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Theoretical insights into the C-C bond formation through isonitrile insertion into Cp*Ti complex

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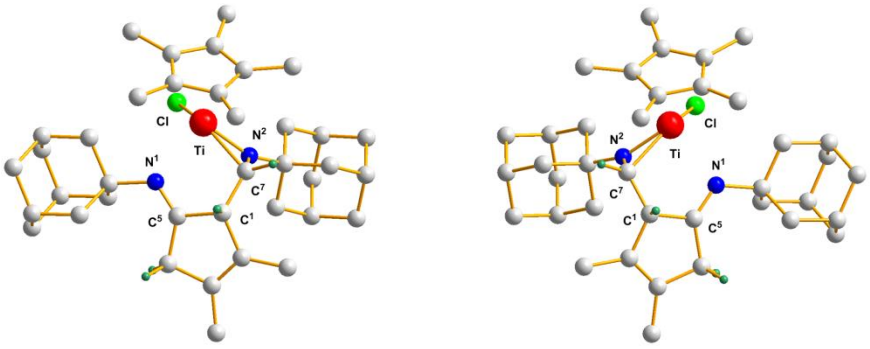
S1. Choice of calculation method

The geometrical structures of the enantiomers of titanaaziridine, **10**$^{1\text{-Ad}}$ and **10**$^{1\text{-Ad}}$**IS**, were estimated by examining four theoretical models, B3LYP/BS1, B3LYP/def2-SVP, BP86/BS2, and BP86/LANL2DZ, and by comparing the calculated bond parameters to their X-ray crystal structures in order to predict the geometrical structures of the molecules accurately.[1] In BS1, the Ti and Cl atoms are described with the LANL2DZ basis sets improved with a set of f- or d-polarization function (α = 1.506 for Ti; α = 0.640 for Cl) with effective core potentials (ECPs),[2-6] while the other atoms are represented by the 6-311+G(d,p) basis sets, except for the atoms in the methyl and 1-adamantyl substituent groups, which are described with the 6-31G basis sets.[7-9] In BS2, the Ti atom is represented by the LANL2DZ basis set with ECP, Cl atom by the 6-311+G(d,p) basis set, and other atoms by the same basis sets as in BS1. These calculation methods have been applied to study titanium complexes and the complexes of the same group metals (Zr and Hf).[10-18] Moreover, the theoretical models, B3LYP/BS3 and B3LYP/BS4, were also examined. In BS3, the Cl atom is described with the 6-311+G(d,p) basis set instead of the improved LANL2DZ basis set used in BS1. Since Ti atom can be represented by a full basis set, the 6-311G basis set is adopted for the Ti atom in BS4 instead of the LANL2DZ basis set with ECP used in BS2. As shown in **Table 1**, the calculated results at the levels of B3LYP/BS1 and BP86/BS2 are closer to the experimental ones. However, BP86/BS2 is less accurate in predicting the Ti-N^2 bond length with the largest error of 0.031 Å. In addition, it is found that B3LYP/BS1 is much better than BP86/BS2 in predicting the Hf complex **16** (**Table 2**). For **16**, the Hf and Cl atoms are represented by the LANL2DZ basis sets improved with a set of f- or d-polarization function (α = 0.784 for Hf; α = 0.640 for Cl) with ECP in BS1,[4] while the other atoms are described with the 6-311+G(d,p) basis sets, except for the atoms in the methyl and 2,6-dimethylphenyl (Ar) substituent groups, which are described with the 6-31G basis sets. Further, in BS2, the Hf atom is described with the LANL2DZ basis sets with ECP, Cl atom with the 6-311+G(d,p) basis set, and other atoms with the same basis sets as in BS1. In order to compare with the on-going study of the reaction of Cp*(Cl)Hf(diene) with isonitriles, the B3LYP/BS1 model is adopted in this work. All the calculations were performed in n-pentane with the G09 program, and the polarizable continuum model (PCM) using the integral equation formalism variant (IEFPCM) was adopted for the SCRF calculations.[19]



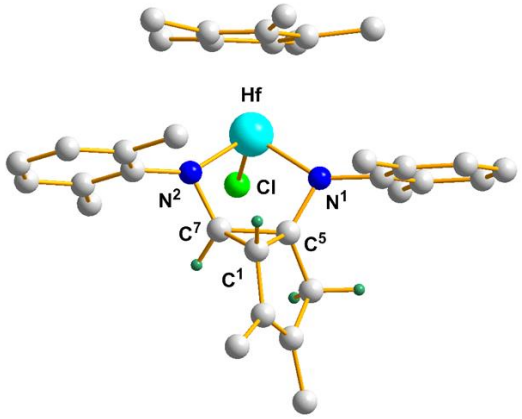
10$^{1\text{-Ad}}$ **10**$^{1\text{-Ad}}$**IS**

Atomic numbering for **10**$^{1\text{-Ad}}$ and **10**$^{1\text{-Ad}}$**IS**

(The H atoms on the methyl and 1-Ad groups were omitted for clarity.)

Table 1. Calculated main bond parameters and corresponding experimental values (bond length in Angstrom, angle and dihedral angle in Degree) for **$10^{1\text{-Ad}}$** and **$10^{1\text{-Ad}}$IS** (in parentheses)

	Bond Parameters									
Methods	**Ti-N^1**	**Ti-N^2**	**Ti-C^7**	**Ti-Cl**	**C^5-N^1**	**C^5-C^1**	**C^7-C^1**	**C^7-N^2**	**Ti-N^2-C^7**	**Ti-N^2-C^7-C^1**
B3LYP/BS1	2.348	1.874	2.092	2.426	1.285	1.513	1.530	1.396	78.1	98.7
	(2.348)	(1.874)	(2.092)	(2.426)	(1.285)	(1.513)	(1.530)	(1.396)	(78.1)	(-98.7)
B3LYP/def2-SVP	2.355	1.877	2.099	2.413	1.288	1.513	1.530	1.395	78.3	98.4
BP86/BS2	2.341	1.893	2.110	2.415	1.298	1.516	1.537	1.407	78.0	98.6
BP86/LANL2DZ	2.292	1.881	2.112	2.465	1.318	1.526	1.554	1.434	77.9	98.6
B3LYP/BS3	2.349	1.875	2.091	2.433	1.285	1.513	1.530	1.396	78.0	98.7
B3LYP/BS4	2.360	1.890	2.106	2.430	1.286	1.514	1.531	1.397	78.1	98.8
Exp.[1]	2.250	1.862	2.118	2.411	1.302	1.475	1.506	1.406	79.4	96.8
	(2.273)	(1.881)	(2.118)	(2.412)	(1.291)	(1.503)	(1.526)	(1.380)	(79.4)	(-96.4)



16

Atomic numbering for **16**

(The H atoms on the methyl and Ar groups were omitted for clarity.)

Table 2. Calculated main bond parameters and corresponding experimental values (bond length in Angstrom, angle and dihedral angle in Degree) for **16**

	Bond Parameters									
Methods	**Hf-N^1**	**Hf-N^2**	**Hf-C^5**	**Hf- C^7**	**C^5-N^1**	**C^7-N^2**	**C^7-C^5**	**C^5-C^1**	**C^7-C^1**	**N^1-Hf-N^2**
B3LYP/BS1	2.037	2.028	2.628	2.588	1.451	1.449	1.576	1.525	1.524	93.5
BP86/BS2	2.052	2.045	2.622	2.583	1.454	1.451	1.594	1.535	1.535	93.7
Exp.[1]	2.010	1.991	2.527	2.490	1.423	1.444	1.552	1.493	1.507	95.0

References

1 N. Valadez, J. R. Norton and M. C. Neary, *J. Am. Chem. Soc.*, 2015, **137**, 10152-10155.

2 P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 270-283.

3 W. R. Wadt and P. J. Hay, *J. Chem. Phys.*, 1985, **82**, 284-298.

4 A. W. Ehlers, M. Böhme, S. Dapprich, A. Gobbi, A. Höllwarth, V. Jonas, K. F. Köhler, R. Stegmann, A. Veldkamp and G. Frenking, *Chem. Phys. Lett.*, 1993, **208**, 111-114.

5 A. Höllwarth, M. Böhme, S. Dapprich, A. W. Ehlers, A. Gobbi, V. Jonas, K. F. Köhler, R. Stegmann, A. Veldkamp and G. Frenking, *Chem. Phys. Lett.*, 1993, **208**, 237-240.

6 P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 299-310.

7 W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257-2261.

8 R. Krishnan, J. S. Binkley, R. Seeger and J. A. Pople, *J. Chem. Phys.*, 1972, **72**, 650-654.

9 V. A. Rassolov, M. A. Ratner, J. A. Pople, P. C. Redfern and L. A. Curtiss, *J. Comput. Chem.*, 2001, **22**, 976-984.

10 M. Haehnel, M. Ruhmann, O. Theilmann, S. Roy, T. Beweries, P. Arndt, A. Spannenberg, A. Villinger, E. D. Jemmis, A. Schulz and U. Rosenthal, *J. Am. Chem. Soc.*, 2012, **134**, 15979-15991.

11 Y.-D. Wu and Z.-X. Yu, *J. Am. Chem. Soc.*, 2001, **123**, 5777-5786.

12 S. Roy, U. Rosenthal and E. D. Jemmis, *Acc. Chem. Res.*, 2014, **47**, 2917-2930.

13 S. Niu and M. B. Hall, *Chem. Rev.*, 2000, **100**, 353-405.

14 B. Flemmig, P. Strauch and J. Reinhold, *Organometallics*, 2003, **22**, 1196-1202.

15 S. Roy, E. D. Jemmis, M. Ruhmann, A. Schulz, K. Kaleta, T. Beweries and U. Rosenthal, *Organometallics*, 2011, **30**, 2670-2679.

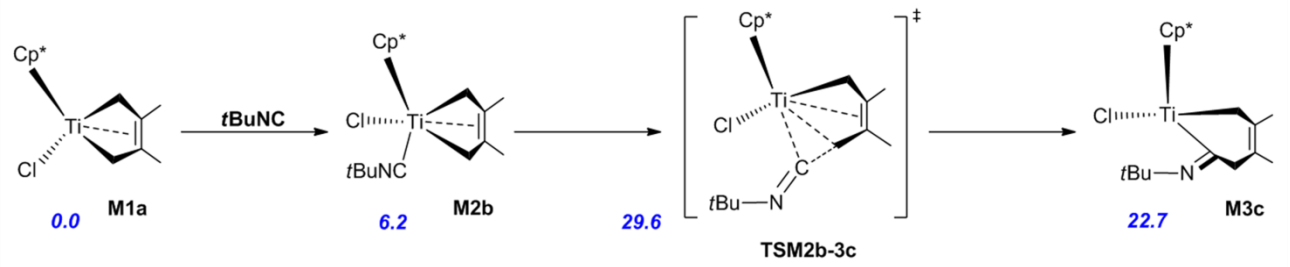
16 K. Kaleta, M. Ruhmann, O. Theilmann, T. Beweries, S. Roy, P. Arndt, A. Villinger, E. D. Jemmis, A. Schulz and U. Rosenthal, *J. Am. Chem. Soc.*, 2011, **133**, 5463-5473.

17 L. A. Watson, D. V. Yandulov and K. G. Caulton, *J. Am. Chem. Soc.*, 2001, **123**, 603-611.

18 E. Clot, C. Mégret, B. M. Kraft, O. Eisenstein and W. D. Jones, *J. Am. Chem. Soc.*, 2004, **126**, 5647-5653.

19 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09 Revision A.02, Gaussian, Inc., Wallingford, CT 2009.

S2. **Scheme S1.** Summary of the calculated reaction pathways and results for (a) coordination of *t*BuNC to **M1a** and subsequent insertion into Ti-C bond, (b) coordination of *t*BuNC to **M3a** and subsequent insertion into Ti-C bond. Values denote Gibbs free energies in kcal mol^{-1}. Solvent: n-pentane



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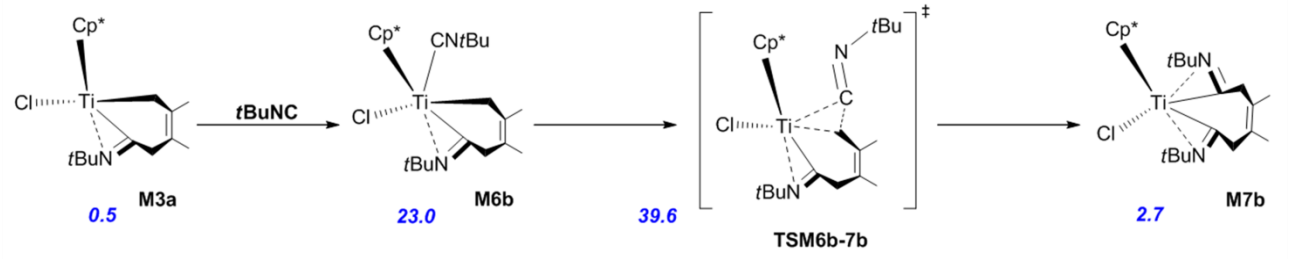
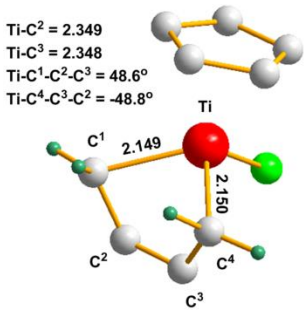


(b)

S3. **Figure S1.** Optimised structures (the methyl groups and the H atoms except for that involved in reaction were omitted for clarity, distances and angles are given in Å and degree, respectively; in n-pentane)



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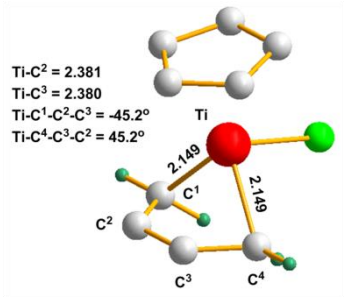

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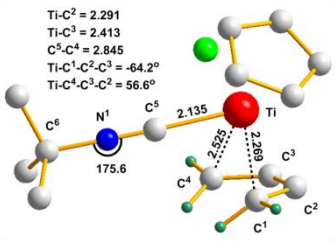

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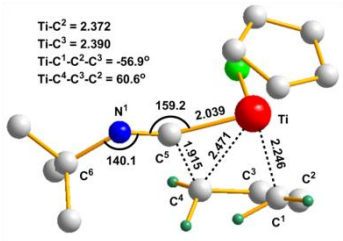

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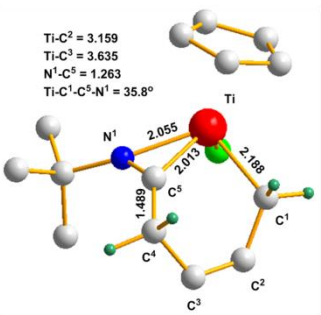

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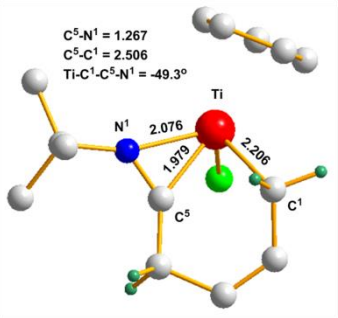

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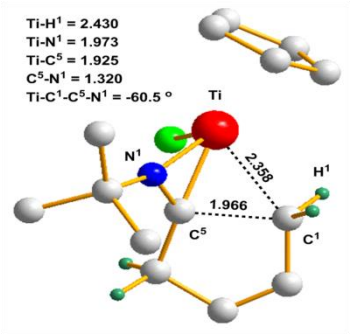

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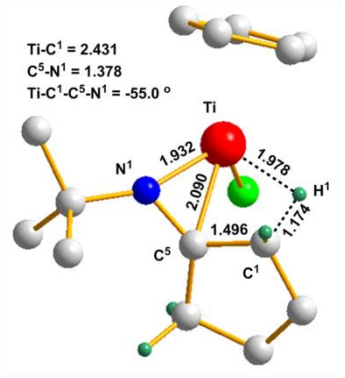

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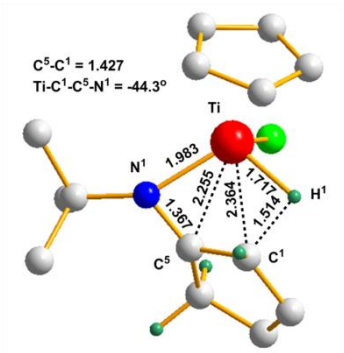

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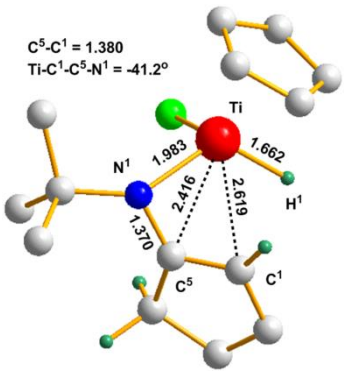

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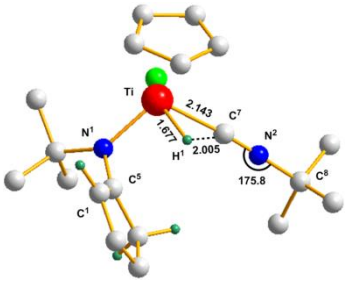

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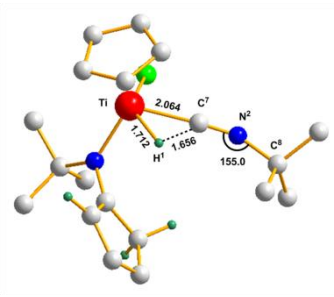

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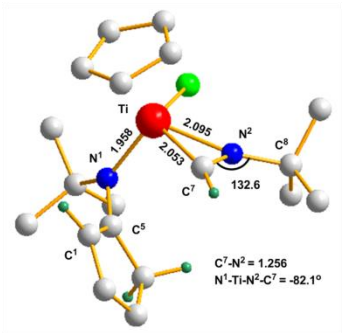

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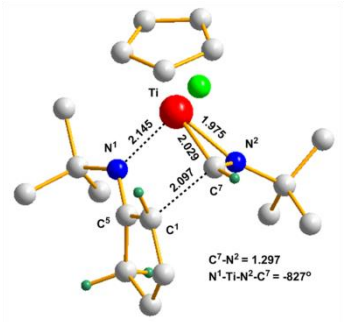

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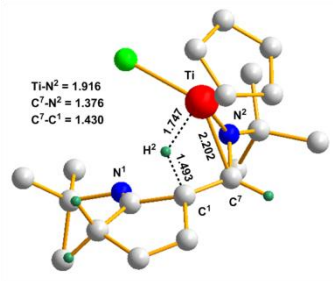

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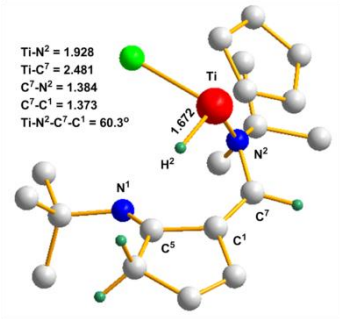

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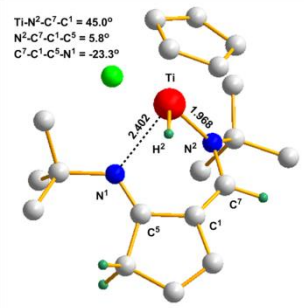

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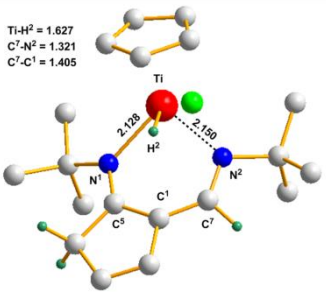

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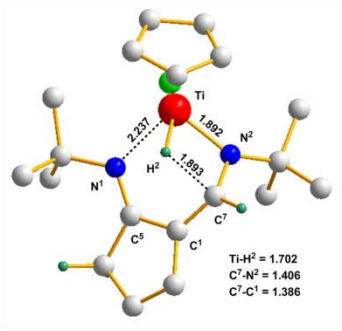

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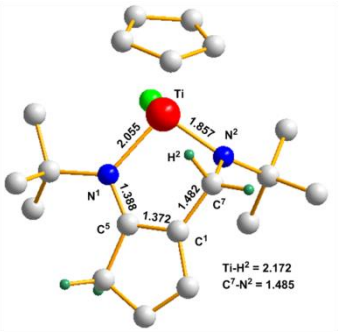

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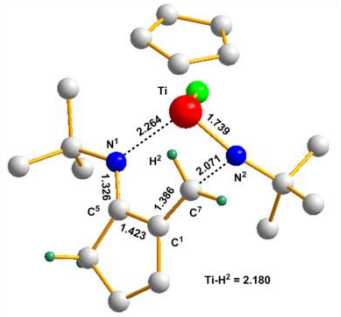

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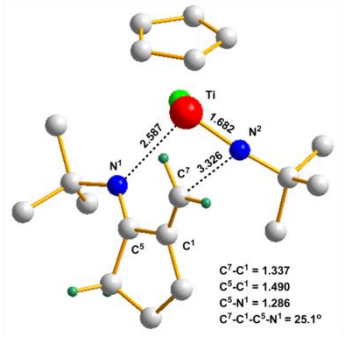
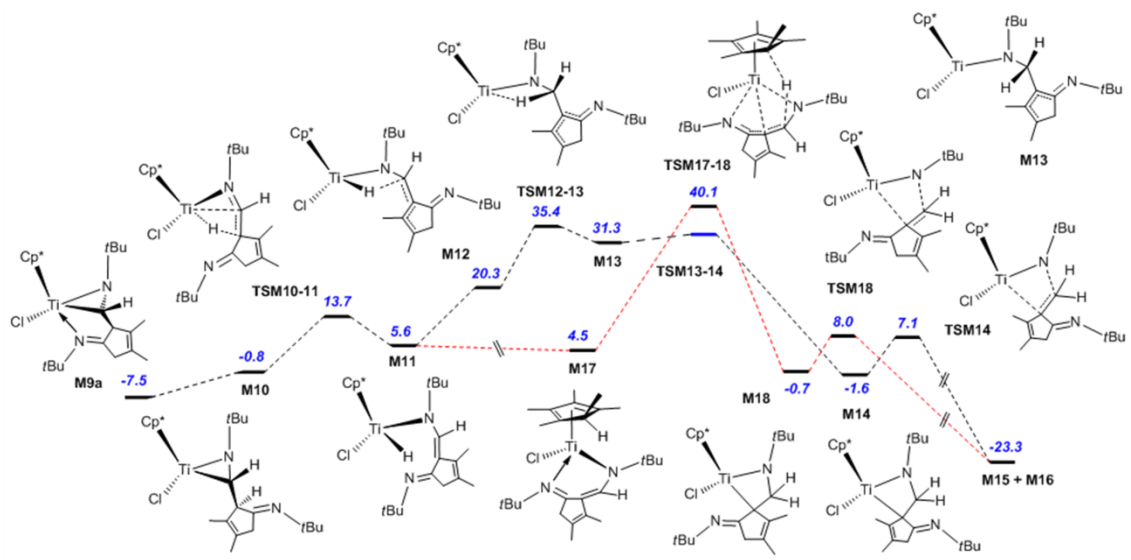


M21

S4. **Figure S2.** Energetic profiles for the fragmentation of the titanaaziridine **M9a** (a) involving four-membered titanacycles, and (b) for breaking the Ti-C bond in **M9a**, and γ-H elimination in **M23**. The Gibbs free energies are given in kcal mol^{-1}. Blue italics: reaction in n-pentane, black: reaction in benzene.



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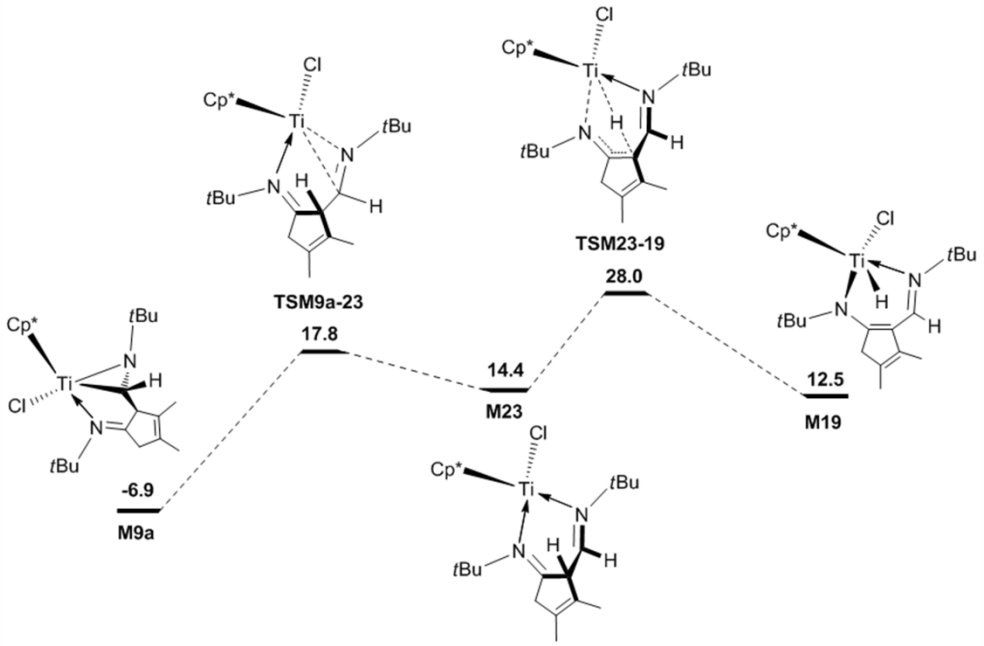
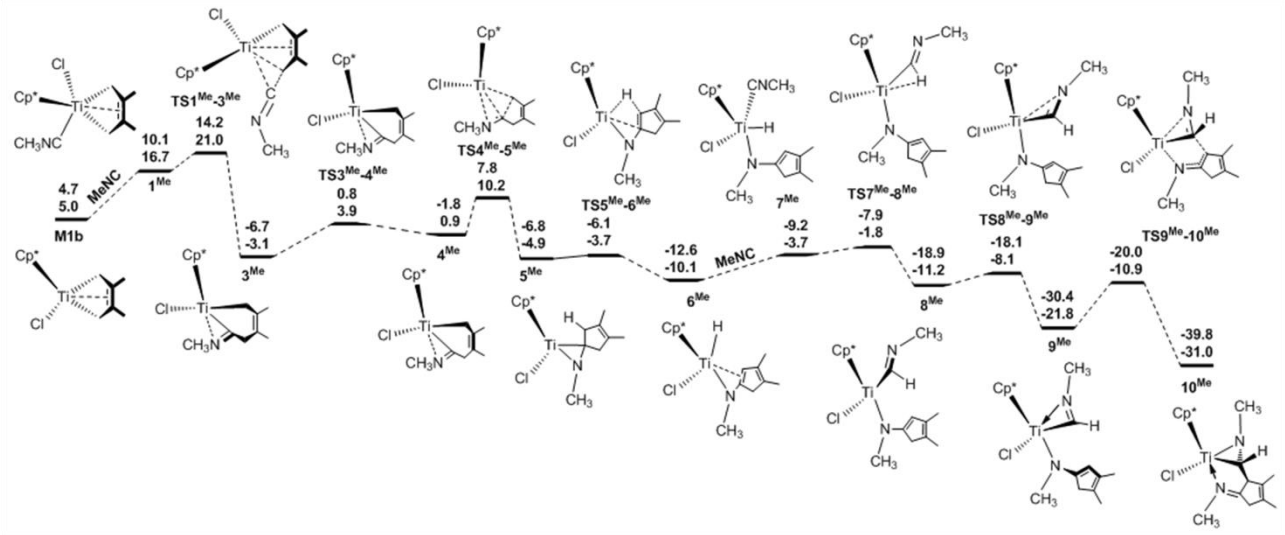
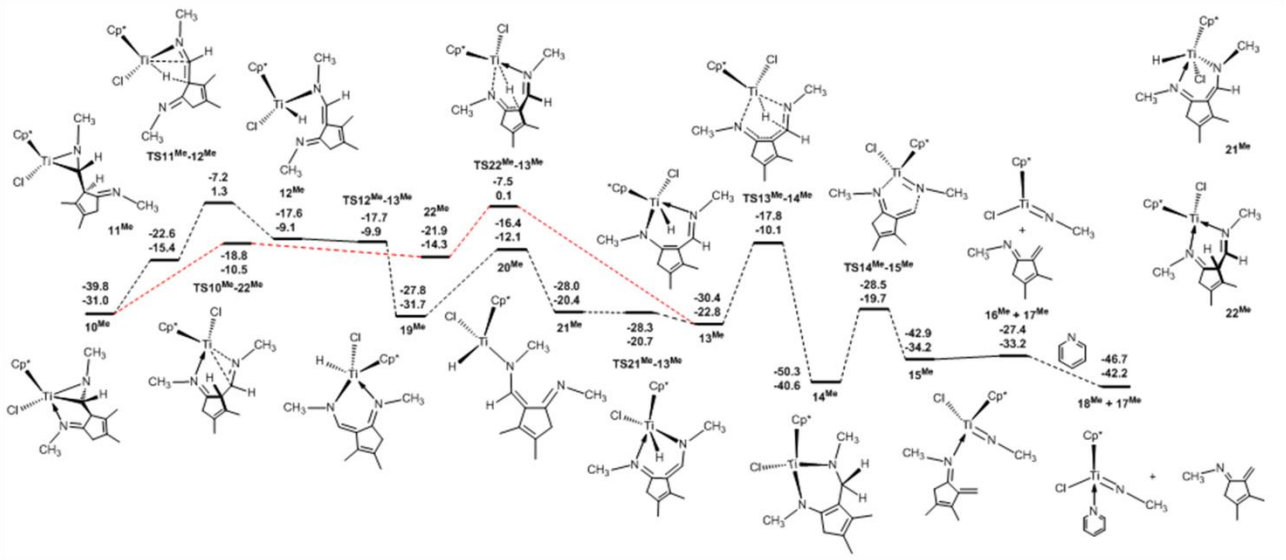


(b)

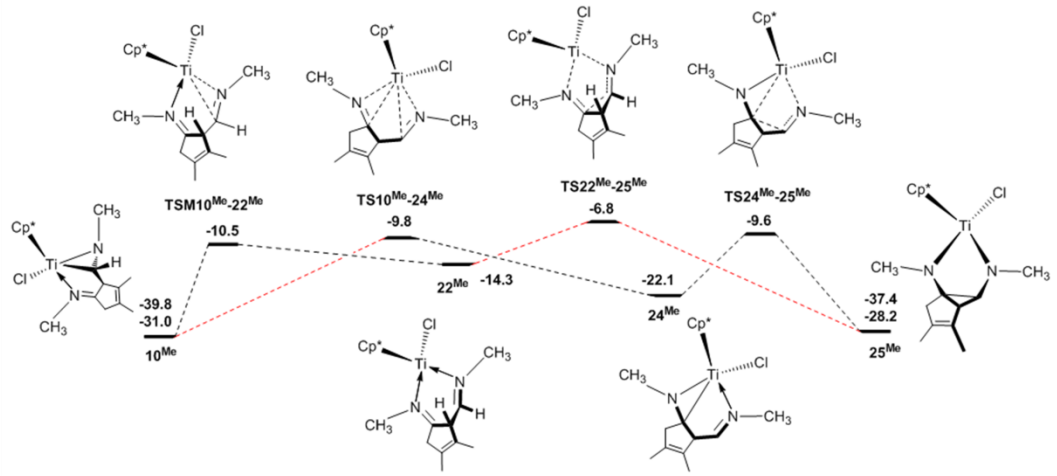
S5. **Figure S3.** Energetic profile for the formation of the titanaaziridine **10^{Me}**. The Gibbs free energies are given in kcal mol^{-1} and the above values include the dispersion correction. Solvent: benzene



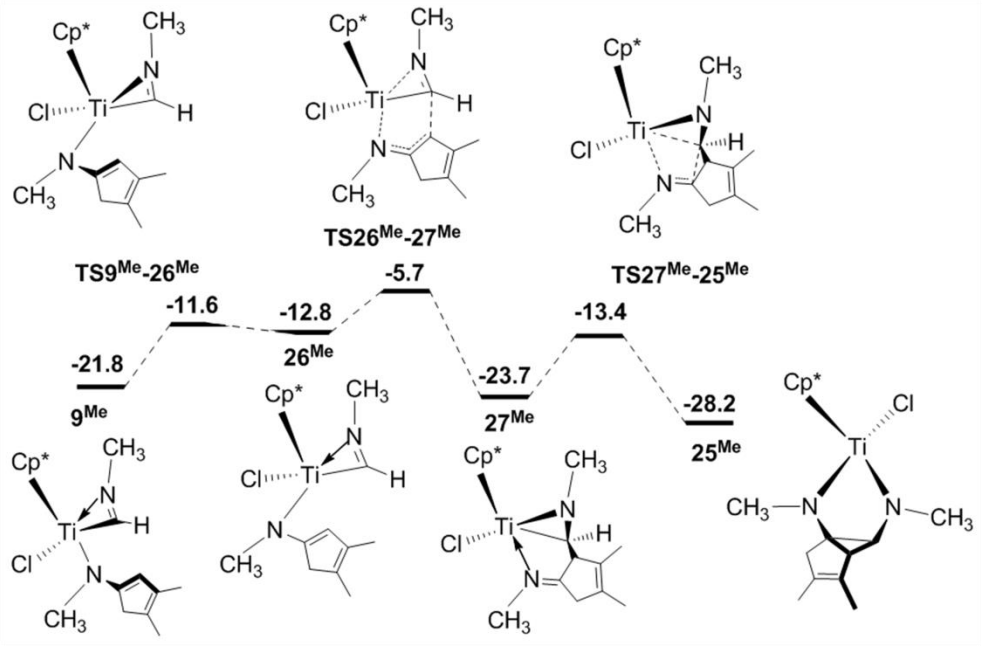
S6. **Figure S4.** Energetic profiles for the fragmentation of the titanaaziridine **10^{Me}** via the β-H elimination and the γ-H elimination reaction pathways. The Gibbs free energies are given in kcal mol^{-1} and the above values include the dispersion correction. Solvent: benzene



S7. **Figure S5.** Energetic profiles for the formation of the diazatitanacyclopentane **25^{Me}** (a) via the insertion and the C-C coupling reaction pathways, and (b) via the isomerisation reaction pathway. The Gibbs free energies are given in kcal mol^{-1} and the above values include the dispersion correction. Solvent: benzene

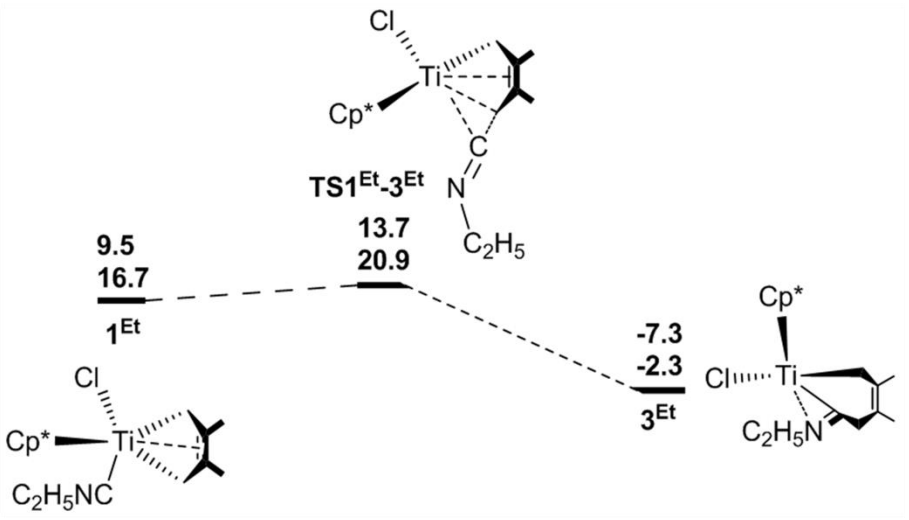


(a)

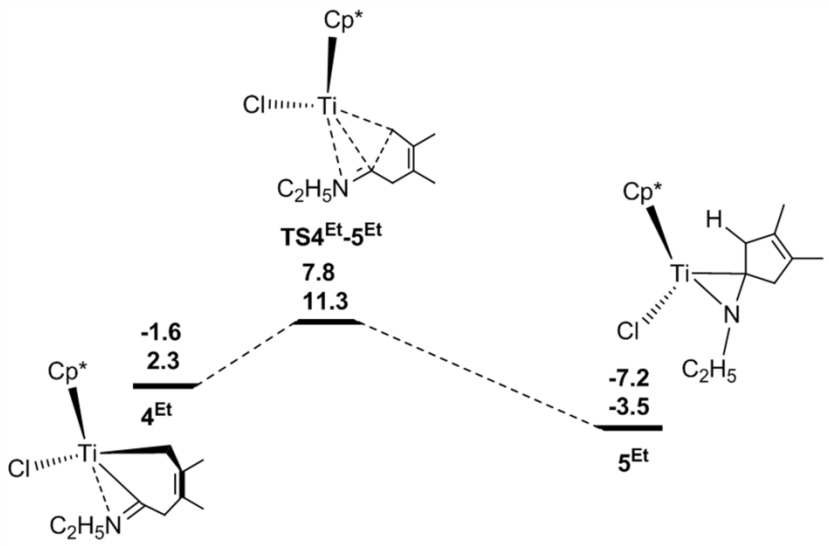


(b)

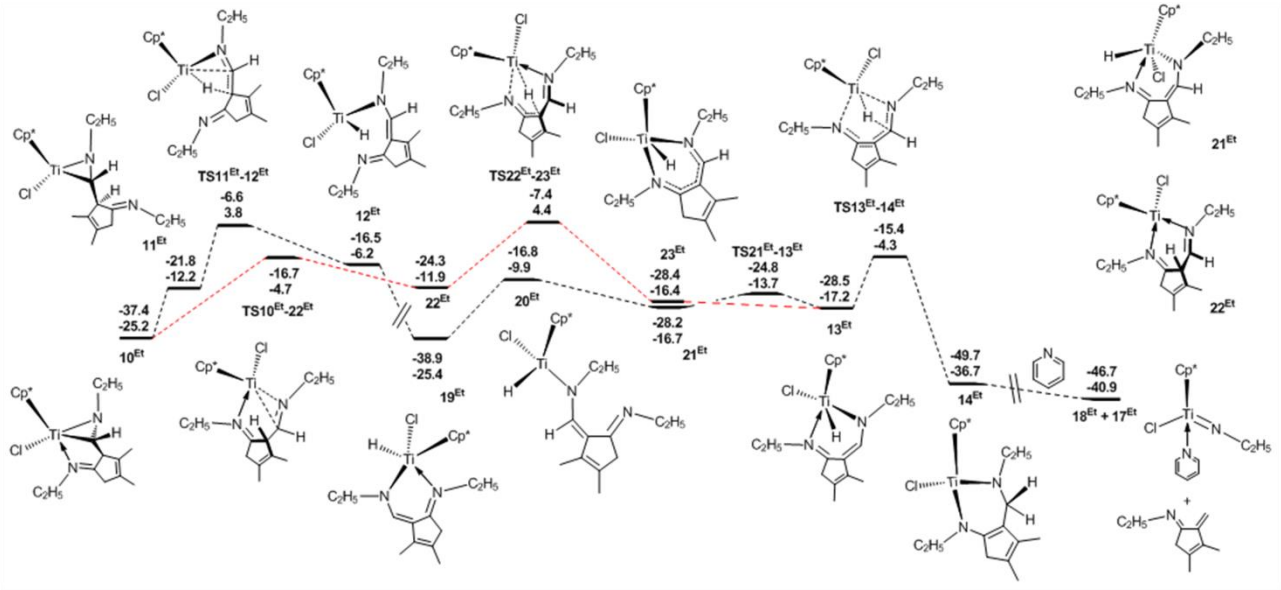
S8. **Figure S6.** Energy profiles for (a) migratory insertion of an Et-substituted isonitrile (EtNC) into the Ti–C bond in Ti complex $\mathbf{1}^{Et}$. (b) C–C reductive elimination in Ti complex $\mathbf{4}^{Et}$. (c) Fragmentation of titanaaziridine $\mathbf{10}^{Et}$. Formation of diazatitanacyclopentane $\mathbf{25}^{Et}$ via (d) via the insertion and the C-C coupling reaction pathways, and (e) via the isomerisation reaction pathway. The Gibbs free energies are given in kcal mol^{-1} and the above values include the dispersion correction. Solvent: benzene



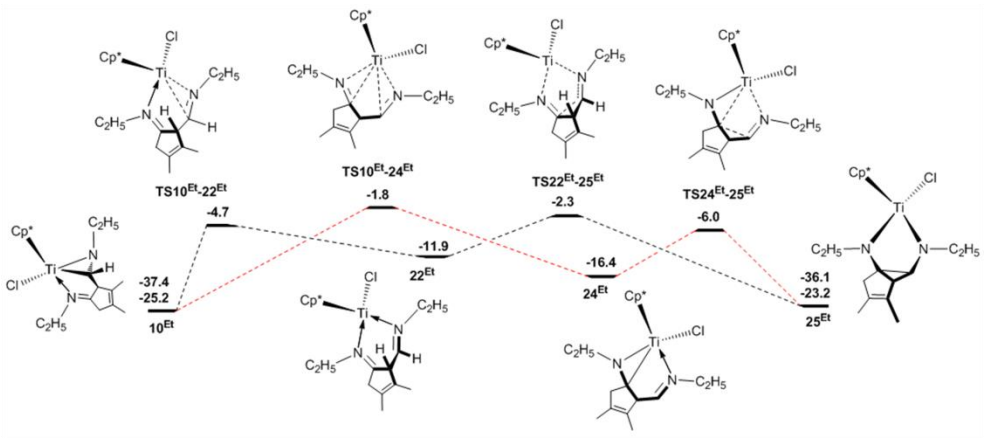
(a)


Cp*
Cl
Ti
C_2H_5N
$TS4^{Et}$-5^{Et}
7.8
11.3
-1.6
2.3
4^{Et}
-7.2
-3.5
5^{Et}
H
N
C_2H_5

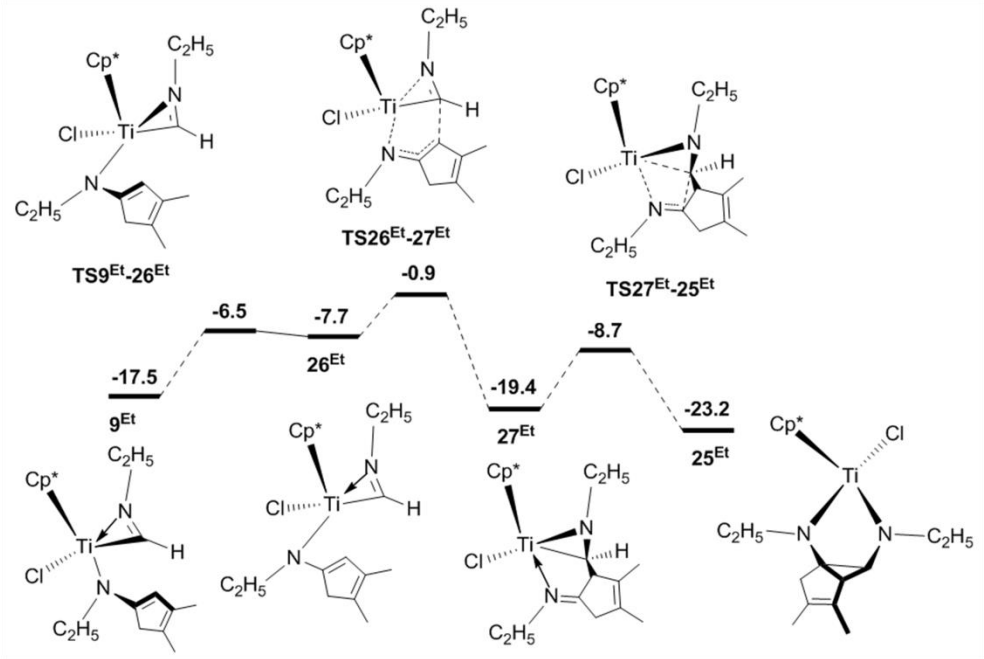
(b)


$TS11^{Et}$-12^{Et}
-6.6
3.8
11^{Et}
-21.8
-12.2
12^{Et}
-16.5
-6.2
$TS22^{Et}$-23^{Et}
-7.4
4.4
23^{Et}
-28.4
-16.4
$TS13^{Et}$-14^{Et}
-15.4
-4.3
21^{Et}
22^{Et}
-24.3
-11.9
22^{Et}
-16.8
-9.9
20^{Et}
$TS21^{Et}$-13^{Et}
-24.8
-13.7
-28.5
-17.2
13^{Et}
-49.7
-36.7
14^{Et}
-46.7
-40.9
18^{Et} + 17^{Et}
-37.4
-25.2
10^{Et}
-16.7
-4.7
$TS10^{Et}$-22^{Et}
-38.9
-25.4
19^{Et}
-28.2
-16.7
21^{Et}

(c)

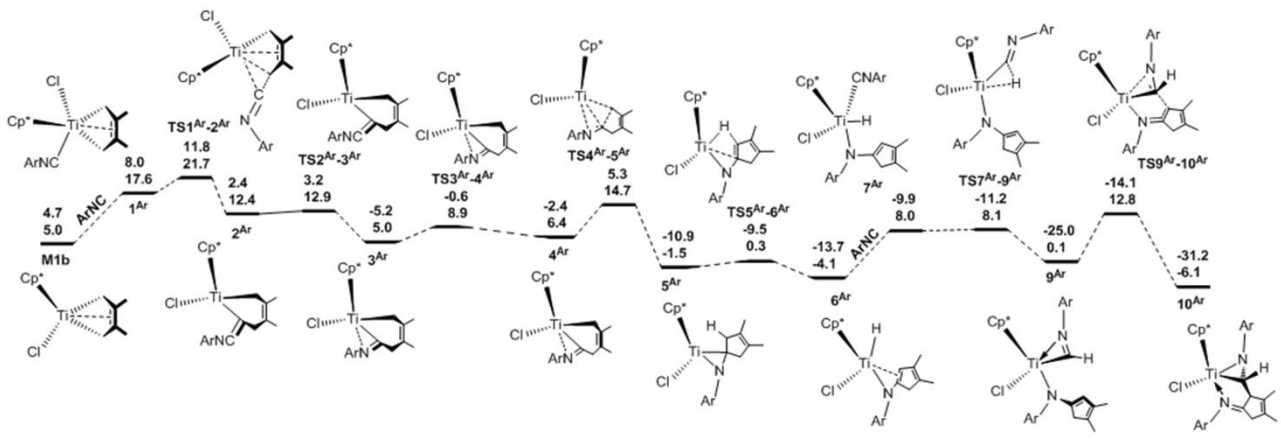

$TS10^{Et}$-22^{Et}
-4.7
$TS10^{Et}$-24^{Et}
-1.8
$TS22^{Et}$-25^{Et}
-2.3
$TS24^{Et}$-25^{Et}
-6.0
-37.4
-25.2
10^{Et}
-11.9
22^{Et}
-16.4
24^{Et}
-36.1
-23.2
25^{Et}

(d)

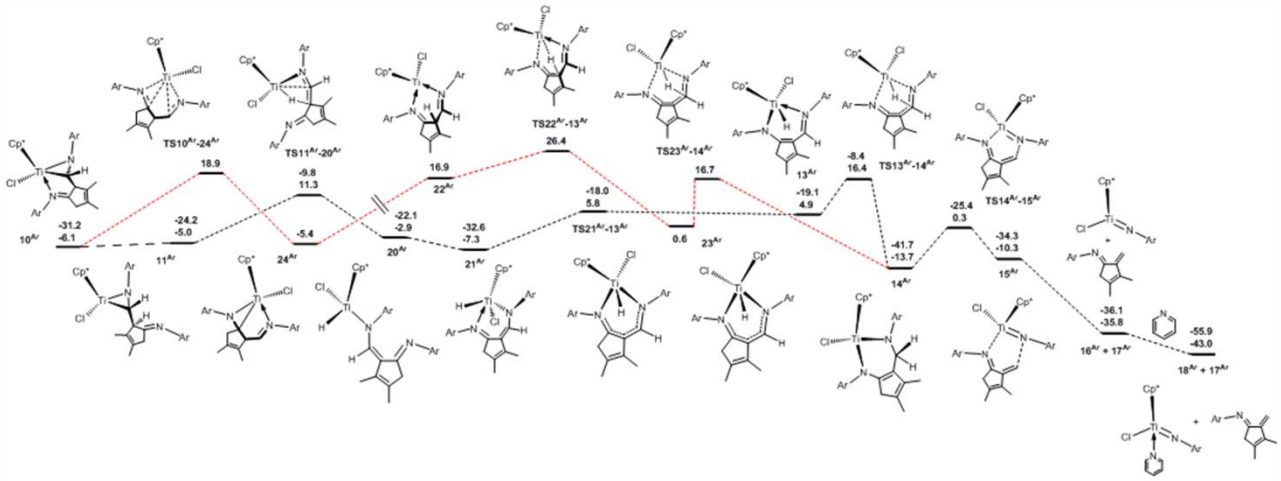


(e)

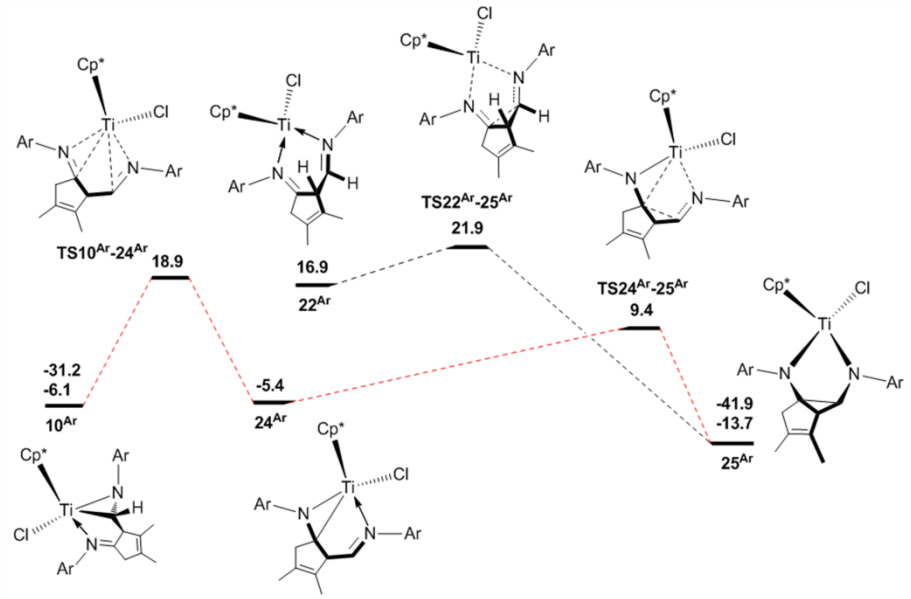
S9. **Figure S7.** Energetic profile of forming the titanaaziridine **10^{Ar}**. The Gibbs free energies are given in kcal mol^{-1} and the above values include the dispersion correction. Solvent: benzene



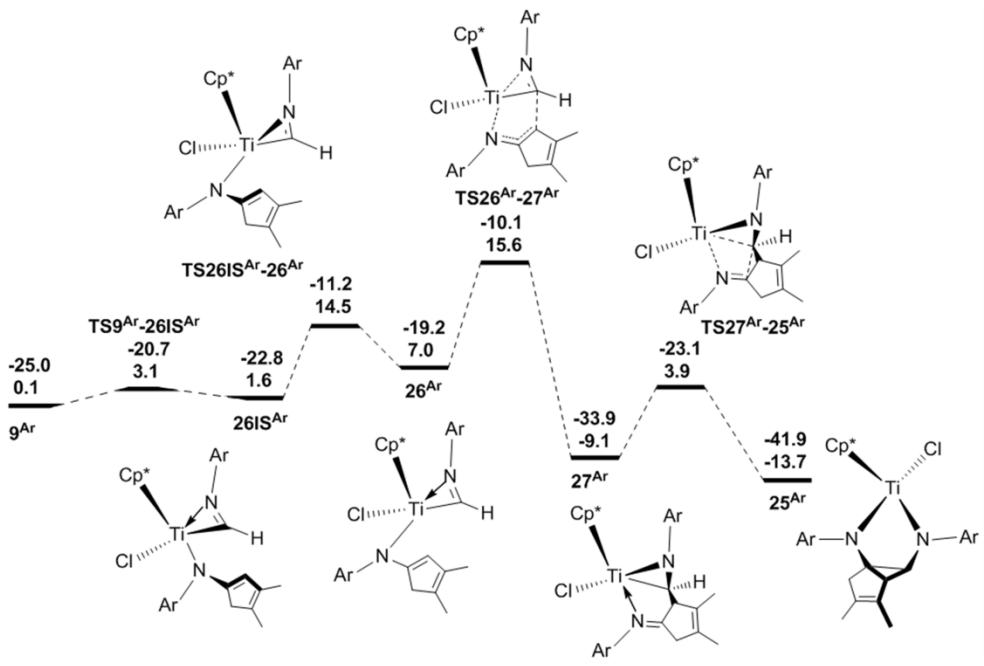
S10. **Figure S8.** Energetic profiles for the fragmentation of the titanaaziridine **10^{Ar}** via the β-H and γ-H elimination reaction pathways. The Gibbs free energies are given in kcal mol^{-1} and the above values include the dispersion correction. Solvent: benzene



S11. **Figure S9.** Energetic profiles for the formation of diazatitanacyclopentane **25^{Ar}** (a) via the insertion and the C-C coupling reaction pathways, and (b) via the isomerisation reaction pathway. The Gibbs free energies are given in kcal mol^{-1} and the above values include the dispersion correction. Solvent: benzene

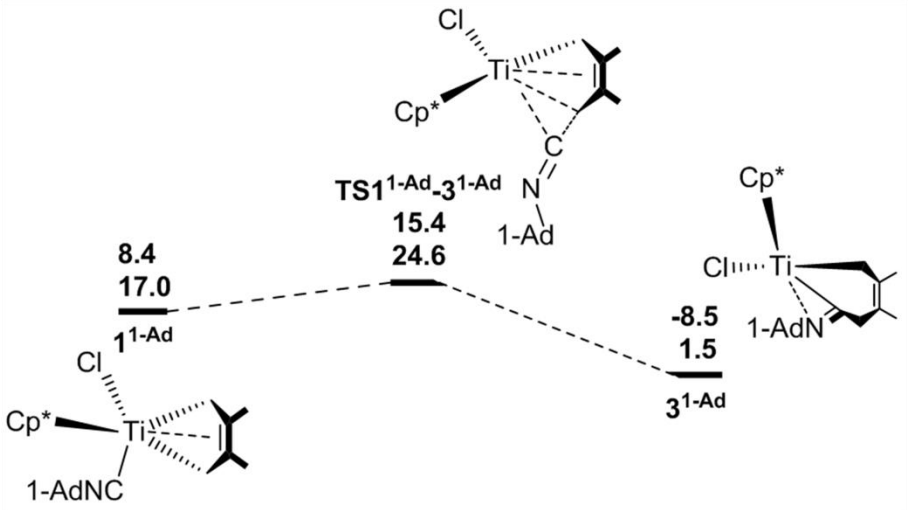


(a)

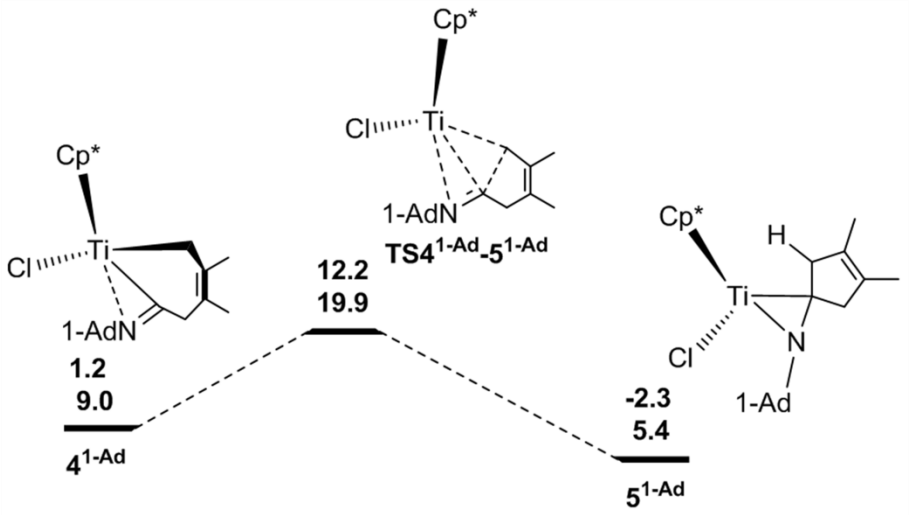


(b)

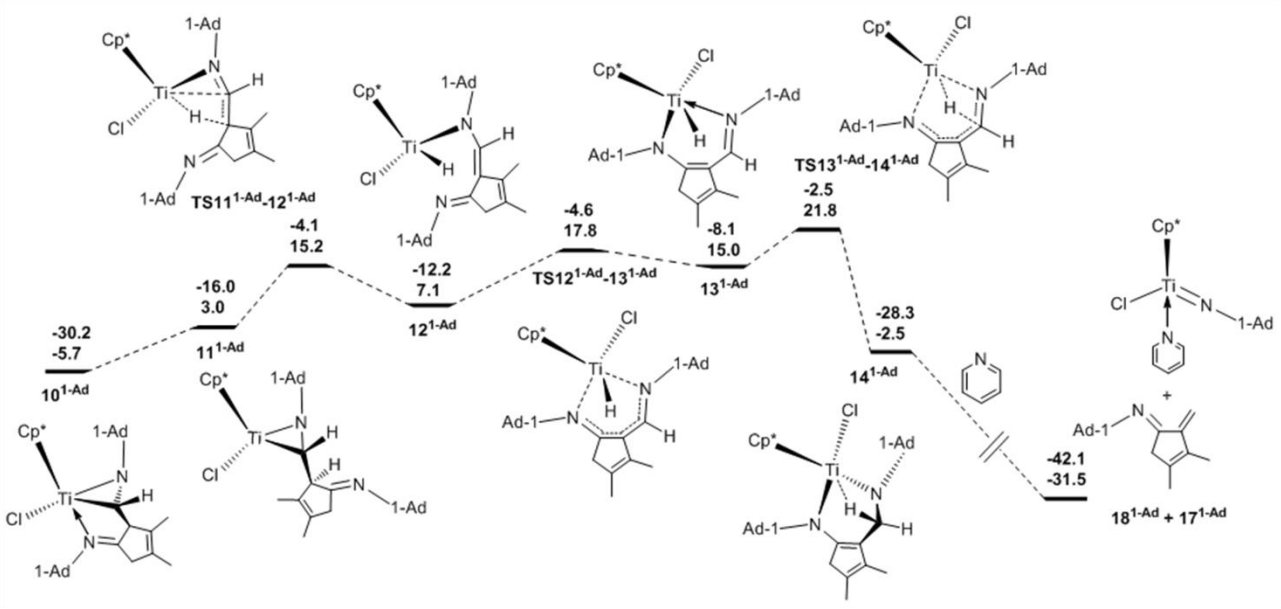
S12. **Figure S10.** Energy profiles for (a) migratory insertion of an 1-Ad-substituted isonitrile (1-AdNC) into the Ti–C bond in Ti complex $\mathbf{1}^{\mathbf{1\text{-}Ad}}$. (b) C–C reductive elimination in Ti complex $\mathbf{4}^{\mathbf{1\text{-}Ad}}$. (c) Fragmentation of titanaaziridine $\mathbf{10}^{\mathbf{1\text{-}Ad}}$. Formation of diazatitanacyclopentane $\mathbf{25}^{\mathbf{1\text{-}Ad}}$ via (d) via the insertion and the C-C coupling reaction pathways, and (e) via the isomerisation reaction pathway. The Gibbs free energies are given in kcal mol^{-1} and the above values include the dispersion correction. Solvent: benzene



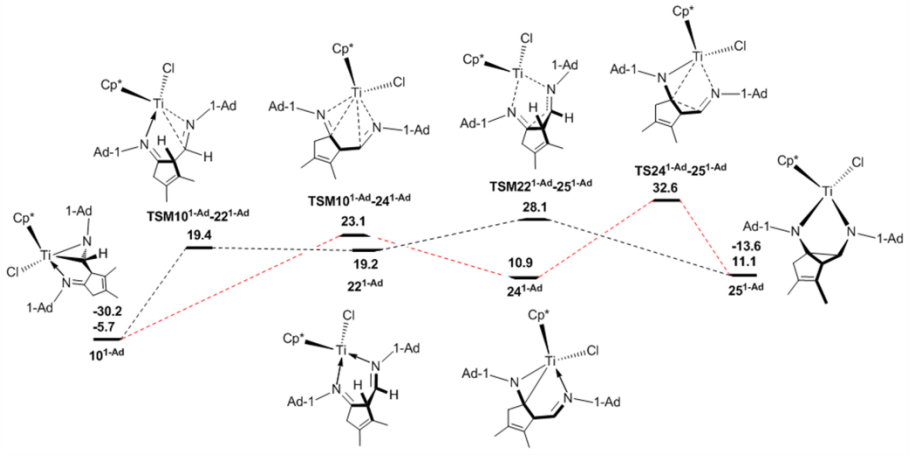
(a)


Cp*
Cl
Ti
1-AdN
TS4^1-Ad-5^1-Ad
12.2
19.9
Cp*
Cl
Ti
1-AdN
1.2
9.0
4^1-Ad
Cp*
H
Ti
Cl
N
1-Ad
-2.3
5.4
5^1-Ad

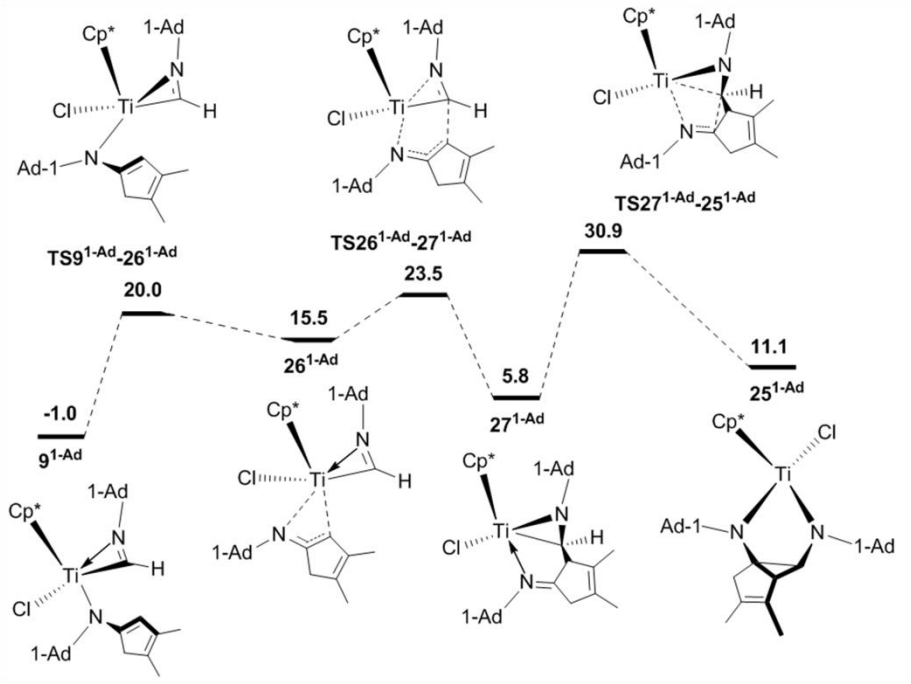
(b)


TS11^1-Ad-12^1-Ad
-4.1
15.2
-16.0
3.0
11^1-Ad
-30.2
-5.7
10^1-Ad
-12.2
7.1
12^1-Ad
-4.6
17.8
TS12^1-Ad-13^1-Ad
-8.1
15.0
13^1-Ad
TS13^1-Ad-14^1-Ad
-2.5
21.8
-28.3
-2.5
14^1-Ad
-42.1
-31.5
18^1-Ad + 17^1-Ad

(c)

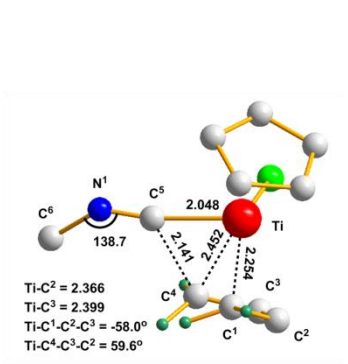

TSM10^1-Ad-22^1-Ad
19.4
TSM10^1-Ad-24^1-Ad
23.1
19.2
22^1-Ad
TSM22^1-Ad-25^1-Ad
28.1
10.9
24^1-Ad
TS24^1-Ad-25^1-Ad
32.6
-13.6
11.1
25^1-Ad
-30.2
-5.7
10^1-Ad

(d)

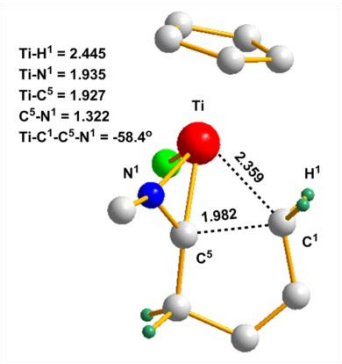


(e)

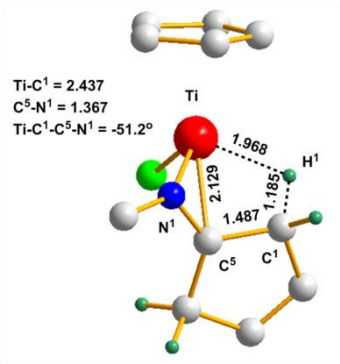
S13. **Figure S11.** Optimised structures (the methyl groups and the H atoms except for that involved in reaction were omitted for clarity, distances and angles are given in Å and degree, respectively; in benzene)



