	0.988924
25	15	-1.302329	0.033867	1.699816
26	8	-1.860328	0.377761	3.152117
27	8	-1.116675	1.428602	0.961302
28	8	0.117595	-0.587060	2.009380
29	15	-1.258930	1.641945	-0.742751
30	8	-1.1711071	3.246463	-0.793818
31	8	-2.711068	1.236747	-1.039058
32	8	-0.114022	0.960614	-1.384086
33	6	1.466131	-1.935245	-1.494794
34	1	1.006718	-2.833725	-1.068010
35	1	0.683344	-1.260921	-1.858142
36	1	2.059663	-2.239442	-2.368123
37	12	-3.504159	-0.446943	-0.498540
38	8	-4.282719	-1.923796	-1.668062
39	8	-5.520716	-0.716379	-0.280340
40	6	-5.405479	-1.638280	-1.145449
41	1	-6.296793	-2.205474	-1.451213
42	1	-1.212396	0.829686	3.718484
43	1	-2.053944	3.642848	-0.706312

Figure S14c.

TS(S19)



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.3495333 hartrees (-1249591.74564108 kcal/mol)

Imaginary Frequencies: 1 (-388.0038 1/cm)

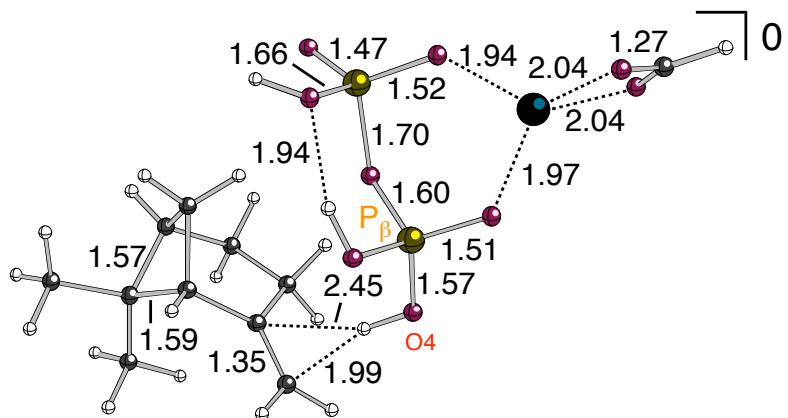
Zero-point correction = 0.324501 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3.252183	0.510102	0.430601
2	6	2.369375	0.807925	-0.712354
3	6	2.053645	-0.355686	-1.592890
4	6	3.167464	-1.448123	-1.597547
5	6	4.053370	-1.324114	-0.350198
6	6	3.140157	-0.983735	0.858059
7	1	1.152131	-0.808080	-1.149658
8	1	3.265541	1.302825	1.183483
9	1	2.687311	-2.431068	-1.611346
10	1	3.770912	-1.366534	-2.508559
11	1	2.143056	-1.430007	0.869245
12	1	3.622267	-1.148437	1.822503
13	1	4.745557	-2.168467	-0.262153
14	6	4.675846	0.106700	-0.231740
15	6	5.143484	0.838651	-1.492623

16	1	6.061290	0.372516	-1.871634
17	1	4.413167	0.831736	-2.306654
18	1	5.378053	1.886171	-1.268278
19	6	5.787524	0.194033	0.822350
20	1	6.694734	-0.286050	0.434994
21	1	6.033349	1.239693	1.041238
22	1	5.532138	-0.295500	1.765432
23	1	1.773725	-0.028066	-2.598719
24	8	-2.477379	-1.537344	-0.139289
25	15	-1.120156	-1.534012	0.557915
26	8	-1.449053	-1.602039	2.174350
27	8	-0.533155	0.018001	0.435054
28	8	-0.014869	-2.450211	0.175210
29	15	-1.260200	1.399477	0.944352
30	8	-1.176376	1.304156	2.549977
31	8	-2.713506	1.370865	0.479389
32	8	-0.373711	2.531867	0.470384
33	6	1.850387	2.096896	-0.927071
34	1	1.499824	2.326497	-1.934693
35	1	0.798698	2.148821	-0.246249
36	1	2.388642	2.914246	-0.439775
37	12	-3.673419	-0.040192	-0.454082
38	8	-4.570735	0.279671	-2.272080
39	8	-5.714806	-0.181458	-0.428544
40	6	-5.670463	0.083262	-1.669748
41	1	-6.611244	0.144095	-2.237601
42	1	-0.788254	-2.168275	2.606045
43	1	-1.523633	0.440670	2.850718

3-PPi-Mg²⁺-HCOO⁻



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.3665818 hartrees (-1249602.44374532 kcal/mol)
 Imaginary Frequencies: none found
 Zero-point correction = 0.328789 (Hartree/Particle)

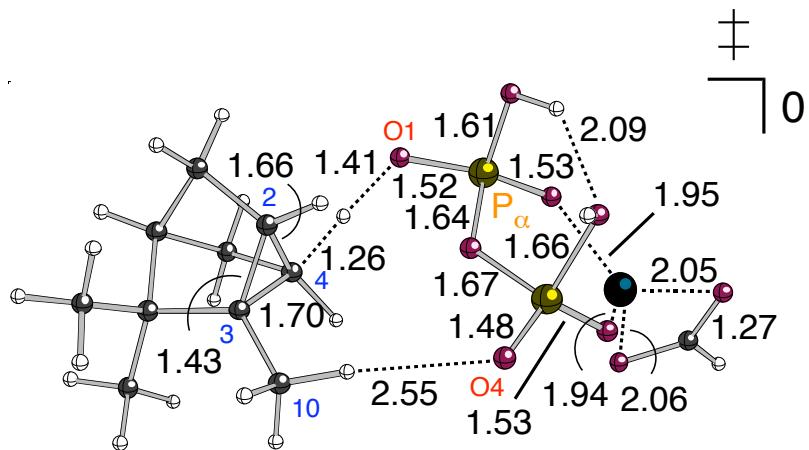
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3.338563	-0.100874	-0.614165
2	6	2.874478	-1.289553	0.184928
3	6	2.747454	-1.014381	1.676300
4	6	3.706556	0.109704	2.168436
5	6	4.097286	1.049402	1.015703
6	6	2.876535	1.222989	0.070139
7	1	1.714617	-0.687248	1.854599
8	1	3.179719	-0.235379	-1.690120
9	1	3.207568	0.683969	2.957235
10	1	4.606676	-0.323413	2.619660
11	1	1.881178	1.257311	0.519973
12	1	2.977998	2.080782	-0.596996
13	1	4.600877	1.949572	1.386595
14	6	4.810089	0.264535	-0.141423
15	6	5.777155	-0.871600	0.201607
16	1	6.687515	-0.468669	0.663407
17	1	5.358320	-1.615065	0.884505
18	1	6.079779	-1.404124	-0.708812
19	6	5.507165	1.202096	-1.139546
20	1	6.427078	1.604700	-0.697288
21	1	5.789217	0.656340	-2.048502
22	1	4.889474	2.052883	-1.441160
23	1	2.877627	-1.936124	2.253335
24	8	-2.869389	1.500312	0.271327
25	15	-1.391465	1.733146	-0.016851
26	8	-1.279287	1.905949	-1.663387
27	8	-0.688870	0.187831	0.105382
28	8	-0.540087	2.697165	0.702063
29	15	-1.205586	-1.091603	-0.711761
30	8	-0.832505	-0.802607	-2.236203
31	8	-2.670295	-1.364263	-0.469953
32	8	-0.329335	-2.308514	-0.255357
33	6	2.627867	-2.493489	-0.366515
34	1	2.416164	-3.369162	0.245249
35	1	0.658132	-2.185747	-0.339356
36	1	2.736877	-2.659791	-1.436392
37	12	-3.982936	-0.085432	0.263287

38	8	-5.284289	-0.632833	1.737001
39	8	-5.937116	-0.133971	-0.322454
40	6	-6.199785	-0.491706	0.867908
41	1	-7.244543	-0.683826	1.152542
42	1	-0.646947	2.618379	-1.858652
43	1	-0.977149	0.151369	-2.437693

Figure S15.

TS(S20)



B3LYP/6-31G(d)//B3LYP/6-31G(d)

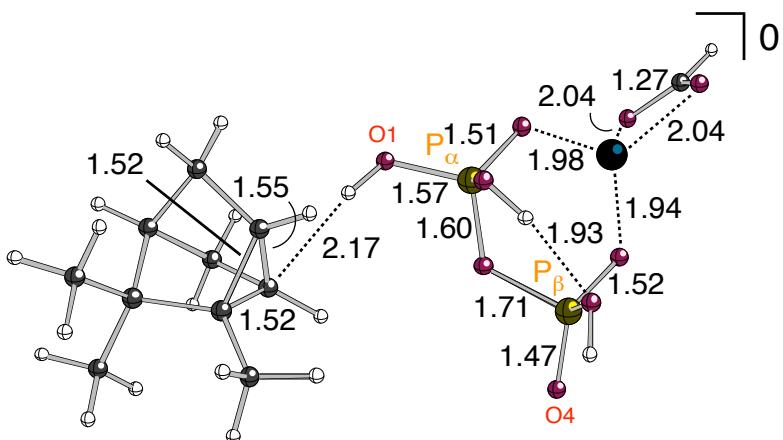
HF = -1991.3520641 hartrees (-1249593.33374339 kcal/mol)
 Imaginary Frequencies: 1 (-601.6371 1/cm)
 Zero-point correction = 0.325215 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.583723	0.483497	0.648659
2	6	3.027394	0.193874	-0.681972
3	6	2.021072	-0.961196	0.059031
4	6	2.990364	-2.039388	0.554643
5	6	4.226921	-1.144986	0.779196
6	6	3.623355	-0.007543	1.646289
7	1	1.160271	-0.795237	0.957561
8	1	2.635846	-2.497584	1.483375
9	1	3.149226	-2.835802	-0.174118

10	1	3.168135	-0.362782	2.575306
11	1	4.333601	0.786994	1.890679
12	6	2.490877	0.877095	-1.913095
13	1	1.474046	1.257066	-1.770640
14	1	3.131109	1.735301	-2.152408
15	1	2.499553	0.208050	-2.779816
16	1	5.109177	-1.637565	1.193162
17	6	4.430075	-0.449376	-0.604989
18	6	4.728683	-1.410667	-1.768655
19	1	5.645229	-1.977140	-1.567251
20	1	3.925148	-2.126641	-1.959241
21	1	4.888707	-0.849480	-2.695682
22	6	5.531825	0.632013	-0.589577
23	1	6.508503	0.168619	-0.408791
24	1	5.585688	1.139844	-1.558645
25	1	5.378023	1.400058	0.173271
26	1	1.282899	-1.114361	-0.725564
27	8	-2.218743	2.780317	0.425338
28	15	-1.620956	1.774362	-0.745131
29	8	-2.794761	0.893137	-1.166972
30	8	-0.640753	0.802330	0.196607
31	8	-0.759234	2.495240	-1.709872
32	15	-1.069288	-0.014978	1.553888
33	8	-2.362221	-0.774485	1.271484
34	8	-1.307787	1.145256	2.642578
35	8	0.161423	-0.811381	1.946910
36	1	1.821052	1.218163	0.878124
37	12	-3.471541	-0.715742	-0.329638
38	8	-3.853991	-2.425584	-1.402746
39	8	-5.434966	-1.290142	-0.338756
40	6	-5.066269	-2.265790	-1.063502
41	1	-5.819424	-2.991577	-1.406016
42	1	-1.872972	1.846794	2.257020
43	1	-1.831524	3.662729	0.301247

5-PPi-Mg²⁺-HCOO⁻



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.3813027 hartrees (-1249611.68125728 kcal/mol)

Imaginary Frequencies: none found

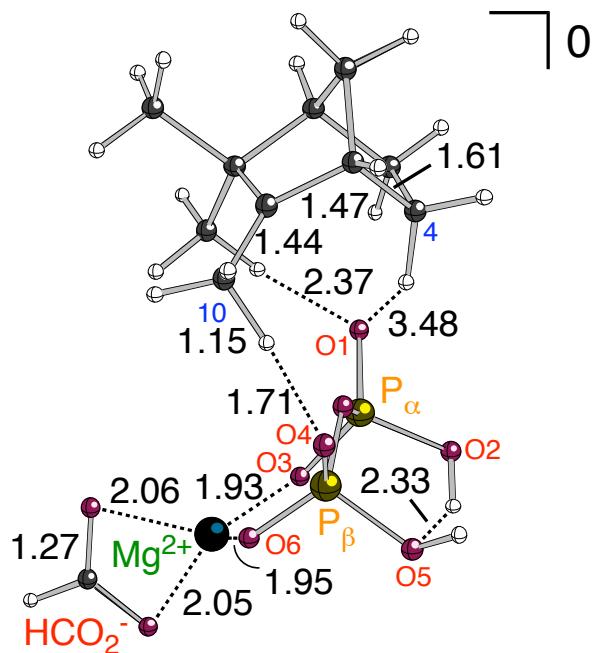
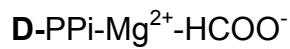
Zero-point correction = 0.329339 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.964458	-0.505501	-0.814376
2	6	-3.916324	0.516742	-0.219546
3	6	-2.752298	0.033016	0.624377
4	6	-3.268296	-1.061338	1.559300
5	6	-4.399805	-1.574021	0.632796
6	6	-3.595964	-1.889070	-0.653942
7	1	-1.011659	-1.028609	-0.107747
8	1	-2.519242	-1.836590	1.763334
9	1	-3.619056	-0.676286	2.520103
10	1	-2.854793	-2.681893	-0.492658
11	1	-4.215533	-2.181760	-1.505217
12	6	-3.991004	1.932356	-0.737651
13	1	-2.998328	2.302814	-1.018343
14	1	-4.631494	2.001620	-1.625347
15	1	-4.392763	2.615461	0.020263
16	1	-5.015232	-2.385938	1.027476
17	6	-5.167246	-0.261028	0.255204
18	6	-5.868753	0.408317	1.451015
19	1	-6.636349	-0.254530	1.869128
20	1	-5.179150	0.676306	2.255513
21	1	-6.372437	1.329307	1.134959
22	6	-6.210068	-0.456670	-0.860884

23	1	-6.988764	-1.160523	-0.542206
24	1	-6.706112	0.492946	-1.093261
25	1	-5.777171	-0.831517	-1.792303
26	1	-1.943520	0.708616	0.891135
27	8	1.977501	2.397321	-1.210865
28	15	2.240445	1.975445	0.372519
29	8	3.577748	1.245696	0.382680
30	8	1.081987	0.724635	0.465857
31	8	1.863967	3.051482	1.303297
32	15	1.067958	-0.537215	-0.518147
33	8	2.365762	-1.304502	-0.492465
34	8	0.665156	0.044611	-1.950341
35	8	-0.124138	-1.461481	-0.071641
36	1	-2.319642	-0.239048	-1.648091
37	12	4.107094	-0.598018	0.122939
38	8	5.318211	-1.687339	1.350812
39	8	5.851396	-1.201992	-0.745845
40	6	6.120395	-1.750756	0.367995
41	1	7.069853	-2.293347	0.483856
42	1	1.069999	0.936073	-2.074334
43	1	1.592414	3.289939	-1.234748

Figure S16a.



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.3626722 hartrees (-1249599.99043222 kcal/mol)

Imaginary Frequencies: none found

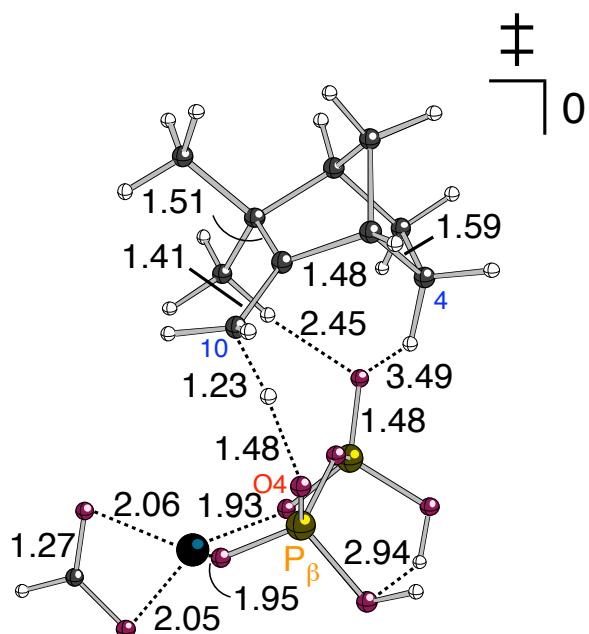
Zero-point correction = 0.328216 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3.792019	-0.413287	0.949543
2	6	2.860684	0.719518	0.986302
3	6	2.971076	-1.436955	0.018099
4	6	3.142629	-0.853151	-1.409721
5	6	3.882016	0.480117	-1.139068
6	6	4.884903	0.035165	-0.053441
7	1	3.460635	-2.406450	0.155319
8	1	3.779519	-1.501849	-2.019842
9	1	2.186208	-0.750054	-1.926556
10	1	5.507567	-0.808816	-0.364344
11	1	5.537882	0.821049	0.334495
12	6	1.991545	1.035170	2.083133
13	1	2.473350	0.887527	3.056549
14	1	1.491319	2.002444	2.007904
15	1	1.160277	0.236418	2.122088
16	1	4.306355	0.955889	-2.026371
17	6	2.942275	1.438477	-0.330642
18	6	1.593729	1.782089	-0.990974
19	1	1.787260	2.386927	-1.883799
20	1	1.034590	0.898313	-1.300734
21	1	0.965887	2.378951	-0.320764
22	6	3.667644	2.792905	-0.007888
23	1	3.906257	3.272322	-0.962614
24	1	3.001080	3.453450	0.553519
25	1	4.595280	2.682603	0.558976
26	1	1.927999	-1.538022	0.321760
27	8	-1.400054	-2.785389	-1.452272
28	15	-1.096482	-1.194033	-1.475359
29	8	-0.046857	-0.857685	-2.466848
30	8	-0.414700	-0.957267	0.046915
31	8	-2.435225	-0.438890	-1.439147
32	15	-1.138828	-1.013023	1.508020
33	8	-0.037518	-0.918995	2.529489
34	8	-1.831787	-2.497579	1.540614
35	8	-2.292991	-0.015764	1.511592

36	1	4.076431	-0.839529	1.912190
37	12	-3.159507	0.710916	-0.072442
38	8	-5.065649	1.456701	-0.059478
39	6	-4.538935	2.605235	-0.186649
40	1	-5.193486	3.488980	-0.238850
41	8	-3.282060	2.761848	-0.254580
42	1	-2.014405	-3.003275	-0.727984
43	1	-1.229049	-3.129558	1.966001

TS(S21)



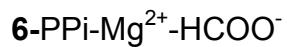
B3LYP/6-31G(d)//B3LYP/6-31G(d)

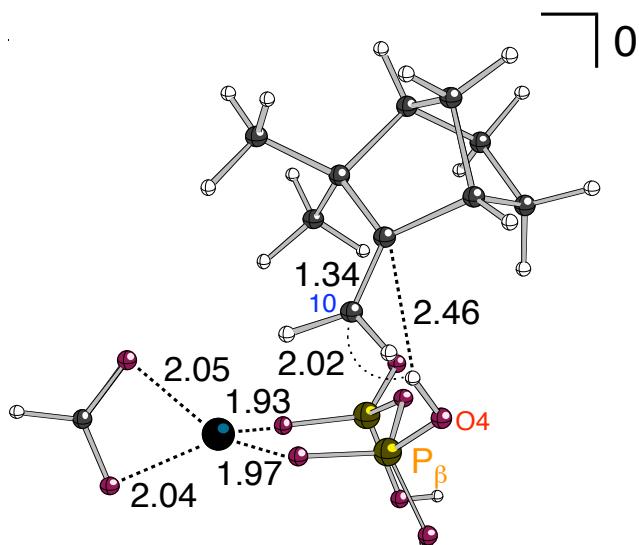
HF = -1991.3623475 hartrees (-1249599.78667972 kcal/mol)
 Imaginary Frequencies: 1 (-171.1044 1/cm)
 Zero-point correction = 0.325852 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3.827867	-0.420011	0.885300
2	6	2.898788	0.729719	0.959680
3	6	3.041678	-1.462597	-0.023785
4	6	3.158009	-0.864003	-1.454944

5	6	3.866922	0.487849	-1.197681
6	6	4.897577	0.069254	-0.126082
7	1	3.559593	-2.421559	0.079739
8	1	3.795163	-1.491462	-2.086902
9	1	2.187244	-0.785387	-1.948027
10	1	5.544063	-0.752507	-0.449011
11	1	5.529084	0.875301	0.256563
12	6	2.094717	1.056547	2.068487
13	1	2.530372	0.806593	3.040695
14	1	1.601962	2.029877	2.044599
15	1	1.172633	0.250408	2.091915
16	1	4.268450	0.966755	-2.094339
17	6	2.927507	1.437390	-0.378126
18	6	1.541930	1.706933	-0.997356
19	1	1.675343	2.266437	-1.929899
20	1	0.995318	0.793528	-1.234202
21	1	0.927793	2.322813	-0.331044
22	6	3.611530	2.820777	-0.135614
23	1	3.763853	3.298847	-1.108821
24	1	2.964155	3.466160	0.465560
25	1	4.581004	2.753958	0.364700
26	1	2.008293	-1.601339	0.298788
27	8	-1.505312	-2.914173	-1.332924
28	15	-1.151533	-1.332522	-1.403132
29	8	-0.109496	-1.045828	-2.414505
30	8	-0.426239	-1.068622	0.095003
31	8	-2.484477	-0.566734	-1.357310
32	15	-1.080263	-0.875825	1.566020
33	8	0.093432	-0.677734	2.509436
34	8	-1.824499	-2.279403	1.898860
35	8	-2.177252	0.177880	1.501792
36	1	4.149331	-0.829595	1.844411
37	12	-3.145227	0.731780	-0.094107
38	8	-5.074018	1.414864	-0.056814
39	6	-4.594347	2.558155	-0.332013
40	1	-5.279784	3.412215	-0.442957
41	8	-3.347866	2.741914	-0.481877
42	1	-2.356101	-3.052409	-0.884833
43	1	-1.185356	-2.942196	2.208533





B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.3885094 hartrees (-1249616.20353359 kcal/mol)

Imaginary Frequencies: none found

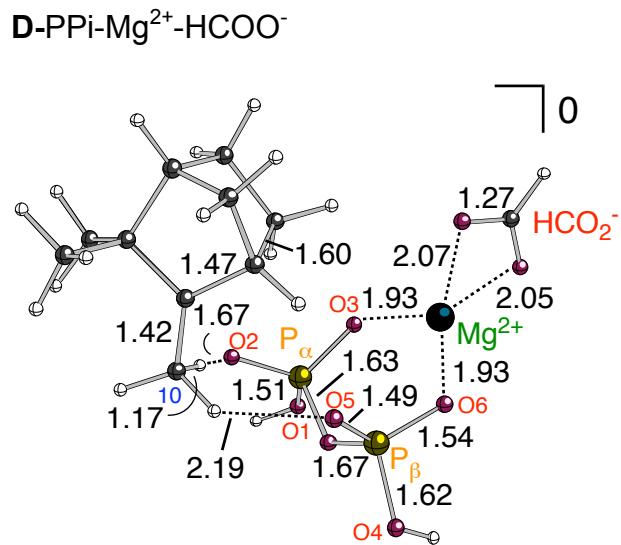
Zero-point correction = 0.329647 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	4.134846	-0.662809	0.852166
2	6	3.077382	0.421741	0.861487
3	6	3.577292	-1.876001	0.045896
4	6	3.588661	-1.359269	-1.428473
5	6	4.085327	0.099312	-1.283410
6	6	5.142399	-0.076237	-0.167247
7	1	4.242329	-2.737052	0.173862
8	1	4.298034	-1.930917	-2.036728
9	1	2.615168	-1.441762	-1.917267
10	1	5.931700	-0.787817	-0.434037
11	1	5.610371	0.854047	0.166603
12	6	2.373525	0.840479	1.925905
13	1	2.561285	0.440556	2.921238
14	1	1.659691	1.659518	1.860817
15	1	1.025052	-0.640642	1.689025
16	1	4.440187	0.539624	-2.220195
17	6	3.008046	0.990131	-0.572127
18	6	1.598252	0.905226	-1.188095
19	1	1.626559	1.184419	-2.248094

20	1	1.163190	-0.095980	-1.119860
21	1	0.920484	1.605811	-0.686618
22	6	3.439373	2.475452	-0.587952
23	1	3.429505	2.856470	-1.616121
24	1	2.746360	3.085349	0.001495
25	1	4.443143	2.627739	-0.180556
26	1	2.583374	-2.181183	0.386080
27	8	-3.603611	-2.286362	-0.169020
28	15	-2.609665	-1.430413	-1.181902
29	8	-2.385279	-2.117854	-2.463892
30	8	-1.191611	-1.524209	-0.242904
31	8	-3.055409	0.022709	-1.048577
32	15	-1.085421	-1.002384	1.267321
33	8	0.354435	-1.373172	1.779848
34	8	-2.039932	-1.934649	2.126854
35	8	-1.390091	0.480370	1.360942
36	1	4.516449	-0.924674	1.842589
37	12	-2.443122	1.497017	0.036769
38	8	-3.526633	3.140100	0.567967
39	6	-2.649415	3.822314	-0.047719
40	1	-2.749872	4.916852	-0.084518
41	8	-1.659657	3.269821	-0.620912
42	1	-3.799101	-3.146939	-0.577957
43	1	-2.791984	-2.251733	1.572714

Figure S16b.



B3LYP/6-31G(d)//B3LYP/6-31G(d)

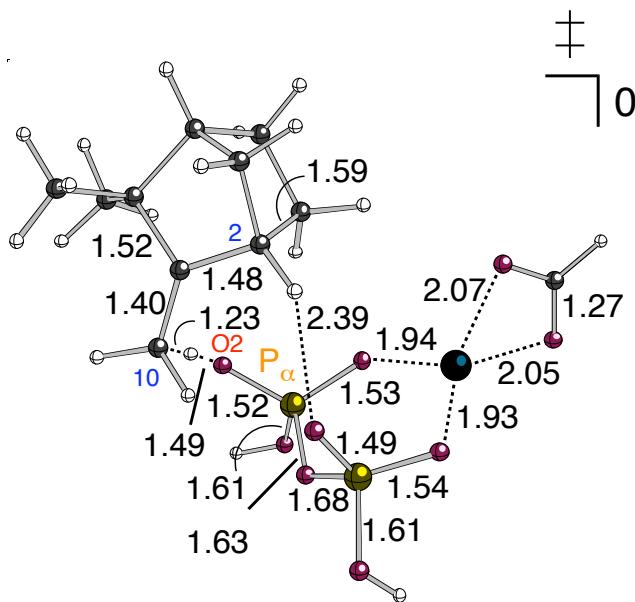
HF = -1991.368993 hartrees (-1249603.95679743 kcal/mol)
 Imaginary Frequencies: none found
 Zero-point correction = 0.327542 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.975083	0.705550	-1.080045
2	6	2.618063	-0.491345	-0.516404
3	6	1.456683	1.452456	0.239483
4	6	2.748687	2.055892	0.854989
5	6	3.858522	1.481308	-0.054485
6	6	3.184516	1.607757	-1.437656
7	1	0.748537	2.214075	-0.100568
8	1	2.743348	3.148424	0.788465
9	1	2.873863	1.797975	1.909232
10	1	2.865202	2.628109	-1.669591
11	1	3.776692	1.233216	-2.276952
12	6	2.045560	-1.789777	-0.457001
13	1	1.291900	-1.686759	0.428523
14	1	1.351714	-2.005448	-1.277080
15	1	2.729699	-2.595710	-0.183901
16	1	4.835361	1.959648	0.057906
17	6	3.923939	-0.074741	0.122464
18	6	4.054122	-0.584443	1.574348
19	1	4.920443	-0.109973	2.048741
20	1	3.166651	-0.371686	2.175369
21	1	4.213400	-1.667026	1.594602
22	6	5.095300	-0.674313	-0.709944
23	1	6.038988	-0.336174	-0.268554
24	1	5.074920	-1.767831	-0.677211
25	1	5.081816	-0.365753	-1.758133
26	1	0.921442	0.782285	0.914136
27	8	-2.114275	-2.049806	2.595666
28	15	-1.258695	-1.258098	1.474854
29	8	-1.743568	0.192376	1.493254
30	8	-1.790202	-1.960443	0.097668
31	8	0.217872	-1.514764	1.677821
32	15	-1.867846	-1.272047	-1.419910
33	8	-2.807996	-0.059358	-1.280780
34	8	-2.671328	-2.429783	-2.208503
35	8	-0.500912	-1.083008	-1.981291
36	1	1.181519	0.512138	-1.800437
37	12	-2.594877	1.252500	0.119770

38	8	-3.837925	2.838972	0.470031
39	8	-1.757555	3.112214	-0.249472
40	6	-2.876824	3.587406	0.111302
41	1	-3.021974	4.678731	0.113957
42	1	-3.623049	-2.366320	-2.026074
43	1	-1.588630	-2.785433	2.948704

TS(S22)



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.3688466 hartrees (-1249603.86492997 kcal/mol)

Imaginary Frequencies: 1 (-140.8724 1/cm)

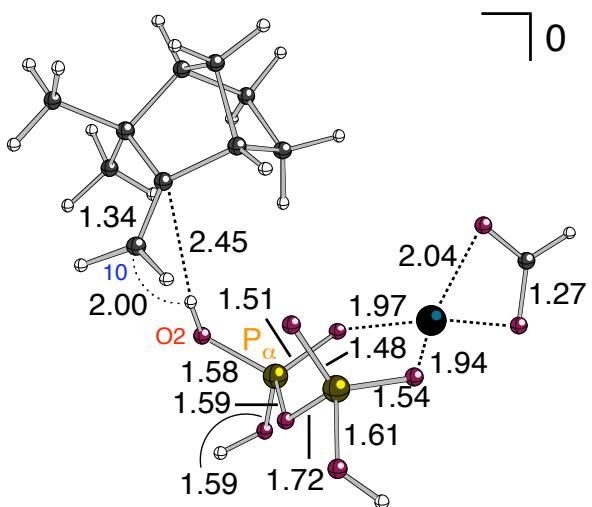
Zero-point correction = 0.325881 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.014546	0.706629	-1.158735
2	6	2.618695	-0.486802	-0.519171
3	6	1.465912	1.561718	0.061513
4	6	2.751362	2.158430	0.703527
5	6	3.881214	1.488889	-0.111355
6	6	3.272138	1.536399	-1.530253
7	1	0.805096	2.330188	-0.350562

8	1	2.791092	3.244148	0.568935
9	1	2.816413	1.966145	1.777143
10	1	3.004316	2.547770	-1.851456
11	1	3.886255	1.078747	-2.310686
12	6	2.039278	-1.759798	-0.451184
13	1	1.246562	-1.585509	0.469240
14	1	1.320408	-1.994252	-1.242003
15	1	2.674309	-2.577133	-0.105171
16	1	4.864681	1.951097	0.012070
17	6	3.901403	-0.053213	0.169592
18	6	3.924309	-0.462243	1.658457
19	1	4.768974	0.024687	2.158937
20	1	3.004428	-0.191678	2.182336
21	1	4.053847	-1.544385	1.761225
22	6	5.112285	-0.723476	-0.536754
23	1	6.034021	-0.377107	-0.056508
24	1	5.065422	-1.812524	-0.438383
25	1	5.175168	-0.483481	-1.601301
26	1	0.875077	0.962451	0.756558
27	8	-1.968486	-2.031297	2.631877
28	15	-1.183362	-1.249716	1.459035
29	8	-1.670762	0.196269	1.480160
30	8	-1.742611	-1.978862	0.117465
31	8	0.311199	-1.492258	1.617933
32	15	-1.879802	-1.301198	-1.410594
33	8	-2.833603	-0.104213	-1.243519
34	8	-2.693279	-2.478372	-2.156547
35	8	-0.530716	-1.102013	-2.005236
36	1	1.255843	0.487837	-1.908948
37	12	-2.612468	1.229813	0.136019
38	8	-3.932779	2.734469	0.553348
39	8	-1.903333	3.132317	-0.248533
40	6	-3.032156	3.540104	0.161880
41	1	-3.239539	4.620995	0.180259
42	1	-3.643359	-2.407305	-1.968128
43	1	-1.440901	-2.782887	2.946930

6-PPi-Mg²⁺-HCOO⁻



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.3856877 hartrees (-1249614.43288863 kcal/mol)
 Imaginary Frequencies: none found
 Zero-point correction = 0.328733 (Hartree/Particle)

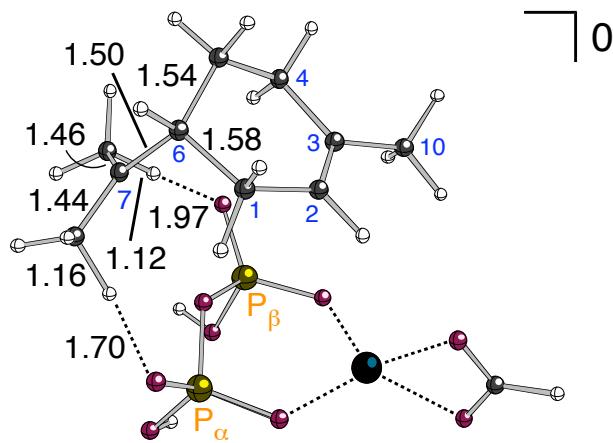
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.186753	0.698759	-1.248167
2	6	2.739889	-0.532517	-0.560486
3	6	1.599147	1.644622	-0.154831
4	6	2.868947	2.201277	0.564083
5	6	4.021494	1.444364	-0.135961
6	6	3.501860	1.439761	-1.593982
7	1	1.019914	2.445700	-0.626808
8	1	2.976071	3.277748	0.390622
9	1	2.845987	2.056289	1.647160
10	1	3.327403	2.447713	-1.987019
11	1	4.135416	0.896060	-2.301068
12	6	2.267521	-1.785295	-0.670377
13	1	0.902142	-1.474831	0.759018
14	1	1.427149	-2.010754	-1.323848
15	1	2.765514	-2.624063	-0.185554
16	1	5.006660	1.893400	0.026097
17	6	3.990787	-0.082256	0.224546
18	6	3.882706	-0.386629	1.731770
19	1	4.709035	0.081333	2.281300
20	1	2.942910	-0.037240	2.168747

21	1	3.940989	-1.467148	1.907033
22	6	5.258797	-0.783910	-0.312434
23	1	6.142716	-0.437996	0.237729
24	1	5.186560	-1.869605	-0.184496
25	1	5.425178	-0.587866	-1.375695
26	1	0.925738	1.120724	0.529514
27	8	-1.850801	-1.813211	2.759069
28	15	-1.217491	-1.199910	1.432243
29	8	-1.517645	0.278476	1.372631
30	8	-1.866912	-1.999495	0.222346
31	8	0.309870	-1.584529	1.559370
32	15	-2.045609	-1.363588	-1.370174
33	8	-2.958891	-0.144180	-1.175200
34	8	-2.925886	-2.548258	-2.006048
35	8	-0.696670	-1.237869	-1.963345
36	1	1.492919	0.477340	-2.060661
37	12	-2.601987	1.293498	0.073150
38	8	-3.979430	2.669248	0.689047
39	8	-2.113069	3.228468	-0.368898
40	6	-3.206280	3.547107	0.193196
41	1	-3.490817	4.607842	0.252196
42	1	-3.874280	-2.386098	-1.870348
43	1	-1.511133	-2.698944	2.971349

Figure S17.

A-PPi-Mg²⁺-HCOO⁻



0

B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.3620115 hartrees (-1249599.57583637 kcal/mol)
Imaginary Frequencies: none found

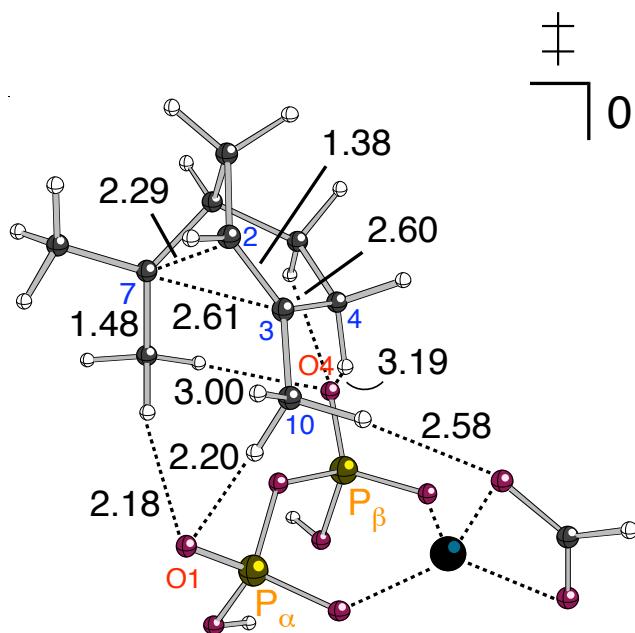
Zero-point correction = 0.325867 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3.149935	-0.667670	-0.477004
2	6	3.247956	-1.027159	0.938188
3	6	2.949800	-1.700720	-1.463761
4	6	3.264768	0.751542	-0.943713
5	6	3.624345	1.830135	0.094798
6	6	2.457064	2.248105	0.999434
7	6	1.179544	2.488386	0.227155
8	6	1.017204	2.013916	-1.015162
9	6	0.109672	3.272521	0.940589
10	6	2.029351	1.217895	-1.802122
11	1	3.990341	-0.417899	1.464560
12	1	3.431627	-2.091533	1.095021
13	1	2.279271	-0.772125	1.437564
14	1	1.810030	-1.840343	-1.589528
15	1	3.318274	-2.681719	-1.155148
16	1	3.273697	-1.430826	-2.472323
17	1	4.100541	0.677751	-1.660802
18	1	3.948919	2.706493	-0.479752
19	1	4.492245	1.524299	0.692169
20	1	2.740146	3.167692	1.530138
21	1	2.259567	1.507212	1.785482
22	1	0.088182	2.219206	-1.546191
23	1	-0.178009	2.770514	1.873058
24	1	-0.786919	3.387850	0.325264
25	1	0.477381	4.271824	1.213201
26	1	2.416813	1.830418	-2.628117
27	1	1.536255	0.360198	-2.271735
28	8	-1.142813	-3.408160	-0.431224
29	15	-0.766934	-1.943625	-0.997525
30	8	0.209176	-2.054017	-2.130508
31	8	0.077154	-1.271596	0.263454
32	8	-2.040236	-1.111853	-1.175020
33	15	-0.492202	-0.789428	1.733341
34	8	0.697279	-0.445895	2.568837
35	8	-1.233023	-2.160032	2.266983
36	8	-1.618044	0.209598	1.482033
37	1	-1.577489	-3.331520	0.440297
38	1	-0.665629	-2.594703	2.924751
39	12	-2.576465	0.463528	-0.187004

40	8	-4.446267	1.298125	-0.261446
41	6	-3.912026	2.272805	-0.872773
42	1	-4.543429	3.115520	-1.192630
43	8	-2.667334	2.300908	-1.124638

TS(S24)



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.3372833 hartrees (-1249584.05864358 kcal/mol)

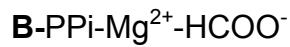
Imaginary Frequencies: 1 (-123.0867 1/cm)

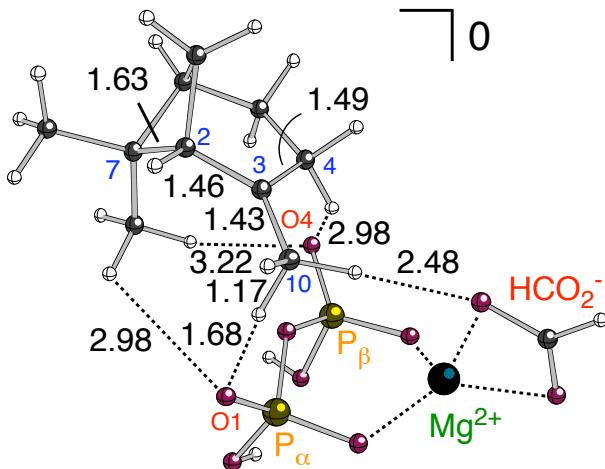
Zero-point correction = 0.327097 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3.583815	1.570790	-0.453942
2	6	2.211625	1.553897	-0.361055
3	6	1.561125	1.233133	0.958143
4	6	2.424761	0.320461	1.880523
5	6	3.740080	-0.058052	1.181849
6	6	4.437058	1.247970	0.760191
7	1	1.353594	2.192269	1.453379
8	1	4.047787	1.897825	-1.382241

9	1	2.683492	0.843597	2.806628
10	1	1.835860	-0.552964	2.174492
11	1	4.403713	2.021371	1.536546
12	1	5.485333	1.109883	0.486567
13	1	0.583886	0.783024	0.775855
14	6	1.334241	1.872798	-1.524190
15	1	0.824784	0.963678	-1.886296
16	1	0.537753	2.561557	-1.213666
17	1	1.894274	2.311915	-2.355210
18	1	4.334273	-0.730560	1.819574
19	6	3.504384	-0.703533	-0.185917
20	6	2.312614	-1.541288	-0.461020
21	1	2.663055	-2.557217	-0.698982
22	1	1.596305	-1.584980	0.355787
23	1	1.749598	-1.230745	-1.360287
24	6	4.674980	-1.005523	-1.079692
25	1	5.051510	-1.992008	-0.764109
26	1	4.356767	-1.110911	-2.121068
27	1	5.504432	-0.302883	-1.015222
28	8	-2.018436	-2.553940	-1.757966
29	15	-1.296325	-1.123078	-1.548170
30	8	-0.117406	-0.966367	-2.448748
31	8	-0.705654	-1.252231	0.002746
32	8	-2.361632	-0.012836	-1.492358
33	15	-1.494465	-1.337802	1.447754
34	8	-0.490815	-1.677603	2.490459
35	8	-2.551330	-2.574967	1.170042
36	8	-2.360521	-0.075486	1.536156
37	1	-2.580499	-2.756945	-0.984251
38	1	-2.222187	-3.369737	1.621244
39	12	-2.669784	1.113581	0.042896
40	8	-3.872545	2.765675	0.049991
41	6	-2.815085	3.467385	0.061885
42	1	-2.905608	4.564830	0.058727
43	8	-1.661218	2.940378	0.077598





B3LYP/6-31G(d)//B3LYP/6-31G(d)

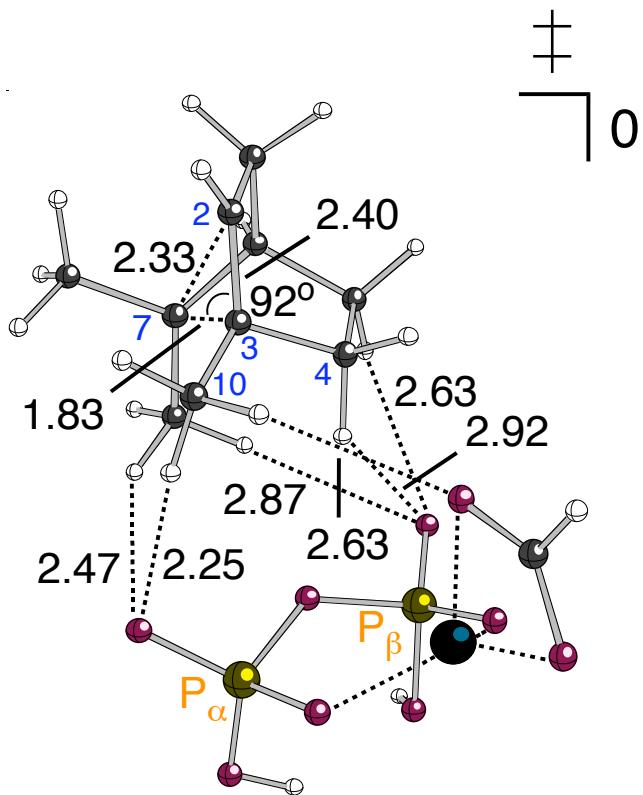
HF = -1991.3457249 hartrees (-1249589.355832 kcal/mol)
 Imaginary Frequencies: none found
 Zero-point correction = 0.326801 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3.409835	1.119943	-0.728138
2	6	2.006275	1.410396	-0.442287
3	6	1.577564	1.303677	0.980729
4	6	2.545914	0.515896	1.903451
5	6	3.901143	0.300301	1.213121
6	6	4.286553	1.608169	0.478058
7	1	1.488110	2.356109	1.304513
8	1	3.710194	1.353374	-1.751994
9	1	2.695889	1.074223	2.833775
10	1	2.075491	-0.432490	2.179853
11	1	4.004162	2.558182	0.941960
12	1	5.334812	1.659120	0.183982
13	1	0.553794	0.922602	1.030716
14	6	1.065961	1.746164	-1.466510
15	1	0.647194	0.719232	-1.836170
16	1	0.171999	2.269598	-1.111322
17	1	1.509478	2.191382	-2.360824
18	1	4.634656	-0.147156	1.891708
19	6	3.729456	-0.381860	-0.184036
20	6	2.674917	-1.469875	-0.376257
21	1	3.043656	-2.407271	0.058528

22	1	1.712808	-1.251738	0.088862
23	1	2.486402	-1.648319	-1.440706
24	6	5.054735	-0.862378	-0.790638
25	1	5.381558	-1.763630	-0.258048
26	1	4.919068	-1.131273	-1.844044
27	1	5.865160	-0.131052	-0.728987
28	8	-1.665089	-2.578463	-1.779405
29	15	-1.272264	-1.036599	-1.542894
30	8	-0.136262	-0.639758	-2.442955
31	8	-0.671344	-1.025131	0.004714
32	8	-2.530381	-0.155469	-1.505417
33	15	-1.452235	-1.354950	1.435154
34	8	-0.422442	-1.475154	2.496033
35	8	-2.161719	-2.802143	1.078280
36	8	-2.602927	-0.345670	1.516603
37	1	-2.137618	-2.925304	-0.994799
38	1	-1.660251	-3.509062	1.517785
39	12	-2.945790	0.890863	0.070242
40	8	-4.139609	2.541521	0.089151
41	6	-3.082212	3.243694	0.114781
42	1	-3.173626	4.340658	0.119873
43	8	-1.928579	2.715385	0.134857

TS(S23)



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.3193929 hartrees (-1249572.83223868 kcal/mol)

Imaginary Frequencies: 1 (-341.3778 1/cm)

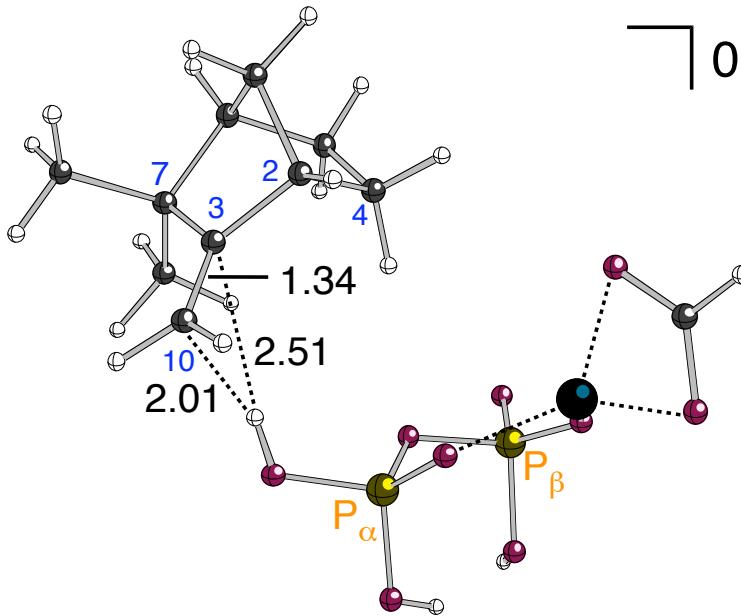
Zero-point correction = 0.327341 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3.687323	1.530492	-0.262104
2	6	2.456928	0.891708	-0.478911
3	6	1.629982	0.814682	0.874988
4	6	2.478324	0.063423	1.922757
5	6	3.738591	-0.350798	1.137051
6	6	4.519150	0.936623	0.816778
7	1	1.354254	1.832122	1.159994
8	1	4.074403	2.315553	-0.915742
9	1	2.744154	0.699088	2.773242
10	1	1.918848	-0.786498	2.319888
11	1	4.648374	1.632787	1.660240

12	1	5.531911	0.755457	0.431985
13	1	0.715328	0.280052	0.626118
14	6	1.657585	1.205953	-1.724916
15	1	1.005362	0.370300	-2.007736
16	1	1.004658	2.065949	-1.533775
17	1	2.308404	1.442049	-2.574281
18	1	4.342912	-1.121759	1.623951
19	6	3.222140	-0.754602	-0.274928
20	6	2.130677	-1.807364	-0.344330
21	1	2.639977	-2.781894	-0.299762
22	1	1.405485	-1.769735	0.465117
23	1	1.574580	-1.774720	-1.287567
24	6	4.267207	-1.049494	-1.353469
25	1	4.692414	-2.042921	-1.167946
26	1	3.790418	-1.084582	-2.338172
27	1	5.096855	-0.339034	-1.404324
28	8	-2.613260	-2.361345	-1.565829
29	15	-1.614798	-1.090018	-1.515404
30	8	-0.506453	-1.216224	-2.499328
31	8	-0.944075	-1.235924	0.008438
32	8	-2.445669	0.209030	-1.462476
33	15	-1.625928	-1.120494	1.504081
34	8	-0.598292	-1.529680	2.498760
35	8	-2.865034	-2.202653	1.394740
36	8	-2.300818	0.256327	1.565332
37	1	-3.131427	-2.413780	-0.738998
38	1	-2.586019	-3.036451	1.808047
39	12	-2.394011	1.424243	0.027600
40	8	-3.146420	3.325761	0.033200
41	6	-1.951559	3.747892	-0.016240
42	1	-1.773945	4.834721	-0.043213
43	8	-0.959480	2.957079	-0.035145

6-PPi-Mg²⁺-HCOO⁻



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.3875988 hartrees (-1249615.63212299 kcal/mol)

Imaginary Frequencies: none found

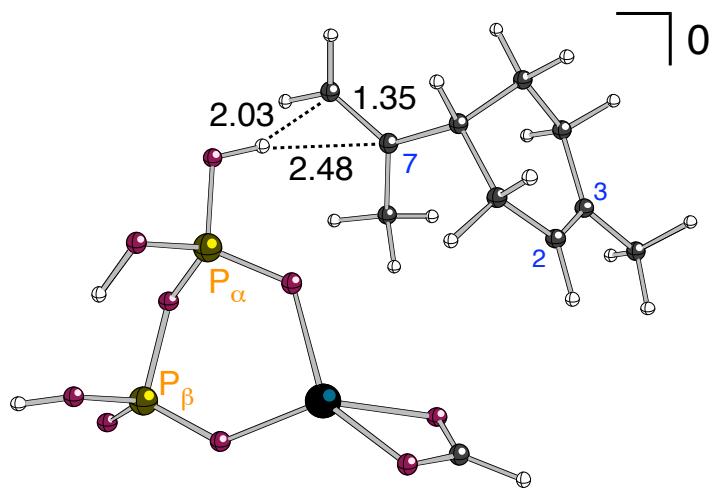
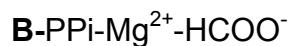
Zero-point correction = 0.329487 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.631963	1.551237	-0.118206
2	6	2.975149	0.276826	-0.860098
3	6	1.608685	1.210431	1.007711
4	6	2.469526	0.438179	2.056492
5	6	3.850778	0.344240	1.366591
6	6	3.926332	1.743728	0.711161
7	1	1.188761	2.133807	1.418931
8	1	2.321468	2.375969	-0.764470
9	1	2.560726	1.013275	2.984186
10	1	2.044691	-0.531384	2.325970
11	1	3.843213	2.560570	1.436522
12	1	4.815809	1.911893	0.096866
13	1	0.771133	0.613713	0.633490
14	6	2.683770	-0.001211	-2.141183
15	1	1.018712	-1.050343	-1.727766
16	1	2.168059	0.719233	-2.773288
17	1	3.041773	-0.906052	-2.630269
18	1	4.667212	0.084854	2.047506

19	6	3.793533	-0.599002	0.113745
20	6	3.136530	-1.969162	0.373392
21	1	3.664107	-2.500157	1.175007
22	1	2.083870	-1.890915	0.658548
23	1	3.186221	-2.595382	-0.524838
24	6	5.216612	-0.848306	-0.435414
25	1	5.794446	-1.447409	0.278702
26	1	5.178310	-1.399312	-1.381480
27	1	5.764298	0.081215	-0.617002
28	8	-2.179791	-2.077035	-1.947086
29	15	-1.104311	-1.156076	-1.231098
30	8	0.267887	-1.704136	-1.766272
31	8	-1.173167	-1.512781	0.329497
32	8	-1.287010	0.332548	-1.457038
33	15	-2.542675	-1.236777	1.303107
34	8	-2.290259	-1.773139	2.650402
35	8	-3.618318	-2.156697	0.441461
36	8	-2.931744	0.208783	1.007011
37	1	-2.910848	-2.297714	-1.321653
38	1	-3.812352	-2.966845	0.943517
39	12	-2.254893	1.534976	-0.223296
40	8	-3.256929	3.178928	-0.894493
41	6	-2.351545	3.867445	-0.328657
42	1	-2.402810	4.964929	-0.377635
43	8	-1.389583	3.317618	0.292189

Figure S18.