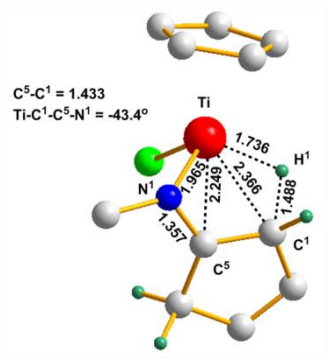
TS1^{Me}-3^{Me}



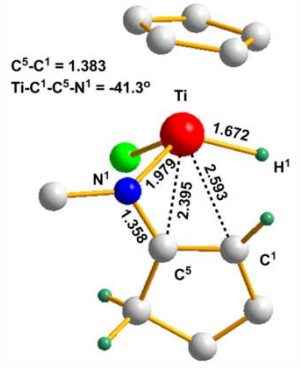
TS4^{Me}-5^{Me}



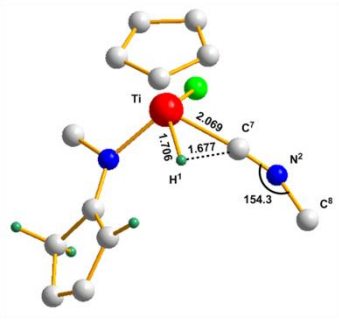
5^{Me}



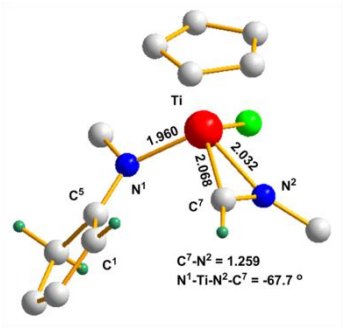
TS5^{Me}-6^{Me}



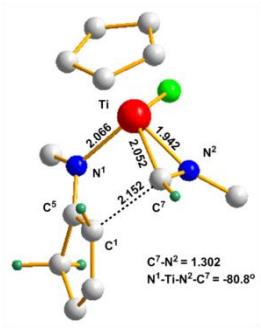
6^{Me}



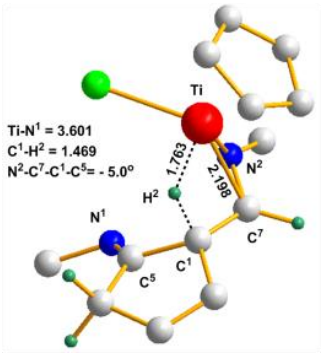
TS7^{Me}-8^{Me}



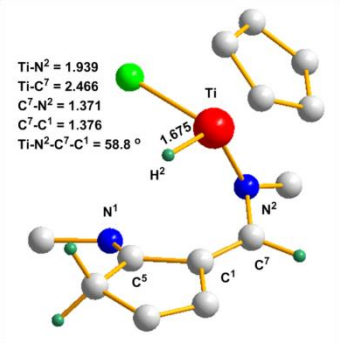
9^{Me}



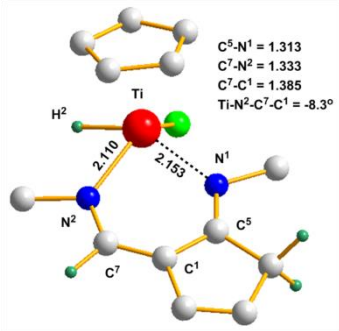
TS9^{Me}-10^{Me}



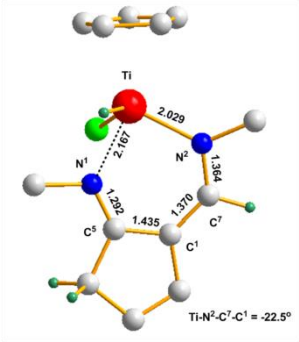
TS11^{Me}-12^{Me}



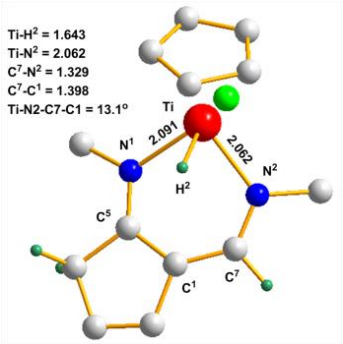
12^{Me}



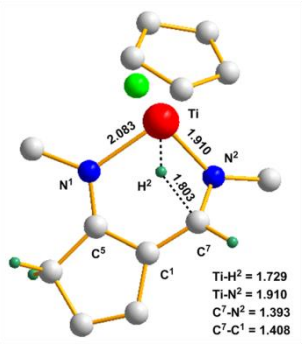
19^{Me}



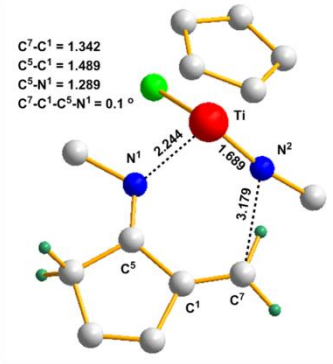
21^{Me}



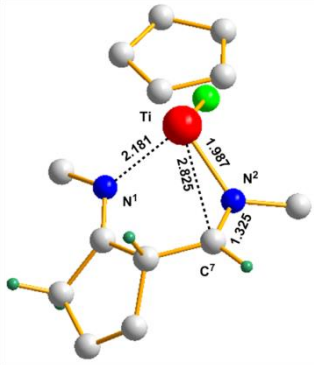
13^{Me}



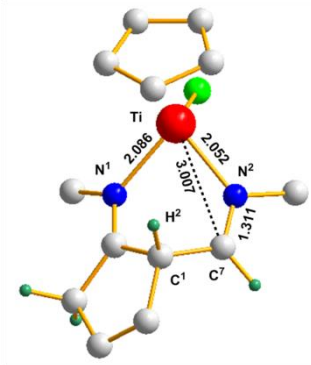
TS13^{Me}-14^{Me}



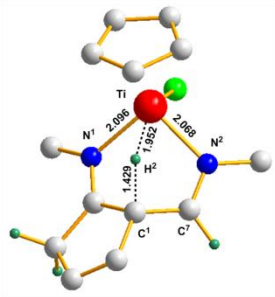
15^{Me}



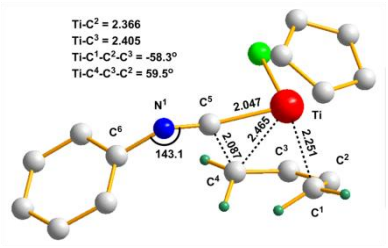
TS10^{Me}-22^{Me}



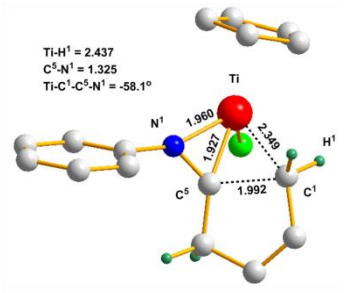
22^{Me}



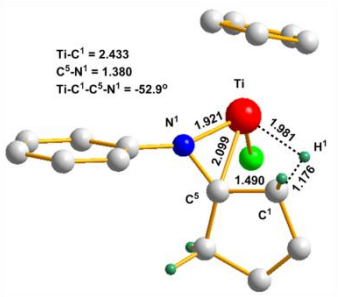
TS22^{Me}-13^{Me}



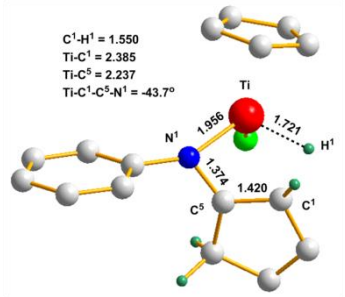
TS1^{Ar}-2^{Ar}



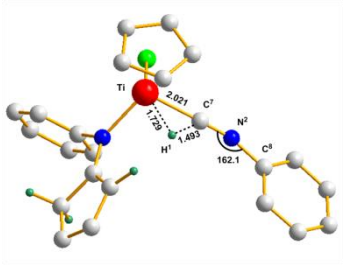
TS4^{Ar}-5^{Ar}



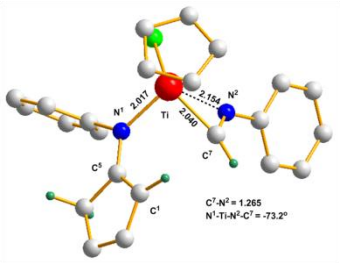
5^{Ar}



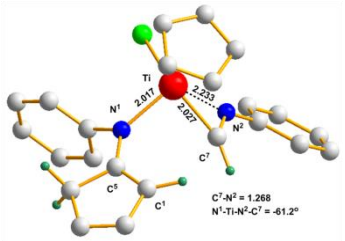
TS5^{Ar}-6^{Ar}



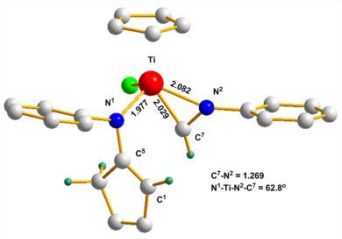
TS7^{Ar}-9^{Ar}



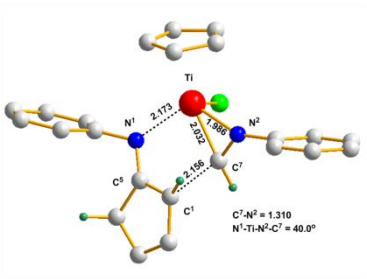
9^{Ar}



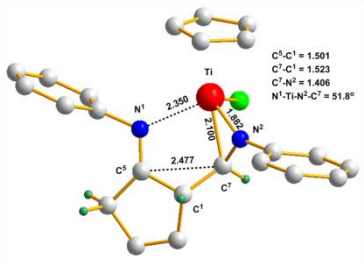
26IS^{Ar}



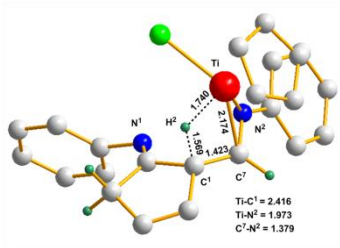
26^{Ar}



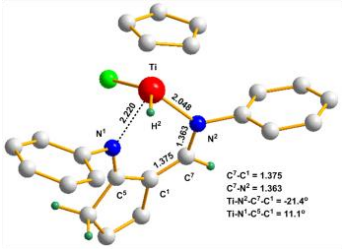
TS26^{Ar}-27^{Ar}



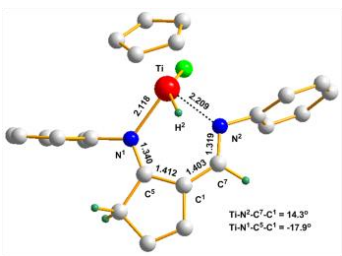
27^{Ar}



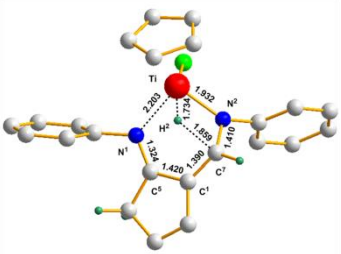
TS11^{Ar}-20^{Ar}



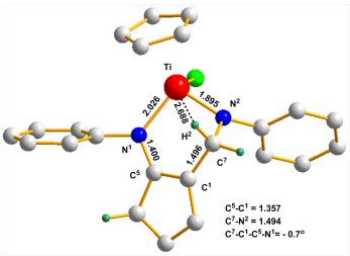
21^{Ar}



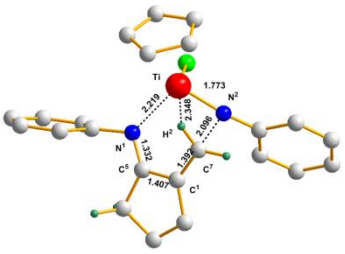
13^{Ar}



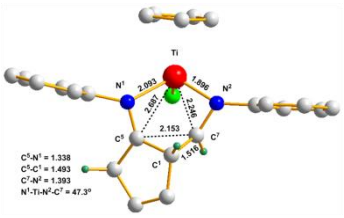
TS13^{Ar}-14^{Ar}



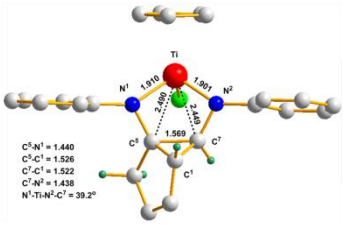
14^{Ar}



TS14^{Ar}-15^{Ar}

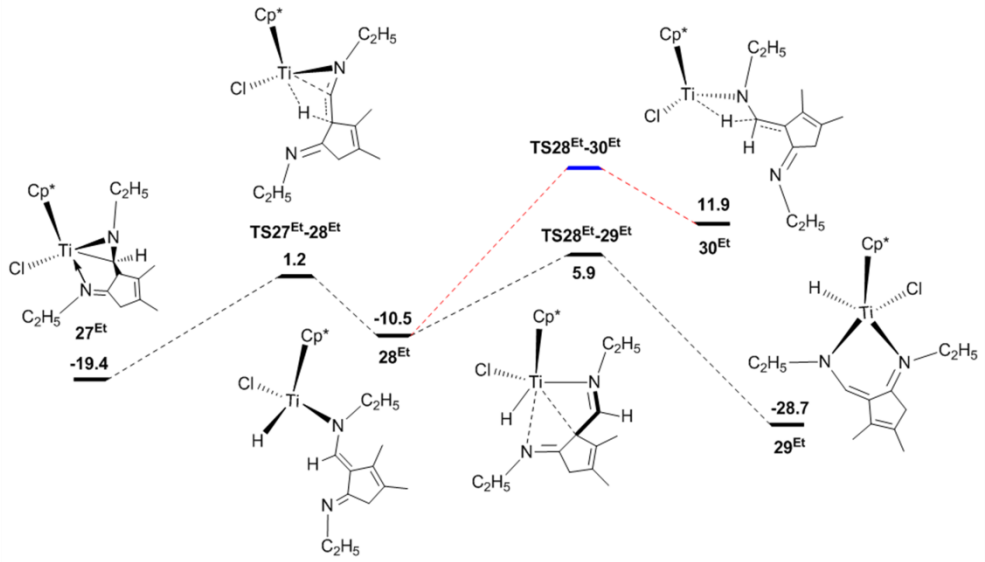


TS27^{Ar}-25^{Ar}

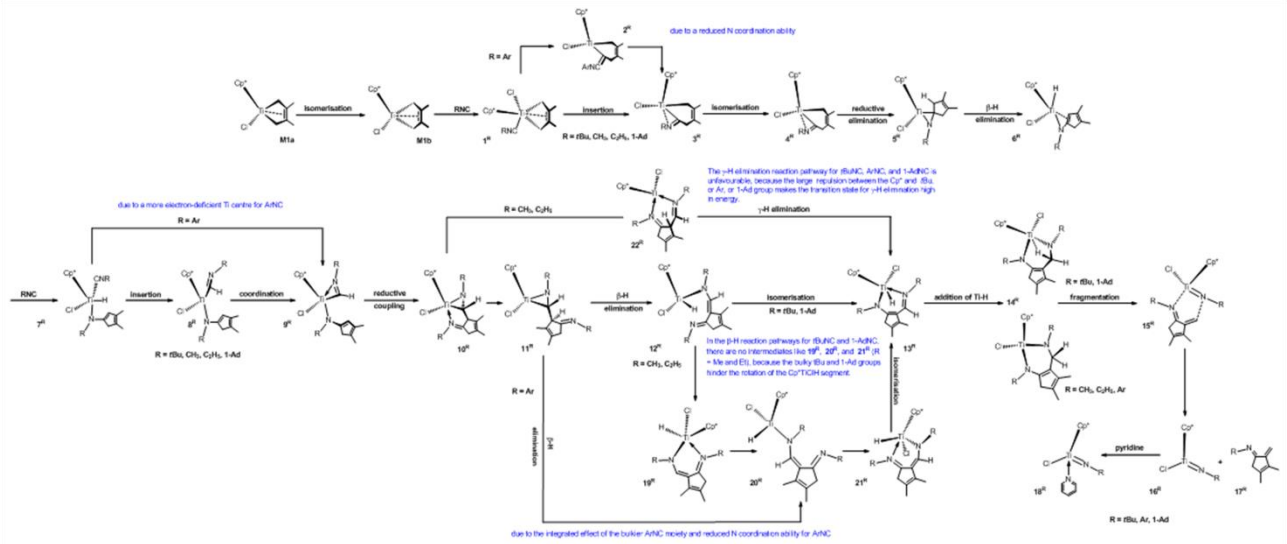


25^{Ar}

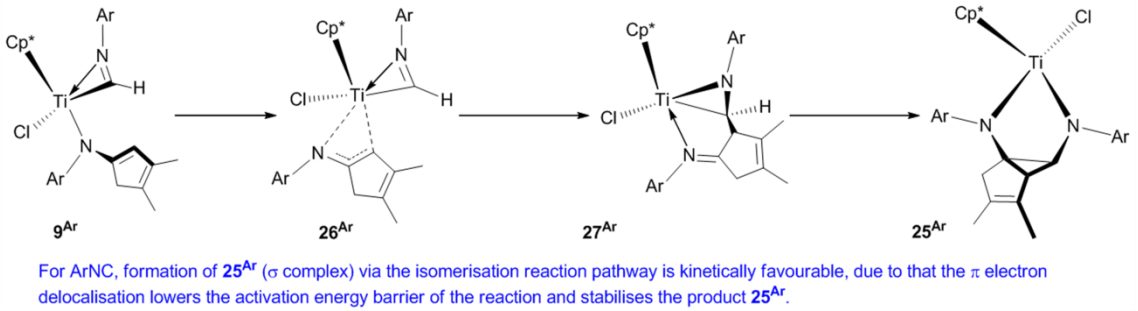
S14. **Figure S12.** Energetic profiles for γ-H elimination, rotation of Cp*ClH, and addition of Ti-H across the azaallyl double bond, starting from **27^{Et}**. The Gibbs free energies are given in kcal mol^{-1}. Solvent: benzene



S15. **Scheme 2.** Summary of the optimum reaction pathways for *t*BuNC, MeNC, EtNC, ArNC, and 1-AdNC, and substituent effects on the reaction pathways.



(a)



(b)

S16. **Table S1.** The calculated energies for species in the reaction pathways of bis-insertion and fragmentation of bis-insertion product in the case of *t*BuNC [referred to **M1a** and *t*BuNC (or 2 *t*BuNC)]. Note: 1) $\Delta E_{1(B.-O.)}$ and $\Delta E_{2(B.-O.)}$ denote the Born-Oppenheimer energy in pentane and benzene, respectively; 2) ΔG denotes the Gibbs free energy in benzene; 3) energies are given in kcal mol^{-1}.

Mol.	$\Delta E_{1(B.-O.)}$	$\Delta E_{2(B.-O.)}$	ΔG
TSM1a-1b	16.8	16.8	16.6
M1b	5.6	5.5	5.0
M2a	4.9	4.9	17.1
TSM2a-3a	10.6	10.8	24.4

M2b	-6.3		
TSM2b-3c	16.1		
M3c	8.6		
M3a	-12.4	-12.0	1.0
TSM3a-3b	-3.5	-3.2	10.8
M3b	-4.9	-4.7	8.0
TSM3b-4	5.5	5.8	19.5
M4	-9.1	-8.7	5.2
TSM4-5	-7.7	-7.3	6.8
M5	-12.3	-12.0	1.4
M6b	-2.8		
TSM6b-7b	11.8		
M6a	-11.1	-10.6	14.1
TSM6a-7a	-10.3	-9.7	15.9
M7a	-22.0	-21.4	4.5
TSM7a-8a	-22.0	-21.3	5.5
M8a	-29.0	-28.2	-1.0
TSM8a-9a	-18.8	-18.0	10.7
M9a	-37.1	-36.3	-6.9
M10	-27.2	-26.6	-0.1
TSM10-11	-14.2	-13.5	14.5
M11	-21.8	-21.0	6.5
M12	-5.7		
TSM12-13	9.1		
M13	5.4		
M14	-29.1		
TSM14	-20.9		
M15 + M16	34.3	-34.5	-23.6
M17	-24.6		
TSM17-18	11.9		
M18	-28.8		
TSM18	-19.9		
TSM11-19	-15.1	-14.3	15.7
M19	-17.9	-17.2	12.6
TSM19-20	-10.7	-10.0	19.8
M20	-34.5	-34.0	-4.8
TSM20-21	-20.5	-19.7	9.9
M21	-31.8	-31.1	-4.1
M22 + M16	-57.0	-56.5	-32.2
TSM9a-23		-11.6	17.8
M23		-13.7	14.4
TSM23-19		-1.5	28.0
M24	-21.8	-21.0	7.6
M25	-22.3	-21.6	5.4
M26	-11.3	-10.7	18.0
TSM23-27		-3.7	25.6
M27		-20.9	8.9
TSM9a-28		-8.5	21.3
M28		-18.7	10.4
TSM28-27		1.3	31.0
M8a		-28.2	-1.0
TSM8a-8b		-10.0	18.6

M8b	-14.4	13.9
TSM8b-9b	-6.9	21.9
M9b	-24.9	4.5
TSM9b-27	-0.4	29.7

S17. **Table S2.** The calculated Born-Oppenheimer energies ($\Delta E_{2(B.-O.)}$; in kcal mol^{-1}) for species in the reaction pathways of bis-insertion and fragmentation of bis-insertion product in the case of *t*BuNC, MeNC, EtNC, ArNC, and 1-AdNC [referred to **M1a** and RNC (or 2RNC)]. Note: 1) **TSA-B** denotes a transition state connected species **A** and **B**; 2) $\mathbf{23^R}$ is an isomer of $\mathbf{13^R}$.

Mol.	$\Delta E_{2(B.-O.)}$				
	*t*Bu	Me	Et	Ar	1-Ad
$\mathbf{1^R}$	4.9	5.3	5.1	4.3	4.6
$\mathbf{TS1^R\text{-}3^R}$ **(for R = Ar,** $\mathbf{TS1^R\text{-}2^R}$**)**	10.8	8.1	7.8	7.8	10.8
$\mathbf{2^R}$				-0.9	
$\mathbf{TS2^R\text{-}3^R}$				-0.8	
$\mathbf{3^R}$	-12.0	-14.8	-14.4	-8.5	-11.8
$\mathbf{TS3^R\text{-}4^R}$	-3.2	-8.9		-5.5	
$\mathbf{4^R}$	-4.7	-10.4	-10.0	-6.8	-4.4
$\mathbf{TS4^R\text{-}5^R}$	5.8	-1.7	-1.0	0.4	-6.0
$\mathbf{5^R}$	-8.7	-17.1	-16.2	-15.7	-8.6
$\mathbf{TS5^R\text{-}6^R}$	-7.3	-16.7		-14.2	
$\mathbf{6^R}$	-12.0	-22.5		-17.9	
$\mathbf{7^R}$	-10.6	-25.3		-18.4	
$\mathbf{TS7^R\text{-}8^R}$ **(for R=Ar,** $\mathbf{TS7^R\text{-}9^R}$**)**	-9.7	-24.8		-18.4	
$\mathbf{8^R}$	-21.4	-33.7			
$\mathbf{TS8^R\text{-}9^R}$	-21.3	-33.0			
$\mathbf{9^R}$	-28.2	-45.8	-42.7	-28.5	-28.0
$\mathbf{TS9^R\text{-}10^R}$	-18.0	-36.1		-17.1	
$\mathbf{10^R}$	-36.3	-56.1	-52.0	-35.7	-35.4
$\mathbf{11^R}$	-26.6	-38.7	-36.7	-32.4	-24.6
$\mathbf{TS11^R\text{-}12^R}$ **(for R = Ar,** $\mathbf{TS11^R\text{-}20^R}$**)**	-13.5	-23.9	-22.1	-17.4	-13.1
$\mathbf{12^R}$	-21.0	-33.6	-31.2		-21.0
$\mathbf{TS12^R\text{-}13^R}$ **(for R = Me, Et,** $\mathbf{TS12^R\text{-}19^R}$**)**	-14.3	-33.8			-12.8
$\mathbf{13^R}$	-17.2	-48.0	-44.3	-24.8	-15.4
$\mathbf{TS13^R\text{-}14^R}$	-10.0	-35.8	-31.6	-13.6	-8.7
$\mathbf{14^R}$	-34.0	-65.5	-62.6	-43.3	-32.6
$\mathbf{TS14^R\text{-}15^R}$	-19.7	-45.0		-28.7	
$\mathbf{15^R}$	-31.1	-52.2		-38.4	
$\mathbf{16^R + 17^R}$	-34.5	-41.7		-47.3	
$\mathbf{18^R + 17^R}$	-56.7	-64.1	-63.7	-68.5	-56.1
$\mathbf{19^R}$	-21.0	-57.6	-52.8		
$\mathbf{20^R}$		-35.5	-34.6	-29.9	
$\mathbf{21^R}$	-10.7	-46.0	-43.5	-36.4	
$\mathbf{TS21^R\text{-}13^R}$		-46.6	-41.3	-24.5	
$\mathbf{TS10^R\text{-}22^R}$	-11.6	-35.9	-31.7		
$\mathbf{22^R}$	-13.7	-39.3	-38.1	-12.8	

TS22^{R}-13^{R} (for R = Et, Ar, TS22^{R}-23^{R})	-1.5	-24.8	-22.9	-2.9
23^{R}			-43.7	-29.1
TS23^{R}-14^{R}				-13.3

S18. **Table S3.** The calculated Born-Oppenheimer energies ($\Delta E_{2(B.-O.)}$; in kcal mol^{-1}) for species in the reaction pathways of forming diazatitanacyclopentane **25^{R}** in the case of *t*BuNC, MeNC, EtNC, ArNC, and 1-AdNC [referred to **M1a** and RNC (or 2RNC)]. Note: 1) **TSA-B** denotes a transition state connected species **A** and **B**; 2) **26IS^{R}** is an isomer of **26^{R}**.

Mol.	$\Delta E_{2(B.-O.)}$				
	*t*Bu	Me	Et	Ar	1-Ad
10^{R}	-36.3	-56.1	-52.0	-35.7	-35.4
TS10^{R}-24^{R}	-8.5	-36.3	-29.1	-11.0	-7.6
24^{R}	-18.7	-47.7	-43.1	-35.3	-18.2
TS24^{R}-25^{R}	1.3	-35.9	-33.6	-20.9	2.3
25^{R}	-20.9	-54.3	-50.5	-43.7	-19.8
TS10^{R}-22^{R}	-11.6	-35.9	-31.7		-10.3
22^{R}	-13.7	-39.3	-38.1	-12.8	-9.9
TS22^{R}-25^{R}	-3.7	-31.5	-29.3	-7.9	-1.7
9^{R}	-28.2	-45.8	-42.7	-28.5	-28.0
TS9^{R}-26^{R} (R = Ar, TS9^{R}-26IS^{R})	-10.0	-37.5	-33.7	-25.8	-9.3
26IS^{R}				-26.7	
TS26IS^{R}-26^{R}				-15.7	
26^{R}	-14.4	-37.7	-33.8	-21.3	-13.7
TS26^{R}-27^{R}	-6.9	-31.4	-28.3	-13.9	-5.7
27^{R}	-24.9	-49.1	-47.2	-38.2	-24.1
TS27^{R}-25^{R}	-0.4	-40.2	-36.3	-26.8	-0.2

S19. **Table S4.** Imaginary frequencies for transition states on the optimum reaction pathways, values in and outside parentheses denote imaginary frequencies calculated in n-pentane and benzene, respectively.

Species	**Imaginary Frequency**	**Species**	**Imaginary Frequency**	**Species**	**Imaginary Frequency**
TSM1a-1b	-49.6904 (-49.7248)	**TSM2a-3a**	-207.3180 (-205.3061)	**TSM3a-3b**	-40.9766 (-40.7349)
TSM3b-4	-386.2885 (-384.5758)	**TSM4-5**	-675.5377 (-673.9984)	**TSM6a-7a**	-131.7989 (-142.6350)
TSM7a-8a	-42.1885 (-37.0399)	**TSM8a-9a**	-408.7640 (-407.5426)	**TSM10-11**	-689.1489 (-686.2643)
TSM11-19	-28.3850	**TSM19-20**	-509.5880	**TSM20-21**	-324.8016
TS1^{Me}-3^{Me}	-93.0918	**TS3^{Me}-4^{Me}**	-57.6638	**TS4^{Me}-5^{Me}**	-368.2559
TS5^{Me}-6^{Me}	-715.9386	**TS7^{Me}-8^{Me}**	-186.8282	**TS8^{Me}-9^{Me}**	-56.4152

TS9^{Me}-10^{Me}	-383.2096	**TS11^{Me}-12^{Me}**	-697.7267	**TS12^{Me}-13^{Me}**	-29.6233
TS21^{Me}-13^{Me}	-77.7236	**TS10^{Me}-22^{Me}**	-156.6364	**TS22^{Me}-13^{Me}**	-1098.0768
TS13^{Me}-14^{Me}	-659.9720	**TS14^{Me}-15^{Me}**	-360.8384	**TS1^{Et}-3^{Et}**	-94.3736
TS4^{Et}-5^{Et}	-370.8034	**TS11^{Et}-12^{Et}**	-704.9099	**TS21^{Et}-13^{Et}**	-126.6873
TS10^{Et}-22^{Et}	-177.9423	**TS22^{t}-23^{Et}**	-1105.7016	**TS13^{Et}-14^{Et}**	-596.2601
TS1^{Ar}-2^{Ar}	-122.9318	**TS2^{Ar}-3^{Ar}**	-23.1846	**TS3^{Ar}-4^{Ar}**	-40.5931
TS4^{Ar}-5^{Ar}	-358.5559	**TS5^{Ar}-6^{Ar}**	-711.5665	**TS7^{Ar}-9^{Ar}**	-268.8599
TS9^{Ar}-10^{Ar}	-333.7148	**TS10^{Ar}-24^{Ar}**	-209.8823	**TS11^{Ar}-20^{Ar}**	-717.8056
TS21^{Ar}-13^{Ar}	-42.8225	**TS13^{Ar}-14^{Ar}**	-552.8481	**TS14^{Ar}-15^{Ar}**	-308.7239
TS9^{Ar}-26IS^{Ar}	-43.7087	**TS26IS^{Ar}-26^{Ar}**	-17.0680	**TS26^{Ar}-27^{Ar}**	-391.5094
TS27^{Ar}-25^{Ar}	-186.8926	**TS1$^{1\text{-}Ad}$-3$^{1\text{-}Ad}$**	-204.3237	**TS4$^{1\text{-}Ad}$-5$^{1\text{-}Ad}$**	-381.4905
TS11$^{1\text{-}Ad}$-12$^{1\text{-}Ad}$	-690.2560	**TS12$^{1\text{-}Ad}$-13$^{1\text{-}Ad}$**	-30.0561	**TS13$^{1\text{-}Ad}$-14$^{1\text{-}Ad}$**	-498.2074

S20. Calculated Cartesian coordinates and electronic energies (E) for relevant species in the calculation method and on the optimum reaction pathways.

In n-pentane

By B3LYP/BS1

$10^{1\text{-Ad}}$ (E = -1663.743672 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.033362	1.199635	0.227001
2	7	1.513135	0.146133	0.129758
3	6	1.152685	0.006920	1.471418
4	7	-1.468195	-0.628764	0.563920
5	6	0.910773	3.160465	1.189608
6	6	-0.026889	2.645287	2.136819
7	6	0.179768	3.607108	0.054983
8	17	-0.396084	1.203410	-2.172012
9	6	-1.335047	2.793743	1.585930
10	6	-1.207745	3.390415	0.301993
11	6	2.775698	-0.249703	-0.530793
12	6	-0.845412	-1.538931	1.223532
13	6	-2.764036	-0.912126	-0.180997
14	6	0.384383	-1.190927	2.033582
15	1	1.818513	0.443971	2.219218
16	6	1.040871	-2.541837	2.298611
17	1	0.005920	-0.830177	3.007456
18	6	-1.053176	-3.044131	1.327252
19	6	0.255122	-3.550109	1.896437
20	1	-1.870642	-3.278717	2.020661
21	1	-1.316672	-3.502119	0.371366
22	6	0.479357	-5.034088	2.009379
23	6	2.341677	-2.629714	3.047264
24	1	2.627237	-3.664769	3.257100
25	1	2.266641	-2.097988	4.007011
26	1	3.160348	-2.160288	2.490742
27	1	1.443630	-5.274139	2.466400
28	1	0.449772	-5.509517	1.018663
29	1	-0.308631	-5.507385	2.613025
30	6	3.000044	0.588615	-1.816553
31	6	4.005273	-0.046059	0.399434
32	6	2.691155	-1.751905	-0.936828
33	6	3.993045	-2.196132	-1.647743
34	1	1.826331	-1.882912	-1.600249
35	1	2.515269	-2.363908	-0.042999
36	6	4.196935	-1.344965	-2.924702
37	6	5.196911	-1.993383	-0.695064
38	1	3.913000	-3.257875	-1.919887
39	6	5.305801	-0.496916	-0.311590
40	1	6.124459	-2.324253	-1.183020
41	1	5.070941	-2.606731	0.209018
42	6	5.512418	0.349329	-1.590871
43	1	6.156256	-0.352183	0.369277
44	1	3.871579	-0.615305	1.326923
45	1	4.077288	1.013730	0.676155
46	6	4.301168	0.149815	-2.532881
47	1	3.056073	1.652706	-1.547450
48	1	2.138791	0.472347	-2.479652
49	1	4.432969	0.758191	-3.438026
50	1	5.615424	1.411722	-1.327297
51	1	6.441215	0.049363	-2.096413
52	1	3.355240	-1.494810	-3.614851
53	1	5.109296	-1.662621	-3.449145
54	6	-3.798960	-1.703912	0.672959

55	6	-3.417163	0.453620	-0.521911
56	6	-2.484445	-1.675283	-1.508017
57	6	-3.808090	-1.876493	-2.290122
58	1	-1.769153	-1.100437	-2.103814
59	1	-2.032775	-2.652425	-1.299595
60	6	-4.420343	-0.498257	-2.637110
61	6	-4.808943	-2.683559	-1.427553
62	1	-3.589645	-2.426909	-3.215001
63	6	-5.116023	-1.902969	-0.124958
64	1	-5.738099	-2.854627	-1.988279
65	1	-4.390938	-3.672100	-1.187179
66	6	-5.739184	-0.534666	-0.479126
67	1	-5.814521	-2.480931	0.495473
68	1	-3.423153	-2.690976	0.946653
69	1	-3.995756	-1.153874	1.604322
70	6	-4.725818	0.266373	-1.326908
71	1	-3.632174	0.982281	0.412905
72	1	-2.714271	1.054711	-1.101501
73	1	-5.138907	1.255958	-1.565197
74	1	-6.675627	-0.678713	-1.035528
75	1	-5.988178	0.017588	0.438272
76	1	-5.342403	-0.631189	-3.220018
77	1	-3.720781	0.078400	-3.255855
78	6	0.252041	2.296484	3.577404
79	6	2.383677	3.369637	1.438782
80	6	0.742885	4.316092	-1.150372
81	6	-2.311227	3.840540	-0.620834
82	6	-2.605873	2.537233	2.362113
83	1	0.046121	3.163443	4.223217
84	1	1.295984	2.011813	3.734856
85	1	-0.377410	1.471730	3.929656
86	1	2.552190	4.325583	1.956042
87	1	2.953467	3.395434	0.505358
88	1	2.807917	2.579012	2.065321
89	1	0.664885	5.405851	-1.021699
90	1	0.205420	4.040709	-2.061775
91	1	1.799447	4.076288	-1.305472
92	1	-2.339733	4.937937	-0.673977
93	1	-3.293398	3.500587	-0.280324
94	1	-2.156082	3.463241	-1.638025
95	1	-2.644536	3.187301	3.247443
96	1	-2.680212	1.502070	2.715854
97	1	-3.495003	2.750727	1.762857

$10^{1\text{-Ad}}$IS (E = -1663.7436724 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.033098	1.199254	0.226921
2	7	-1.513152	0.145455	0.129640
3	6	-1.152531	0.006098	1.471301
4	7	1.468429	-0.628864	0.563692
5	6	-0.911186	3.159892	1.189632
6	6	0.026252	2.644681	2.137026
7	6	-0.179909	3.606719	0.055237
8	17	0.396371	1.203612	-2.171911
9	6	1.334544	2.793347	1.586508
10	6	1.207548	3.390188	0.302634
11	6	-2.776068	-0.249875	-0.530610
12	6	0.845801	-1.539334	1.223047
13	6	2.764475	-0.911855	-0.181108
14	6	-0.384127	-1.191791	2.033082
15	1	-1.818373	0.442948	2.219186
16	6	-1.040471	-2.542886	2.297539
17	1	-0.005768	-0.831367	3.007130
18	6	1.053849	-3.044501	1.326446

19	6	-0.254489	-3.550901	1.895174
20	1	1.317791	-3.502251	0.370576
21	1	1.871136	-3.279041	2.020087
22	6	-0.478528	-5.034937	2.007626
23	6	-2.341343	-2.631167	3.046004
24	1	-2.627718	-3.666380	3.253949
25	1	-3.159620	-2.160066	2.490334
26	1	-2.265907	-2.101270	4.006736
27	1	-1.443050	-5.275256	2.463976
28	1	0.309137	-5.508256	2.611676
29	1	-0.448213	-5.510141	1.016822
30	6	-4.005418	-0.045732	0.399750
31	6	-3.000138	0.588501	-1.816366
32	6	-2.692166	-1.752098	-0.936642
33	6	-3.994300	-2.195811	-1.647458
34	1	-2.516446	-2.364196	-0.042857
35	1	-1.827448	-1.883472	-1.600129
36	6	-5.197986	-1.992568	-0.694670
37	6	-4.197953	-1.344574	-2.924407
38	1	-3.914691	-3.257584	-1.919600
39	6	-5.306202	-0.496065	-0.311177
40	1	-5.072192	-2.605977	0.209394
41	1	-6.125726	-2.323039	-1.182528
42	6	-5.512570	0.350280	-1.590439
43	1	-6.156536	-0.350967	0.369757
44	1	-4.077029	1.014069	0.676475
45	1	-3.871883	-0.615040	1.327230
46	6	-4.301510	0.150248	-2.532592
47	1	-2.138959	0.471848	-2.479508
48	1	-3.055695	1.652623	-1.547316
49	1	-4.433154	0.758686	-3.437715
50	1	-6.441552	0.050723	-2.095883
51	1	-5.615090	1.412713	-1.326847
52	1	-3.356390	-1.494790	-3.614635
53	1	-5.110495	-1.661854	-3.448757
54	6	3.799409	-1.703649	0.672801
55	6	2.485247	-1.674675	-1.508387
56	6	3.417390	0.454110	-0.521533
57	6	3.809071	-1.875398	-2.290339
58	1	2.033731	-2.651963	-1.300340
59	1	1.769949	-1.099797	-2.104146
60	6	4.809933	-2.682510	-1.427826
61	6	4.421113	-0.496942	-2.636826
62	1	3.590889	-2.425591	-3.215410
63	6	5.116646	-1.902229	-0.124963
64	1	5.739218	-2.853248	-1.988437
65	1	4.392078	-3.671200	-1.187804
66	6	5.739605	-0.533713	-0.478641
67	1	5.815146	-2.480236	0.495420
68	1	3.995962	-1.153817	1.604339
69	1	3.423799	-2.690866	0.946189
70	6	4.726217	0.267369	-1.326358
71	1	2.714464	1.055215	-1.101057
72	1	3.632119	0.982536	0.413474
73	1	5.139157	1.257100	-1.564291
74	1	5.988345	0.018334	0.438948
75	1	6.676165	-0.677422	-1.034933
76	1	5.343290	-0.629534	-3.219623
77	1	3.721545	0.079756	-3.255524
78	6	-2.384108	3.369182	1.438576
79	6	-0.742878	4.315866	-1.150086
80	6	2.311270	3.840565	-0.619772
81	6	2.605182	2.536933	2.363009
82	6	-0.253012	2.295825	3.577527

83	1	-2.552582	4.325059	1.955986
84	1	-2.808562	2.578512	2.064906
85	1	-2.953740	3.395255	0.505066
86	1	-0.666282	5.405630	-1.020617
87	1	-1.799024	4.074913	-1.306234
88	1	-0.204368	4.041735	-2.061243
89	1	2.340034	4.937985	-0.672325
90	1	2.156209	3.463846	-1.637188
91	1	3.293318	3.500219	-0.279313
92	1	2.643707	3.187200	3.248204
93	1	3.494467	2.750219	1.763917
94	1	2.679357	1.501846	2.717005
95	1	-0.047307	3.162787	4.223403
96	1	0.376396	1.471101	3.929921
97	1	-1.296974	2.011084	3.734726

By B3LYP/def2-SVP

10$^{1\text{-Ad}}$ (E = -2899.1469483 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.036284	1.199370	0.230315
2	7	1.519500	0.153455	0.145818
3	6	1.152469	0.006067	1.483612
4	7	-1.472868	-0.636113	0.566559
5	6	0.929851	3.165720	1.185010
6	6	-0.004175	2.659016	2.145189
7	6	0.188930	3.608694	0.049193
8	17	-0.397234	1.187580	-2.155260
9	6	-1.319759	2.803471	1.600495
10	6	-1.200695	3.396013	0.308938
11	6	2.758720	-0.247084	-0.526588
12	6	-0.843469	-1.544925	1.227829
13	6	-2.752061	-0.910576	-0.177528
14	6	0.382899	-1.193318	2.041713
15	1	1.813484	0.451289	2.244007
16	6	1.041109	-2.542395	2.316474
17	1	-0.006403	-0.827282	3.017816
18	6	-1.049515	-3.049725	1.329601
19	6	0.253743	-3.558069	1.909362
20	1	-1.882533	-3.286013	2.017366
21	1	-1.311621	-3.509879	0.364254
22	6	0.477482	-5.034303	2.031209
23	6	2.333395	-2.627381	3.066392
24	1	2.629160	-3.664405	3.278259
25	1	2.256946	-2.092778	4.030423
26	1	3.156925	-2.148072	2.513734
27	1	1.443109	-5.278067	2.495764
28	1	0.448492	-5.521589	1.040158
29	1	-0.318104	-5.509216	2.633671
30	6	3.001716	0.615601	-1.786577
31	6	3.994806	-0.099198	0.396007
32	6	2.648229	-1.729327	-0.976519
33	6	3.931941	-2.178329	-1.701692
34	1	1.772774	-1.825658	-1.639692
35	1	2.459942	-2.368058	-0.097991
36	6	4.148465	-1.299844	-2.948518
37	6	5.136601	-2.028241	-0.752302
38	1	3.827869	-3.234901	-2.004441
39	6	5.277541	-0.552853	-0.329175
40	1	6.060415	-2.369394	-1.251502
41	1	5.000662	-2.667394	0.137882
42	6	5.496709	0.320893	-1.578386
43	1	6.136481	-0.444702	0.355886
44	1	3.853809	-0.694476	1.311280

45	1	4.089560	0.952479	0.712087
46	6	4.284889	0.173161	-2.516684
47	1	3.078139	1.675320	-1.488704
48	1	2.131368	0.537886	-2.451884
49	1	4.425943	0.807475	-3.408650
50	1	5.623638	1.377490	-1.284377
51	1	6.423860	0.019521	-2.096944
52	1	3.299227	-1.413303	-3.643921
53	1	5.054008	-1.623982	-3.491086
54	6	-3.788913	-1.711511	0.654993
55	6	-3.409077	0.449317	-0.508859
56	6	-2.473963	-1.658773	-1.507597
57	6	-3.787384	-1.849974	-2.294176
58	1	-1.749400	-1.078834	-2.096468
59	1	-2.021175	-2.642492	-1.307178
60	6	-4.395074	-0.474644	-2.627401
61	6	-4.787011	-2.663014	-1.449266
62	1	-3.562476	-2.392442	-3.228126
63	6	-5.096959	-1.900962	-0.145349
64	1	-5.717936	-2.832123	-2.017488
65	1	-4.369852	-3.659202	-1.218766
66	6	-5.717931	-0.536236	-0.484903
67	1	-5.799282	-2.489179	0.469881
68	1	-3.413490	-2.706428	0.918627
69	1	-3.989430	-1.177741	1.600283
70	6	-4.707592	0.270835	-1.316667
71	1	-3.625875	0.974199	0.433027
72	1	-2.701050	1.058461	-1.082852
73	1	-5.121020	1.267726	-1.545849
74	1	-6.659238	-0.674415	-1.044653
75	1	-5.972101	0.008385	0.441162
76	1	-5.315468	-0.599465	-3.224038
77	1	-3.688923	0.112252	-3.237516
78	6	0.283475	2.308908	3.577314
79	6	2.401619	3.359000	1.415759
80	6	0.740240	4.300550	-1.164262
81	6	-2.304339	3.836381	-0.608614
82	6	-2.580244	2.541765	2.379300
83	1	0.058594	3.168561	4.235544
84	1	1.338010	2.046495	3.738174
85	1	-0.328806	1.466101	3.933374
86	1	2.593513	4.314901	1.936304
87	1	2.966782	3.383338	0.473384
88	1	2.830522	2.561183	2.039219
89	1	0.632256	5.396322	-1.068040
90	1	0.217715	3.987831	-2.078978
91	1	1.809945	4.089394	-1.306993
92	1	-2.341535	4.938373	-0.670609
93	1	-3.290830	3.493760	-0.267105
94	1	-2.148424	3.455890	-1.630290
95	1	-2.637871	3.210710	3.256156
96	1	-2.634528	1.509763	2.761217
97	1	-3.480984	2.721713	1.777094

By BP86/BS2

$10^{1\text{-Ad}}$ (E = -2109.1775863 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.070716	1.225691	0.207231
2	7	1.507177	0.185353	0.094659
3	6	1.163140	0.051095	1.451987
4	7	-1.455954	-0.627526	0.562994
5	6	0.868132	3.175944	1.195197
6	6	-0.071879	2.639447	2.141170

7	6	0.130475	3.629494	0.055545
8	17	-0.410468	1.254351	-2.183508
9	6	-1.388531	2.780170	1.585542
10	6	-1.264206	3.396297	0.299339
11	6	2.785365	-0.225395	-0.553836
12	6	-0.819864	-1.532617	1.241349
13	6	-2.758589	-0.941298	-0.179247
14	6	0.415638	-1.158008	2.036136
15	1	1.841382	0.505082	2.193907
16	6	1.092733	-2.500518	2.319125
17	1	0.038482	-0.781855	3.016600
18	6	-1.008924	-3.043746	1.360175
19	6	0.311797	-3.532095	1.928212
20	1	-1.827571	-3.282243	2.067436
21	1	-1.280463	-3.522191	0.404521
22	6	0.560425	-5.016591	2.053983
23	6	2.401416	-2.562119	3.065630
24	1	2.738844	-3.600012	3.227879
25	1	2.304737	-2.072730	4.056672
26	1	3.200012	-2.021934	2.523650
27	1	1.546063	-5.234429	2.499196
28	1	0.519547	-5.509380	1.061385
29	1	-0.213800	-5.500747	2.683424
30	6	2.990898	0.548511	-1.886296
31	6	4.016031	0.051376	0.362154
32	6	2.729120	-1.752549	-0.875533
33	6	4.044150	-2.214646	-1.569219
34	1	1.860206	-1.938638	-1.535284
35	1	2.565742	-2.320451	0.060618
36	6	4.229164	-1.428972	-2.899208
37	6	5.253328	-1.938693	-0.630750
38	1	3.977197	-3.301187	-1.782899
39	6	5.331210	-0.414677	-0.328483
40	1	6.194231	-2.279303	-1.109587
41	1	5.140488	-2.509403	0.314412
42	6	5.520961	0.369347	-1.658666
43	1	6.185552	-0.212219	0.349896
44	1	3.890547	-0.474067	1.328442
45	1	4.068153	1.135897	0.579771
46	6	4.304863	0.093868	-2.587285
47	1	3.027361	1.635845	-1.671987
48	1	2.120972	0.376057	-2.543820
49	1	4.420947	0.661032	-3.533028
50	1	5.602876	1.456040	-1.450235
51	1	6.462533	0.056493	-2.155058
52	1	3.379297	-1.634012	-3.581073
53	1	5.155090	-1.759853	-3.412937
54	6	-3.778254	-1.757905	0.675400
55	6	-3.440552	0.414849	-0.518125
56	6	-2.463628	-1.703028	-1.507105
57	6	-3.788397	-1.929264	-2.297292
58	1	-1.750192	-1.113442	-2.109271
59	1	-1.994219	-2.681437	-1.290457
60	6	-4.428740	-0.556797	-2.647631
61	6	-4.780231	-2.760052	-1.434089
62	1	-3.551087	-2.480056	-3.229428
63	6	-5.100239	-1.981712	-0.124885
64	1	-5.715083	-2.946734	-2.000373
65	1	-4.339954	-3.749569	-1.192123
66	6	-5.754393	-0.619565	-0.478653
67	1	-5.790213	-2.579179	0.505049
68	1	-3.377909	-2.748583	0.943827
69	1	-3.987456	-1.210279	1.616203
70	6	-4.750370	0.203702	-1.330533

71	1	-3.671408	0.937751	0.427874
72	1	-2.739183	1.037719	-1.097938
73	1	-5.183013	1.196193	-1.568932
74	1	-6.696692	-0.782846	-1.040005
75	1	-6.012338	-0.067453	0.448276
76	1	-5.356293	-0.708479	-3.236326
77	1	-3.731758	0.038511	-3.269547
78	6	0.212312	2.280211	3.583164
79	6	2.343334	3.392342	1.448789
80	6	0.694836	4.348187	-1.149703
81	6	-2.375455	3.837455	-0.626244
82	6	-2.664865	2.516173	2.359263
83	1	0.004111	3.150042	4.240832
84	1	1.267099	1.994001	3.735841
85	1	-0.420904	1.444262	3.932612
86	1	2.505682	4.341230	2.000429
87	1	2.913724	3.452367	0.505978
88	1	2.778455	2.578175	2.055052
89	1	0.626570	5.446800	-1.008124
90	1	0.144895	4.083818	-2.069023
91	1	1.757284	4.096350	-1.313611
92	1	-2.448101	4.944147	-0.642711
93	1	-3.355847	3.441522	-0.310146
94	1	-2.186726	3.497739	-1.662379
95	1	-2.730866	3.201976	3.228163
96	1	-2.715300	1.483629	2.751600
97	1	-3.559801	2.686791	1.737467

By BP86/LANL2DZ

$10^{1\text{-Ad}}$ (E = -1663.7923218 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.081882	1.200414	0.245863
2	7	1.503807	0.195554	0.126912
3	6	1.162416	0.056842	1.512999
4	7	-1.423741	-0.625645	0.588713
5	6	0.819006	3.186284	1.240011
6	6	-0.129741	2.636524	2.192889
7	6	0.073496	3.634666	0.086004
8	17	-0.410783	1.244914	-2.197107
9	6	-1.457869	2.756104	1.622962
10	6	-1.332451	3.376096	0.323553
11	6	2.768617	-0.196457	-0.559103
12	6	-0.801552	-1.545176	1.299563
13	6	-2.713295	-0.938313	-0.191230
14	6	0.435995	-1.168837	2.108328
15	1	1.834404	0.537797	2.246051
16	6	1.123536	-2.521949	2.376422
17	1	0.071258	-0.787567	3.095189
18	6	-1.007388	-3.064330	1.418782
19	6	0.326487	-3.562154	1.986568
20	1	-1.829973	-3.302787	2.127225
21	1	-1.273431	-3.537928	0.455291
22	6	0.576215	-5.049359	2.104187
23	6	2.453902	-2.585457	3.089305
24	1	2.758663	-3.622174	3.319129
25	1	2.412292	-2.021068	4.044200
26	1	3.257654	-2.121234	2.485115
27	1	1.549915	-5.275153	2.574482
28	1	0.563679	-5.534589	1.106136
29	1	-0.215007	-5.542664	2.706635
30	6	2.975796	0.648099	-1.852387
31	6	4.010797	0.016903	0.367715
32	6	2.686481	-1.709428	-0.961729

33	6	3.992394	-2.148040	-1.690127
34	1	1.806659	-1.848389	-1.622156
35	1	2.524100	-2.326116	-0.054365
36	6	4.179827	-1.290828	-2.977358
37	6	5.210944	-1.937127	-0.741792
38	1	3.914235	-3.221220	-1.963437
39	6	5.315695	-0.430043	-0.358424
40	1	6.145605	-2.266890	-1.242007
41	1	5.090738	-2.555102	0.173527
42	6	5.507582	0.421818	-1.648172
43	1	6.179613	-0.278476	0.322300
44	1	3.883642	-0.559493	1.305754
45	1	4.078897	1.088802	0.645783
46	6	4.280577	0.214207	-2.584579
47	1	3.025804	1.723514	-1.579482
48	1	2.098017	0.526510	-2.512330
49	1	4.400564	0.829046	-3.500371
50	1	5.606836	1.495748	-1.383132
51	1	6.442143	0.122068	-2.167778
52	1	3.321882	-1.446033	-3.664157
53	1	5.098181	-1.606548	-3.516201
54	6	-3.753897	-1.755245	0.646734
55	6	-3.390941	0.414685	-0.561985
56	6	-2.368759	-1.711947	-1.507412
57	6	-3.670105	-1.956107	-2.331882
58	1	-1.643613	-1.115929	-2.092465
59	1	-1.894072	-2.685596	-1.273250
60	6	-4.307613	-0.587710	-2.713009
61	6	-4.681651	-2.786424	-1.486312
62	1	-3.404979	-2.514268	-3.253026
63	6	-5.049314	-1.996085	-0.193516
64	1	-5.598231	-2.988372	-2.078287
65	1	-4.239092	-3.769698	-1.219587
66	6	-5.700865	-0.639360	-0.582557
67	1	-5.757237	-2.592047	0.418966
68	1	-3.357909	-2.742156	0.938235
69	1	-3.995382	-1.199366	1.577340
70	6	-4.675447	0.184769	-1.411556
71	1	-3.650904	0.950719	0.370556
72	1	-2.677351	1.035278	-1.131363
73	1	-5.108597	1.171509	-1.674359
74	1	-6.623790	-0.815811	-1.173291
75	1	-5.994067	-0.079490	0.330490
76	1	-5.216551	-0.748532	-3.329585
77	1	-3.593200	0.006235	-3.317639
78	6	0.153440	2.275670	3.634771
79	6	2.294103	3.408094	1.495024
80	6	0.632521	4.360430	-1.118159
81	6	-2.441457	3.794248	-0.616642
82	6	-2.735121	2.448230	2.381097
83	1	-0.039688	3.148693	4.293682
84	1	1.205257	1.974707	3.788368
85	1	-0.492631	1.450399	3.989878
86	1	2.453621	4.337497	2.080801
87	1	2.861031	3.509667	0.551815
88	1	2.742710	2.576457	2.070193
89	1	0.534667	5.458791	-0.987663
90	1	0.098570	4.074129	-2.041301
91	1	1.704233	4.137081	-1.271861
92	1	-2.507059	4.900264	-0.669667
93	1	-3.426952	3.417014	-0.290749
94	1	-2.253245	3.421764	-1.642599
95	1	-2.796230	3.070659	3.297124
96	1	-2.793809	1.389448	2.700941

97	1	-3.631788	2.669160	1.775466

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10$^{1\text{-Ad}}$ (E = -2109.0121412 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.031903	1.199125	0.222067
2	7	1.513890	0.143227	0.122866
3	6	1.151131	0.002649	1.463901
4	7	-1.470949	-0.627974	0.554586
5	6	0.917581	3.155684	1.189408
6	6	-0.016089	2.637314	2.138641
7	6	0.181664	3.605184	0.058879
8	17	-0.390842	1.207758	-2.184449
9	6	-1.326479	2.785864	1.593287
10	6	-1.204832	3.387241	0.310785
11	6	-0.849229	-1.539950	1.212898
12	6	0.380671	-1.194663	2.023784
13	1	1.816698	0.437762	2.212910
14	6	1.035280	-2.546530	2.288032
15	1	0.001906	-0.834216	2.997669
16	6	-1.059037	-3.044963	1.315308
17	6	0.248450	-3.553304	1.884263
18	1	-1.876603	-3.279509	2.008539
19	1	-1.323240	-3.501466	0.358911
20	6	0.470661	-5.037670	1.995777
21	6	2.335224	-2.636845	3.037883
22	1	2.618727	-3.672451	3.247737
23	1	2.260132	-2.105241	3.997698
24	1	3.155348	-2.168787	2.482349
25	1	1.434284	-5.279423	2.453245
26	1	0.441207	-5.511965	1.004522
27	1	-0.318386	-5.510618	2.598302
28	6	0.268233	2.285505	3.577388
29	6	2.391104	3.366078	1.433256
30	6	0.740829	4.316690	-1.147017
31	6	-2.312971	3.840939	-0.604928
32	6	-2.593873	2.526615	2.374061
33	1	0.059984	3.149798	4.225983
34	1	1.313883	2.005370	3.731609
35	1	-0.356458	1.456939	3.929141
36	1	2.560202	4.321046	1.952118
37	1	2.957137	3.395173	0.497654
38	1	2.818903	2.574689	2.056329
39	1	0.682727	5.406276	-1.006625
40	1	0.187026	4.060060	-2.054134
41	1	1.791021	4.060958	-1.319113
42	1	-2.350824	4.938751	-0.641955
43	1	-3.291974	3.487813	-0.268911
44	1	-2.156446	3.480590	-1.628106
45	1	-2.631103	3.177439	3.258913
46	1	-2.663788	1.491615	2.729143
47	1	-3.485869	2.736960	1.778030
48	6	2.780157	-0.251401	-0.532203
49	6	3.009505	0.585304	-1.818099
50	6	4.005137	-0.045081	0.403460
51	6	2.699263	-1.754032	-0.937138
52	6	4.315187	0.147752	-2.527204
53	1	2.152871	0.465186	-2.486587
54	1	3.061440	1.650075	-1.550820
55	6	5.309577	-0.495536	-0.300511
56	1	4.074735	1.015201	0.678627
57	1	3.867730	-0.612847	1.331319
58	6	4.005173	-2.197550	-1.641221

59	1	2.519743	-2.365594	-0.043786
60	1	1.837724	-1.886642	-1.604472
61	6	4.214856	-1.347571	-2.918001
62	6	5.521526	0.349710	-1.579549
63	1	4.450539	0.755348	-3.432308
64	6	5.204092	-1.992537	-0.682797
65	1	6.156461	-0.349167	0.384435
66	1	3.927610	-3.259690	-1.912599
67	1	5.130545	-1.664632	-3.436978
68	1	3.377343	-1.499263	-3.612799
69	1	6.453078	0.050310	-2.080295
70	1	5.622106	1.412486	-1.316480
71	1	6.134352	-2.323004	-1.165799
72	1	5.074323	-2.604990	0.221355
73	6	-2.770850	-0.908003	-0.185011
74	6	-2.501065	-1.672958	-1.512908
75	6	-3.803758	-1.697048	0.674215
76	6	-3.422203	0.459587	-0.521508
77	6	-3.829528	-1.869336	-2.288189
78	1	-1.786425	-1.102989	-2.114023
79	1	-2.052581	-2.651793	-1.305790
80	6	-5.125951	-1.891758	-0.116260
81	1	-3.429450	-2.685474	0.944879
82	1	-3.993464	-1.147219	1.607164
83	6	-4.735406	0.276467	-1.319961
84	1	-3.631141	0.987528	0.415061
85	1	-2.721584	1.060949	-1.103353
86	6	-4.439060	-0.489033	-2.631691
87	6	-4.828549	-2.673192	-1.420560
88	1	-3.617647	-2.420195	-3.214274
89	6	-5.746773	-0.521540	-0.466908
90	1	-5.822722	-2.467574	0.508068
91	1	-5.146793	1.267285	-1.556039
92	1	-5.364608	-0.619072	-3.209694
93	1	-3.741232	0.085621	-3.254449
94	1	-5.761223	-2.840871	-1.976407
95	1	-4.412734	-3.663240	-1.182623
96	1	-6.686507	-0.662619	-1.018452
97	1	-5.989278	0.031419	0.451822

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10$^{\text{1-Ad}}$ (E = -2900.3828701 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.034850	1.199794	0.209716
2	7	1.522321	0.132175	0.122543
3	6	1.151986	-0.006945	1.462147
4	7	-1.478356	-0.636046	0.551724
5	6	0.915915	3.175352	1.184416
6	6	-0.021996	2.666244	2.134063
7	6	0.185023	3.619838	0.047751
8	17	-0.393225	1.194979	-2.193819
9	6	-1.330214	2.814397	1.583287
10	6	-1.202926	3.406454	0.296670
11	6	-0.853468	-1.548237	1.207438
12	6	0.377620	-1.203971	2.019190
13	1	1.810369	0.432448	2.215420
14	6	1.032368	-2.556538	2.279970
15	1	-0.001218	-0.845362	2.993782
16	6	-1.060286	-3.054316	1.303570
17	6	0.247548	-3.562840	1.871427
18	1	-1.878299	-3.294350	1.994273
19	1	-1.322176	-3.506429	0.344382
20	6	0.471617	-5.047344	1.977348

21	6	2.331501	-2.647536	3.031149
22	1	2.621812	-3.683705	3.228514
23	1	2.250924	-2.128624	3.997488
24	1	3.149172	-2.166570	2.483099
25	1	1.435648	-5.289560	2.433718
26	1	0.442479	-5.518032	0.984366
27	1	-0.316633	-5.523480	2.578421
28	6	0.259300	2.314215	3.573898
29	6	2.390053	3.381382	1.432246
30	6	0.750247	4.323275	-1.161037
31	6	-2.308590	3.855295	-0.625627
32	6	-2.601861	2.565771	2.361292
33	1	0.064091	3.182092	4.221606
34	1	1.301155	2.019292	3.726945
35	1	-0.376027	1.494695	3.928023
36	1	2.561803	4.336729	1.949322
37	1	2.959122	3.405793	0.498271
38	1	2.813048	2.589614	2.058255
39	1	0.687434	5.413783	-1.032379
40	1	0.204440	4.055890	-2.070120
41	1	1.802569	4.069440	-1.323024
42	1	-2.351003	4.952623	-0.665901
43	1	-3.287671	3.498594	-0.293166
44	1	-2.147115	3.492688	-1.647308
45	1	-2.647819	3.233957	3.232656
46	1	-2.670099	1.537874	2.736768
47	1	-3.490775	2.760039	1.755218
48	6	2.794651	-0.260703	-0.525615
49	6	3.019292	0.567521	-1.817684
50	6	4.015728	-0.036351	0.411042
51	6	2.728215	-1.767393	-0.918505
52	6	4.330104	0.135880	-2.521030
53	1	2.164660	0.435477	-2.486967
54	1	3.062347	1.634783	-1.558759
55	6	5.325739	-0.480532	-0.286892
56	1	4.075490	1.026629	0.678211
57	1	3.881123	-0.598187	1.343088
58	6	4.039686	-2.204734	-1.616576
59	1	2.552843	-2.373520	-0.020732
60	1	1.869618	-1.914795	-1.586515
61	6	4.244087	-1.363355	-2.899830
62	6	5.532418	0.356424	-1.572315
63	1	4.461849	0.737420	-3.430623
64	6	5.234758	-1.981361	-0.657510
65	1	6.169873	-0.320880	0.398480
66	1	3.971926	-3.269679	-1.879354
67	1	5.163580	-1.676299	-3.414618
68	1	3.409418	-1.528399	-3.594897
69	1	6.467800	0.061724	-2.068729
70	1	5.622756	1.422054	-1.317595
71	1	6.168985	-2.307212	-1.136024
72	1	5.108751	-2.587846	0.251184
73	6	-2.781829	-0.915841	-0.183144
74	6	-2.520441	-1.677514	-1.514807
75	6	-3.809674	-1.706458	0.680643
76	6	-3.435389	0.452560	-0.513721
77	6	-3.854220	-1.872387	-2.281737
78	1	-1.810096	-1.105950	-2.119813
79	1	-2.070298	-2.656719	-1.313204
80	6	-5.136761	-1.899977	-0.101655
81	1	-3.433424	-2.695318	0.946798
82	1	-3.993699	-1.158647	1.615838
83	6	-4.754471	0.270878	-1.302841
84	1	-3.636374	0.980690	0.424604

85	1	-2.740487	1.054173	-1.102356
86	6	-4.466751	-0.491683	-2.618132
87	6	-4.847397	-2.678472	-1.409483
88	1	-3.648144	-2.421033	-3.210334
89	6	-5.759972	-0.529026	-0.444832
90	1	-5.829257	-2.477410	0.525935
91	1	-5.167400	1.262143	-1.533936
92	1	-5.396173	-0.620993	-3.189992
93	1	-3.773808	0.084660	-3.244732
94	1	-5.783504	-2.845335	-1.959769
95	1	-4.429757	-3.668865	-1.176257
96	1	-6.703349	-0.668612	-0.990483
97	1	-5.996399	0.021667	0.476766

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M1a (E = -697.941082 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.297529	0.029112	0.003551
2	6	-1.807569	0.872691	0.719875
3	6	-1.734119	-0.479638	1.157761
4	6	-1.803312	0.878015	-0.707358
5	17	1.105643	2.224380	0.093527
6	6	-1.687569	-1.307960	-0.000904
7	6	-1.731772	-0.471639	-1.154354
8	6	1.257483	-1.347472	1.347512
9	6	2.400562	-0.789971	0.652963
10	1	0.869144	-2.305378	1.002719
11	6	1.244740	-1.205672	-1.478571
12	6	2.395158	-0.721359	-0.741931
13	1	0.858374	-2.193611	-1.228562
14	1	1.234698	-1.014635	-2.546721
15	6	3.482645	0.037103	-1.480282
16	6	3.493139	-0.106949	1.454360
17	1	3.665978	0.924024	1.129785
18	1	4.439087	-0.655092	1.343396
19	1	3.239560	-0.091451	2.518309
20	1	3.632372	1.044748	-1.079135
21	1	3.238232	0.126130	-2.542720
22	1	4.437828	-0.499789	-1.399437
23	6	-1.845324	-0.953562	2.585444
24	6	-1.990822	2.080946	1.602707
25	6	-1.969835	2.094938	-1.581949
26	6	-1.855136	-0.940660	-2.582344
27	6	-1.738386	-2.815142	-0.009613
28	1	-2.900531	-1.076514	2.868508
29	1	-1.398492	-0.240168	3.285181
30	1	-1.350052	-1.918133	2.733544
31	1	-3.060718	2.298914	1.731868
32	1	-1.513801	2.966484	1.174499
33	1	-1.563486	1.925062	2.598419
34	1	-3.035984	2.330793	-1.710286
35	1	-1.544780	1.939059	-2.578736
36	1	-1.479889	2.970429	-1.147096
37	1	-2.912500	-1.079450	-2.849772
38	1	-1.347622	-1.897121	-2.742300
39	1	-1.430163	-0.217415	-3.285321
40	1	-2.781182	-3.158002	-0.068979
41	1	-1.307092	-3.246048	0.899380
42	1	-1.209684	-3.241863	-0.868529
43	1	1.256946	-1.264091	2.429436