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.3838426 hartrees (-1249613.27506993 kcal/mol)

Imaginary Frequencies: none found

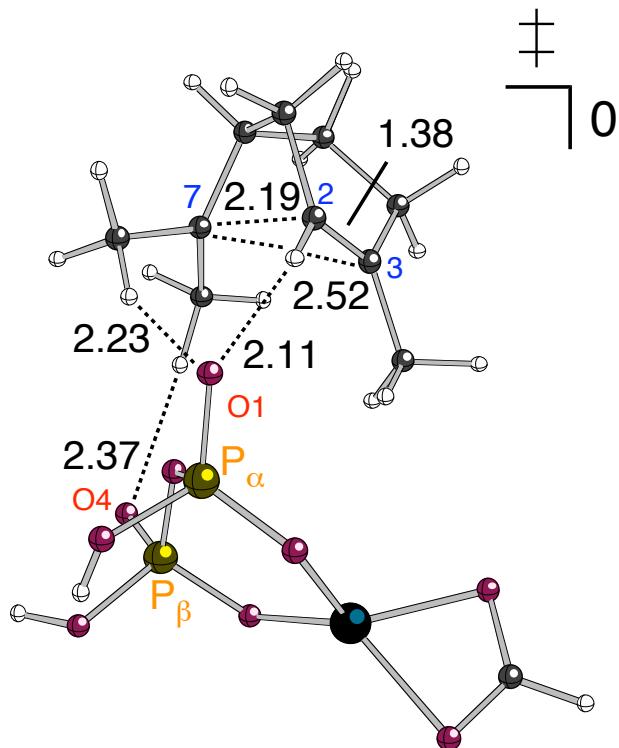
Zero-point correction = 0.327602 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.156515	-1.836317	0.346436
2	6	1.865449	-0.990822	1.563569
3	6	1.705788	-3.105254	0.278420
4	6	2.993050	-1.275856	-0.803573
5	6	4.509598	-1.542147	-0.615399
6	6	5.150491	-0.696577	0.493478
7	6	4.693952	0.747051	0.481891
8	6	3.627520	1.136382	-0.229660
9	6	5.488900	1.704628	1.331430
10	6	2.779900	0.227739	-1.086047
11	1	1.411255	-0.031804	1.290770
12	1	2.785785	-0.744478	2.103558
13	1	1.194352	-1.511984	2.253294
14	1	-0.078380	-2.506784	-0.485276
15	1	1.180204	-3.570369	1.110199
16	1	1.932267	-3.746201	-0.572163
17	1	2.689373	-1.833607	-1.698194
18	1	4.997841	-1.299785	-1.568684
19	1	4.682802	-2.608580	-0.431079
20	1	6.244674	-0.736192	0.391034
21	1	4.944366	-1.135958	1.482587
22	1	3.323115	2.181871	-0.201582
23	1	5.507026	1.382996	2.382706
24	1	5.075603	2.717565	1.296286
25	1	6.537055	1.751440	1.003858
26	1	3.009199	0.413853	-2.146921
27	1	1.722097	0.494549	-0.973792
28	8	-3.041777	-1.548690	-1.785271
29	15	-1.850572	-1.254770	-0.779072
30	8	-1.020540	-2.587950	-0.797412
31	8	-2.507939	-1.120928	0.674937
32	8	-1.025926	-0.026394	-1.118038
33	15	-3.608629	0.103330	1.108374
34	8	-4.088526	-0.139548	2.478099
35	8	-4.762686	-0.218449	-0.036765

36	8	-2.940481	1.395526	0.644883
37	1	-3.883879	-1.168499	-1.438451
38	1	-5.532929	-0.621797	0.399315
39	12	-1.352874	1.774676	-0.381185
40	8	-0.991115	3.462867	-1.465866
41	6	0.038048	3.621308	-0.739328
42	1	0.689316	4.490019	-0.913600
43	8	0.333500	2.798369	0.183375

TS(S25)



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.3427485 hartrees (-1249587.48811123 kcal/mol)

Imaginary Frequencies: 1 (-68.1762 1/cm)

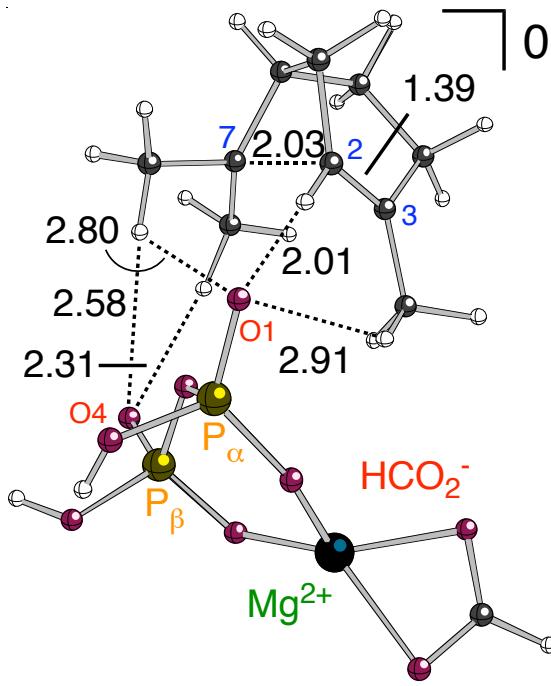
Zero-point correction = 0.327563 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-3.049815	-0.717628	-0.393510
2	6	-2.375167	-0.648051	-1.725013

3	6	-2.708856	-1.948113	0.396286
4	6	-4.398564	-0.033982	-0.135580
5	6	-4.563892	1.232961	-0.978475
6	6	-3.400469	2.232355	-0.670520
7	6	-2.325679	1.624518	0.197326
8	6	-2.693680	0.745273	1.190501
9	6	-0.908594	2.039304	-0.021046
10	6	-4.165927	0.389035	1.330668
11	1	-2.422969	0.324572	-2.215561
12	1	-2.934039	-1.354439	-2.364223
13	1	-1.341981	-1.008945	-1.702815
14	1	-1.733109	-1.845330	0.889819
15	1	-2.617979	-2.785725	-0.307714
16	1	-3.456785	-2.193484	1.152347
17	1	-5.230074	-0.732559	-0.306571
18	1	-5.530306	1.690334	-0.745090
19	1	-4.580366	0.990989	-2.045532
20	1	-3.799796	3.098401	-0.123779
21	1	-2.963623	2.635438	-1.589974
22	1	-1.938808	0.349155	1.871143
23	1	-0.557457	1.719947	-1.012229
24	1	-0.238862	1.639788	0.741185
25	1	-0.830933	3.134446	-0.014980
26	1	-4.799956	1.225831	1.648088
27	1	-4.307710	-0.425181	2.042157
28	8	1.764968	-2.376173	1.918651
29	15	0.976643	-1.016726	1.543918
30	8	-0.298332	-0.897863	2.308801
31	8	0.562790	-1.271183	-0.048932
32	8	1.954460	0.172287	1.541314
33	15	1.552590	-1.435739	-1.359265
34	8	0.715922	-1.847663	-2.514986
35	8	2.551121	-2.653900	-0.850280
36	8	2.441248	-0.188956	-1.402551
37	1	2.346946	-2.644440	1.177985
38	1	2.279143	-3.479336	-1.284335
39	12	2.770926	1.058143	0.035359
40	8	4.391582	2.302591	0.145995
41	6	3.591735	3.257673	-0.097857
42	1	3.989421	4.282687	-0.158540
43	8	2.350376	3.064242	-0.273282

B-PPi-Mg²⁺-HCOO⁻



B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1991.3431952 hartrees (-1249587.76841995 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.328086 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-3.042558	-0.632591	-0.444144
2	6	-2.436431	-0.465773	-1.812969
3	6	-2.693044	-1.970264	0.164078
4	6	-4.416501	-0.023957	-0.105185
5	6	-4.608837	1.314680	-0.820016
6	6	-3.424285	2.272358	-0.461915
7	6	-2.308127	1.560461	0.256112
8	6	-2.633029	0.556010	1.155302
9	6	-0.901325	1.977067	0.002015
10	6	-4.111189	0.265077	1.380417
11	1	-2.507070	0.539693	-2.231334
12	1	-3.020452	-1.126033	-2.474811
13	1	-1.400441	-0.817662	-1.863793
14	1	-1.613813	-2.063339	0.300638

15	1	-3.001754	-2.735802	-0.563712
16	1	-3.193935	-2.176008	1.110398
17	1	-5.245044	-0.712983	-0.314193
18	1	-5.560843	1.757393	-0.511645
19	1	-4.659654	1.173888	-1.903809
20	1	-3.781860	3.055021	0.223164
21	1	-3.041959	2.795959	-1.343696
22	1	-1.842698	0.104006	1.762579
23	1	-0.596708	1.714454	-1.020934
24	1	-0.204434	1.529347	0.709782
25	1	-0.819667	3.069784	0.065857
26	1	-4.676881	1.103327	1.803309
27	1	-4.250425	-0.598463	2.030949
28	8	1.779488	-2.421153	1.892879
29	15	1.041058	-1.020469	1.572919
30	8	-0.194713	-0.853426	2.385690
31	8	0.557633	-1.230382	-0.012945
32	8	2.075758	0.119812	1.541296
33	15	1.492701	-1.411381	-1.360414
34	8	0.601577	-1.779169	-2.491042
35	8	2.467959	-2.668966	-0.908192
36	8	2.420221	-0.194137	-1.424226
37	1	2.339413	-2.688106	1.135383
38	1	2.150231	-3.478607	-1.340911
39	12	2.810692	1.034657	0.013805
40	8	4.396159	2.324501	0.052822
41	6	3.559156	3.259383	-0.140795
42	1	3.926225	4.295200	-0.210823
43	8	2.316430	3.033681	-0.255410

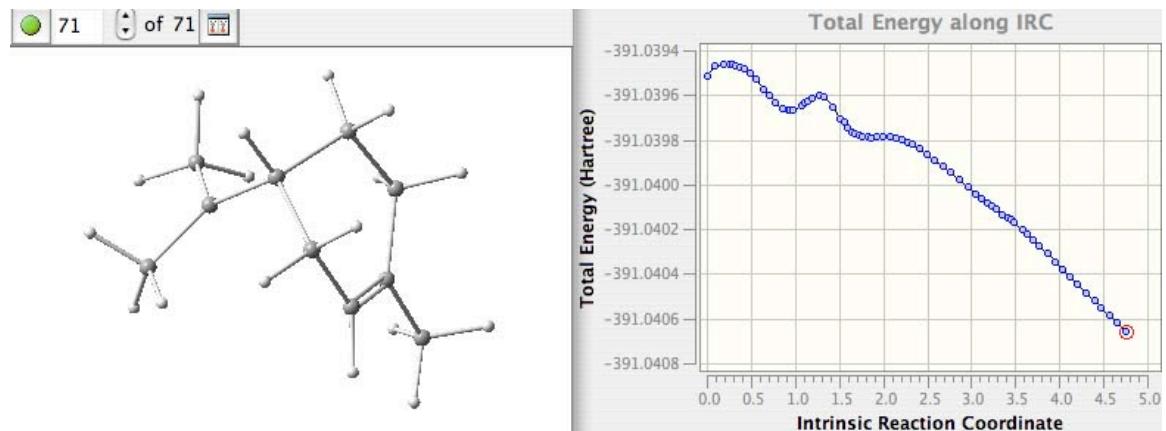
IX. IRC Plots

Figure 1.

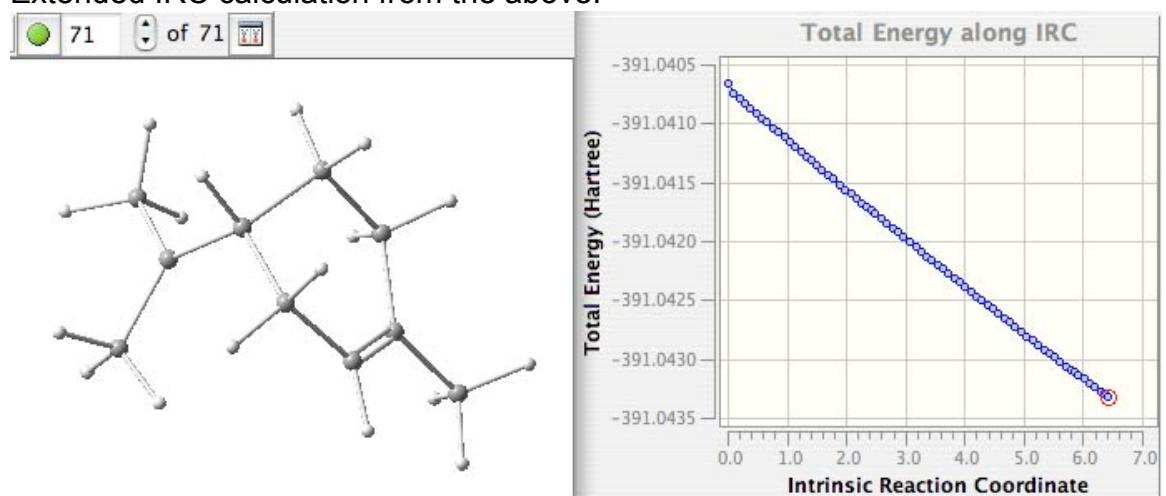
TS(A-to-B)

B3LYP

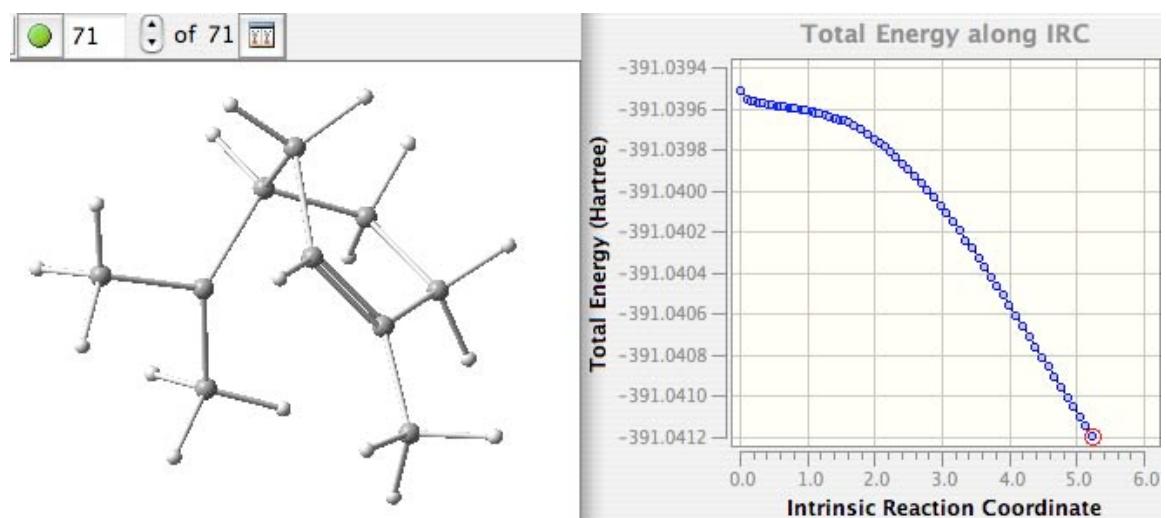
Toward A:



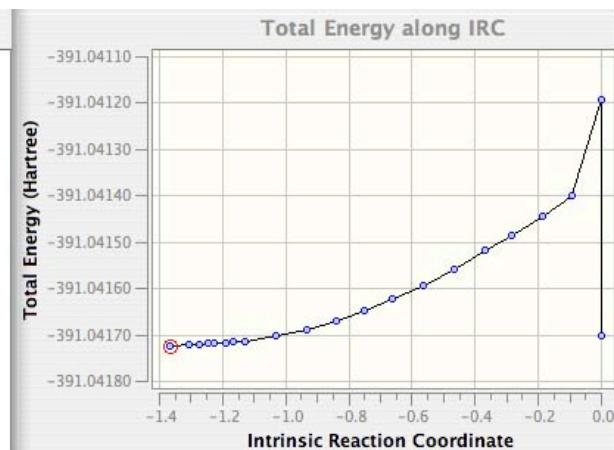
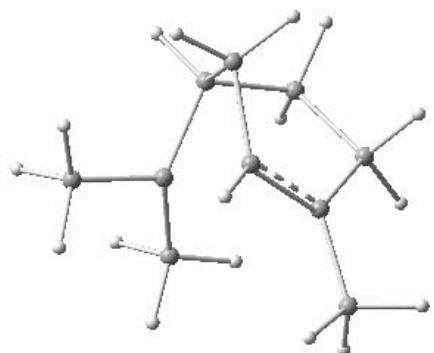
Extended IRC calculation from the above.



Toward **B**:

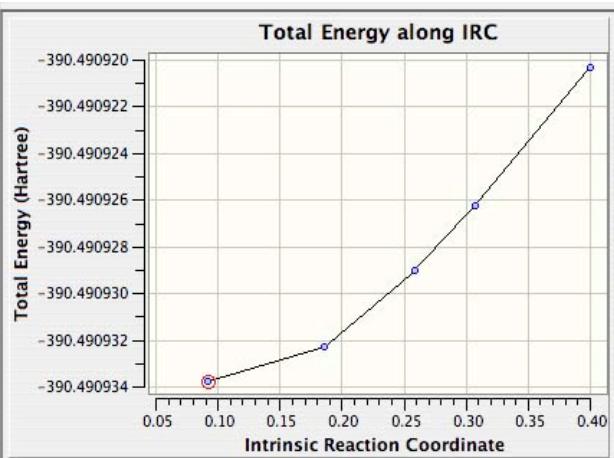
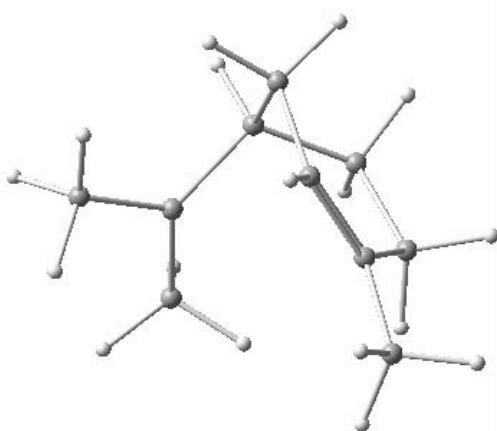


Extended IRC calculation from the above.

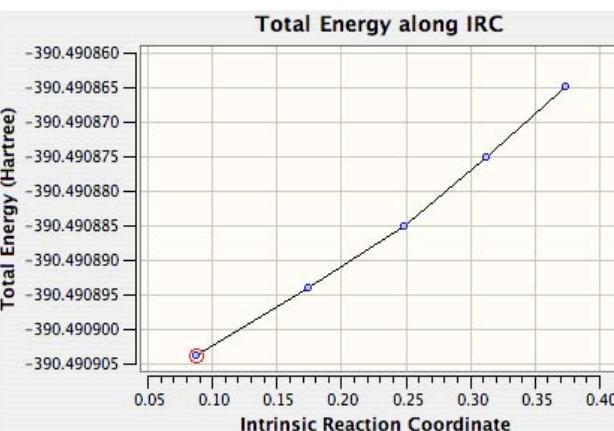
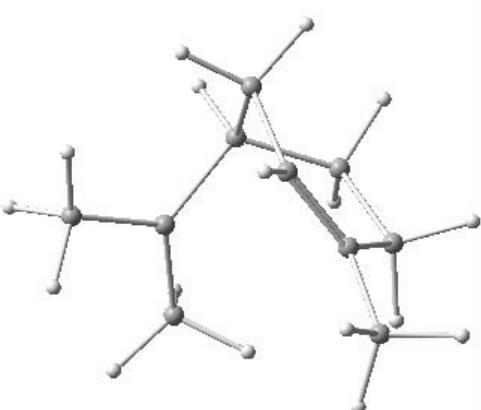


PBE

Toward **A**:



Toward **B**:

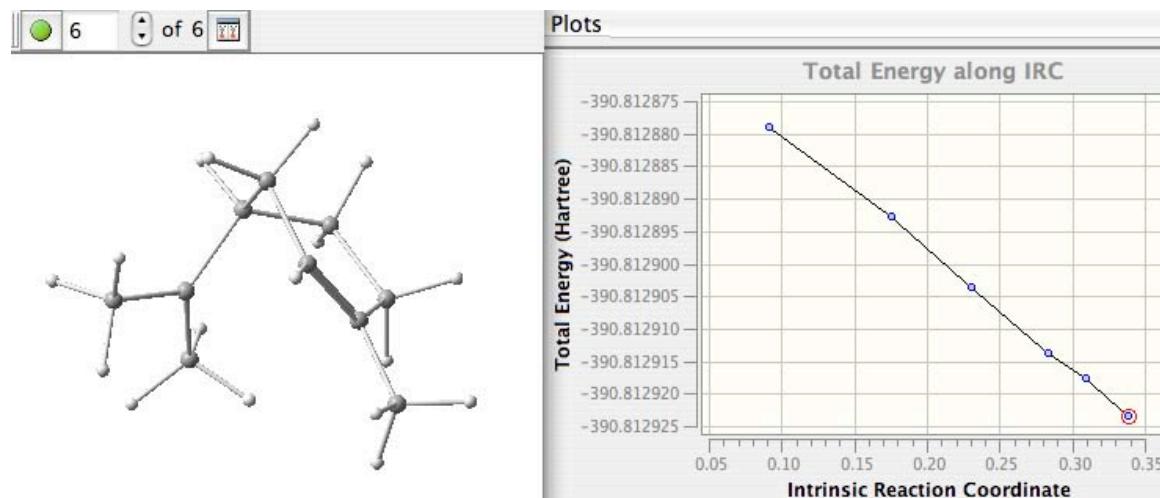


mPW1PW91

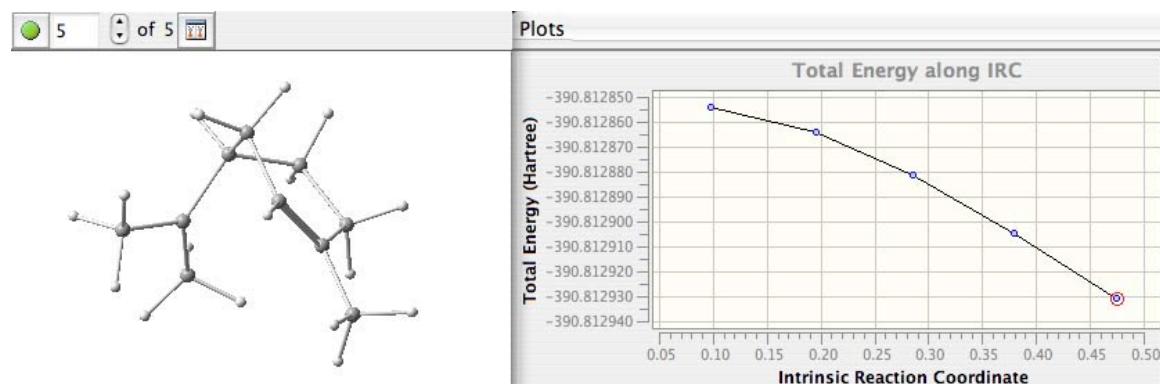
unsuccessful.

BB1K

Toward A:

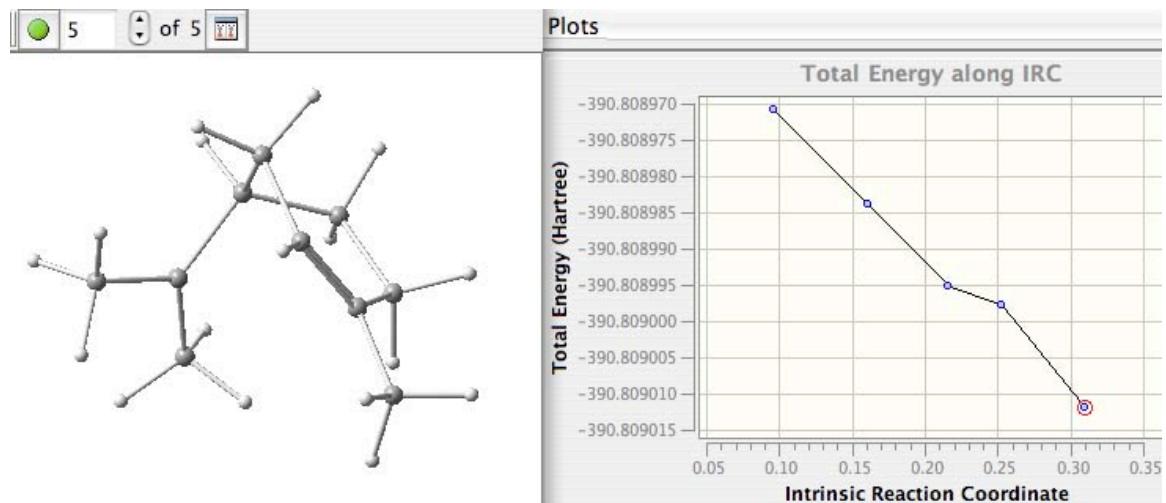


Toward B:

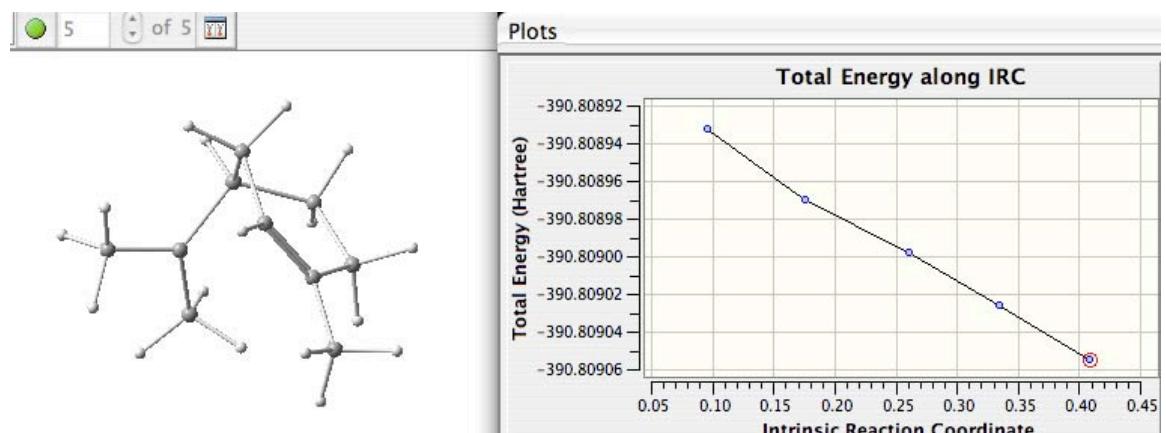


mPWB1K

Toward A:

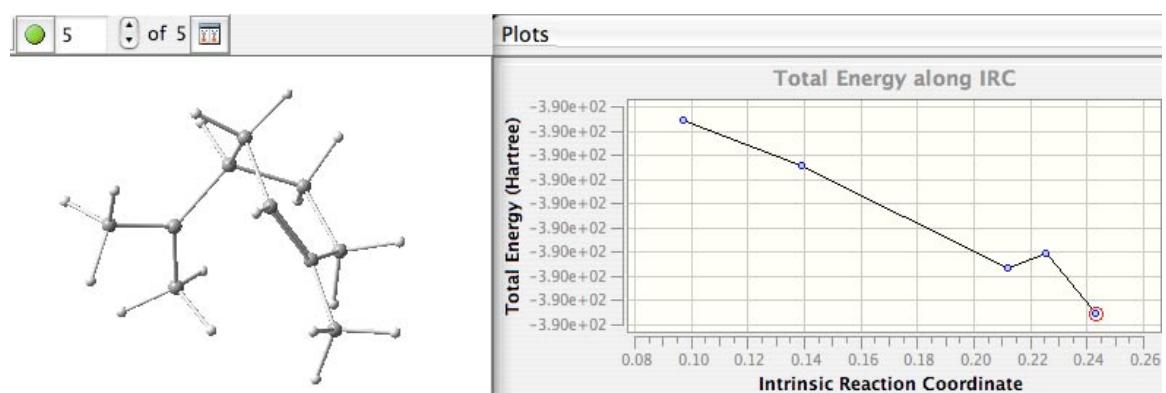


Toward **B**:

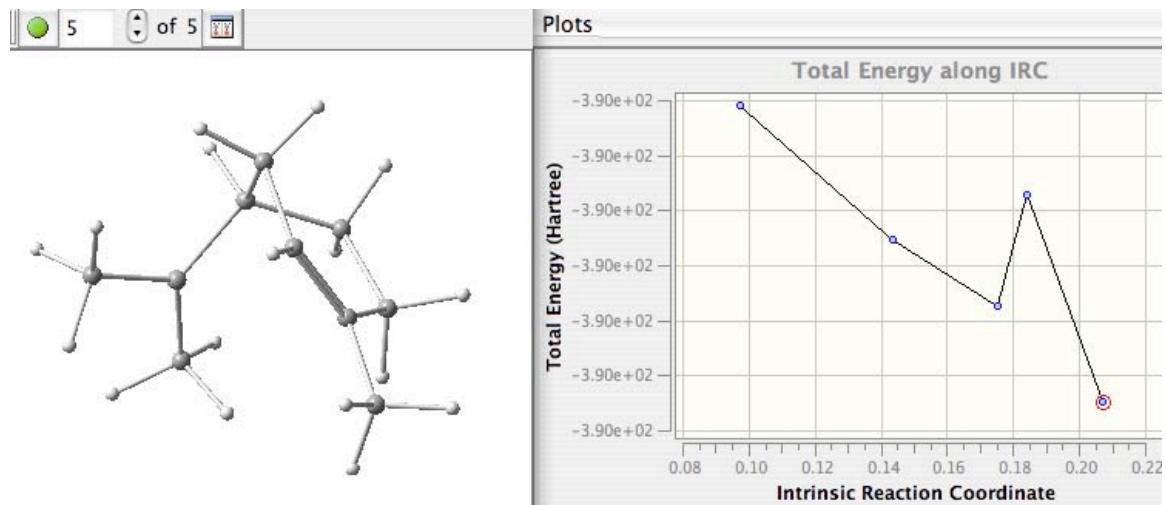


MP2

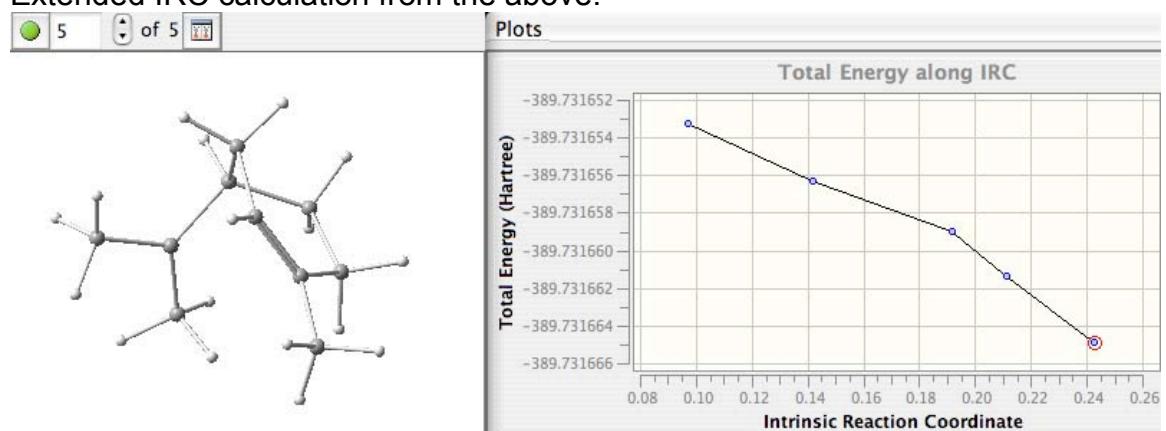
Toward **A**:



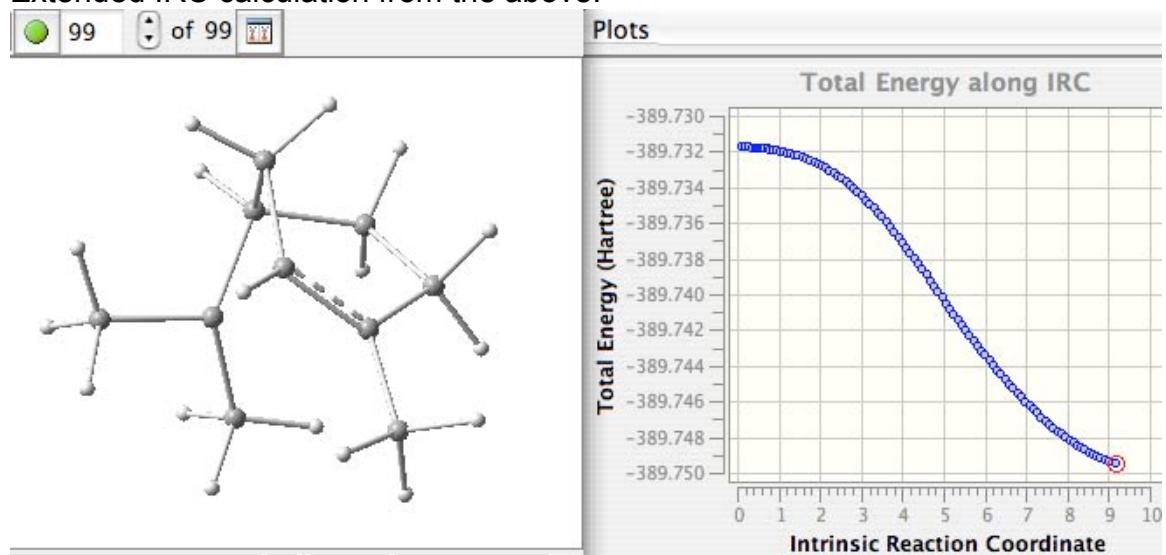
Toward **B**:



Extended IRC calculation from the above.



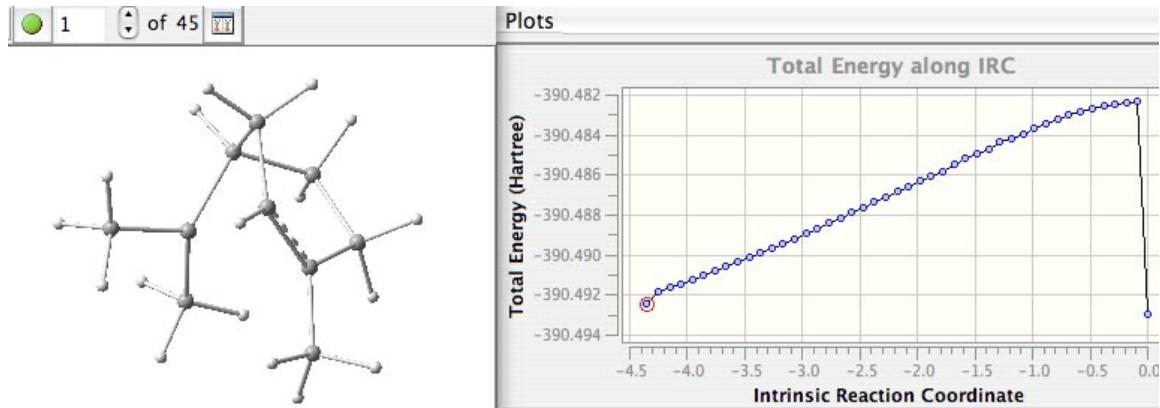
Extended IRC calculation from the above.



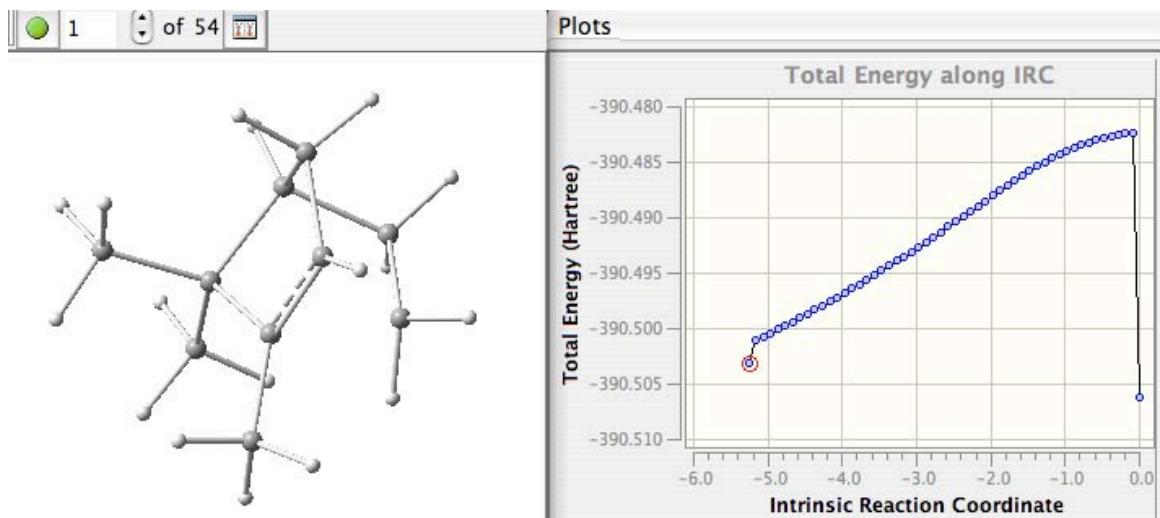
TS(B-to-D)

PBE

Toward B:

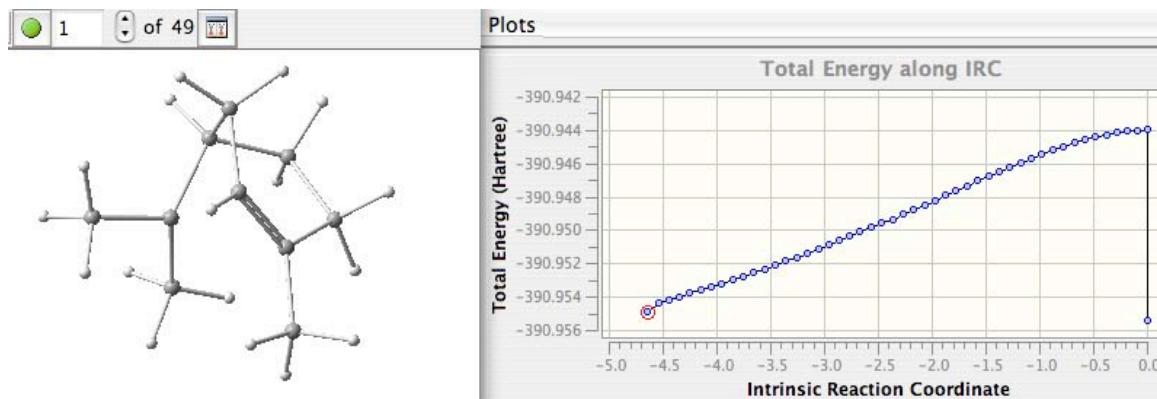


Toward D:

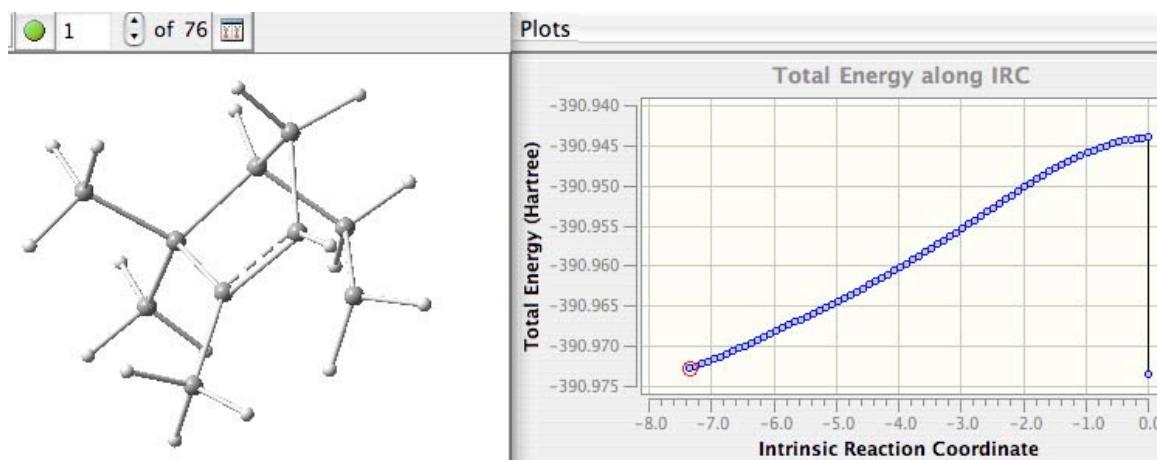


mPW1PW91

Toward B:

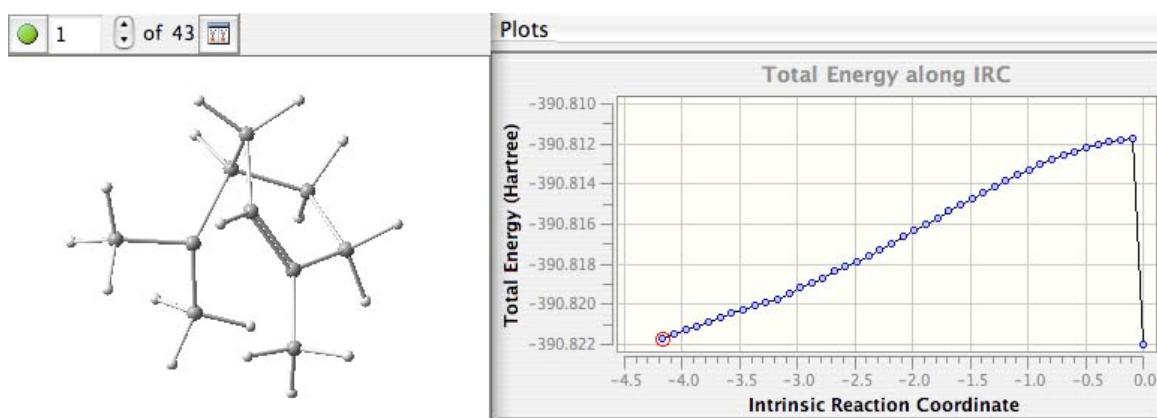


Toward D:



BB1K

Toward B:



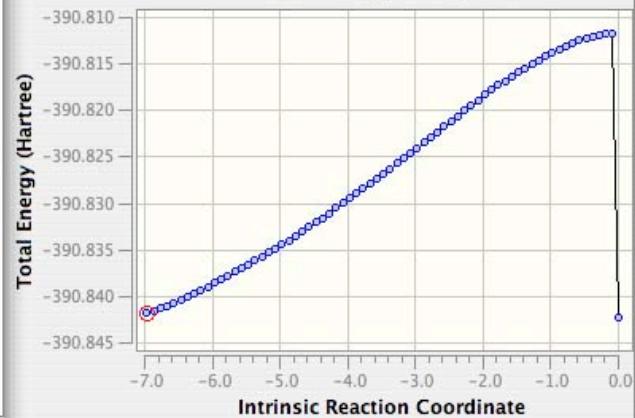
Toward D:

1 of 71



Plots

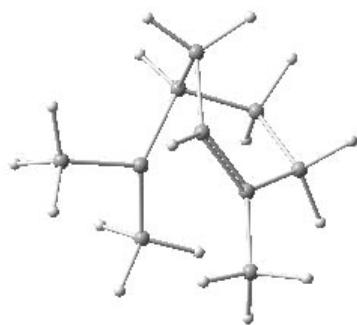
Total Energy along IRC



mPWB1K

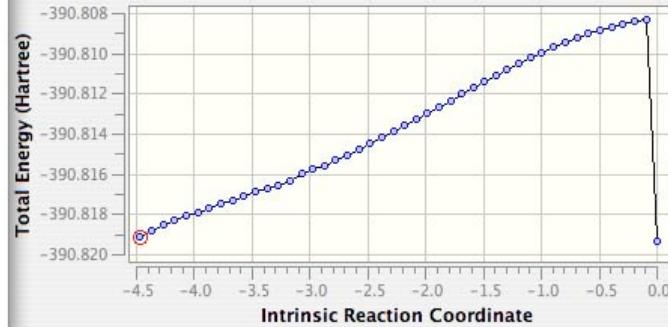
Toward B:

1 of 46



Plots

Total Energy along IRC



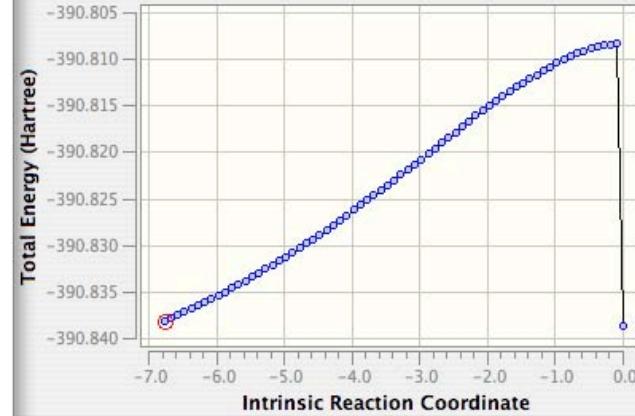
Toward D:

1 of 69



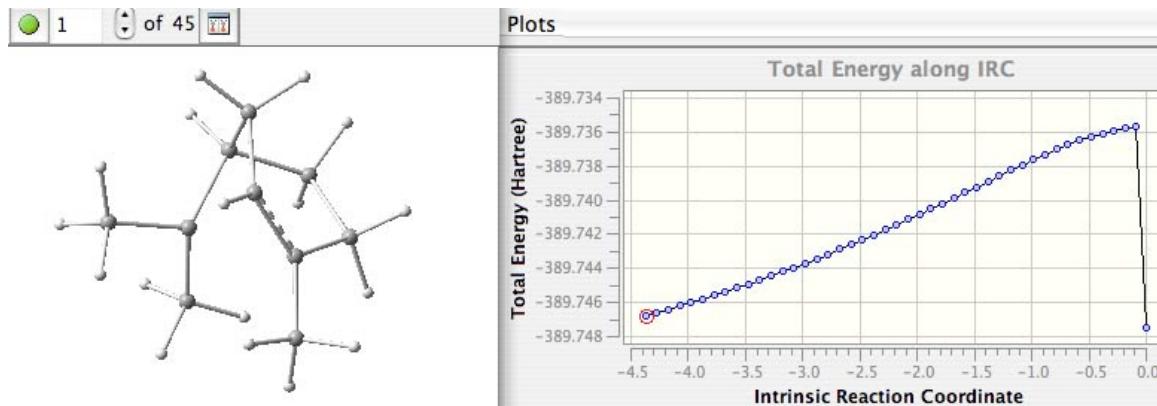
Plots

Total Energy along IRC



MP2

Toward B:



Toward D:

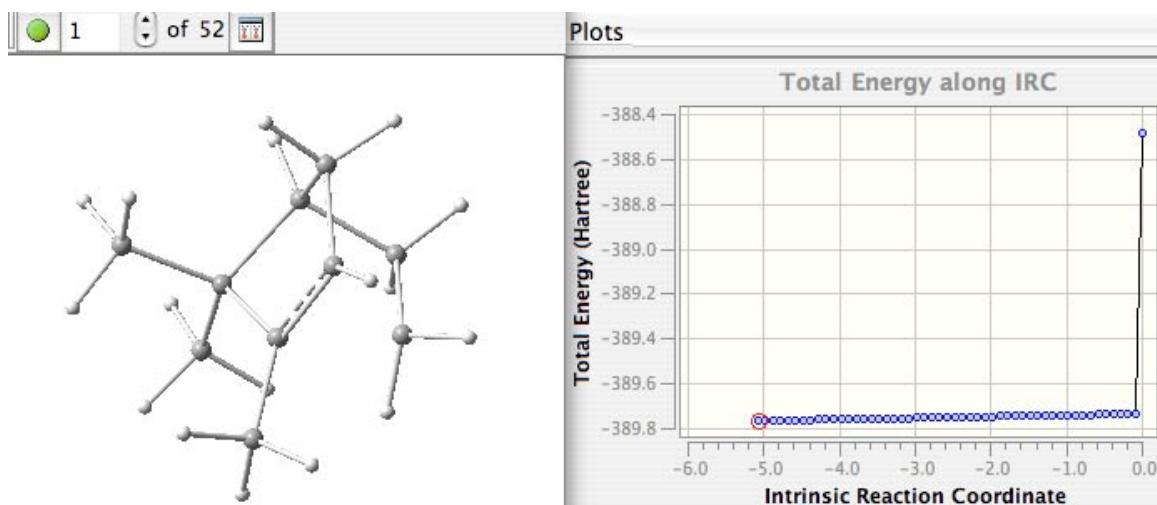
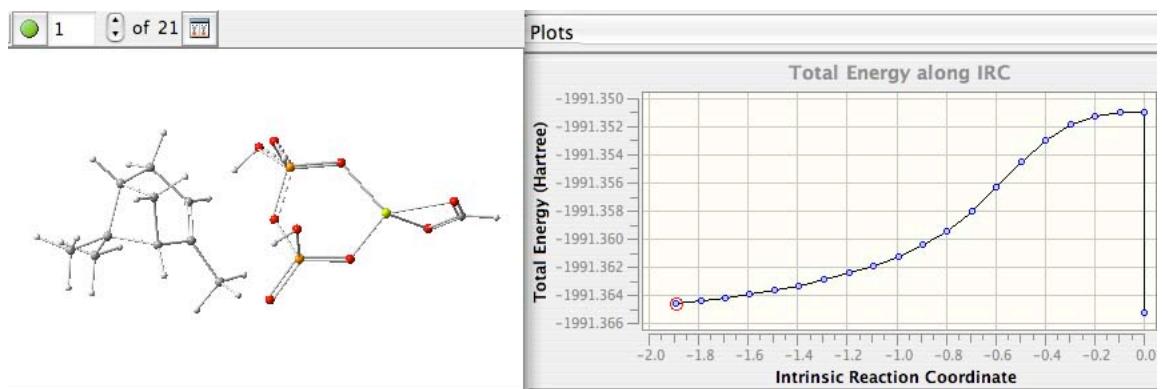
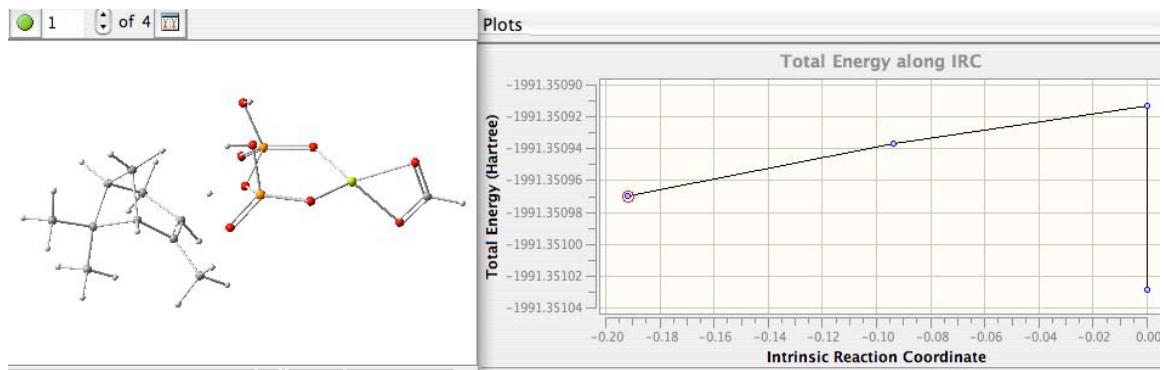


Figure 10.