TSM1a-1b (E = -697.9123803 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	22	-0.441026	-0.974421	-0.097242
2	6	-2.581739	-1.920780	-0.513619
3	6	-2.121401	-2.405530	0.743391
4	6	-1.704297	-2.418312	-1.521519
5	17	-1.296329	1.138710	0.090158
6	6	-0.968550	-3.213929	0.513076
7	6	-0.712106	-3.219963	-0.889441
8	6	1.053075	-1.129934	1.366574
9	6	2.388247	-1.071438	0.647309
10	1	1.028129	-1.933404	2.105616
11	6	1.133234	-0.858274	-1.482696
12	6	2.425834	-0.940932	-0.693518
13	1	1.145167	-1.532867	-2.342588
14	1	0.997615	0.159542	-1.888087
15	6	3.684893	-0.825998	-1.532203
16	6	3.598867	-1.128672	1.560085
17	1	4.552694	-1.086000	1.027036
18	1	3.584930	-2.053216	2.154748
19	1	3.574098	-0.294257	2.275810
20	1	3.690509	0.128472	-2.078200
21	1	3.712309	-1.621683	-2.290436
22	1	4.608166	-0.884989	-0.949210
23	6	-2.769935	-2.152497	2.082016
24	6	-3.831167	-1.110996	-0.752152
25	6	-1.849003	-2.170431	-3.002033
26	6	0.343497	-4.056753	-1.563644
27	6	-0.282387	-4.098710	1.520288
28	1	-3.514658	-2.930504	2.301372
29	1	-3.284412	-1.187060	2.106626
30	1	-2.037273	-2.161635	2.895530
31	1	-4.685220	-1.780423	-0.927416
32	1	-3.734467	-0.459739	-1.625812
33	1	-4.073122	-0.475435	0.103876
34	1	-2.562354	-2.881659	-3.441530
35	1	-0.897899	-2.288307	-3.528936
36	1	-2.223254	-1.162565	-3.210536
37	1	0.061018	-5.118303	-1.531407
38	1	1.316906	-3.957011	-1.071477
39	1	0.469300	-3.782804	-2.614466
40	1	-0.719583	-5.107094	1.491667
41	1	-0.395194	-3.721475	2.541068
42	1	0.788114	-4.196561	1.313881
43	1	0.881803	-0.190608	1.921975

M1b (E = -697.9317757 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-1.182855	-0.939098	-0.949716
2	6	1.088193	-1.590767	-0.779217
3	6	0.718867	-1.030945	0.481562
4	6	1.040872	-0.544932	-1.750402
5	17	-1.968147	-0.112817	-3.010048
6	6	0.387952	0.343019	0.275478
7	6	0.610900	0.642313	-1.102853
8	6	-2.099647	-2.864047	-1.219294
9	6	-2.172304	-2.764176	0.214846
10	1	-2.910819	-2.438659	-1.809657
11	6	-2.984629	-0.417114	0.098987
12	6	-2.600160	-1.581853	0.851807
13	1	-3.589558	-0.555871	-0.796727
14	1	-3.251343	0.474907	0.652855
15	6	-2.588355	-1.435033	2.365421
16	6	-1.674617	-3.966370	1.001721
17	1	-2.514823	-4.658312	1.154876
18	1	-1.265945	-3.727278	1.984627

19	1	-0.912581	-4.510019	0.433903
20	1	-3.574818	-1.723688	2.755003
21	1	-2.425455	-0.390333	2.649325
22	1	-1.844365	-2.049446	2.874810
23	6	0.930961	-1.686000	1.822253
24	6	1.634008	-2.978285	-1.014812
25	6	1.433338	-0.682511	-3.198063
26	6	0.458303	2.000633	-1.735722
27	6	0.063293	1.353587	1.348766
28	1	1.962581	-1.502386	2.155741
29	1	0.791139	-2.768907	1.782040
30	1	0.265844	-1.283584	2.589991
31	1	2.732089	-2.973671	-0.956923
32	1	1.358485	-3.359577	-2.003086
33	1	1.269030	-3.690986	-0.269704
34	1	2.518165	-0.544710	-3.311379
35	1	0.928740	0.057772	-3.823226
36	1	1.182145	-1.672246	-3.592915
37	1	1.387164	2.577964	-1.623732
38	1	-0.347376	2.576176	-1.268620
39	1	0.231136	1.923725	-2.801626
40	1	0.977997	1.860853	1.688024
41	1	-0.395673	0.884215	2.223556
42	1	-0.624316	2.123790	0.985556
43	1	-1.710311	-3.783354	-1.640073

M2a (E = -948.594597 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-1.036437	-1.354815	-0.934276
2	7	-2.530625	0.021602	-3.534721
3	6	1.360818	-1.427787	-0.763526
4	6	0.894042	-0.920956	0.489943
5	6	1.057888	-0.475155	-1.771823
6	17	-0.596732	-3.267047	-2.391002
7	6	0.325744	0.360483	0.249305
8	6	0.396690	0.624059	-1.146130
9	6	-2.002956	-0.429708	-2.598016
10	6	-3.232503	0.483413	-4.728273
11	6	-3.274059	-2.509101	-1.130873
12	6	-2.732490	-2.696148	0.137037
13	1	-3.900250	-1.659072	-1.354196
14	6	-2.630270	-0.271262	0.263819
15	6	-2.397190	-1.541018	0.900407
16	1	-3.539767	-0.121556	-0.310977
17	1	-2.372324	0.604116	0.846896
18	6	-2.066430	-1.653027	2.376549
19	6	-2.409029	-4.095366	0.629332
20	1	-3.182310	-4.428620	1.336604
21	1	-1.444235	-4.153542	1.144238
22	1	-2.390220	-4.797497	-0.208155
23	1	-2.996150	-1.818961	2.942753
24	1	-1.624101	-0.728283	2.754513
25	1	-1.389429	-2.479450	2.611629
26	6	-4.275037	-0.593004	-5.103156
27	6	-3.918223	1.824058	-4.387892
28	1	-3.786880	-1.551133	-5.304249
29	1	-4.998558	-0.730369	-4.293723
30	1	-4.635009	1.696846	-3.570749
31	1	-3.179293	2.575953	-4.093849
32	6	1.265196	-1.510381	1.829736
33	6	2.223426	-2.653809	-0.920230
34	6	1.459648	-0.570795	-3.220782
35	6	0.018499	1.931811	-1.797531
36	6	-0.025671	1.388715	1.293478

37	1	2.337274	-1.357987	2.023270
38	1	1.081109	-2.589597	1.873442
39	1	0.714900	-1.043963	2.649965
40	1	3.259085	-2.417783	-0.632193
41	1	2.226596	-3.015022	-1.950164
42	1	1.882451	-3.478818	-0.286474
43	1	2.502396	-0.248437	-3.354598
44	1	0.834229	0.063661	-3.856938
45	1	1.369869	-1.597894	-3.585821
46	1	0.796815	2.687724	-1.618901
47	1	-0.922692	2.327345	-1.400885
48	1	-0.093616	1.826357	-2.880303
49	1	0.874473	1.962700	1.559301
50	1	-0.408015	0.942021	2.215230
51	1	-0.771461	2.103275	0.931870
52	1	-4.454850	2.189565	-5.268954
53	1	-4.812886	-0.276975	-6.002612
54	1	-3.345163	-3.347138	-1.810190
55	6	-2.193535	0.662384	-5.856211
56	1	-2.700101	1.000307	-6.765779
57	1	-1.443476	1.409691	-5.578631
58	1	-1.686847	-0.283724	-6.068703

TSM2a-3a (E = -948.5858409 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-1.101495	-0.608586	-0.596541
2	7	-3.104139	1.228348	-2.289278
3	6	1.272129	-1.061212	-0.894803
4	6	1.135788	-0.281022	0.281516
5	6	0.825661	-0.277631	-1.999434
6	17	-1.462848	-2.451974	-2.127535
7	6	0.604380	0.995197	-0.093048
8	6	0.417286	0.993957	-1.504410
9	6	-2.578712	0.426788	-1.546041
10	6	-4.457587	1.710947	-2.674210
11	6	-1.784335	0.144362	1.405747
12	6	-2.078583	-1.257939	1.464639
13	1	-2.592196	0.843598	1.202211
14	6	-3.560514	-0.776086	-0.425926
15	6	-2.912283	-1.752027	0.463477
16	1	-4.154007	-1.254505	-1.195772
17	1	-4.094915	0.017134	0.096754
18	6	-3.334173	-3.202806	0.385710
19	6	-1.481579	-2.153784	2.534126
20	1	-1.091975	-3.096254	2.135390
21	1	-2.253542	-2.405998	3.275073
22	1	-0.673994	-1.643381	3.064506
23	1	-4.193660	-3.375768	1.051390
24	1	-2.535582	-3.887939	0.684331
25	1	-3.630913	-3.465209	-0.632103
26	6	-5.358816	0.529765	-3.095262
27	6	-5.066666	2.480876	-1.481295
28	1	-4.864348	-0.081842	-3.856805
29	1	-5.615116	-0.108102	-2.245587
30	1	-5.230066	1.821661	-0.623107
31	1	-4.407393	3.299289	-1.173569
32	6	1.651365	-0.654251	1.648929
33	6	1.864210	-2.444791	-0.984981
34	6	0.930241	-0.649433	-3.454609
35	6	0.064936	2.194232	-2.345810
36	6	0.515178	2.224722	0.776609
37	1	2.702980	-0.350038	1.751924
38	1	1.605856	-1.733507	1.824250
39	1	1.092956	-0.160284	2.449887

40	1	2.927963	-2.389170	-1.257417
41	1	1.351947	-3.046899	-1.740571
42	1	1.796647	-2.978453	-0.031314
43	1	1.873652	-0.268679	-3.873367
44	1	0.108767	-0.225029	-4.040180
45	1	0.905926	-1.732057	-3.595014
46	1	0.979985	2.729361	-2.639415
47	1	-0.573604	2.896902	-1.802781
48	1	-0.466556	1.909627	-3.257491
49	1	1.353648	2.901659	0.557803
50	1	0.564971	1.978171	1.840664
51	1	-0.411635	2.783414	0.606415
52	1	-6.032274	2.907467	-1.774301
53	1	-6.291028	0.919700	-3.518582
54	1	-1.082045	0.523487	2.136932
55	6	-4.256139	2.665040	-3.870046
56	1	-5.217923	3.078441	-4.192217
57	1	-3.594384	3.491931	-3.593054
58	1	-3.805688	2.131438	-4.713369

M3a (E = -948.6243643 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.459792	-0.177472	-0.277276
2	7	-1.016288	1.186728	0.151765
3	6	2.578461	0.932015	-0.135476
4	6	2.834471	-0.436009	-0.451088
5	6	2.000525	0.983647	1.163197
6	17	0.220843	-0.074546	-2.605965
7	6	2.410349	-1.229144	0.651397
8	6	1.875148	-0.350550	1.645403
9	6	-1.164878	0.153847	0.863339
10	6	-1.897220	2.356779	-0.186342
11	6	-0.405022	-2.169124	-0.008147
12	6	-1.888893	-2.288234	-0.198432
13	1	-0.136255	-2.440643	1.016326
14	6	-2.274278	-0.550021	1.563223
15	6	-2.774282	-1.607765	0.565683
16	1	-3.099414	0.107241	1.856548
17	1	-1.885383	-1.016328	2.477393
18	6	-4.280052	-1.767477	0.556199
19	6	-2.305586	-3.244454	-1.301456
20	1	-3.374473	-3.223600	-1.527537
21	1	-2.028351	-4.276602	-1.044921
22	1	-1.763370	-2.987730	-2.221023
23	1	-4.644353	-2.041927	1.557627
24	1	-4.619312	-2.540164	-0.136853
25	1	-4.785408	-0.828353	0.284596
26	6	-3.106322	1.833581	-0.991807
27	6	-2.351077	3.048670	1.115928
28	1	-2.768533	1.294583	-1.881793
29	1	-3.723058	1.159723	-0.390178
30	1	-2.947097	2.376293	1.740889
31	1	-1.487193	3.390100	1.696220
32	6	3.532353	-0.932607	-1.692067
33	6	2.940534	2.107026	-1.009722
34	6	1.659842	2.231023	1.938979
35	6	1.434221	-0.758090	3.029263
36	6	2.657467	-2.706358	0.819701
37	1	4.623129	-0.857615	-1.575159
38	1	3.246246	-0.351563	-2.573488
39	1	3.292748	-1.980219	-1.898659
40	1	4.007441	2.350072	-0.903023
41	1	2.371083	3.002953	-0.744541
42	1	2.751996	1.893635	-2.066512

43	1	2.499397	2.519177	2.587182
44	1	0.784725	2.085892	2.580555
45	1	1.450496	3.076606	1.277185
46	1	2.303156	-0.880123	3.691738
47	1	0.893760	-1.710634	3.022051
48	1	0.779013	-0.007374	3.482405
49	1	3.656285	-2.876130	1.246351
50	1	2.612261	-3.240393	-0.134759
51	1	1.930002	-3.170356	1.492021
52	1	-2.966968	3.921961	0.873837
53	1	-3.728179	2.678675	-1.308309
54	1	0.130796	-2.839708	-0.687760
55	6	-1.066394	3.323258	-1.048455
56	1	-1.677923	4.183437	-1.341865
57	1	-0.199025	3.693737	-0.491463
58	1	-0.710161	2.819864	-1.951876

TSM3a-3b (E = -948.6104305 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.248393	-0.284724	-0.250795
2	7	-0.885209	1.447495	-0.619577
3	6	2.366214	-1.473869	0.275440
4	6	1.923115	-0.790054	1.439996
5	6	2.691514	-0.499922	-0.711937
6	17	0.001893	-1.443424	-2.248869
7	6	1.917800	0.606728	1.154133
8	6	2.415924	0.785153	-0.176030
9	6	-1.601676	0.501258	-0.190378
10	6	-1.208656	2.832568	-1.124684
11	6	-0.897784	-1.626559	1.072916
12	6	-2.195412	-2.141152	0.519728
13	1	-1.058946	-1.020613	1.974667
14	6	-3.015718	0.174758	0.143921
15	6	-3.209267	-1.333994	0.143304
16	1	-3.219008	0.614552	1.134553
17	1	-3.728170	0.646947	-0.539034
18	6	-4.579250	-1.769454	-0.331524
19	6	-2.253920	-3.654872	0.409041
20	1	-3.133704	-4.025378	-0.122285
21	1	-2.233089	-4.121012	1.404382
22	1	-1.366065	-4.010823	-0.130717
23	1	-4.719006	-2.852011	-0.307165
24	1	-4.765992	-1.429159	-1.361887
25	1	-5.367548	-1.324127	0.294663
26	6	-0.718138	3.847322	-0.072465
27	6	-0.453610	3.005688	-2.457390
28	1	-1.227524	3.693516	0.885424
29	1	0.358741	3.760542	0.088950
30	1	0.621148	2.871565	-2.318670
31	1	-0.799243	2.272200	-3.193234
32	6	1.709957	-1.390229	2.805964
33	6	2.545752	-2.962795	0.123632
34	6	3.315035	-0.790170	-2.051969
35	6	2.829355	2.091021	-0.808914
36	6	1.665167	1.689866	2.177443
37	1	2.625758	-1.280596	3.404533
38	1	1.477678	-2.457469	2.756531
39	1	0.899232	-0.899796	3.354617
40	1	3.581268	-3.258739	0.345163
41	1	2.318250	-3.288121	-0.896718
42	1	1.892718	-3.520866	0.802371
43	1	4.401992	-0.921064	-1.948323
44	1	3.144212	0.022967	-2.764125
45	1	2.906528	-1.703401	-2.494271

46	1	3.891315	2.288495	-0.602006
47	1	2.260801	2.938632	-0.418385
48	1	2.709025	2.076921	-1.896842
49	1	2.540034	1.809767	2.832967
50	1	0.809144	1.455911	2.821202
51	1	1.472402	2.658140	1.708687
52	1	-0.630918	4.010290	-2.857318
53	1	-0.931277	4.865741	-0.415752
54	1	-0.264171	-2.467578	1.359091
55	6	-2.721482	3.013640	-1.357291
56	1	-2.903560	4.015247	-1.762201
57	1	-3.101437	2.284515	-2.079964
58	1	-3.288213	2.921528	-0.425537

M3b (E = -948.6127734 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.287057	-0.173494	-0.190348
2	7	-0.854020	1.557349	-0.077235
3	6	2.310801	-1.525013	0.209237
4	6	2.022625	-0.780783	1.387940
5	6	2.646009	-0.602484	-0.819262
6	17	-0.110880	-1.019901	-2.345913
7	6	2.147829	0.605023	1.076628
8	6	2.533582	0.714278	-0.293789
9	6	-1.568100	0.516854	-0.191676
10	6	-1.265815	3.002942	0.076486
11	6	-0.881794	-1.498863	1.129506
12	6	-2.181805	-2.080451	0.626817
13	1	-1.050185	-0.867602	2.014842
14	6	-2.996611	0.131736	-0.194772
15	6	-3.172722	-1.352940	0.075340
16	1	-3.576969	0.743065	0.512851
17	1	-3.406720	0.366791	-1.187608
18	6	-4.533291	-1.862966	-0.351723
19	6	-2.268692	-3.587713	0.804200
20	1	-3.167960	-4.034050	0.373898
21	1	-2.228038	-3.857209	1.869121
22	1	-1.401491	-4.060704	0.322978
23	1	-4.713047	-2.904325	-0.078659
24	1	-4.659809	-1.772862	-1.441655
25	1	-5.331942	-1.261507	0.108602
26	6	-1.695283	3.220157	1.543299
27	6	-0.061779	3.891529	-0.271981
28	1	-2.552648	2.589889	1.802282
29	1	-0.873412	2.985486	2.227536
30	1	0.767344	3.716697	0.416577
31	1	0.283509	3.693358	-1.291645
32	6	1.846045	-1.330302	2.781099
33	6	2.348641	-3.027196	0.082552
34	6	3.159350	-0.953103	-2.190402
35	6	2.947545	1.962952	-1.036219
36	6	2.117256	1.704704	2.112154
37	1	2.794712	-1.259720	3.332742
38	1	1.551217	-2.383158	2.774330
39	1	1.092716	-0.778456	3.353947
40	1	3.366128	-3.409748	0.247340
41	1	2.030654	-3.351447	-0.913872
42	1	1.694163	-3.513132	0.813399
43	1	4.253497	-1.064923	-2.166438
44	1	2.917130	-0.178033	-2.923555
45	1	2.731854	-1.890760	-2.555344
46	1	4.030204	1.950362	-1.224402
47	1	2.724154	2.867933	-0.466773
48	1	2.450232	2.049622	-2.009429

49	1	2.992625	1.624937	2.772585
50	1	1.227196	1.653309	2.750075
51	1	2.144608	2.696798	1.655223
52	1	-0.347078	4.946902	-0.202464
53	1	-1.981697	4.266801	1.696195
54	1	-0.235759	-2.312998	1.459074
55	6	-2.426496	3.315651	-0.892979
56	1	-2.660210	4.385033	-0.848209
57	1	-2.146786	3.069952	-1.923259
58	1	-3.334113	2.763381	-0.636206

TSM3b-4 (E = -948.5954742 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.677413	0.035662	-0.662299
2	7	-0.617761	1.507884	-0.444284
3	6	2.830654	-1.089002	-0.563315
4	6	2.497443	-0.635054	0.741803
5	6	3.020069	0.056725	-1.392813
6	17	0.243202	-1.206636	-2.630221
7	6	2.465642	0.793503	0.715809
8	6	2.806680	1.219264	-0.605820
9	6	-1.217381	0.332491	-0.492621
10	6	-1.213443	2.856027	-0.189648
11	6	-0.759364	-0.943998	0.930080
12	6	-2.138497	-1.545863	1.005136
13	1	-0.472007	-0.437972	1.858307
14	6	-2.610071	-0.086550	-0.845956
15	6	-3.051626	-1.170170	0.099679
16	1	-3.316374	0.749687	-0.809739
17	1	-2.602692	-0.446159	-1.884545
18	6	-4.452777	-1.700293	-0.075952
19	6	-2.336219	-2.585209	2.087794
20	1	-3.358234	-2.972772	2.122010
21	1	-2.103502	-2.161082	3.074420
22	1	-1.656031	-3.435738	1.939424
23	1	-4.706604	-2.476101	0.650503
24	1	-4.578263	-2.127048	-1.081058
25	1	-5.191921	-0.892288	0.020790
26	6	-2.079626	2.801878	1.089678
27	6	-0.079256	3.877146	-0.004189
28	1	-2.900036	2.084353	0.991279
29	1	-1.470661	2.509768	1.952535
30	1	0.539344	3.621025	0.859483
31	1	0.554901	3.912546	-0.894178
32	6	2.399876	-1.480690	1.988336
33	6	3.058801	-2.517524	-0.989456
34	6	3.485149	0.031136	-2.826300
35	6	3.105392	2.627806	-1.062699
36	6	2.342090	1.655819	1.951023
37	1	3.372385	-1.515086	2.500203
38	1	2.114302	-2.513548	1.763625
39	1	1.671681	-1.082309	2.703100
40	1	4.132509	-2.754186	-0.984473
41	1	2.678810	-2.695632	-2.000003
42	1	2.562573	-3.226843	-0.319035
43	1	4.574020	-0.115481	-2.875702
44	1	3.253951	0.969163	-3.341270
45	1	3.009645	-0.780110	-3.385634
46	1	4.187561	2.755415	-1.206325
47	1	2.782025	3.370129	-0.329785
48	1	2.620821	2.867374	-2.015917
49	1	3.208740	1.500037	2.608994
50	1	1.445465	1.424783	2.538458
51	1	2.309714	2.718925	1.700802

52	1	-0.500138	4.875733	0.158537
53	1	-2.511630	3.788568	1.292463
54	1	-0.050563	-1.771465	0.790539
55	6	-2.059173	3.281507	-1.415827
56	1	-2.439899	4.299141	-1.269805
57	1	-1.443448	3.268221	-2.321494
58	1	-2.914424v	2.619610	-1.574075

M4 (E = -948.6194269 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.362855	-0.240263	-0.153593
2	7	-0.539266	1.442955	0.141009
3	6	2.173574	-1.804055	0.092552
4	6	1.977202	-1.123212	1.327373
5	6	2.616190	-0.848292	-0.864229
6	17	-0.306423	-1.306579	-2.140024
7	6	2.315549	0.251407	1.133278
8	6	2.710586	0.423457	-0.226936
9	6	-1.564699	0.522074	0.117217
10	6	-0.746637	2.912781	0.013708
11	6	-1.647087	-0.522367	1.184405
12	6	-2.892113	-1.313077	0.861426
13	1	-1.572723	-0.159666	2.216209
14	6	-2.804747	0.418909	-0.754141
15	6	-3.522284	-0.793320	-0.203746
16	1	-3.452834	1.303593	-0.677037
17	1	-2.559106	0.298255	-1.815355
18	6	-4.789536	-1.273307	-0.857350
19	6	-3.264712	-2.511063	1.692892
20	1	-4.209413	-2.958298	1.370428
21	1	-3.365218	-2.239502	2.753224
22	1	-2.489328	-3.288135	1.632464
23	1	-5.235683	-2.122967	-0.332103
24	1	-4.595419	-1.580467	-1.894043
25	1	-5.536648	-0.468297	-0.896429
26	6	-1.821398	3.363390	1.032114
27	6	0.570213	3.645014	0.320199
28	1	-2.782412	2.874951	0.842741
29	1	-1.506251	3.116762	2.052484
30	1	0.899879	3.440574	1.342195
31	1	1.354274	3.335486	-0.373701
32	6	1.647105	-1.751756	2.661854
33	6	2.009585	-3.283066	-0.153934
34	6	3.054702	-1.148104	-2.274138
35	6	3.370468	1.631660	-0.850141
36	6	2.443377	1.251012	2.258108
37	1	2.568867	-1.983799	3.214846
38	1	1.091011	-2.687782	2.546405
39	1	1.051546	-1.082766	3.293473
40	1	2.978715	-3.797285	-0.082595
41	1	1.599049	-3.478319	-1.149433
42	1	1.338654	-3.744503	0.578248
43	1	4.119261	-1.424827	-2.290795
44	1	2.926595	-0.280401	-2.929069
45	1	2.483049	-1.973565	-2.706313
46	1	4.419689	1.406540	-1.087878
47	1	3.367440	2.489155	-0.172914
48	1	2.886197	1.940135	-1.783717
49	1	3.230217	0.930687	2.955498
50	1	1.517793	1.355892	2.835383
51	1	2.715312	2.241652	1.887550
52	1	0.426911	4.726400	0.214595
53	1	-1.970571	4.447460	0.969709
54	1	-0.731301	-1.255650	1.144746

55	6	-1.185294	3.271319	-1.430128
56	1	-1.294655	4.358177	-1.528334
57	1	-0.431418	2.931432	-2.148360
58	1	-2.140497	2.809598	-1.692032

TSM4-5 (E = -948.6142426 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.380511	-0.196944	-0.192838
2	7	-0.611085	1.445556	0.307767
3	6	2.103123	-1.786310	0.218317
4	6	1.937513	-1.015262	1.407929
5	6	2.575079	-0.912850	-0.795973
6	17	-0.216037	-0.655994	-2.390616
7	6	2.354962	0.319980	1.137091
8	6	2.728519	0.396082	-0.231276
9	6	-1.675973	0.588879	0.293670
10	6	-0.779277	2.913803	0.083449
11	6	-1.597356	-0.633321	1.026253
12	6	-2.808930	-1.441576	0.699296
13	1	-1.198675	-0.627064	2.038683
14	6	-2.918120	0.528330	-0.591709
15	6	-3.556863	-0.788413	-0.208569
16	1	-3.602457	1.365180	-0.403781
17	1	-2.663328	0.553723	-1.655687
18	6	-4.860340	-1.211725	-0.827988
19	6	-3.046046	-2.781147	1.340362
20	1	-3.990083	-3.229618	1.017733
21	1	-3.069934	-2.696611	2.435742
22	1	-2.237310	-3.481250	1.087924
23	1	-5.212940	-2.170207	-0.435129
24	1	-4.761938	-1.310658	-1.917799
25	1	-5.643654	-0.462835	-0.644187
26	6	-1.788386	3.466617	1.118295
27	6	0.578692	3.603296	0.296367
28	1	-2.774471	3.005710	1.001988
29	1	-1.436077	3.268602	2.136849
30	1	0.937392	3.447992	1.316383
31	1	1.322354	3.215017	-0.403339
32	6	1.550599	-1.544367	2.768097
33	6	1.902948	-3.274663	0.076585
34	6	3.024331	-1.316105	-2.176992
35	6	3.398627	1.546195	-0.945055
36	6	2.519187	1.379858	2.198020
37	1	2.443004	-1.862677	3.326246
38	1	0.884923	-2.410536	2.694371
39	1	1.046111	-0.781991	3.372083
40	1	2.860743	-3.804286	0.182528
41	1	1.487544	-3.534457	-0.902484
42	1	1.222371	-3.664184	0.839949
43	1	4.098418	-1.553772	-2.170206
44	1	2.861861	-0.515991	-2.905109
45	1	2.486519	-2.197704	-2.536109
46	1	4.439131	1.285930	-1.185445
47	1	3.421799	2.448757	-0.328988
48	1	2.902062	1.796567	-1.889686
49	1	3.269321	1.055758	2.932571
50	1	1.588464	1.574065	2.742403
51	1	2.861069	2.326556	1.774165
52	1	0.477882	4.681155	0.127378
53	1	-1.901184	4.549855	0.995221
54	1	-0.488451	-1.512456	0.487379
55	6	-1.260840	3.221041	-1.358368
56	1	-1.256359	4.305090	-1.522710
57	1	-0.593965	2.755674	-2.091447

58	1	-2.275963	2.860942	-1.540607

M5 (E = -948.6222201 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.451624	-0.154950	-0.346251
2	7	-0.723544	1.238060	0.435998
3	6	2.038444	-1.916442	0.024969
4	6	1.740988	-1.324146	1.289776
5	6	2.665226	-0.923253	-0.776863
6	17	0.346006	0.530542	-2.550789
7	6	2.224977	0.016693	1.282823
8	6	2.782894	0.271051	0.001174
9	6	-1.793241	0.385619	0.365165
10	6	-0.891779	2.725529	0.444937
11	6	-1.728502	-0.880522	0.910098
12	6	-2.857457	-1.697729	0.449490
13	1	-1.057699	-1.162362	1.708937
14	6	-3.041147	0.429788	-0.516205
15	6	-3.642769	-0.947444	-0.355584
16	1	-3.747828	1.209380	-0.208756
17	1	-2.768517	0.639358	-1.555450
18	6	-4.938508	-1.312092	-1.024816
19	6	-3.038560	-3.129273	0.877690
20	1	-3.977726	-3.552391	0.509215
21	1	-3.034956	-3.218100	1.972607
22	1	-2.217501	-3.752603	0.498137
23	1	-5.255498	-2.329626	-0.775754
24	1	-4.852964	-1.247200	-2.118703
25	1	-5.745201	-0.626913	-0.727036
26	6	-1.677802	3.118117	1.718241
27	6	0.508000	3.364865	0.487953
28	1	-2.669440	2.651398	1.727008
29	1	-1.139956	2.794661	2.616381
30	1	1.064840	3.022978	1.362455
31	1	1.074629	3.117528	-0.414776
32	6	1.230671	-2.054467	2.508040
33	6	1.901234	-3.375865	-0.328275
34	6	3.245400	-1.138316	-2.150865
35	6	3.513091	1.512191	-0.449112
36	6	2.268401	0.904625	2.501967
37	1	2.071126	-2.492438	3.066171
38	1	0.555111	-2.873924	2.242467
39	1	0.701917	-1.385168	3.195525
40	1	2.824192	-3.915550	-0.070871
41	1	1.719251	-3.515292	-1.397676
42	1	1.075301	-3.847113	0.212231
43	1	4.268527	-1.534684	-2.075408
44	1	3.285190	-0.205925	-2.720185
45	1	2.651851	-1.850076	-2.732591
46	1	4.592997	1.314232	-0.498129
47	1	3.360748	2.348187	0.237896
48	1	3.193414	1.833218	-1.446214
49	1	2.879610	0.433205	3.283666
50	1	1.272789	1.082533	2.923041
51	1	2.717526	1.875519	2.278575
52	1	0.415742	4.455118	0.544076
53	1	-1.810825	4.205258	1.764705
54	1	-0.138611	-1.656012	-0.745613
55	6	-1.621406	3.255057	-0.817347
56	1	-1.550794	4.348839	-0.840862
57	1	-1.156699	2.858163	-1.724479
58	1	-2.682497	2.995156	-0.821184

M6a (E = -1199.2794629 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)

		X	Y	Z
1	22	0.510408	-0.713766	0.083069
2	7	-1.254166	-0.705351	0.917461
3	6	1.969681	-0.900055	-1.915221
4	6	0.639891	-1.357443	-2.201009
5	6	2.534854	-1.760356	-0.944752
6	17	1.898005	-0.755774	2.122544
7	6	0.394107	-2.506848	-1.399185
8	6	1.555612	-2.734934	-0.593084
9	6	-2.197405	0.098118	0.228216
10	6	-1.756807	-1.331149	2.216572
11	6	-3.044476	-0.254339	-0.766804
12	6	-3.844677	0.900216	-1.198908
13	1	-3.132134	-1.245262	-1.194052
14	6	-2.435338	1.569824	0.526807
15	6	-3.501328	1.982306	-0.458897
16	1	-2.766269	1.718261	1.562540
17	1	-1.509735	2.145462	0.415663
18	6	-4.037776	3.386863	-0.518254
19	6	-4.868714	0.801566	-2.300749
20	1	-5.369645	1.757262	-2.483914
21	1	-5.640385	0.059241	-2.054400
22	1	-4.403506	0.480025	-3.242837
23	1	-4.807755	3.496738	-1.289220
24	1	-3.241490	4.112645	-0.739293
25	1	-4.483591	3.687797	0.441027
26	6	-3.275329	-1.619261	2.156057
27	6	-1.031911	-2.674703	2.445139
28	1	-3.867721	-0.704604	2.059084
29	1	-3.521427	-2.272379	1.312068
30	1	-1.267968	-3.376414	1.637406
31	1	0.049848	-2.539901	2.501734
32	6	-0.231326	-0.864611	-3.329375
33	6	2.666675	0.222502	-2.641942
34	6	3.941586	-1.718228	-0.411046
35	6	1.801379	-3.908036	0.322149
36	6	-0.790319	-3.433490	-1.531270
37	1	-0.031243	-1.439476	-4.245663
38	1	-0.045665	0.191280	-3.547020
39	1	-1.294323	-0.967159	-3.093689
40	1	3.050151	-0.126168	-3.611473
41	1	3.516773	0.608098	-2.070956
42	1	1.987082	1.058289	-2.839210
43	1	4.560895	-2.477748	-0.909885
44	1	3.961969	-1.913316	0.664750
45	1	4.411065	-0.743995	-0.578877
46	1	2.442567	-4.651088	-0.173690
47	1	0.869686	-4.409273	0.599038
48	1	2.301848	-3.594575	1.243934
49	1	-0.578757	-4.211657	-2.279217
50	1	-1.686721	-2.898621	-1.856642
51	1	-1.026813	-3.937287	-0.589854
52	1	-1.367685	-3.119374	3.389843
53	1	-3.575720	-2.123547	3.082036
54	1	-0.122009	0.444536	-0.952189
55	6	-1.465573	-0.371789	3.396522
56	1	-1.791406	-0.825786	4.341220
57	1	-0.395469	-0.160160	3.457593
58	1	-2.005723	0.573209	3.273314
59	6	1.908944	4.519421	-0.896362
60	6	2.216366	3.719940	0.387324
61	1	2.412720	4.075717	-1.760831
62	1	0.832310	4.542850	-1.091291
63	1	2.264403	5.547755	-0.777340

64	6	1.473944	4.314897	1.604498
65	6	3.736288	3.648331	0.648950
66	1	1.668261	3.722074	2.503044
67	1	1.823999	5.337889	1.774678
68	1	0.394366	4.340560	1.426442
69	1	4.124104	4.659984	0.805133
70	1	3.946892	3.049173	1.539479
71	1	4.256905	3.204273	-0.205270
72	7	1.727887	2.356669	0.203751
73	6	1.349354	1.257335	0.140880

TSM6a-7a (E = -1199.2773702 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.998379	-0.222670	-0.139267
2	7	0.374776	-1.580727	-0.479768
3	6	-2.228050	1.302470	1.390394
4	6	-1.507525	0.299656	2.124672
5	6	-3.220765	0.655184	0.615453
6	17	-2.020965	-0.111387	-2.331681
7	6	-2.064849	-0.966358	1.794218
8	6	-3.108366	-0.745570	0.834686
9	6	1.658721	-1.320232	0.054443
10	6	0.284346	-2.834666	-1.347616
11	6	2.094286	-1.499392	1.322823
12	6	3.486635	-1.049206	1.463359
13	1	1.506729	-1.914174	2.131955
14	6	2.815320	-0.733868	-0.742119
15	6	3.928739	-0.589851	0.267670
16	1	3.115466	-1.387535	-1.569441
17	1	2.526763	0.217972	-1.202806
18	6	5.284442	-0.054379	-0.106331
19	6	4.232070	-1.136515	2.770548
20	1	5.255630	-0.758259	2.686821
21	1	4.285636	-2.175726	3.123099
22	1	3.722636	-0.558257	3.553722
23	1	5.962237	-0.025887	0.753333
24	1	5.218928	0.965993	-0.511227
25	1	5.759226	-0.671944	-0.882622
26	6	1.225707	-3.941106	-0.814921
27	6	-1.158924	-3.379785	-1.292777
28	1	2.280374	-3.658527	-0.885515
29	1	1.006987	-4.170408	0.233684
30	1	-1.420174	-3.667712	-0.268921
31	1	-1.878359	-2.644272	-1.659368
32	6	-0.528158	0.568083	3.240407
33	6	-2.071018	2.791044	1.571381
34	6	-4.263874	1.319108	-0.242099
35	6	-4.058677	-1.777103	0.280194
36	6	-1.759458	-2.269371	2.493599
37	1	-1.060914	0.674663	4.196826
38	1	0.038406	1.488275	3.069300
39	1	0.194181	-0.245280	3.350176
40	1	-2.702545	3.142492	2.399805
41	1	-2.364090	3.343254	0.673564
42	1	-1.038185	3.063559	1.809936
43	1	-5.222089	1.371657	0.294944
44	1	-4.423091	0.765790	-1.171750
45	1	-3.975948	2.339358	-0.512714
46	1	-5.029132	-1.711380	0.792662
47	1	-3.682690	-2.794601	0.416238
48	1	-4.235419	-1.622050	-0.789106
49	1	-2.387038	-2.372090	3.390916
50	1	-0.715091	-2.324255	2.813344
51	1	-1.955506	-3.134886	1.854956

52	1	-1.240279	-4.271277	-1.926154
53	1	1.077952	-4.851797	-1.407185
54	1	0.286382	0.639623	0.593960
55	6	0.648473	-2.499796	-2.814593
56	1	0.531435	-3.392251	-3.442561
57	1	-0.006036	-1.712637	-3.196314
58	1	1.686904	-2.164796	-2.899614
59	6	2.197790	3.470324	0.331807
60	6	1.356224	3.654255	-0.948264
61	1	1.575432	3.582839	1.225638
62	1	2.663549	2.480066	0.357675
63	1	2.987060	4.228778	0.363686
64	6	2.225637	3.498293	-2.215156
65	6	0.639933	5.020956	-0.951048
66	1	1.612484	3.586883	-3.116922
67	1	2.989450	4.282512	-2.230997
68	1	2.725470	2.524669	-2.228209
69	1	1.384257	5.823684	-0.938018
70	1	0.022098	5.130196	-1.847486
71	1	-0.000342	5.126897	-0.069652
72	7	0.324110	2.610172	-0.998616
73	6	-0.197015	1.606689	-0.660367

M7a (E = -1199.3003885 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.859885	-0.189267	-0.193568
2	7	0.556008	1.694385	-0.452361
3	6	1.402946	-2.146506	1.254793
4	6	1.358086	-0.969596	2.063916
5	6	2.452757	-1.996476	0.320154
6	17	1.463679	-0.660789	-2.398477
7	6	2.401756	-0.097437	1.637712
8	6	3.070464	-0.727334	0.548469
9	6	-0.709224	1.821273	0.126883
10	6	1.106183	2.837164	-1.268430
11	6	-0.996354	1.666019	1.451804
12	6	-2.440025	1.731786	1.684146
13	1	-0.257266	1.557192	2.231234
14	6	-2.032291	2.017634	-0.600182
15	6	-3.063730	1.951517	0.499559
16	1	-2.089137	2.974188	-1.131262
17	1	-2.168301	1.233525	-1.352848
18	6	-4.525248	2.170487	0.225852
19	6	-3.046062	1.612117	3.059199
20	1	-4.131821	1.744566	3.040670
21	1	-2.627202	2.365687	3.739693
22	1	-2.836507	0.628496	3.500359
23	1	-5.128347	2.101337	1.136527
24	1	-4.912672	1.432000	-0.489542
25	1	-4.700041	3.161326	-0.217251
26	6	0.844131	4.172531	-0.534187
27	6	2.628090	2.641390	-1.410434
28	1	-0.226469	4.374068	-0.423387
29	1	1.293024	4.157580	0.465412
30	1	3.110415	2.649516	-0.428168
31	1	2.855157	1.698784	-1.913349
32	6	0.514641	-0.823474	3.307053
33	6	0.590978	-3.396209	1.474159
34	6	2.929350	-3.046865	-0.647222
35	6	4.331386	-0.259650	-0.133351
36	6	2.834399	1.167909	2.338268
37	1	0.827941	-1.562985	4.057319
38	1	-0.551405	-0.988557	3.114917
39	1	0.626939	0.165201	3.760902

40	1	1.140603	-4.095248	2.121096
41	1	0.379650	-3.912063	0.532580
42	1	-0.365408	-3.182470	1.960375
43	1	3.657296	-3.711141	-0.158567
44	1	3.410212	-2.598588	-1.519868
45	1	2.102994	-3.664686	-1.011920
46	1	5.191374	-0.833078	0.241133
47	1	4.532950	0.797459	0.055587
48	1	4.281356	-0.405353	-1.216839
49	1	3.469739	0.924563	3.201907
50	1	1.985173	1.750844	2.707781
51	1	3.412618	1.818529	1.677385
52	1	3.050356	3.460247	-2.004073
53	1	1.287585	4.999563	-1.100264
54	1	-1.511985	-1.273670	1.009597
55	6	0.470958	2.861030	-2.680853
56	1	0.956377	3.632748	-3.290637
57	1	0.602658	1.892283	-3.169611
58	1	-0.597484	3.090469	-2.641492
59	6	-2.580445	-3.745713	-1.579546
60	6	-2.874682	-2.314754	-1.074883
61	1	-2.029992	-3.706176	-2.524726
62	1	-1.973534	-4.295665	-0.851003
63	1	-3.515744	-4.295819	-1.737405
64	6	-3.626495	-2.370344	0.269498
65	6	-3.721174	-1.562144	-2.124524
66	1	-3.821436	-1.365056	0.661381
67	1	-4.590341	-2.872808	0.129244
68	1	-3.065086	-2.931867	1.025725
69	1	-4.667402	-2.086231	-2.303615
70	1	-3.949897	-0.545832	-1.783271
71	1	-3.171560	-1.491816	-3.068392
72	7	-1.546300	-1.615198	-1.035002
73	6	-1.012619	-1.185703	0.027281

TSM7a-8a (E = -1199.300333 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.970218	-0.156976	-0.293146
2	7	0.662961	1.739566	-0.471228
3	6	1.489363	-2.163349	1.105405
4	6	1.353779	-1.022828	1.956546
5	6	2.588600	-1.942584	0.247141
6	17	1.794520	-0.486734	-2.473208
7	6	2.393678	-0.103182	1.634150
8	6	3.147463	-0.663902	0.563387
9	6	-0.632953	1.841947	0.043277
10	6	1.248751	2.926082	-1.197887
11	6	-0.999619	1.624758	1.339079
12	6	-2.455079	1.681615	1.486447
13	1	-0.310141	1.472422	2.155505
14	6	-1.910095	2.074408	-0.751862
15	6	-3.007007	1.955579	0.277955
16	1	-1.936510	3.055694	-1.238275
17	1	-1.995782	1.328512	-1.549023
18	6	-4.450089	2.187285	-0.073109
19	6	-3.142353	1.499306	2.815747
20	1	-4.226605	1.621259	2.735942
21	1	-2.775361	2.228556	3.550613
22	1	-2.947381	0.500684	3.229032
23	1	-5.106381	2.077592	0.795929
24	1	-4.792871	1.481969	-0.842875
25	1	-4.600691	3.197169	-0.480758
26	6	0.922219	4.224577	-0.424001
27	6	2.779384	2.757916	-1.252301

28	1	-0.155293	4.412657	-0.374983
29	1	1.304844	4.168705	0.601374
30	1	3.200577	2.734984	-0.242642
31	1	3.052065	1.839346	-1.775791
32	6	0.426043	-0.955548	3.144989
33	6	0.699594	-3.441897	1.217304
34	6	3.169314	-2.935632	-0.723816
35	6	4.441160	-0.141892	-0.007899
36	6	2.746287	1.140594	2.413459
37	1	0.695931	-1.733888	3.872354
38	1	-0.622803	-1.117370	2.871444
39	1	0.494929	0.006543	3.660338
40	1	1.230460	-4.159435	1.859499
41	1	0.554990	-3.916621	0.241782
42	1	-0.287469	-3.275943	1.658834
43	1	3.945238	-3.539338	-0.230281
44	1	3.621514	-2.435809	-1.583849
45	1	2.406529	-3.620271	-1.107262
46	1	5.284123	-0.726234	0.388157
47	1	4.613773	0.904563	0.254121
48	1	4.461590	-0.226112	-1.098896
49	1	3.369898	0.879448	3.280501
50	1	1.860734	1.661513	2.789760
51	1	3.308661	1.853541	1.805421
52	1	3.222699	3.606137	-1.786594
53	1	1.392632	5.079736	-0.922538
54	1	-1.469710	-1.405605	0.740328
55	6	0.704106	3.005547	-2.645809
56	1	1.209212	3.815517	-3.186164
57	1	0.889943	2.064148	-3.169099
58	1	-0.369811	3.210526	-2.664990
59	6	-2.112575	-3.496651	-2.296120
60	6	-2.551433	-2.161597	-1.652636
61	1	-1.449904	-3.307068	-3.146334
62	1	-1.573056	-4.116591	-1.570883
63	1	-2.987766	-4.055960	-2.647327
64	6	-3.460031	-2.427645	-0.436881
65	6	-3.297541	-1.305404	-2.698277
66	1	-3.749925	-1.492486	0.056785
67	1	-4.373679	-2.935529	-0.765879
68	1	-2.969394	-3.070540	0.303434
69	1	-4.179040	-1.839622	-3.071699
70	1	-3.631295	-0.357799	-2.260012
71	1	-2.637033	-1.081501	-3.541956
72	7	-1.281637	-1.425169	-1.332227
73	6	-0.887410	-1.156436	-0.163405

M8a (E = -1199.3125154 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.731591	-0.121609	-0.049552
2	7	-0.278580	1.918372	-0.203223
3	6	0.260212	1.446784	0.828076
4	7	0.801028	-1.102343	-0.772532
5	6	-2.275172	0.323673	1.882630
6	6	-1.313149	-0.682296	2.221476
7	6	-3.081839	-0.172432	0.843145
8	17	-1.902766	0.179526	-2.177260
9	6	-1.574726	-1.830859	1.416558
10	6	-2.642554	-1.506660	0.537455
11	6	-0.298999	3.292796	-0.797215
12	6	1.987884	-0.677623	-0.140140
13	6	0.993165	-2.054641	-1.946591
14	6	2.396846	-0.942967	1.125862
15	1	0.884391	1.969989	1.556695

16	6	3.664418	-0.264673	1.422417
17	1	1.872631	-1.576650	1.827449
18	6	3.039046	0.233881	-0.765896
19	6	4.060579	0.430404	0.328503
20	1	3.499075	-0.205648	-1.657286
21	1	2.587966	1.176932	-1.094359
22	6	5.303273	1.251741	0.119771
23	6	4.358591	-0.399713	2.753717
24	1	5.293996	0.167038	2.788668
25	1	4.594551	-1.451055	2.967875
26	1	3.718018	-0.042295	3.571500
27	1	5.928144	1.281752	1.018324
28	1	5.059485	2.288999	-0.151417
29	1	5.916560	0.847240	-0.698376
30	6	-1.776909	3.729391	-0.878927
31	6	0.516084	4.270187	0.068014
32	6	0.299613	3.181886	-2.215617
33	1	-0.251047	2.441468	-2.800865
34	1	1.352870	2.882477	-2.172720
35	1	1.563321	3.955603	0.146783
36	1	0.099930	4.351127	1.079088
37	1	-2.213051	3.818839	0.122171
38	1	-2.354421	3.000184	-1.452611
39	6	2.181909	-3.009933	-1.678273
40	6	-0.272572	-2.919851	-2.112541
41	6	1.231574	-1.259583	-3.253632
42	1	0.392256	-0.584552	-3.437634
43	1	2.152704	-0.671006	-3.205879
44	1	3.138793	-2.483165	-1.615220
45	1	2.034711	-3.558083	-0.741224
46	1	-0.439183	-3.530731	-1.220644
47	1	-1.151590	-2.301119	-2.297315
48	6	-0.402663	-0.630793	3.423245
49	6	-2.433102	1.637576	2.603881
50	6	-4.285555	0.492197	0.229834
51	6	-3.380478	-2.433275	-0.393699
52	6	-0.944947	-3.188880	1.616413
53	1	-0.993231	-0.706918	4.347918
54	1	0.168995	0.302085	3.475235
55	1	0.311041	-1.458975	3.423814
56	1	-3.040161	1.506024	3.511091
57	1	-2.930774	2.387459	1.981792
58	1	-1.468105	2.049525	2.919388
59	1	-5.209495	0.026422	0.602212
60	1	-4.274248	0.399332	-0.860324
61	1	-4.329637	1.557721	0.476018
62	1	-4.370500	-2.671951	0.020957
63	1	-2.848060	-3.375996	-0.543033
64	1	-3.530990	-1.970092	-1.374352
65	1	-1.273604	-3.619230	2.572968
66	1	0.148613	-3.147009	1.628224
67	1	-1.237523	-3.885489	0.826965
68	1	0.496010	5.266265	-0.386416
69	1	-1.845388	4.705752	-1.371565
70	1	0.239918	4.154242	-2.717401
71	1	-0.141906	-3.594657	-2.967092
72	1	2.250988	-3.736493	-2.496096
73	1	1.319647	-1.952124	-4.100258

TSM8a-9a (E = -1199.2971545 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	22	-0.571511	-0.362104	0.102567
2	7	-1.930066	0.982321	-0.393046
3	6	-2.104262	0.725379	0.866617
4	7	0.811368	1.067419	0.905166
5	6	-2.048710	-2.275000	0.470352
6	6	-1.330305	-1.996429	1.677425
7	6	-1.117493	-2.692870	-0.504524
8	17	0.198348	-0.264082	-2.221148
9	6	0.047967	-2.278377	1.446059
10	6	0.186703	-2.685365	0.089202
11	6	-2.727612	1.800728	-1.354335
12	6	0.175239	2.014428	1.598015
13	6	2.269442	1.268081	0.514031
14	6	-1.013407	1.765560	2.324270
15	1	-3.042374	0.761302	1.414567
16	6	-1.571212	3.052324	2.784992
17	1	-1.101900	0.880159	2.937857
18	6	0.363535	3.532098	1.552348
19	6	-0.813580	4.073914	2.333619
20	1	1.309660	3.874150	1.981457
21	1	0.355983	3.875361	0.512734
22	6	-0.984598	5.554458	2.536101
23	6	-2.809780	3.114603	3.640087
24	1	-3.056963	4.139070	3.934244
25	1	-2.679028	2.522584	4.556644
26	1	-3.679045	2.698975	3.112229
27	1	-1.861868	5.783896	3.149357
28	1	-1.102107	6.081563	1.577997
29	1	-0.105934	5.992346	3.032215
30	6	-3.268499	0.860986	-2.453875
31	6	-3.894106	2.495737	-0.624240
32	6	-1.783876	2.854263	-1.974742
33	1	-0.933552	2.360884	-2.451874
34	1	-1.409349	3.535210	-1.201986
35	1	-3.524528	3.137448	0.183747
36	1	-4.590348	1.763878	-0.197938
37	1	-3.949989	0.117537	-2.024289
38	1	-2.444168	0.339565	-2.946184
39	6	3.103375	1.704107	1.745830
40	6	2.834725	-0.092583	0.057451
41	6	2.419549	2.276976	-0.649450
42	1	1.775436	1.986154	-1.483806
43	1	2.176767	3.299080	-0.349101
44	1	2.847807	2.701422	2.108378
45	1	2.965341	0.993021	2.568277
46	1	2.763979	-0.826225	0.864207
47	1	2.309863	-0.466057	-0.822555
48	6	-1.950349	-1.739105	3.027288
49	6	-3.548709	-2.239623	0.322783
50	6	-1.428082	-3.198916	-1.888405
51	6	1.418187	-3.221328	-0.595106
52	6	1.106392	-2.300810	2.524595
53	1	-2.255902	-2.688822	3.490747
54	1	-2.842754	-1.108819	2.958750
55	1	-1.246421	-1.257086	3.713580
56	1	-3.991867	-3.178166	0.685490
57	1	-3.850632	-2.114629	-0.721297
58	1	-3.996695	-1.424279	0.900648
59	1	-1.445780	-4.298720	-1.892966
60	1	-0.677979	-2.865322	-2.610021
61	1	-2.403889	-2.849641	-2.239436
62	1	1.307001	-4.298551	-0.783217
63	1	2.317996	-3.083315	0.010209
64	1	1.580417	-2.730660	-1.561199

65	1	0.880071	-3.086839	3.258379
66	1	1.171083	-1.351540	3.068074
67	1	2.095890	-2.516297	2.113060
68	1	-4.452033	3.119802	-1.330905
69	1	-3.820738	1.442247	-3.201660
70	1	-2.322149	3.446636	-2.724428
71	1	3.893314	0.024771	-0.201189
72	1	4.165620	1.713553	1.476977
73	1	3.458970	2.273541	-0.998647

M9a (E = -1199.3296348 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.877953	-0.083393	-0.125737
2	7	-0.332591	-1.448272	-0.544534
3	6	-0.698890	-1.136659	0.764916
4	7	-0.760430	1.581490	-0.051058
5	6	2.446430	-1.338039	1.147355
6	6	1.875483	-0.370414	2.030455
7	6	3.215177	-0.638850	0.177091
8	17	1.431319	0.399340	-2.435857
9	6	2.312148	0.921390	1.608808
10	6	3.142349	0.755504	0.467161
11	6	-0.755333	-2.610690	-1.370752
12	6	-1.862499	1.083008	0.379546
13	6	-0.720303	2.942818	-0.743395
14	6	-1.869163	-0.224587	1.137806
15	1	-0.521242	-1.895763	1.530691
16	6	-3.327421	-0.669929	1.075960
17	1	-1.670069	0.042245	2.191831
18	6	-3.307318	1.532214	0.218560
19	6	-4.106950	0.294502	0.567256
20	1	-3.542548	2.342340	0.920497
21	1	-3.523469	1.916314	-0.780775
22	6	-5.600032	0.309263	0.377989
23	6	-3.754038	-1.987186	1.661904
24	1	-4.841407	-2.107303	1.657236
25	1	-3.408057	-2.073921	2.702033
26	1	-3.320150	-2.831564	1.114444
27	1	-6.066743	-0.629711	0.689029
28	1	-5.857981	0.478934	-0.677012
29	1	-6.062469	1.124089	0.953693
30	6	0.295213	-2.870143	-2.468619
31	6	-0.896023	-3.883038	-0.503089
32	6	-2.112779	-2.265320	-2.032580
33	1	-2.000287	-1.385106	-2.674212
34	1	-2.874100	-2.046081	-1.276907
35	1	-1.625557	-3.746660	0.300596
36	1	0.064726	-4.152325	-0.051945
37	1	1.267982	-3.109578	-2.024160
38	1	0.423185	-1.990903	-3.102148
39	6	-1.538670	4.012459	0.024888
40	6	0.745001	3.421429	-0.754087
41	6	-1.217951	2.803588	-2.200928
42	1	-0.605321	2.079697	-2.742571
43	1	-2.263156	2.484900	-2.250923
44	1	-2.615019	3.930154	-0.132910
45	1	-1.332831	3.964516	1.100787
46	1	1.103688	3.589042	0.264701
47	1	1.391932	2.701847	-1.255588
48	6	1.197145	-0.648451	3.348466
49	6	2.395515	-2.833827	1.335695
50	6	4.074973	-1.252874	-0.898244
51	6	3.921960	1.814065	-0.269986
52	6	2.069759	2.188326	2.395843

53	1	1.928087	-0.592872	4.169252
54	1	0.749685	-1.645759	3.375711
55	1	0.407866	0.079732	3.566156
56	1	3.174333	-3.156923	2.041860
57	1	2.563132	-3.367229	0.395341
58	1	1.432257	-3.162541	1.738037
59	1	5.115419	-1.338849	-0.551601
60	1	4.067275	-0.646085	-1.807712
61	1	3.732572	-2.256688	-1.168483
62	1	5.000134	1.672848	-0.110860
63	1	3.666843	2.821578	0.070548
64	1	3.736623	1.764093	-1.349009
65	1	2.514178	2.101640	3.397206
66	1	1.002642	2.400824	2.531675
67	1	2.525079	3.056753	1.912279
68	1	-1.228180	-4.721584	-1.126074
69	1	-0.018366	-3.718548	-3.088880
70	1	-2.463370	-3.103819	-2.647257
71	1	0.808325	4.371279	-1.296710
72	1	-1.235671	5.003565	-0.329005
73	1	-1.138894	3.775419	-2.702057

M10 (E = -1199.3110758 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	1.678618	-0.267901	-0.417038
2	7	0.180628	-1.312868	-0.256650
3	6	-0.325083	-0.054701	0.144625
4	7	-3.536840	-0.397071	-0.393256
5	6	2.494242	-0.300567	1.794391
6	6	2.363546	1.077252	1.431107
7	6	3.504211	-0.874877	0.972334
8	17	2.118716	0.009221	-2.689965
9	6	3.314534	1.348900	0.399432
10	6	4.010163	0.145447	0.110106
11	6	-0.420000	-2.671906	-0.278049
12	6	-2.794164	0.591727	-0.121792
13	6	-4.941518	-0.578059	0.085023
14	6	-1.372430	0.711481	-0.708740
15	1	-0.536529	0.060352	1.214745
16	6	-1.154239	2.218167	-0.683188
17	1	-1.346305	0.310532	-1.725913
18	6	-3.058751	1.874357	0.672407
19	6	-2.048800	2.842022	0.098883
20	1	-4.083768	2.235620	0.557408
21	1	-2.906408	1.714288	1.748911
22	6	-2.160029	4.307505	0.425244
23	6	-0.047553	2.842638	-1.483611
24	1	0.000196	3.927815	-1.351774
25	1	-0.177716	2.631237	-2.553232
26	1	0.931448	2.428706	-1.212140
27	1	-1.376060	4.903762	-0.050644
28	1	-2.096685	4.471189	1.510878
29	1	-3.131455	4.707917	0.101581
30	6	0.738785	-3.685130	-0.393694
31	6	-1.218160	-2.924485	1.018341
32	6	-1.339120	-2.800609	-1.515956
33	1	-0.768205	-2.601285	-2.429568
34	1	-2.172757	-2.096745	-1.450680
35	1	-2.036926	-2.205383	1.109501
36	1	-0.570311	-2.838788	1.898224
37	1	1.397827	-3.628436	0.479454
38	1	1.328537	-3.493995	-1.298287
39	6	-5.880737	0.342231	-0.731010
40	6	-5.293704	-2.050690	-0.230215

41	6	-5.117221	-0.348058	1.605502
42	1	-4.372989	-0.924251	2.167928
43	1	-5.024237	0.703737	1.886487
44	1	-5.688211	1.401236	-0.532326
45	1	-5.744317	0.164943	-1.803292
46	1	-5.160319	-2.250287	-1.298321
47	1	-4.638297	-2.729211	0.326714
48	6	1.532919	2.099745	2.166017
49	6	1.789014	-0.963686	2.951121
50	6	4.043177	-2.284238	1.050545
51	6	5.152674	0.003152	-0.862480
52	6	3.610765	2.687286	-0.231920
53	1	2.109741	2.534470	2.995178
54	1	0.628237	1.654405	2.589746
55	1	1.218657	2.919603	1.513544
56	1	2.280577	-0.701659	3.898714
57	1	1.801086	-2.053802	2.863414
58	1	0.743349	-0.648942	3.027118
59	1	5.025743	-2.285879	1.542493
60	1	4.178036	-2.734055	0.059971
61	1	3.385839	-2.939445	1.628331
62	1	6.092528	0.338539	-0.400646
63	1	4.988749	0.600218	-1.764402
64	1	5.291233	-1.036309	-1.175611
65	1	4.569444	3.077702	0.137279
66	1	2.842297	3.428150	0.006241
67	1	3.684545	2.614345	-1.322785
68	1	-1.645839	-3.933903	1.003427
69	1	0.345002	-4.705770	-0.458126
70	1	-1.743942	-3.819127	-1.573593
71	1	-6.332968	-2.268457	0.042287
72	1	-6.926434	0.132740	-0.477213
73	1	-6.111787	-0.688582	1.916029

TSM10-11 (E = -1199.2861808 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	1.012038	-0.047417	-0.214004
2	7	0.282992	-0.888331	1.345036
3	6	-0.323343	0.337992	1.493305
4	7	-2.471663	-1.110521	-0.130661
5	6	3.261432	0.349082	0.339291
6	6	2.579211	1.590629	0.513625
7	6	3.246620	0.039664	-1.054324
8	17	0.584848	-1.611796	-1.908556
9	6	2.143983	2.040370	-0.772920
10	6	2.561550	1.081740	-1.736872
11	6	0.415834	-1.874309	2.443671
12	6	-2.218534	0.105093	-0.334716
13	6	-3.547289	-1.886054	-0.819538
14	6	-1.131102	0.871284	0.440231
15	1	-0.092419	0.976958	2.346818
16	6	-1.691701	2.267736	0.528538
17	1	-0.263949	1.010561	-0.766901
18	6	-2.910235	1.177867	-1.177705
19	6	-2.665352	2.439657	-0.383647
20	1	-2.456100	1.235588	-2.177185
21	1	-3.973354	0.986225	-1.321906
22	6	-3.488718	3.665931	-0.663038
23	6	-1.244911	3.257455	1.571128
24	1	-1.706846	4.236506	1.417045
25	1	-0.159670	3.393427	1.572805
26	1	-1.523924	2.914406	2.576822
27	1	-3.194407	4.522047	-0.049750
28	1	-4.554839	3.470054	-0.480848

29	1	-3.397182	3.958057	-1.718727
30	6	1.293136	-3.028542	1.924668
31	6	1.049756	-1.235044	3.702593
32	6	-0.992104	-2.407812	2.798809
33	1	-1.463019	-2.844834	1.916601
34	1	-1.633223	-1.592531	3.152926
35	1	0.427548	-0.422097	4.094381
36	1	2.045974	-0.839474	3.484557
37	1	2.299890	-2.674941	1.679513
38	1	0.851542	-3.461268	1.021680
39	6	-3.522332	-1.713965	-2.357752
40	6	-3.254617	-3.368586	-0.492193
41	6	-4.925137	-1.506355	-0.226661
42	1	-4.914320	-1.624113	0.862661
43	1	-5.200932	-0.472206	-0.456447
44	1	-3.859962	-0.724571	-2.677334
45	1	-2.507493	-1.874845	-2.736600
46	1	-2.260770	-3.644616	-0.858595
47	1	-3.278707	-3.530960	0.590250
48	6	2.586124	2.387842	1.796770
49	6	4.113565	-0.340536	1.376706
50	6	3.951087	-1.126238	-1.699718
51	6	2.353354	1.170395	-3.226315
52	6	1.519458	3.376047	-1.097895
53	1	3.595542	2.779533	1.987935
54	1	2.301042	1.785407	2.665884
55	1	1.911781	3.246485	1.748908
56	1	5.145337	0.038824	1.328261
57	1	4.158743	-1.422898	1.222019
58	1	3.747318	-0.161677	2.391031
59	1	4.991125	-0.856492	-1.934856
60	1	3.459035	-1.427918	-2.627553
61	1	3.976455	-2.001030	-1.042091
62	1	3.245928	1.581029	-3.719886
63	1	1.508171	1.819620	-3.476274
64	1	2.151844	0.185023	-3.657056
65	1	2.292982	4.085705	-1.424438
66	1	1.015039	3.816430	-0.234767
67	1	0.783669	3.296087	-1.904251
68	1	1.146157	-1.989021	4.492156
69	1	1.380028	-3.812429	2.685477
70	1	-0.918954	-3.164662	3.588968
71	1	-3.999229	-4.022699	-0.960778
72	1	-4.184320	-2.455640	-2.819506
73	1	-5.701116	-2.163618	-0.635856

M11 (E = -1199.2996804 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.956665	-0.145739	-0.335736
2	7	0.305045	-0.840555	1.340430
3	6	-0.367874	0.310566	1.712215
4	7	-2.495126	-0.975276	-0.107958
5	6	3.142040	0.519042	0.314242
6	6	2.381133	1.698901	0.071483
7	6	3.283246	-0.165111	-0.927624
8	17	0.640357	-1.944948	-1.764272
9	6	2.081942	1.760101	-1.325927
10	6	2.643381	0.609662	-1.939087
11	6	0.539516	-1.921180	2.345124
12	6	-2.301703	0.273718	-0.032886
13	6	-3.458317	-1.638334	-1.033641
14	6	-1.391899	0.884554	1.000938
15	1	-0.004213	0.854191	2.587358
16	6	-1.892373	2.249634	1.231638

17	1	-0.077925	0.847343	-1.195554
18	6	-2.997905	1.460413	-0.705557
19	6	-2.787269	2.587068	0.275487
20	1	-2.522862	1.683900	-1.669934
21	1	-4.056187	1.280892	-0.901677
22	6	-3.529664	3.880156	0.097964
23	6	-1.460229	3.088070	2.407415
24	1	-1.956691	4.062150	2.412686
25	1	-0.378432	3.262656	2.408719
26	1	-1.705831	2.583455	3.351605
27	1	-3.272682	4.624195	0.856992
28	1	-4.615569	3.713865	0.139953
29	1	-3.316682	4.314332	-0.889398
30	6	1.509704	-2.948615	1.733508
31	6	1.115945	-1.369642	3.671523
32	6	-0.821714	-2.604685	2.624363
33	1	-1.250643	-2.985356	1.694725
34	1	-1.532098	-1.889296	3.053665
35	1	0.418454	-0.680957	4.161343
36	1	2.064451	-0.850420	3.507513
37	1	2.490839	-2.502201	1.541203
38	1	1.115768	-3.331773	0.788258
39	6	-3.335789	-1.149233	-2.497153
40	6	-3.094274	-3.140867	-0.986849
41	6	-4.899603	-1.458337	-0.497561
42	1	-4.961833	-1.799063	0.542001
43	1	-5.225760	-0.414039	-0.536567
44	1	-3.709041	-0.130699	-2.633819
45	1	-2.289712	-1.186065	-2.818247
46	1	-2.062968	-3.286244	-1.322060
47	1	-3.177800	-3.516237	0.038726
48	6	2.142794	2.814419	1.058383
49	6	3.883389	0.202062	1.588600
50	6	4.086148	-1.419148	-1.161072
51	6	2.615438	0.291308	-3.410393
52	6	1.457300	2.931847	-2.041104
53	1	2.988459	3.517583	1.045581
54	1	2.041659	2.444297	2.083238
55	1	1.241660	3.383372	0.812702
56	1	4.890725	0.642133	1.550935
57	1	4.004627	-0.873343	1.745313
58	1	3.380000	0.615422	2.466935
59	1	5.107812	-1.162385	-1.476194
60	1	3.638497	-2.041582	-1.940785
61	1	4.163369	-2.027566	-0.254706
62	1	3.485925	0.733001	-3.916701
63	1	1.714200	0.686008	-3.890119
64	1	2.633060	-0.787635	-3.585210
65	1	2.226935	3.672423	-2.303058
66	1	0.708368	3.432226	-1.420252
67	1	0.964706	2.619830	-2.966441
68	1	1.296847	-2.200814	4.362468
69	1	1.648455	-3.788282	2.423779
70	1	-0.688905	-3.432100	3.331995
71	1	-3.764939	-3.722811	-1.630194
72	1	-3.919051	-1.807016	-3.152153
73	1	-5.597295	-2.054404	-1.097286