TS5



TS6

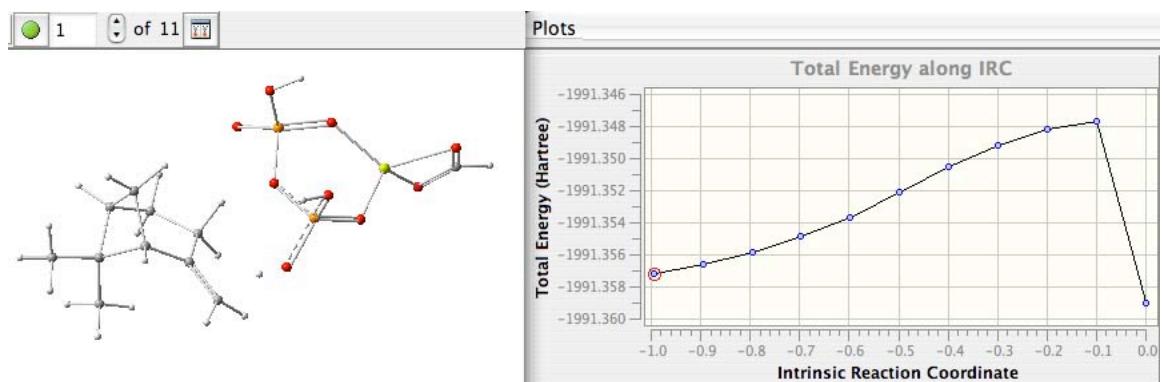
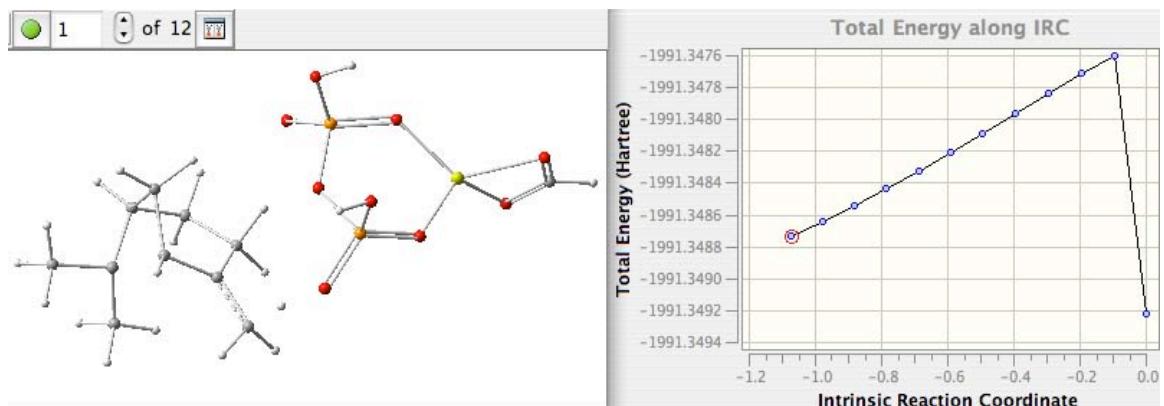
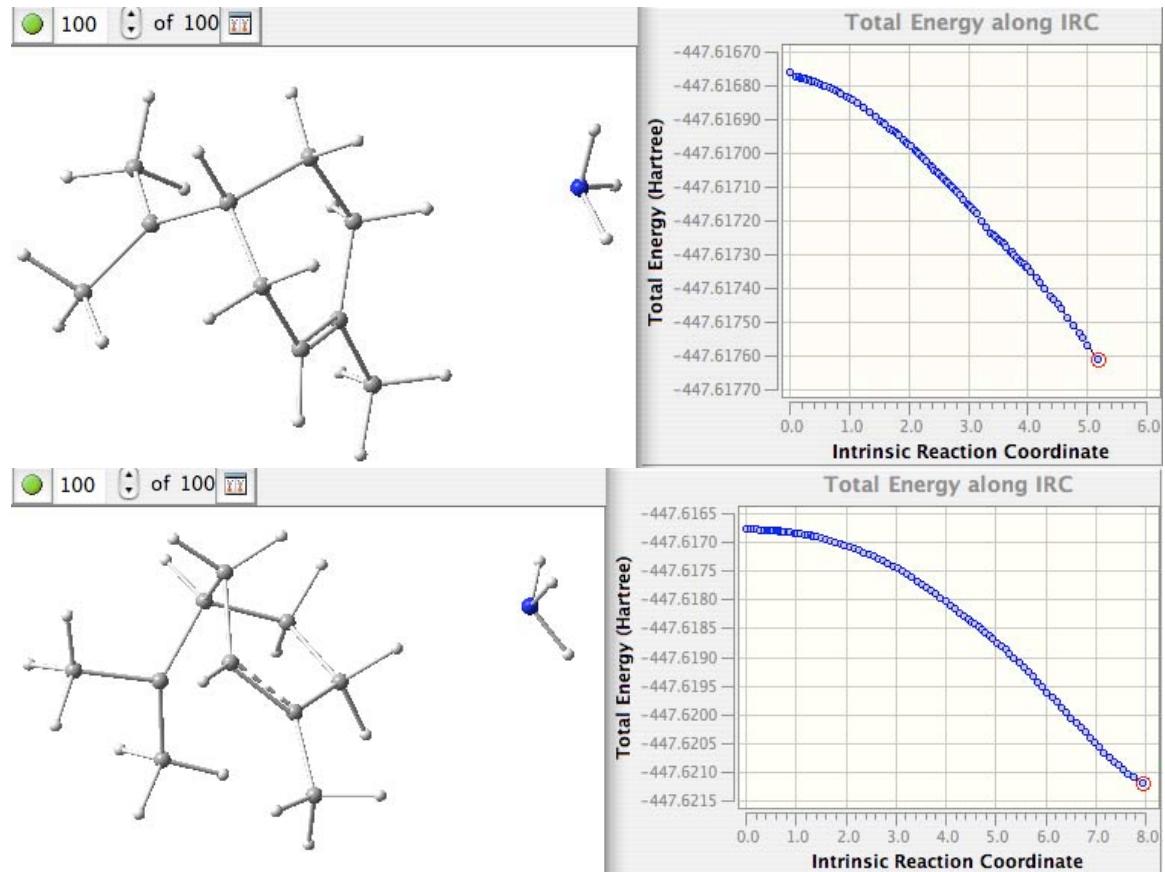
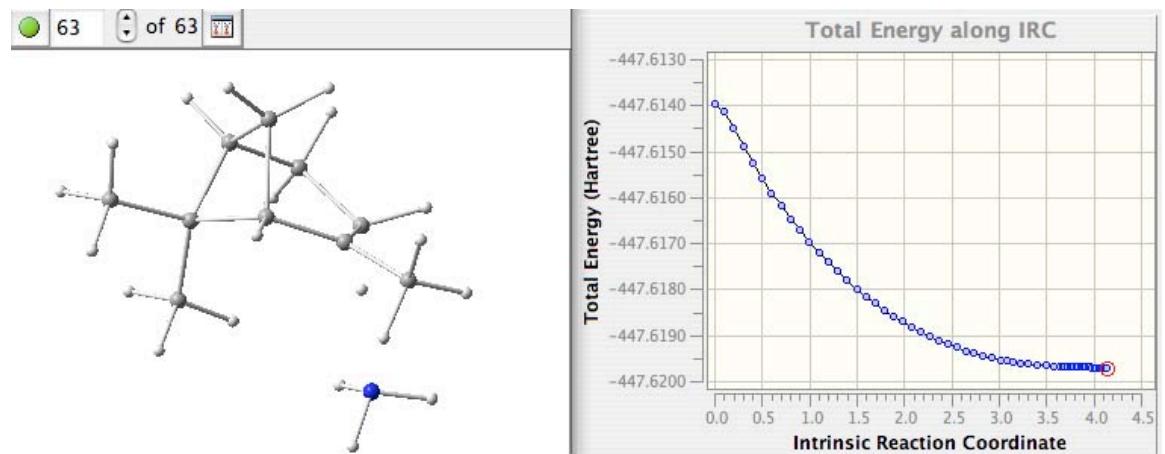


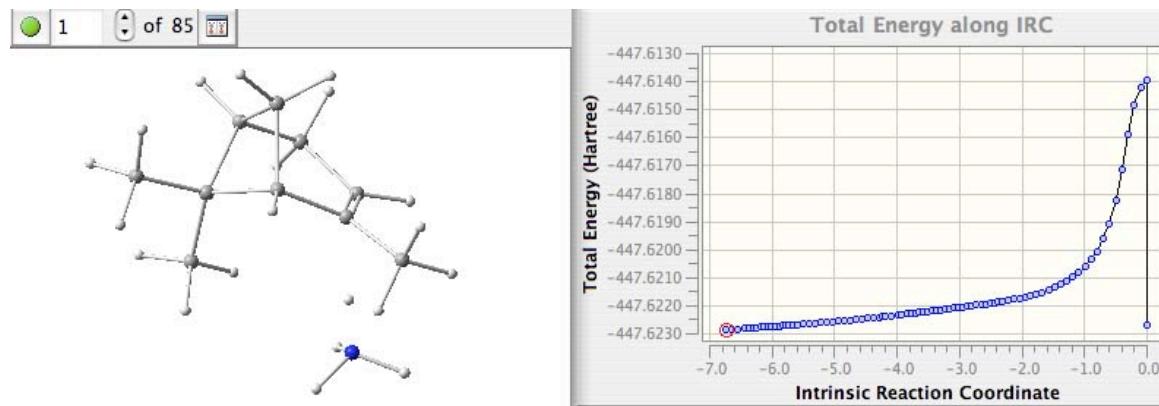
Figure S3.

TS(S1)



TS(S2)





TS(S3)

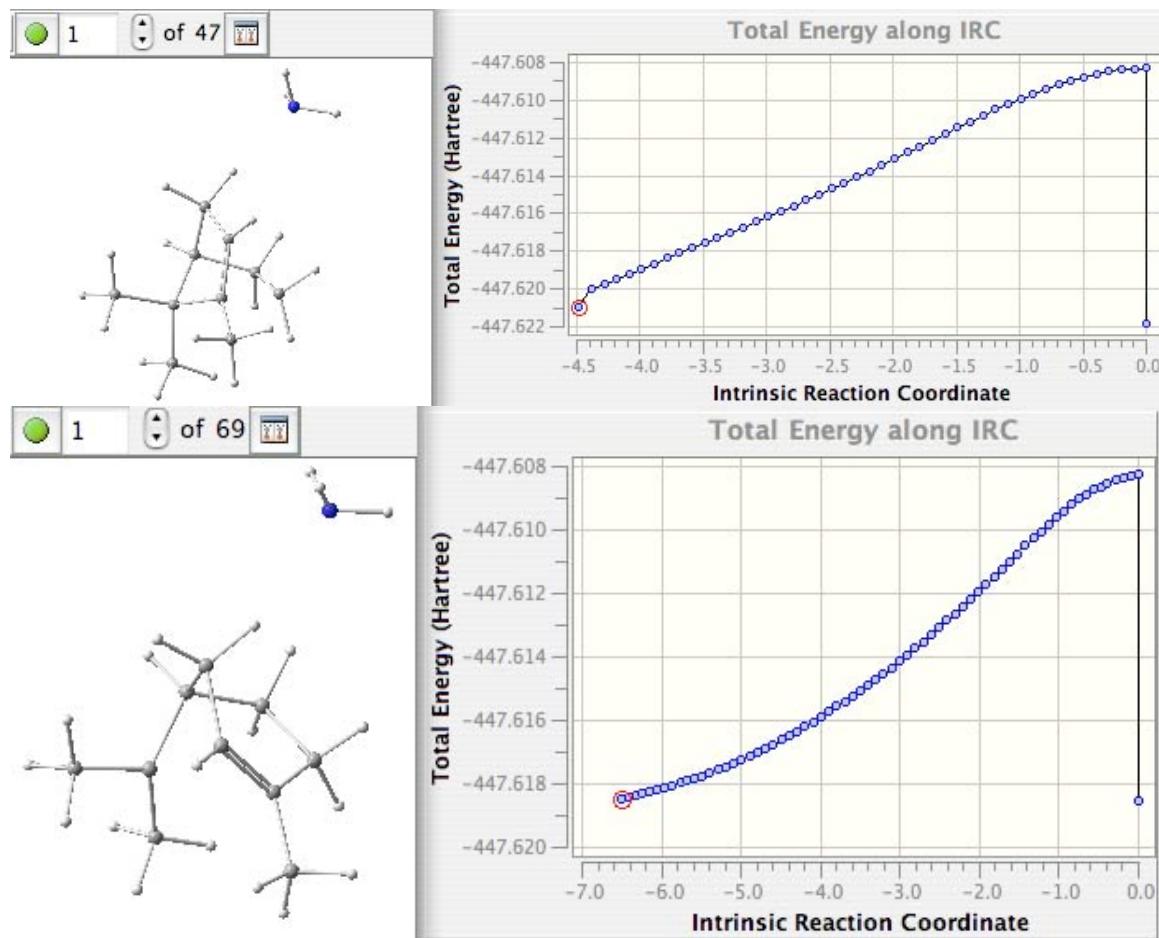
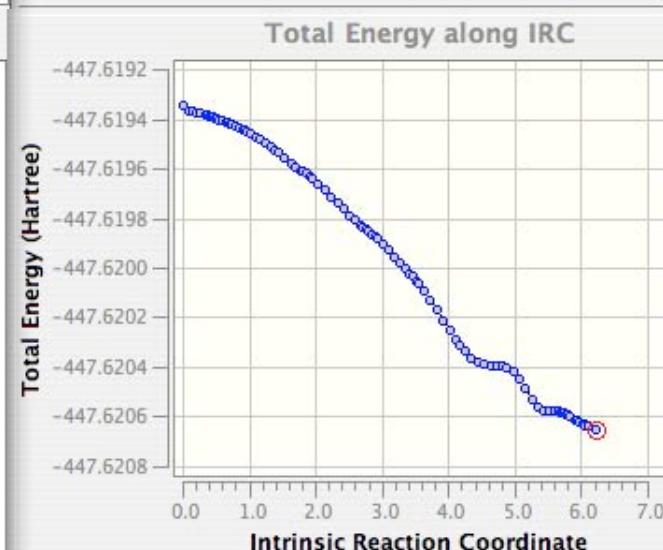
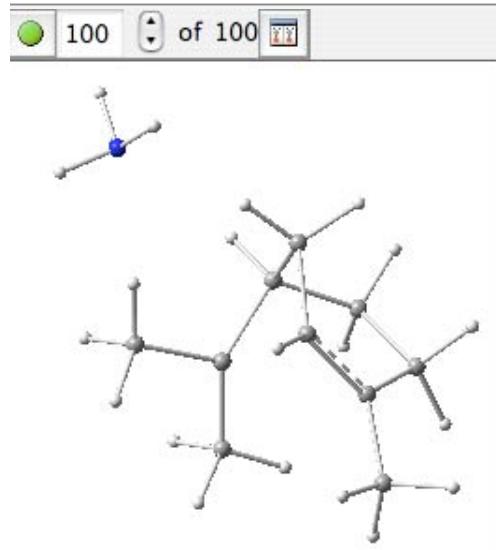
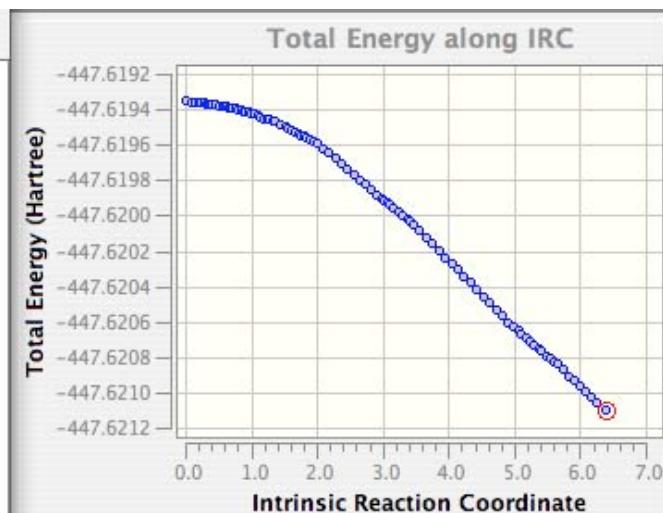
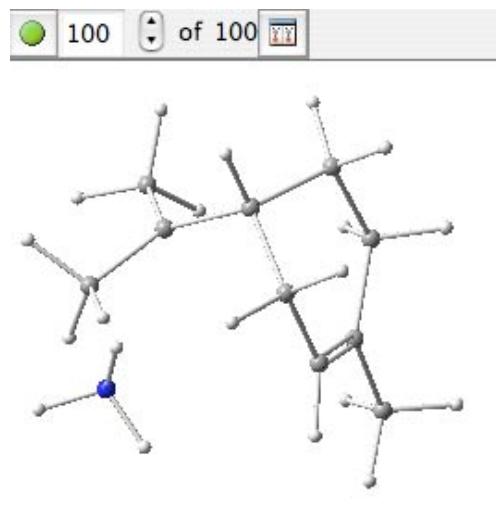
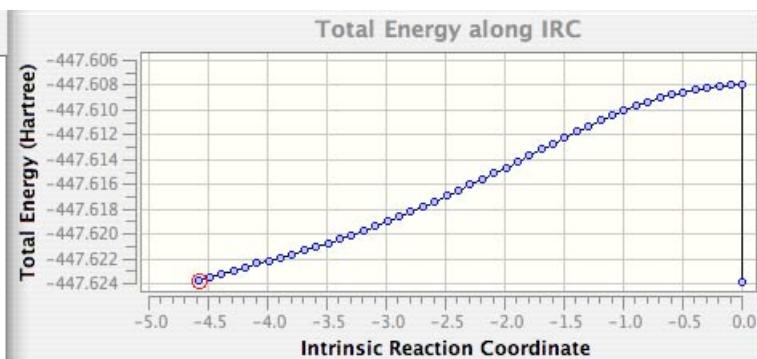
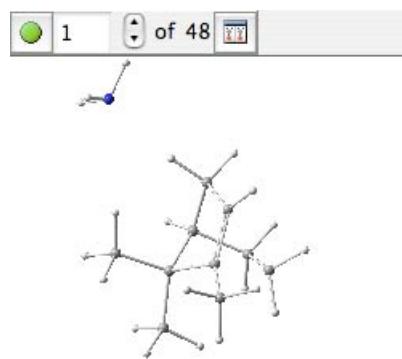


Figure S4.

TS(S4)



TS(S5)



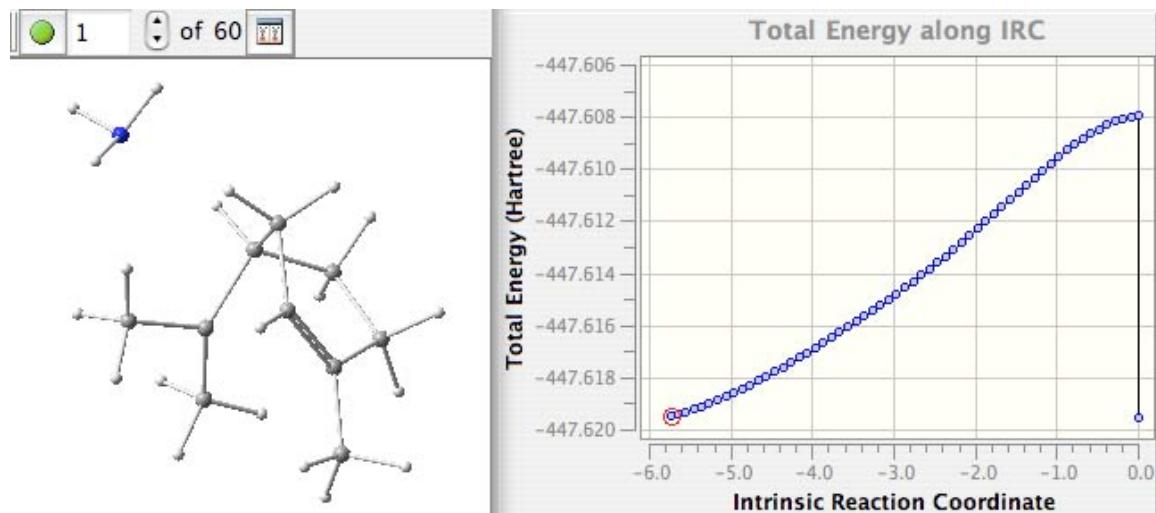


Figure S5.

TS(S7)

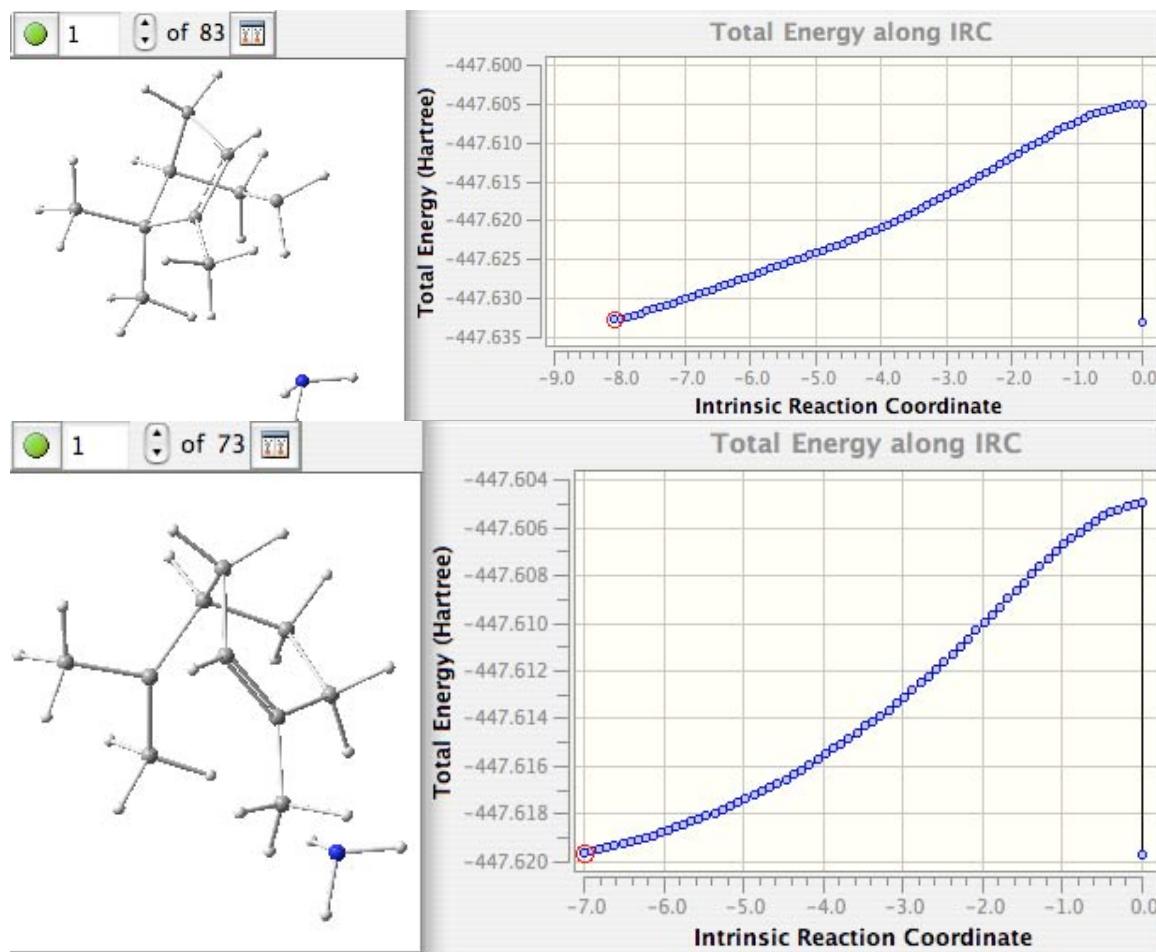


Figure S6b.

TS(S10)

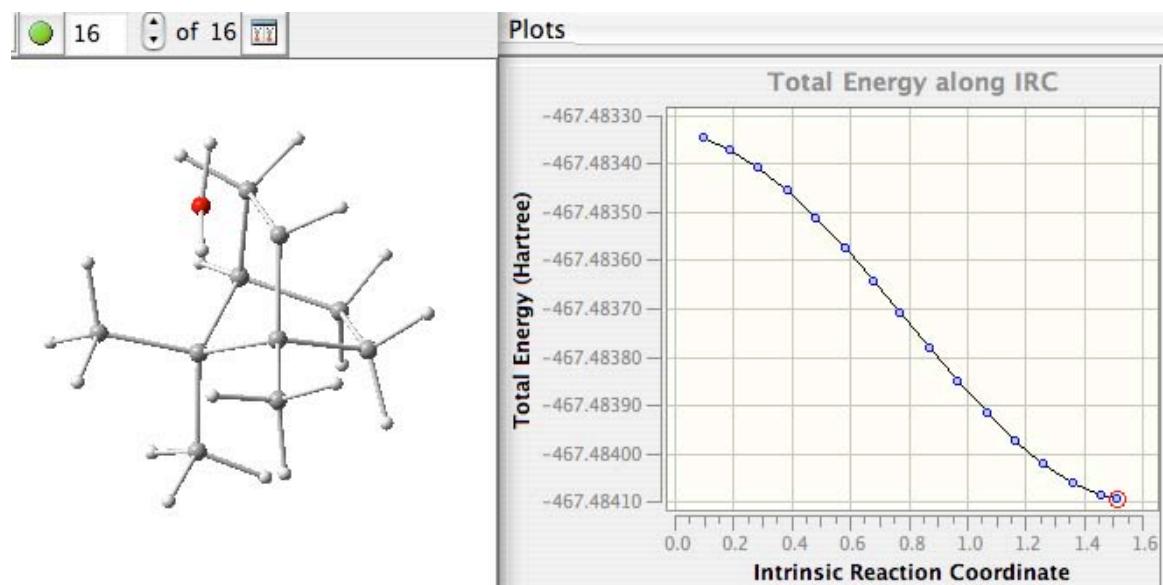
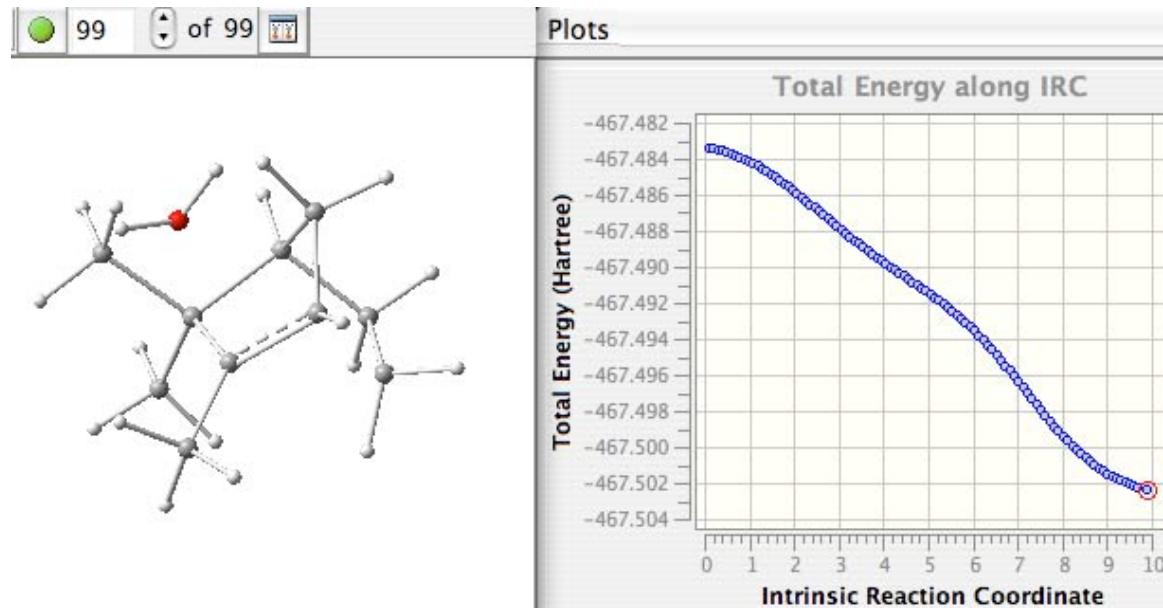
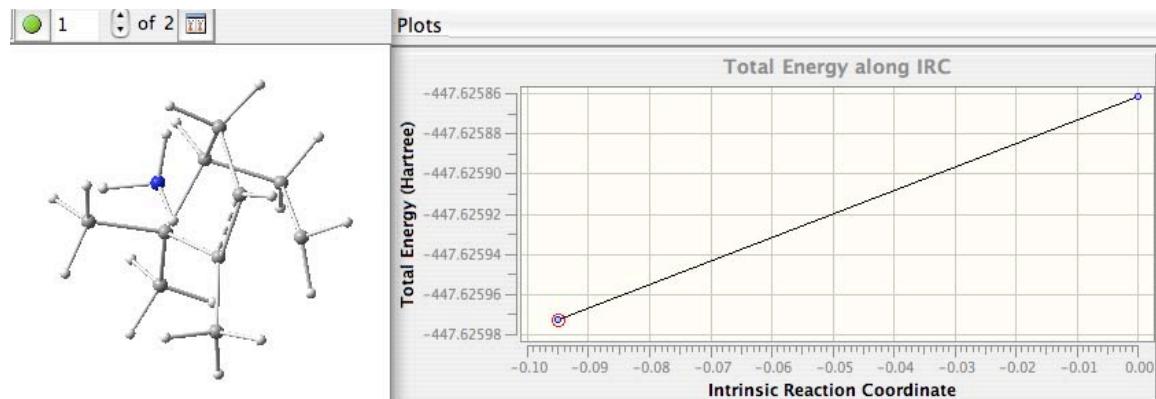
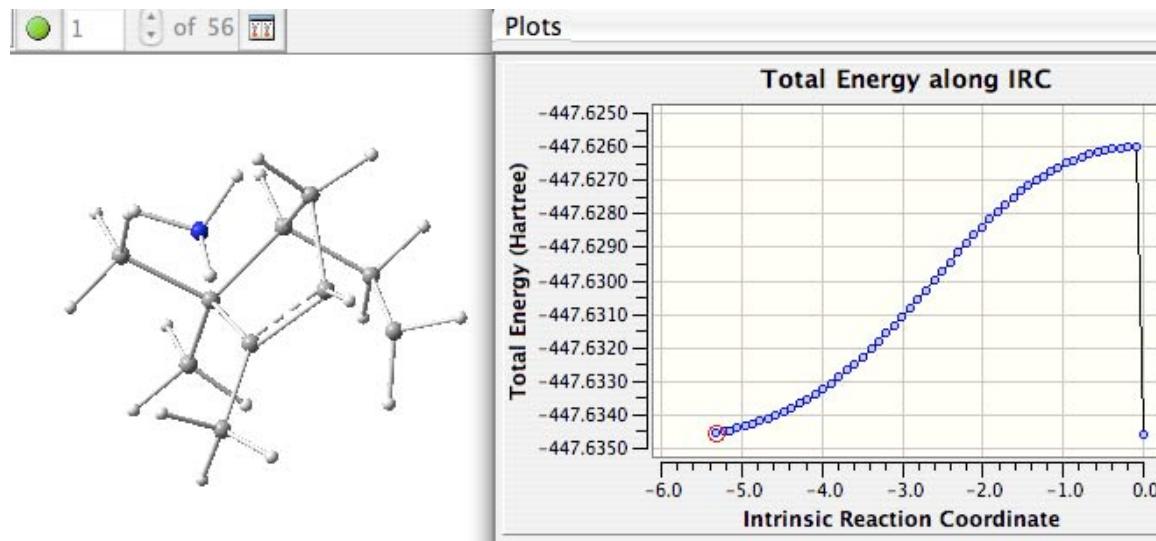


Figure S8.

TS(S11)



Extended IRC calculation from the above.

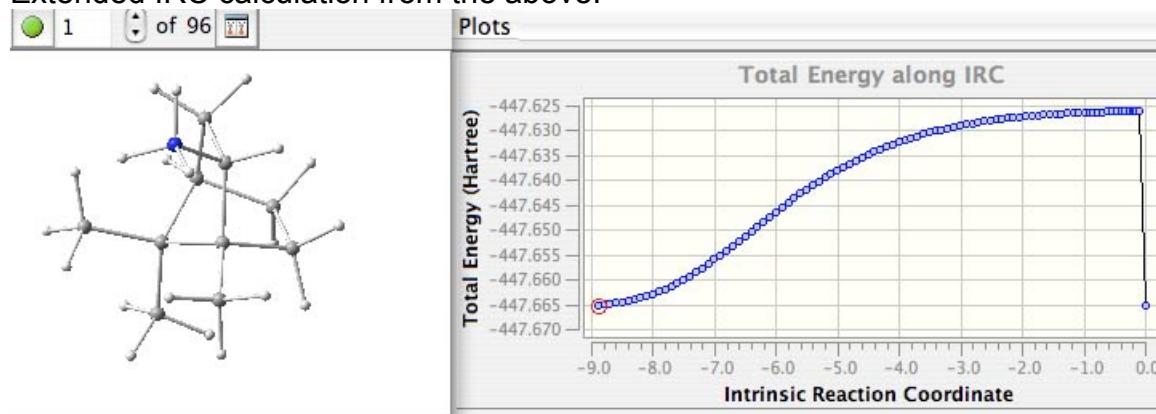


Figure S9b.

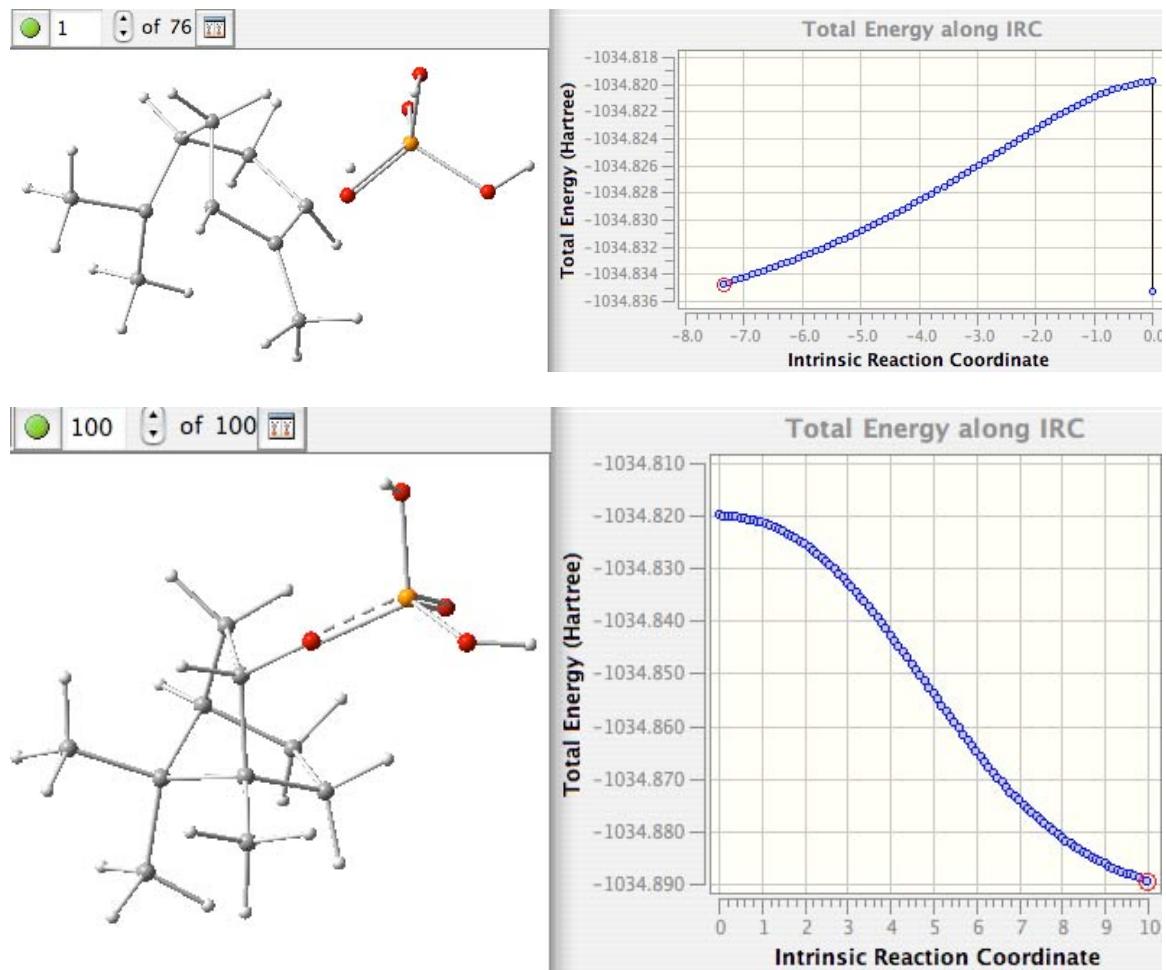
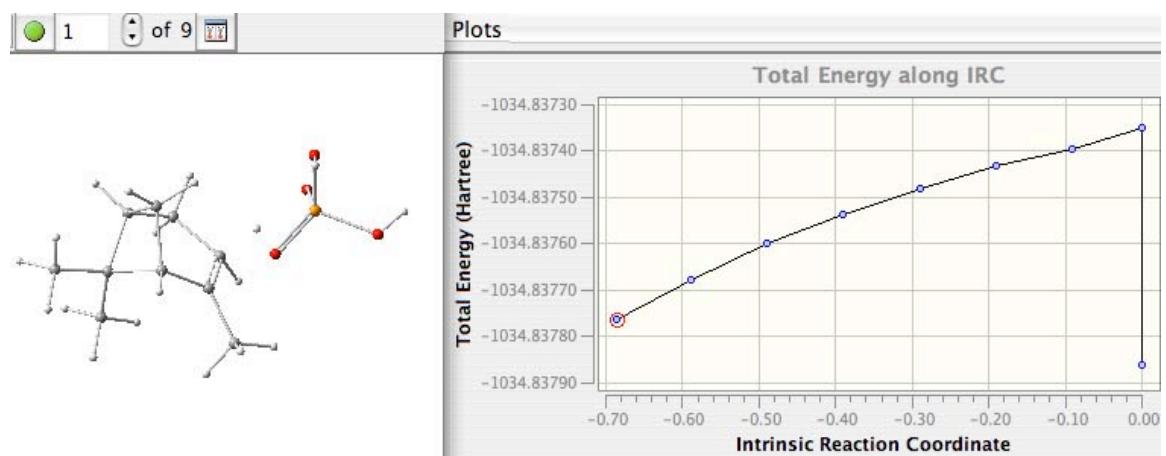


Figure S9c.



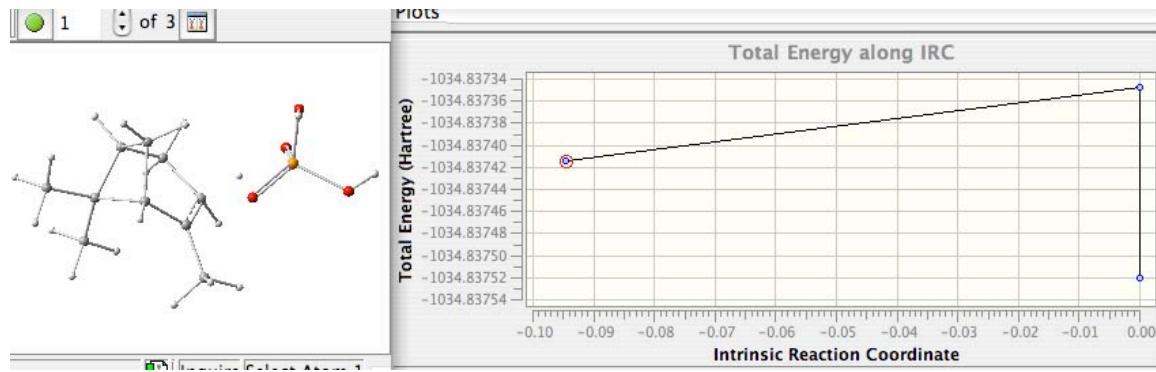
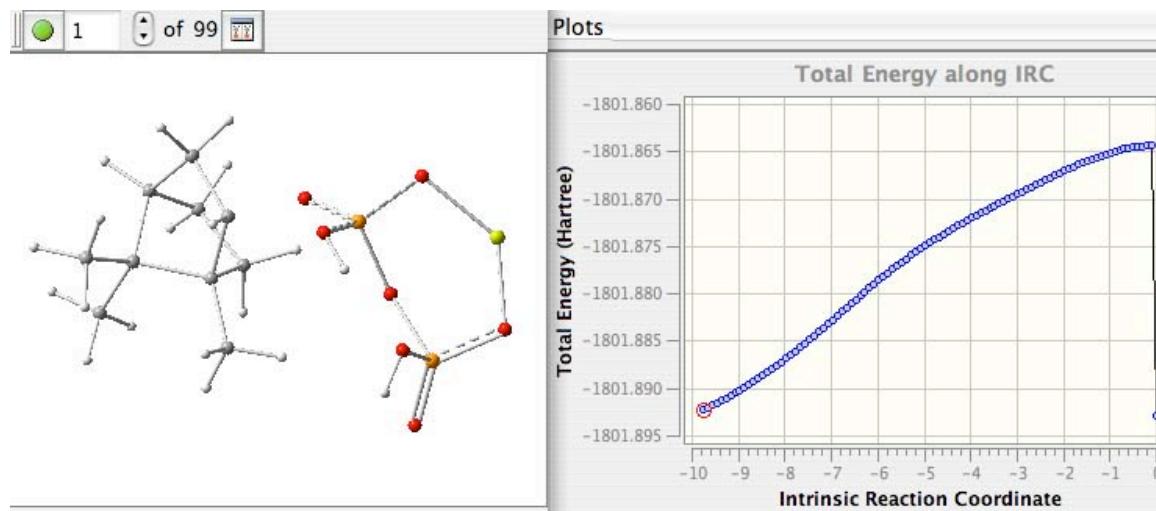
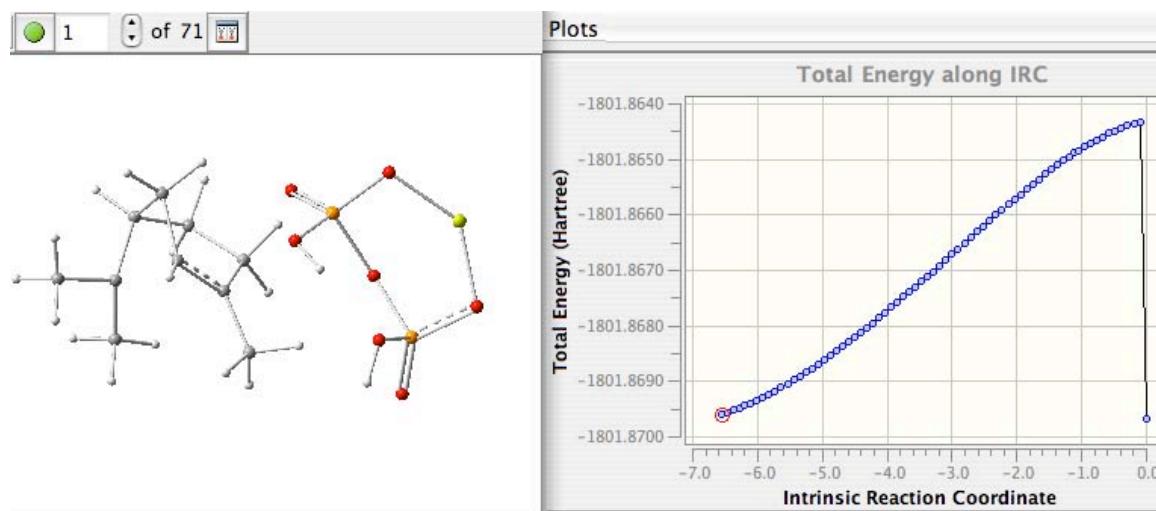
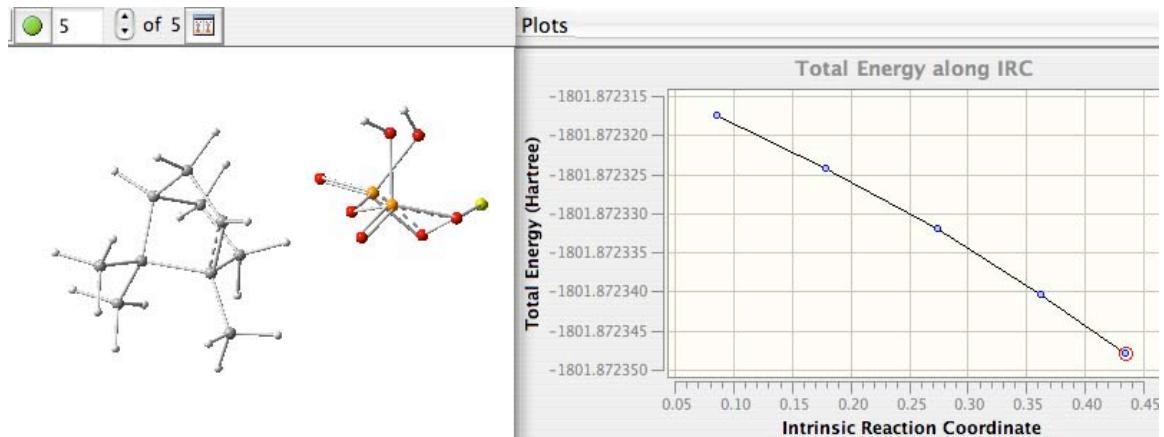


Figure S11b.

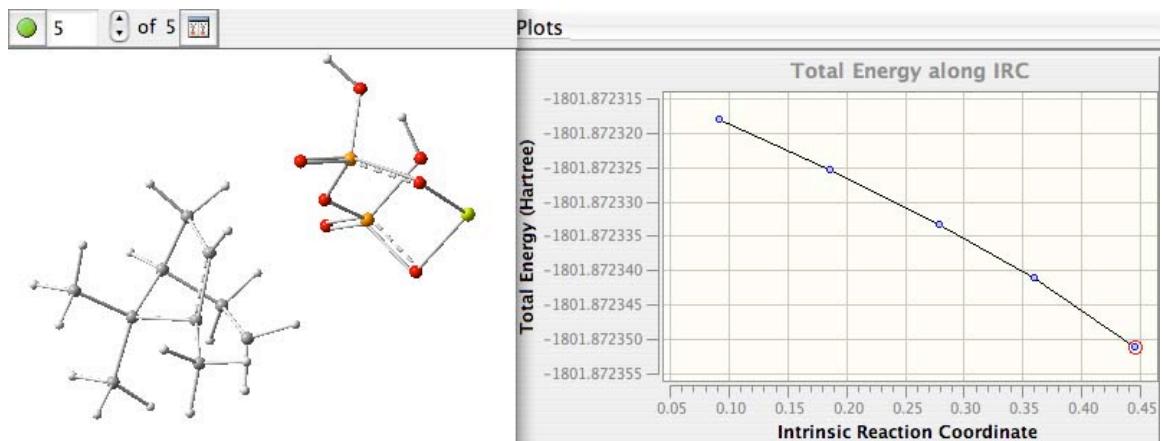
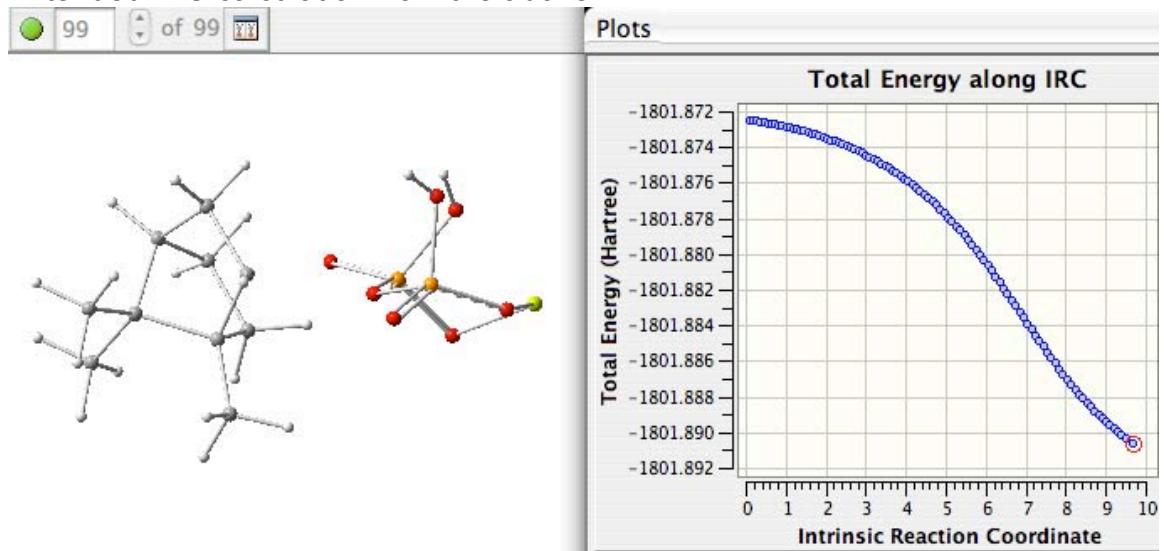
TS(S12)



TS(S13)



Extended IRC calculation from the above.



Extended IRC calculation from the above.

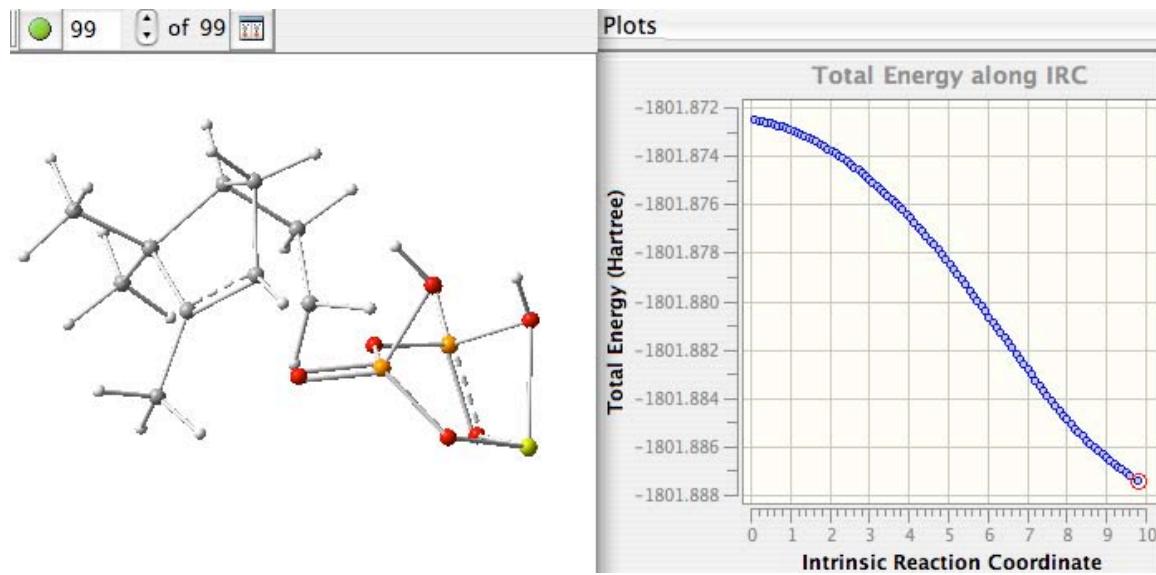
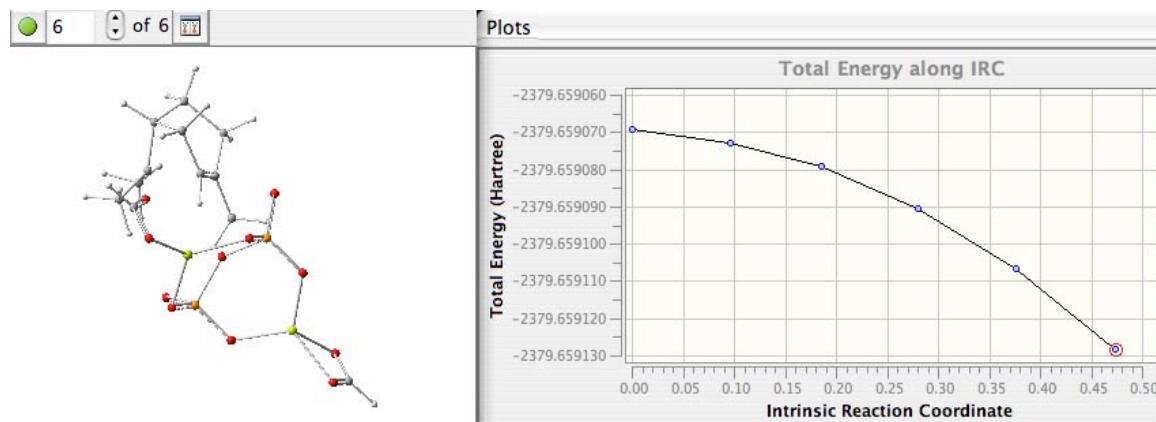
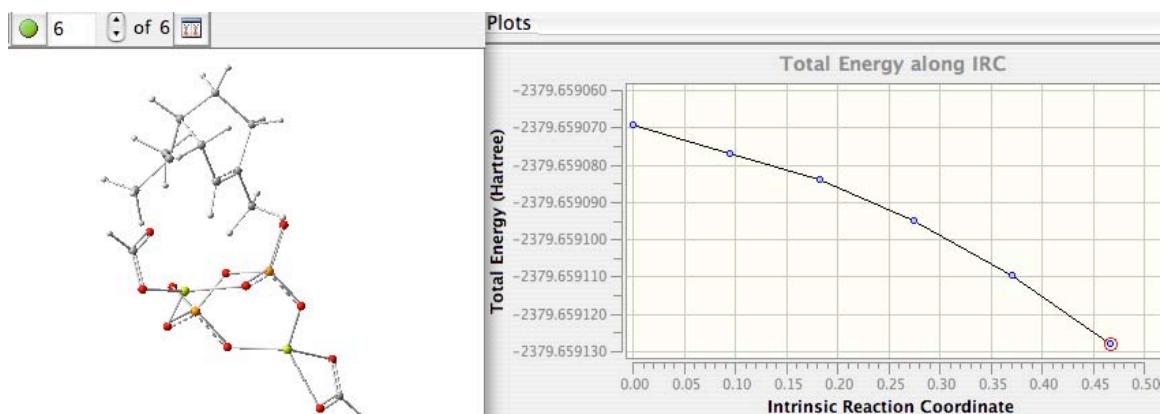
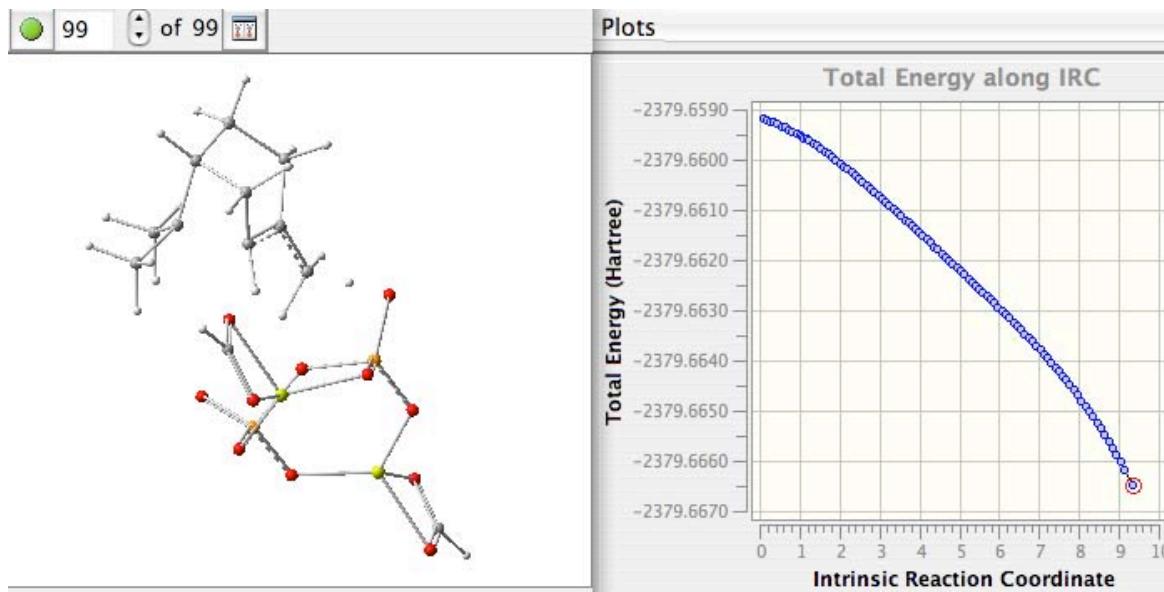


Figure S12b.