TSM11-19 (E = -1199.2913712 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	22	0.782641	-0.103788	-0.235918
2	7	0.448253	-1.233202	1.340639
3	6	-0.376696	-0.529330	2.179622
4	7	-1.589888	0.088096	-0.560817
5	6	3.057831	0.414196	0.477412
6	6	2.329771	1.626373	0.318631
7	6	3.175478	-0.194856	-0.797523
8	17	0.640779	-1.933877	-1.870823
9	6	2.077342	1.815574	-1.081060
10	6	2.574073	0.688067	-1.761952
11	6	0.827588	-2.614159	1.845757
12	6	-2.180777	0.301446	0.570256
13	6	-2.305231	0.120736	-1.901287
14	6	-1.501286	0.189812	1.864780
15	1	-0.155789	-0.596289	3.242660
16	6	-2.367887	0.786940	2.897041
17	1	0.082550	1.349367	0.087479
18	6	-3.600205	0.782764	0.894841
19	6	-3.568688	1.095053	2.369020
20	1	-3.874973	1.668195	0.324236
21	1	-4.345844	0.011676	0.662946
22	6	-4.788671	1.657061	3.042467
23	6	-1.936910	0.937371	4.332562
24	1	-2.681500	1.480439	4.921069
25	1	-0.986541	1.482284	4.403465
26	1	-1.786560	-0.040118	4.811231
27	1	-4.615143	1.879821	4.099307
28	1	-5.631000	0.952315	2.983308
29	1	-5.117706	2.584214	2.551430
30	6	2.063670	-3.148121	1.104602
31	6	1.122924	-2.639919	3.367947
32	6	-0.383485	-3.530728	1.537400
33	1	-0.564364	-3.559442	0.459302
34	1	-1.287160	-3.159437	2.034470
35	1	0.228003	-2.483517	3.978811
36	1	1.873968	-1.890138	3.641395
37	1	2.961694	-2.595698	1.387075
38	1	1.927496	-3.085822	0.024767
39	6	-3.521393	1.078995	-2.020709
40	6	-1.290186	0.606035	-2.962116
41	6	-2.776818	-1.322082	-2.201061
42	1	-1.932752	-2.012743	-2.183353
43	1	-3.515438	-1.644506	-1.456845
44	1	-4.405927	0.724845	-1.489145
45	1	-3.274575	2.093400	-1.689158
46	1	-0.994002	1.640434	-2.753016
47	1	-0.405531	-0.028096	-2.989727
48	6	2.098007	2.647928	1.402844
49	6	3.725235	0.003137	1.767015
50	6	4.001589	-1.394373	-1.180305
51	6	2.633163	0.478583	-3.252315
52	6	1.478850	3.057691	-1.690000
53	1	2.983906	3.289262	1.524161
54	1	1.900958	2.172222	2.369444
55	1	1.244549	3.291764	1.170721
56	1	4.457805	0.766472	2.063923
57	1	4.263256	-0.942098	1.662988
58	1	3.012677	-0.104023	2.591719
59	1	4.850436	-1.082224	-1.805097
60	1	3.410555	-2.114611	-1.756381
61	1	4.407001	-1.909876	-0.306013
62	1	3.651208	0.671167	-3.621128
63	1	1.955837	1.151913	-3.786447
64	1	2.366521	-0.548947	-3.516946

65	1	2.229738	3.859456	-1.735352
66	1	0.632542	3.427469	-1.101402
67	1	1.126098	2.880872	-2.710261
68	1	1.522164	-3.626346	3.627114
69	1	2.216658	-4.199135	1.376210
70	1	-0.187050	-4.549738	1.892348
71	1	-1.757006	0.579898	-3.953313
72	1	-3.788435	1.137397	-3.081530
73	1	-3.248211	-1.359113	-3.190759

M19 (E = -1199.2976994 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.815172	-0.151827	-0.030131
2	7	0.042226	1.790954	-0.364902
3	6	1.330527	1.863126	-0.079688
4	7	0.988831	-1.179562	-0.496395
5	6	-2.362942	0.481897	1.710036
6	6	-1.457750	-0.512486	2.205823
7	6	-3.162775	-0.115097	0.701131
8	17	-1.619321	-0.047673	-2.371539
9	6	-1.718772	-1.727502	1.500700
10	6	-2.758966	-1.473994	0.558237
11	6	2.097856	-0.559598	-0.070718
12	6	2.227722	0.825695	0.223561
13	1	1.799166	2.842456	-0.128971
14	6	3.608179	1.101108	0.677413
15	1	0.190329	0.194725	1.201368
16	6	3.480584	-1.170206	0.173437
17	6	4.334252	-0.033197	0.666001
18	1	3.412736	-1.973464	0.913175
19	1	3.910198	-1.613583	-0.729284
20	6	5.773497	-0.259263	1.038173
21	6	4.073114	2.477294	1.080126
22	1	5.087712	2.453830	1.488163
23	1	3.412016	2.911325	1.842117
24	1	4.079255	3.168098	0.225486
25	1	6.251570	0.654197	1.405399
26	1	6.357361	-0.615317	0.176512
27	1	5.868048	-1.024412	1.822485
28	6	-0.661378	-0.403077	3.482822
29	6	-2.533403	1.837410	2.352367
30	6	-4.323949	0.492957	-0.040781
31	6	-3.467055	-2.462463	-0.332358
32	6	-1.150999	-3.065035	1.914816
33	1	-1.287670	-0.687189	4.341889
34	1	-0.304342	0.617456	3.647875
35	1	0.211158	-1.062766	3.470658
36	1	-2.828598	1.716141	3.403778
37	1	-3.314115	2.424216	1.861770
38	1	-1.607961	2.423500	2.338458
39	1	-5.258566	-0.002869	0.256944
40	1	-4.210594	0.368957	-1.123010
41	1	-4.432350	1.559818	0.169134
42	1	-4.512002	-2.575752	-0.011485
43	1	-3.003235	-3.451439	-0.299580
44	1	-3.473430	-2.124299	-1.374415
45	1	-1.506400	-3.320857	2.922973
46	1	-0.056623	-3.062144	1.945598
47	1	-1.467795	-3.870091	1.246992
48	6	-0.518306	3.081286	-0.969139
49	6	-0.127243	4.318778	-0.114957
50	6	0.040252	3.223758	-2.405306
51	6	-2.055004	3.037972	-1.024409
52	1	-0.398776	4.166533	0.935687

53	1	0.937821	4.564392	-0.166089
54	1	1.134150	3.295174	-2.396890
55	1	-0.247254	2.357011	-3.006115
56	1	-2.407441	2.178421	-1.592680
57	1	-2.480555	3.009504	-0.019492
58	6	1.131587	-2.466002	-1.312957
59	6	-0.263013	-3.062863	-1.591233
60	6	1.774051	-2.096766	-2.672630
61	6	1.937857	-3.589354	-0.596963
62	1	-0.724975	-3.418334	-0.669002
63	1	-0.922746	-2.345909	-2.077068
64	1	1.138567	-1.377081	-3.197321
65	1	2.767696	-1.654276	-2.550875
66	1	3.018390	-3.471089	-0.676806
67	1	1.667094	-3.653253	0.462262
68	1	1.685368	-4.548391	-1.062631
69	1	1.875760	-2.993958	-3.294847
70	1	-0.149466	-3.925114	-2.258060
71	1	-0.675214	5.191661	-0.485979
72	1	-2.418649	3.948405	-1.514753
73	1	-0.358332	4.130369	-2.876258

TSM19-20 (E = -1199.2660566 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	1.341330	-0.179089	-0.633995
2	7	0.454886	-0.755579	0.893712
3	6	-0.188815	0.537262	1.114323
4	7	-2.473195	-0.626100	-0.526082
5	6	3.127277	1.010622	0.286664
6	6	2.576103	1.845643	-0.736638
7	6	3.680494	-0.143354	-0.339662
8	17	0.694198	-1.427548	-2.468713
9	6	2.826393	1.217644	-1.994389
10	6	3.507081	-0.001500	-1.751926
11	6	0.335900	-1.842471	1.909866
12	6	-2.661477	0.266432	0.371244
13	6	-3.510934	-1.135527	-1.461918
14	6	-1.568905	0.815495	1.184417
15	1	0.384282	1.178484	1.786023
16	6	-2.097237	1.933026	1.961571
17	1	0.247867	1.108608	-0.176054
18	6	-3.926026	1.041210	0.779032
19	6	-3.432732	2.073521	1.756285
20	1	-4.415553	1.498552	-0.087816
21	1	-4.668316	0.382000	1.242463
22	6	-4.391521	3.048863	2.376542
23	6	-1.245387	2.780424	2.874758
24	1	-1.844117	3.521511	3.411068
25	1	-0.474653	3.324607	2.312338
26	1	-0.727676	2.164307	3.622122
27	1	-3.906094	3.723121	3.088346
28	1	-5.198213	2.522371	2.908537
29	1	-4.876999	3.667596	1.607189
30	6	1.168779	-3.028577	1.381825
31	6	0.892687	-1.368299	3.273404
32	6	-1.132321	-2.293257	2.078698
33	1	-1.550468	-2.589565	1.114828
34	1	-1.750098	-1.488004	2.486127
35	1	0.328285	-0.509248	3.653328
36	1	1.946664	-1.083997	3.188222
37	1	2.221396	-2.747572	1.270831
38	1	0.789157	-3.356778	0.408688
39	6	-3.614373	-0.143746	-2.647973
40	6	-2.970641	-2.489814	-1.979970

41	6	-4.911361	-1.383137	-0.842752
42	1	-4.825794	-1.931646	0.102937
43	1	-5.467637	-0.459608	-0.664372
44	1	-3.980375	0.834675	-2.315413
45	1	-2.631139	-0.007393	-3.109439
46	1	-1.962970	-2.361845	-2.382134
47	1	-2.921030	-3.217250	-1.160594
48	6	2.040124	3.243157	-0.541117
49	6	3.278886	1.391906	1.738661
50	6	4.485136	-1.227922	0.334920
51	6	4.035543	-0.942334	-2.802225
52	6	2.443157	1.759919	-3.347788
53	1	2.855005	3.977604	-0.617003
54	1	1.576401	3.367601	0.442438
55	1	1.290669	3.500142	-1.295997
56	1	4.181719	2.004169	1.875517
57	1	3.375588	0.514025	2.382903
58	1	2.432144	1.981976	2.104115
59	1	5.558475	-0.995712	0.278647
60	1	4.337525	-2.203362	-0.140240
61	1	4.226437	-1.328161	1.393116
62	1	5.034787	-0.621087	-3.129669
63	1	3.384546	-0.971587	-3.679979
64	1	4.122730	-1.965322	-2.423940
65	1	3.274102	2.327830	-3.789855
66	1	1.582130	2.433109	-3.283328
67	1	2.183078	0.954134	-4.041116
68	1	0.812945	-2.175663	4.010403
69	1	1.111316	-3.871038	2.080391
70	1	-1.172488	-3.142486	2.771467
71	1	-3.625910	-2.894071	-2.761072
72	1	-4.305951	-0.529618	-3.406539
73	1	-5.504625	-1.995290	-1.532091

M20 (E = -1199.3258323 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.605295	-0.419064	-0.322981
2	7	0.528819	-0.331454	1.529893
3	6	-0.041755	1.039606	1.539741
4	7	-1.382492	-0.052472	-0.695977
5	6	2.850225	0.514306	-0.266122
6	6	2.053787	1.399598	-1.055820
7	6	2.968468	-0.704442	-0.976812
8	17	0.459121	-2.765581	-0.548224
9	6	1.754149	0.747050	-2.294322
10	6	2.299136	-0.553536	-2.238974
11	6	0.633050	-1.097927	2.810159
12	6	-2.108154	0.503579	0.348954
13	6	-2.147511	-0.399258	-1.964977
14	6	-1.520543	1.068550	1.452409
15	1	0.392481	1.650825	2.332916
16	6	-2.522620	1.598057	2.378986
17	1	0.319554	1.524520	0.602566
18	6	-3.615714	0.579843	0.587513
19	6	-3.756829	1.336648	1.887369
20	1	-4.182386	1.053048	-0.217071
21	1	-4.025436	-0.428671	0.706633
22	6	-5.108656	1.679152	2.450370
23	6	-2.174468	2.336805	3.646581
24	1	-3.063901	2.764118	4.119312
25	1	-1.475602	3.160513	3.446723
26	1	-1.694896	1.677633	4.382222
27	1	-5.029032	2.227211	3.395050
28	1	-5.706473	0.776091	2.643264

29	1	-5.690730	2.301056	1.754084
30	6	1.738035	-2.166600	2.665411
31	6	1.006269	-0.177784	3.997685
32	6	-0.721872	-1.797060	3.090827
33	1	-0.971302	-2.471007	2.266232
34	1	-1.528397	-1.065037	3.196557
35	1	0.213807	0.538479	4.233332
36	1	1.931339	0.373503	3.793449
37	1	2.717349	-1.696691	2.528670
38	1	1.540384	-2.821091	1.815385
39	6	-2.705935	0.890747	-2.620222
40	6	-1.205222	-1.066812	-2.988517
41	6	-3.282206	-1.428864	-1.699454
42	1	-2.924178	-2.218378	-1.030653
43	1	-4.181812	-0.982440	-1.275307
44	1	-3.363439	1.451972	-1.953338
45	1	-1.884131	1.551261	-2.914973
46	1	-0.325771	-0.455755	-3.177328
47	1	-0.882251	-2.051701	-2.649463
48	6	1.852772	2.877856	-0.810298
49	6	3.567861	0.893998	1.004823
50	6	3.802540	-1.901586	-0.601288
51	6	2.318066	-1.595647	-3.325791
52	6	1.192555	1.469809	-3.495216
53	1	2.590046	3.457252	-1.385633
54	1	1.985919	3.141855	0.243437
55	1	0.858885	3.218795	-1.122026
56	1	4.477832	1.464535	0.769611
57	1	3.869477	0.013467	1.577463
58	1	2.949927	1.517256	1.658880
59	1	4.724330	-1.926481	-1.200566
60	1	3.260270	-2.835479	-0.780350
61	1	4.093511	-1.881068	0.452640
62	1	3.348602	-1.781525	-3.658885
63	1	1.738081	-1.286632	-4.200142
64	1	1.909697	-2.547706	-2.967016
65	1	1.912044	2.226932	-3.838837
66	1	0.256724	1.993035	-3.271717
67	1	1.007936	0.794851	-4.335322
68	1	1.168981	-0.793210	4.889050
69	1	1.776216	-2.775046	3.576407
70	1	-0.657599	-2.381264	4.017329
71	1	-1.740715	-1.184832	-3.937527
72	1	-3.277130	0.633039	-3.520235
73	1	-3.569280	-1.894425	-2.649334

TSM20-21 (E = -1199.3008203 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.383353	-0.202641	-0.108014
2	7	0.407286	-0.337662	1.626035
3	6	-0.361095	1.584527	1.553017
4	7	-1.771197	0.330612	-0.553765
5	6	2.689288	0.522083	-0.155218
6	6	1.960130	1.527548	-0.854076
7	6	2.639556	-0.661558	-0.932203
8	17	0.012853	-2.537991	-0.494942
9	6	1.531955	0.982337	-2.108581
10	6	1.943332	-0.365111	-2.155108
11	6	0.479308	-0.952777	2.958834
12	6	-2.413037	0.994363	0.398026
13	6	-2.564120	-0.196611	-1.747883
14	6	-1.746262	1.545868	1.527438
15	1	0.187260	1.980297	2.395066
16	6	-2.725912	1.924127	2.549121

17	1	0.113058	1.839962	0.603387
18	6	-3.904702	1.232591	0.639130
19	6	-3.973409	1.749713	2.058982
20	1	-4.290994	1.995883	-0.044210
21	1	-4.513044	0.339182	0.487625
22	6	-5.300022	2.063349	2.691550
23	6	-2.328866	2.493449	3.885445
24	1	-3.200024	2.803856	4.469249
25	1	-1.678695	3.370187	3.758740
26	1	-1.771131	1.761876	4.484134
27	1	-5.188235	2.462364	3.704467
28	1	-5.931809	1.165594	2.755742
29	1	-5.860336	2.802845	2.100311
30	6	1.407362	-2.191477	2.855048
31	6	1.053678	0.008658	4.028860
32	6	-0.941536	-1.419504	3.368847
33	1	-1.323556	-2.135141	2.634719
34	1	-1.634165	-0.574228	3.418822
35	1	0.381244	0.850413	4.220780
36	1	2.027618	0.399734	3.717989
37	1	2.433901	-1.888315	2.625202
38	1	1.058264	-2.864502	2.068959
39	6	-3.533562	0.858366	-2.347759
40	6	-1.584186	-0.570555	-2.876345
41	6	-3.329113	-1.476913	-1.328373
42	1	-2.625656	-2.236583	-0.979765
43	1	-4.054220	-1.285014	-0.533294
44	1	-4.467652	0.954394	-1.793044
45	1	-3.052348	1.841904	-2.404854
46	1	-1.094049	0.319529	-3.272694
47	1	-0.834555	-1.283504	-2.536957
48	6	1.931990	3.001442	-0.517235
49	6	3.511404	0.746538	1.088236
50	6	3.379384	-1.947336	-0.664826
51	6	1.822252	-1.332110	-3.302663
52	6	0.953703	1.820841	-3.223078
53	1	2.734066	3.525985	-1.057321
54	1	2.090269	3.183494	0.550526
55	1	0.987012	3.477545	-0.804842
56	1	4.501848	1.142918	0.820911
57	1	3.666124	-0.181120	1.645191
58	1	3.041012	1.465410	1.766173
59	1	4.307392	-1.983932	-1.254623
60	1	2.772794	-2.817556	-0.931959
61	1	3.652909	-2.045612	0.389817
62	1	2.816321	-1.574370	-3.704066
63	1	1.223659	-0.923069	-4.121713
64	1	1.360239	-2.272737	-2.979768
65	1	1.676004	2.593650	-3.522433
66	1	0.032539	2.338602	-2.929318
67	1	0.733912	1.221141	-4.110394
68	1	1.187091	-0.531321	4.973433
69	1	1.411857	-2.728092	3.811702
70	1	-0.910617	-1.904646	4.352427
71	1	-2.145634	-1.038752	-3.692959
72	1	-3.796653	0.555005	-3.366959
73	1	-3.875121	-1.873970	-2.192638

M21 (E = -1199.3179596 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	22	1.003076	-0.080074	-0.239777
2	7	0.209958	-1.493708	-0.687211
3	6	-1.503424	-0.757126	2.066858
4	7	-1.074873	1.436162	0.035400
5	6	2.894227	-1.160479	0.734446
6	6	2.109392	-0.657360	1.813783
7	6	3.474796	-0.051726	0.065153
8	17	1.580382	0.670945	-2.428202
9	6	2.224856	0.770407	1.813641
10	6	3.067961	1.140857	0.734434
11	6	-0.312854	-2.706370	-1.302039
12	6	-2.210238	0.921327	0.349741
13	6	-1.019045	2.822006	-0.613586
14	6	-2.390047	-0.306884	1.173194
15	1	-1.693981	-1.630274	2.678097
16	6	-3.752649	-0.807772	0.940823
17	1	-0.563058	-0.249500	2.211815
18	6	-3.629958	1.328357	-0.057586
19	6	-4.455175	0.094510	0.227010
20	1	-3.992723	2.156283	0.560740
21	1	-3.695752	1.653102	-1.096593
22	6	-5.885883	0.037297	-0.222868
23	6	-4.228662	-2.114610	1.513194
24	1	-5.255108	-2.341877	1.213585
25	1	-4.195836	-2.094121	2.611148
26	1	-3.588245	-2.943356	1.186820
27	1	-6.373549	-0.900231	0.057477
28	1	-5.952907	0.141309	-1.314953
29	1	-6.465968	0.864866	0.209904
30	6	0.716173	-3.242618	-2.329601
31	6	-0.593875	-3.781660	-0.223997
32	6	-1.627561	-2.347606	-2.043124
33	1	-1.428610	-1.584010	-2.802052
34	1	-2.371294	-1.955562	-1.341754
35	1	-1.301611	-3.399896	0.518780
36	1	0.330420	-4.060575	0.292858
37	1	1.647146	-3.527172	-1.829906
38	1	0.943208	-2.470017	-3.070149
39	6	-1.973833	3.840472	0.065834
40	6	0.411169	3.349069	-0.393855
41	6	-1.307421	2.729654	-2.130000
42	1	-0.611205	2.041943	-2.613711
43	1	-2.329237	2.398744	-2.335998
44	1	-3.007513	3.760028	-0.273283
45	1	-1.947093	3.738359	1.157083
46	1	0.623592	3.440011	0.675607
47	1	1.150653	2.696778	-0.857647
48	6	1.582734	-1.513765	2.943601
49	6	3.246638	-2.610551	0.519028
50	6	4.492963	-0.116609	-1.043468
51	6	3.598084	2.512892	0.400348
52	6	1.680566	1.686396	2.885672
53	1	2.423476	-1.935827	3.513603
54	1	0.976989	-2.352218	2.583885
55	1	0.975967	-0.936886	3.648334
56	1	4.105049	-2.891915	1.147750
57	1	3.520968	-2.811577	-0.520791
58	1	2.414860	-3.271156	0.779002
59	1	5.510123	-0.097778	-0.623782
60	1	4.393227	0.727260	-1.731262
61	1	4.391907	-1.032168	-1.633786
62	1	4.665219	2.581313	0.655869
63	1	3.079064	3.301339	0.952603
64	1	3.507374	2.734234	-0.669698

65	1	2.278096	1.599426	3.804633
66	1	0.642838	1.454971	3.152213
67	1	1.712873	2.734810	2.575398
68	1	-1.017960	-4.684283	-0.681645
69	1	0.315619	-4.124268	-2.845907
70	1	-2.044676	-3.234691	-2.536545
71	1	0.510338	4.340464	-0.849494
72	1	-1.634814	4.851524	-0.182743
73	1	-1.181220	3.722344	-2.578117

M15 (E = -675.8581344 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.554670	-0.165500	-0.476379
2	7	-0.928568	1.471232	-0.303342
3	6	-2.020948	-1.137328	1.061152
4	6	-0.752852	-0.998552	1.698523
5	6	-1.877692	-2.099094	0.012451
6	17	0.361515	-0.583409	-2.581625
7	6	0.163567	-1.886223	1.047074
8	6	-0.535188	-2.580347	0.020732
9	6	-1.292278	2.874421	-0.175032
10	6	-2.670487	3.091851	-0.849255
11	6	-1.364580	3.272713	1.318790
12	6	-0.215168	3.724739	-0.895131
13	1	-0.146700	3.435605	-1.948590
14	1	0.765218	3.570927	-0.430865
15	1	-0.401025	3.095302	1.808767
16	1	-2.132017	2.688045	1.837353
17	1	-3.438522	2.486971	-0.354503
18	1	-2.625366	2.803696	-1.904778
19	6	-0.469994	-0.204367	2.951381
20	6	-3.318511	-0.513725	1.515038
21	6	-2.976432	-2.590490	-0.899490
22	6	0.017038	-3.659183	-0.873906
23	6	1.609134	-2.094335	1.434062
24	1	-0.619294	-0.830291	3.842724
25	1	-1.131827	0.661272	3.036753
26	1	0.560801	0.164254	2.980051
27	1	-3.829919	-1.172869	2.230938
28	1	-4.004029	-0.342577	0.678761
29	1	-3.152022	0.447973	2.007953
30	1	-3.457802	-3.482204	-0.473426
31	1	-2.590071	-2.865857	-1.886164
32	1	-3.757349	-1.836268	-1.041760
33	1	-0.296899	-4.651449	-0.520792
34	1	1.110552	-3.644285	-0.893459
35	1	-0.327892	-3.545000	-1.906433
36	1	1.696552	-2.903130	2.173042
37	1	2.043450	-1.196242	1.886127
38	1	2.226956	-2.369218	0.573043
39	1	-1.614771	4.335664	1.420697
40	1	-2.965841	4.146286	-0.787358
41	1	-0.465123	4.791165	-0.836545

M16 (E = -523.4592199 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	2.075137	-1.274408	-0.526310
2	6	1.564146	-0.157600	-0.843236
3	6	3.157126	-1.484522	0.474456
4	6	0.511370	-0.054930	-1.910305
5	6	0.234186	1.372844	-2.118885
6	6	1.825767	1.274815	-0.363914
7	6	0.969485	2.126109	-1.272684
8	1	1.531395	1.405044	0.683234

9	1	2.886292	1.543588	-0.424355
10	6	1.004389	3.621857	-1.138613
11	6	-0.752521	1.841691	-3.154084
12	1	-0.831348	2.931646	-3.186262
13	1	-1.752424	1.435890	-2.949823
14	1	-0.462482	1.492731	-4.154084
15	1	0.336959	4.122813	-1.845238
16	1	2.022130	4.002966	-1.304910
17	1	0.714958	3.928225	-0.123094
18	6	2.968388	-0.709436	1.801209
19	6	3.136866	-2.999561	0.782819
20	6	4.508371	-1.116798	-0.185449
21	1	4.643634	-1.679524	-1.115137
22	1	4.561147	-0.047828	-0.419182
23	1	3.171567	0.359404	1.696371
24	1	1.948694	-0.837848	2.182837
25	1	2.184229	-3.281287	1.245664
26	1	3.247255	-3.573729	-0.142405
27	1	3.950242	-3.268694	1.466651
28	1	3.661139	-1.103215	2.553685
29	1	5.336283	-1.360567	0.490341
30	6	-0.051229	-1.097721	-2.538078
31	1	-0.805698	-0.964907	-3.304353
32	1	0.245155	-2.108474	-2.285797

M22 (E = -924.1524042 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.297764	-0.073262	-0.371971
2	7	-0.824365	1.527225	-0.222760
3	6	-1.893915	-1.062652	1.064522
4	6	-0.648237	-1.048388	1.758292
5	6	-1.771845	-1.972919	-0.023338
6	17	-0.216779	-0.525687	-2.696343
7	6	0.218494	-1.998456	1.126474
8	6	-0.472112	-2.563364	0.026704
9	6	-1.351062	2.882770	-0.200123
10	6	-2.761548	2.893205	-0.841747
11	6	-1.431488	3.404010	1.256617
12	6	-0.400949	3.788288	-1.026733
13	1	-0.326626	3.415078	-2.052983
14	1	0.603251	3.790712	-0.587754
15	1	-0.439195	3.393959	1.722671
16	1	-2.100195	2.775264	1.854147
17	1	-3.446808	2.258623	-0.269812
18	1	-2.710076	2.512046	-1.866722
19	6	-0.371370	-0.332980	3.059952
20	6	-3.161792	-0.372646	1.503142
21	6	-2.859873	-2.356727	-0.995440
22	6	0.024003	-3.633358	-0.912206
23	6	1.580422	-2.407045	1.631679
24	1	-0.663677	-0.955358	3.918472
25	1	-0.927857	0.607020	3.128236
26	1	0.692642	-0.099214	3.179641
27	1	-3.733474	-1.019325	2.185013
28	1	-3.809575	-0.134685	0.653764
29	1	-2.950987	0.562332	2.029807
30	1	-3.383562	-3.260488	-0.650357
31	1	-2.451485	-2.563320	-1.989248
32	1	-3.606583	-1.563519	-1.102941
33	1	-0.505674	-4.581149	-0.741349
34	1	1.093110	-3.826953	-0.775258
35	1	-0.133633	-3.347062	-1.958523
36	1	1.487581	-3.199270	2.388127
37	1	2.111751	-1.571959	2.100635

38	1	2.215783	-2.795939	0.829153
39	1	-1.812084	4.432853	1.280585
40	1	-3.168652	3.912040	-0.864920
41	1	-0.772851	4.820470	-1.050523
42	7	1.868589	0.311090	-0.132583
43	6	2.774825	-0.285525	-0.941753
44	6	2.317333	1.188931	0.794965
45	6	4.144232	-0.032369	-0.848166
46	1	2.373709	-0.960605	-1.687836
47	6	3.670543	1.486671	0.954496
48	1	1.557943	1.664800	1.402168
49	6	4.604906	0.866516	0.118213
50	1	4.828349	-0.529961	-1.524913
51	1	3.978813	2.197042	1.712265
52	1	5.663136	1.083031	0.213754

***t*BuNC** (E = -250.6576605 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.759878	1.394223	-0.463256
2	6	0.285381	-0.000045	-0.000046
3	1	0.397322	1.611376	-1.472537
4	1	0.396566	2.172243	0.214967
5	1	1.854255	1.421516	-0.471796
6	6	0.759950	-0.295622	1.439076
7	6	0.759572	-1.098393	-0.976076
8	1	0.398318	-1.272684	1.773482
9	1	1.854306	-0.299632	1.467642
10	1	0.395560	0.469089	2.131669
11	1	1.853925	-1.119738	-0.996122
12	1	0.397000	-2.080998	-0.659419
13	1	0.395743	-0.899989	-1.988761
14	7	-1.175731	-0.000054	0.000231
15	6	-2.344783	-0.000389	0.000578

pyridine (E = -248.2540483 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.845126	-0.064010	0.000229
2	6	0.554105	-0.065633	0.000123
3	6	1.224743	1.161383	-0.000068
4	6	0.466485	2.336263	-0.000206
5	6	-0.928907	2.232679	-0.000131
6	7	-1.591345	1.058636	0.000117
7	1	2.309100	1.200923	-0.000148
8	1	-1.397143	-0.999164	0.000384
9	1	1.098109	-1.003510	0.000220
10	1	0.940673	3.311304	-0.000360
11	1	-1.547605	3.125115	-0.000183

In Benzene

By B3LYP/BS1

M1a (E = -697.9418212 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.297474	0.029992	0.005020
2	6	1.804546	0.883626	-0.695800
3	6	1.732578	-0.462048	-1.154845
4	6	1.806451	0.865623	0.731345
5	17	-1.107365	2.229029	0.103364
6	6	1.686623	-1.308604	-0.008899
7	6	1.731883	-0.490613	1.157157
8	6	-1.243107	-1.200293	-1.482429
9	6	-2.394177	-0.717758	-0.745598
10	1	-0.857380	-2.189361	-1.236305
11	6	-1.258211	-1.353993	1.341180

12	6	-2.400701	-0.792225	0.649016
13	1	-0.870079	-2.310554	0.992605
14	1	-1.256935	-1.274142	2.423397
15	6	-3.493963	-0.114529	1.453846
16	6	-3.481048	0.042372	-1.483091
17	1	-3.638229	1.045649	-1.074071
18	1	-4.434085	-0.499739	-1.412196
19	1	-3.231315	0.141718	-2.543396
20	1	-3.678982	0.912951	1.125286
21	1	-3.233711	-0.091412	2.516075
22	1	-4.435475	-0.672085	1.351932
23	6	1.857070	-0.918042	-2.586963
24	6	1.974905	2.107465	-1.559956
25	6	1.988926	2.065399	1.625900
26	6	1.841612	-0.977129	2.580704
27	6	1.736746	-2.815638	-0.030671
28	1	2.914757	-1.052363	-2.855325
29	1	1.430881	-0.189342	-3.283539
30	1	1.351547	-1.874048	-2.755391
31	1	3.041966	2.338439	-1.689503
32	1	1.491645	2.981883	-1.115618
33	1	1.546073	1.962903	-2.556832
34	1	3.058806	2.277783	1.764037
35	1	1.554610	1.902483	2.617483
36	1	1.518826	2.956784	1.202176
37	1	2.896610	-1.101780	2.863748
38	1	1.347118	-1.943439	2.719564
39	1	1.393532	-0.270323	3.286286
40	1	2.779738	-3.158197	-0.087882
41	1	1.212280	-3.234409	-0.895984
42	1	1.300937	-3.254480	0.872333
43	1	-1.230532	-1.003614	-2.549561

TSM1a-1b (E = -697.9131394 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.442954	-0.971817	-0.099940
2	6	-2.582747	-1.920721	-0.513068
3	6	-2.119791	-2.405359	0.743082
4	6	-1.706693	-2.417448	-1.522669
5	17	-1.294336	1.147936	0.083838
6	6	-0.965913	-3.211662	0.510818
7	6	-0.712063	-3.217476	-0.892338
8	6	1.051062	-1.125092	1.365271
9	6	2.388215	-1.070035	0.649758
10	1	1.022866	-1.926374	2.106559
11	6	1.136156	-0.861190	-1.481111
12	6	2.428144	-0.943439	-0.691349
13	1	1.147811	-1.536403	-2.340455
14	1	1.001009	0.156427	-1.887623
15	6	3.688339	-0.833473	-1.529020
16	6	3.597041	-1.126716	1.564939
17	1	4.551859	-1.086336	1.033427
18	1	3.580919	-2.049927	2.161600
19	1	3.572095	-0.290717	2.278846
20	1	3.696051	0.118796	-2.078869
21	1	3.715468	-1.632178	-2.284086
22	1	4.610840	-0.891517	-0.944668
23	6	-2.766885	-2.154693	2.082836
24	6	-3.833899	-1.112981	-0.749649
25	6	-1.853858	-2.169263	-3.002836
26	6	0.341554	-4.054992	-1.568602
27	6	-0.277079	-4.095774	1.516767
28	1	-3.507071	-2.936490	2.303907
29	1	-3.286613	-1.192109	2.107983

30	1	-2.032645	-2.159818	2.894935
31	1	-4.686373	-1.783920	-0.926594
32	1	-3.738777	-0.459678	-1.621955
33	1	-4.077711	-0.480521	0.108158
34	1	-2.566239	-2.881959	-3.441478
35	1	-0.903278	-2.285094	-3.531122
36	1	-2.230871	-1.162263	-3.210423
37	1	0.057154	-5.116029	-1.536967
38	1	1.315501	-3.957748	-1.077084
39	1	0.466687	-3.780349	-2.619304
40	1	-0.712262	-5.104971	1.487488
41	1	-0.390060	-3.719667	2.537912
42	1	0.793421	-4.191389	1.309386
43	1	0.878950	-0.184016	1.917634

M1b (E = -697.9327466 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.064924	0.672100	-0.000123
2	6	1.847347	-0.760882	0.710107
3	6	1.847873	-0.760878	-0.708942
4	6	0.611856	-1.321777	1.155696
5	17	1.619016	2.450660	-0.000514
6	6	0.612719	-1.321756	-1.155459
7	6	-0.135467	-1.702398	-0.000174
8	6	-1.207185	1.606869	-1.459011
9	6	-2.198012	0.885140	-0.704985
10	1	-1.233998	1.518639	-2.538437
11	6	-1.207215	1.607923	1.458163
12	6	-2.197972	0.885573	0.704694
13	1	-1.233887	1.520449	2.537648
14	1	-0.925296	2.604988	1.120393
15	6	-3.182519	0.049599	1.507241
16	6	-3.182849	0.049056	-1.507022
17	1	-3.539778	-0.845875	-0.995136
18	1	-2.742724	-0.252370	-2.462922
19	1	-4.061949	0.666910	-1.738689
20	1	-4.063022	0.666380	1.736416
21	1	-2.743083	-0.249033	2.464322
22	1	-3.537182	-0.847082	0.996830
23	6	2.966625	-0.299377	-1.605603
24	6	2.965452	-0.299172	1.607473
25	6	0.263760	-1.640908	2.589443
26	6	-1.340388	-2.607710	-0.000737
27	6	0.265778	-1.640800	-2.589500
28	1	3.601581	-1.150968	-1.888727
29	1	3.595753	0.445313	-1.112690
30	1	2.585582	0.150379	-2.528247
31	1	3.602550	-1.150003	1.888054
32	1	2.583733	0.147210	2.531466
33	1	3.592586	0.448334	1.116262
34	1	0.723329	-2.592621	2.892981
35	1	-0.816089	-1.736861	2.734135
36	1	0.624323	-0.868230	3.275702
37	1	-1.005119	-3.654958	-0.001613
38	1	-1.965214	-2.467067	-0.885869
39	1	-1.964911	-2.468458	0.884829
40	1	0.725527	-2.592540	-2.892696
41	1	0.627014	-0.868116	-3.275402
42	1	-0.813957	-1.736672	-2.735125
43	1	-0.925250	2.604202	-1.122020

M2a (E = -948.5958698 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	22	0.541546	0.293778	0.126413
2	7	-2.739430	0.155835	-0.222914
3	6	1.748233	-1.554093	1.071473
4	6	2.454013	-1.195823	-0.120194
5	6	0.471674	-2.054028	0.701630
6	17	0.106227	0.711270	2.500893
7	6	1.613691	-1.504352	-1.225149
8	6	0.380597	-2.001962	-0.721868
9	6	-1.577490	0.191069	-0.136875
10	6	-4.199004	0.188254	-0.255402
11	6	-0.254902	2.699651	0.199718
12	6	1.107528	2.635711	-0.068883
13	1	-0.988047	2.662020	-0.591043
14	6	0.503273	1.212320	-1.944944
15	6	1.538457	1.873534	-1.193834
16	1	-0.428351	1.734672	-2.143679
17	1	0.834018	0.636602	-2.800537
18	6	2.962008	1.985832	-1.706026
19	6	2.103807	3.269041	0.885744
20	1	2.485108	4.207060	0.456997
21	1	2.966392	2.625448	1.088764
22	1	1.622131	3.503410	1.838530
23	1	3.080130	2.942956	-2.237637
24	1	3.189064	1.193304	-2.422759
25	1	3.714922	1.958495	-0.912894
26	6	-4.649834	1.526678	0.369849
27	6	-4.644738	0.088160	-1.729992
28	1	-4.298679	1.609555	1.402577
29	1	-4.259621	2.373077	-0.203587
30	1	-4.249369	0.925909	-2.312682
31	1	-4.298826	-0.847896	-2.179329
32	6	3.929701	-0.878849	-0.165906
33	6	2.364525	-1.603711	2.445964
34	6	-0.551170	-2.633743	1.643837
35	6	-0.734952	-2.560206	-1.571197
36	6	2.032826	-1.573450	-2.670940
37	1	4.515608	-1.784096	0.051526
38	1	4.215670	-0.125423	0.576477
39	1	4.240868	-0.515633	-1.147931
40	1	2.983082	-2.508877	2.542357
41	1	1.603149	-1.622646	3.227712
42	1	3.008625	-0.739677	2.638480
43	1	-0.305842	-3.678239	1.884533
44	1	-1.555203	-2.623155	1.208078
45	1	-0.588484	-2.068293	2.579336
46	1	-0.474704	-3.565578	-1.932483
47	1	-0.930382	-1.934771	-2.448834
48	1	-1.668291	-2.645755	-1.007720
49	1	2.471205	-2.561151	-2.877266
50	1	2.786802	-0.825237	-2.929120
51	1	1.185400	-1.446168	-3.351486
52	1	-5.737750	0.114619	-1.778815
53	1	-5.743217	1.576008	0.365235
54	1	-0.594890	3.088463	1.149466
55	6	-4.722942	-1.009727	0.565542
56	1	-5.817402	-1.000418	0.561931
57	1	-4.382612	-1.955926	0.133202
58	1	-4.376157	-0.950049	1.601459

TSM2a-3a (E = -948.5868182 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	22	-1.101113	-0.609815	-0.598997
2	7	-3.105101	1.229240	-2.287967
3	6	1.273189	-1.060977	-0.891671
4	6	1.134738	-0.278256	0.282603
5	6	0.828013	-0.280066	-1.998913
6	17	-1.463467	-2.453011	-2.137946
7	6	0.602240	0.996525	-0.095507
8	6	0.417666	0.992216	-1.507305
9	6	-2.579500	0.425864	-1.546764
10	6	-4.459111	1.714069	-2.670080
11	6	-1.784065	0.140333	1.403762
12	6	-2.078259	-1.262010	1.461299
13	1	-2.591565	0.839791	1.199517
14	6	-3.560029	-0.778223	-0.429399
15	6	-2.911386	-1.754967	0.459045
16	1	-4.153749	-1.256020	-1.199446
17	1	-4.094997	0.014023	0.094159
18	6	-3.333738	-3.205636	0.380861
19	6	-1.481564	-2.158932	2.530009
20	1	-1.090911	-3.100557	2.130348
21	1	-2.254101	-2.412845	3.269769
22	1	-0.674841	-1.648757	3.061854
23	1	-4.190798	-3.379257	1.049438
24	1	-2.534355	-3.891302	0.676238
25	1	-3.634829	-3.466677	-0.636018
26	6	-5.365017	0.534469	-3.085270
27	6	-5.061655	2.488046	-1.476484
28	1	-4.875193	-0.080231	-3.847349
29	1	-5.620703	-0.100555	-2.233314
30	1	-5.223057	1.831157	-0.616120
31	1	-4.399641	3.305966	-1.173406
32	6	1.648421	-0.648375	1.651549
33	6	1.866710	-2.444277	-0.977245
34	6	0.938090	-0.653526	-3.453312
35	6	0.066867	2.190679	-2.351920
36	6	0.509218	2.227610	0.771548
37	1	2.699702	-0.343305	1.755195
38	1	1.603368	-1.727266	1.829029
39	1	1.088863	-0.152945	2.450739
40	1	2.932481	-2.388267	-1.241558
41	1	1.360973	-3.046753	-1.736909
42	1	1.792286	-2.977841	-0.024041
43	1	1.880085	-0.267576	-3.870438
44	1	0.115575	-0.235013	-4.041672
45	1	0.921343	-1.736514	-3.592135
46	1	0.982220	2.727836	-2.640818
47	1	-0.576507	2.892368	-1.813418
48	1	-0.458223	1.903618	-3.266558
49	1	1.347339	2.905194	0.553491
50	1	0.556637	1.983242	1.836184
51	1	-0.417786	2.784807	0.597619
52	1	-6.027517	2.915737	-1.766871
53	1	-6.297322	0.926463	-3.506353
54	1	-1.081822	0.519059	2.135146
55	6	-4.259227	2.664957	-3.868648
56	1	-5.221124	3.080017	-4.188142
57	1	-3.594593	3.490925	-3.595778
58	1	-3.813400	2.128399	-4.712592

M3a (E = -948.6252462 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.460715	-0.177701	-0.280075
2	7	-1.015668	1.187930	0.143260
3	6	2.580097	0.929649	-0.129739

4	6	2.835983	-0.438849	-0.443728
5	6	1.996242	0.982454	1.166168
6	17	0.232254	-0.080151	-2.614392
7	6	2.405877	-1.231170	0.657031
8	6	1.866908	-0.351565	1.648264
9	6	-1.166050	0.155816	0.855442
10	6	-1.893994	2.361893	-0.189870
11	6	-0.408370	-2.168383	-0.012481
12	6	-1.892800	-2.288804	-0.199718
13	1	-0.137891	-2.439226	1.011693
14	6	-2.276065	-0.544894	1.557002
15	6	-2.777129	-1.605888	0.563399
16	1	-1.887840	-1.008499	2.472778
17	1	-3.100370	0.114309	1.848013
18	6	-4.282949	-1.765982	0.557215
19	6	-2.311419	-3.250916	-1.297100
20	1	-3.380572	-3.230676	-1.521936
21	1	-2.034639	-4.281881	-1.035201
22	1	-1.770160	-3.000455	-2.218996
23	1	-4.623626	-2.541324	-0.132169
24	1	-4.788502	-0.827813	0.282994
25	1	-4.645271	-2.036272	1.560455
26	6	-3.115512	1.844327	-0.979927
27	6	-2.329352	3.059580	1.115744
28	1	-2.792282	1.301328	-1.872922
29	1	-3.729947	1.176265	-0.369614
30	1	-2.920441	2.391326	1.749801
31	1	-1.457251	3.399391	1.684419
32	6	3.540476	-0.936740	-1.680430
33	6	2.947847	2.104126	-1.002349
34	6	1.653920	2.230533	1.940079
35	6	1.419786	-0.757861	3.030527
36	6	2.651295	-2.708496	0.826963
37	1	4.630635	-0.864292	-1.556518
38	1	3.261878	-0.354453	-2.563444
39	1	3.299965	-1.983811	-1.888723
40	1	4.013860	2.347668	-0.888234
41	1	2.376239	3.000047	-0.741939
42	1	2.767389	1.889892	-2.060385
43	1	2.491636	2.518078	2.590905
44	1	0.776710	2.086469	2.578900
45	1	1.447660	3.076054	1.277276
46	1	2.285941	-0.879769	3.696616
47	1	0.879004	-1.710180	3.021854
48	1	0.763100	-0.006488	3.480322
49	1	3.649005	-2.878696	1.255984
50	1	2.607874	-3.243254	-0.127183
51	1	1.922154	-3.171256	1.498285
52	1	-2.944693	3.934444	0.878171
53	1	-3.735354	2.692791	-1.291142
54	1	0.126733	-2.839643	-0.692109
55	6	-1.067045	3.321238	-1.063445
56	1	-1.676457	4.184735	-1.351275
57	1	-0.190879	3.687037	-0.517321
58	1	-0.724460	2.814225	-1.970143

TSM3a-3b (E = -948.6114725 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.249380	-0.285664	-0.250869
2	7	-0.885027	1.445398	-0.620983
3	6	2.367643	-1.472894	0.276544
4	6	1.922531	-0.789796	1.440848
5	6	2.692799	-0.498267	-0.710303
6	17	0.003766	-1.446345	-2.252918

7	6	1.916267	0.607162	1.155413
8	6	2.415561	0.786491	-0.174249
9	6	-1.600163	0.502217	-0.183499
10	6	-1.208674	2.829533	-1.129353
11	6	-0.895033	-1.633927	1.067630
12	6	-2.195700	-2.142588	0.516383
13	1	-1.051406	-1.031628	1.972540
14	6	-3.012507	0.177695	0.159571
15	6	-3.209524	-1.330769	0.149281
16	1	-3.205017	0.610186	1.155466
17	1	-3.729719	0.657101	-0.513051
18	6	-4.582529	-1.760267	-0.322537
19	6	-2.258265	-3.655627	0.397051
20	1	-3.138609	-4.020692	-0.137169
21	1	-2.239810	-4.127557	1.389749
22	1	-1.370655	-4.011361	-0.143253
23	1	-4.723364	-2.842894	-0.308107
24	1	-4.774474	-1.409410	-1.348345
25	1	-5.366934	-1.320101	0.312089
26	6	-0.718725	3.846382	-0.078848
27	6	-0.453375	3.000307	-2.462130
28	1	-1.227390	3.693358	0.879510
29	1	0.358418	3.761762	0.081888
30	1	0.621263	2.865113	-2.323384
31	1	-0.800295	2.267009	-3.197595
32	6	1.708455	-1.391084	2.806172
33	6	2.549880	-2.961629	0.125912
34	6	3.319016	-0.786447	-2.049577
35	6	2.828720	2.092717	-0.806528
36	6	1.660002	1.690040	2.178100
37	1	2.625959	-1.287592	3.403193
38	1	1.469979	-2.456901	2.755586
39	1	0.901831	-0.896461	3.357026
40	1	3.584039	-3.256408	0.355129
41	1	2.330648	-3.287317	-0.896098
42	1	1.892627	-3.520489	0.799911
43	1	4.407435	-0.904532	-1.945913
44	1	3.138945	0.022121	-2.764686
45	1	2.921307	-1.706211	-2.488087
46	1	3.890547	2.290256	-0.599053
47	1	2.259928	2.940016	-0.415878
48	1	2.708967	2.079022	-1.894493
49	1	2.534419	1.813015	2.833603
50	1	0.804700	1.453511	2.821795
51	1	1.464138	2.657388	1.708805
52	1	-0.629473	4.004796	-2.862713
53	1	-0.933755	4.863776	-0.423811
54	1	-0.261771	-2.477606	1.347018
55	6	-2.721528	3.009305	-1.362359
56	1	-2.903329	4.008724	-1.772657
57	1	-3.101925	2.276284	-2.080876
58	1	-3.287818	2.922783	-0.429829

M3b (E = -948.6138898 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.286570	-0.174147	-0.190295
2	7	-0.850112	1.558699	-0.078000
3	6	2.306870	-1.530031	0.210431
4	6	2.019838	-0.784537	1.388602
5	6	2.644564	-0.608618	-0.818423
6	17	-0.114242	-1.022433	-2.350798
7	6	2.148825	0.600967	1.076717
8	6	2.535547	0.708744	-0.293474
9	6	-1.566961	0.520319	-0.192512

10	6	-1.257420	3.005871	0.076049
11	6	-0.885753	-1.496794	1.129849
12	6	-2.187515	-2.075251	0.627593
13	1	-1.052091	-0.863771	2.014248
14	6	-2.996474	0.138904	-0.195150
15	6	-3.176340	-1.345383	0.075120
16	1	-3.574557	0.751471	0.513038
17	1	-3.407069	0.375633	-1.187323
18	6	-4.538582	-1.851880	-0.351150
19	6	-2.279065	-3.582140	0.806967
20	1	-3.179117	-4.026341	0.376058
21	1	-2.240845	-3.850230	1.872354
22	1	-1.412447	-4.058742	0.328222
23	1	-4.720948	-2.892887	-0.078420
24	1	-4.665816	-1.760763	-1.440897
25	1	-5.335098	-1.248206	0.109858
26	6	-1.684772	3.224039	1.543354
27	6	-0.051200	3.890890	-0.273661
28	1	-2.543938	2.596564	1.803079
29	1	-0.862964	2.987018	2.226817
30	1	0.777876	3.714412	0.414482
31	1	0.292728	3.691709	-1.293599
32	6	1.841254	-1.332877	2.781985
33	6	2.342345	-3.032406	0.084987
34	6	3.159286	-0.960963	-2.188644
35	6	2.952996	1.956153	-1.036086
36	6	2.120058	1.701032	2.111880
37	1	2.789731	-1.263807	3.334087
38	1	1.544364	-2.385149	2.775704
39	1	1.088958	-0.778815	3.353989
40	1	3.359010	-3.416408	0.251411
41	1	2.025530	-3.357225	-0.911631
42	1	1.686297	-3.516690	0.815477
43	1	4.253301	-1.073616	-2.163180
44	1	2.919216	-0.186046	-2.922701
45	1	2.732081	-1.898983	-2.553047
46	1	4.035516	1.940137	-1.224749
47	1	2.732654	2.861710	-0.466485
48	1	2.455582	2.044579	-2.009058
49	1	2.994397	1.618652	2.773309
50	1	1.229156	1.652177	2.748701
51	1	2.150819	2.692922	1.654900
52	1	-0.333927	4.946892	-0.204204
53	1	-1.967765	4.271555	1.696220
54	1	-0.241874	-2.312403	1.459970
55	6	-2.418213	3.321735	-0.892183
56	1	-2.648602	4.391755	-0.846695
57	1	-2.140288	3.075777	-1.922885
58	1	-3.327207	2.772195	-0.634504

TSM3b-4 (E = -948.5964941 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.676302	0.035695	-0.662055
2	7	-0.617453	1.508662	-0.445162
3	6	2.828600	-1.089456	-0.561374
4	6	2.495696	-0.633099	0.743069
5	6	3.018280	0.054859	-1.392849
6	17	0.239028	-1.210366	-2.633387
7	6	2.464849	0.795514	0.714719
8	6	2.805777	1.218930	-0.607702
9	6	-1.218312	0.333711	-0.492203
10	6	-1.211416	2.857472	-0.187992
11	6	-0.761053	-0.941460	0.932319
12	6	-2.138097	-1.548918	1.002119

13	1	-0.480385	-0.430771	1.859983
14	6	-2.612336	-0.082862	-0.843146
15	6	-3.051395	-1.172079	0.097219
16	1	-3.318235	0.753301	-0.799257
17	1	-2.609394	-0.435630	-1.884075
18	6	-4.451282	-1.704632	-0.081437
19	6	-2.333914	-2.593303	2.080323
20	1	-3.354476	-2.984912	2.111035
21	1	-2.104544	-2.172224	3.069022
22	1	-1.650128	-3.440552	1.929808
23	1	-4.703804	-2.484046	0.641581
24	1	-4.575371	-2.127223	-1.088466
25	1	-5.192099	-0.898555	0.018282
26	6	-2.073116	2.803280	1.094339
27	6	-0.076017	3.877841	-0.006334
28	1	-2.895223	2.087391	0.998027
29	1	-1.461568	2.509533	1.954797
30	1	0.545291	3.621554	0.855275
31	1	0.555123	3.913162	-0.898483
32	6	2.397896	-1.476442	1.991163
33	6	3.056650	-2.519061	-0.984054
34	6	3.484241	0.027868	-2.826060
35	6	3.104962	2.626406	-1.067523
36	6	2.341705	1.659582	1.948805
37	1	3.370406	-1.509968	2.503057
38	1	2.112170	-2.509662	1.768390
39	1	1.669917	-1.076342	2.705143
40	1	4.129798	-2.757940	-0.971561
41	1	2.683502	-2.697905	-1.997005
42	1	2.554552	-3.226393	-0.315930
43	1	4.574805	-0.106060	-2.874325
44	1	3.242419	0.960684	-3.345642
45	1	3.019086	-0.791774	-3.381736
46	1	4.186938	2.752464	-1.213902
47	1	2.784156	3.370262	-0.335100
48	1	2.618559	2.864979	-2.020044
49	1	3.204766	1.498596	2.610156
50	1	1.441415	1.434695	2.532936
51	1	2.317233	2.722648	1.697663
52	1	-0.496054	4.876516	0.157804
53	1	-2.502757	3.790494	1.299359
54	1	-0.048179	-1.766438	0.800275
55	6	-2.061248	3.283684	-1.411050
56	1	-2.441449	4.301118	-1.262642
57	1	-1.448499	3.271681	-2.318792
58	1	-2.917082	2.622002	-1.567008

M4 (E = -948.6203282 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.363126	-0.240805	-0.153345
2	7	-0.539483	1.441695	0.139279
3	6	2.173925	-1.803774	0.095797
4	6	1.976783	-1.120934	1.329423
5	6	2.617303	-0.849549	-0.862284
6	17	-0.303077	-1.303817	-2.148259
7	6	2.315704	0.253388	1.133308
8	6	2.711410	0.423254	-0.226946
9	6	-1.564095	0.519567	0.114643
10	6	-0.747859	2.911690	0.014025
11	6	-1.648298	-0.522679	1.184667
12	6	-2.892992	-1.313921	0.861308
13	1	-1.576643	-0.156963	2.215567
14	6	-2.804866	0.416925	-0.755759
15	6	-3.522662	-0.794993	-0.204720

16	1	-3.452530	1.301801	-0.677805
17	1	-2.560696	0.296888	-1.817373
18	6	-4.790790	-1.274304	-0.857299
19	6	-3.267015	-2.510022	1.694943
20	1	-4.210640	-2.958722	1.371403
21	1	-3.370141	-2.235511	2.754241
22	1	-2.490878	-3.286607	1.638820
23	1	-5.236299	-2.124448	-0.332333
24	1	-4.598364	-1.580246	-1.894674
25	1	-5.537802	-0.469120	-0.894540
26	6	-1.822033	3.360285	1.033932
27	6	0.568747	3.644627	0.319804
28	1	-2.782976	2.871630	0.844627
29	1	-1.505865	3.112701	2.053757
30	1	0.899432	3.440129	1.341426
31	1	1.352517	3.336050	-0.374895
32	6	1.645788	-1.747299	2.664719
33	6	2.009975	-3.283351	-0.147639
34	6	3.058587	-1.151376	-2.270921
35	6	3.370445	1.630862	-0.852220
36	6	2.443833	1.254352	2.256876
37	1	2.567225	-1.977279	3.219079
38	1	1.090795	-2.684085	2.550393
39	1	1.048930	-1.077659	3.294341
40	1	2.977880	-3.798576	-0.067581
41	1	1.607049	-3.481311	-1.145714
42	1	1.333136	-3.741863	0.580921
43	1	4.124331	-1.423532	-2.285508
44	1	2.927895	-0.285941	-2.928356
45	1	2.491416	-1.980779	-2.701441
46	1	4.419709	1.406022	-1.090007
47	1	3.367085	2.489385	-0.176339
48	1	2.885681	1.937513	-1.786130
49	1	3.230813	0.934500	2.954299
50	1	1.518568	1.359618	2.834505
51	1	2.715833	2.244546	1.885247
52	1	0.424427	4.725908	0.214717
53	1	-1.971762	4.444330	0.972883
54	1	-0.732748	-1.254888	1.149552
55	6	-1.188325	3.271542	-1.428947
56	1	-1.299724	4.358340	-1.525140
57	1	-0.434186	2.934548	-2.148314
58	1	-2.142933	2.808591	-1.690845

TSM4-5 (E = -948.6150644 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.381513	-0.196601	-0.194824
2	7	-0.611104	1.445247	0.303968
3	6	2.103170	-1.786350	0.218325
4	6	1.936129	-1.015366	1.407770
5	6	2.576054	-0.912602	-0.795467
6	17	-0.218439	-0.661971	-2.394780
7	6	2.354060	0.320030	1.137546
8	6	2.729364	0.396247	-0.230295
9	6	-1.676069	0.588571	0.291056
10	6	-0.779332	2.914038	0.081990
11	6	-1.596622	-0.633678	1.023577
12	6	-2.808686	-1.441966	0.698118
13	1	-1.196766	-0.627740	2.035533
14	6	-2.919470	0.528339	-0.592463
15	6	-3.557752	-0.788610	-0.208834
16	1	-3.603527	1.365033	-0.403024
17	1	-2.666808	0.554697	-1.656914
18	6	-4.862822	-1.211092	-0.825587

19	6	-3.045495	-2.781103	1.340310
20	1	-3.989629	-3.229863	1.018422
21	1	-3.068756	-2.695586	2.435597
22	1	-2.236774	-3.481353	1.088317
23	1	-5.214484	-2.170014	-0.433023
24	1	-4.767349	-1.308540	-1.915789
25	1	-5.645481	-0.462252	-0.638911
26	6	-1.785000	3.465731	1.120746
27	6	0.579628	3.602668	0.290975
28	1	-2.771522	3.005051	1.007015
29	1	-1.429306	3.266801	2.137956
30	1	0.941990	3.445947	1.309439
31	1	1.320696	3.215159	-0.411940
32	6	1.547724	-1.544592	2.767464
33	6	1.904064	-3.274894	0.077076
34	6	3.028236	-1.315695	-2.175623
35	6	3.400651	1.546366	-0.942978
36	6	2.517822	1.379537	2.198944
37	1	2.439715	-1.862543	3.326432
38	1	0.882489	-2.410996	2.693033
39	1	1.042465	-0.782354	3.370889
40	1	2.861584	-3.803976	0.187993
41	1	1.493583	-3.536111	-0.903685
42	1	1.220221	-3.663924	0.837724
43	1	4.102674	-1.551583	-2.166878
44	1	2.866337	-0.515885	-2.904246
45	1	2.492849	-2.198605	-2.535183
46	1	4.441613	1.286135	-1.181396
47	1	3.422522	2.448974	-0.327005
48	1	2.905960	1.796614	-1.888610
49	1	3.267228	1.054667	2.933870
50	1	1.586964	1.573775	2.743005
51	1	2.860500	2.326226	1.775770
52	1	0.478458	4.680752	0.123792
53	1	-1.898030	4.549077	0.999134
54	1	-0.488182	-1.512393	0.483697
55	6	-1.265734	3.223268	-1.357755
56	1	-1.262492	4.307592	-1.520046
57	1	-0.600453	2.760128	-2.093744
58	1	-2.281160	2.862802	-1.537484

M5 (E = -948.6231051 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.455264	-0.151595	-0.348724
2	7	-0.723934	1.236447	0.431006
3	6	2.039056	-1.917194	0.020254
4	6	1.735188	-1.331552	1.286728
5	6	2.670525	-0.920013	-0.772966
6	17	0.359367	0.539222	-2.556169
7	6	2.219767	0.009199	1.289504
8	6	2.784653	0.270110	0.012132
9	6	-1.794256	0.383932	0.359172
10	6	-0.893209	2.723999	0.447833
11	6	-1.733623	-0.880891	0.906766
12	6	-2.863706	-1.696412	0.446134
13	1	-1.062560	-1.164239	1.704821
14	6	-3.040864	0.429952	-0.523535
15	6	-3.646013	-0.945606	-0.361782
16	1	-3.746217	1.211433	-0.217918
17	1	-2.767160	0.638005	-1.562813
18	6	-4.942242	-1.307870	-1.031391
19	6	-3.049928	-3.126304	0.878090
20	1	-3.989626	-3.547580	0.508928
21	1	-3.048714	-3.211825	1.973240

22	1	-2.230087	-3.753526	0.502404
23	1	-5.261762	-2.324437	-0.781736
24	1	-4.855923	-1.243842	-2.125247
25	1	-5.747315	-0.620389	-0.734655
26	6	-1.689363	3.109288	1.717032
27	6	0.505751	3.363912	0.506006
28	1	-2.681470	2.643565	1.715100
29	1	-1.158862	2.780394	2.617572
30	1	1.054610	3.019212	1.384487
31	1	1.081380	3.120343	-0.392037
32	6	1.219880	-2.068864	2.498650
33	6	1.903347	-3.374790	-0.341022
34	6	3.259585	-1.128349	-2.144193
35	6	3.517890	1.513335	-0.427304
36	6	2.258581	0.890472	2.513633
37	1	2.058326	-2.510683	3.056694
38	1	0.544733	-2.886249	2.225895
39	1	0.689570	-1.403412	3.188579
40	1	2.824323	-3.916062	-0.079990
41	1	1.728793	-3.509181	-1.412311
42	1	1.073798	-3.848310	0.191837
43	1	4.283108	-1.522634	-2.063779
44	1	3.301283	-0.193588	-2.709488
45	1	2.671644	-1.839590	-2.732208
46	1	4.597970	1.315126	-0.470784
47	1	3.361780	2.345750	0.263127
48	1	3.204743	1.839741	-1.424721
49	1	2.870019	0.416284	3.293462
50	1	1.261987	1.062845	2.934508
51	1	2.705029	1.863970	2.296537
52	1	0.412213	4.453859	0.565175
53	1	-1.821866	4.196217	1.768690
54	1	-0.136542	-1.649556	-0.760130
55	6	-1.613520	3.259195	-0.817292
56	1	-1.547355	4.353377	-0.832713
57	1	-1.139008	2.870287	-1.722813
58	1	-2.673347	2.994581	-0.832656

M6a (E = -1199.2807284 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.523937	-0.708355	0.086050
2	7	-1.248381	-0.742070	0.904389
3	6	2.008679	-0.844637	-1.897967
4	6	0.689586	-1.319484	-2.204699
5	6	2.576557	-1.708294	-0.932039
6	17	1.894047	-0.749155	2.142258
7	6	0.453295	-2.483093	-1.420507
8	6	1.609300	-2.703036	-0.604248
9	6	-2.199402	0.056716	0.220260
10	6	-1.751986	-1.395891	2.189265
11	6	-3.024824	-0.291179	-0.794354
12	6	-3.843362	0.855796	-1.212430
13	1	-3.084895	-1.273816	-1.244873
14	6	-2.471924	1.516271	0.547239
15	6	-3.533448	1.928055	-0.443651
16	1	-2.819001	1.636459	1.581268
17	1	-1.557047	2.113064	0.460833
18	6	-4.099369	3.321888	-0.478794
19	6	-4.850020	0.760301	-2.330540
20	1	-5.368245	1.709276	-2.499930
21	1	-5.609239	-0.003104	-2.111440
22	1	-4.365342	0.469144	-3.272674
23	1	-4.860843	3.433045	-1.257961
24	1	-3.315964	4.069346	-0.671573

25	1	-4.564624	3.590929	0.480700
26	6	-3.264424	-1.710094	2.109217
27	6	-1.005537	-2.729725	2.404699
28	1	-3.872113	-0.804656	2.020611
29	1	-3.490293	-2.354072	1.252644
30	1	-1.224570	-3.424833	1.586601
31	1	0.073417	-2.577190	2.469441
32	6	-0.175740	-0.826758	-3.337661
33	6	2.696368	0.296991	-2.603637
34	6	3.976949	-1.651108	-0.383342
35	6	1.863773	-3.885473	0.296549
36	6	-0.713889	-3.427583	-1.578355
37	1	0.048348	-1.383788	-4.259367
38	1	-0.007888	0.235631	-3.537375
39	1	-1.239618	-0.954141	-3.118763
40	1	3.096211	-0.034901	-3.572435
41	1	3.533759	0.689412	-2.018751
42	1	2.006310	1.124361	-2.799821
43	1	4.613772	-2.392370	-0.887535
44	1	3.990181	-1.862991	0.689351
45	1	4.431681	-0.666776	-0.531389
46	1	2.514443	-4.615208	-0.206688
47	1	0.936430	-4.400024	0.563357
48	1	2.357928	-3.579560	1.224197
49	1	-0.479707	-4.193682	-2.331956
50	1	-1.614785	-2.904060	-1.909683
51	1	-0.954223	-3.945809	-0.645794
52	1	-1.339057	-3.192447	3.341491
53	1	-3.564792	-2.234176	3.024143
54	1	-0.119833	0.449184	-0.941884
55	6	-1.489255	-0.449951	3.386625
56	1	-1.814970	-0.924779	4.321056
57	1	-0.423768	-0.219847	3.460556
58	1	-2.045419	0.486888	3.273460
59	6	1.793082	4.542527	-0.880135
60	6	2.135084	3.762349	0.406730
61	1	2.301380	4.106698	-1.745936
62	1	0.714434	4.534080	-1.064789
63	1	2.120376	5.581275	-0.771813
64	6	1.387279	4.345354	1.626210
65	6	3.658700	3.735706	0.654238
66	1	1.606056	3.765269	2.527449
67	1	1.710644	5.378749	1.785448
68	1	0.305913	4.340132	1.457665
69	1	4.018738	4.759392	0.797555
70	1	3.894779	3.151556	1.548378
71	1	4.183592	3.298799	-0.201023
72	7	1.683535	2.384070	0.237138
73	6	1.325590	1.278517	0.167176