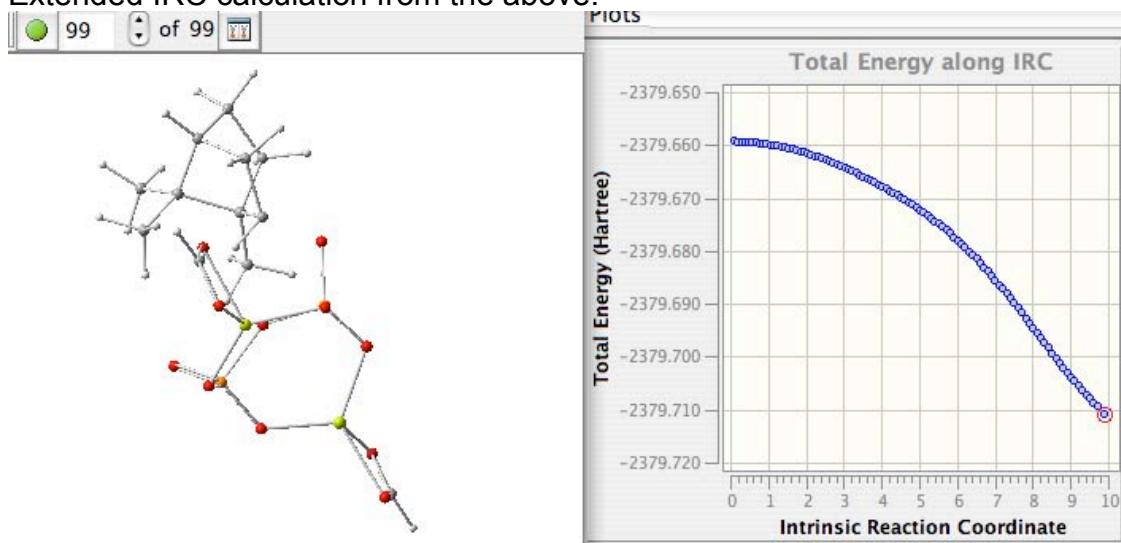
TS(S14)



Extended IRC calculation from the above.



Extended IRC calculation from the above.



TS(S15)

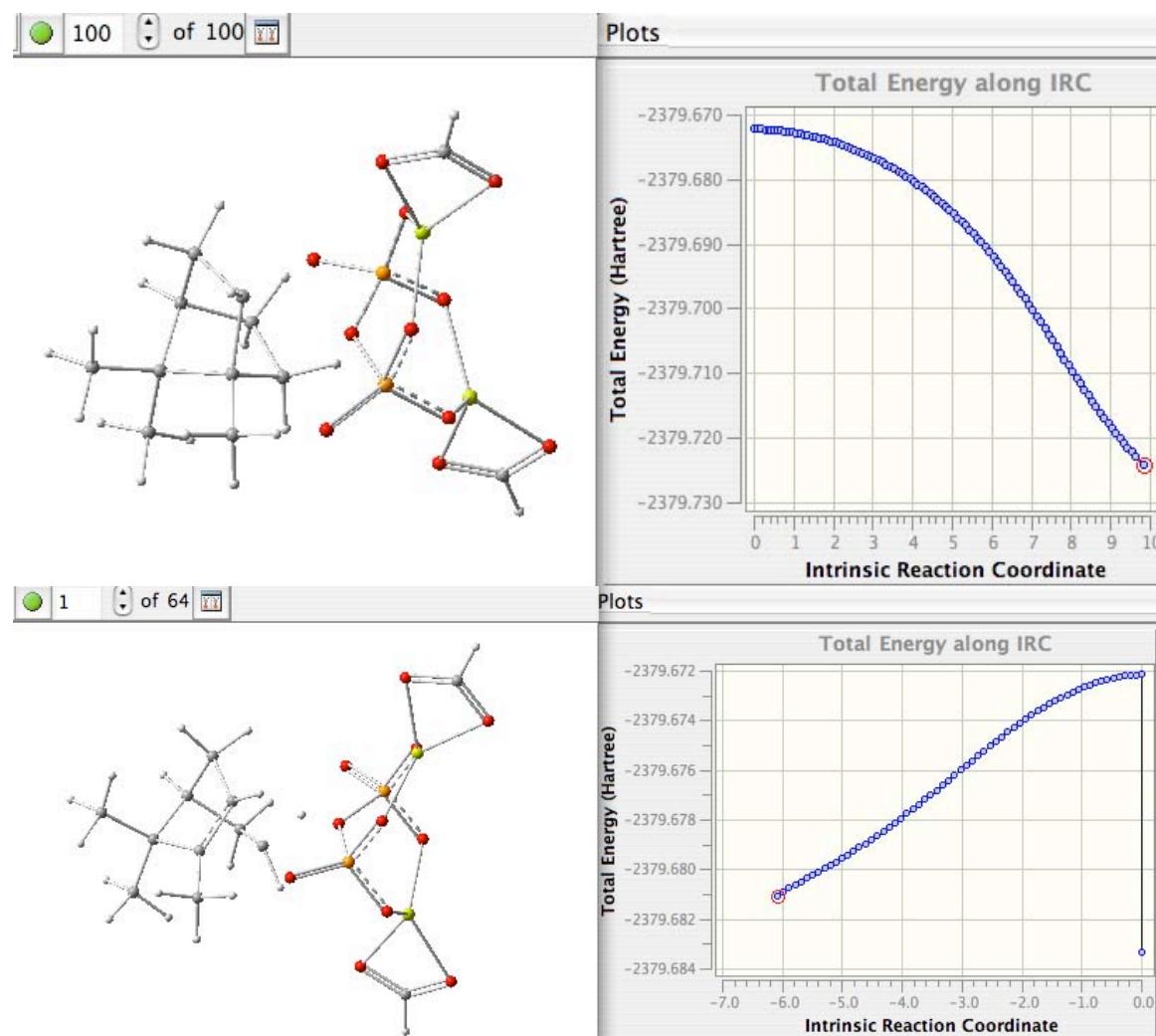


Figure S13b.

TS(S16)

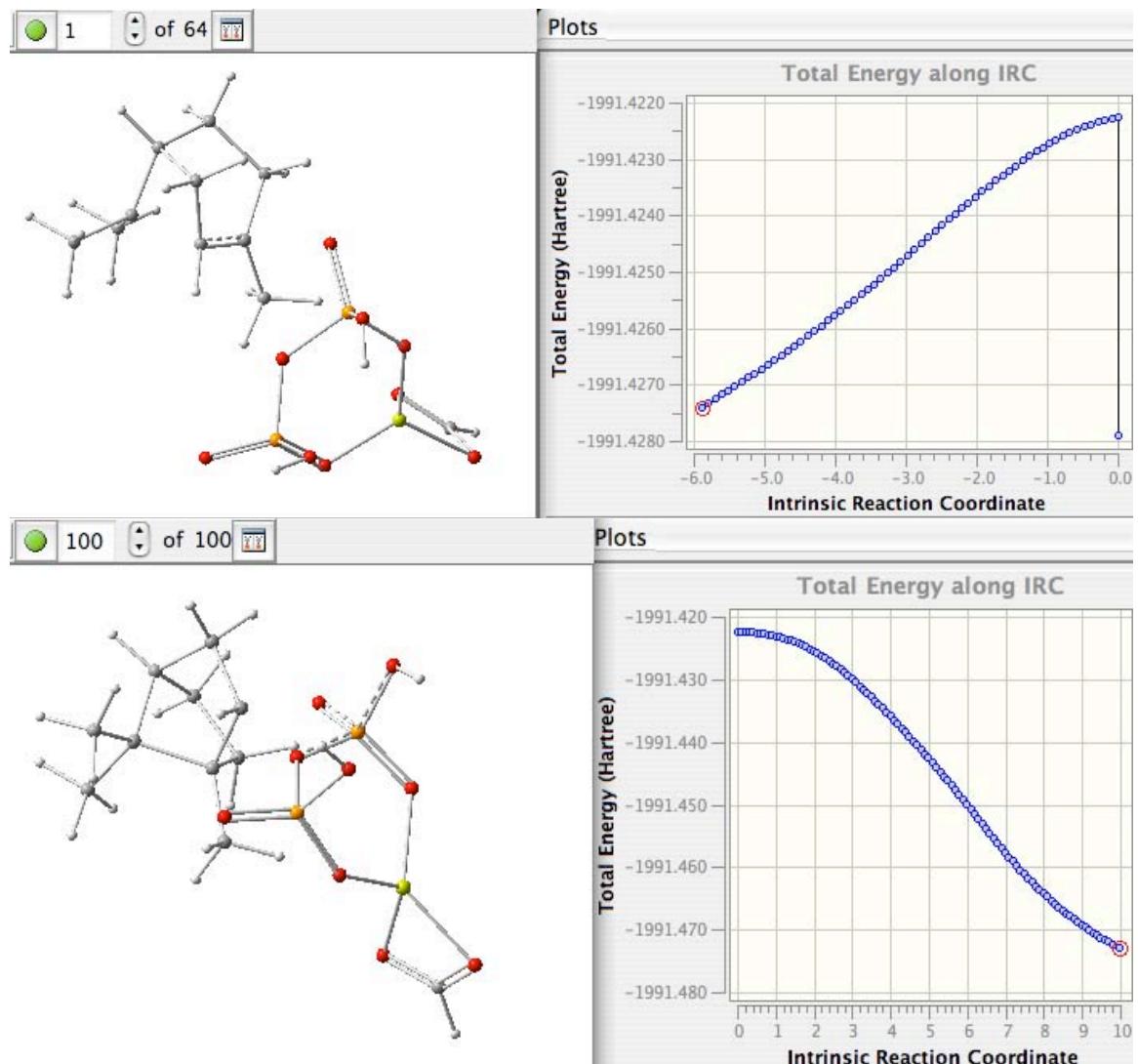
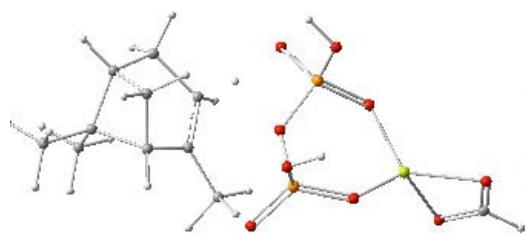


Figure S14b.

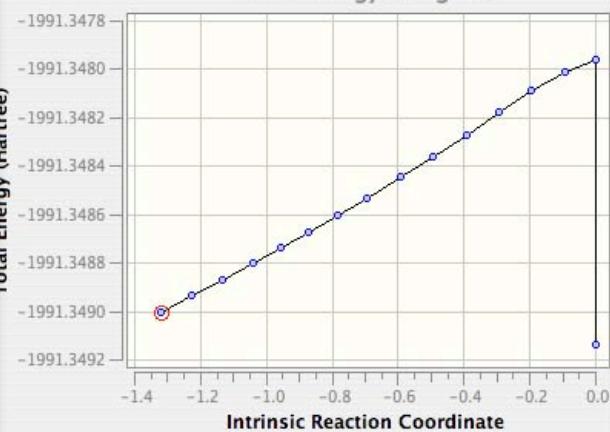
TS(S18)

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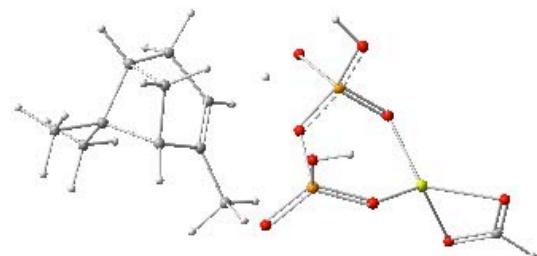


Plots

Total Energy along IRC

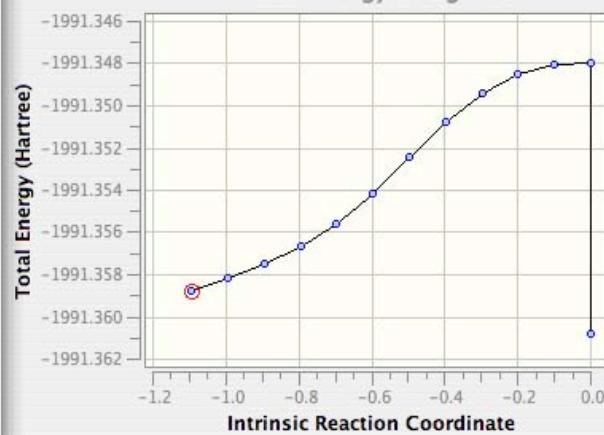


1 of 13



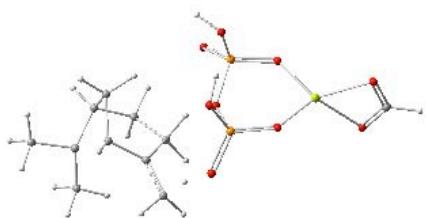
Plots

Total Energy along IRC



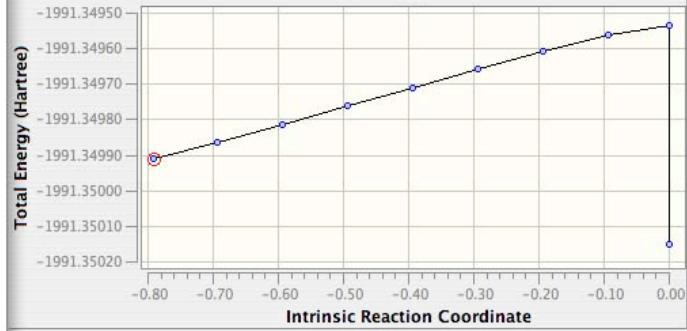
TS(S19)

1 of 10



Plots

Total Energy along IRC



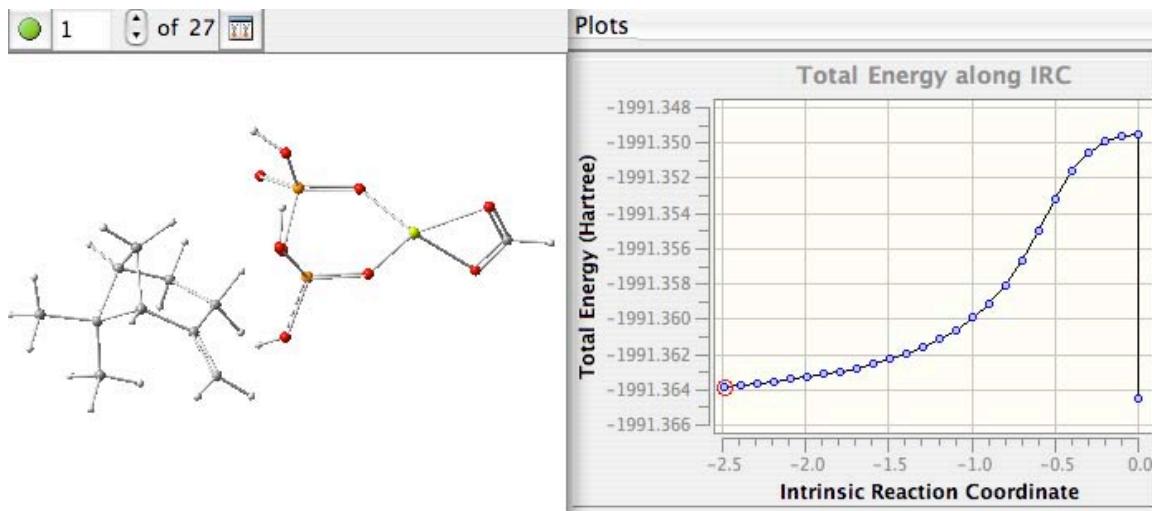
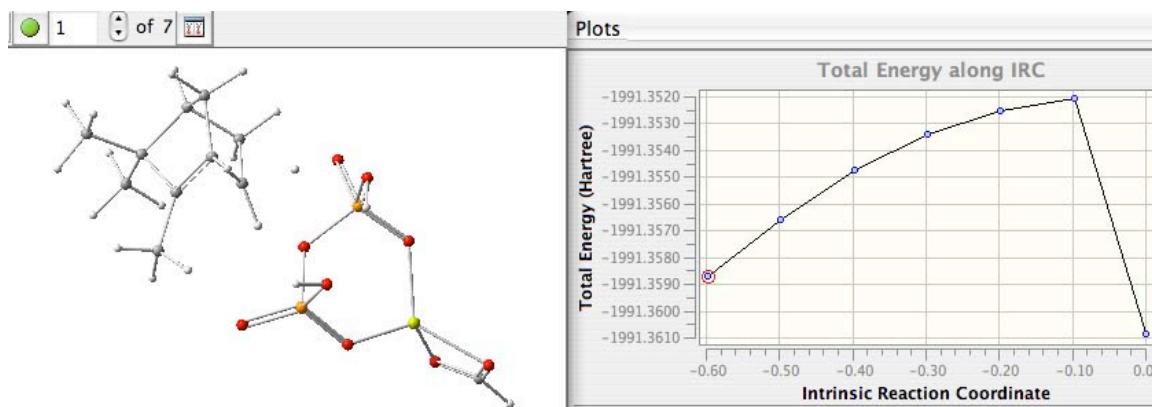


Figure S15.

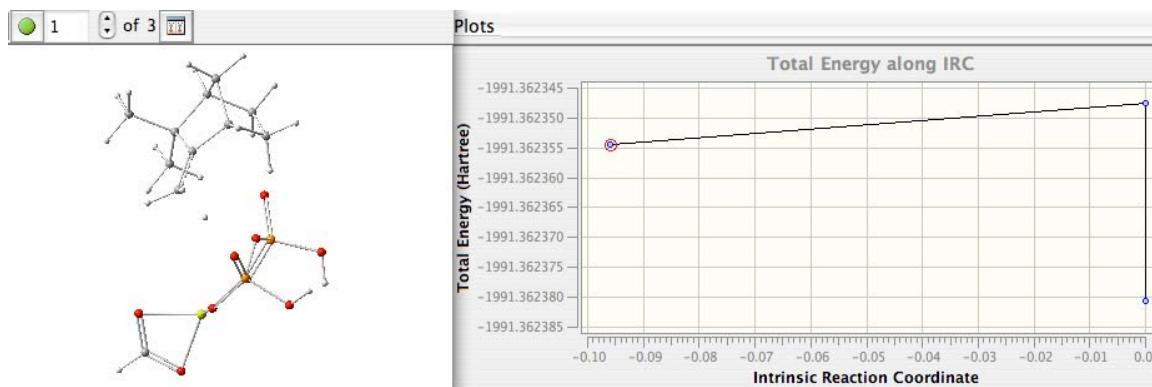
TS(S20)



IRC calculation to the other direction was unsuccessful.

Figure S16a.

TS(S21)



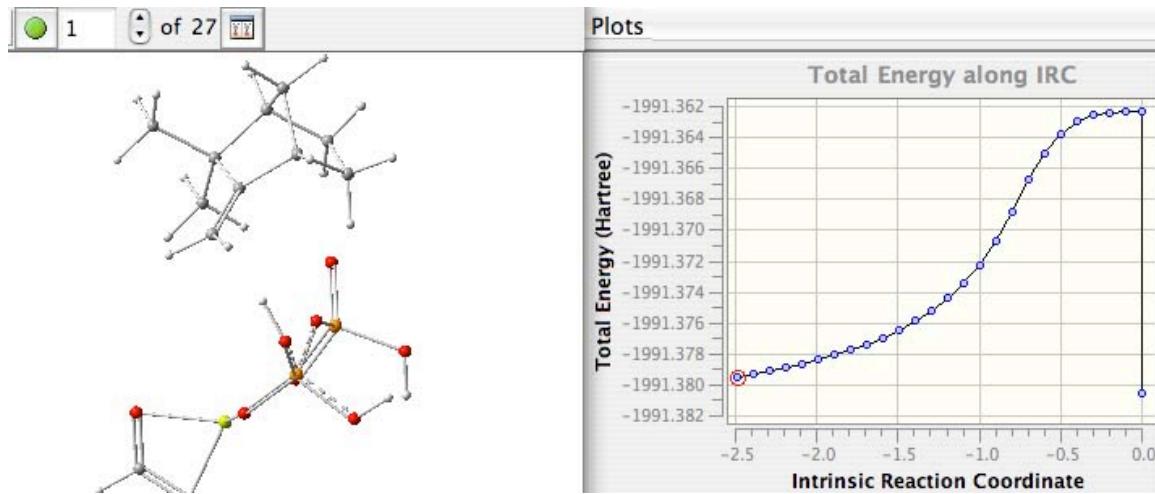
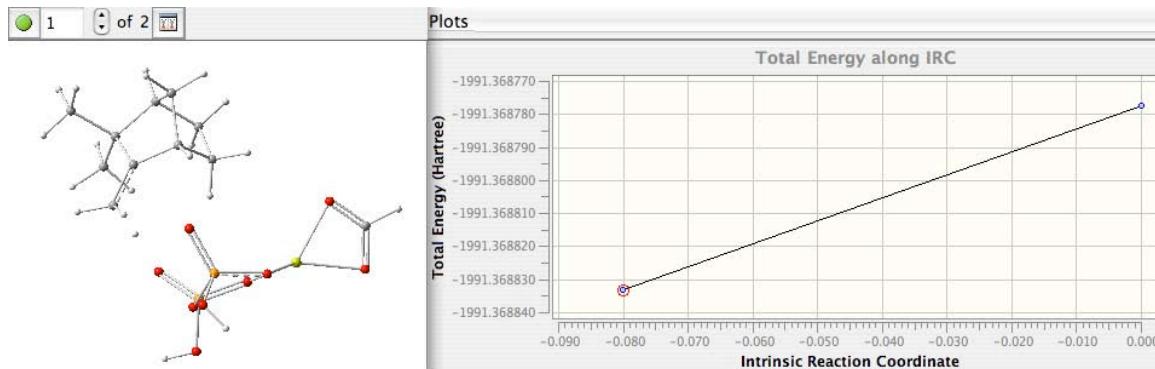
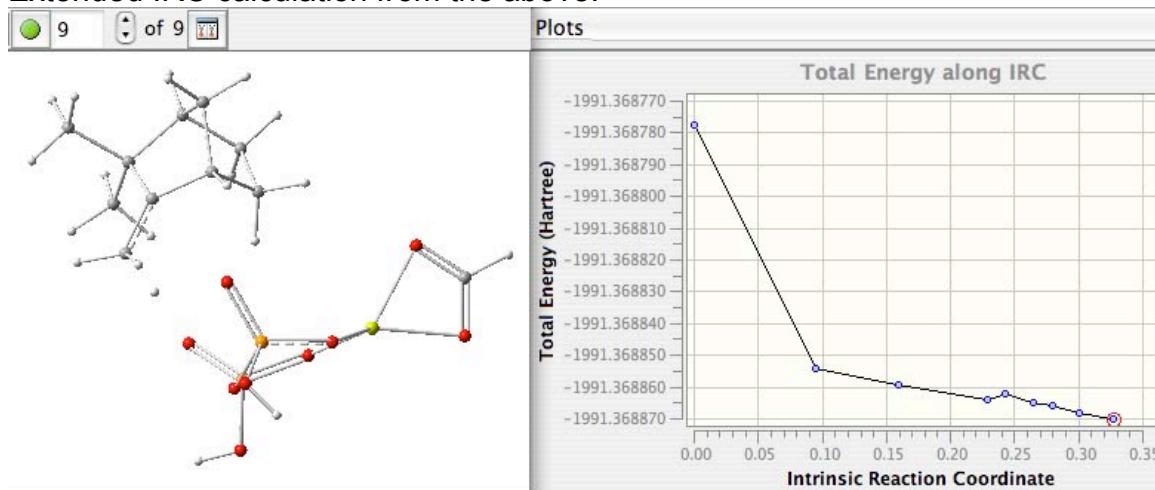


Figure S16b.

TS(S22)



Extended IRC calculation from the above.



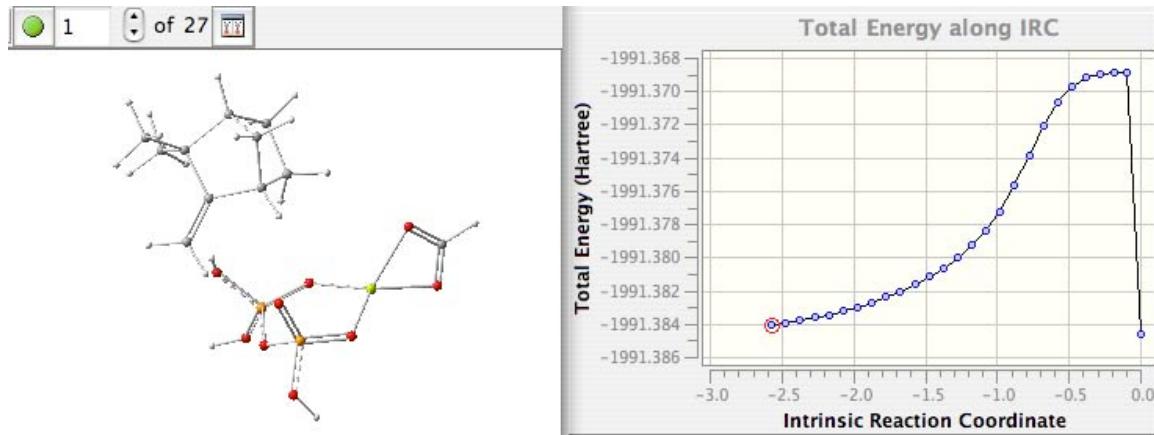
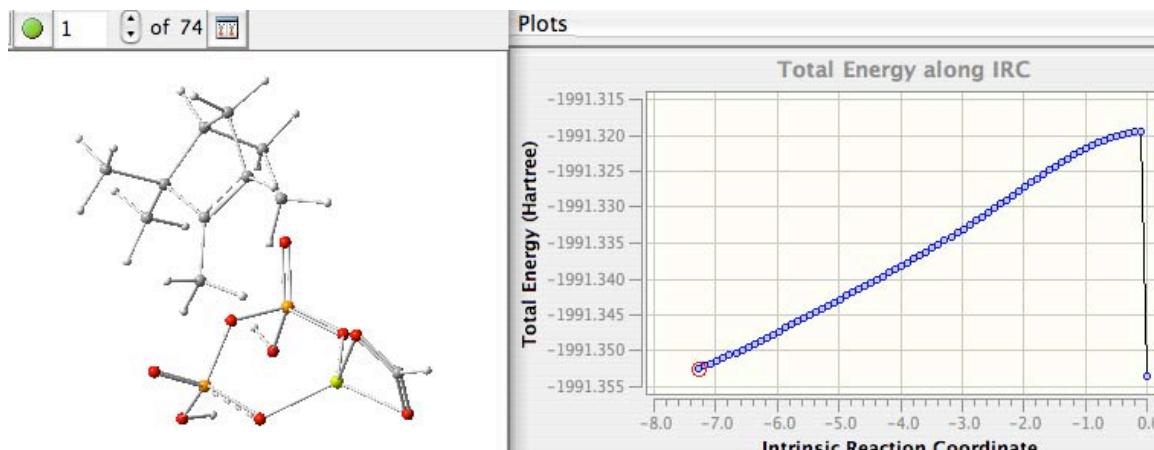
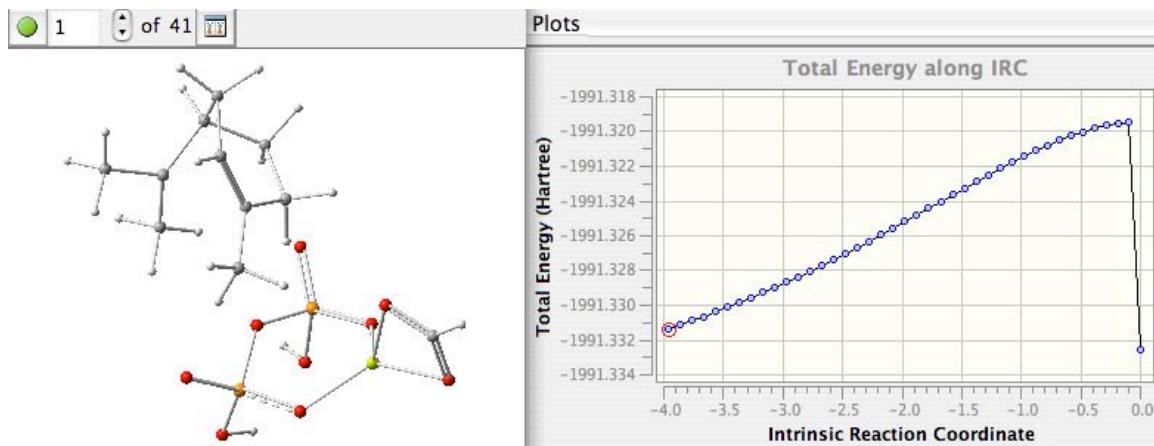
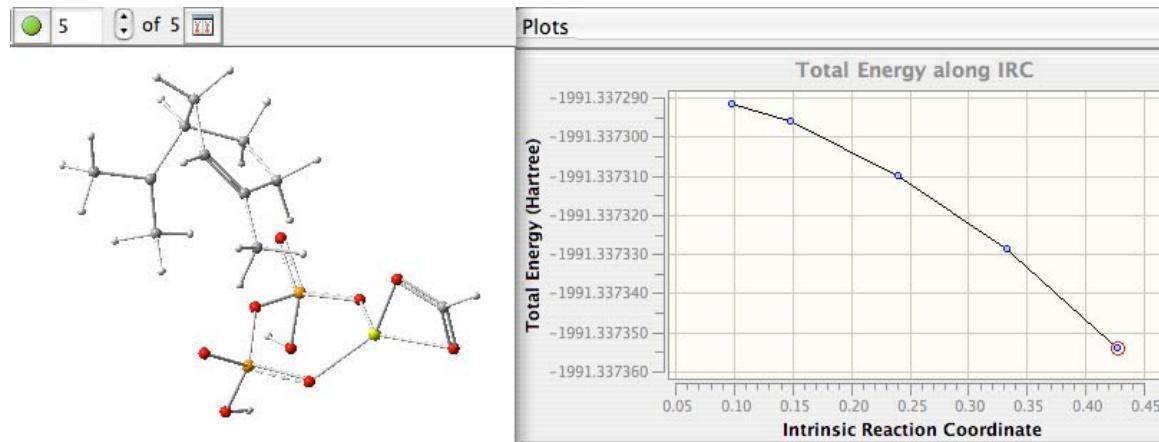


Figure S17.