TSM6a-7a (E = -1199.2786235 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-1.000797	-0.224892	-0.139255
2	7	0.377454	-1.579387	-0.479767
3	6	-2.242649	1.299904	1.380637
4	6	-1.521331	0.301797	2.120787
5	6	-3.229373	0.646444	0.603358
6	17	-2.010802	-0.099478	-2.343499
7	6	-2.072030	-0.967579	1.791178
8	6	-3.112788	-0.753300	0.827010
9	6	1.666143	-1.317434	0.041961
10	6	0.279929	-2.836472	-1.341943
11	6	2.103309	-1.466385	1.313730
12	6	3.498199	-1.019765	1.440498

13	1	1.514390	-1.855412	2.134576
14	6	2.823953	-0.756212	-0.771157
15	6	3.940072	-0.592603	0.232796
16	1	3.121456	-1.429978	-1.583017
17	1	2.538694	0.185692	-1.253981
18	6	5.297642	-0.073871	-0.157678
19	6	4.245761	-1.077957	2.748158
20	1	5.270905	-0.706759	2.653081
21	1	4.295049	-2.108220	3.126660
22	1	3.740489	-0.477946	3.517525
23	1	5.977215	-0.025912	0.699702
24	1	5.235797	0.935595	-0.589458
25	1	5.767838	-0.714019	-0.918297
26	6	1.214545	-3.945476	-0.802640
27	6	-1.166609	-3.372262	-1.283613
28	1	2.270891	-3.669889	-0.875718
29	1	0.994604	-4.165973	0.247629
30	1	-1.429016	-3.654282	-0.258574
31	1	-1.881818	-2.633817	-1.652922
32	6	-0.550987	0.577547	3.242639
33	6	-2.093700	2.789658	1.558930
34	6	-4.273065	1.304759	-0.257789
35	6	-4.059431	-1.788971	0.273699
36	6	-1.763893	-2.266983	2.496305
37	1	-1.092016	0.690117	4.193686
38	1	0.016850	1.496790	3.070759
39	1	0.169965	-0.235355	3.364270
40	1	-2.734324	3.140300	2.380672
41	1	-2.381217	3.338379	0.657185
42	1	-1.064446	3.067554	1.806193
43	1	-5.228831	1.367298	0.282569
44	1	-4.438894	0.741461	-1.180158
45	1	-3.982285	2.320773	-0.540999
46	1	-5.032574	-1.720109	0.780541
47	1	-3.684137	-2.805424	0.418437
48	1	-4.231412	-1.640985	-0.797422
49	1	-2.386348	-2.363807	3.397799
50	1	-0.717755	-2.321714	2.810372
51	1	-1.964999	-3.135872	1.863900
52	1	-1.254302	-4.265710	-1.913320
53	1	1.060955	-4.859366	-1.388472
54	1	0.277215	0.628524	0.608145
55	6	0.644254	-2.512986	-2.811497
56	1	0.518855	-3.408324	-3.433692
57	1	-0.005209	-1.723243	-3.196630
58	1	1.684804	-2.186500	-2.901232
59	6	2.206018	3.456074	0.367417
60	6	1.371461	3.650403	-0.915699
61	1	1.579229	3.563648	1.258725
62	1	2.670376	2.464994	0.388501
63	1	2.996075	4.213175	0.408282
64	6	2.246728	3.501021	-2.179194
65	6	0.657139	5.018061	-0.912989
66	1	1.638592	3.597151	-3.083591
67	1	3.011818	4.284055	-2.185607
68	1	2.745151	2.526759	-2.195968
69	1	1.403066	5.819030	-0.891210
70	1	0.044066	5.134553	-1.811785
71	1	0.013053	5.119512	-0.033885
72	7	0.337872	2.607568	-0.976772
73	6	-0.190908	1.605447	-0.648194

M7a (E = -1199.3015263 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	22	0.859708	-0.194799	-0.195658
2	7	0.577784	1.691659	-0.450863
3	6	1.378370	-2.163260	1.245211
4	6	1.343124	-0.989571	2.059536
5	6	2.432545	-2.019499	0.314257
6	17	1.457046	-0.669037	-2.405538
7	6	2.397051	-0.126064	1.640429
8	6	3.062776	-0.757966	0.550555
9	6	-0.688114	1.828262	0.125022
10	6	1.144226	2.833809	-1.256614
11	6	-0.979887	1.670507	1.448771
12	6	-2.423144	1.751519	1.678420
13	1	-0.243815	1.550930	2.229491
14	6	-2.007186	2.042380	-0.604115
15	6	-3.041527	1.983948	0.493295
16	1	-2.052232	3.001127	-1.132273
17	1	-2.151438	1.262314	-1.359509
18	6	-4.499700	2.221384	0.217397
19	6	-3.033544	1.632604	3.051636
20	1	-4.117423	1.779246	3.031547
21	1	-2.606263	2.377045	3.736870
22	1	-2.837573	0.644115	3.488068
23	1	-5.105752	2.154422	1.126217
24	1	-4.893767	1.491373	-0.502986
25	1	-4.661595	3.216476	-0.220958
26	6	0.893779	4.167016	-0.514599
27	6	2.664364	2.621984	-1.394185
28	1	-0.175059	4.379684	-0.407642
29	1	1.337964	4.140468	0.486853
30	1	3.143379	2.618846	-0.410344
31	1	2.883067	1.679934	-1.901985
32	6	0.497956	-0.840611	3.301196
33	6	0.554298	-3.406147	1.457789
34	6	2.902248	-3.070998	-0.655294
35	6	4.330958	-0.300333	-0.124678
36	6	2.840276	1.131624	2.348176
37	1	0.803177	-1.585777	4.049155
38	1	-0.568951	-0.996016	3.106126
39	1	0.617764	0.145195	3.759255
40	1	1.094664	-4.111178	2.105993
41	1	0.343134	-3.918290	0.514196
42	1	-0.402417	-3.185023	1.939956
43	1	3.616983	-3.747912	-0.164552
44	1	3.396893	-2.624634	-1.521186
45	1	2.070546	-3.675589	-1.029854
46	1	5.182988	-0.886436	0.248279
47	1	4.544403	0.752913	0.072361
48	1	4.282985	-0.438035	-1.209316
49	1	3.470030	0.877651	3.212793
50	1	1.995879	1.721351	2.717855
51	1	3.427491	1.779303	1.692377
52	1	3.097748	3.439584	-1.981457
53	1	1.349085	4.992694	-1.073137
54	1	-1.521893	-1.254202	0.997040
55	6	0.514901	2.874234	-2.671255
56	1	1.009417	3.646489	-3.272932
57	1	0.640471	1.908228	-3.167041
58	1	-0.551708	3.112268	-2.634352
59	6	-2.632940	-3.725495	-1.577765
60	6	-2.905119	-2.291244	-1.069884
61	1	-2.093902	-3.692735	-2.529848
62	1	-2.023419	-4.282131	-0.856532
63	1	-3.576234	-4.264996	-1.724052
64	6	-3.643722	-2.339160	0.282136

65	6	-3.754935	-1.528797	-2.109741
66	1	-3.825746	-1.332022	0.675449
67	1	-4.613522	-2.832616	0.151460
68	1	-3.080089	-2.905638	1.032978
69	1	-4.709017	-2.042128	-2.277779
70	1	-3.968024	-0.510034	-1.765813
71	1	-3.216109	-1.464680	-3.060224
72	7	-1.568085	-1.606715	-1.044111
73	6	-1.024281	-1.176285	0.013123

TSM7a-8a (E = -1199.3014325 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.964655	-0.159621	-0.294091
2	7	0.661017	1.737242	-0.474314
3	6	1.486677	-2.163659	1.105860
4	6	1.350896	-1.022501	1.956178
5	6	2.584596	-1.942458	0.246061
6	17	1.795681	-0.489415	-2.479661
7	6	2.389889	-0.102257	1.632020
8	6	3.143047	-0.663050	0.560922
9	6	-0.634004	1.841476	0.042685
10	6	1.247598	2.924452	-1.199447
11	6	-0.998413	1.625993	1.339459
12	6	-2.453504	1.685164	1.489818
13	1	-0.307720	1.473124	2.154728
14	6	-1.912247	2.076186	-0.749873
15	6	-3.007352	1.959232	0.282105
16	1	-1.937998	3.057766	-1.235717
17	1	-2.001513	1.331211	-1.547429
18	6	-4.450798	2.192122	-0.066613
19	6	-3.138377	1.504443	2.820612
20	1	-4.222531	1.628439	2.742975
21	1	-2.768385	2.233073	3.554551
22	1	-2.944290	0.505597	3.233712
23	1	-5.105620	2.084395	0.803739
24	1	-4.795579	1.486105	-0.834835
25	1	-4.600792	3.201523	-0.475580
26	6	0.922931	4.222317	-0.423749
27	6	2.777979	2.755179	-1.255621
28	1	-0.154299	4.411890	-0.374401
29	1	1.305925	4.164646	0.601386
30	1	3.200475	2.732332	-0.246571
31	1	3.049354	1.836117	-1.778888
32	6	0.424520	-0.955251	3.145653
33	6	0.698671	-3.443112	1.219826
34	6	3.165692	-2.937276	-0.722935
35	6	4.436709	-0.141093	-0.010502
36	6	2.742869	1.141756	2.410778
37	1	0.695929	-1.733180	3.872844
38	1	-0.624503	-1.118170	2.873612
39	1	0.493283	0.007008	3.660603
40	1	1.230588	-4.158497	1.863538
41	1	0.555390	-3.920151	0.245234
42	1	-0.288690	-3.278047	1.660968
43	1	3.928731	-3.552020	-0.222981
44	1	3.634361	-2.438453	-1.574566
45	1	2.400160	-3.611693	-1.118904
46	1	5.279288	-0.728013	0.382456
47	1	4.611158	0.904145	0.254961
48	1	4.455709	-0.221689	-1.101782
49	1	3.368550	0.880756	3.276336
50	1	1.857719	1.661456	2.789553
51	1	3.303317	1.855483	1.801935
52	1	3.221126	3.602921	-1.790794

53	1	1.394466	5.077377	-0.921361
54	1	-1.478235	-1.403914	0.746767
55	6	0.701418	3.006442	-2.646653
56	1	1.205407	3.817865	-3.185836
57	1	0.887637	2.066174	-3.171871
58	1	-0.372679	3.210479	-2.664381
59	6	-2.102409	-3.497093	-2.297935
60	6	-2.545555	-2.163604	-1.654283
61	1	-1.437734	-3.305991	-3.146312
62	1	-1.564329	-4.117183	-1.571799
63	1	-2.975801	-4.057075	-2.652399
64	6	-3.458942	-2.432745	-0.442883
65	6	-3.288180	-1.306302	-2.701431
66	1	-3.753143	-1.498760	0.050430
67	1	-4.370009	-2.941997	-0.776768
68	1	-2.970296	-3.075483	0.298843
69	1	-4.167752	-1.840906	-3.078709
70	1	-3.624511	-0.359692	-2.263056
71	1	-2.625259	-1.080668	-3.542797
72	7	-1.278079	-1.425920	-1.325194
73	6	-0.891832	-1.155691	-0.154103

M8a (E = -1199.3133687 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.731354	-0.120680	-0.049551
2	7	-0.271838	1.918303	-0.209715
3	6	0.261014	1.447803	0.825038
4	7	0.797563	-1.108594	-0.770174
5	6	-2.275947	0.335212	1.879296
6	6	-1.317189	-0.672236	2.222948
7	6	-3.081994	-0.162070	0.839782
8	17	-1.900511	0.177807	-2.183987
9	6	-1.580452	-1.822806	1.421310
10	6	-2.645915	-1.498640	0.539263
11	6	-0.285208	3.292716	-0.804890
12	6	1.984592	-0.682991	-0.138560
13	6	0.988711	-2.067635	-1.938618
14	6	2.390625	-0.942255	1.129757
15	1	0.883629	1.970090	1.555415
16	6	3.659152	-0.265085	1.424909
17	1	1.863637	-1.570696	1.833973
18	6	3.038689	0.222744	-0.767465
19	6	4.058773	0.422931	0.327638
20	1	3.499514	-0.222203	-1.655757
21	1	2.590277	1.165126	-1.101391
22	6	5.303396	1.240757	0.116527
23	6	4.350338	-0.393706	2.758460
24	1	5.287894	0.169575	2.791232
25	1	4.581598	-1.444463	2.980403
26	1	3.709634	-0.028157	3.572520
27	1	5.927362	1.273730	1.015583
28	1	5.061773	2.277122	-0.159847
29	1	5.916537	0.831247	-0.699198
30	6	-1.760796	3.736977	-0.886800
31	6	0.534725	4.266396	0.059853
32	6	0.313049	3.178294	-2.223062
33	1	-0.241480	2.440922	-2.808557
34	1	1.364661	2.873305	-2.179893
35	1	1.580260	3.946361	0.138909
36	1	0.118804	4.350166	1.070750
37	1	-2.196685	3.828634	0.114156
38	1	-2.342203	3.011101	-1.460771
39	6	2.174083	-3.025074	-1.663498
40	6	-0.279533	-2.929489	-2.102165

41	6	1.231922	-1.280342	-3.249511
42	1	0.394752	-0.604001	-3.438593
43	1	2.154492	-0.693987	-3.203111
44	1	3.132373	-2.500636	-1.602212
45	1	2.023880	-3.567653	-0.723671
46	1	-0.449150	-3.536030	-1.207928
47	1	-1.156308	-2.308471	-2.289983
48	6	-0.408454	-0.619139	3.425981
49	6	-2.431789	1.651740	2.596212
50	6	-4.283713	0.503689	0.223650
51	6	-3.385734	-2.427121	-0.388628
52	6	-0.955116	-3.181956	1.627504
53	1	-1.000816	-0.691321	4.349787
54	1	0.164742	0.312843	3.476325
55	1	0.303517	-1.448785	3.430292
56	1	-3.040004	1.524099	3.503187
57	1	-2.927340	2.400706	1.971385
58	1	-1.466355	2.062649	2.911560
59	1	-5.209268	0.047181	0.603464
60	1	-4.276623	0.399950	-0.865502
61	1	-4.320639	1.571859	0.459296
62	1	-4.376497	-2.661801	0.026522
63	1	-2.855521	-3.371680	-0.534004
64	1	-3.535000	-1.967560	-1.371167
65	1	-1.287899	-3.608020	2.584527
66	1	0.138490	-3.143124	1.643035
67	1	-1.247138	-3.880527	0.839599
68	1	0.519789	5.262175	-0.395375
69	1	-1.823857	4.713682	-1.379390
70	1	0.258675	4.150913	-2.724846
71	1	-0.150259	-3.608251	-2.953794
72	1	2.242095	-3.756339	-2.477209
73	1	1.319676	-1.977726	-4.092183

TSM8a-9a (E = -1199.2979755 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.571625	-0.361634	0.101395
2	7	-1.929529	0.983771	-0.395177
3	6	-2.104221	0.725590	0.864208
4	7	0.812186	1.067251	0.902320
5	6	-2.048428	-2.274873	0.469659
6	6	-1.331521	-1.994427	1.677254
7	6	-1.115785	-2.693222	-0.503637
8	17	0.197918	-0.265555	-2.227387
9	6	0.047328	-2.275465	1.447741
10	6	0.187874	-2.683965	0.091439
11	6	-2.728515	1.802888	-1.354955
12	6	0.176054	2.013442	1.596399
13	6	2.270417	1.268028	0.511902
14	6	-1.012579	1.763032	2.322339
15	1	-3.042264	0.760605	1.412156
16	6	-1.570940	3.049062	2.784799
17	1	-1.100568	0.876971	2.935039
18	6	0.364119	3.531058	1.553011
19	6	-0.813210	4.071402	2.335067
20	1	1.310112	3.872733	1.982651
21	1	0.356538	3.876268	0.514033
22	6	-0.984316	5.551653	2.539846
23	6	-2.809766	3.109756	3.639685
24	1	-3.056986	4.133683	3.935634
25	1	-2.679344	2.515915	4.555092
26	1	-3.678814	2.695049	3.110792
27	1	-1.861634	5.780166	3.153353
28	1	-1.101585	6.080031	1.582436

29	1	-0.105573	5.988687	3.036507
30	6	-3.274185	0.863432	-2.452394
31	6	-3.892029	2.500124	-0.622215
32	6	-1.785085	2.854757	-1.978547
33	1	-0.936997	2.360010	-2.458328
34	1	-1.406832	3.535205	-1.207181
35	1	-3.519321	3.141510	0.184576
36	1	-4.588322	1.769634	-0.193771
37	1	-3.954993	0.120850	-2.020330
38	1	-2.452242	0.340851	-2.947485
39	6	3.104295	1.702954	1.744078
40	6	2.835322	-0.092381	0.054283
41	6	2.420665	2.278167	-0.650469
42	1	1.776971	1.987990	-1.485416
43	1	2.177062	3.299779	-0.349199
44	1	2.849185	2.700238	2.106978
45	1	2.965805	0.991430	2.566067
46	1	2.765923	-0.826172	0.860993
47	1	2.309050	-0.466037	-0.824819
48	6	-1.953531	-1.736629	3.026133
49	6	-3.548303	-2.240647	0.320413
50	6	-1.425140	-3.202443	-1.886642
51	6	1.420340	-3.221520	-0.589997
52	6	1.104637	-2.295634	2.527434
53	1	-2.260014	-2.686308	3.488984
54	1	-2.845707	-1.106214	2.956261
55	1	-1.250475	-1.254998	3.713522
56	1	-3.991134	-3.179072	0.683788
57	1	-3.849274	-2.117140	-0.724112
58	1	-3.997442	-1.425072	0.896997
59	1	-1.448192	-4.302158	-1.887550
60	1	-0.671315	-2.875357	-2.607302
61	1	-2.398310	-2.849690	-2.241516
62	1	1.309273	-4.299128	-0.775961
63	1	2.319211	-3.082377	0.016392
64	1	1.584298	-2.733269	-1.556998
65	1	0.879220	-3.082257	3.260836
66	1	1.166264	-1.346386	3.071235
67	1	2.095180	-2.508616	2.117169
68	1	-4.450609	3.124804	-1.327797
69	1	-3.828219	1.445199	-3.198434
70	1	-2.324819	3.447840	-2.726584
71	1	3.893484	0.025232	-0.205916
72	1	4.166563	1.711946	1.475352
73	1	3.460274	2.275625	-0.999073

M9a (E = -1199.3305563 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.877845	-0.083160	-0.126242
2	7	-0.332132	-1.448883	-0.546176
3	6	-0.698873	-1.136828	0.763059
4	7	-0.759836	1.580253	-0.054449
5	6	2.444727	-1.336001	1.150994
6	6	1.870534	-0.368355	2.032123
7	6	3.215071	-0.636592	0.182205
8	17	1.437464	0.395096	-2.441320
9	6	2.306675	0.923721	1.610600
10	6	3.139786	0.757977	0.470926
11	6	-0.753563	-2.613439	-1.370142
12	6	-1.862144	1.082881	0.377300
13	6	-0.719364	2.941855	-0.746545
14	6	-1.869099	-0.224570	1.135495
15	1	-0.521256	-1.895770	1.528870
16	6	-3.327558	-0.669572	1.073801

17	1	-1.670213	0.042573	2.189426
18	6	-3.306504	1.533400	0.218142
19	6	-4.106745	0.295872	0.566335
20	1	-3.540254	2.342746	0.921426
21	1	-3.523740	1.918902	-0.780348
22	6	-5.600024	0.312196	0.378770
23	6	-3.754778	-1.986694	1.659750
24	1	-4.842311	-2.105241	1.656967
25	1	-3.407000	-2.074507	2.699178
26	1	-3.323253	-2.831512	1.111065
27	1	-6.067225	-0.626955	0.688510
28	1	-5.858867	0.484378	-0.675574
29	1	-6.060844	1.126431	0.956544
30	6	0.298484	-2.875820	-2.465892
31	6	-0.895514	-3.883870	-0.499929
32	6	-2.110100	-2.269385	-2.034521
33	1	-1.996743	-1.390438	-2.677811
34	1	-2.872136	-2.048305	-1.280129
35	1	-1.626540	-3.745904	0.302066
36	1	0.064499	-4.152007	-0.046545
37	1	1.270355	-3.115153	-2.019368
38	1	0.427928	-1.997891	-3.100971
39	6	-1.536355	4.011938	0.022417
40	6	0.746188	3.419538	-0.758560
41	6	-1.218407	2.802938	-2.203609
42	1	-0.605753	2.079764	-2.746199
43	1	-2.263369	2.483519	-2.252739
44	1	-2.612835	3.930562	-0.134580
45	1	-1.329745	3.963555	1.098111
46	1	1.105346	3.588828	0.259714
47	1	1.392763	2.698812	-1.258926
48	6	1.189908	-0.646176	3.349011
49	6	2.395187	-2.831740	1.340251
50	6	4.078957	-1.250968	-0.889647
51	6	3.920730	1.817069	-0.264168
52	6	2.060355	2.190920	2.396057
53	1	1.919215	-0.588426	4.171070
54	1	0.744155	-1.644223	3.376471
55	1	0.399120	0.080978	3.564377
56	1	3.172997	-3.153422	2.048160
57	1	2.565256	-3.365727	0.400663
58	1	1.431620	-3.161185	1.741187
59	1	5.117054	-1.341612	-0.537207
60	1	4.079208	-0.641542	-1.797356
61	1	3.734666	-2.252900	-1.164534
62	1	4.998558	1.676632	-0.102076
63	1	3.663884	2.824342	0.075621
64	1	3.738682	1.767062	-1.343732
65	1	2.499807	2.104407	3.399594
66	1	0.992603	2.403301	2.526610
67	1	2.517954	3.059285	1.914585
68	1	-1.226434	-4.723739	-1.121800
69	1	-0.014773	-3.725199	-3.084963
70	1	-2.460134	-3.109140	-2.647794
71	1	0.809751	4.368437	-1.302800
72	1	-1.232693	5.002792	-0.331616
73	1	-1.140446	3.775027	-2.704362

M10 (E = -1199.3122662 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	22	1.680478	-0.272988	-0.420040
2	7	0.179727	-1.315297	-0.261540
3	6	-0.324008	-0.056485	0.139132
4	7	-3.539001	-0.393125	-0.403396
5	6	2.488144	-0.294243	1.794714
6	6	2.359761	1.081826	1.423323
7	6	3.500644	-0.873598	0.979692
8	17	2.122307	0.013199	-2.696411
9	6	3.314231	1.347099	0.393276
10	6	4.009570	0.141205	0.112753
11	6	-0.420484	-2.674729	-0.272985
12	6	-2.792116	0.590514	-0.124272
13	6	-4.942716	-0.573867	0.078821
14	6	-1.371221	0.711392	-0.712976
15	1	-0.534584	0.059230	1.209270
16	6	-1.152985	2.218091	-0.682342
17	1	-1.345791	0.312623	-1.731038
18	6	-3.050594	1.867186	0.681207
19	6	-2.043500	2.837988	0.107553
20	1	-4.075861	2.230357	0.576094
21	1	-2.890652	1.699185	1.755380
22	6	-2.152451	4.301560	0.443028
23	6	-0.050020	2.846408	-1.484961
24	1	0.001315	3.930309	-1.344481
25	1	-0.188252	2.644523	-2.555499
26	1	0.929585	2.427688	-1.223456
27	1	-1.371041	4.900423	-0.033763
28	1	-2.082897	4.458606	1.529244
29	1	-3.125671	4.703971	0.127453
30	6	0.737496	-3.689310	-0.384872
31	6	-1.215986	-2.919554	1.026562
32	6	-1.342542	-2.810236	-1.507964
33	1	-0.773125	-2.618923	-2.424275
34	1	-2.173940	-2.103377	-1.446131
35	1	-2.034357	-2.199708	1.115790
36	1	-0.566220	-2.829171	1.904496
37	1	1.400528	-3.625192	0.484627
38	1	1.323251	-3.507311	-1.293861
39	6	-5.882426	0.357505	-0.723942
40	6	-5.301513	-2.042185	-0.248844
41	6	-5.110927	-0.358140	1.602253
42	1	-4.367164	-0.943462	2.155793
43	1	-5.011751	0.690313	1.893286
44	1	-5.685150	1.413851	-0.516152
45	1	-5.752260	0.189866	-1.798599
46	1	-5.175185	-2.232133	-1.319627
47	1	-4.645409	-2.728227	0.298018
48	6	1.528600	2.108885	2.151136
49	6	1.779588	-0.949753	2.953731
50	6	4.037937	-2.283062	1.066531
51	6	5.155615	-0.008450	-0.854628
52	6	3.613697	2.682083	-0.243679
53	1	2.102959	2.544172	2.981689
54	1	0.620712	1.667489	2.572087
55	1	1.220178	2.927841	1.494857
56	1	2.268449	-0.681068	3.900831
57	1	1.792291	-2.040408	2.873611
58	1	0.733758	-0.634501	3.024857
59	1	5.021234	-2.282510	1.556945
60	1	4.170997	-2.739535	0.078746
61	1	3.380733	-2.933620	1.649643
62	1	6.096396	0.315377	-0.386503
63	1	5.002739	0.594651	-1.754426
64	1	5.285619	-1.047929	-1.171492

65	1	4.571076	3.073792	0.127425
66	1	2.844710	3.424516	-0.012393
67	1	3.691924	2.603685	-1.333820
68	1	-1.643950	-3.928895	1.018164
69	1	0.342663	-4.710205	-0.438217
70	1	-1.750076	-3.828069	-1.557565
71	1	-6.339975	-2.258940	0.027398
72	1	-6.927559	0.149295	-0.466874
73	1	-6.105823	-0.697049	1.913416

TSM10-11 (E = -1199.2872637 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	1.013713	-0.048371	-0.216503
2	7	0.283291	-0.892830	1.341212
3	6	-0.323181	0.333670	1.489745
4	7	-2.475216	-1.112350	-0.131341
5	6	3.261934	0.348769	0.339596
6	6	2.578447	1.589322	0.516289
7	6	3.248048	0.042385	-1.054740
8	17	0.582168	-1.602235	-1.926307
9	6	2.143671	2.041620	-0.769642
10	6	2.562933	1.085665	-1.735526
11	6	0.419144	-1.874921	2.443489
12	6	-2.218450	0.102256	-0.338357
13	6	-3.553590	-1.886071	-0.818346
14	6	-1.131322	0.867593	0.437663
15	1	-0.092519	0.971806	2.343813
16	6	-1.691966	2.263923	0.526262
17	1	-0.261635	1.008043	-0.770788
18	6	-2.907343	1.175054	-1.183122
19	6	-2.663872	2.436454	-0.387850
20	1	-2.450321	1.233043	-2.181248
21	1	-3.970111	0.984365	-1.330458
22	6	-3.486463	3.662875	-0.668470
23	6	-1.247274	3.252669	1.570690
24	1	-1.708889	4.231810	1.416495
25	1	-0.162091	3.388814	1.574872
26	1	-1.528327	2.908714	2.575500
27	1	-3.193510	4.518606	-0.054079
28	1	-4.552974	3.466783	-0.489026
29	1	-3.392368	3.955260	-1.723835
30	6	1.294930	-3.031471	1.927180
31	6	1.056505	-1.231316	3.698472
32	6	-0.987815	-2.406918	2.805025
33	1	-1.461805	-2.848248	1.926536
34	1	-1.627712	-1.590098	3.157847
35	1	0.435809	-0.416705	4.089055
36	1	2.052287	-0.837084	3.476562
37	1	2.299524	-2.678102	1.673093
38	1	0.848167	-3.472161	1.030548
39	6	-3.526248	-1.719747	-2.357099
40	6	-3.267048	-3.368407	-0.484846
41	6	-4.930768	-1.499068	-0.228646
42	1	-4.922039	-1.613160	0.861111
43	1	-5.202504	-0.464837	-0.462528
44	1	-3.857440	-0.729442	-2.680404
45	1	-2.512012	-1.887872	-2.734532
46	1	-2.273437	-3.649427	-0.848255
47	1	-3.293584	-3.526656	0.598181
48	6	2.583617	2.383910	1.801085
49	6	4.115153	-0.342353	1.375146
50	6	3.954354	-1.121771	-1.701346
51	6	2.357468	1.179643	-3.224988
52	6	1.518557	3.377506	-1.092528

53	1	3.592880	2.774921	1.994218
54	1	2.297364	1.779906	2.668661
55	1	1.909606	3.242789	1.753922
56	1	5.147965	0.033491	1.322306
57	1	4.156288	-1.425135	1.222244
58	1	3.753283	-0.160240	2.390393
59	1	4.996479	-0.853087	-1.928199
60	1	3.468269	-1.417545	-2.634221
61	1	3.973965	-1.999792	-1.047775
62	1	3.247642	1.600495	-3.714245
63	1	1.507336	1.822752	-3.473954
64	1	2.166001	0.194725	-3.661144
65	1	2.291919	4.087866	-1.417856
66	1	1.014040	3.816415	-0.228796
67	1	0.783071	3.298545	-1.899246
68	1	1.154444	-1.982683	4.490297
69	1	1.387827	-3.809613	2.693122
70	1	-0.912144	-3.160254	3.598254
71	1	-4.013025	-4.021647	-0.952378
72	1	-4.192233	-2.459128	-2.816742
73	1	-5.708498	-2.155015	-0.636575

M11 (E = -1199.3007068 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.957871	-0.146659	-0.336310
2	7	0.305442	-0.846008	1.337549
3	6	-0.365512	0.305811	1.711350
4	7	-2.500390	-0.972862	-0.107251
5	6	3.144222	0.514407	0.313079
6	6	2.384137	1.695579	0.073825
7	6	3.283382	-0.167125	-0.930527
8	17	0.632076	-1.940884	-1.775470
9	6	2.083639	1.760341	-1.323228
10	6	2.643319	0.610670	-1.939637
11	6	0.542828	-1.926582	2.341886
12	6	-2.302618	0.275581	-0.031321
13	6	-3.468282	-1.631572	-1.031450
14	6	-1.389636	0.882627	1.002142
15	1	0.000218	0.847738	2.586511
16	6	-1.887277	2.248233	1.236095
17	1	-0.077631	0.847533	-1.194157
18	6	-2.996572	1.464771	-0.701457
19	6	-2.782471	2.589227	0.281328
20	1	-2.522001	1.689040	-1.665878
21	1	-4.055430	1.288418	-0.896985
22	6	-3.522248	3.884091	0.106545
23	6	-1.452366	3.083667	2.412995
24	1	-1.947173	4.058524	2.420480
25	1	-0.370330	3.256467	2.413512
26	1	-1.697776	2.577750	3.356523
27	1	-3.263149	4.626327	0.866541
28	1	-4.608402	3.719773	0.148918
29	1	-3.309069	4.319164	-0.880343
30	6	1.510881	-2.954255	1.727163
31	6	1.123398	-1.375120	3.666434
32	6	-0.817371	-2.610202	2.626058
33	1	-1.249895	-2.991549	1.698230
34	1	-1.526041	-1.894939	3.058453
35	1	0.427468	-0.686421	4.158388
36	1	2.071331	-0.855949	3.499572
37	1	2.491002	-2.507650	1.530470
38	1	1.113080	-3.338569	0.783905
39	6	-3.347247	-1.142131	-2.494915
40	6	-3.109901	-3.135530	-0.986404

41	6	-4.907870	-1.446701	-0.492473
42	1	-4.969810	-1.788804	0.546681
43	1	-5.229974	-0.401136	-0.529507
44	1	-3.715045	-0.121458	-2.629830
45	1	-2.302300	-1.184554	-2.818990
46	1	-2.080020	-3.284719	-1.324450
47	1	-3.192058	-3.511195	0.039186
48	6	2.148654	2.809213	1.063516
49	6	3.887791	0.194341	1.585371
50	6	4.084994	-1.421474	-1.166881
51	6	2.615023	0.297323	-3.412048
52	6	1.460277	2.934662	-2.035320
53	1	2.996335	3.509908	1.052270
54	1	2.046649	2.436941	2.087463
55	1	1.249261	3.381403	0.819194
56	1	4.896361	0.631261	1.544973
57	1	4.006252	-0.881460	1.741398
58	1	3.388236	0.609290	2.465083
59	1	5.109041	-1.164960	-1.474316
60	1	3.641117	-2.038166	-1.953273
61	1	4.155790	-2.035463	-0.263756
62	1	3.483186	0.744432	-3.917525
63	1	1.711861	0.690249	-3.889633
64	1	2.637452	-0.780866	-3.590856
65	1	2.231144	3.674071	-2.296836
66	1	0.713532	3.435653	-1.412391
67	1	0.965843	2.625627	-2.960681
68	1	1.306327	-2.206431	4.356653
69	1	1.652703	-3.793273	2.417541
70	1	-0.681663	-3.437487	3.333218
71	1	-3.784418	-3.714548	-1.628312
72	1	-3.935996	-1.796264	-3.148650
73	1	-5.608872	-2.039220	-1.091832

TSM11-19 (E = -1199.2922563 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.782460	-0.103127	-0.236785
2	7	0.447274	-1.236705	1.335173
3	6	-0.374672	-0.529623	2.174934
4	7	-1.592676	0.085767	-0.564271
5	6	3.056397	0.413965	0.482429
6	6	2.328352	1.626298	0.323993
7	6	3.176490	-0.193229	-0.793143
8	17	0.644140	-1.933000	-1.878351
9	6	2.078687	1.817702	-1.075965
10	6	2.576614	0.691051	-1.757458
11	6	0.826494	-2.617093	1.841585
12	6	-2.181411	0.300894	0.567576
13	6	-2.310968	0.115849	-1.903556
14	6	-1.498724	0.190784	1.860936
15	1	-0.150638	-0.593729	3.237427
16	6	-2.361573	0.792124	2.893979
17	1	0.081191	1.350160	0.082771
18	6	-3.599511	0.783886	0.894862
19	6	-3.563379	1.100363	2.368062
20	1	-3.875792	1.667681	0.322554
21	1	-4.346218	0.012446	0.667830
22	6	-4.780967	1.665499	3.043166
23	6	-1.926702	0.945243	4.328078
24	1	-2.668876	1.491079	4.917021
25	1	-0.975131	1.488488	4.395426
26	1	-1.776942	-0.031364	4.808709
27	1	-4.604524	1.891053	4.098896
28	1	-5.624023	0.961366	2.987854

29	1	-5.110263	2.591419	2.550072
30	6	2.062967	-3.151331	1.101296
31	6	1.120599	-2.642209	3.363919
32	6	-0.384534	-3.533696	1.533169
33	1	-0.564480	-3.563585	0.454937
34	1	-1.288510	-3.161679	2.029116
35	1	0.225284	-2.484249	3.973745
36	1	1.872267	-1.893206	3.637597
37	1	2.961004	-2.599649	1.385088
38	1	1.928106	-3.087747	0.021351
39	6	-3.530397	1.070000	-2.021425
40	6	-1.299915	0.602611	-2.967642
41	6	-2.779245	-1.328632	-2.200716
42	1	-1.933249	-2.016981	-2.183804
43	1	-3.515635	-1.652061	-1.454775
44	1	-4.411939	0.714606	-1.485816
45	1	-3.285659	2.086099	-1.693701
46	1	-1.005055	1.637753	-2.760197
47	1	-0.413750	-0.029452	-2.996931
48	6	2.094005	2.645803	1.409598
49	6	3.721233	0.001234	1.772809
50	6	4.004827	-1.391295	-1.175863
51	6	2.639122	0.485005	-3.248192
52	6	1.480907	3.060075	-1.685142
53	1	2.979702	3.286725	1.534208
54	1	1.894780	2.168319	2.374852
55	1	1.241379	3.290428	1.176611
56	1	4.454434	0.763396	2.071142
57	1	4.257955	-0.944777	1.669442
58	1	3.007274	-0.104903	2.596375
59	1	4.854626	-1.077274	-1.798419
60	1	3.416121	-2.111507	-1.754296
61	1	4.408956	-1.907465	-0.301396
62	1	3.656512	0.684466	-3.615200
63	1	1.958501	1.155373	-3.781855
64	1	2.379196	-0.543506	-3.515459
65	1	2.234279	3.859071	-1.737611
66	1	0.639616	3.434707	-1.092570
67	1	1.121125	2.881413	-2.702648
68	1	1.518413	-3.628987	3.623908
69	1	2.215043	-4.202609	1.372330
70	1	-0.188620	-4.552333	1.889384
71	1	-1.769657	0.574828	-3.957376
72	1	-3.801152	1.124413	-3.081511
73	1	-3.252357	-1.368054	-3.189482

M19 (E = -1199.2986638 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.814706	-0.152079	-0.030642
2	7	0.041899	1.790889	-0.366090
3	6	1.330352	1.863747	-0.081043
4	7	0.989289	-1.178753	-0.497778
5	6	-2.362567	0.481013	1.710157
6	6	-1.456735	-0.513225	2.205417
7	6	-3.162094	-0.116002	0.701112
8	17	-1.621768	-0.047121	-2.377284
9	6	-1.717419	-1.728291	1.500102
10	6	-2.757605	-1.474790	0.557618
11	6	2.098288	-0.558891	-0.071655
12	6	2.228067	0.826667	0.221705
13	1	1.798245	2.843426	-0.129500
14	6	3.608634	1.102425	0.675471
15	1	0.190130	0.194871	1.200853
16	6	3.480496	-1.169611	0.173719

17	6	4.334379	-0.032208	0.665120
18	1	3.412095	-1.971669	0.914713
19	1	3.910422	-1.614759	-0.727917
20	6	5.773522	-0.258348	1.037757
21	6	4.073675	2.478986	1.076919
22	1	5.088286	2.455770	1.484895
23	1	3.412672	2.913858	1.838508
24	1	4.079690	3.169043	0.221697
25	1	6.251669	0.655127	1.404776
26	1	6.357334	-0.614963	0.176333
27	1	5.867500	-1.023378	1.822204
28	6	-0.660781	-0.403978	3.482696
29	6	-2.533997	1.835924	2.353526
30	6	-4.324279	0.491535	-0.039647
31	6	-3.466576	-2.463722	-0.331779
32	6	-1.149989	-3.065837	1.914707
33	1	-1.287674	-0.688056	4.341285
34	1	-0.303916	0.616530	3.648232
35	1	0.211442	-1.064072	3.471076
36	1	-2.828076	1.713343	3.405072
37	1	-3.315848	2.422210	1.864171
38	1	-1.609326	2.423159	2.339596
39	1	-5.258234	-0.005202	0.258576
40	1	-4.211878	0.367914	-1.121991
41	1	-4.433339	1.558178	0.170831
42	1	-4.510662	-2.578156	-0.008544
43	1	-3.001666	-3.452187	-0.300449
44	1	-3.475985	-2.125223	-1.373675
45	1	-1.506260	-3.321280	2.922629
46	1	-0.055695	-3.063080	1.946636
47	1	-1.466308	-3.871056	1.246903
48	6	-0.519647	3.082650	-0.966865
49	6	-0.130396	4.317710	-0.108490
50	6	0.040129	3.230462	-2.401991
51	6	-2.056214	3.037968	-1.023473
52	1	-0.403037	4.162030	0.941332
53	1	0.934546	4.564128	-0.157689
54	1	1.133911	3.303168	-2.392421
55	1	-0.245878	2.365475	-3.006100
56	1	-2.407467	2.179066	-1.593455
57	1	-2.482552	3.007205	-0.019015
58	6	1.132469	-2.466916	-1.311728
59	6	-0.262324	-3.062619	-1.591211
60	6	1.777908	-2.101196	-2.670953
61	6	1.936571	-3.589491	-0.592315
62	1	-0.725391	-3.417658	-0.669430
63	1	-0.921036	-2.345017	-2.077550
64	1	1.143862	-1.382825	-3.199243
65	1	2.771425	-1.658743	-2.548399
66	1	3.017299	-3.472281	-0.670814
67	1	1.664261	-3.651068	0.466600
68	1	1.683847	-4.549122	-1.056604
69	1	1.880638	-3.000098	-3.290479
70	1	-0.148989	-3.925023	-2.257843
71	1	-0.678636	5.191275	-0.477477
72	1	-2.420289	3.949023	-1.512299
73	1	-0.359059	4.138172	-2.870242

TSM19-20 (E = -1199.2840759 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	22	0.743107	0.259274	0.077380
2	7	0.053413	0.103031	-1.677478
3	6	-0.987783	-0.811591	-1.436783
4	7	-1.230972	0.770465	0.995681
5	6	2.616337	-1.151383	-0.360804
6	6	1.902053	-1.728391	0.732110
7	6	3.158902	0.085392	0.078087
8	17	1.073924	2.705547	-0.093374
9	6	2.071673	-0.873350	1.870853
10	6	2.833757	0.243970	1.466343
11	6	-2.282726	0.429173	0.274815
12	6	-2.189258	-0.468253	-0.837420
13	1	-0.966695	-1.734297	-2.020349
14	6	-3.506954	-1.063033	-1.085374
15	1	-0.204053	-1.143339	0.251284
16	6	-3.779251	0.645545	0.503238
17	6	-4.438190	-0.411615	-0.353252
18	1	-4.096299	0.586220	1.542164
19	1	-4.062957	1.645193	0.148663
20	6	-5.933091	-0.562472	-0.362372
21	6	-3.722381	-2.169136	-2.084608
22	1	-4.776811	-2.450293	-2.155700
23	1	-3.155622	-3.068125	-1.807678
24	1	-3.383740	-1.869961	-3.085745
25	1	-6.264334	-1.344155	-1.052655
26	1	-6.423373	0.376284	-0.659352
27	1	-6.314014	-0.815393	0.637536
28	6	1.384348	-3.145285	0.784443
29	6	2.890930	-1.866611	-1.660716
30	6	4.099301	0.995866	-0.668489
31	6	3.350250	1.373091	2.319081
32	6	1.645904	-1.255592	3.267817
33	1	2.191852	-3.832886	1.078048
34	1	1.006785	-3.473589	-0.188778
35	1	0.572337	-3.253127	1.510011
36	1	3.592030	-2.696292	-1.490812
37	1	3.342388	-1.203827	-2.402624
38	1	1.981367	-2.289526	-2.099119
39	1	5.110359	0.928031	-0.241631
40	1	3.775110	2.039607	-0.601732
41	1	4.168991	0.731504	-1.726730
42	1	4.447047	1.332152	2.375425
43	1	2.964734	1.325957	3.341425
44	1	3.074963	2.345041	1.894535
45	1	2.200789	-2.145232	3.597218
46	1	0.579244	-1.501842	3.325362
47	1	1.848094	-0.460762	3.991023
48	6	0.172914	0.626500	-3.088283
49	6	-0.022435	-0.500062	-4.132565
50	6	-0.916113	1.710933	-3.277616
51	6	1.561580	1.257954	-3.289973
52	1	0.677529	-1.325138	-3.958715
53	1	-1.042844	-0.897610	-4.127116
54	1	-1.915833	1.295072	-3.112906
55	1	-0.756363	2.528267	-2.568882
56	1	1.758622	2.009309	-2.523503
57	1	2.346245	0.497544	-3.255911
58	6	-1.448889	1.494026	2.323209
59	6	-0.089660	1.905695	2.921455
60	6	-2.270141	2.795378	2.144422
61	6	-2.101794	0.518245	3.339328
62	1	0.581092	1.049518	2.988789
63	1	0.391361	2.679860	2.325322
64	1	-1.843922	3.389933	1.330164

65	1	-3.327607	2.622441	1.941668
66	1	-3.074030	0.139367	3.021775
67	1	-1.444947	-0.341918	3.504800
68	1	-2.238604	1.032619	4.297437
69	1	-2.205623	3.385203	3.065771
70	1	-0.250170	2.286157	3.936723
71	1	0.169532	-0.096975	-5.132904
72	1	1.600363	1.739763	-4.273907
73	1	-0.872264	2.111012	-4.298058

M20 (E = -1199.3265871 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.812927	-0.024518	-0.156309
2	7	-0.246723	-1.547044	-0.221232
3	6	-1.040663	-1.160524	0.972984
4	7	-0.696967	1.368125	-0.238737
5	6	2.400436	-1.198069	1.263240
6	6	1.957369	-0.054312	1.996186
7	6	3.154942	-0.733329	0.159010
8	17	1.355821	0.091064	-2.456270
9	6	2.516483	1.113057	1.384276
10	6	3.236312	0.698614	0.243281
11	6	-0.650547	-2.745780	-1.019656
12	6	-1.972075	0.903554	0.053918
13	6	-0.568872	2.825399	-0.658283
14	6	-2.208590	-0.304920	0.658827
15	1	-1.246660	-2.018909	1.614605
16	6	-3.640528	-0.526912	0.867293
17	1	-0.365902	-0.523304	1.592223
18	6	-3.345780	1.504449	-0.241445
19	6	-4.326001	0.525541	0.361220
20	1	-3.495471	2.513890	0.147250
21	1	-3.504600	1.559951	-1.323453
22	6	-5.807277	0.784070	0.331946
23	6	-4.200383	-1.739530	1.567201
24	1	-5.277507	-1.644914	1.734558
25	1	-3.723264	-1.889245	2.545305
26	1	-4.036643	-2.655732	0.984575
27	1	-6.370702	-0.022100	0.813325
28	1	-6.180682	0.876884	-0.698627
29	1	-6.063935	1.721812	0.846790
30	6	0.579112	-3.269680	-1.792359
31	6	-1.171841	-3.887488	-0.113379
32	6	-1.751486	-2.332503	-2.029934
33	1	-1.372946	-1.552243	-2.696530
34	1	-2.636585	-1.948385	-1.513645
35	1	-2.112187	-3.628777	0.382039
36	1	-0.432071	-4.153761	0.650106
37	1	1.347480	-3.629763	-1.100852
38	1	1.009608	-2.487575	-2.419188
39	6	-0.980799	3.755249	0.512587
40	6	0.897535	3.149047	-1.012522
41	6	-1.393521	3.140024	-1.938477
42	1	-1.270785	2.336437	-2.671870
43	1	-2.456173	3.286450	-1.744249
44	1	-2.002087	3.575407	0.854276
45	1	-0.310774	3.609002	1.365924
46	1	1.570433	2.882711	-0.201077
47	1	1.213507	2.626784	-1.916304
48	6	1.318815	-0.066663	3.366647
49	6	2.233659	-2.629601	1.707454
50	6	3.921511	-1.565463	-0.835907
51	6	4.069134	1.545188	-0.682767
52	6	2.521638	2.471097	2.044468

53	1	2.089633	0.065150	4.140403
54	1	0.810536	-1.013198	3.575172
55	1	0.591726	0.743525	3.493238
56	1	2.967048	-2.870053	2.490520
57	1	2.390013	-3.330100	0.883406
58	1	1.238525	-2.821740	2.120509
59	1	4.994923	-1.551129	-0.597033
60	1	3.799096	-1.181268	-1.853562
61	1	3.595340	-2.609190	-0.831252
62	1	5.130239	1.272251	-0.598613
63	1	3.982212	2.611023	-0.453196
64	1	3.772100	1.397992	-1.727716
65	1	3.114376	2.427911	2.969513
66	1	1.517396	2.808735	2.321658
67	1	2.970752	3.238722	1.408541
68	1	-1.357714	-4.774647	-0.728318
69	1	0.276428	-4.106882	-2.431857
70	1	-2.049007	-3.198619	-2.634135
71	1	0.990350	4.227520	-1.184250
72	1	-0.909326	4.803249	0.197513
73	1	-1.015738	4.066779	-2.385409

TSM20-21 (E = -1199.3016712 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.382438	-0.202737	-0.107557
2	7	0.406673	-0.338286	1.626492
3	6	-0.362907	1.581627	1.551450
4	7	-1.772112	0.326977	-0.553973
5	6	2.689589	0.518506	-0.154611
6	6	1.960665	1.525931	-0.850947
7	6	2.637380	-0.663850	-0.933360
8	17	0.011191	-2.543285	-0.493495
9	6	1.530368	0.983323	-2.105973
10	6	1.940157	-0.364593	-2.155155
11	6	0.481833	-0.948955	2.961332
12	6	-2.414883	0.990328	0.397767
13	6	-2.564080	-0.197598	-1.749991
14	6	-1.748242	1.542267	1.526865
15	1	0.186027	1.979683	2.391993
16	6	-2.727875	1.921982	2.548156
17	1	0.109489	1.837423	0.600751
18	6	-3.906466	1.228658	0.638340
19	6	-3.975325	1.747241	2.057708
20	1	-4.292869	1.991273	-0.045611
21	1	-4.515032	0.335278	0.487722
22	6	-5.302080	2.061779	2.689579
23	6	-2.330937	2.493070	3.883815
24	1	-3.202238	2.803375	4.467420
25	1	-1.681403	3.370118	3.756106
26	1	-1.772399	1.762696	4.483199
27	1	-5.190634	2.460833	3.702495
28	1	-5.934353	1.164367	2.753229
29	1	-5.861520	2.801409	2.097745
30	6	1.409832	-2.187835	2.859326
31	6	1.058342	0.015588	4.027386
32	6	-0.937936	-1.414614	3.376323
33	1	-1.321731	-2.133379	2.646133
34	1	-1.630627	-0.569340	3.424704
35	1	0.385828	0.857240	4.219245
36	1	2.031106	0.406641	3.713049
37	1	2.435970	-1.885276	2.627062
38	1	1.059472	-2.863021	2.075629
39	6	-3.530434	0.859876	-2.350275
40	6	-1.582912	-0.572463	-2.876965

41	6	-3.332339	-1.476840	-1.333342
42	1	-2.630773	-2.238644	-0.985507
43	1	-4.057818	-1.284862	-0.538705
44	1	-4.465132	0.957217	-1.796849
45	1	-3.047108	1.842453	-2.405622
46	1	-1.090753	0.316960	-3.272173
47	1	-0.834785	-1.286505	-2.536517
48	6	1.934408	2.999217	-0.511356
49	6	3.514287	0.740324	1.087602
50	6	3.377412	-1.950206	-0.669221
51	6	1.818297	-1.328821	-3.305045
52	6	0.951569	1.824524	-3.218218
53	1	2.737550	3.523426	-1.050119
54	1	2.092321	3.179090	0.556788
55	1	0.990356	3.477091	-0.798878
56	1	4.504736	1.135576	0.818645
57	1	3.669024	-0.188091	1.643267
58	1	3.046393	1.459326	1.767028
59	1	4.309242	-1.981898	-1.253264
60	1	2.773914	-2.819525	-0.945986
61	1	3.644310	-2.054803	0.386523
62	1	2.812213	-1.570828	-3.706969
63	1	1.220035	-0.917350	-4.123058
64	1	1.355746	-2.270016	-2.984684
65	1	1.673206	2.598956	-3.514821
66	1	0.029864	2.340540	-2.923234
67	1	0.732709	1.227326	-4.107432
68	1	1.194603	-0.522216	4.972772
69	1	1.415852	-2.721851	3.817387
70	1	-0.904450	-1.895815	4.361711
71	1	-2.143724	-1.039397	-3.694717
72	1	-3.792536	0.558004	-3.370167
73	1	-3.878277	-1.871147	-2.198884

M21 (E = -1199.3190574 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.844799	-0.529151	-0.303692
2	7	0.741679	-0.588946	1.373608
3	6	-0.442598	2.475965	0.876663
4	7	-1.573575	0.220721	-0.790205
5	6	3.185780	-0.087931	-0.392830
6	6	2.526288	1.137074	-0.708298
7	6	2.997077	-0.976843	-1.483583
8	17	0.501698	-2.856162	-0.724055
9	6	1.939377	0.998397	-2.007421
10	6	2.233186	-0.305835	-2.483429
11	6	0.732252	-0.899696	2.797089
12	6	-2.227041	0.913071	0.074330
13	6	-2.328764	-0.539836	-1.884513
14	6	-1.615476	1.858030	1.050173
15	1	-0.057250	3.191492	1.592148
16	6	-2.596752	2.097000	2.118726
17	1	0.156641	2.282520	0.001369
18	6	-3.722517	0.925140	0.406023
19	6	-3.783289	1.555159	1.778460
20	1	-4.275121	1.550225	-0.303379
21	1	-4.172068	-0.067823	0.373970
22	6	-5.080800	1.570167	2.532524
23	6	-2.258315	2.899739	3.344746
24	1	-3.095185	2.945687	4.046515
25	1	-1.989724	3.930084	3.074147
26	1	-1.397047	2.469772	3.870917
27	1	-4.992936	2.065513	3.503189
28	1	-5.440021	0.545953	2.705255

29	1	-5.862193	2.086505	1.956857
30	6	1.624385	-2.140604	3.056526
31	6	1.253257	0.305917	3.617217
32	6	-0.725410	-1.229119	3.213772
33	1	-1.094589	-2.081123	2.633411
34	1	-1.382397	-0.372736	3.030366
35	1	0.640887	1.192114	3.422512
36	1	2.289194	0.537130	3.347490
37	1	2.665312	-1.928749	2.793781
38	1	1.279642	-2.983858	2.450701
39	6	-3.471295	0.297619	-2.520351
40	6	-1.311433	-0.813323	-3.007676
41	6	-2.871530	-1.881780	-1.340781
42	1	-2.061575	-2.487057	-0.929362
43	1	-3.629605	-1.735895	-0.566206
44	1	-4.392192	0.291190	-1.935780
45	1	-3.157094	1.335677	-2.680326
46	1	-0.937414	0.128389	-3.420448
47	1	-0.473948	-1.411880	-2.650036
48	6	2.747982	2.431542	0.041933
49	6	4.127511	-0.294954	0.766555
50	6	3.642124	-2.327715	-1.651754
51	6	1.957081	-0.875517	-3.852714
52	6	1.282041	2.111514	-2.790527
53	1	3.795399	2.749110	-0.066667
54	1	2.544524	2.334172	1.113444
55	1	2.125775	3.243312	-0.347036
56	1	5.137213	0.057419	0.506553
57	1	4.207938	-1.351085	1.040487
58	1	3.802250	0.255923	1.653381
59	1	4.584566	-2.228831	-2.211329
60	1	2.993998	-3.018436	-2.197738
61	1	3.873251	-2.789495	-0.687506
62	1	2.889203	-0.940568	-4.432222
63	1	1.260510	-0.255978	-4.424390
64	1	1.540857	-1.888351	-3.797309
65	1	2.041728	2.789008	-3.206608
66	1	0.609891	2.719818	-2.174861
67	1	0.696905	1.724789	-3.629992
68	1	1.218666	0.084399	4.691321
69	1	1.584175	-2.423722	4.115993
70	1	-0.771215	-1.483717	4.280276
71	1	-1.798142	-1.372430	-3.814392
72	1	-3.711918	-0.132144	-3.498249
73	1	-3.336441	-2.438233	-2.163125

M15 (E = -675.8599464 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.034526	0.539374	-0.204746
2	7	1.641083	0.343435	-0.144968
3	6	-0.774656	-1.363046	0.929390
4	6	-0.813250	-1.651525	-0.466362
5	6	-1.756801	-0.356883	1.192998
6	17	-0.602186	2.770382	-0.617693
7	6	-1.825089	-0.827349	-1.055563
8	6	-2.421993	-0.043876	-0.028340
9	6	3.085174	0.179514	-0.066015
10	6	3.550715	0.579561	1.356845
11	6	3.473970	-1.290149	-0.356052
12	6	3.740810	1.112774	-1.115401
13	1	3.458692	2.153393	-0.926475
14	1	3.410247	0.843159	-2.124596
15	1	3.128327	-1.587810	-1.351907
16	1	3.025339	-1.961366	0.384070

17	1	3.085950	-0.068883	2.107908
18	1	3.271041	1.616768	1.569776
19	6	-0.057970	-2.754154	-1.168945
20	6	0.030615	-2.102469	1.970521
21	6	-2.091362	0.216410	2.549770
22	6	-3.577841	0.908048	-0.191520
23	6	-2.237467	-0.840406	-2.508406
24	1	-0.654810	-3.677260	-1.182298
25	1	0.888236	-2.975678	-0.669000
26	1	0.170041	-2.497111	-2.208671
27	1	-0.550969	-2.940608	2.380071
28	1	0.308434	-1.455350	2.808838
29	1	0.952839	-2.511664	1.549345
30	1	-2.897272	-0.362527	3.022459
31	1	-2.431517	1.254766	2.480244
32	1	-1.231592	0.188581	3.227333
33	1	-4.532787	0.385298	-0.039601
34	1	-3.596479	1.352746	-1.190878
35	1	-3.529194	1.729868	0.528965
36	1	-3.055428	-1.556911	-2.668541
37	1	-1.412771	-1.139206	-3.163911
38	1	-2.592683	0.140907	-2.839553
39	1	4.563065	-1.413083	-0.316356
40	1	4.640012	0.486567	1.444292
41	1	4.833736	1.029967	-1.073226

M16 (E = -523.4597698 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.249944	0.738935	-0.017703
2	6	0.070473	0.274765	-0.070148
3	6	2.501607	-0.067052	0.020534
4	6	-1.127978	1.181243	-0.049075
5	6	-2.323176	0.328718	0.010750
6	6	-0.478240	-1.155528	-0.117870
7	6	-1.975106	-0.976150	-0.013793
8	1	-0.210180	-1.654518	-1.055488
9	1	-0.079703	-1.778334	0.690652
10	6	-2.866066	-2.184722	0.027941
11	6	-3.707422	0.914992	0.083805
12	1	-4.480652	0.143725	0.132924
13	1	-3.910739	1.542681	-0.794187
14	1	-3.811879	1.557105	0.968499
15	1	-3.925765	-1.923675	0.095265
16	1	-2.617664	-2.820344	0.889844
17	1	-2.725082	-2.802635	-0.870464
18	6	2.546967	-1.236391	-0.992979
19	6	3.635696	0.926022	-0.323660
20	6	2.701178	-0.587861	1.464660
21	1	2.685326	0.244941	2.175696
22	1	1.914588	-1.296367	1.746283
23	1	1.910929	-2.074465	-0.696933
24	1	2.240674	-0.897262	-1.989511
25	1	3.509011	1.311162	-1.341911
26	1	3.615120	1.775835	0.365835
27	1	4.614581	0.437585	-0.254896
28	1	3.573488	-1.613115	-1.066715
29	1	3.667690	-1.097710	1.550596
30	6	-1.080383	2.521162	-0.080026
31	1	-1.979288	3.125799	-0.059313
32	1	-0.125980	3.031197	-0.126254

M22 (E = -924.1538813 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	22	-0.292612	-0.075288	-0.377424
2	7	-0.824011	1.524750	-0.237695
3	6	-1.895595	-1.063152	1.053921
4	6	-0.654983	-1.037711	1.756564
5	6	-1.761137	-1.980210	-0.026827
6	17	-0.203662	-0.537238	-2.704592
7	6	0.221420	-1.986776	1.136853
8	6	-0.458436	-2.562708	0.035824
9	6	-1.357265	2.877892	-0.206771
10	6	-2.766621	2.886902	-0.850996
11	6	-1.442503	3.389279	1.253204
12	6	-0.410120	3.794246	-1.024840
13	1	-0.334134	3.431375	-2.054674
14	1	0.593838	3.796740	-0.585457
15	1	-0.451159	3.380078	1.721183
16	1	-2.110098	2.754542	1.845510
17	1	-3.449679	2.243448	-0.286514
18	1	-2.711583	2.516165	-1.879694
19	6	-0.390429	-0.313227	3.055779
20	6	-3.171134	-0.378918	1.479287
21	6	-2.841688	-2.376996	-1.002092
22	6	0.050780	-3.636941	-0.891248
23	6	1.581586	-2.385025	1.654812
24	1	-0.676538	-0.935996	3.916082
25	1	-0.959381	0.619503	3.119024
26	1	0.670039	-0.064833	3.176846
27	1	-3.744540	-1.026479	2.158871
28	1	-3.813445	-0.148250	0.623764
29	1	-2.970498	0.559115	2.004355
30	1	-3.369269	-3.275024	-0.648103
31	1	-2.425735	-2.599152	-1.989356
32	1	-3.586691	-1.584754	-1.127282
33	1	-0.463571	-4.590611	-0.706576
34	1	1.123223	-3.812183	-0.755991
35	1	-0.114900	-3.366844	-1.940527
36	1	1.486823	-3.172423	2.416043
37	1	2.105121	-1.544071	2.121892
38	1	2.224721	-2.776341	0.859792
39	1	-1.827021	4.416493	1.282574
40	1	-3.178794	3.903839	-0.865285
41	1	-0.786249	4.825041	-1.039428
42	7	1.871238	0.314209	-0.130313
43	6	2.783213	-0.292240	-0.925864
44	6	2.313891	1.203477	0.789573
45	6	4.151835	-0.037508	-0.826635
46	1	2.388254	-0.977989	-1.665401
47	6	3.665980	1.503358	0.954261
48	1	1.550945	1.686446	1.386515
49	6	4.605938	0.873421	0.131642
50	1	4.840460	-0.543394	-1.492475
51	1	3.969171	2.222760	1.705444
52	1	5.663396	1.091382	0.231492

1^{Me} (E = -830.6734761 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.001867	0.332183	0.065924
2	7	-3.128708	1.018424	-0.726470
3	6	1.453943	-1.618229	0.113252
4	6	0.700049	-1.763875	-1.083535
5	6	0.540367	-1.703638	1.211357
6	17	-0.600823	0.998823	2.344349
7	6	-0.672500	-1.887184	-0.733513
8	6	-0.769803	-1.872807	0.690689
9	6	-2.018843	0.765003	-0.478742

10	6	0.445571	1.100908	-2.021346
11	6	1.525341	1.509955	-1.162209
12	1	-0.281877	1.836593	-2.352195
13	6	-0.126606	2.869047	-0.034394
14	6	1.187993	2.428343	-0.124202
15	1	-0.456152	3.392649	0.852244
16	1	-0.748005	2.974046	-0.910306
17	6	2.198441	2.827974	0.936177
18	6	2.976195	1.211787	-1.490634
19	1	3.596233	1.032484	-0.607463
20	1	3.408921	2.071083	-2.026222
21	1	3.063230	0.347349	-2.152829
22	1	2.858439	3.615072	0.543948
23	1	2.833382	1.994229	1.254077
24	1	1.687446	3.222157	1.818360
25	6	1.254019	-2.030214	-2.459339
26	6	2.954910	-1.702813	0.253999
27	6	0.950860	-1.826800	2.656393
28	6	-2.016358	-2.102131	1.505538
29	6	-1.786997	-2.184248	-1.706991
30	1	1.431485	-3.109327	-2.578698
31	1	2.206679	-1.524680	-2.637183
32	1	0.559213	-1.726825	-3.248436
33	1	3.246572	-2.716286	0.566734
34	1	3.340025	-1.010104	1.010555
35	1	3.467965	-1.490101	-0.686511
36	1	1.289670	-2.854032	2.859116
37	1	0.123196	-1.598309	3.330215
38	1	1.773570	-1.150197	2.908857
39	1	-2.086796	-3.154861	1.814932
40	1	-2.921253	-1.865588	0.936543
41	1	-2.017417	-1.481371	2.406125
42	1	-1.765043	-3.243033	-2.002461
43	1	-1.700429	-1.585559	-2.620115
44	1	-2.770044	-1.987023	-1.270027
45	1	0.705023	0.405947	-2.810341
46	6	-4.491267	1.375817	-0.978344
47	1	-4.661008	2.408423	-0.663572
48	1	-4.704285	1.286215	-2.046298
49	1	-5.159043	0.715356	-0.419855

TS1^{Me}-3^{Me} (E = -830.669533 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-1.151381	-0.548876	-0.646017
2	7	-3.170645	1.347574	-2.316808
3	6	1.225520	-1.092852	-0.868639
4	6	1.093479	-0.298542	0.298187
5	6	0.831228	-0.303088	-1.988951
6	17	-1.538490	-2.344000	-2.240448
7	6	0.608336	0.990335	-0.095938
8	6	0.455985	0.985943	-1.511397
9	6	-2.529348	0.600833	-1.633418
10	6	-1.822390	0.188380	1.375307
11	6	-2.055559	-1.226485	1.433167
12	1	-2.662720	0.856978	1.205190
13	6	-3.578413	-0.805908	-0.407430
14	6	-2.909447	-1.752084	0.457332
15	1	-4.155804	-1.247772	-1.212263
16	1	-4.065652	0.035545	0.080751
17	6	-3.241243	-3.226178	0.370385
18	6	-1.431829	-2.105924	2.500871
19	1	-0.973482	-3.015128	2.097131
20	1	-2.208994	-2.421736	3.211620
21	1	-0.674718	-1.559562	3.066821

22	1	-4.037362	-3.466613	1.091340
23	1	-2.382068	-3.865469	0.593636
24	1	-3.597260	-3.482364	-0.629598
25	6	1.601774	-0.661237	1.670415
26	6	1.769965	-2.496824	-0.938534
27	6	0.978609	-0.681308	-3.438861
28	6	0.170119	2.194718	-2.367758
29	6	0.542122	2.229480	0.762249
30	1	2.656675	-0.366296	1.767394
31	1	1.545374	-1.737083	1.859895
32	1	1.050546	-0.149873	2.465087
33	1	2.835749	-2.483296	-1.208218
34	1	1.239296	-3.089809	-1.689085
35	1	1.680125	-3.014517	0.021856
36	1	1.944646	-0.321241	-3.823000
37	1	0.188651	-0.242345	-4.056176
38	1	0.937347	-1.763452	-3.577903
39	1	1.109588	2.709285	-2.617249
40	1	-0.475942	2.913437	-1.855038
41	1	-0.319706	1.922118	-3.306663
42	1	1.409084	2.874796	0.559231
43	1	0.557020	1.990151	1.828889
44	1	-0.360046	2.818854	0.565435
45	1	-1.117117	0.586570	2.093541
46	6	-4.566703	1.656754	-2.586664
47	1	-4.747663	2.710470	-2.359293
48	1	-4.761733	1.500581	-3.650609
49	1	-5.242224	1.031408	-1.994849