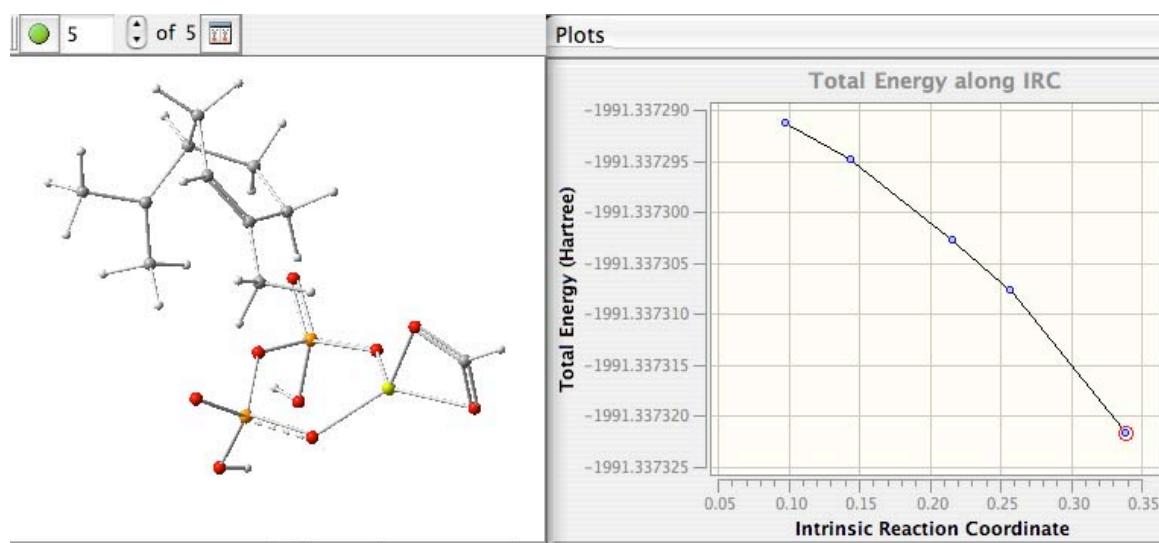
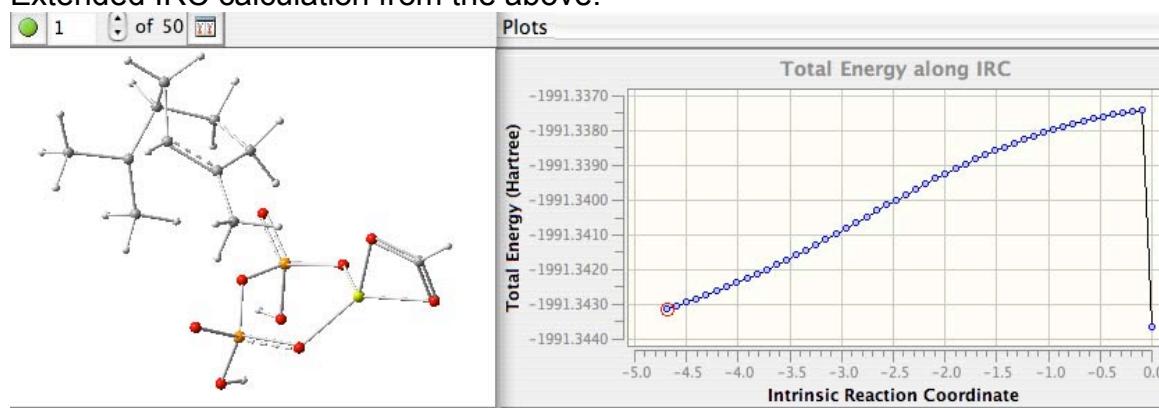
TS(S23)



TS(S24)



Extended IRC calculation from the above.



Extended IRC calculation from the above.

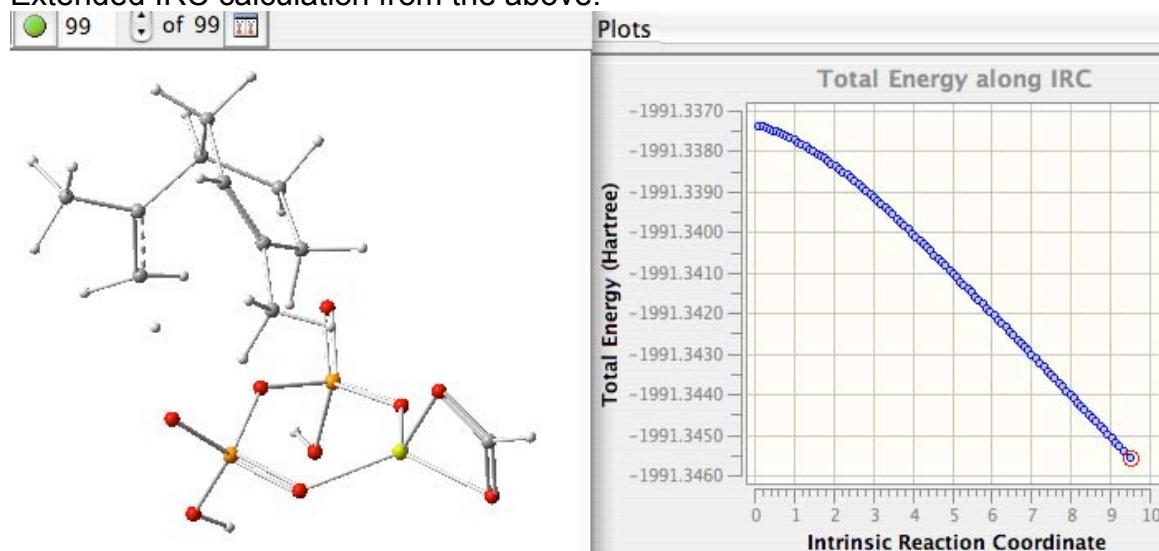
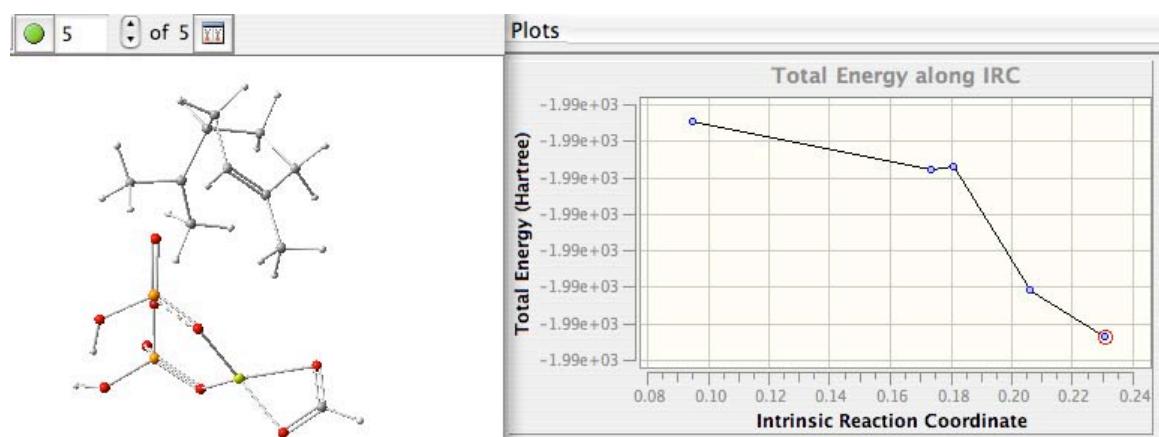
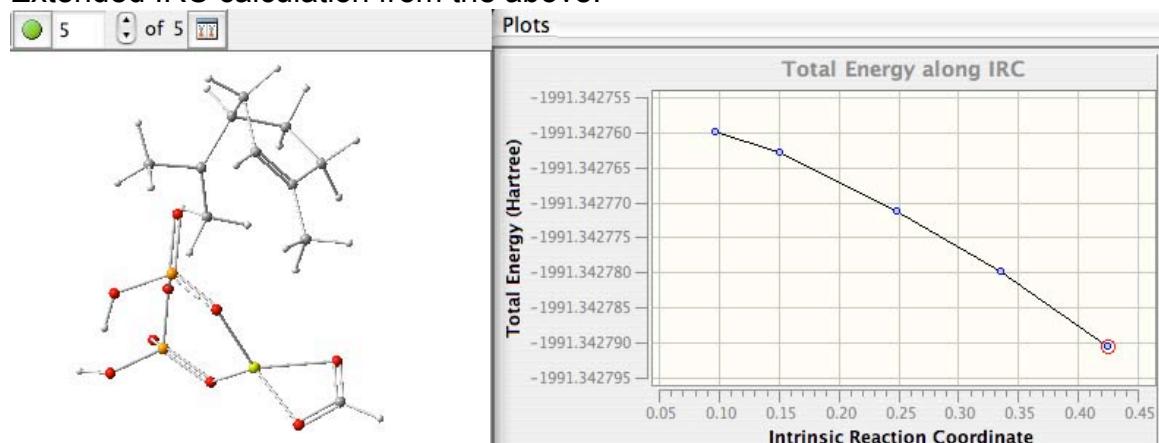


Figure S18.

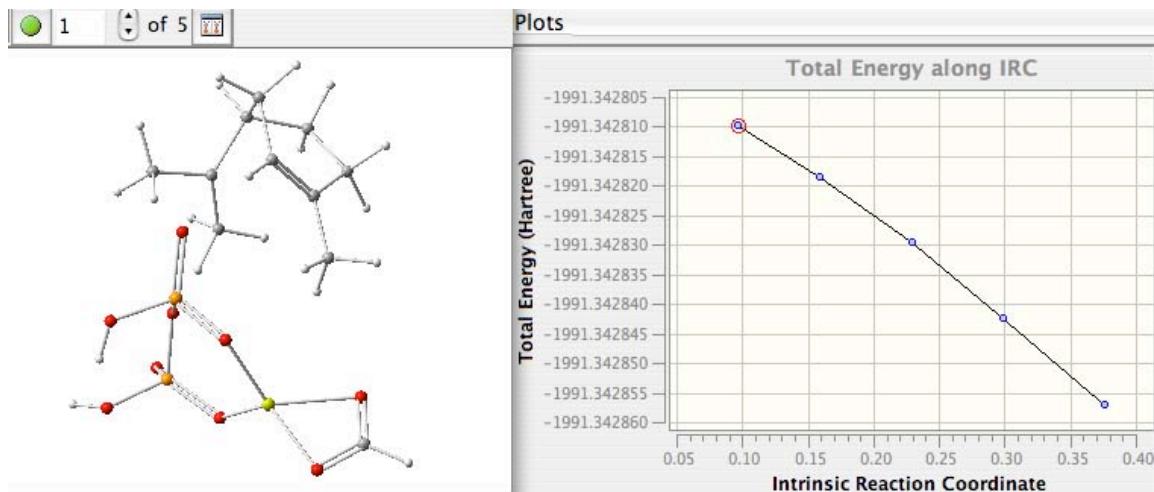
TS(S25)



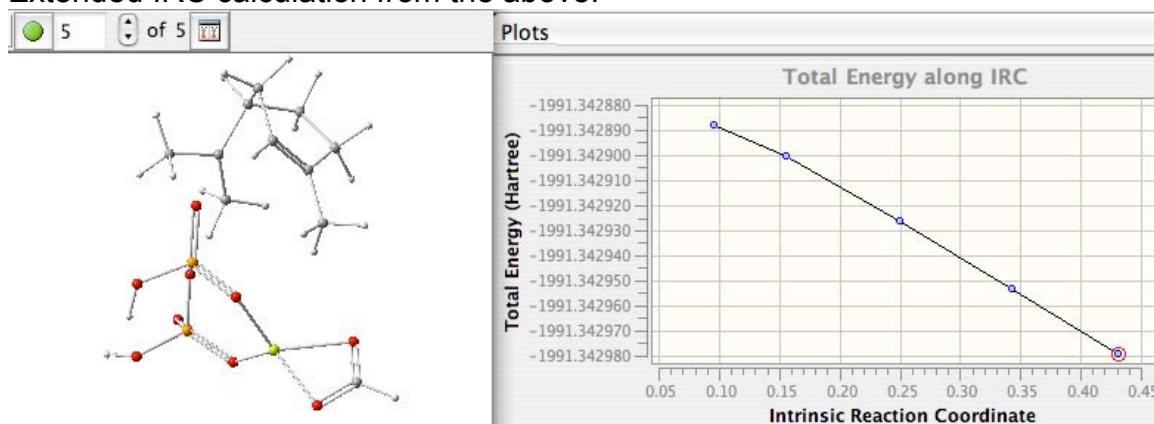
Extended IRC calculation from the above.



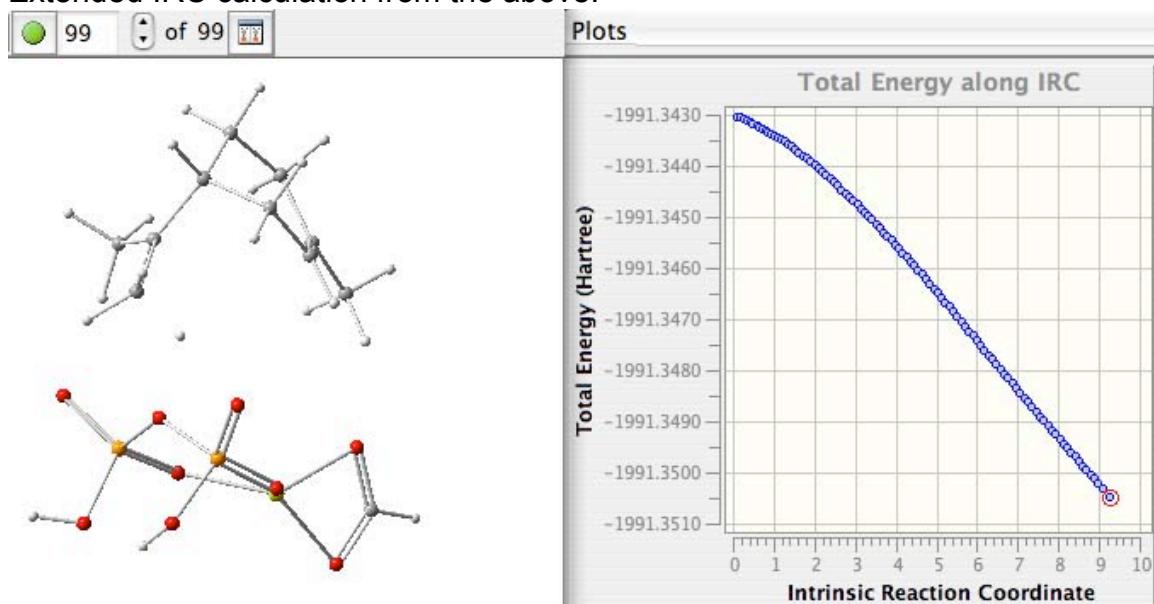
Extended IRC calculation from the above.



Extended IRC calculation from the above.

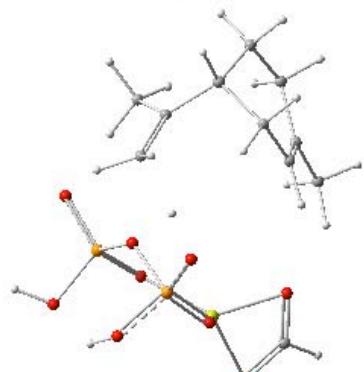


Extended IRC calculation from the above.



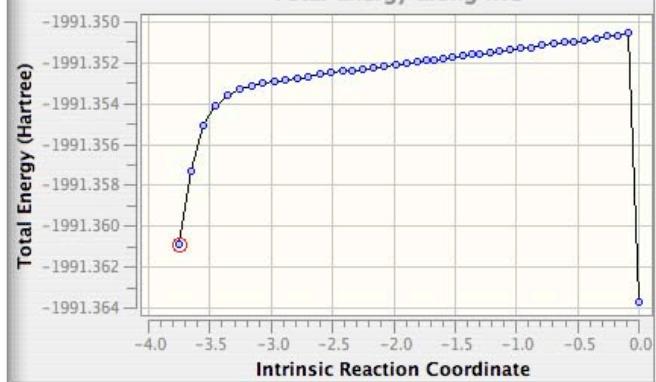
Extended IRC calculation from the above.

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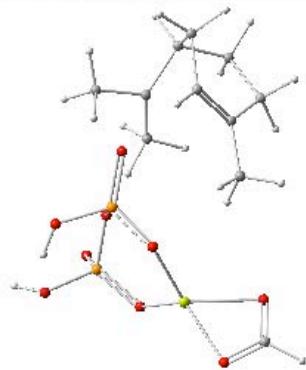


Plots

Total Energy along IRC

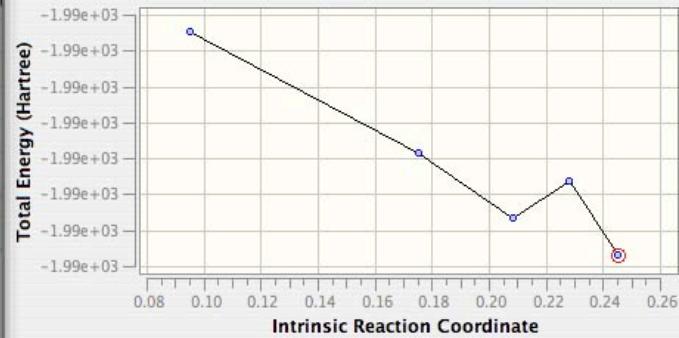


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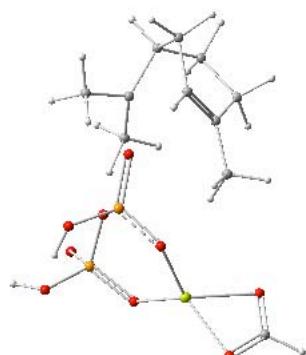
Plots

Total Energy along IRC



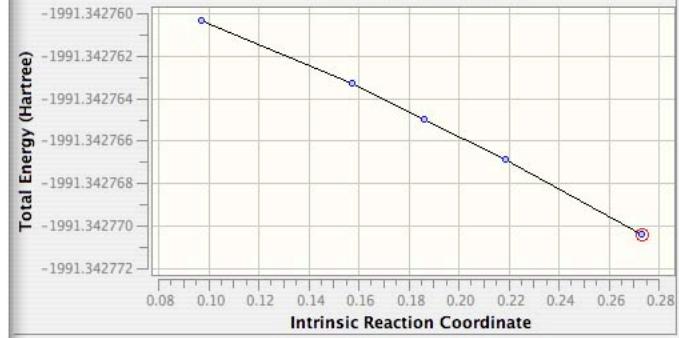
Extended IRC calculation from the above.

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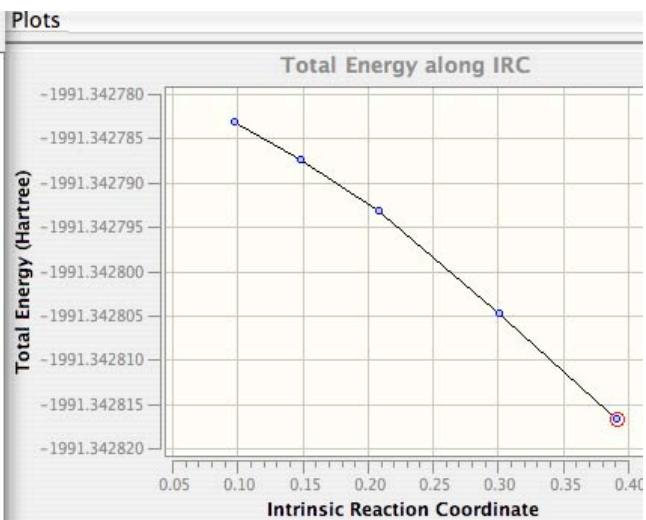
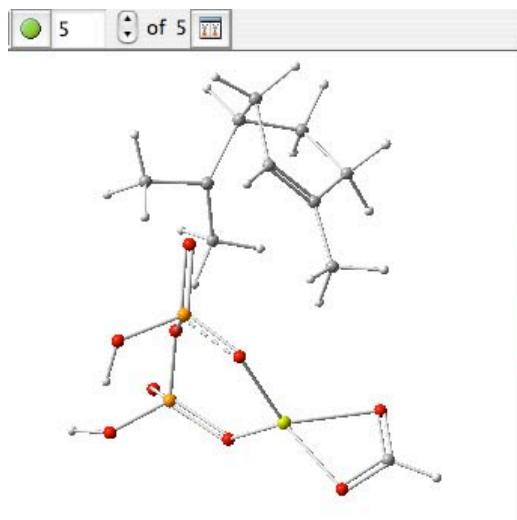


Plots

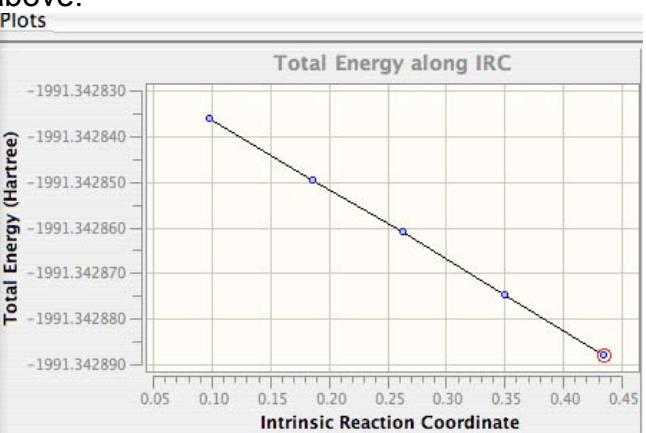
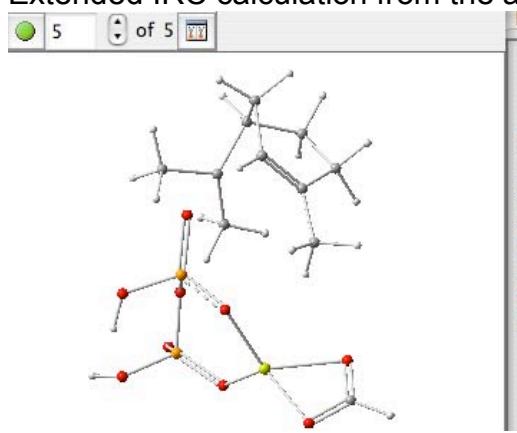
Total Energy along IRC



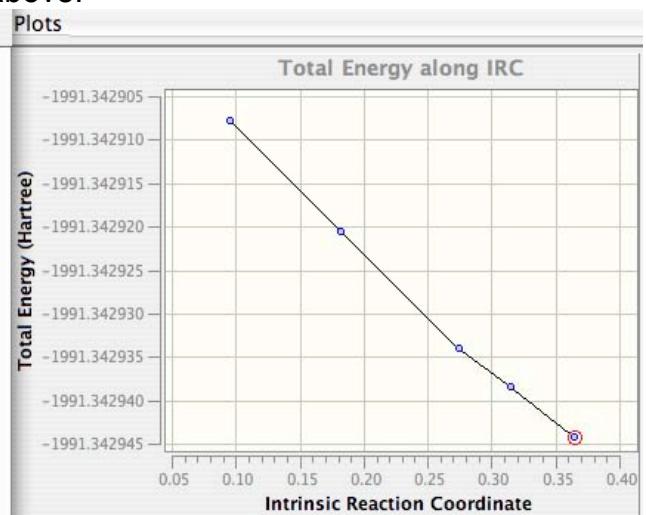
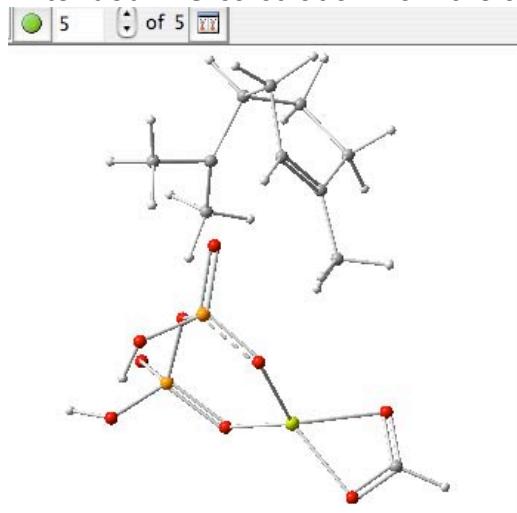
Extended IRC calculation from the above.



Extended IRC calculation from the above.

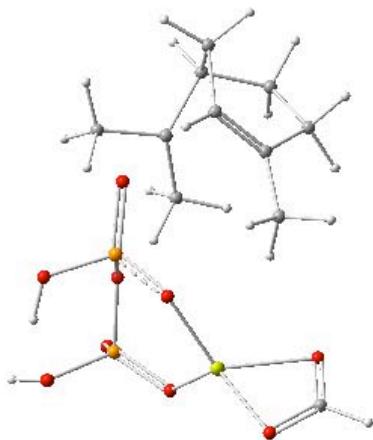


Extended IRC calculation from the above.



Extended IRC calculation from the above.

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Plots