3^{Me} (E = -830.7077649 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.467417	-0.775951	-0.324679
2	7	-0.644604	0.662488	-1.282985
3	6	2.695206	-1.391866	0.279847
4	6	2.022068	-1.013309	1.476354
5	6	2.785971	-0.241235	-0.558617
6	17	0.366172	-2.318911	-2.084291
7	6	1.683342	0.372599	1.371150
8	6	2.171308	0.848058	0.120147
9	6	-1.077393	0.494049	-0.109001
10	6	-1.237820	1.290933	-2.467165
11	6	-0.894539	-1.809891	1.041440
12	6	-2.330597	-1.842851	0.601960
13	1	-0.795323	-1.280035	1.992523
14	6	-2.397339	0.660485	0.553446
15	6	-3.066401	-0.718818	0.433671
16	1	-2.252744	0.950401	1.601136
17	1	-3.024250	1.426239	0.081236
18	6	-4.539818	-0.647950	0.090845
19	6	-2.880864	-3.238448	0.368549
20	1	-3.875098	-3.254291	-0.084174
21	1	-2.924473	-3.799329	1.312740
22	1	-2.200671	-3.785983	-0.296968
23	1	-5.009584	-1.631833	0.030212
24	1	-4.701768	-0.138241	-0.870969
25	1	-5.086068	-0.069013	0.850418
26	6	1.870541	-1.868886	2.707860
27	6	3.292366	-2.745690	-0.011965
28	6	3.471843	-0.184136	-1.900911
29	6	2.105214	2.273712	-0.367285
30	6	1.082116	1.213565	2.469863
31	1	2.777299	-1.805393	3.326037
32	1	1.716007	-2.923403	2.458054
33	1	1.027593	-1.549192	3.327321

34	1	4.343677	-2.779182	0.308103
35	1	3.258368	-2.978658	-1.080016
36	1	2.760977	-3.543945	0.515648
37	1	4.544116	0.023717	-1.775458
38	1	3.056433	0.604018	-2.537034
39	1	3.376007	-1.130432	-2.441094
40	1	2.961213	2.849446	0.011725
41	1	1.194344	2.777644	-0.028164
42	1	2.129354	2.329660	-1.460042
43	1	1.856532	1.524802	3.185440
44	1	0.318945	0.665490	3.032308
45	1	0.616158	2.121705	2.074754
46	1	-0.503762	-2.824213	1.174854
47	1	-0.539169	2.028284	-2.872398
48	1	-2.188408	1.780189	-2.229866
49	1	-1.399161	0.519995	-3.226426

TS3^{Me}-4^{Me} (E = -830.6981749 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.307741	-0.418734	-0.299960
2	7	-0.746711	1.337527	-0.624382
3	6	2.469196	-1.468286	0.312607
4	6	1.944076	-0.792581	1.449264
5	6	2.749840	-0.496521	-0.690312
6	17	0.124603	-1.547954	-2.318159
7	6	1.851180	0.594690	1.130374
8	6	2.359860	0.776176	-0.195325
9	6	-1.497772	0.439095	-0.158967
10	6	-1.037891	2.715783	-1.046719
11	6	-0.873506	-1.754898	0.997416
12	6	-2.230199	-2.152485	0.478649
13	1	-0.959680	-1.202246	1.940991
14	6	-2.915718	0.229507	0.210495
15	6	-3.206132	-1.267191	0.173358
16	1	-3.065813	0.656684	1.215364
17	1	-3.600029	0.778211	-0.451490
18	6	-4.622779	-1.597037	-0.246653
19	6	-2.404132	-3.654457	0.325790
20	1	-3.326911	-3.944458	-0.181978
21	1	-2.381277	-4.152076	1.305656
22	1	-1.564127	-4.056726	-0.256389
23	1	-4.833095	-2.668233	-0.253523
24	1	-4.836544	-1.205258	-1.253114
25	1	-5.348005	-1.125648	0.434197
26	6	1.714419	-1.396827	2.810418
27	6	2.757491	-2.944313	0.207388
28	6	3.420593	-0.766272	-2.011811
29	6	2.584256	2.093182	-0.898368
30	6	1.450364	1.690311	2.090914
31	1	2.647758	-1.374672	3.390838
32	1	1.389875	-2.439675	2.750949
33	1	0.959968	-0.847445	3.382253
34	1	3.800152	-3.161865	0.480377
35	1	2.599085	-3.310321	-0.812343
36	1	2.115789	-3.529582	0.874005
37	1	4.512422	-0.799929	-1.885552
38	1	3.194824	0.012910	-2.746302
39	1	3.102210	-1.722099	-2.438049
40	1	3.638810	2.394035	-0.824739
41	1	1.985147	2.894286	-0.456144
42	1	2.333569	2.036974	-1.963499
43	1	2.310104	2.008749	2.697678
44	1	0.668167	1.360045	2.783408
45	1	1.076312	2.575155	1.566126

46	1	-0.276644	-2.648766	1.200579
47	1	-0.544909	3.415941	-0.365473
48	1	-2.115330	2.910851	-1.047501
49	1	-0.634439	2.873410	-2.050265

4^{Me} (E = -830.7008941 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.341341	-0.386986	-0.378123
2	7	-0.725371	1.333570	-0.537358
3	6	2.492033	-1.484738	0.175113
4	6	1.986075	-0.871214	1.351990
5	6	2.770597	-0.456964	-0.774082
6	17	0.196128	-1.633152	-2.364721
7	6	1.904299	0.534874	1.113436
8	6	2.406430	0.789429	-0.199773
9	6	-1.489479	0.323790	-0.614482
10	6	-1.041869	2.767202	-0.477419
11	6	-0.952424	-1.493196	1.021188
12	6	-2.308725	-2.023658	0.603859
13	1	-1.060631	-0.788259	1.859422
14	6	-2.939777	0.070075	-0.616657
15	6	-3.238211	-1.320721	-0.075164
16	1	-3.490001	0.852255	-0.068939
17	1	-3.294620	0.133928	-1.656332
18	6	-4.645997	-1.774116	-0.404194
19	6	-2.538609	-3.458702	1.053406
20	1	-3.485982	-3.885267	0.716563
21	1	-2.499648	-3.532786	2.149401
22	1	-1.731455	-4.094553	0.664024
23	1	-4.916762	-2.726586	0.054395
24	1	-4.780248	-1.872504	-1.492309
25	1	-5.378227	-1.026496	-0.063565
26	6	1.771404	-1.535045	2.687517
27	6	2.772671	-2.951734	-0.029573
28	6	3.434703	-0.661058	-2.110635
29	6	2.628152	2.142578	-0.832614
30	6	1.537183	1.565469	2.155193
31	1	2.662294	-1.402207	3.317826
32	1	1.599431	-2.610987	2.588470
33	1	0.919969	-1.111608	3.230354
34	1	3.840092	-3.171760	0.114826
35	1	2.501674	-3.268118	-1.042408
36	1	2.209936	-3.573613	0.673895
37	1	4.521333	-0.770814	-1.982646
38	1	3.263986	0.186638	-2.781625
39	1	3.061077	-1.559131	-2.611095
40	1	3.682406	2.440827	-0.746508
41	1	2.028661	2.919124	-0.348808
42	1	2.374929	2.142356	-1.898702
43	1	2.375757	1.730230	2.846754
44	1	0.676865	1.252477	2.758124
45	1	1.294932	2.532271	1.703895
46	1	-0.354801	-2.322555	1.405015
47	1	-0.590106	3.206847	0.415876
48	1	-2.124158	2.932635	-0.456737
49	1	-0.618470	3.263064	-1.355663

TS4^{Me}-5^{Me} (E = -830.6862308 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	22	0.727945	-0.140872	-0.750833
2	7	-0.467373	1.370362	-0.570204
3	6	2.955165	-1.098614	-0.546702
4	6	2.524729	-0.667950	0.739764
5	6	3.075635	0.052948	-1.381972
6	17	0.394166	-1.444902	-2.695183
7	6	2.356129	0.750274	0.691709
8	6	2.707987	1.194060	-0.620602
9	6	-1.154448	0.241407	-0.591465
10	6	-0.896939	2.702305	-0.151604
11	6	-0.740542	-1.044152	0.859760
12	6	-2.163531	-1.533805	0.972075
13	1	-0.404698	-0.567080	1.786735
14	6	-2.609561	0.012554	-0.818734
15	6	-3.091791	-1.046888	0.136456
16	1	-3.187379	0.939447	-0.689962
17	1	-2.757490	-0.302337	-1.861241
18	6	-4.546288	-1.435567	0.042008
19	6	-2.397072	-2.588304	2.033581
20	1	-3.443395	-2.898056	2.103143
21	1	-2.089216	-2.215603	3.020413
22	1	-1.792064	-3.482758	1.829264
23	1	-4.832273	-2.193269	0.775381
24	1	-4.774289	-1.831704	-0.957635
25	1	-5.193753	-0.559868	0.191903
26	6	2.434324	-1.523638	1.979742
27	6	3.328407	-2.503534	-0.947495
28	6	3.590116	0.052055	-2.798849
29	6	2.793144	2.627152	-1.087905
30	6	2.039365	1.631660	1.876643
31	1	3.396746	-1.528246	2.510674
32	1	2.187475	-2.563966	1.743242
33	1	1.679105	-1.155223	2.681799
34	1	4.418894	-2.638774	-0.912342
35	1	2.995041	-2.728125	-1.965475
36	1	2.882919	-3.248376	-0.280315
37	1	4.688318	-0.001160	-2.809715
38	1	3.298381	0.960734	-3.334991
39	1	3.206097	-0.803843	-3.362251
40	1	3.829024	2.990657	-1.033709
41	1	2.182159	3.290575	-0.469111
42	1	2.460046	2.739215	-2.125362
43	1	2.950369	1.840897	2.455233
44	1	1.323145	1.161389	2.559732
45	1	1.620103	2.593655	1.567638
46	1	-0.095047	-1.921546	0.708382
47	1	-0.216753	3.452020	-0.561806
48	1	-0.891209	2.787706	0.943873
49	1	-1.911152	2.919294	-0.509044

5^{Me} (E = -830.7116004 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.694786	-0.108999	-0.395838
2	7	-0.383057	1.417211	0.004553
3	6	2.870575	-1.132057	-0.499570
4	6	2.647005	-0.637913	0.817256
5	6	2.894066	-0.018806	-1.389002
6	17	-0.018868	-1.324050	-2.279653
7	6	2.531122	0.784991	0.735938
8	6	2.686012	1.168664	-0.631812
9	6	-1.299330	0.411093	0.137454
10	6	-0.738237	2.815185	-0.193080
11	6	-1.102465	-0.652273	1.157964
12	6	-2.288122	-1.572154	0.976124

13	1	-0.927815	-0.311458	2.185335
14	6	-2.617470	0.193502	-0.572739
15	6	-3.119703	-1.100397	0.032385
16	1	-3.331885	1.011023	-0.391336
17	1	-2.499579	0.112594	-1.660752
18	6	-4.411643	-1.701830	-0.450115
19	6	-2.406489	-2.823228	1.804047
20	1	-3.331157	-3.369101	1.596038
21	1	-2.387632	-2.588797	2.877715
22	1	-1.565085	-3.503097	1.608750
23	1	-4.677762	-2.612847	0.093858
24	1	-4.346129	-1.952483	-1.517679
25	1	-5.238759	-0.986732	-0.339410
26	6	2.674122	-1.449402	2.092185
27	6	3.113051	-2.568359	-0.889388
28	6	3.187941	-0.082824	-2.865922
29	6	2.812700	2.577228	-1.160449
30	6	2.411969	1.722188	1.914096
31	1	3.693798	-1.490050	2.501201
32	1	2.346336	-2.480402	1.924537
33	1	2.032079	-1.016605	2.867304
34	1	4.190355	-2.769461	-0.977597
35	1	2.649108	-2.803860	-1.852231
36	1	2.708053	-3.263870	-0.147248
37	1	4.273630	-0.097344	-3.040145
38	1	2.779047	0.783370	-3.395794
39	1	2.761117	-0.981014	-3.321306
40	1	3.870061	2.837574	-1.312891
41	1	2.397011	3.308648	-0.461505
42	1	2.302783	2.704537	-2.121573
43	1	3.407204	1.975709	2.306752
44	1	1.841147	1.275113	2.735010
45	1	1.914101	2.656575	1.639630
46	1	-0.111532	-1.274648	0.969368
47	1	0.139502	3.380103	-0.512448
48	1	-1.121036	3.256251	0.738889
49	1	-1.516253	2.924707	-0.962264

TS5^{Me}-6^{Me} (E = -830.7083392 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.389559	-0.241346	-0.077127
2	7	-0.580596	1.144596	0.922141
3	6	2.125673	-1.741266	0.454803
4	6	2.037153	-0.749611	1.480896
5	6	2.521265	-1.081443	-0.742743
6	17	-0.182701	0.018581	-2.322657
7	6	2.423707	0.509601	0.923245
8	6	2.708611	0.305860	-0.450012
9	6	-1.653360	0.361518	0.643600
10	6	-0.723654	2.596429	1.001489
11	6	-1.598266	-1.042159	0.926254
12	6	-2.821716	-1.650063	0.314683
13	1	-1.263896	-1.376458	1.906760
14	6	-2.886518	0.656933	-0.191073
15	6	-3.545570	-0.701454	-0.309249
16	1	-3.548910	1.377845	0.308042
17	1	-2.636852	1.076449	-1.172183
18	6	-4.845976	-0.853489	-1.049398
19	6	-3.094582	-3.123910	0.437036
20	1	-4.040100	-3.407963	-0.033553
21	1	-3.136600	-3.430971	1.491308
22	1	-2.293264	-3.707654	-0.037048
23	1	-5.218836	-1.881767	-1.024438
24	1	-4.732608	-0.562182	-2.102672

25	1	-5.620024	-0.202669	-0.618899
26	6	1.743474	-1.003045	2.941043
27	6	1.991850	-3.233923	0.639658
28	6	2.810175	-1.744213	-2.065620
29	6	3.190476	1.341790	-1.434446
30	6	2.618668	1.778796	1.711272
31	1	2.677282	-1.143899	3.504310
32	1	1.139783	-1.905510	3.084097
33	1	1.206189	-0.165097	3.397142
34	1	2.969790	-3.680412	0.871023
35	1	1.610713	-3.720674	-0.263341
36	1	1.314152	-3.482983	1.462331
37	1	3.874524	-2.011256	-2.137507
38	1	2.571329	-1.084930	-2.905042
39	1	2.228393	-2.662495	-2.193487
40	1	4.280089	1.273774	-1.563257
41	1	2.960419	2.357822	-1.098886
42	1	2.730082	1.203829	-2.417816
43	1	3.584147	1.756389	2.236415
44	1	1.837076	1.909616	2.466613
45	1	2.618409	2.663822	1.067482
46	1	-0.476331	-1.716885	0.218204
47	1	0.261771	3.063966	0.980748
48	1	-1.228202	2.887005	1.933442
49	1	-1.309187	2.990720	0.158645

6^{Me} (E = -830.7181998 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.315048	-0.031718	0.177926
2	7	-0.541419	-1.212533	-1.160023
3	6	2.034211	1.596329	0.250176
4	6	1.899062	1.132770	-1.094168
5	6	2.455154	0.491270	1.042137
6	17	-0.181353	-1.171710	2.124639
7	6	2.304940	-0.235359	-1.140579
8	6	2.626566	-0.638842	0.180012
9	6	-1.747230	-0.660270	-0.865940
10	6	-0.456074	-2.651992	-1.416288
11	6	-1.932570	0.710179	-0.880893
12	6	-3.217550	1.034493	-0.241150
13	1	-1.360868	1.400653	-1.486573
14	6	-2.961731	-1.300732	-0.216219
15	6	-3.835246	-0.112629	0.125259
16	1	-3.468391	-1.994406	-0.900537
17	1	-2.678801	-1.875922	0.671842
18	6	-5.184381	-0.299501	0.761496
19	6	-3.693736	2.453538	-0.086085
20	1	-4.694374	2.506394	0.352743
21	1	-3.722077	2.968249	-1.056200
22	1	-3.009825	3.019524	0.560594
23	1	-5.700829	0.653444	0.912856
24	1	-5.096993	-0.791578	1.740413
25	1	-5.830579	-0.936603	0.140618
26	6	1.540396	1.975382	-2.294162
27	6	1.934709	3.027767	0.714036
28	6	2.795868	0.537906	2.509531
29	6	3.143629	-1.987439	0.614611
30	6	2.452174	-1.040048	-2.405504
31	1	2.446029	2.393914	-2.756507
32	1	0.895576	2.816864	-2.020466
33	1	1.023792	1.387840	-3.060565
34	1	2.918937	3.513700	0.648628
35	1	1.597495	3.092856	1.752318
36	1	1.235263	3.604250	0.101917

37	1	3.849360	0.820259	2.649234
38	1	2.640829	-0.432853	2.988105
39	1	2.181116	1.269263	3.043304
40	1	4.235589	-1.957969	0.735277
41	1	2.913400	-2.767455	-0.117345
42	1	2.711189	-2.292397	1.572496
43	1	3.282912	-0.646283	-3.006739
44	1	1.546336	-0.998456	-3.019620
45	1	2.670933	-2.090959	-2.196198
46	1	-0.297213	1.447632	0.658942
47	1	0.591103	-2.946145	-1.503181
48	1	-0.966281	-2.912544	-2.353382
49	1	-0.906725	-3.236714	-0.601182

7^{Me} (E = -963.4610289 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.781852	-0.044633	-0.340699
2	7	1.022954	-0.699538	-0.706757
3	6	-2.515537	0.322509	1.361854
4	6	-1.386533	-0.357802	1.928566
5	6	-3.089767	-0.517746	0.373538
6	17	-1.629633	0.047727	-2.621288
7	6	-1.269741	-1.620203	1.284370
8	6	-2.309910	-1.706729	0.300679
9	6	2.309333	-0.355010	-0.329523
10	6	0.938098	-1.885072	-1.594435
11	6	2.731970	0.520190	0.627744
12	6	4.194649	0.594362	0.635872
13	1	2.089136	1.087020	1.286565
14	6	3.553639	-0.925702	-0.999875
15	6	4.702457	-0.238032	-0.306234
16	1	3.613207	-2.016140	-0.887077
17	1	3.549065	-0.730573	-2.080263
18	6	6.134560	-0.518756	-0.671276
19	6	4.943349	1.487437	1.592614
20	1	6.027722	1.410164	1.465357
21	1	4.707205	1.231083	2.634698
22	1	4.661505	2.539794	1.449634
23	1	6.830345	0.065476	-0.059521
24	1	6.338795	-0.277884	-1.725173
25	1	6.386638	-1.581237	-0.535144
26	6	-0.621256	0.076667	3.153722
27	6	-3.075668	1.630536	1.862971
28	6	-4.333656	-0.246525	-0.430358
29	6	-2.640833	-2.901131	-0.560516
30	6	-0.309950	-2.717198	1.676735
31	1	-1.117984	-0.291984	4.063202
32	1	-0.557860	1.166512	3.225501
33	1	0.399901	-0.315321	3.149523
34	1	-3.731554	1.457681	2.727916
35	1	-3.668265	2.140017	1.097105
36	1	-2.282886	2.313447	2.184804
37	1	-5.185980	-0.804257	-0.016591
38	1	-4.204873	-0.547836	-1.474175
39	1	-4.596806	0.815526	-0.423504
40	1	-3.492248	-3.451116	-0.135176
41	1	-1.802430	-3.601067	-0.627574
42	1	-2.912705	-2.599817	-1.577215
43	1	-0.711830	-3.292536	2.522970
44	1	0.661543	-2.313674	1.977936
45	1	-0.136668	-3.420122	0.856524
46	1	0.093931	0.946857	0.674874
47	6	-1.080772	4.640185	-0.922102
48	7	-1.087865	3.226290	-0.701766

49	6	-1.052333	2.074031	-0.552334
50	1	-2.058151	5.055497	-0.665880
51	1	-0.312728	5.108630	-0.302204
52	1	-0.871431	4.840053	-1.975460
53	1	-0.107555	-2.134076	-1.797580
54	1	1.415124	-2.763953	-1.140353
55	1	1.404129	-1.688919	-2.568851

TS7^{Me}-8^{Me} (E = -963.4593184 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-1.006066	0.185486	-0.105173
2	7	0.524273	-1.011061	-0.330699
3	6	-2.553377	1.215930	1.499204
4	6	-1.714741	0.252107	2.155716
5	6	-3.352872	0.531178	0.546926
6	17	-1.714949	0.378031	-2.388779
7	6	-2.001095	-1.025107	1.602890
8	6	-3.000731	-0.846593	0.588372
9	6	1.843326	-1.028577	0.087275
10	6	0.128102	-2.176122	-1.159624
11	6	2.448556	-0.322060	1.084308
12	6	3.882397	-0.623581	1.121027
13	1	1.955005	0.363755	1.758961
14	6	2.916305	-1.882103	-0.577658
15	6	4.184374	-1.530390	0.159805
16	1	2.693738	-2.954156	-0.498292
17	1	2.987367	-1.662985	-1.651036
18	6	5.505089	-2.162676	-0.184785
19	6	4.808216	0.016575	2.124141
20	1	5.838846	-0.335446	2.015999
21	1	4.484201	-0.200658	3.151417
22	1	4.812999	1.109852	2.013651
23	1	6.311040	-1.794438	0.458959
24	1	5.793185	-1.956144	-1.226151
25	1	5.469779	-3.257194	-0.077408
26	6	-0.862801	0.509407	3.373981
27	6	-2.689309	2.665010	1.894784
28	6	-4.422420	1.134676	-0.324068
29	6	-3.677502	-1.936547	-0.205875
30	6	-1.453789	-2.340745	2.100834
31	1	-1.461903	0.390340	4.288477
32	1	-0.451947	1.523529	3.376225
33	1	-0.024142	-0.190396	3.433975
34	1	-3.440401	2.771437	2.690143
35	1	-3.006492	3.288710	1.053792
36	1	-1.747935	3.071877	2.277085
37	1	-5.414472	0.979562	0.123761
38	1	-4.425239	0.683477	-1.320397
39	1	-4.278841	2.211713	-0.451809
40	1	-4.645289	-2.190758	0.249136
41	1	-3.080914	-2.853491	-0.234513
42	1	-3.865410	-1.623130	-1.237351
43	1	-2.039473	-2.697958	2.959827
44	1	-0.411631	-2.248810	2.421112
45	1	-1.495823	-3.117019	1.331140
46	1	0.154599	1.018630	0.827505
47	6	0.907132	4.330965	-0.063539
48	7	-0.021231	3.266001	-0.340392
49	6	-0.447343	2.173316	-0.229735
50	1	0.356690	5.225432	0.237163
51	1	1.600227	4.038692	0.731508
52	1	1.469775	4.559257	-0.971895
53	1	-0.940468	-2.132539	-1.390322
54	1	0.325296	-3.123673	-0.640250

55	1	0.654398	-2.179542	-2.122843

8^{Me} (E = -963.4776729 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.908005	-0.169752	-0.522631
2	7	0.879325	-0.860348	-0.899100
3	6	-2.412661	0.674892	1.238004
4	6	-1.129017	0.403943	1.807588
5	6	-2.944478	-0.543203	0.752382
6	17	-2.167121	-0.663222	-2.396815
7	6	-0.870814	-0.990139	1.678344
8	6	-1.985453	-1.574235	1.000587
9	6	2.135459	-0.461072	-0.481569
10	6	0.868781	-2.092081	-1.731115
11	6	2.482562	0.560549	0.355803
12	6	3.937921	0.627798	0.498257
13	1	1.806404	1.234774	0.857608
14	6	3.424783	-1.134289	-0.930512
15	6	4.513336	-0.349428	-0.244664
16	1	3.448741	-2.193528	-0.643922
17	1	3.534018	-1.110592	-2.022273
18	6	5.967900	-0.679659	-0.435549
19	6	4.610201	1.667668	1.357776
20	1	5.699754	1.568222	1.345292
21	1	4.277463	1.590872	2.401916
22	1	4.360583	2.680840	1.014472
23	1	6.614844	-0.007384	0.137315
24	1	6.262901	-0.602558	-1.492293
25	1	6.193536	-1.708115	-0.117598
26	6	-0.309943	1.394279	2.597694
27	6	-3.131143	1.997110	1.247562
28	6	-4.324282	-0.725034	0.177503
29	6	-2.181954	-3.041999	0.711528
30	6	0.289588	-1.743512	2.279306
31	1	-0.814112	1.618252	3.548112
32	1	-0.179181	2.343197	2.066752
33	1	0.679733	0.997637	2.838015
34	1	-4.035576	1.932806	1.867645
35	1	-3.425451	2.302121	0.237934
36	1	-2.498810	2.790474	1.654518
37	1	-5.045191	-0.916840	0.985379
38	1	-4.367864	-1.565925	-0.519490
39	1	-4.653892	0.167782	-0.361769
40	1	-2.695898	-3.530613	1.551332
41	1	-1.229667	-3.561811	0.565674
42	1	-2.790870	-3.197515	-0.184314
43	1	0.083532	-1.979147	3.332868
44	1	1.218493	-1.167746	2.237870
45	1	0.466255	-2.689494	1.758831
46	1	0.632995	2.178722	-0.703954
47	6	-0.862349	4.014600	-1.700187
48	7	-1.289384	2.676984	-1.257772
49	6	-0.432516	1.870265	-0.793385
50	1	-1.444887	4.773411	-1.165091
51	1	0.212287	4.195304	-1.535885
52	1	-1.085417	4.123965	-2.767504
53	1	-0.151115	-2.347236	-2.020430
54	1	1.295687	-2.941974	-1.183110
55	1	1.442773	-1.943746	-2.654191

TS8^{Me}-9^{Me} (E = -963.477474 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.689283	-0.191634	0.163658
2	7	0.661195	1.732337	0.510852
3	6	1.683752	-2.174821	1.106851
4	6	1.806707	-1.113889	2.051885
5	6	2.423738	-1.809059	-0.049468
6	17	0.787712	0.109161	-2.162834
7	6	2.705244	-0.141709	1.517204
8	6	3.072969	-0.558200	0.213500
9	6	-0.698374	1.915610	0.460980
10	6	1.502687	2.799006	-0.042567
11	6	-1.594841	1.305926	1.300600
12	6	-2.962554	1.559694	0.846194
13	1	-1.336486	0.805264	2.223853
14	6	-1.486220	2.647220	-0.612424
15	6	-2.923318	2.354936	-0.252742
16	1	-1.282518	3.725762	-0.620147
17	1	-1.218875	2.267154	-1.605283
18	6	-4.062376	2.938920	-1.039700
19	6	-4.166391	1.016452	1.571442
20	1	-5.103718	1.358875	1.123299
21	1	-4.163224	1.326489	2.625294
22	1	-4.169265	-0.081416	1.557651
23	1	-5.034882	2.652479	-0.627513
24	1	-4.031655	2.607282	-2.087019
25	1	-4.013396	4.037224	-1.052420
26	6	1.230394	-1.082024	3.445435
27	6	1.039790	-3.515658	1.343214
28	6	2.642271	-2.666654	-1.269217
29	6	4.065580	0.094776	-0.714177
30	6	3.226902	1.040356	2.292766
31	1	1.940766	-1.509480	4.167806
32	1	0.304229	-1.660757	3.517236
33	1	1.015243	-0.057362	3.767305
34	1	1.797359	-4.231280	1.693268
35	1	0.595859	-3.919608	0.428824
36	1	0.254908	-3.469018	2.103743
37	1	3.516764	-3.318285	-1.126679
38	1	2.815122	-2.055207	-2.158571
39	1	1.777951	-3.305731	-1.473140
40	1	4.969478	-0.524459	-0.795786
41	1	4.373531	1.080890	-0.355308
42	1	3.651874	0.216131	-1.720399
43	1	3.741633	0.694728	3.198974
44	1	2.419093	1.712784	2.601672
45	1	3.946248	1.622984	1.711009
46	1	-1.431678	-1.655786	1.618562
47	6	-2.629823	-2.787658	-0.383182
48	7	-1.454033	-1.904313	-0.430393
49	6	-0.977801	-1.413809	0.633116
50	1	1.323306	3.748833	0.478728
51	1	2.553539	2.534001	0.071858
52	1	1.308914	2.939257	-1.115660
53	1	-3.434314	-2.352363	-0.986475
54	1	-2.374585	-3.756159	-0.828625
55	1	-2.994519	-2.947461	0.645667

9^{Me} (E = -963.4983595 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	22	0.779327	-0.072158	0.364759
2	7	-0.922504	-0.984753	0.026503
3	6	2.584885	1.262774	-0.656573
4	6	1.535977	1.016384	-1.602078
5	6	3.159178	0.022517	-0.306015
6	17	1.537456	-1.522477	2.140619
7	6	1.501454	-0.385835	-1.866487
8	6	2.481833	-1.005451	-1.043585
9	6	-2.221383	-0.522360	-0.060243
10	6	-0.794260	-2.460172	-0.049391
11	6	-2.687427	0.693463	-0.467616
12	6	-4.146518	0.749018	-0.329724
13	1	-2.088991	1.494116	-0.876016
14	6	-3.429015	-1.357016	0.349813
15	6	-4.605064	-0.432813	0.149129
16	1	-3.528681	-2.262328	-0.262764
17	1	-3.336932	-1.698175	1.389068
18	6	-6.014960	-0.869486	0.438835
19	6	-4.938374	1.975713	-0.705177
20	1	-6.013474	1.831938	-0.559820
21	1	-4.773691	2.241613	-1.758562
22	1	-4.630947	2.842372	-0.103619
23	1	-6.738379	-0.076914	0.220126
24	1	-6.142064	-1.151613	1.494359
25	1	-6.295659	-1.748924	-0.159734
26	6	0.768404	2.064123	-2.368624
27	6	3.020691	2.624164	-0.176974
28	6	4.339690	-0.211542	0.599030
29	6	2.891937	-2.456702	-1.045372
30	6	0.656802	-1.047733	-2.927269
31	1	1.289583	2.311231	-3.304892
32	1	0.662637	2.991714	-1.797579
33	1	-0.235207	1.716639	-2.633145
34	1	3.707159	3.087149	-0.899502
35	1	3.542918	2.568217	0.783136
36	1	2.171136	3.305500	-0.055911
37	1	5.238573	-0.428463	0.004319
38	1	4.162924	-1.059082	1.268023
39	1	4.556215	0.663863	1.218906
40	1	3.872431	-2.572352	-1.528464
41	1	2.181498	-3.081021	-1.595610
42	1	2.973801	-2.849826	-0.026397
43	1	1.120395	-0.921438	-3.915963
44	1	-0.348241	-0.617191	-2.972269
45	1	0.548895	-2.121483	-2.750485
46	1	-0.690857	2.673684	0.695553
47	6	0.724824	1.939337	3.109317
48	7	0.518050	1.357140	1.785124
49	6	-0.122101	1.743438	0.772619
50	1	-1.295184	-2.856420	-0.942872
51	1	0.257477	-2.747348	-0.088999
52	1	-1.218707	-2.939456	0.842214
53	1	0.406228	1.215515	3.863598
54	1	1.792355	2.127202	3.255210
55	1	0.162575	2.873220	3.219786

TS9^{Me}-10^{Me} (E = -963.482729 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.834987	-0.427205	0.062009
2	7	-2.163443	0.917322	-0.385571
3	6	-2.350791	0.686769	0.881607
4	7	0.498787	0.924319	0.875023
5	6	-2.032971	-2.472840	0.454475
6	6	-1.375050	-2.082732	1.666363

7	6	-1.037874	-2.794606	-0.499914
8	17	0.008026	-0.175746	-2.199162
9	6	0.032339	-2.182756	1.453251
10	6	0.242619	-2.599413	0.109175
11	6	-2.868402	1.781742	-1.323608
12	6	0.003484	1.891129	1.628313
13	6	1.860659	1.096566	0.330847
14	6	-1.228954	1.824484	2.323540
15	1	-3.300811	0.769491	1.407745
16	6	-1.543081	3.191645	2.794245
17	1	-1.470593	0.973475	2.944672
18	6	0.531776	3.310646	1.704598
19	6	-0.566432	4.055144	2.434108
20	1	1.480988	3.352162	2.258420
21	1	0.743511	3.714158	0.706585
22	6	-0.458398	5.534456	2.683010
23	6	-2.799792	3.482939	3.572225
24	1	-2.856376	4.527343	3.893252
25	1	-2.856843	2.850450	4.469176
26	1	-3.693424	3.266247	2.971168
27	1	-1.308876	5.915809	3.256938
28	1	-0.414406	6.098338	1.739554
29	1	0.457848	5.778441	3.240483
30	6	-2.052069	-1.860083	2.995174
31	6	-3.526661	-2.598587	0.279722
32	6	-1.258870	-3.349815	-1.882872
33	6	1.561980	-2.913707	-0.548989
34	6	1.095452	-1.977571	2.505220
35	1	-2.222978	-2.821490	3.501254
36	1	-3.024640	-1.371602	2.880641
37	1	-1.442622	-1.245438	3.665502
38	1	-3.886554	-3.551260	0.693727
39	1	-3.815347	-2.567832	-0.775358
40	1	-4.063406	-1.795051	0.796099
41	1	-1.120327	-4.440676	-1.878412
42	1	-0.555216	-2.919576	-2.600751
43	1	-2.270721	-3.145727	-2.246263
44	1	1.698139	-4.000630	-0.640948
45	1	2.406830	-2.526318	0.029439
46	1	1.613930	-2.482305	-1.554188
47	1	1.261931	-2.905447	3.070598
48	1	0.812621	-1.199970	3.221727
49	1	2.053442	-1.686031	2.064016
50	1	2.217046	0.143906	-0.062211
51	1	2.556599	1.440737	1.105562
52	1	1.861713	1.813389	-0.499225
53	1	-2.604277	2.829222	-1.129832
54	1	-2.567793	1.528122	-2.341739
55	1	-3.955799	1.672323	-1.218266

10^{Me} (E = -963.5174613 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.670747	-0.010072	-0.345370
2	7	0.532145	1.220923	-1.056566
3	6	0.913232	1.250386	0.283311
4	7	0.800699	-1.507865	0.309042
5	6	-2.318419	1.461166	0.479525
6	6	-1.773986	0.772454	1.608249
7	6	-3.007654	0.506430	-0.321052
8	17	-0.952393	-1.228545	-2.407457
9	6	-2.141235	-0.603496	1.500872
10	6	-2.906564	-0.766814	0.314589
11	6	0.837520	2.212324	-2.073541
12	6	1.962978	-1.007049	0.503238

13	6	0.661708	-2.955591	0.052843
14	6	2.121873	0.461548	0.783641
15	1	0.749201	2.185023	0.830431
16	6	3.554084	0.719993	0.316148
17	1	2.108990	0.578761	1.882127
18	6	3.320792	-1.643267	0.327720
19	6	4.208932	-0.431176	0.088950
20	1	3.625575	-2.202234	1.225139
21	1	3.335112	-2.355999	-0.504049
22	6	5.640669	-0.640249	-0.323905
23	6	4.083759	2.124769	0.245834
24	1	5.126924	2.161543	-0.081193
25	1	4.018725	2.611863	1.229615
26	1	3.487353	2.732259	-0.446288
27	1	6.172233	0.304724	-0.467600
28	1	5.696968	-1.205758	-1.264670
29	1	6.186245	-1.223420	0.431854
30	6	-1.160633	1.406398	2.831896
31	6	-2.276816	2.953351	0.255870
32	6	-3.794988	0.790996	-1.575817
33	6	-3.567795	-2.030581	-0.173365
34	6	-1.857905	-1.653674	2.548193
35	1	-1.926421	1.552855	3.608208
36	1	-0.727517	2.385237	2.608238
37	1	-0.370570	0.782644	3.263933
38	1	-3.075495	3.453545	0.822409
39	1	-2.414152	3.207106	-0.799829
40	1	-1.324638	3.387020	0.579500
41	1	-4.856186	0.949351	-1.334491
42	1	-3.728977	-0.039646	-2.284059
43	1	-3.435458	1.690320	-2.086115
44	1	-4.651622	-1.993118	0.006155
45	1	-3.180316	-2.916150	0.340578
46	1	-3.407846	-2.172631	-1.247063
47	1	-2.551973	-1.552927	3.394764
48	1	-0.841278	-1.566294	2.947303
49	1	-1.975609	-2.667011	2.151798
50	1	-0.295300	-3.291737	0.456695
51	1	1.465005	-3.532941	0.521065
52	1	1.906501	2.195687	-2.330016
53	1	0.264991	1.995705	-2.980713
54	1	0.649892	-3.135457	-1.025902
55	1	0.589563	3.229636	-1.729465

11^{Me} (E = -963.4887044 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-1.075504	0.241129	-0.518622
2	7	0.165511	1.591511	-0.353214
3	6	0.875906	0.481601	0.169876
4	7	3.532195	1.926834	-0.728415
5	6	-3.056792	0.954733	0.548178
6	6	-2.099119	0.684860	1.563261
7	6	-3.382533	-0.281641	-0.097547
8	17	-1.145570	-0.605048	-2.687945
9	6	-1.798561	-0.712290	1.524118
10	6	-2.612922	-1.307675	0.506906
11	6	0.437264	2.983229	-0.012460
12	6	3.368293	0.737106	-0.321573
13	6	4.770600	2.646616	-0.412927
14	6	2.089450	-0.060413	-0.614836
15	1	1.085108	0.535096	1.247622
16	6	2.479505	-1.473704	-0.215141
17	1	1.851113	0.007478	-1.681938
18	6	4.326928	-0.157608	0.463151

19	6	3.675988	-1.519655	0.392270
20	1	5.330209	-0.163224	0.019046
21	1	4.455658	0.189847	1.498372
22	6	4.404914	-2.714711	0.946948
23	6	1.563609	-2.624902	-0.525432
24	1	1.966143	-3.582750	-0.182789
25	1	1.384000	-2.694224	-1.606490
26	1	0.582376	-2.481627	-0.055579
27	1	3.835004	-3.641820	0.837144
28	1	4.622960	-2.576740	2.015769
29	1	5.371966	-2.850719	0.441842
30	6	-1.583784	1.653151	2.596478
31	6	-3.681498	2.294059	0.234655
32	6	-4.418270	-0.469797	-1.176961
33	6	-2.683404	-2.774901	0.161316
34	6	-0.954623	-1.451308	2.533220
35	1	-2.144617	1.538880	3.534702
36	1	-1.693188	2.691693	2.272148
37	1	-0.526806	1.483725	2.826052
38	1	-4.660284	2.385970	0.725827
39	1	-3.846460	2.428664	-0.840296
40	1	-3.059758	3.123788	0.584141
41	1	-5.392470	-0.715615	-0.730806
42	1	-4.146801	-1.280413	-1.858938
43	1	-4.550563	0.435938	-1.777001
44	1	-3.541958	-3.246416	0.659776
45	1	-1.785107	-3.311530	0.481460
46	1	-2.798664	-2.930901	-0.916138
47	1	-1.557472	-1.714124	3.414469
48	1	-0.110942	-0.845904	2.877352
49	1	-0.548301	-2.381475	2.124741
50	1	5.269834	2.919051	-1.350329
51	1	5.481811	2.095141	0.216604
52	1	4.512074	3.583088	0.095718
53	1	-0.403709	3.615084	-0.316466
54	1	0.601573	3.100445	1.069219
55	1	1.343424	3.315654	-0.530087

TS11^{Me}-12^{Me} (E = -963.4604818 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.990432	0.033892	-0.345796
2	7	0.302974	-0.849834	1.206870
3	6	-0.283999	0.371020	1.413144
4	7	-2.408198	-1.126587	-0.087791
5	6	3.190296	0.306084	0.370466
6	6	2.567078	1.584395	0.497240
7	6	3.263847	-0.001370	-1.020923
8	17	0.532500	-1.458079	-2.102300
9	6	2.252254	2.057476	-0.817999
10	6	2.687954	1.078439	-1.750038
11	6	0.584837	-1.750555	2.310636
12	6	-2.222865	0.102199	-0.300464
13	6	-3.502595	-1.844157	-0.740290
14	6	-1.125006	0.917687	0.389932
15	1	-0.022496	0.969749	2.288971
16	6	-1.744385	2.289012	0.508768
17	1	-0.310879	1.126650	-0.815122
18	6	-3.062806	1.114348	-1.069393
19	6	-2.800280	2.400353	-0.318263
20	1	-2.742164	1.182469	-2.118971
21	1	-4.124598	0.855728	-1.080017
22	6	-3.692783	3.587925	-0.547938
23	6	-1.235700	3.326984	1.471487
24	1	-1.834249	4.240559	1.425356

25	1	-0.195137	3.598760	1.267719
26	1	-1.274544	2.957389	2.504553
27	1	-3.394808	4.461738	0.037754
28	1	-4.734453	3.347408	-0.293190
29	1	-3.684756	3.873784	-1.609252
30	6	2.534965	2.390985	1.773638
31	6	3.839318	-0.477445	1.485342
32	6	3.932758	-1.212759	-1.619301
33	6	2.602559	1.180360	-3.250704
34	6	1.728601	3.426879	-1.179259
35	1	3.522614	2.839369	1.954759
36	1	2.292854	1.776204	2.646628
37	1	1.811447	3.208443	1.730187
38	1	4.887707	-0.170770	1.612833
39	1	3.836394	-1.553068	1.281184
40	1	3.332405	-0.319534	2.442140
41	1	4.999564	-1.008902	-1.791561
42	1	3.480473	-1.489227	-2.574864
43	1	3.865452	-2.083157	-0.958724
44	1	3.546909	1.559114	-3.667394
45	1	1.805205	1.862252	-3.562666
46	1	2.400019	0.205825	-3.704441
47	1	2.562881	4.102970	-1.415099
48	1	1.163203	3.880342	-0.361369
49	1	1.073538	3.393199	-2.055412
50	1	-3.063103	-2.583244	-1.420434
51	1	-4.200390	-1.218438	-1.312886
52	1	-4.063656	-2.397723	0.020568
53	1	1.342725	-2.478885	2.011476
54	1	0.943474	-1.204712	3.198612
55	1	-0.326213	-2.294605	2.592083

12^{Me} (E = -963.4773152 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.712706	0.398773	0.060462
2	7	-0.078977	0.550535	1.886545
3	6	0.965544	-0.320785	1.717640
4	7	2.102974	2.298598	0.619888
5	6	-2.709199	-0.755196	0.548142
6	6	-1.722789	-1.734859	0.238889
7	6	-2.975760	-0.016098	-0.643869
8	17	-1.129851	2.580188	-0.581453
9	6	-1.361361	-1.583136	-1.133234
10	6	-2.142642	-0.521241	-1.676449
11	6	-0.645489	0.703060	3.221755
12	6	2.428730	1.153241	0.181192
13	6	2.626405	3.505553	-0.013491
14	6	1.966381	-0.132182	0.792246
15	1	0.945266	-1.256126	2.287293
16	6	2.905663	-1.171093	0.342873
17	1	0.370930	0.120019	-1.185932
18	6	3.444175	0.773100	-0.894626
19	6	3.730749	-0.680608	-0.610041
20	1	3.026480	0.911264	-1.901315
21	1	4.349886	1.385747	-0.841546
22	6	4.813242	-1.391228	-1.370088
23	6	2.899950	-2.567225	0.908714
24	1	3.687631	-3.185026	0.469746
25	1	1.941192	-3.069800	0.728809
26	1	3.055228	-2.551215	1.995708
27	1	4.912452	-2.441876	-1.083595
28	1	5.785369	-0.903195	-1.211167
29	1	4.614438	-1.351464	-2.450727
30	6	-1.293746	-2.861439	1.146160

31	6	-3.504567	-0.658550	1.826534
32	6	-4.051774	1.025397	-0.802588
33	6	-2.111903	-0.029182	-3.099422
34	6	-0.444717	-2.497006	-1.906660
35	1	-2.005451	-3.695840	1.068569
36	1	-1.261791	-2.558052	2.197260
37	1	-0.307456	-3.249892	0.877839
38	1	-4.452710	-1.205390	1.723091
39	1	-3.753817	0.377666	2.078182
40	1	-2.967697	-1.090537	2.675311
41	1	-4.999825	0.542583	-1.080894
42	1	-3.799265	1.750913	-1.579583
43	1	-4.220107	1.581814	0.124292
44	1	-2.893202	-0.518370	-3.698384
45	1	-1.147847	-0.236051	-3.573646
46	1	-2.279272	1.051220	-3.149090
47	1	-0.991344	-3.389881	-2.242647
48	1	0.401753	-2.834108	-1.300945
49	1	-0.037706	-1.999217	-2.790841
50	1	1.786934	4.025872	-0.491380
51	1	3.408074	3.339609	-0.767746
52	1	3.018923	4.171643	0.763158
53	1	-1.627087	1.176876	3.158878
54	1	-0.746344	-0.266646	3.736898
55	1	0.004019	1.344196	3.831855

TS12^{Me}-19^{Me} (E = -963.477027 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.788753	0.449633	0.160730
2	7	-0.011314	0.388167	1.929054
3	6	1.094101	-0.407072	1.729618
4	7	1.947181	2.254096	0.478184
5	6	-2.802004	-0.713998	0.499297
6	6	-1.778914	-1.692672	0.348806
7	6	-2.973069	-0.060437	-0.763050
8	17	-1.471601	2.636472	-0.090402
9	6	-1.274697	-1.596672	-0.980068
10	6	-2.027187	-0.594214	-1.668309
11	6	-0.564216	0.435433	3.281619
12	6	2.495567	1.141208	0.209681
13	6	2.399814	3.476986	-0.177560
14	6	2.116601	-0.151461	0.852926
15	1	1.119843	-1.351593	2.282604
16	6	3.140991	-1.135105	0.474474
17	1	0.260643	0.365131	-1.139162
18	6	3.679606	0.840488	-0.709622
19	6	4.013763	-0.598897	-0.409603
20	1	3.412142	0.984725	-1.765094
21	1	4.528145	1.505039	-0.510387
22	6	5.191911	-1.247784	-1.077234
23	6	3.164542	-2.533421	1.035504
24	1	3.991994	-3.120280	0.628455
25	1	2.232353	-3.069209	0.813604
26	1	3.273663	-2.516949	2.128221
27	1	5.310807	-2.298468	-0.798401
28	1	6.123231	-0.722397	-0.821278
29	1	5.092544	-1.196029	-2.171025
30	6	-1.407325	-2.747446	1.360851
31	6	-3.698063	-0.524850	1.698811
32	6	-4.060856	0.925617	-1.094404
33	6	-1.876909	-0.205790	-3.116011
34	6	-0.246817	-2.505008	-1.604768
35	1	-2.062448	-3.622765	1.247253
36	1	-1.515758	-2.389797	2.388930

37	1	-0.377493	-3.093196	1.232654
38	1	-4.662083	-1.027432	1.536312
39	1	-3.910393	0.533126	1.887659
40	1	-3.257396	-0.947111	2.606211
41	1	-4.960220	0.388705	-1.429615
42	1	-3.758736	1.609050	-1.892373
43	1	-4.334912	1.534389	-0.228567
44	1	-2.592839	-0.756596	-3.742669
45	1	-0.870881	-0.423169	-3.486033
46	1	-2.060328	0.863268	-3.264178
47	1	-0.734223	-3.386678	-2.045410
48	1	0.480886	-2.862664	-0.870585
49	1	0.308369	-1.996243	-2.397732
50	1	1.576160	3.858698	-0.793352
51	1	3.291196	3.366958	-0.810975
52	1	2.602658	4.234300	0.588564
53	1	-1.566565	0.868275	3.259540
54	1	-0.614026	-0.566591	3.738530
55	1	0.064597	1.068041	3.921892

19^{Me} (E = -963.5188804 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.974159	0.010110	-0.611772
2	7	-0.352863	1.609495	-0.974307
3	6	-1.661681	1.642123	-0.725016
4	7	-0.805965	-1.188277	-0.433086
5	6	2.700926	1.178816	0.576992
6	6	3.174304	-0.155458	0.404745
7	6	1.522809	1.120318	1.380886
8	17	1.779790	-1.479664	-2.253309
9	6	2.310800	-1.030741	1.115260
10	6	1.277609	-0.248119	1.707517
11	6	0.165315	2.876142	-1.547404
12	6	-2.032795	-0.759119	-0.245188
13	6	-0.639887	-2.659101	-0.385997
14	6	-2.464860	0.587341	-0.323591
15	1	-2.160817	2.599611	-0.882323
16	6	-3.911130	0.632708	-0.044586
17	1	1.776622	1.052330	-1.621726
18	6	-3.249086	-1.613434	0.067829
19	6	-4.376557	-0.614673	0.189715
20	1	-3.430924	-2.346097	-0.729811
21	1	-3.102339	-2.198016	0.985761
22	6	-5.772841	-1.068219	0.513803
23	6	-4.691024	1.921071	-0.048425
24	1	-5.741270	1.760215	0.210380
25	1	-4.660919	2.399337	-1.037176
26	1	-4.272979	2.639376	0.670167
27	1	-6.473590	-0.229839	0.575999
28	1	-5.806184	-1.602930	1.474438
29	1	-6.153049	-1.763783	-0.248754
30	6	4.439139	-0.549421	-0.308904
31	6	3.470293	2.419798	0.199910
32	6	0.770051	2.292847	1.958380
33	6	0.211099	-0.730404	2.658950
34	6	2.531094	-2.513570	1.275496
35	1	5.292961	-0.521542	0.383839
36	1	4.658093	0.128458	-1.139237
37	1	4.368393	-1.559681	-0.720201
38	1	4.264764	2.601949	0.937850
39	1	2.834760	3.309467	0.182474
40	1	3.940654	2.323561	-0.782563
41	1	1.149662	2.530359	2.962441
42	1	-0.299796	2.081545	2.050387

43	1	0.878724	3.190786	1.344052
44	1	0.527962	-0.566882	3.698699
45	1	0.011745	-1.798987	2.540031
46	1	-0.733727	-0.196659	2.515101
47	1	3.355140	-2.694440	1.979710
48	1	2.800078	-2.987178	0.325718
49	1	1.646013	-3.019836	1.670180
50	1	0.348379	2.756562	-2.620228
51	1	1.110109	3.153250	-1.081063
52	1	-0.554187	3.693476	-1.401597
53	1	-0.970219	-3.066009	0.578872
54	1	0.402923	-2.919537	-0.545468
55	1	-1.224587	-3.138943	-1.181199

20^{Me} (E = -963.4813566 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-1.299456	-0.453906	0.060875
2	7	0.268873	0.594814	0.490669
3	6	1.312575	-0.306965	0.375824
4	7	3.108705	2.082534	-0.668186
5	6	-2.852274	1.038619	1.084516
6	6	-3.412160	-0.277358	1.094591
7	6	-2.696849	1.441697	-0.269446
8	17	-0.904654	-2.118812	-1.472322
9	6	-3.632998	-0.670034	-0.258111
10	6	-3.165052	0.375206	-1.100002
11	6	0.577134	1.957423	0.938452
12	6	3.516471	0.977767	-0.168692
13	6	4.120217	3.070523	-1.068912
14	6	2.665005	-0.172861	0.214854
15	1	0.981479	-1.341006	0.473335
16	6	3.574313	-1.329197	0.372006
17	1	-1.319930	-1.364783	1.463871
18	6	4.966933	0.527434	-0.018939
19	6	4.866364	-0.948404	0.265077
20	1	5.541628	0.738379	-0.929335
21	1	5.471090	1.073002	0.792457
22	6	6.113119	-1.776708	0.399729
23	6	3.065790	-2.720113	0.649958
24	1	3.884428	-3.440646	0.724293
25	1	2.391849	-3.061977	-0.146591
26	1	2.499988	-2.756960	1.590769
27	1	5.898177	-2.826660	0.618109
28	1	6.754774	-1.389636	1.204999
29	1	6.709893	-1.741008	-0.523409
30	6	-3.911241	-1.002223	2.318916
31	6	-2.627558	1.859377	2.331075
32	6	-2.272534	2.792292	-0.795597
33	6	-3.243116	0.425225	-2.604982
34	6	-4.293716	-1.950780	-0.698355
35	1	-4.946761	-0.703729	2.538112
36	1	-3.300910	-0.773829	3.197005
37	1	-3.898491	-2.086689	2.178569
38	1	-3.565066	1.938434	2.896669
39	1	-2.301970	2.876375	2.097824
40	1	-1.881254	1.409505	2.995890
41	1	-3.093398	3.238358	-1.372292
42	1	-1.402441	2.730484	-1.458536
43	1	-2.025544	3.484900	0.012611
44	1	-4.174820	0.916235	-2.920207
45	1	-3.224506	-0.575539	-3.044047
46	1	-2.410632	0.992385	-3.033993
47	1	-5.386914	-1.842421	-0.660357
48	1	-4.021181	-2.790420	-0.051287

49	1	-4.016228	-2.217780	-1.720887
50	1	1.175179	1.909287	1.858990
51	1	-0.346854	2.487817	1.148914
52	1	1.167808	2.495266	0.191048
53	1	4.886799	3.239782	-0.298614
54	1	3.622542	4.022805	-1.271802
55	1	4.632836	2.758839	-1.991025

21^{Me} (E = -963.5003545 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.715149	-0.146697	-0.155434
2	7	-0.290685	1.605832	-0.340498
3	6	-1.627492	1.672380	-0.079591
4	7	-1.115410	-1.175334	-0.692128
5	6	2.824639	0.788792	-0.953545
6	6	2.855147	-0.636813	-1.056407
7	6	2.807161	1.131508	0.431483
8	17	-0.047838	-1.077731	1.952566
9	6	2.812972	-1.165642	0.262765
10	6	2.793571	-0.070064	1.179451
11	6	0.228358	2.961818	-0.641837
12	6	-2.294667	-0.694159	-0.475502
13	6	-1.010983	-2.591815	-1.083513
14	6	-2.554629	0.663934	-0.089991
15	1	-2.009698	2.675123	0.116770
16	6	-4.003365	0.798714	0.134807
17	1	0.765567	-0.723357	-1.706656
18	6	-3.621796	-1.422684	-0.550563
19	6	-4.624891	-0.374401	-0.122755
20	1	-3.822013	-1.797913	-1.563453
21	1	-3.623943	-2.299643	0.109527
22	6	-6.086598	-0.712619	-0.040532
23	6	-4.630681	2.094438	0.574926
24	1	-5.709781	1.995214	0.720273
25	1	-4.465150	2.887202	-0.167712
26	1	-4.192761	2.440256	1.520799
27	1	-6.690023	0.135828	0.295587
28	1	-6.259671	-1.544696	0.657257
29	1	-6.474764	-1.033292	-1.018409
30	6	3.167927	-1.410772	-2.313542
31	6	3.026058	1.703875	-2.140170
32	6	2.969428	2.496135	1.059734
33	6	2.943830	-0.152346	2.674188
34	6	2.911661	-2.625495	0.633533
35	1	4.257418	-1.495357	-2.441093
36	1	2.759764	-0.919540	-3.201425
37	1	2.759731	-2.425551	-2.278726
38	1	3.917688	1.395984	-2.701802
39	1	3.183426	2.742627	-1.834581
40	1	2.179343	1.681491	-2.837155
41	1	3.848621	2.496223	1.717188
42	1	2.106930	2.780739	1.672956
43	1	3.123459	3.278892	0.311874
44	1	4.002913	-0.033591	2.949087
45	1	2.595872	-1.111539	3.062073
46	1	2.374282	0.631320	3.182991
47	1	3.962548	-2.916367	0.775336
48	1	2.498303	-3.271781	-0.148507
49	1	2.373593	-2.838833	1.561365
50	1	-0.295462	3.384492	-1.509010
51	1	1.283259	2.926785	-0.875423
52	1	0.081383	3.637138	0.212406
53	1	-1.145563	-3.234630	-0.204902
54	1	-0.018677	-2.774737	-1.500338

55	1	-1.757858	-2.861918	-1.839622

TS21^{Me}-13^{Me} (E = -963.4996556 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.099926	0.039280	-0.189637
2	7	0.018648	0.070345	1.804591
3	6	1.151679	0.028658	2.550342
4	7	1.924672	1.233101	-0.068955
5	6	-1.329876	-1.901761	-0.124640
6	6	-0.240930	-2.152725	-1.011435
7	6	-2.127772	-0.866889	-0.687905
8	17	-0.798534	2.277853	-0.648463
9	6	-0.389712	-1.287087	-2.142476
10	6	-1.553684	-0.508791	-1.947515
11	6	-1.213223	0.145947	2.612273
12	6	2.714942	1.144263	0.951961
13	6	2.397265	1.999879	-1.237579
14	6	2.403164	0.459395	2.179857
15	1	1.028232	-0.321790	3.577939
16	6	3.609025	0.480469	3.024501
17	1	1.468719	-0.876568	-0.405296
18	6	4.124381	1.690721	1.071172
19	6	4.595192	1.175007	2.412599
20	1	4.755195	1.347345	0.240810
21	1	4.132831	2.788518	1.027341
22	1	-1.208822	-0.601360	3.418702
23	1	-2.088575	-0.012533	1.988092
24	1	-1.301298	1.143421	3.061520
25	1	1.564034	2.158724	-1.921502
26	1	3.193508	1.449713	-1.756935
27	1	2.784599	2.982300	-0.943805
28	6	5.983319	1.482193	2.899240
29	1	6.740235	1.118298	2.189395
30	1	6.137288	2.566790	2.997368
31	1	6.191518	1.027327	3.872263
32	6	3.650689	-0.173110	4.380405
33	1	2.926720	0.289676	5.065194
34	1	3.394850	-1.238963	4.311513
35	1	4.639533	-0.093066	4.840044
36	6	0.521769	-1.263536	-3.344844
37	1	0.265934	-2.071543	-4.044826
38	1	0.444656	-0.319349	-3.893419
39	1	1.569959	-1.400596	-3.055782
40	6	-2.187611	0.422968	-2.944301
41	1	-2.979670	-0.107696	-3.493176
42	1	-2.631256	1.292220	-2.453401
43	1	-1.464578	0.791327	-3.677949
44	6	-3.452503	-0.338351	-0.195509
45	1	-4.241721	-0.550966	-0.929350
46	1	-3.755215	-0.803829	0.747381
47	1	-3.424703	0.748208	-0.050758
48	6	-1.633807	-2.745059	1.089927
49	1	-1.894671	-3.766413	0.780190
50	1	-0.774649	-2.816842	1.765795
51	1	-2.478184	-2.351616	1.661492
52	6	0.707507	-3.320421	-0.903410
53	1	0.221935	-4.237127	-1.269733
54	1	1.612874	-3.159144	-1.495508
55	1	1.015409	-3.497374	0.132037

13^{Me} (E = -963.5024612 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.771747	0.077087	-0.236662
2	7	0.356458	1.771101	-0.565932

3	6	1.657701	1.759786	-0.295646
4	7	0.869851	-1.168111	-0.595262
5	6	-2.378328	0.949788	1.253108
6	6	-1.692036	-0.122357	1.909263
7	6	-3.122653	0.400292	0.169490
8	17	-1.249943	-0.029394	-2.641648
9	6	-2.007091	-1.330627	1.207459
10	6	-2.896597	-1.005024	0.143806
11	6	-0.168628	2.980196	-1.227964
12	6	2.074281	-0.723263	-0.303732
13	6	0.751308	-2.534346	-1.135769
14	6	2.440890	0.630835	-0.035898
15	1	2.182201	2.716896	-0.357156
16	6	3.886436	0.657911	0.264118
17	1	0.219392	0.225010	1.065226
18	6	3.336699	-1.561397	-0.248527
19	6	4.411998	-0.583014	0.159074
20	1	3.221014	-2.392936	0.459198
21	1	3.554014	-2.020408	-1.222812
22	6	5.830796	-1.039447	0.356072
23	6	4.611177	1.932495	0.610547
24	1	5.653696	1.744678	0.882210
25	1	4.127735	2.443308	1.454026
26	1	4.611194	2.634040	-0.235170
27	1	6.487021	-0.221453	0.668829
28	1	6.245304	-1.462012	-0.571077
29	1	5.893020	-1.828759	1.119319
30	6	-1.042176	-0.042125	3.268195
31	6	-2.404686	2.378595	1.741416
32	6	-4.048564	1.142039	-0.759990
33	6	-3.554852	-1.968749	-0.809175
34	6	-1.579345	-2.713919	1.636805
35	1	-1.799111	-0.184712	4.053508
36	1	-0.566688	0.929373	3.430732
37	1	-0.275922	-0.812207	3.395638
38	1	-3.081621	2.479036	2.601537
39	1	-2.759225	3.066689	0.967978
40	1	-1.413004	2.715633	2.061716
41	1	-5.095202	0.976266	-0.467972
42	1	-3.926325	0.803433	-1.793209
43	1	-3.868080	2.221181	-0.738954
44	1	-4.592683	-2.159144	-0.500761
45	1	-3.037737	-2.932979	-0.835190
46	1	-3.570429	-1.570845	-1.828082
47	1	-2.226135	-3.084247	2.444794
48	1	-0.550290	-2.720242	2.011593
49	1	-1.640836	-3.433014	0.814459
50	1	-0.254361	-2.675911	-1.534415
51	1	0.931913	-3.287721	-0.357065
52	1	1.460993	-2.704322	-1.954564
53	1	-1.149430	3.244677	-0.823683
54	1	0.508517	3.832263	-1.081893
55	1	-0.283598	2.795281	-2.301722

TS13^{Me}-14^{Me} (E = -963.3568035354 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.672980	0.295842	0.073194
2	7	-0.041367	0.264137	-1.697822
3	6	-1.094402	-0.630140	-1.516081
4	7	-1.137063	0.680627	1.030134
5	6	2.496695	-1.136257	-0.427556
6	6	1.753389	-1.731533	0.640128
7	6	3.065616	0.072663	0.057324
8	17	0.990604	2.722992	0.180169

9	6	1.893065	-0.890475	1.793830
10	6	2.709813	0.208881	1.437450
11	6	0.392332	0.517653	-3.068893
12	6	-2.258783	0.400411	0.386592
13	6	-1.255717	1.390619	2.317699
14	6	-2.280287	-0.325186	-0.820720
15	1	-1.132772	-1.460117	-2.232299
16	6	-3.647974	-0.808968	-1.048829
17	1	-0.298025	-1.133950	0.020425
18	6	-3.682158	0.544777	0.878092
19	6	-4.475068	-0.287570	-0.109131
20	1	-3.791343	0.181594	1.906889
21	1	-4.007674	1.593856	0.884880
22	6	-5.969822	-0.396691	0.003627
23	6	-4.010432	-1.688214	-2.216678
24	1	-5.084127	-1.892073	-2.255174
25	1	-3.490231	-2.654188	-2.161782
26	1	-3.720007	-1.218763	-3.166392
27	1	-6.397895	-1.017284	-0.789546
28	1	-6.445375	0.593378	-0.053422
29	1	-6.266327	-0.835466	0.967279
30	6	1.208857	-3.139426	0.654060
31	6	2.742629	-1.773806	-1.773256
32	6	3.986756	1.003366	-0.689196
33	6	3.209554	1.299001	2.348119
34	6	1.335553	-1.208426	3.160439
35	1	1.995210	-3.842301	0.966524
36	1	0.859077	-3.449935	-0.335081
37	1	0.371702	-3.243204	1.350972
38	1	3.571786	-2.492934	-1.711419
39	1	3.008724	-1.032678	-2.532436
40	1	1.863028	-2.318640	-2.131810
41	1	5.030224	0.840331	-0.383571
42	1	3.735283	2.049909	-0.490895
43	1	3.932918	0.845500	-1.771078
44	1	4.261635	1.117863	2.610775
45	1	2.639778	1.344491	3.281382
46	1	3.141586	2.279023	1.867182
47	1	1.945944	-1.972831	3.661740
48	1	0.312088	-1.595543	3.099629
49	1	1.321195	-0.326499	3.807990
50	1	-0.263858	1.553579	2.738618
51	1	-1.852872	0.811489	3.033740
52	1	-1.724418	2.371950	2.179277
53	1	1.329618	1.077746	-3.057547
54	1	0.539968	-0.418626	-3.630486
55	1	-0.356804	1.120066	-3.600627

14^{Me} (E = -963.5326559 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.813103	0.105888	-0.503731
2	7	0.128127	1.731143	-0.754999
3	6	1.555735	1.909599	-0.520773
4	7	0.652808	-1.082206	-0.868843
5	6	-2.160239	0.936555	1.352055
6	6	-1.095186	0.106703	1.820852
7	6	-3.039571	0.124845	0.598669
8	17	-2.040452	-0.067655	-2.501885
9	6	-1.374983	-1.241751	1.423976
10	6	-2.553389	-1.226336	0.642210
11	6	1.921292	-0.647671	-0.527182
12	6	2.337043	0.639663	-0.336673
13	1	1.990270	2.474184	-1.365324
14	6	3.762960	0.633965	0.038490

15	1	1.697571	2.562842	0.359306
16	6	3.095966	-1.572909	-0.272091
17	6	4.225574	-0.639563	0.077891
18	1	2.880348	-2.280586	0.539070
19	1	3.335925	-2.180671	-1.154085
20	6	5.608621	-1.148842	0.376115
21	6	4.534741	1.902224	0.305519
22	1	5.581744	1.694563	0.544465
23	1	4.104987	2.461731	1.147492
24	1	4.517824	2.570430	-0.565999
25	1	6.304323	-0.333713	0.599732
26	1	6.020115	-1.711445	-0.474717
27	1	5.610255	-1.831893	1.238008
28	6	0.012336	0.530610	2.754887
29	6	-2.349983	2.393283	1.694363
30	6	-4.340232	0.542410	-0.035240
31	6	-3.264907	-2.404521	0.026666
32	6	-0.597486	-2.450399	1.880816
33	1	-0.299488	0.410598	3.802805
34	1	0.282169	1.581556	2.611028
35	1	0.917644	-0.067474	2.610367
36	1	-2.873805	2.492650	2.655674
37	1	-2.947666	2.917855	0.942671
38	1	-1.393983	2.917258	1.787128
39	1	-5.188638	0.202193	0.575745
40	1	-4.451580	0.112286	-1.035559
41	1	-4.415968	1.630028	-0.130056
42	1	-4.206759	-2.607673	0.555517
43	1	-2.659713	-3.315202	0.073547
44	1	-3.510934	-2.215819	-1.024666
45	1	-0.856295	-2.695941	2.920328
46	1	0.483222	-2.278215	1.844467
47	1	-0.817756	-3.331384	1.271562
48	6	-0.520359	2.995253	-1.121917
49	6	0.516987	-2.457733	-1.367166
50	1	-0.345058	3.774878	-0.363577
51	1	-0.124805	3.358974	-2.082469
52	1	-1.598125	2.859635	-1.238346
53	1	0.877367	-3.201491	-0.644423
54	1	1.079767	-2.580758	-2.302549
55	1	-0.533078	-2.663672	-1.584917

TS14^{Me}-15^{Me} (E = -963.4971736 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.493812	-0.128256	0.016477
2	7	0.547808	-0.093412	1.759180
3	6	-0.364185	1.816716	1.805345
4	7	-1.456359	0.506912	-0.465285
5	6	2.807977	0.415691	-0.248753
6	6	2.044657	1.471851	-0.832053
7	6	2.599740	-0.746526	-1.032721
8	17	-0.114760	-2.414133	-0.259338
9	6	1.418085	0.969005	-2.019370
10	6	1.752503	-0.397724	-2.140029
11	6	-2.225288	1.121289	0.413888
12	6	-1.733959	1.666709	1.622815
13	1	0.049379	2.123381	2.758758
14	6	-2.874103	1.892056	2.521434
15	1	0.214779	2.160195	0.957482
16	6	-3.736525	1.187596	0.443726
17	6	-4.030847	1.653734	1.857004
18	1	-4.126340	1.887812	-0.308263
19	1	-4.184787	0.212448	0.220058
20	6	-5.448308	1.822850	2.326721

21	6	-2.696356	2.378816	3.934531
22	1	-3.654394	2.529222	4.439778
23	1	-2.149099	3.331388	3.955071
24	1	-2.114579	1.659959	4.527191
25	1	-5.498753	2.174131	3.361889
26	1	-6.001986	0.874593	2.269018
27	1	-5.992128	2.546025	1.701257
28	6	2.118480	2.932361	-0.450447
29	6	3.747532	0.549937	0.923715
30	6	3.270773	-2.084366	-0.853662
31	6	1.381333	-1.342699	-3.253353
32	6	0.638957	1.815006	-2.997134
33	1	2.911497	3.433236	-1.024800
34	1	2.353351	3.069377	0.610259
35	1	1.184288	3.465050	-0.663340
36	1	4.742667	0.874069	0.586747
37	1	3.870832	-0.400121	1.452473
38	1	3.387264	1.286842	1.648660
39	1	4.140432	-2.168871	-1.521825
40	1	2.586079	-2.906229	-1.082165
41	1	3.626348	-2.224810	0.171918
42	1	2.273210	-1.633723	-3.825485
43	1	0.675334	-0.888137	-3.955738
44	1	0.925696	-2.258059	-2.858261
45	1	1.313209	2.488891	-3.544214
46	1	-0.109279	2.439532	-2.495452
47	1	0.117812	1.203115	-3.739116
48	6	0.847642	-0.490268	3.111220
49	1	1.692386	0.072540	3.537783
50	1	-0.023993	-0.346647	3.767188
51	1	1.103678	-1.558413	3.131323
52	6	-2.109065	-0.010912	-1.684492
53	1	-1.349098	-0.314795	-2.403863
54	1	-2.709565	-0.897580	-1.446663
55	1	-2.752936	0.744502	-2.151162

15^{Me} (E = -963.5190324 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.791381	-0.605131	0.157556
2	7	1.148929	-0.681605	1.806949
3	6	-0.645646	1.844855	2.515282
4	7	-1.332809	0.105721	0.024661
5	6	2.896621	0.337943	-0.382013
6	6	1.914392	1.345288	-0.604390
7	6	2.687085	-0.688525	-1.344674
8	17	0.357084	-2.893763	-0.346447
9	6	1.139494	0.964539	-1.748531
10	6	1.613527	-0.290227	-2.202514
11	6	-2.131718	0.842424	0.717135
12	6	-1.831994	1.681377	1.909814
13	1	-0.556928	2.489453	3.382125
14	6	-3.101074	2.315929	2.316591
15	1	0.237272	1.320327	2.178193
16	6	-3.615223	1.004295	0.429526
17	6	-4.107796	1.940656	1.502409
18	1	-3.785306	1.408966	-0.576767
19	1	-4.128236	0.034191	0.453507
20	6	-5.557551	2.326431	1.549166
21	6	-3.168430	3.237248	3.503554
22	1	-4.180120	3.616092	3.668962
23	1	-2.502196	4.099799	3.369103
24	1	-2.847149	2.720899	4.417819
25	1	-5.781342	3.011297	2.371175
26	1	-6.192190	1.436689	1.666442

27	1	-5.862548	2.810685	0.610705
28	6	1.851275	2.688977	0.082193
29	6	4.030085	0.407313	0.609756
30	6	3.537132	-1.919344	-1.538385
31	6	1.149598	-1.072061	-3.405596
32	6	0.105700	1.840185	-2.414164
33	1	2.443453	3.433409	-0.470670
34	1	2.252118	2.641844	1.099617
35	1	0.826593	3.069920	0.148193
36	1	4.907721	0.893616	0.159805
37	1	4.338740	-0.588852	0.942164
38	1	3.752708	0.981574	1.499030
39	1	4.315419	-1.732813	-2.293234
40	1	2.937023	-2.770058	-1.873529
41	1	4.038840	-2.214812	-0.611538
42	1	1.935750	-1.108329	-4.172515
43	1	0.264879	-0.621706	-3.867595
44	1	0.903594	-2.106575	-3.136613
45	1	0.594796	2.622384	-3.012010
46	1	-0.534949	2.345513	-1.682844
47	1	-0.539610	1.270614	-3.089977
48	6	1.681064	-0.836277	3.133749
49	1	2.769673	-0.676876	3.157954
50	1	1.223187	-0.121006	3.835811
51	1	1.481911	-1.848525	3.516165
52	6	-1.953356	-0.604398	-1.128745
53	1	-1.178120	-1.064177	-1.736907
54	1	-2.608236	-1.405827	-0.770671
55	1	-2.532981	0.083535	-1.752433

16^{Me} (E = -675.8581344 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.554670	-0.165500	-0.476379
2	7	-0.928568	1.471232	-0.303342
3	6	-2.020948	-1.137328	1.061152
4	6	-0.752852	-0.998552	1.698523
5	6	-1.877692	-2.099094	0.012451
6	17	0.361515	-0.583409	-2.581625
7	6	0.163567	-1.886223	1.047074
8	6	-0.535188	-2.580347	0.020732
9	6	-1.292278	2.874421	-0.175032
10	6	-2.670487	3.091851	-0.849255
11	6	-1.364580	3.272713	1.318790
12	6	-0.215168	3.724739	-0.895131
13	1	-0.146700	3.435605	-1.948590
14	1	0.765218	3.570927	-0.430865
15	1	-0.401025	3.095302	1.808767
16	1	-2.132017	2.688045	1.837353
17	1	-3.438522	2.486971	-0.354503
18	1	-2.625366	2.803696	-1.904778
19	6	-0.469994	-0.204367	2.951381
20	6	-3.318511	-0.513725	1.515038
21	6	-2.976432	-2.590490	-0.899490
22	6	0.017038	-3.659183	-0.873906
23	6	1.609134	-2.094335	1.434062
24	1	-0.619294	-0.830291	3.842724
25	1	-1.131827	0.661272	3.036753
26	1	0.560801	0.164254	2.980051
27	1	-3.829919	-1.172869	2.230938
28	1	-4.004029	-0.342577	0.678761
29	1	-3.152022	0.447973	2.007953
30	1	-3.457802	-3.482204	-0.473426
31	1	-2.590071	-2.865857	-1.886164
32	1	-3.757349	-1.836268	-1.041760

33	1	-0.296899	-4.651449	-0.520792
34	1	1.110552	-3.644285	-0.893459
35	1	-0.327892	-3.545000	-1.906433
36	1	1.696552	-2.903130	2.173042
37	1	2.043450	-1.196242	1.886127
38	1	2.226956	-2.369218	0.573043
39	1	-1.614771	4.335664	1.420697
40	1	-2.965841	4.146286	-0.787358
41	1	-0.465123	4.791165	-0.836545

17^{Me} (E = -523.4592199 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	2.075137	-1.274408	-0.526310
2	6	1.564146	-0.157600	-0.843236
3	6	3.157126	-1.484522	0.474456
4	6	0.511370	-0.054930	-1.910305
5	6	0.234186	1.372844	-2.118885
6	6	1.825767	1.274815	-0.363914
7	6	0.969485	2.126109	-1.272684
8	1	1.531395	1.405044	0.683234
9	1	2.886292	1.543588	-0.424355
10	6	1.004389	3.621857	-1.138613
11	6	-0.752521	1.841691	-3.154084
12	1	-0.831348	2.931646	-3.186262
13	1	-1.752424	1.435890	-2.949823
14	1	-0.462482	1.492731	-4.154084
15	1	0.336959	4.122813	-1.845238
16	1	2.022130	4.002966	-1.304910
17	1	0.714958	3.928225	-0.123094
18	6	2.968388	-0.709436	1.801209
19	6	3.136866	-2.999561	0.782819
20	6	4.508371	-1.116798	-0.185449
21	1	4.643634	-1.679524	-1.115137
22	1	4.561147	-0.047828	-0.419182
23	1	3.171567	0.359404	1.696371
24	1	1.948694	-0.837848	2.182837
25	1	2.184229	-3.281287	1.245664
26	1	3.247255	-3.573729	-0.142405
27	1	3.950242	-3.268694	1.466651
28	1	3.661139	-1.103215	2.553685
29	1	5.336283	-1.360567	0.490341
30	6	-0.051229	-1.097721	-2.538078
31	1	-0.805698	-0.964907	-3.304353
32	1	0.245155	-2.108474	-2.285797

18^{Me} (E = -924.1524042 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.297764	-0.073262	-0.371971
2	7	-0.824365	1.527225	-0.222760
3	6	-1.893915	-1.062652	1.064522
4	6	-0.648237	-1.048388	1.758292
5	6	-1.771845	-1.972919	-0.023338
6	17	-0.216779	-0.525687	-2.696343
7	6	0.218494	-1.998456	1.126474
8	6	-0.472112	-2.563364	0.026704
9	6	-1.351062	2.882770	-0.200123
10	6	-2.761548	2.893205	-0.841747
11	6	-1.431488	3.404010	1.256617
12	6	-0.400949	3.788288	-1.026733
13	1	-0.326626	3.415078	-2.052983
14	1	0.603251	3.790712	-0.587754
15	1	-0.439195	3.393959	1.722671
16	1	-2.100195	2.775264	1.854147
17	1	-3.446808	2.258623	-0.269812

18	1	-2.710076	2.512046	-1.866722
19	6	-0.371370	-0.332980	3.059952
20	6	-3.161792	-0.372646	1.503142
21	6	-2.859873	-2.356727	-0.995440
22	6	0.024003	-3.633358	-0.912206
23	6	1.580422	-2.407045	1.631679
24	1	-0.663677	-0.955358	3.918472
25	1	-0.927857	0.607020	3.128236
26	1	0.692642	-0.099214	3.179641
27	1	-3.733474	-1.019325	2.185013
28	1	-3.809575	-0.134685	0.653764
29	1	-2.950987	0.562332	2.029807
30	1	-3.383562	-3.260488	-0.650357
31	1	-2.451485	-2.563320	-1.989248
32	1	-3.606583	-1.563519	-1.102941
33	1	-0.505674	-4.581149	-0.741349
34	1	1.093110	-3.826953	-0.775258
35	1	-0.133633	-3.347062	-1.958523
36	1	1.487581	-3.199270	2.388127
37	1	2.111751	-1.571959	2.100635
38	1	2.215783	-2.795939	0.829153
39	1	-1.812084	4.432853	1.280585
40	1	-3.168652	3.912040	-0.864920
41	1	-0.772851	4.820470	-1.050523
42	7	1.868589	0.311090	-0.132583
43	6	2.774825	-0.285525	-0.941753
44	6	2.317333	1.188931	0.794965
45	6	4.144232	-0.032369	-0.848166
46	1	2.373709	-0.960605	-1.687836
47	6	3.670543	1.486671	0.954496
48	1	1.557943	1.664800	1.402168
49	6	4.604906	0.866516	0.118213
50	1	4.828349	-0.529961	-1.524913
51	1	3.978813	2.197042	1.712265
52	1	5.663136	1.083031	0.213754

TS10^{Me}-22^{Me} (E = -963.4845347 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.736612	-0.026416	-0.441759
2	7	0.678604	1.341794	-0.715571
3	6	1.394911	1.646881	0.357019
4	7	0.854560	-1.291867	0.348602
5	6	-2.283295	1.451967	0.477893
6	6	-1.861004	0.533680	1.495751
7	6	-3.010054	0.698269	-0.488330
8	17	-0.872553	-0.918571	-2.639579
9	6	-2.345408	-0.776121	1.154422
10	6	-3.061429	-0.663672	-0.062871
11	6	0.718533	2.299576	-1.835176
12	6	1.851056	-0.782260	0.968175
13	6	0.875261	-2.714257	-0.048360
14	6	1.879672	0.667746	1.410457
15	1	1.706863	2.681869	0.504657
16	6	3.336277	0.864407	1.839675
17	1	1.272726	0.759157	2.329668
18	6	3.162656	-1.440405	1.344493
19	6	4.019866	-0.288661	1.817157
20	1	3.015873	-2.191580	2.134107
21	1	3.607521	-1.974724	0.496538
22	6	5.453259	-0.544733	2.198401
23	6	3.815116	2.216472	2.293519
24	1	4.833356	2.178557	2.690704
25	1	3.159786	2.615670	3.080757
26	1	3.806657	2.941897	1.469763

27	1	5.958090	0.359264	2.550007
28	1	6.020732	-0.935127	1.341833
29	1	5.517391	-1.300133	2.994290
30	6	-1.293691	0.915955	2.841921
31	6	-2.118462	2.949461	0.531493
32	6	-3.673024	1.242860	-1.729829
33	6	-3.781050	-1.772444	-0.787910
34	6	-2.250630	-1.996736	2.037480
35	1	-2.105115	1.033226	3.576026
36	1	-0.751440	1.865896	2.800512
37	1	-0.613652	0.153955	3.240849
38	1	-2.818701	3.400804	1.249842
39	1	-2.307285	3.408423	-0.444138
40	1	-1.104133	3.232272	0.841770
41	1	-4.736554	1.449341	-1.541541
42	1	-3.611752	0.532959	-2.560603
43	1	-3.209302	2.178511	-2.059408
44	1	-4.861898	-1.726140	-0.591376
45	1	-3.428647	-2.758545	-0.468539
46	1	-3.633454	-1.704874	-1.870534
47	1	-3.046229	-1.994542	2.797503
48	1	-1.293968	-2.038558	2.570610
49	1	-2.352912	-2.922363	1.461374
50	1	0.158296	-3.260317	0.573260
51	1	1.861469	-3.175674	0.057120
52	1	1.725936	2.322169	-2.271355
53	1	0.008742	1.987926	-2.604247
54	1	0.547331	-2.788228	-1.087282
55	1	0.461621	3.313363	-1.497873

22^{Me} (E = -963.4905322 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.912101	-0.197286	-0.434534
2	7	0.408136	0.866478	-1.590105
3	6	1.654150	1.124567	-1.275597
4	7	0.789973	-1.375266	-0.173686
5	6	-2.023276	1.623282	0.630510
6	6	-1.159005	0.986240	1.577527
7	6	-3.045914	0.694657	0.305094
8	17	-2.092307	-1.442360	-2.058426
9	6	-1.658581	-0.330256	1.841657
10	6	-2.823469	-0.505897	1.054088
11	6	-0.033427	1.286766	-2.939021
12	6	1.975416	-0.873881	0.017306
13	6	0.677001	-2.843096	-0.314518
14	6	2.218739	0.624179	0.029596
15	1	2.317626	1.599275	-1.996286
16	6	3.729086	0.729580	0.153347
17	1	1.745239	1.123052	0.885644
18	6	3.291708	-1.598990	0.171601
19	6	4.308054	-0.478380	0.235358
20	1	3.307064	-2.208878	1.088848
21	1	3.497886	-2.298850	-0.650025
22	6	5.769199	-0.809928	0.378256
23	6	4.382668	2.085053	0.205212
24	1	5.465932	2.017198	0.340055
25	1	3.975220	2.679818	1.034784
26	1	4.194789	2.654531	-0.714951
27	1	6.397014	0.084183	0.428757
28	1	6.115333	-1.417440	-0.469699
29	1	5.948433	-1.401400	1.287126
30	6	-0.116800	1.696782	2.409932
31	6	-1.942998	3.067810	0.199921
32	6	-4.228319	0.942566	-0.598026

33	6	-3.736181	-1.706405	1.053178
34	6	-1.126339	-1.275321	2.891576
35	1	-0.593837	2.147348	3.293384
36	1	0.371359	2.508869	1.860819
37	1	0.658777	1.016480	2.777447
38	1	-2.410638	3.728373	0.945398
39	1	-2.457340	3.232503	-0.752467
40	1	-0.905017	3.396162	0.075795
41	1	-5.116560	1.206471	-0.005682
42	1	-4.472464	0.056050	-1.191573
43	1	-4.039930	1.766037	-1.294464
44	1	-4.618991	-1.519588	1.681802
45	1	-3.234153	-2.596366	1.446240
46	1	-4.088314	-1.942057	0.043886
47	1	-1.523287	-1.022940	3.886233
48	1	-0.033319	-1.234631	2.955587
49	1	-1.406779	-2.312189	2.679704
50	1	-0.343721	-3.097342	-0.600696
51	1	0.914519	-3.344352	0.632117
52	1	0.813728	1.286475	-3.637460
53	1	-0.797971	0.598958	-3.304757
54	1	1.358984	-3.214584	-1.089309
55	1	-0.461175	2.294789	-2.898700

TS22^{Me}-13^{Me} (E = -963.462804 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.655673	-0.204751	-0.395428
2	7	0.845775	0.916023	-1.269959
3	6	2.018665	0.760532	-0.693964
4	7	0.583714	-1.846645	0.008296
5	6	-2.032597	1.515260	0.446034
6	6	-1.469524	0.836641	1.569134
7	6	-2.895548	0.609091	-0.241520
8	17	-1.171122	-1.139966	-2.583723
9	6	-1.976354	-0.501005	1.556072
10	6	-2.861725	-0.635080	0.446506
11	6	0.784843	1.637942	-2.550756
12	6	1.773589	-1.477068	0.400244
13	6	0.280209	-3.277818	-0.158350
14	6	2.079616	-0.050463	0.508732
15	1	2.912511	1.218284	-1.118147
16	6	3.316244	0.004903	1.366455
17	1	0.741321	0.292873	0.874444
18	6	2.896019	-2.292645	0.987509
19	6	3.763009	-1.235316	1.649346
20	1	2.518815	-3.040676	1.695973
21	1	3.462877	-2.847942	0.226525
22	6	4.962817	-1.648750	2.457083
23	6	3.899508	1.322924	1.802856
24	1	4.804180	1.195746	2.404479
25	1	3.171471	1.890976	2.397722
26	1	4.158395	1.948928	0.938491
27	1	5.501181	-0.788828	2.866444
28	1	5.669949	-2.225558	1.843778
29	1	4.672422	-2.294874	3.298032
30	6	-0.733286	1.491192	2.712409
31	6	-1.833857	2.977400	0.121121
32	6	-3.776476	0.924035	-1.423747
33	6	-3.673165	-1.851164	0.074837
34	6	-1.711610	-1.536011	2.623282
35	1	-1.449413	1.915138	3.432848
36	1	-0.089541	2.306210	2.366796
37	1	-0.103561	0.776282	3.250551
38	1	-2.551260	3.599293	0.675615

39	1	-1.982627	3.182384	-0.944239
40	1	-0.827532	3.316223	0.388470
41	1	-4.809648	1.104382	-1.093536
42	1	-3.787209	0.099764	-2.142891
43	1	-3.439474	1.820330	-1.953977
44	1	-4.721205	-1.724701	0.381826
45	1	-3.296138	-2.755676	0.562608
46	1	-3.659000	-2.022164	-1.006542
47	1	-2.379111	-1.384375	3.483662
48	1	-0.681761	-1.480483	2.991552
49	1	-1.880059	-2.552808	2.254979
50	1	-0.501247	-3.386130	-0.912743
51	1	-0.074658	-3.708848	0.786580
52	1	1.720109	2.178327	-2.743714
53	1	0.594966	0.929666	-3.362702
54	1	1.161012	-3.839444	-0.489657
55	1	-0.039312	2.357782	-2.532061

TS10^{Me}-24^{Me} (E = -963.4858526 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.189399	-0.471367	0.152911
2	7	1.661081	0.244479	-0.172515
3	6	1.655828	0.631854	-1.433792
4	7	-1.479966	0.706733	-0.840758
5	6	-0.331235	-2.397446	-1.187458
6	6	-1.660261	-2.281963	-0.664714
7	6	0.548784	-2.704457	-0.103944
8	17	-0.571188	0.412951	2.324400
9	6	-1.592714	-2.429403	0.735441
10	6	-0.222176	-2.673475	1.089439
11	6	-0.583624	1.675835	-0.997858
12	6	0.600195	1.565033	-1.947961
13	1	2.476540	0.338965	-2.097053
14	6	1.100071	3.002327	-2.078106
15	1	0.236263	1.195087	-2.918499
16	6	-0.697317	3.111546	-0.520980
17	6	0.386982	3.829682	-1.298842
18	1	-1.691223	3.535026	-0.723413
19	1	-0.546991	3.201194	0.563750
20	6	0.539468	5.318053	-1.136996
21	6	2.237747	3.333877	-3.006698
22	1	2.484660	4.399368	-2.991091
23	1	1.988780	3.061132	-4.042334
24	1	3.146835	2.779018	-2.738767
25	1	1.360028	5.725254	-1.734618
26	1	0.727028	5.571902	-0.084096
27	1	-0.383971	5.838147	-1.428473
28	6	-2.888005	-2.131282	-1.524192
29	6	0.008848	-2.456180	-2.658860
30	6	1.969251	-3.192421	-0.249176
31	6	0.257819	-3.007863	2.479892
32	6	-2.735158	-2.412018	1.719055
33	1	-3.008567	-3.011049	-2.171288
34	1	-2.819862	-1.250601	-2.173954
35	1	-3.798539	-2.041492	-0.924146
36	1	-0.220480	-3.451821	-3.068774
37	1	1.071210	-2.264475	-2.838777
38	1	-0.565823	-1.724289	-3.236618
39	1	1.974507	-4.255645	-0.529738
40	1	2.533185	-3.101179	0.683637
41	1	2.516089	-2.650394	-1.028179
42	1	0.029112	-4.055186	2.726037
43	1	-0.223004	-2.372373	3.229737
44	1	1.340224	-2.875366	2.580201

45	1	-2.906905	-3.416591	2.130811
46	1	-3.668525	-2.082894	1.251622
47	1	-2.526099	-1.739684	2.558539
48	6	2.947345	-0.112256	0.442938
49	6	-2.835433	1.064615	-0.388850
50	1	2.791411	-0.800630	1.274114
51	1	3.636748	-0.561944	-0.284056
52	1	3.408481	0.801701	0.836000
53	1	-3.403726	0.152704	-0.208058
54	1	-2.810641	1.639612	0.545426
55	1	-3.351893	1.656029	-1.156759

24^{Me} (E = -963.5050994 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.202102	-0.727763	-0.455446
2	7	-1.460439	0.754897	-0.352983
3	6	-1.125105	1.925314	0.041850
4	7	1.564361	0.061777	0.541064
5	6	0.062363	-2.375531	1.288625
6	6	0.873803	-2.935839	0.262220
7	6	-1.261546	-2.235026	0.775888
8	17	0.452195	-0.649739	-2.824689
9	6	0.045393	-3.149649	-0.877803
10	6	-1.271075	-2.716774	-0.566427
11	6	1.201302	1.136591	-0.265481
12	6	0.307167	2.251571	0.315240
13	1	-1.891023	2.702131	0.139900
14	6	0.766677	3.525704	-0.386445
15	1	0.417417	2.366401	1.410459
16	6	2.192390	1.812393	-1.215438
17	6	1.794697	3.269869	-1.211339
18	1	3.236118	1.703672	-0.877420
19	1	2.157912	1.392767	-2.227788
20	6	2.552733	4.248489	-2.069055
21	6	0.120860	4.853582	-0.079243
22	1	0.620658	5.679915	-0.593566
23	1	0.152772	5.062506	1.000020
24	1	-0.936808	4.876378	-0.377420
25	1	2.184548	5.274368	-1.972614
26	1	2.483682	3.961206	-3.127398
27	1	3.620774	4.244121	-1.809429
28	6	2.309726	-3.394218	0.369304
29	6	0.426782	-2.153973	2.736836
30	6	-2.447499	-1.866131	1.638106
31	6	-2.458432	-2.885459	-1.483493
32	6	0.455730	-3.866119	-2.137451
33	1	2.367236	-4.489664	0.304499
34	1	2.760532	-3.099604	1.320814
35	1	2.934843	-2.986979	-0.433874
36	1	-0.142939	-2.840740	3.379143
37	1	0.206923	-1.133769	3.071591
38	1	1.487194	-2.342231	2.922436
39	1	-2.499479	-2.537897	2.505887
40	1	-3.392225	-1.970565	1.096497
41	1	-2.390807	-0.842919	2.030274
42	1	-2.640596	-3.950409	-1.682726
43	1	-2.294682	-2.397406	-2.451849
44	1	-3.374315	-2.474868	-1.048504
45	1	0.262098	-4.944976	-2.039297
46	1	1.521555	-3.735853	-2.347956
47	1	-0.096040	-3.498189	-3.006376
48	6	-2.853577	0.545204	-0.785942
49	6	2.697526	0.058285	1.453665
50	1	-3.432672	1.474782	-0.731407

51	1	-3.335044	-0.212958	-0.169608
52	1	-2.843404	0.193141	-1.821100
53	1	2.524760	0.746371	2.295803
54	1	2.872343	-0.939926	1.857234
55	1	3.613368	0.384722	0.939363

TS24^{Me}-25^{Me} (E = -963.4851424 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.681196	0.166012	-0.402093
2	7	-0.143331	2.045823	-0.205379
3	6	0.882696	1.433184	-0.725734
4	7	0.896281	-1.220959	-0.389635
5	6	-1.651199	-0.082850	1.706568
6	6	-1.653381	-1.412731	1.176749
7	6	-2.611099	0.684792	0.973250
8	17	-1.246340	-0.028519	-2.684672
9	6	-2.541027	-1.438320	0.073817
10	6	-3.135744	-0.140573	-0.046999
11	6	2.060804	-0.778130	0.036556
12	6	2.239207	0.483495	0.667890
13	1	1.628902	1.891391	-1.373354
14	6	3.691609	0.738915	0.732303
15	1	1.597090	0.831904	1.466387
16	6	3.423167	-1.367833	-0.271002
17	6	4.382729	-0.286333	0.181287
18	1	3.585530	-2.309213	0.274341
19	1	3.521946	-1.612913	-1.336108
20	6	5.867445	-0.454250	0.008157
21	6	4.239316	2.001579	1.345390
22	1	5.333200	2.024545	1.342490
23	1	3.902458	2.105364	2.386417
24	1	3.881012	2.887906	0.804195
25	1	6.424784	0.398354	0.409086
26	1	6.139458	-0.559643	-1.052461
27	1	6.228549	-1.359361	0.518777
28	6	-0.944127	-2.586106	1.804588
29	6	-0.954541	0.351042	2.975430
30	6	-3.105154	2.060068	1.342751
31	6	-4.226652	0.212309	-1.022634
32	6	-2.930953	-2.623237	-0.773404
33	1	-1.478112	-2.906120	2.710393
34	1	0.081415	-2.337364	2.095944
35	1	-0.898999	-3.445089	1.129993
36	1	-1.594968	0.168708	3.850823
37	1	-0.714065	1.419368	2.963570
38	1	-0.021899	-0.200095	3.135675
39	1	-3.980362	1.979270	2.003239
40	1	-3.412506	2.637974	0.465246
41	1	-2.345499	2.635611	1.878514
42	1	-5.181197	-0.233960	-0.707791
43	1	-3.995654	-0.158884	-2.026076
44	1	-4.372993	1.294456	-1.093287
45	1	-3.991712	-2.868285	-0.624561
46	1	-2.351696	-3.516070	-0.519235
47	1	-2.788878	-2.414738	-1.840529
48	6	-0.331668	3.480073	0.011385
49	6	0.848230	-2.536253	-1.047720
50	1	-1.384981	3.747901	-0.087835
51	1	0.006217	3.763539	1.017099
52	1	0.252334	4.048243	-0.723403
53	1	1.371930	-2.499206	-2.012170
54	1	-0.187649	-2.806856	-1.249103
55	1	1.304885	-3.323510	-0.433582

25^{Me} (E = -963.515535 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.647766	-0.093770	-0.236420
2	7	0.318391	1.485469	-0.597003
3	6	1.596531	0.854745	-0.616106
4	7	0.602318	-0.896409	0.929919
5	6	-2.218228	0.108030	1.553920
6	6	-2.592743	-1.049787	0.814592
7	6	-2.388369	1.246402	0.707619
8	17	-0.376495	-1.284472	-2.274218
9	6	-2.976508	-0.628625	-0.489895
10	6	-2.853446	0.790768	-0.556752
11	6	1.764117	-0.432453	0.239623
12	6	2.507471	0.848559	0.613296
13	1	2.098990	0.823977	-1.584750
14	6	3.950783	0.580356	0.333829
15	1	2.192106	1.447401	1.461434
16	6	2.819094	-1.408909	-0.293507
17	6	4.126258	-0.644251	-0.197671
18	1	2.851442	-2.325136	0.309165
19	1	2.584868	-1.721492	-1.316196
20	6	5.401200	-1.280722	-0.682330
21	6	4.982942	1.644437	0.602708
22	1	5.997902	1.303861	0.376966
23	1	4.957829	1.953595	1.656964
24	1	4.785285	2.543610	0.002305
25	1	6.273648	-0.639713	-0.522737
26	1	5.344399	-1.510638	-1.755574
27	1	5.581889	-2.233452	-0.163906
28	6	-2.685273	-2.471745	1.313809
29	6	-1.899777	0.202608	3.025728
30	6	-2.267330	2.671116	1.188094
31	6	-3.241448	1.631272	-1.748836
32	6	-3.578499	-1.511349	-1.551391
33	1	-3.736962	-2.782723	1.379699
34	1	-2.249285	-2.584382	2.310111
35	1	-2.178272	-3.175700	0.644473
36	1	-2.714325	0.720319	3.551493
37	1	-0.979045	0.765724	3.213570
38	1	-1.790251	-0.782241	3.486247
39	1	-3.028997	2.871116	1.954646
40	1	-2.424756	3.389661	0.379768
41	1	-1.288716	2.875171	1.635577
42	1	-4.334447	1.660627	-1.858300
43	1	-2.828931	1.227371	-2.679863
44	1	-2.893772	2.663525	-1.650680
45	1	-4.666094	-1.584928	-1.403178
46	1	-3.164495	-2.523001	-1.519678
47	1	-3.398945	-1.117055	-2.554728
48	6	0.310617	2.868819	-1.048289
49	6	0.838784	-1.635231	2.162355
50	1	-0.709753	3.250753	-1.082752
51	1	0.739924	2.948489	-2.059400
52	1	0.903750	3.511987	-0.379777
53	1	-0.106441	-1.993969	2.568095
54	1	1.329321	-1.001747	2.918341
55	1	1.481392	-2.509720	1.990417

1^{Et} (E = -869.9811052 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	22	0.202229	0.330779	0.070231
2	7	-2.958169	0.773369	-0.764510
3	6	1.817952	-1.488757	0.130613
4	6	1.083075	-1.700632	-1.068461
5	6	0.911147	-1.648376	1.225796
6	17	-0.485121	0.941524	2.341229
7	6	-0.275135	-1.939919	-0.722153
8	6	-0.378064	-1.930549	0.701400
9	6	-1.836145	0.599622	-0.500954
10	6	0.605303	1.135607	-2.012536
11	6	1.643796	1.626137	-1.145420
12	1	-0.175386	1.812361	-2.347934
13	6	-0.115241	2.849931	-0.025231
14	6	1.229957	2.512803	-0.107576
15	1	-0.489490	3.346156	0.859350
16	1	-0.738241	2.906343	-0.904480
17	6	2.200796	2.988992	0.958248
18	6	3.115462	1.443833	-1.465864
19	1	3.742533	1.310262	-0.579678
20	1	3.482439	2.336452	-1.996050
21	1	3.273680	0.591436	-2.130418
22	1	2.803685	3.821187	0.567107
23	1	2.893810	2.205675	1.283222
24	1	1.656591	3.348101	1.835575
25	6	1.661323	-1.922906	-2.442188
26	6	3.320199	-1.444564	0.277958
27	6	1.326932	-1.730138	2.672332
28	6	-1.603128	-2.267329	1.511109
29	6	-1.357580	-2.333181	-1.697619
30	1	1.923684	-2.984737	-2.560274
31	1	2.571740	-1.343847	-2.617353
32	1	0.947405	-1.675509	-3.233817
33	1	3.692470	-2.419756	0.624671
34	1	3.644163	-0.697804	1.011561
35	1	3.818258	-1.221373	-0.668227
36	1	1.755955	-2.722315	2.878966
37	1	0.480554	-1.575242	3.343792
38	1	2.085435	-0.982219	2.924961
39	1	-1.598333	-3.329937	1.793860
40	1	-2.524078	-2.080104	0.949696
41	1	-1.645700	-1.670884	2.426750
42	1	-1.248080	-3.388468	-1.986212
43	1	-1.316577	-1.734895	-2.614223
44	1	-2.354973	-2.213882	-1.265005
45	1	0.924046	0.464018	-2.800157
46	6	-4.356359	1.025758	-1.003745
47	1	-4.571566	0.748270	-2.040862
48	1	-4.517457	2.104608	-0.907484
49	6	-5.254336	0.250890	-0.030008
50	1	-5.037352	0.530180	1.004942
51	1	-6.302462	0.484358	-0.241700
52	1	-5.111261	-0.828393	-0.139185

TS1^{Et}-3^{Et} (E = -869.977135 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-1.144079	-0.556523	-0.643137
2	7	-3.158742	1.334027	-2.322893
3	6	1.232412	-1.099572	-0.863065
4	6	1.099271	-0.300481	0.300333
5	6	0.838061	-0.314696	-1.986898
6	17	-1.529914	-2.361587	-2.226805
7	6	0.613732	0.986521	-0.099491
8	6	0.462090	0.976143	-1.514958
9	6	-2.523699	0.584673	-1.633930

10	6	-1.817318	0.190198	1.373596
11	6	-2.057834	-1.223141	1.435718
12	1	-2.653579	0.862363	1.197464
13	6	-3.573866	-0.800651	-0.411512
14	6	-2.910273	-1.747767	0.458547
15	1	-4.153355	-1.245704	-1.213190
16	1	-4.062138	0.041080	0.075363
17	6	-3.251517	-3.219964	0.376856
18	6	-1.439857	-2.101522	2.507583
19	1	-0.991821	-3.017938	2.108683
20	1	-2.217996	-2.404689	3.222790
21	1	-0.675645	-1.558868	3.067633
22	1	-4.050527	-3.452660	1.097157
23	1	-2.396773	-3.863693	0.604177
24	1	-3.606961	-3.478022	-0.622853
25	6	1.604843	-0.658014	1.674954
26	6	1.777387	-2.503660	-0.926565
27	6	0.984929	-0.699269	-3.435211
28	6	0.175618	2.181075	-2.376388
29	6	0.545538	2.229068	0.753591
30	1	2.659155	-0.361558	1.773674
31	1	1.549224	-1.733340	1.867736
32	1	1.051022	-0.144772	2.466644
33	1	2.843761	-2.490866	-1.193961
34	1	1.248440	-3.099615	-1.675950
35	1	1.685550	-3.017811	0.035550
36	1	1.950081	-0.339521	-3.821866
37	1	0.193719	-0.264301	-4.053754
38	1	0.945174	-1.782106	-3.569296
39	1	1.114792	2.695472	-2.627415
40	1	-0.471584	2.901135	-1.867051
41	1	-0.313640	1.904134	-3.314258
42	1	1.411394	2.875014	0.547887
43	1	0.560865	1.994114	1.821206
44	1	-0.357634	2.816079	0.554316
45	1	-1.112203	0.587776	2.092339
46	6	-4.566704	1.630177	-2.600261
47	1	-4.749780	2.657982	-2.268514
48	1	-5.208107	0.961728	-2.013621
49	6	-4.864281	1.498976	-4.097940
50	1	-4.684233	0.475829	-4.442629
51	1	-5.912755	1.749912	-4.289547
52	1	-4.232244	2.176461	-4.680485

3^{Et} (E = -870.0144956 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.246369	-0.083200	-0.283007
2	7	-0.833011	1.642537	0.019354
3	6	2.583550	0.402816	-0.211290
4	6	2.444897	-1.002979	-0.412172
5	6	2.056503	0.718705	1.072296
6	17	0.002445	-0.038563	-2.615035
7	6	1.829588	-1.554795	0.747592
8	6	1.574224	-0.484997	1.661486
9	6	-1.210436	0.746763	0.827296
10	6	-1.145430	-1.726743	0.104519
11	6	-2.594526	-1.417189	-0.142896
12	1	-0.983907	-1.991201	1.152976
13	6	-2.494422	0.452632	1.518123
14	6	-3.259425	-0.459709	0.545041
15	1	-3.083562	1.352397	1.731378
16	1	-2.297552	-0.049222	2.472965
17	6	-4.736044	-0.138303	0.446570
18	6	-3.241477	-2.269485	-1.219656

19	1	-4.251922	-1.953115	-1.489321
20	1	-3.283384	-3.322082	-0.906214
21	1	-2.624355	-2.230758	-2.126856
22	1	-5.215279	-0.216467	1.433847
23	1	-5.271890	-0.807059	-0.230321
24	1	-4.897776	0.892981	0.098234
25	6	2.954835	-1.777841	-1.601167
26	6	3.235975	1.364051	-1.173637
27	6	2.077058	2.073154	1.734709
28	6	1.053584	-0.639700	3.068586
29	6	1.656802	-3.023683	1.037369
30	1	4.011329	-2.047461	-1.459768
31	1	2.876033	-1.195867	-2.523703
32	1	2.393548	-2.705595	-1.749649
33	1	4.326115	1.369791	-1.031499
34	1	2.879878	2.388850	-1.028611
35	1	3.036535	1.087145	-2.213114
36	1	2.964027	2.171053	2.376345
37	1	1.196200	2.231988	2.365297
38	1	2.109875	2.882728	1.000101
39	1	1.861932	-0.946806	3.747521
40	1	0.267615	-1.399589	3.132135
41	1	0.641078	0.298827	3.451723
42	1	2.574953	-3.431190	1.483867
43	1	1.449694	-3.598641	0.129201
44	1	0.839355	-3.209567	1.740058
45	1	-0.815177	-2.568493	-0.513040
46	6	-1.491938	2.878905	-0.441774
47	1	-2.336744	3.110647	0.219463
48	1	-1.889701	2.665524	-1.441249
49	6	-0.510877	4.051853	-0.508789
50	1	0.332691	3.811390	-1.163933
51	1	-1.013844	4.938449	-0.909241
52	1	-0.121021	4.298835	0.484453

4^{Et} (E = -870.0077525 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.193135	0.011469	-0.192439
2	7	-0.438666	1.895492	0.241104
3	6	2.026169	-1.655797	-0.173585
4	6	1.669267	-1.370673	1.171047
5	6	2.541467	-0.459853	-0.756759
6	17	-0.244033	-0.510696	-2.439425
7	6	1.916539	0.016771	1.406312
8	6	2.476700	0.572419	0.215418
9	6	-1.417543	1.153528	-0.079740
10	6	-0.431546	3.285573	0.742511
11	6	-1.329559	-1.148769	0.898962
12	6	-2.772860	-1.205754	0.443118
13	1	-1.266920	-0.732217	1.915886
14	6	-2.886926	1.244553	-0.053174
15	6	-3.508357	-0.138467	0.071073
16	1	-3.235710	1.926562	0.739586
17	1	-3.215333	1.702365	-0.998410
18	6	-4.983150	-0.138859	-0.276262
19	6	-3.336708	-2.618579	0.463790
20	1	-4.359530	-2.696377	0.088637
21	1	-3.313239	-3.030374	1.482643
22	1	-2.705471	-3.270374	-0.155988
23	1	-5.471844	-1.099792	-0.107039
24	1	-5.135838	0.136723	-1.330969
25	1	-5.518412	0.611430	0.325183
26	6	1.298241	-2.374455	2.231755
27	6	1.963162	-2.995803	-0.861489

28	6	3.145360	-0.350251	-2.132649
29	6	3.031312	1.966924	0.048829
30	6	1.787096	0.702096	2.746486
31	1	2.191222	-2.655131	2.808284
32	1	0.885520	-3.292208	1.802188
33	1	0.562190	-1.979239	2.939475
34	1	2.954027	-3.471436	-0.885918
35	1	1.617443	-2.893080	-1.895645
36	1	1.280613	-3.681959	-0.350165
37	1	4.183667	-0.712366	-2.123624
38	1	3.158794	0.684950	-2.488074
39	1	2.587456	-0.943104	-2.863296
40	1	4.121873	1.965073	0.186144
41	1	2.612059	2.661268	0.782645
42	1	2.829000	2.372144	-0.948539
43	1	2.652004	0.470378	3.384482
44	1	0.889797	0.378860	3.286448
45	1	1.740415	1.790612	2.645115
46	1	-0.946106	-2.168341	0.970798
47	1	0.394238	3.385417	1.452544
48	1	-1.369006	3.472917	1.282458
49	6	-0.267468	4.284587	-0.411145
50	1	-0.240295	5.307325	-0.020246
51	1	0.661968	4.098578	-0.958694
52	1	-1.101498	4.207306	-1.116754

TS4^{Et}-5^{Et} (E = -869.9924161 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.821120	-0.113967	-0.679711
2	7	-0.315704	1.439165	-0.458980
3	6	3.012757	-1.164343	-0.529752
4	6	2.592618	-0.795866	0.778722
5	6	3.177416	0.030023	-1.295356
6	17	0.441061	-1.356603	-2.656187
7	6	2.477286	0.627917	0.815231
8	6	2.851830	1.136716	-0.467155
9	6	-1.047632	0.339634	-0.511354
10	6	-0.714165	2.804614	-0.094631
11	6	-0.705669	-1.005879	0.886067
12	6	-2.144266	-1.454741	0.963821
13	1	-0.362596	-0.577154	1.833955
14	6	-2.510341	0.183755	-0.756824
15	6	-3.043444	-0.903286	0.136870
16	1	-3.047962	1.126849	-0.577334
17	1	-2.665013	-0.061916	-1.816869
18	6	-4.507759	-1.239870	0.004219
19	6	-2.425051	-2.544729	1.976500
20	1	-3.482279	-2.820084	2.022747
21	1	-2.115233	-2.225332	2.981226
22	1	-1.849281	-3.450378	1.739584
23	1	-4.830280	-2.015642	0.702774
24	1	-4.731317	-1.589490	-1.013607
25	1	-5.129296	-0.349897	0.178071
26	6	2.460685	-1.718819	1.965747
27	6	3.339396	-2.555037	-1.012142
28	6	3.692436	0.090554	-2.711001
29	6	3.002737	2.591661	-0.841383
30	6	2.193148	1.445881	2.052974
31	1	3.413068	-1.777889	2.511400
32	1	2.193430	-2.737285	1.665117
33	1	1.702006	-1.372702	2.675565
34	1	4.425003	-2.727002	-0.987345
35	1	2.997960	-2.709942	-2.040318
36	1	2.870085	-3.322181	-0.388025

37	1	4.786561	-0.016866	-2.728656
38	1	3.446827	1.043631	-3.190100
39	1	3.266443	-0.709345	-3.324604
40	1	4.042023	2.920926	-0.700028
41	1	2.368957	3.236821	-0.226306
42	1	2.741410	2.771372	-1.889413
43	1	3.106832	1.565839	2.652520
44	1	1.442973	0.972972	2.696540
45	1	1.832347	2.448369	1.805089
46	1	-0.088936	-1.897723	0.703212
47	1	0.068878	3.243248	0.534734
48	1	-1.633093	2.763815	0.506880
49	6	-0.933736	3.682548	-1.335919
50	1	-1.207893	4.701152	-1.038080
51	1	-0.021494	3.731004	-1.939740
52	1	-1.734753	3.277581	-1.964008

5^{Et} (E = -870.0172275 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.300886	-0.056048	0.108581
2	7	0.407151	1.550101	-0.635070
3	6	-2.147897	-1.581239	0.360995
4	6	-1.904158	-1.363909	-1.025434
5	6	-2.555975	-0.342335	0.934650
6	17	0.455835	-0.542923	2.283264
7	6	-2.163804	0.014194	-1.304369
8	6	-2.567299	0.647704	-0.088901
9	6	1.548111	0.819074	-0.430589
10	6	0.345586	2.991332	-0.883161
11	6	1.745904	-0.464689	-1.163328
12	6	3.089714	-0.967804	-0.689512
13	1	1.622428	-0.422263	-2.252245
14	6	2.793074	1.132020	0.371046
15	6	3.664564	-0.084554	0.143456
16	1	3.299733	2.043519	0.017597
17	1	2.577554	1.282615	1.436192
18	6	4.999197	-0.189809	0.830087
19	6	3.607113	-2.299771	-1.161900
20	1	4.607474	-2.514189	-0.775016
21	1	3.654649	-2.337604	-2.259348
22	1	2.942393	-3.114301	-0.840851
23	1	5.543918	-1.096039	0.549491
24	1	4.872609	-0.195530	1.921311
25	1	5.631440	0.675288	0.585816
26	6	-1.577437	-2.424150	-2.052185
27	6	-2.060038	-2.896792	1.092877
28	6	-2.998077	-0.141751	2.361546
29	6	-3.107847	2.050034	0.057922
30	6	-2.158277	0.642892	-2.677155
31	1	-2.499198	-2.830304	-2.492718
32	1	-1.027988	-3.261861	-1.610758
33	1	-0.974096	-2.025877	-2.875399
34	1	-3.055173	-3.353815	1.190549
35	1	-1.651801	-2.765472	2.099882
36	1	-1.419837	-3.611677	0.566047
37	1	-4.061434	-0.399320	2.472330
38	1	-2.874539	0.898188	2.680119
39	1	-2.425471	-0.768881	3.050659
40	1	-4.207287	2.043451	0.034063
41	1	-2.768231	2.702095	-0.751425
42	1	-2.804459	2.508746	1.004878
43	1	-3.133424	0.505958	-3.166346
44	1	-1.400168	0.195029	-3.328362
45	1	-1.959107	1.717336	-2.631757

46	1	0.923441	-1.262629	-0.885289
47	1	-0.628066	3.212456	-1.334566
48	1	1.114344	3.257948	-1.623556
49	6	0.520325	3.848417	0.383551
50	1	0.429899	4.912956	0.135603
51	1	-0.246824	3.596919	1.123727
52	1	1.500797	3.686124	0.843019

10^{Et} (E = -1042.1258594 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.769089	0.061485	-0.269275
2	7	0.446048	1.323311	-0.881416
3	6	0.823632	1.240962	0.457942
4	7	0.748472	-1.507855	0.079977
5	6	-2.411573	1.288062	0.909156
6	6	-1.756126	0.449250	1.863835
7	6	-3.134589	0.448607	0.015175
8	17	-1.262964	-0.618146	-2.534934
9	6	-2.082458	-0.904441	1.553412
10	6	-2.931950	-0.905433	0.412019
11	6	0.965327	2.180184	-1.941259
12	6	1.876330	-1.042720	0.469669
13	6	0.641984	-2.938655	-0.324992
14	6	2.004112	0.385943	0.919239
15	1	0.661387	2.117800	1.091880
16	6	3.470767	0.684538	0.596456
17	1	1.921222	0.372156	2.021195
18	6	3.250000	-1.672454	0.439224
19	6	4.152219	-0.448844	0.358696
20	1	3.433706	-2.245603	1.361349
21	1	3.389668	-2.366864	-0.392111
22	6	5.619231	-0.632347	0.078765
23	6	3.992924	2.091492	0.669240
24	1	5.061057	2.151787	0.441179
25	1	3.835264	2.511575	1.673161
26	1	3.456511	2.742889	-0.032006
27	1	6.155215	0.320393	0.042361
28	1	5.773749	-1.143512	-0.881859
29	1	6.091801	-1.256031	0.851263
30	6	-1.069052	0.906819	3.125979
31	6	-2.442052	2.797270	0.942535
32	6	-4.049647	0.899471	-1.095060
33	6	-3.582013	-2.100229	-0.238773
34	6	-1.692842	-2.099083	2.391038
35	1	-1.786814	0.943416	3.959056
36	1	-0.641351	1.907338	3.015946
37	1	-0.261148	0.228435	3.421163
38	1	-3.208302	3.154131	1.645988
39	1	-2.675218	3.217599	-0.040436
40	1	-1.482275	3.216312	1.262492
41	1	-5.089100	0.942262	-0.738063
42	1	-4.009799	0.214304	-1.946199
43	1	-3.784680	1.896398	-1.461054
44	1	-4.654363	-2.136694	0.000004
45	1	-3.138875	-3.041133	0.103671
46	1	-3.482153	-2.059382	-1.328718
47	1	-2.343673	-2.180386	3.273304
48	1	-0.661372	-2.024470	2.752616
49	1	-1.783958	-3.036604	1.833939
50	1	-0.401387	-3.228633	-0.174412
51	1	1.251781	-3.546502	0.355952
52	1	2.044630	1.990941	-2.058225
53	1	0.477696	1.875774	-2.873714
54	6	1.035839	-3.208724	-1.785571

55	1	0.900745	-4.274408	-2.004070
56	1	0.407954	-2.627570	-2.463635
57	1	2.082263	-2.952816	-1.980015
58	6	0.731729	3.679089	-1.687774
59	1	1.158748	4.276395	-2.502417
60	1	-0.340504	3.896299	-1.626335
61	1	1.199535	3.999484	-0.748959

11^{Et} (E = -1042.0995569 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	1.270741	-0.297590	-0.523382
2	7	-0.205042	-1.368924	-0.390479
3	6	-0.690708	-0.160795	0.173199
4	7	-3.699419	-0.934799	-0.591517
5	6	3.090038	-1.235834	0.642054
6	6	2.212402	-0.680701	1.612423
7	6	3.636544	-0.159971	-0.128057
8	17	1.460659	0.516882	-2.699281
9	6	2.190472	0.736341	1.428906
10	6	3.089488	1.055210	0.363566
11	6	-0.883402	-2.662615	-0.522805
12	6	-3.201423	0.167623	-0.209424
13	6	-5.078448	-1.268757	-0.181316
14	6	-1.786122	0.626760	-0.586020
15	1	-0.878271	-0.169133	1.254535
16	6	-1.823630	2.108072	-0.233763
17	1	-1.619909	0.473172	-1.657945
18	6	-3.865620	1.264617	0.610848
19	6	-2.934729	2.442429	0.443243
20	1	-4.876946	1.480918	0.241697
21	1	-3.989309	0.965453	1.662595
22	6	-3.339994	3.787974	0.983918
23	6	-0.712417	3.025517	-0.665258
24	1	-0.927126	4.071910	-0.428285
25	1	-0.546303	2.944909	-1.747047
26	1	0.237452	2.762479	-0.184074
27	1	-2.592000	4.561700	0.788831
28	1	-3.498087	3.738926	2.070938
29	1	-4.290936	4.116538	0.540584
30	6	1.528702	-1.413147	2.738079
31	6	3.449565	-2.694952	0.484849
32	6	4.680545	-0.282309	-1.209448
33	6	3.449623	2.433007	-0.134055
34	6	1.504756	1.713324	2.351653
35	1	2.079170	-1.260160	3.677164
36	1	1.484003	-2.489496	2.552891
37	1	0.505254	-1.058613	2.897854
38	1	4.391640	-2.917477	1.005164
39	1	3.589540	-2.973158	-0.566051
40	1	2.679364	-3.349591	0.903771
41	1	5.687266	-0.165883	-0.783197
42	1	4.552295	0.482801	-1.980542
43	1	4.644878	-1.259127	-1.702387
44	1	4.430535	2.738816	0.255735
45	1	2.721114	3.183948	0.185923
46	1	3.501451	2.463985	-1.227409
47	1	2.102314	1.860282	3.262871
48	1	0.516200	1.356924	2.657677
49	1	1.373415	2.693884	1.885106
50	1	-5.782806	-0.573639	-0.665434
51	1	-5.203169	-1.139215	0.905527
52	1	-0.213076	-3.332688	-1.075126
53	1	-1.787050	-2.509503	-1.124908
54	6	-5.423961	-2.706492	-0.576201

55	1	-6.453240	-2.953612	-0.291304
56	1	-5.322432	-2.841940	-1.658498
57	1	-4.750419	-3.415860	-0.082407
58	6	-1.273164	-3.298083	0.820057
59	1	-1.939101	-2.635193	1.382621
60	1	-1.802302	-4.242685	0.646308
61	1	-0.390792	-3.506942	1.434303

$TS11^{Et}$-12^{Et} (E = -1042.0720963 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	1.025500	0.062830	-0.311288
2	7	0.352194	-0.787512	1.250282
3	6	-0.249712	0.433508	1.444697
4	7	-2.377903	-1.106280	-0.012200
5	6	3.246361	0.358722	0.328322
6	6	2.618355	1.633893	0.462178
7	6	3.281367	0.038879	-1.061926
8	17	0.552887	-1.483397	-2.017643
9	6	2.262820	2.092181	-0.847758
10	6	2.677699	1.107130	-1.783617
11	6	0.532509	-1.804441	2.283925
12	6	-2.191644	0.116782	-0.257873
13	6	-3.473163	-1.849808	-0.643285
14	6	-1.099818	0.950160	0.416958
15	1	0.009122	1.062968	2.296150
16	6	-1.716093	2.323842	0.495616
17	1	-0.279735	1.128104	-0.814360
18	6	-3.025842	1.109033	-1.058866
19	6	-2.767518	2.414495	-0.339888
20	1	-2.697058	1.149399	-2.107374
21	1	-4.087656	0.850611	-1.071588
22	6	-3.657999	3.596062	-0.605173
23	6	-1.212142	3.383325	1.437328
24	1	-1.784693	4.309569	1.340226
25	1	-0.158545	3.620361	1.259381
26	1	-1.293762	3.050991	2.480765
27	1	-3.358650	4.486289	-0.045372
28	1	-4.700271	3.365263	-0.343765
29	1	-3.649267	3.850120	-1.674551
30	6	2.603012	2.448591	1.733805
31	6	3.940142	-0.413912	1.423956
32	6	3.946939	-1.171096	-1.666453
33	6	2.544057	1.190260	-3.281905
34	6	1.718104	3.453754	-1.207685
35	1	3.591829	2.899633	1.900678
36	1	2.370904	1.839557	2.613602
37	1	1.877651	3.264851	1.693354
38	1	5.009200	-0.157965	1.458376
39	1	3.868958	-1.495756	1.269026
40	1	3.516772	-0.190315	2.407238
41	1	5.009009	-0.960952	-1.859711
42	1	3.478564	-1.455790	-2.611826
43	1	3.897763	-2.038272	-1.000023
44	1	3.481426	1.540949	-3.737008
45	1	1.751784	1.885565	-3.576749
46	1	2.304464	0.213346	-3.712733
47	1	2.538240	4.126928	-1.495565
48	1	1.192126	3.920826	-0.371506
49	1	1.021309	3.403728	-2.050298
50	1	-3.005725	-2.542496	-1.356378
51	1	-4.162759	-1.212060	-1.216347
52	1	1.372551	-2.437666	1.977651
53	1	-0.364938	-2.440629	2.278891
54	6	-4.249845	-2.651873	0.409393

55	1	-5.019335	-3.269447	-0.067433
56	1	-3.572182	-3.307430	0.966418
57	1	-4.741059	-1.982878	1.125779
58	6	0.763882	-1.266554	3.704493
59	1	-0.092915	-0.679035	4.053524
60	1	0.899928	-2.103852	4.398223
61	1	1.658595	-0.635744	3.756283

12^{Et} (E = -1042.0877979 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.765822	-0.352079	-0.191031
2	7	0.043536	-0.780827	1.540654
3	6	-0.805963	0.299382	1.609818
4	7	-2.439539	-1.709947	-0.018615
5	6	2.937514	0.241777	0.480708
6	6	2.177841	1.444824	0.408202
7	6	3.084846	-0.258658	-0.849182
8	17	0.763298	-2.397532	-1.276046
9	6	1.831408	1.668758	-0.958018
10	6	2.399726	0.615330	-1.732419
11	6	0.423988	-1.551874	2.731265
12	6	-2.485236	-0.455170	-0.202229
13	6	-3.181570	-2.620690	-0.892307
14	6	-1.791748	0.535646	0.680397
15	1	-0.621155	1.061716	2.369639
16	6	-2.480926	1.820500	0.486248
17	1	-0.216446	0.394422	-1.328226
18	6	-3.341883	0.361389	-1.167377
19	6	-3.342657	1.739872	-0.553270
20	1	-2.904708	0.371207	-2.175163
21	1	-4.354119	-0.043325	-1.266016
22	6	-4.222499	2.812492	-1.127357
23	6	-2.216402	3.020513	1.357587
24	1	-2.832863	3.875569	1.068128
25	1	-1.165420	3.331152	1.302942
26	1	-2.430459	2.795973	2.411040
27	1	-4.119049	3.768838	-0.607344
28	1	-5.279614	2.514352	-1.081841
29	1	-3.987445	2.975737	-2.188922
30	6	1.959786	2.415920	1.542156
31	6	3.651714	-0.295339	1.696138
32	6	3.933162	-1.436341	-1.250528
33	6	2.304916	0.456628	-3.226979
34	6	1.135394	2.892579	-1.498131
35	1	2.822341	3.092400	1.626926
36	1	1.847183	1.908782	2.505043
37	1	1.074158	3.037684	1.383825
38	1	4.689374	0.067448	1.719053
39	1	3.690876	-1.389829	1.698039
40	1	3.171861	0.024861	2.624888
41	1	4.964813	-1.105810	-1.439862
42	1	3.557270	-1.912905	-2.159149
43	1	3.965697	-2.200429	-0.468244
44	1	3.184602	0.890298	-3.723583
45	1	1.416259	0.954585	-3.626454
46	1	2.247585	-0.598908	-3.510739
47	1	1.858311	3.707023	-1.650146
48	1	0.362987	3.257711	-0.814543
49	1	0.653600	2.687401	-2.457921
50	1	-2.433509	-3.121281	-1.523295
51	1	-3.883766	-2.106321	-1.566188
52	1	1.382590	-2.035895	2.517801
53	1	-0.316222	-2.358652	2.843858
54	6	-3.927408	-3.672490	-0.059842

55	1	-4.418291	-4.403922	-0.711894
56	1	-3.229712	-4.202944	0.596692
57	1	-4.693823	-3.202192	0.567565
58	6	0.511939	-0.764011	4.047645
59	1	-0.457641	-0.338381	4.329738
60	1	0.826666	-1.436112	4.853810
61	1	1.240280	0.052724	3.986572

19^{Et} (E = -1042.1256169 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-1.015902	0.067743	0.490370
2	7	0.211863	1.726968	0.808506
3	6	1.479410	1.759022	0.402442
4	7	0.786862	-1.089153	0.912390
5	6	-2.414895	1.169273	-1.139671
6	6	-3.074401	-0.056585	-0.838587
7	6	-1.157219	0.852909	-1.728574
8	17	-2.184491	-1.260687	2.068284
9	6	-2.238085	-1.126749	-1.251189
10	6	-1.036034	-0.570545	-1.779655
11	6	-0.271595	3.005676	1.391767
12	6	1.953509	-0.670279	0.469621
13	6	0.786843	-2.414324	1.597567
14	6	2.269962	0.663082	0.087067
15	1	1.955433	2.741061	0.353987
16	6	3.668775	0.704703	-0.377868
17	1	-1.982539	1.172758	1.255342
18	6	3.234721	-1.486120	0.333132
19	6	4.228837	-0.519301	-0.267134
20	1	3.580940	-1.844166	1.311660
21	1	3.082032	-2.379637	-0.281804
22	6	5.621923	-0.967443	-0.611721
23	6	4.315595	1.973478	-0.868734
24	1	5.327164	1.794115	-1.243639
25	1	4.388332	2.719222	-0.064883
26	1	3.729588	2.429040	-1.678277
27	1	6.216812	-0.160655	-1.050952
28	1	5.606550	-1.800576	-1.329350
29	1	6.156586	-1.327745	0.279508
30	6	-4.464422	-0.196334	-0.280149
31	6	-3.035435	2.540175	-1.057422
32	6	-0.224805	1.833000	-2.393038
33	6	0.071399	-1.321995	-2.476612
34	6	-2.639805	-2.578928	-1.225526
35	1	-5.200528	-0.241758	-1.096220
36	1	-4.726040	0.650541	0.361155
37	1	-4.563030	-1.105947	0.318007
38	1	-3.630915	2.738131	-1.960437
39	1	-2.278775	3.326829	-0.987343
40	1	-3.699038	2.633003	-0.192891
41	1	-0.517154	1.974713	-3.443541
42	1	0.810867	1.481917	-2.381465
43	1	-0.249605	2.812679	-1.907058
44	1	-0.116841	-1.358558	-3.559129
45	1	0.152189	-2.351652	-2.118522
46	1	1.043423	-0.841031	-2.327916
47	1	-3.500058	-2.738201	-1.890127
48	1	-2.934394	-2.899356	-0.220329
49	1	-1.832982	-3.229844	-1.572308
50	1	-1.309622	3.156349	1.092144
51	1	0.327310	3.834680	0.982997
52	1	0.039328	-2.358883	2.389212
53	1	1.761642	-2.568671	2.075274
54	6	0.462922	-3.606042	0.686291

55	1	1.161064	-3.681864	-0.154736
56	1	0.526024	-4.536631	1.263224
57	1	-0.551672	-3.525004	0.290684
58	6	-0.174404	3.004723	2.923458
59	1	-0.537439	3.956514	3.330521
60	1	-0.779708	2.193763	3.341430
61	1	0.863387	2.863134	3.247737

20^{Et} (E = -1042.0936899 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-1.502023	-0.529382	0.053245
2	7	0.124467	0.411143	0.513595
3	6	1.077764	-0.589680	0.421534
4	7	3.160199	1.590732	-0.577129
5	6	-2.976045	1.141782	0.899615
6	6	-3.637202	-0.124377	0.975110
7	6	-2.739483	1.434869	-0.470794
8	17	-1.213617	-2.316612	-1.373547
9	6	-3.835891	-0.594642	-0.355638
10	6	-3.256503	0.349946	-1.245891
11	6	0.528518	1.765489	0.939907
12	6	3.421191	0.411798	-0.154001
13	6	4.283198	2.453439	-0.982635
14	6	2.433035	-0.623904	0.227757
15	1	0.642983	-1.581337	0.555132
16	6	3.186403	-1.891243	0.360749
17	1	-1.661520	-1.359277	1.496963
18	6	4.799711	-0.238104	-0.081352
19	6	4.513169	-1.687292	0.208016
20	1	5.348463	-0.101660	-1.022118
21	1	5.417454	0.229875	0.699068
22	6	5.641387	-2.676520	0.293398
23	6	2.507973	-3.204384	0.654450
24	1	3.226085	-4.027553	0.693228
25	1	1.763395	-3.446634	-0.114986
26	1	1.980552	-3.174509	1.617640
27	1	5.295999	-3.689085	0.520669
28	1	6.360675	-2.383362	1.072286
29	1	6.200640	-2.716849	-0.652815
30	6	-4.240436	-0.719408	2.222287
31	6	-2.752765	2.038051	2.092528
32	6	-2.195445	2.710821	-1.068556
33	6	-3.275862	0.298760	-2.752685
34	6	-4.578481	-1.849390	-0.735532
35	1	-5.255706	-0.325231	2.375056
36	1	-3.648384	-0.478112	3.109472
37	1	-4.310816	-1.808718	2.156013
38	1	-3.720148	2.319189	2.530156
39	1	-2.235770	2.962019	1.822897
40	1	-2.171012	1.542605	2.877118
41	1	-2.960394	3.175877	-1.704256
42	1	-1.311331	2.539264	-1.692590
43	1	-1.924145	3.437741	-0.299153
44	1	-4.161234	0.824069	-3.138371
45	1	-3.306574	-0.729668	-3.121414
46	1	-2.392818	0.780939	-3.184468
47	1	-5.660762	-1.657247	-0.746014
48	1	-4.392735	-2.661024	-0.025072
49	1	-4.288856	-2.205277	-1.727049
50	1	-0.346955	2.406636	0.857447
51	1	1.304285	2.138868	0.263335
52	1	5.057554	2.484712	-0.199063
53	1	4.763725	2.033737	-1.881609
54	6	1.053713	1.787143	2.384764

55	1	1.960962	1.182795	2.483873
56	1	1.298863	2.816300	2.673797
57	1	0.306135	1.399115	3.085803
58	6	3.792774	3.872552	-1.281128
59	1	3.342202	4.322775	-0.389291
60	1	4.622085	4.511304	-1.606184
61	1	3.036095	3.859179	-2.073292

21^{Et} (E = -1042.1103718 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.758656	-0.138007	-0.103240
2	7	-0.182992	1.643311	-0.121745
3	6	-1.494655	1.683502	0.249606
4	7	-1.089192	-1.040732	-0.864576
5	6	2.931777	0.790482	-0.712075
6	6	2.929788	-0.621859	-0.939502
7	6	2.852382	1.010894	0.693999
8	17	-0.127172	-1.225747	1.876883
9	6	2.810404	-1.262232	0.322738
10	6	2.768292	-0.250500	1.331258
11	6	0.328213	3.006349	-0.416868
12	6	-2.243923	-0.563864	-0.525132
13	6	-1.057172	-2.290534	-1.664059
14	6	-2.437601	0.695044	0.143943
15	1	-1.840406	2.648215	0.626014
16	6	-3.866697	0.818052	0.477372
17	1	0.863338	-0.474723	-1.721326
18	6	-3.615802	-1.183487	-0.738339
19	6	-4.549838	-0.238546	-0.015551
20	1	-3.861497	-1.254907	-1.806953
21	1	-3.662607	-2.202612	-0.340136
22	6	-6.020534	-0.537309	0.059250
23	6	-4.415841	1.995240	1.238320
24	1	-5.484433	1.884796	1.442128
25	1	-4.278878	2.930378	0.677704
26	1	-3.897972	2.114834	2.199116
27	1	-6.568316	0.220319	0.627479
28	1	-6.200795	-1.510961	0.537346
29	1	-6.466294	-0.590023	-0.944935
30	6	3.272564	-1.292159	-2.247149
31	6	3.218716	1.799475	-1.799770
32	6	3.001605	2.312976	1.445870
33	6	2.841674	-0.468052	2.818286
34	6	2.866548	-2.749541	0.572629
35	1	4.362064	-1.420054	-2.330824
36	1	2.934199	-0.700536	-3.102637
37	1	2.816692	-2.283844	-2.328889
38	1	4.172506	1.560448	-2.289162
39	1	3.305367	2.816161	-1.405866
40	1	2.446689	1.804022	-2.577991
41	1	3.820147	2.227957	2.172325
42	1	2.097912	2.579530	2.006030
43	1	3.244441	3.146470	0.780433
44	1	3.886348	-0.387296	3.155412
45	1	2.467468	-1.454142	3.099717
46	1	2.252358	0.272939	3.366983
47	1	3.898191	-3.063386	0.788065
48	1	2.528908	-3.320684	-0.298717
49	1	2.242749	-3.035189	1.424583
50	1	1.411585	2.983384	-0.419601
51	1	0.016139	3.690374	0.388188
52	1	-0.177498	-2.225357	-2.310873
53	1	-1.938316	-2.336494	-2.317358
54	6	-0.179132	3.533060	-1.768818

55	1	-1.272552	3.607560	-1.779123
56	1	0.233356	4.529222	-1.970178
57	1	0.120129	2.861019	-2.580422
58	6	-0.977648	-3.567528	-0.809858
59	1	-0.929304	-4.443973	-1.467222
60	1	-0.092374	-3.561321	-0.168624
61	1	-1.851284	-3.673096	-0.159077

TS21^{Et}-13^{Et} (E = -1042.1056904 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.740446	0.074858	-0.214654
2	7	0.504621	-0.991112	1.458756
3	6	-0.450281	-0.631947	2.348871
4	7	-1.440678	0.230673	-0.333520
5	6	3.026349	0.499940	0.475287
6	6	2.410957	1.731454	0.106321
7	6	3.127135	-0.308882	-0.688838
8	17	0.312791	-1.705952	-1.833571
9	6	2.173205	1.697503	-1.306308
10	6	2.620046	0.449696	-1.792718
11	6	1.276377	-2.227129	1.756067
12	6	-2.127990	0.340857	0.760653
13	6	-2.109013	0.507458	-1.629949
14	6	-1.617366	0.048120	2.075470
15	1	-0.307527	-0.956440	3.377812
16	6	-2.646342	0.428930	3.058053
17	1	0.179426	1.572894	0.225566
18	6	-3.553379	0.844051	0.926374
19	6	-3.748801	0.887987	2.425426
20	1	-3.678048	1.830026	0.459207
21	1	-4.282633	0.182799	0.445221
22	6	-5.047215	1.371317	3.007605
23	6	-2.434421	0.279157	4.541529
24	1	-3.283579	0.662119	5.114155
25	1	-1.535319	0.819370	4.867214
26	1	-2.295694	-0.775282	4.817911
27	1	-5.037638	1.366003	4.101705
28	1	-5.887909	0.743398	2.677885
29	1	-5.270526	2.396687	2.678845
30	6	1.595470	-2.515985	3.232107
31	1	0.705288	-2.780219	3.812290
32	1	2.084482	-1.663344	3.715868
33	6	-3.000463	-0.641661	-2.127716
34	1	-2.401272	-1.545231	-2.257651
35	1	-3.814697	-0.859417	-1.428955
36	6	2.297850	2.941536	0.999104
37	6	3.615353	0.227990	1.837167
38	6	3.811174	-1.644533	-0.838329
39	6	2.707056	0.028415	-3.234829
40	6	1.600766	2.830174	-2.121984
41	1	3.265691	3.460993	1.060084
42	1	2.003376	2.667720	2.017521
43	1	1.557135	3.651706	0.620754
44	1	4.510892	0.847108	1.987644
45	1	3.917967	-0.815748	1.954236
46	1	2.912817	0.467461	2.642168
47	1	4.678576	-1.555891	-1.506800
48	1	3.135310	-2.390876	-1.272275
49	1	4.178043	-2.027338	0.118990
50	1	3.723285	0.212530	-3.613703
51	1	2.011386	0.588164	-3.867380
52	1	2.482316	-1.034015	-3.354736
53	1	2.384886	3.552441	-2.390243
54	1	0.828393	3.372931	-1.566320

55	1	1.153475	2.472516	-3.055208
56	1	2.278937	-3.371337	3.282667
57	1	-3.445831	-0.371350	-3.092884
58	1	-2.694653	1.433505	-1.539502
59	1	-1.324808	0.691139	-2.370896
60	1	0.710081	-3.070191	1.333796
61	1	2.205507	-2.174564	1.189498

13^{Et} (E = -1042.1114608 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.807710	0.042407	-0.150145
2	7	0.310126	1.699160	-0.725903
3	6	1.610896	1.731045	-0.474713
4	7	0.833877	-1.199838	-0.383883
5	6	-3.186594	0.072429	0.247182
6	6	-2.537285	0.856425	1.242897
7	6	-2.767306	-1.279486	0.401254
8	17	-1.390090	-0.204382	-2.537618
9	6	-1.709410	-0.012273	2.020873
10	6	-1.848185	-1.335182	1.486655
11	6	-0.225536	2.836207	-1.522584
12	6	2.028342	-0.716634	-0.081981
13	6	0.734649	-2.616617	-0.813797
14	6	2.390550	0.658876	-0.020680
15	1	2.146255	2.653359	-0.709899
16	6	3.822475	0.743647	0.329430
17	1	0.164183	0.448083	1.112246
18	6	3.279384	-1.531725	0.205249
19	6	4.342802	-0.494418	0.476642
20	1	3.110786	-2.195881	1.063689
21	1	3.554665	-2.180689	-0.633599
22	6	5.745548	-0.906318	0.826922
23	6	4.536412	2.061992	0.477826
24	1	5.566933	1.928580	0.818692
25	1	4.021241	2.709212	1.200229
26	1	4.571702	2.606390	-0.476025
27	1	6.393955	-0.044083	1.010385
28	1	6.200231	-1.498097	0.018931
29	1	5.762841	-1.535620	1.728672
30	6	-2.796220	2.313708	1.543123
31	6	-4.227639	0.550426	-0.730705
32	6	-3.280904	-2.433784	-0.420951
33	6	-1.240217	-2.570591	2.106408
34	6	-1.077119	0.327837	3.347547
35	1	-3.617947	2.416416	2.266547
36	1	-3.081434	2.872174	0.645968
37	1	-1.916175	2.799422	1.976060
38	1	-5.235184	0.339504	-0.343934
39	1	-4.120859	0.053327	-1.698538
40	1	-4.159455	1.629195	-0.902575
41	1	-4.327518	-2.648620	-0.163795
42	1	-2.706800	-3.348590	-0.244869
43	1	-3.237473	-2.206798	-1.491226
44	1	-1.782277	-2.845484	3.022191
45	1	-0.191647	-2.412314	2.380396
46	1	-1.283877	-3.430420	1.432010
47	1	-1.806247	0.182610	4.158321
48	1	-0.740137	1.367883	3.380389
49	1	-0.211245	-0.307375	3.555195
50	1	-1.233431	2.560762	-1.842390
51	1	0.370579	2.948926	-2.438703
52	1	1.313224	-3.256124	-0.132133
53	1	-0.312027	-2.916646	-0.719868
54	6	-0.256690	4.161097	-0.744515

55	1	0.749026	4.478898	-0.446137
56	1	-0.685768	4.952979	-1.369724
57	1	-0.864666	4.070544	0.160948
58	6	1.181514	-2.830674	-2.269747
59	1	1.064561	-3.885660	-2.545677
60	1	0.568881	-2.220324	-2.938221
61	1	2.231458	-2.555173	-2.416363

TS13^{Et}-14^{Et} (E = -1042.0887794 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-1.027373	-0.189999	0.333175
2	7	0.470339	-1.338626	0.517842
3	6	1.094300	-1.241597	-0.732609
4	7	0.118179	1.442828	-0.369520
5	6	-3.195767	-0.898721	1.071001
6	6	-2.779382	-1.734623	-0.002718
7	6	-3.421747	0.416496	0.550289
8	17	-0.758584	0.712943	2.590473
9	6	-2.701535	-0.929561	-1.178816
10	6	-3.109882	0.402211	-0.827953
11	6	1.106844	-2.163870	1.557530
12	6	1.307235	1.207910	-0.889601
13	6	-0.329284	2.853723	-0.236972
14	6	1.777660	-0.103685	-1.167957
15	1	1.309323	-2.183509	-1.247277
16	6	2.872736	-0.005766	-2.142852
17	1	-0.503637	-0.524308	-1.274608
18	6	2.254042	2.188798	-1.556464
19	6	3.180856	1.295741	-2.354467
20	1	1.715222	2.902717	-2.190496
21	1	2.811613	2.784755	-0.824158
22	6	4.290144	1.887062	-3.178100
23	6	3.542473	-1.221799	-2.726703
24	1	4.370813	-0.952490	-3.387931
25	1	2.832286	-1.822665	-3.310776
26	1	3.937992	-1.870741	-1.933551
27	1	4.893023	1.117809	-3.670121
28	1	4.964469	2.494274	-2.556643
29	1	3.895103	2.552289	-3.959453
30	6	-2.604757	-3.233760	0.043989
31	6	-3.515385	-1.336327	2.477006
32	6	-3.950974	1.572165	1.359366
33	6	-3.269250	1.527176	-1.821426
34	6	-2.547730	-1.442361	-2.590110
35	1	-3.542369	-3.737127	-0.233134
36	1	-2.331632	-3.579211	1.045582
37	1	-1.829800	-3.575002	-0.649523
38	1	-4.595210	-1.514186	2.586414
39	1	-3.218152	-0.576500	3.204995
40	1	-2.999581	-2.265476	2.739679
41	1	-4.995739	1.390354	1.647324
42	1	-3.923375	2.510764	0.797174
43	1	-3.368348	1.708716	2.276685
44	1	-4.121581	1.334101	-2.487720
45	1	-2.380836	1.641252	-2.453509
46	1	-3.453722	2.484835	-1.326040
47	1	-3.529716	-1.727536	-2.995926
48	1	-1.901613	-2.324368	-2.633048
49	1	-2.119413	-0.683363	-3.251844
50	1	0.554994	-1.983940	2.484235
51	1	2.130153	-1.788883	1.715822
52	1	-0.214088	3.363258	-1.204571
53	1	-1.397889	2.830237	-0.011541
54	6	1.149477	-3.669617	1.246153

55	1	1.719942	-3.883003	0.334503
56	1	1.632516	-4.205550	2.071632
57	1	0.139195	-4.072061	1.120242
58	6	0.394190	3.640967	0.867990
59	1	-0.042072	4.643882	0.948441
60	1	0.281402	3.129976	1.826880
61	1	1.461990	3.754493	0.657328

14^{Et} (E = -1042.1420389 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.813270	-0.020400	-0.369014
2	7	0.028696	1.609837	-0.857392
3	6	1.471702	1.807710	-0.824849
4	7	0.655160	-1.214706	-0.677605
5	6	-3.019690	0.077647	0.768312
6	6	-2.121528	0.924945	1.455285
7	6	-2.547920	-1.274196	0.892700
8	17	-2.074313	-0.423281	-2.318230
9	6	-1.055272	0.114807	1.958082
10	6	-1.357029	-1.253535	1.652690
11	6	-0.707656	2.720368	-1.495876
12	6	1.893191	-0.695209	-0.335463
13	6	0.573899	-2.627652	-1.094866
14	6	2.262850	0.619760	-0.346010
15	1	1.827775	2.097790	-1.832316
16	6	3.649520	0.734909	0.146102
17	1	1.710246	2.663869	-0.178260
18	6	3.056475	-1.515752	0.192924
19	6	4.131330	-0.492492	0.457939
20	1	2.775964	-2.060719	1.103497
21	1	3.395364	-2.271916	-0.525588
22	6	5.492922	-0.889802	0.957079
23	6	4.371166	2.056061	0.241891
24	1	5.402833	1.927364	0.581852
25	1	3.871206	2.735136	0.945910
26	1	4.401243	2.566225	-0.730165
27	1	6.152543	-0.024615	1.077942
28	1	5.984712	-1.587664	0.263692
29	1	5.432971	-1.399443	1.929657
30	6	-2.301956	2.399044	1.714457
31	6	-4.325887	0.470666	0.129665
32	6	-3.284904	-2.481574	0.371904
33	6	-0.585484	-2.444198	2.163884
34	6	0.070633	0.586310	2.846809
35	1	-2.901151	2.554678	2.622983
36	1	-2.820100	2.903829	0.892855
37	1	-1.342548	2.901911	1.864304
38	1	-5.168977	0.171848	0.769100
39	1	-4.454286	-0.013152	-0.843921
40	1	-4.394193	1.552367	-0.022704
41	1	-4.216626	-2.638200	0.933686
42	1	-2.688253	-3.394372	0.465776
43	1	-3.551449	-2.359210	-0.684019
44	1	-0.874080	-2.667787	3.200623
45	1	0.493978	-2.263696	2.156632
46	1	-0.777685	-3.341997	1.569457
47	1	-0.233320	0.557407	3.903554
48	1	0.363825	1.615228	2.616091
49	1	0.961357	-0.041216	2.743262
50	1	-1.778556	2.522932	-1.381025
51	1	-0.505982	2.685889	-2.580493
52	1	1.145841	-3.264027	-0.404542
53	1	-0.473506	-2.936543	-1.023778
54	6	-0.388065	4.130975	-0.968691

55	1	0.636779	4.435370	-1.206631
56	1	-1.063812	4.856572	-1.436733
57	1	-0.521706	4.193220	0.116430
58	6	1.061162	-2.828817	-2.539204
59	1	0.981125	-3.884494	-2.825538
60	1	0.452881	-2.232515	-3.225855
61	1	2.107080	-2.521254	-2.651145

18^{Et} (E = -845.5421563 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.175397	-0.168256	-0.492633
2	7	-0.811305	1.399942	-0.485928
3	6	-1.787788	-0.966441	1.037493
4	6	-0.525819	-1.017310	1.695036
5	6	-1.755908	-1.910851	-0.026677
6	17	0.070477	-0.781010	-2.771011
7	6	0.253971	-2.053754	1.080984
8	6	-0.502695	-2.602648	0.021049
9	6	-0.152313	-0.263572	2.949802
10	6	-2.978892	-0.147915	1.466492
11	6	-2.889759	-2.239060	-0.967170
12	6	-0.119514	-3.751095	-0.876432
13	6	1.597928	-2.535985	1.568425
14	1	-0.443807	-0.828631	3.847150
15	1	-0.651495	0.709914	2.997824
16	1	0.927390	-0.088818	3.015814
17	1	-3.587744	-0.705861	2.192622
18	1	-3.624003	0.104835	0.619209
19	1	-2.674067	0.789917	1.941024
20	1	-3.471218	-3.092804	-0.589105
21	1	-2.518772	-2.501835	-1.962668
22	1	-3.578271	-1.395673	-1.081472
23	1	-0.712576	-4.645589	-0.639142
24	1	0.936453	-4.017341	-0.763046
25	1	-0.289114	-3.505734	-1.930723
26	1	1.473760	-3.275655	2.372154
27	1	2.204832	-1.718372	1.972001
28	1	2.174105	-3.016146	0.770722
29	7	1.954189	0.302192	-0.131675
30	6	2.926846	-0.371942	-0.789296
31	6	2.319251	1.307710	0.698323
32	6	4.281094	-0.072455	-0.636567
33	1	2.593370	-1.151553	-1.463197
34	6	3.652408	1.659402	0.909341
35	1	1.510309	1.840773	1.180575
36	6	4.654889	0.958683	0.230505
37	1	5.020763	-0.636852	-1.191326
38	1	3.893251	2.472223	1.583822
39	1	5.699564	1.213970	0.369019
40	6	-1.555107	2.635360	-0.464347
41	1	-2.469295	2.516054	0.140244
42	1	-1.884634	2.875403	-1.488328
43	6	-0.736685	3.818314	0.088350
44	1	-1.327353	4.742191	0.061433
45	1	-0.438942	3.632414	1.127357
46	1	0.168781	3.969718	-0.509674

17^{Et} **M64** (E = -444.8549561 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	7	1.238661	0.918134	0.398652
2	6	0.075039	0.434738	0.239467
3	6	-1.160301	1.275873	0.181600
4	6	-2.296479	0.361318	-0.006071
5	6	-0.369281	-1.019356	0.083253
6	6	-1.870514	-0.920168	-0.063099
7	1	0.094533	-1.495992	-0.789800
8	1	-0.084949	-1.626116	0.952278
9	6	-2.684020	-2.169745	-0.243073
10	6	-3.708488	0.871455	-0.109676
11	1	-4.431295	0.062557	-0.244827
12	1	-3.811260	1.562874	-0.956696
13	1	-3.988050	1.428063	0.794809
14	1	-3.754157	-1.965233	-0.335280
15	1	-2.540530	-2.851775	0.607137
16	1	-2.363713	-2.715083	-1.142300
17	6	-1.190273	2.612837	0.285754
18	1	-2.118365	3.169758	0.236117
19	1	-0.271613	3.170001	0.422730
20	6	2.407222	0.030496	0.449417
21	1	2.755576	0.011725	1.492311
22	1	2.172256	-1.006269	0.165626
23	6	3.529366	0.574653	-0.445206
24	1	4.425938	-0.049901	-0.361389
25	1	3.215994	0.588505	-1.495344
26	1	3.788257	1.598272	-0.155158

TS10^{Et}-22^{Et} (E = -1042.0983571 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.820792	-0.019712	-0.317402
2	7	0.399571	1.415619	-0.807433
3	6	1.157783	1.535579	0.335518
4	7	0.775236	-1.372883	0.023217
5	6	-1.595464	0.271769	1.877628
6	6	-2.011040	-1.050137	1.520048
7	6	-2.303347	1.194418	1.044914
8	17	-1.404048	-0.649756	-2.541459
9	6	-2.959543	-0.945944	0.466873
10	6	-3.128758	0.435898	0.164075
11	6	0.393765	2.450276	-1.861640
12	6	1.932723	-0.913743	0.339587
13	6	0.664580	-2.828287	-0.314719
14	6	2.168633	0.509138	0.778337
15	1	1.150766	2.469519	0.896855
16	6	3.662251	0.698372	0.455691
17	1	2.108416	0.474775	1.883407
18	6	3.270059	-1.625363	0.289419
19	6	4.260186	-0.478706	0.219660
20	1	3.412087	-2.232191	1.197576
21	1	3.355632	-2.313124	-0.554516
22	6	5.710652	-0.768236	-0.058934
23	6	4.278310	2.066509	0.519799
24	1	5.345857	2.051813	0.282135
25	1	4.159300	2.501557	1.522939
26	1	3.779383	2.747670	-0.181037
27	1	6.314040	0.143269	-0.095086
28	1	5.828243	-1.289809	-1.019228
29	1	6.135958	-1.423986	0.714470
30	6	-1.627042	-2.299013	2.276361
31	6	-0.786089	0.615080	3.104716
32	6	-2.308451	2.692140	1.219809
33	6	-4.090903	0.988203	-0.857555
34	6	-3.702231	-2.074523	-0.202414
35	1	-2.167017	-2.346609	3.232876

36	1	-0.556187	-2.326102	2.507323
37	1	-1.874571	-3.208362	1.720088
38	1	-1.413022	0.551016	4.007665
39	1	-0.382917	1.629621	3.047955
40	1	0.056427	-0.071279	3.246375
41	1	-2.940219	2.977272	2.074065
42	1	-2.703889	3.200676	0.335672
43	1	-1.303049	3.082225	1.409324
44	1	-5.101215	1.068910	-0.430693
45	1	-4.147806	0.344079	-1.739990
46	1	-3.794998	1.986396	-1.196238
47	1	-4.748969	-2.101891	0.131965
48	1	-3.257774	-3.047811	0.029740
49	1	-3.700870	-1.959771	-1.291592
50	1	1.308936	-3.404136	0.361498
51	1	1.367733	2.401779	-2.375781
52	1	-0.371066	2.161667	-2.589989
53	1	-0.367704	-3.116380	-0.103452
54	6	0.987656	-3.161732	-1.779940
55	1	0.312398	-2.629010	-2.452119
56	1	2.015601	-2.897041	-2.046371
57	1	0.863383	-4.239380	-1.938333
58	6	0.150871	3.890936	-1.385512
59	1	0.206352	4.577706	-2.238500
60	1	-0.838017	3.994498	-0.928281
61	1	0.903789	4.206998	-0.653890

22^{Et} (E = -1042.1027081 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.975802	-0.180925	0.331267
2	7	-0.285537	1.067662	1.353013
3	6	-1.526414	1.310692	0.998218
4	7	-0.750728	-1.340378	0.297359
5	6	2.563192	1.204287	-0.822022
6	6	1.346919	1.248641	-1.564888
7	6	3.062772	-0.128669	-0.888234
8	17	2.222960	-1.253024	2.006861
9	6	1.088464	-0.061172	-2.070185
10	6	2.142490	-0.917644	-1.639775
11	6	0.132706	1.559910	2.693104
12	6	-1.904856	-0.815960	-0.009811
13	6	-0.710814	-2.771655	0.702232
14	6	-2.055259	0.674588	-0.259246
15	1	-2.208518	1.833308	1.666188
16	6	-3.543638	0.843657	-0.498261
17	1	-1.492035	1.015803	-1.139346
18	6	-3.255523	-1.483169	-0.145404
19	6	-4.192371	-0.329525	-0.438018
20	1	-3.255762	-2.212666	-0.971199
21	1	-3.562887	-2.045839	0.745732
22	6	-5.661359	-0.599177	-0.624798
23	6	-4.106696	2.210032	-0.787035
24	1	-5.183382	2.182261	-0.977745
25	1	-3.618917	2.652799	-1.666716
26	1	-3.931418	2.897671	0.051211
27	1	-6.228423	0.310449	-0.842019
28	1	-6.091053	-1.057192	0.277155
29	1	-5.826854	-1.306490	-1.449724
30	6	0.590802	2.520431	-1.878042
31	6	3.285040	2.394979	-0.238976
32	6	4.407760	-0.585957	-0.383845
33	6	2.330951	-2.360076	-2.042953
34	6	-0.005650	-0.475776	-3.026111
35	1	1.238966	3.221906	-2.420941

36	1	0.238587	3.030586	-0.973969
37	1	-0.279134	2.328355	-2.513332
38	1	4.019954	2.796861	-0.953325
39	1	3.828764	2.134256	0.675662
40	1	2.589358	3.204137	0.005109
41	1	5.173700	-0.425337	-1.156949
42	1	4.406110	-1.649204	-0.128131
43	1	4.714456	-0.035993	0.510752
44	1	2.930861	-2.438052	-2.962388
45	1	1.371364	-2.851411	-2.236066
46	1	2.848376	-2.932761	-1.265730
47	1	0.405246	-0.615732	-4.035977
48	1	-0.797716	0.275174	-3.099265
49	1	-0.472477	-1.421039	-2.728028
50	1	0.304555	-3.134065	0.523216
51	1	-0.656666	1.307351	3.416148
52	1	-1.384297	-3.353550	0.058311
53	1	1.033855	1.012980	2.982622
54	6	0.405932	3.070591	2.713888
55	1	0.741429	3.379945	3.710666
56	1	1.187444	3.332550	1.993099
57	1	-0.496461	3.640394	2.464311
58	6	-1.073337	-2.974662	2.181547
59	1	-0.366850	-2.437025	2.819847
60	1	-2.084513	-2.615450	2.400715
61	1	-1.026444	-4.040420	2.434689

TS22^{Et}-23^{Et} (E = -1042.0741945 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.704114	0.322718	-0.357610
2	7	0.530422	1.816853	-1.138459
3	6	1.805040	1.603085	-0.891541
4	7	0.629928	-1.183090	-0.915040
5	6	-1.838277	1.278721	1.505166
6	6	-0.990501	0.242558	2.000837
7	6	-2.840560	0.681306	0.685580
8	17	-1.826148	0.253604	-2.518127
9	6	-1.473620	-0.996043	1.474044
10	6	-2.616593	-0.725024	0.668963
11	6	0.194979	2.887849	-2.103036
12	6	1.866829	-0.869016	-0.618239
13	6	0.333996	-2.471540	-1.579586
14	6	2.150759	0.455164	-0.074160
15	1	2.574860	2.248516	-1.314641
16	6	3.527433	0.343826	0.517836
17	1	0.913387	0.538381	0.663094
18	6	3.102308	-1.730545	-0.535828
19	6	4.053351	-0.875245	0.282594
20	1	2.886185	-2.697088	-0.062789
21	1	3.532194	-1.961506	-1.519880
22	6	5.399112	-1.418482	0.677913
23	6	4.148031	1.495797	1.263118
24	1	5.154996	1.262105	1.620846
25	1	3.533524	1.772206	2.130564
26	1	4.217264	2.388566	0.627447
27	1	5.983831	-0.694290	1.252812
28	1	5.987352	-1.695915	-0.208567
29	1	5.296937	-2.327783	1.287610
30	6	0.014796	0.390395	3.116983
31	6	-1.760257	2.728879	1.921754
32	6	-4.009018	1.374893	0.032154
33	6	-3.504870	-1.731376	-0.018450
34	6	-0.937673	-2.358301	1.844339
35	1	-0.483781	0.288138	4.093087

36	1	0.502749	1.369667	3.094256
37	1	0.797791	-0.372298	3.062874
38	1	-2.210145	2.865980	2.915734
39	1	-2.295509	3.382269	1.227175
40	1	-0.724510	3.080361	1.977852
41	1	-4.923314	1.223108	0.623799
42	1	-4.187581	0.986082	-0.974916
43	1	-3.847711	2.454226	-0.051503
44	1	-4.446666	-1.855491	0.535007
45	1	-3.030549	-2.716013	-0.080842
46	1	-3.751583	-1.412461	-1.036293
47	1	-1.365670	-2.694230	2.799725
48	1	0.151335	-2.345794	1.957767
49	1	-1.185632	-3.113301	1.092100
50	1	-0.730995	-2.675670	-1.440533
51	1	1.120014	3.396495	-2.409997
52	1	0.892048	-3.278281	-1.082638
53	1	-0.242468	2.411471	-2.986759
54	6	-0.793477	3.905332	-1.524981
55	1	-1.012853	4.679722	-2.269178
56	1	-1.738021	3.420970	-1.256351
57	1	-0.384030	4.390768	-0.631913
58	6	0.654340	-2.444848	-3.081728
59	1	0.076433	-1.655848	-3.570669
60	1	1.719786	-2.259241	-3.258154
61	1	0.394623	-3.406723	-3.539252

23^{Et} (E = -1042.110676 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.775552	0.100707	-0.120046
2	7	0.327647	1.858436	-0.613122
3	6	1.620817	1.877368	-0.350405
4	7	0.861278	-1.029898	-0.576558
5	6	-2.478309	0.524969	1.517160
6	6	-1.535641	-0.409133	2.054190
7	6	-3.144277	-0.097979	0.429180
8	17	-1.547073	0.234887	-2.461676
9	6	-1.632630	-1.612937	1.288867
10	6	-2.619198	-1.416883	0.281050
11	6	-0.187882	3.036494	-1.355770
12	6	2.054615	-0.580516	-0.193614
13	6	0.791551	-2.352919	-1.243836
14	6	2.404953	0.771401	0.024769
15	1	2.152856	2.818244	-0.510466
16	6	3.827937	0.828159	0.415198
17	1	0.181789	0.508783	1.155350
18	6	3.302338	-1.420547	0.025986
19	6	4.353883	-0.416420	0.436220
20	1	3.120787	-2.180671	0.797434
21	1	3.599924	-1.965683	-0.877117
22	6	5.752464	-0.857089	0.767987
23	6	4.526164	2.127174	0.723163
24	1	5.548001	1.964019	1.077135
25	1	3.985403	2.690757	1.495146
26	1	4.583046	2.770557	-0.165791
27	1	6.389001	-0.016525	1.061080
28	1	6.229186	-1.350755	-0.091556
29	1	5.757103	-1.583638	1.593445
30	6	-0.828137	-0.274766	3.379491
31	6	-2.788187	1.867872	2.134190
32	6	-4.285229	0.463872	-0.377435
33	6	-3.134697	-2.431900	-0.707145
34	6	-0.929868	-2.901025	1.644673
35	1	-1.472827	-0.648284	4.189070

36	1	-0.580122	0.767463	3.599724
37	1	0.102828	-0.848875	3.399598
38	1	-3.347658	1.734481	3.071009
39	1	-3.398301	2.489401	1.473599
40	1	-1.877409	2.427309	2.374210
41	1	-5.235473	0.022455	-0.044127
42	1	-4.162015	0.245352	-1.442020
43	1	-4.368659	1.549233	-0.266598
44	1	-4.157518	-2.735531	-0.443600
45	1	-2.519403	-3.336850	-0.722025
46	1	-3.156932	-2.019916	-1.721521
47	1	-1.382573	-3.342939	2.543353
48	1	0.132427	-2.740538	1.857552
49	1	-1.003719	-3.642759	0.844985
50	1	-0.247778	-2.686596	-1.211127
51	1	0.628556	3.761809	-1.482531
52	1	1.384483	-3.090280	-0.684920
53	1	-0.486118	2.689091	-2.350163
54	6	-1.377871	3.714487	-0.672361
55	1	-1.693681	4.588534	-1.254159
56	1	-2.231356	3.032521	-0.607354
57	1	-1.118613	4.048580	0.338529
58	6	1.244717	-2.289481	-2.711717
59	1	0.613609	-1.588020	-3.264232
60	1	2.286005	-1.960239	-2.799199
61	1	1.159984	-3.280093	-3.174497

TS22^{Et}-25^{Et} (E = -1042.0869102 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.905882	-0.089887	-0.366237
2	7	0.271310	1.349764	-0.977621
3	6	1.621954	1.254652	-0.744735
4	7	0.718207	-1.164483	-0.680357
5	6	-2.567166	1.019330	1.029069
6	6	-1.400489	0.743279	1.800829
7	6	-3.164404	-0.220896	0.678441
8	17	-2.107707	-0.582736	-2.320900
9	6	-1.274720	-0.678307	1.919971
10	6	-2.363224	-1.269772	1.216886
11	6	-0.131322	2.308572	-2.031579
12	6	1.941818	-0.560287	-0.507112
13	6	0.690610	-2.458201	-1.400620
14	6	2.137317	0.552212	0.468960
15	1	2.311762	1.864106	-1.322587
16	6	3.626527	0.656311	0.660061
17	1	1.520565	0.600725	1.366793
18	6	3.306788	-1.115517	-0.884408
19	6	4.270717	-0.241042	-0.103882
20	1	3.420150	-2.170309	-0.595362
21	1	3.506305	-1.077562	-1.963213
22	6	5.753561	-0.446626	-0.258601
23	6	4.201064	1.706803	1.572855
24	1	5.295131	1.698016	1.578771
25	1	3.857773	1.558755	2.606234
26	1	3.871958	2.710222	1.268849
27	1	6.336243	0.233603	0.369664
28	1	6.063965	-0.292594	-1.301622
29	1	6.033543	-1.476047	0.006692
30	6	-0.594417	1.790311	2.534924
31	6	-3.127946	2.391276	0.744290
32	6	-4.485179	-0.407831	-0.019317
33	6	-2.703909	-2.738266	1.143488
34	6	-0.282643	-1.416881	2.786861
35	1	-1.218808	2.283539	3.292902

36	1	-0.213003	2.567359	1.863223
37	1	0.259759	1.350524	3.058020
38	1	-3.867932	2.675930	1.506649
39	1	-3.629630	2.434428	-0.228619
40	1	-2.342786	3.153664	0.750870
41	1	-5.281416	-0.580563	0.719410
42	1	-4.465915	-1.263486	-0.700684
43	1	-4.760486	0.472815	-0.606830
44	1	-3.524294	-2.979743	1.834855
45	1	-1.851632	-3.366767	1.417766
46	1	-3.029641	-3.031681	0.138845
47	1	-0.690028	-1.560224	3.798015
48	1	0.661859	-0.873990	2.887671
49	1	-0.046522	-2.404644	2.380733
50	1	1.448659	-2.436909	-2.196209
51	1	0.491672	2.126743	-2.921859
52	1	-0.280102	-2.546718	-1.897675
53	1	-1.162892	2.086053	-2.319219
54	6	-0.015155	3.779952	-1.603582
55	1	-0.330323	4.440217	-2.420821
56	1	-0.649493	3.983624	-0.733871
57	1	1.017225	4.035180	-1.337936
58	6	0.912961	-3.682608	-0.496085
59	1	1.875057	-3.633441	0.025356
60	1	0.123366	-3.752423	0.258928
61	1	0.894537	-4.602232	-1.094294

25^{Et} (E = -1042.1237791 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.706006	-0.038935	0.281655
2	7	-0.279614	1.570239	0.211016
3	6	-1.548566	0.948597	0.400318
4	7	-0.537172	-1.157371	-0.605816
5	6	2.479257	1.102349	-0.874862
6	6	2.301245	-0.170005	-1.499572
7	6	2.924424	0.881094	0.455452
8	17	0.455385	-0.582907	2.578777
9	6	2.672898	-1.176427	-0.562951
10	6	3.040532	-0.529142	0.648632
11	6	-1.702408	-0.534568	-0.059118
12	6	-2.464605	0.582789	-0.768029
13	1	-2.048533	1.174907	1.343973
14	6	-3.902479	0.403203	-0.405176
15	1	-2.161497	0.922285	-1.752482
16	6	-2.749303	-1.321018	0.744142
17	6	-4.060908	-0.613095	0.462846
18	1	-2.797729	-2.363877	0.413684
19	1	-2.495522	-1.344792	1.808940
20	6	-5.323515	-1.087703	1.130788
21	6	-4.946563	1.339049	-0.956991
22	1	-5.956110	1.071288	-0.630931
23	1	-4.934003	1.331816	-2.055799
24	1	-4.753069	2.374494	-0.643255
25	1	-6.203677	-0.524473	0.805642
26	1	-5.250765	-0.996531	2.223646
27	1	-5.502757	-2.150747	0.913626
28	6	2.002215	-0.348893	-2.967778
29	6	2.389096	2.414300	-1.612477
30	6	3.304854	1.919678	1.481979
31	6	3.627824	-1.198787	1.863502
32	6	2.817839	-2.654467	-0.828938
33	1	2.834091	0.042991	-3.570260
34	1	1.096923	0.186692	-3.274878
35	1	1.878609	-1.401636	-3.234723

36	1	3.185594	2.469366	-2.367896
37	1	2.516024	3.270506	-0.945148
38	1	1.433428	2.529468	-2.133750
39	1	4.395276	1.945534	1.615725
40	1	2.858518	1.702646	2.458612
41	1	2.986879	2.922992	1.184521
42	1	4.721869	-1.259508	1.766154
43	1	3.246031	-2.215767	1.992021
44	1	3.397645	-0.646525	2.778011
45	1	3.867508	-2.894861	-1.050639
46	1	2.219773	-2.980653	-1.683556
47	1	2.522951	-3.255795	0.036762
48	6	-0.241588	3.010914	0.467191
49	6	-0.739497	-2.238965	-1.578767
50	1	0.803361	3.327770	0.468634
51	1	-0.630965	3.195985	1.483426
52	1	0.049670	-2.164347	-2.333214
53	1	-1.692615	-2.070258	-2.103517
54	6	-0.718402	-3.659394	-0.981656
55	1	-0.780201	-4.403723	-1.785699
56	1	0.205909	-3.830189	-0.422579
57	1	-1.556135	-3.828235	-0.299294
58	6	-1.042566	3.852671	-0.541401
59	1	-2.102996	3.578923	-0.531169
60	1	-0.964846	4.917148	-0.289926
61	1	-0.663504	3.709961	-1.559473

TS10^{Et}-24^{Et} (E = -1042.0886316 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.091784	-0.426825	0.295562
2	7	1.726461	0.295266	-0.148592
3	6	1.644456	0.699475	-1.403293
4	7	-1.410030	0.844758	-0.569636
5	6	-0.256609	-2.335745	-1.115053
6	6	-1.601167	-2.169557	-0.657266
7	6	0.556635	-2.676380	0.007388
8	17	-0.093277	0.335903	2.551204
9	6	-1.612377	-2.325290	0.745215
10	6	-0.273251	-2.627342	1.163924
11	6	-0.571805	1.823333	-0.867164
12	6	0.578075	1.649482	-1.848663
13	1	2.407511	0.421623	-2.131969
14	6	1.085062	3.072035	-2.078145
15	1	0.139628	1.264361	-2.784509
16	6	-0.704989	3.296344	-0.531486
17	6	0.371554	3.957065	-1.366212
18	1	-1.706310	3.685475	-0.766716
19	1	-0.553423	3.485575	0.540421
20	6	0.520886	5.453964	-1.318626
21	6	2.217772	3.335547	-3.034125
22	1	2.445437	4.402161	-3.116898
23	1	1.975160	2.963944	-4.040155
24	1	3.135668	2.823702	-2.716298
25	1	1.338509	5.815639	-1.948629
26	1	0.712533	5.788199	-0.289104
27	1	-0.404444	5.948991	-1.645737
28	6	-2.777861	-1.981565	-1.579903
29	6	0.154811	-2.401390	-2.567722
30	6	1.956688	-3.234596	-0.062510
31	6	0.121814	-3.038148	2.560367
32	6	-2.803431	-2.269359	1.669902
33	1	-2.873231	-2.849472	-2.247035
34	1	-2.665347	-1.092831	-2.212107
35	1	-3.718978	-1.891228	-1.029366

36	1	-0.071182	-3.393405	-2.988563
37	1	1.227860	-2.228583	-2.694624
38	1	-0.376571	-1.660246	-3.174508
39	1	1.923529	-4.306042	-0.309410
40	1	2.484620	-3.141278	0.891675
41	1	2.560554	-2.744332	-0.832640
42	1	-0.076275	-4.109367	2.714572
43	1	-0.436951	-2.477230	3.314481
44	1	1.186042	-2.866217	2.751047
45	1	-3.059636	-3.273384	2.037342
46	1	-3.689037	-1.866570	1.168301
47	1	-2.600437	-1.642143	2.545449
48	6	3.032214	-0.037863	0.471707
49	6	-2.825088	1.152629	-0.232239
50	1	2.899625	-0.936071	1.078661
51	1	3.228673	0.781701	1.177624
52	1	-3.371464	0.212595	-0.329338
53	1	-3.214714	1.833800	-1.003499
54	6	-3.100041	1.736848	1.162895
55	1	-2.632671	2.715482	1.303158
56	1	-4.182949	1.856814	1.291485
57	1	-2.723819	1.074624	1.945900
58	6	4.234286	-0.200015	-0.465700
59	1	4.445779	0.719238	-1.023155
60	1	5.121310	-0.436482	0.132135
61	1	4.090623	-1.013761	-1.185133

24^{Et} (E = -1042.1123718 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.173832	-0.812490	-0.452612
2	7	-1.458472	0.697905	-0.144481
3	6	-1.059390	1.825817	0.308640
4	7	1.728920	-0.078190	0.277265
5	6	0.152499	-2.442270	1.312256
6	6	0.883942	-3.028107	0.239719
7	6	-1.205760	-2.305033	0.893997
8	17	0.099355	-0.730731	-2.832434
9	6	-0.023026	-3.246714	-0.835883
10	6	-1.312888	-2.803010	-0.436860
11	6	1.183709	1.035181	-0.355368
12	6	0.409362	2.079027	0.482100
13	1	-1.769934	2.626444	0.518305
14	6	0.829552	3.430396	-0.082164
15	1	0.641714	2.019471	1.560005
16	6	1.886887	1.816782	-1.474260
17	6	1.636600	3.271023	-1.144071
18	1	2.960679	1.600525	-1.526020
19	1	1.486078	1.572554	-2.466147
20	6	2.273732	4.345517	-1.985330
21	6	0.371238	4.712495	0.565899
22	1	0.783821	5.595583	0.068463
23	1	0.680028	4.746922	1.620924
24	1	-0.723698	4.810642	0.552810
25	1	2.001863	5.355646	-1.663745
26	1	1.977908	4.232651	-3.037653
27	1	3.369257	4.262155	-1.955597
28	6	2.314883	-3.513541	0.254563
29	6	0.614521	-2.217667	2.733167
30	6	-2.326584	-1.930183	1.836955
31	6	-2.561678	-2.976036	-1.267062
32	6	0.293979	-3.971599	-2.117776
33	1	2.344316	-4.610433	0.195697
34	1	2.834783	-3.222199	1.171048
35	1	2.892190	-3.125208	-0.591983

36	1	0.045650	-2.859763	3.420683
37	1	0.474402	-1.182143	3.065642
38	1	1.671400	-2.465626	2.860109
39	1	-2.316106	-2.597106	2.710087
40	1	-3.307997	-2.037377	1.365621
41	1	-2.242271	-0.904611	2.217743
42	1	-2.760038	-4.042136	-1.443668
43	1	-2.462765	-2.495984	-2.248050
44	1	-3.444375	-2.558809	-0.773326
45	1	0.082399	-5.046086	-2.009226
46	1	1.348227	-3.865958	-2.391952
47	1	-0.301351	-3.589642	-2.951289
48	6	-2.878721	0.499488	-0.532080
49	6	2.840944	-0.095252	1.226611
50	1	-3.255676	-0.354259	0.032390
51	1	-2.846358	0.189784	-1.583250
52	1	2.610144	0.590854	2.060311
53	1	2.913626	-1.098230	1.652695
54	6	4.202689	0.294659	0.623966
55	1	4.208760	1.336581	0.289432
56	1	4.990979	0.177769	1.378102
57	1	4.446127	-0.343847	-0.232430
58	6	-3.829747	1.688526	-0.370118
59	1	-4.822433	1.393138	-0.726583
60	1	-3.933607	1.998483	0.676408
61	1	-3.510684	2.554459	-0.961214

TS24^{Et}-25^{Et} (E = -1042.096092 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.053152	-0.758290	-0.407371
2	7	-1.476315	0.651364	0.176401
3	6	-0.847965	1.754443	-0.150879
4	7	1.667049	-0.049500	0.226380
5	6	0.010073	-2.401190	1.331785
6	6	0.838287	-2.921283	0.296721
7	6	-1.333445	-2.356388	0.840702
8	17	-0.243698	-0.561569	-2.769783
9	6	0.018310	-3.134477	-0.844558
10	6	-1.329428	-2.804640	-0.503008
11	6	1.237998	1.105192	-0.409054
12	6	0.484417	2.176353	0.384385
13	1	-1.281156	2.396187	-0.929989
14	6	0.972427	3.490984	-0.180894
15	1	0.548280	2.080264	1.474289
16	6	1.955904	1.816177	-1.555684
17	6	1.766356	3.288146	-1.247115
18	1	3.017585	1.542695	-1.599576
19	1	1.539700	1.560586	-2.538035
20	6	2.423228	4.323502	-2.120756
21	6	0.523562	4.792954	0.430152
22	1	0.939019	5.662022	-0.088844
23	1	0.825823	4.853660	1.485337
24	1	-0.572493	4.883544	0.410148
25	1	2.199905	5.346666	-1.803473
26	1	2.096209	4.212221	-3.163928
27	1	3.515064	4.197391	-2.117232
28	6	2.281250	-3.359300	0.391808
29	6	0.377361	-2.145933	2.774547
30	6	-2.524035	-2.050332	1.714411
31	6	-2.512214	-3.035126	-1.410207
32	6	0.461473	-3.789808	-2.127414
33	1	2.356701	-4.435237	0.184845
34	1	2.692300	-3.192313	1.391131
35	1	2.925471	-2.841088	-0.326636

36	1	-0.185971	-2.820451	3.434412
37	1	0.147696	-1.120391	3.088441
38	1	1.439935	-2.320990	2.961682
39	1	-2.589591	-2.787287	2.526907
40	1	-3.464758	-2.096714	1.158761
41	1	-2.450212	-1.059110	2.174881
42	1	-2.613058	-4.104459	-1.640975
43	1	-2.396568	-2.501511	-2.360646
44	1	-3.451160	-2.712395	-0.950013
45	1	0.344798	-4.881726	-2.055931
46	1	1.514039	-3.581899	-2.344730
47	1	-0.126613	-3.438913	-2.979156
48	6	-2.848470	0.537103	-0.390820
49	6	2.746443	-0.068498	1.220820
50	1	-3.115891	-0.517336	-0.433115
51	1	-2.847887	0.912046	-1.425168
52	1	2.523024	0.685785	1.994480
53	1	2.738543	-1.041468	1.713679
54	6	4.147849	0.201194	0.646722
55	1	4.227519	1.215662	0.243937
56	1	4.900857	0.093684	1.437178
57	1	4.384922	-0.507481	-0.154469
58	6	-3.873484	1.307482	0.452753
59	1	-4.878906	1.187311	0.032741
60	1	-3.884874	0.943578	1.485832
61	1	-3.638902	2.378746	0.472570

1^{Ar} (E = -1100.9929376 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-1.146858	0.059444	0.327832
2	7	2.127186	-0.141148	0.121180
3	6	-3.039068	0.118836	-1.198779
4	6	-2.119152	-0.780622	-1.804984
5	6	-2.427340	1.412692	-1.178401
6	17	-0.795638	2.233484	1.394963
7	6	-0.932783	-0.061230	-2.116590
8	6	-1.131839	1.303591	-1.748908
9	6	0.958379	-0.095179	0.174563
10	6	-0.966734	-2.191028	0.631006
11	6	-2.059520	-1.722167	1.438050
12	1	-0.028553	-2.463676	1.105032
13	6	-0.389755	-0.506734	2.700498
14	6	-1.724091	-0.831639	2.502983
15	1	-0.128129	0.312864	3.354904
16	1	0.404773	-1.193369	2.453422
17	6	-2.802938	-0.155000	3.330208
18	6	-3.442679	-2.340166	1.357318
19	1	-4.251961	-1.625613	1.531956
20	1	-3.529480	-3.127572	2.122180
21	1	-3.608104	-2.817380	0.388781
22	1	-3.193108	-0.857511	4.080470
23	1	-3.650886	0.183693	2.725104
24	1	-2.393241	0.710463	3.857285
25	6	-2.425621	-2.170911	-2.299089
26	6	-4.506711	-0.123349	-0.938866
27	6	-3.144320	2.688707	-0.817255
28	6	-0.186927	2.445167	-2.018744
29	6	0.234248	-0.614735	-2.896606
30	1	-2.841477	-2.114354	-3.315949
31	1	-3.161330	-2.687610	-1.677364
32	1	-1.529195	-2.796517	-2.349841
33	1	-5.107930	0.321604	-1.745371
34	1	-4.843401	0.330393	-0.000058
35	1	-4.746800	-1.188172	-0.900920

36	1	-3.799320	2.994355	-1.646995
37	1	-2.443365	3.500738	-0.615859
38	1	-3.770760	2.570064	0.072851
39	1	-0.445123	2.943530	-2.964293
40	1	0.849514	2.102038	-2.100378
41	1	-0.229276	3.188564	-1.218000
42	1	-0.001351	-0.637273	-3.970396
43	1	0.478505	-1.637968	-2.592501
44	1	1.133392	-0.004938	-2.771451
45	1	-1.226222	-2.865493	-0.175771
46	6	3.517762	-0.157986	0.087839
47	6	4.216219	1.032169	0.401528
48	6	4.174449	-1.363560	-0.253496
49	6	5.616074	0.987063	0.362328
50	6	5.575025	-1.351569	-0.281389
51	6	6.291055	-0.189736	0.023257
52	1	6.176136	1.885325	0.600514
53	1	6.102942	-2.263175	-0.541509
54	1	7.375659	-0.201862	-0.001951
55	6	3.475853	2.295041	0.765780
56	1	2.823357	2.630732	-0.049700
57	1	2.829396	2.149303	1.639094
58	1	4.178462	3.101216	0.991909
59	6	3.390208	-2.612662	-0.571611
60	1	2.751744	-2.911809	0.269213
61	1	2.729430	-2.466037	-1.435070
62	1	4.063366	-3.443459	-0.798115

TS1^{Ar}-2^{Ar} (E = -1100.9869907 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-1.120175	-0.549627	-0.685044
2	7	-3.157813	1.404796	-2.264645
3	6	1.269382	-1.027620	-0.868668
4	6	1.080271	-0.332165	0.352527
5	6	0.897179	-0.157823	-1.935850
6	17	-1.430742	-2.203204	-2.431450
7	6	0.582523	0.975466	0.044890
8	6	0.476999	1.081172	-1.370938
9	6	-2.511474	0.627832	-1.616282
10	6	-1.880643	0.011683	1.357705
11	6	-2.106227	-1.404391	1.288654
12	1	-2.720797	0.687351	1.214225
13	6	-3.566233	-0.834425	-0.565498
14	6	-2.920054	-1.848755	0.241343
15	1	-4.116281	-1.210349	-1.420919
16	1	-4.085029	-0.045009	-0.026437
17	6	-3.241416	-3.310895	0.019195
18	6	-1.506825	-2.368626	2.295326
19	1	-1.023630	-3.232555	1.826375
20	1	-2.301589	-2.755209	2.949175
21	1	-0.775034	-1.866775	2.931552
22	1	-4.056793	-3.613711	0.693512
23	1	-2.386206	-3.965210	0.212448
24	1	-3.567834	-3.482723	-1.008621
25	6	1.543225	-0.798073	1.709775
26	6	1.846735	-2.410882	-1.030605
27	6	1.101133	-0.417255	-3.404853
28	6	0.185157	2.346435	-2.139194
29	6	0.457837	2.139388	0.996771
30	1	2.588956	-0.498650	1.870584
31	1	1.496694	-1.886433	1.809866
32	1	0.954717	-0.360066	2.521393
33	1	2.920949	-2.354493	-1.257854
34	1	1.357855	-2.951451	-1.846315

35	1	1.734594	-3.006868	-0.119178
36	1	2.075793	-0.018418	-3.723042
37	1	0.328932	0.062644	-4.013973
38	1	1.078735	-1.485173	-3.631131
39	1	1.118155	2.898072	-2.325265
40	1	-0.488209	3.010364	-1.589119
41	1	-0.276381	2.137524	-3.108355
42	1	1.315011	2.817459	0.876140
43	1	0.443513	1.814948	2.040654
44	1	-0.451379	2.723206	0.816878
45	1	-1.206560	0.352343	2.133206
46	6	-4.478014	1.763095	-2.608367
47	6	-5.046444	1.201129	-3.774291
48	6	-5.161638	2.712240	-1.815995
49	6	-6.351871	1.585852	-4.112414
50	6	-6.463430	3.066435	-2.199953
51	6	-7.059380	2.507255	-3.334060
52	1	-6.809588	1.158888	-4.999401
53	1	-7.007070	3.790656	-1.601105
54	1	-8.067384	2.794224	-3.614825
55	6	-4.265041	0.228571	-4.625625
56	1	-3.342212	0.685585	-5.005697
57	1	-3.961134	-0.662331	-4.063509
58	1	-4.860118	-0.097648	-5.483016
59	6	-4.509406	3.325027	-0.599322
60	1	-4.310577	2.576477	0.179112
61	1	-3.546225	3.786693	-0.850234
62	1	-5.152077	4.094719	-0.163221

2^{Ar} (E = -1101.0025418 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	1.306857	0.271352	0.003049
2	7	-1.631422	-0.661490	0.190855
3	6	2.750858	-1.212570	1.231088
4	6	3.349912	-0.927921	-0.033093
5	6	1.531655	-1.896982	0.992341
6	17	1.414044	1.591707	1.926572
7	6	2.525083	-1.485148	-1.052265
8	6	1.390106	-2.070969	-0.419832
9	6	-0.788358	0.056311	-0.434863
10	6	1.697908	1.222519	-1.863049
11	6	1.070659	2.422188	-1.311115
12	1	1.099893	0.638034	-2.564271
13	6	-1.148527	1.240609	-1.341193
14	6	-0.261171	2.423567	-0.996312
15	1	-2.204153	1.505408	-1.234922
16	1	-0.988486	0.933517	-2.383091
17	6	-0.955823	3.567599	-0.301035
18	6	1.972500	3.605941	-0.984467
19	1	1.890980	3.916019	0.061445
20	1	1.715545	4.467023	-1.614981
21	1	3.020216	3.355482	-1.178085
22	1	-1.711737	4.012281	-0.965210
23	1	-0.271232	4.357505	0.011973
24	1	-1.489679	3.208815	0.589123
25	6	4.678432	-0.241689	-0.230959
26	6	3.377023	-0.947213	2.574311
27	6	0.595885	-2.444984	2.038501
28	6	0.365426	-2.948279	-1.088936
29	6	2.875617	-1.617903	-2.511816
30	1	5.503689	-0.950655	-0.074594
31	1	4.819468	0.582640	0.476519
32	1	4.780124	0.161841	-1.242717
33	1	4.019024	-1.794320	2.855887

34	1	2.624246	-0.819226	3.355716
35	1	3.995337	-0.045442	2.565095
36	1	0.800760	-3.511161	2.212769
37	1	-0.445573	-2.340997	1.722502
38	1	0.713607	-1.924038	2.993370
39	1	0.721955	-3.988503	-1.107789
40	1	0.178684	-2.644773	-2.123696
41	1	-0.585038	-2.923501	-0.552596
42	1	3.383304	-2.576508	-2.688812
43	1	3.548215	-0.823957	-2.848656
44	1	1.986911	-1.596616	-3.150752
45	1	2.718901	1.342301	-2.213541
46	6	-3.048550	-0.475649	0.134483
47	6	-3.680383	0.080719	1.274676
48	6	-3.813766	-0.940939	-0.962461
49	6	-5.077769	0.197882	1.282692
50	6	-5.211680	-0.812121	-0.906765
51	6	-5.845341	-0.242608	0.200430
52	1	-5.563105	0.631468	2.152550
53	1	-5.803154	-1.169370	-1.745244
54	1	-6.926627	-0.151636	0.223825
55	6	-2.857537	0.537839	2.456965
56	1	-2.196649	-0.262853	2.810649
57	1	-2.204773	1.382934	2.203908
58	1	-3.503763	0.847314	3.283923
59	6	-3.162175	-1.582967	-2.167805
60	1	-2.539447	-0.875178	-2.729774
61	1	-2.514123	-2.417888	-1.878618
62	1	-3.922871	-1.967671	-2.853817

TS2^{Ar}-3^{Ar} (E = -1101.0022749 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	-1.484197	-0.674642	0.319441
2	6	2.967675	-1.169581	0.807790
3	6	3.380520	-0.776827	-0.500912
4	6	1.766471	-1.916235	0.680830
5	17	1.534118	1.540116	1.841526
6	6	2.454731	-1.311854	-1.438734
7	6	1.446787	-2.009516	-0.709837
8	6	-0.799730	0.007003	-0.510600
9	6	1.488222	1.493609	-1.798669
10	6	0.639169	2.575210	-1.262754
11	1	1.046456	0.914757	-2.611042
12	6	-1.346131	1.064481	-1.468934
13	6	-0.702469	2.392469	-1.100195
14	1	-2.434985	1.134795	-1.405513
15	1	-1.088407	0.776304	-2.495857
16	6	-1.655791	3.414924	-0.528406
17	6	1.363659	3.855445	-0.881777
18	1	0.827901	4.457525	-0.145733
19	1	1.526835	4.472979	-1.776287
20	1	2.347385	3.623317	-0.459611
21	1	-2.398596	3.705550	-1.285913
22	1	-1.160821	4.322681	-0.179874
23	1	-2.219150	2.989155	0.312984
24	6	4.636852	-0.005296	-0.817508
25	6	3.747077	-0.935211	2.075167
26	6	1.007502	-2.585680	1.798196
27	6	0.395843	-2.912909	-1.297460
28	6	2.597984	-1.299676	-2.938523
29	1	5.513403	-0.666369	-0.766343
30	1	4.804060	0.811261	-0.106601
31	1	4.607514	0.424139	-1.822865
32	1	4.482638	-1.740713	2.212819

33	1	3.098258	-0.917397	2.954167
34	1	4.289735	0.013895	2.049666
35	1	1.286725	-3.646853	1.866540
36	1	-0.071368	-2.524461	1.631109
37	1	1.225017	-2.122443	2.765157
38	1	0.807101	-3.923368	-1.435910
39	1	0.048109	-2.559684	-2.272883
40	1	-0.471287	-2.987975	-0.638375
41	1	3.162809	-2.182797	-3.268643
42	1	3.133775	-0.415189	-3.295099
43	1	1.625911	-1.328011	-3.441384
44	1	2.500189	1.804427	-2.055065
45	6	-2.905211	-0.584641	0.473612
46	6	-3.392539	0.013599	1.662505
47	6	-3.796016	-1.171828	-0.458395
48	6	-4.777176	0.051230	1.882029
49	6	-5.174756	-1.117381	-0.192799
50	6	-5.669428	-0.506704	0.961999
51	1	-5.152088	0.516514	2.789275
52	1	-5.861713	-1.566492	-0.904729
53	1	-6.738257	-0.474893	1.147974
54	6	-2.433952	0.598480	2.673834
55	1	-1.667975	-0.132030	2.960552
56	1	-1.892928	1.466947	2.277846
57	1	-2.967386	0.916537	3.574789
58	6	-3.299055	-1.870291	-1.705456
59	1	-2.769718	-1.189689	-2.383661
60	1	-2.603734	-2.681617	-1.462059
61	1	-4.137750	-2.301923	-2.259981
62	22	1.274763	0.273412	-0.078448

3^{Ar} (E = -1101.0159543 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.976439	0.039395	0.244186
2	7	-1.135236	-0.138742	-0.060089
3	6	3.074883	-1.144363	0.341822
4	6	2.926636	-0.651461	-0.982957
5	6	2.031612	-2.086660	0.580585
6	17	1.181918	0.625908	2.493031
7	6	1.778672	-1.277840	-1.563842
8	6	1.241624	-2.180762	-0.598563
9	6	-0.583991	0.683043	-0.856409
10	6	1.627029	1.996354	-0.498409
11	6	0.619704	3.061694	-0.193937
12	1	1.767603	1.879970	-1.575472
13	6	-1.051482	1.872268	-1.619937
14	6	-0.616678	3.059156	-0.748790
15	1	-0.569784	1.893170	-2.605425
16	1	-2.134999	1.892488	-1.770597
17	6	-1.693438	4.106596	-0.561254
18	6	1.095673	4.122077	0.781453
19	1	0.309502	4.804615	1.112789
20	1	1.903008	4.719835	0.335514
21	1	1.511755	3.631177	1.670515
22	1	-1.368792	4.941847	0.062786
23	1	-2.593042	3.671709	-0.100679
24	1	-2.004839	4.521216	-1.531533
25	6	3.926471	0.202750	-1.717868
26	6	4.193121	-0.801484	1.292634
27	6	1.845150	-2.903581	1.834239
28	6	0.108872	-3.155891	-0.803540
29	6	1.380146	-1.161559	-3.015209
30	1	4.729971	-0.428200	-2.123885
31	1	4.391318	0.947833	-1.064901

32	1	3.471437	0.735615	-2.557728
33	1	5.033212	-1.499016	1.163280
34	1	3.866381	-0.857031	2.334557
35	1	4.574102	0.210028	1.120118
36	1	2.431836	-3.831828	1.776857
37	1	0.797676	-3.186267	1.981440
38	1	2.170185	-2.355795	2.723152
39	1	0.506769	-4.163675	-0.987667
40	1	-0.510604	-2.886918	-1.662498
41	1	-0.546754	-3.215738	0.071237
42	1	2.058796	-1.751437	-3.647647
43	1	1.420985	-0.126065	-3.369883
44	1	0.367038	-1.533668	-3.191158
45	1	2.594284	2.226546	-0.043112
46	6	-2.519999	-0.478662	0.116603
47	6	-3.060611	-0.486440	1.426806
48	6	-3.310136	-0.856430	-1.000325
49	6	-4.403859	-0.850709	1.595139
50	6	-4.646194	-1.229859	-0.775126
51	6	-5.196427	-1.221804	0.506305
52	1	-4.824699	-0.844227	2.595827
53	1	-5.253019	-1.531370	-1.623731
54	1	-6.231800	-1.509497	0.657388
55	6	-2.782304	-0.893637	-2.418396
56	1	-2.913323	0.068886	-2.929646
57	1	-1.717711	-1.135191	-2.458775
58	1	-3.322161	-1.644916	-3.003108
59	6	-2.234693	-0.092404	2.625964
60	1	-1.357772	-0.736269	2.747648
61	1	-1.848334	0.928609	2.540755
62	1	-2.834535	-0.154748	3.538678

TS3^{Ar}-4^{Ar} (E = -1101.0107422 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.232519	-0.396319	-0.245994
2	7	-0.836092	1.347960	-0.712791
3	6	2.469334	-1.419185	0.118059
4	6	1.990959	-0.911923	1.353660
5	6	2.642417	-0.319300	-0.776445
6	17	-0.024959	-1.742034	-2.121314
7	6	1.823716	0.500437	1.212336
8	6	2.254924	0.867389	-0.101049
9	6	-1.573218	0.469790	-0.174648
10	6	-0.936275	-1.593783	1.191846
11	6	-2.287063	-2.056437	0.713047
12	1	-1.024164	-0.940735	2.070687
13	6	-2.992191	0.274894	0.195796
14	6	-3.267252	-1.219559	0.305645
15	1	-3.164936	0.791787	1.152496
16	1	-3.666432	0.755030	-0.527009
17	6	-4.674403	-1.606245	-0.096989
18	6	-2.443168	-3.568041	0.720012
19	1	-3.361025	-3.921072	0.244280
20	1	-2.417820	-3.958252	1.747347
21	1	-1.596532	-4.019631	0.185426
22	1	-4.873678	-2.675093	0.001023
23	1	-4.876809	-1.319927	-1.140538
24	1	-5.414384	-1.076906	0.522595
25	6	1.880367	-1.669403	2.651233
26	6	2.817551	-2.851898	-0.193662
27	6	3.227203	-0.415703	-2.162154
28	6	2.418617	2.276341	-0.615715
29	6	1.481530	1.446846	2.339348
30	1	2.802678	-1.542671	3.236112

31	1	1.739609	-2.742384	2.490619
32	1	1.048987	-1.314318	3.268352
33	1	3.902124	-3.015665	-0.118399
34	1	2.508718	-3.123531	-1.208396
35	1	2.330216	-3.546021	0.498148
36	1	4.321272	-0.511665	-2.110987
37	1	3.003239	0.472591	-2.760990
38	1	2.839579	-1.286531	-2.700006
39	1	3.416772	2.659710	-0.360448
40	1	1.682475	2.960296	-0.184089
41	1	2.316749	2.329357	-1.703767
42	1	2.347565	1.580879	3.003593
43	1	0.656192	1.073492	2.956957
44	1	1.202724	2.436443	1.965977
45	1	-0.337901	-2.456614	1.491159
46	6	-1.102946	2.671030	-1.206287
47	6	-0.864370	2.922708	-2.578431
48	6	-1.550811	3.688915	-0.332760
49	6	-1.095087	4.217187	-3.064861
50	6	-1.751625	4.974108	-0.865231
51	6	-1.531716	5.239730	-2.217491
52	1	-0.927100	4.418956	-4.118218
53	1	-2.084258	5.767886	-0.203203
54	1	-1.695708	6.238250	-2.609299
55	6	-1.810946	3.445114	1.137589
56	1	-2.818389	3.043487	1.308301
57	1	-1.101040	2.735837	1.572673
58	1	-1.738564	4.382257	1.697719
59	6	-0.404611	1.825094	-3.509227
60	1	0.534915	1.372513	-3.174032
61	1	-1.132463	1.007878	-3.567364
62	1	-0.253500	2.217882	-4.518745

4^{Ar} (E = -1101.0132089 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.853512	-0.156322	-0.245908
2	7	1.175928	0.118361	-0.251371
3	6	-2.835634	-1.548305	0.233592
4	6	-2.262499	-1.164969	1.475406
5	6	-1.895633	-2.377687	-0.451315
6	17	-1.661378	0.188996	-2.429845
7	6	-0.944375	-1.710889	1.534754
8	6	-0.727550	-2.475927	0.348720
9	6	0.556408	1.180159	-0.584007
10	6	-1.452159	1.672823	0.820584
11	6	-1.256307	3.081556	0.287961
12	1	-0.945693	1.574077	1.793133
13	6	0.915492	2.574390	-0.867791
14	6	-0.192555	3.516039	-0.417287
15	1	1.889497	2.849262	-0.436839
16	1	1.036078	2.666705	-1.958107
17	6	0.061981	4.938062	-0.876404
18	6	-2.412006	3.998011	0.665128
19	1	-2.309399	5.023096	0.302782
20	1	-2.532867	4.032719	1.756939
21	1	-3.348386	3.592925	0.256697
22	1	-0.672458	5.656192	-0.509054
23	1	0.067718	4.994248	-1.975497
24	1	1.052572	5.278149	-0.539485
25	6	-2.974337	-0.486411	2.617031
26	6	-4.225573	-1.230514	-0.256575
27	6	-2.163753	-3.101310	-1.745245
28	6	0.467708	-3.360263	0.088199
29	6	-0.043213	-1.700238	2.746117

30	1	-3.355353	-1.240210	3.320529
31	1	-3.830481	0.102709	2.274820
32	1	-2.315564	0.183378	3.179327
33	1	-4.900029	-2.084910	-0.102504
34	1	-4.223851	-0.995525	-1.326188
35	1	-4.654667	-0.372665	0.270742
36	1	-2.769241	-4.000127	-1.559724
37	1	-1.237919	-3.421202	-2.233268
38	1	-2.707709	-2.467932	-2.452020
39	1	0.359361	-4.314788	0.622925
40	1	1.401519	-2.899845	0.425750
41	1	0.575285	-3.594829	-0.975184
42	1	-0.273482	-2.555299	3.398543
43	1	-0.173883	-0.793212	3.345682
44	1	1.013411	-1.776749	2.471342
45	1	-2.515318	1.535931	1.035141
46	6	2.577459	-0.135896	-0.049849
47	6	3.276137	-0.840249	-1.056044
48	6	3.213490	0.302363	1.132929
49	6	4.634509	-1.121560	-0.843603
50	6	4.573146	-0.007408	1.302276
51	6	5.279869	-0.715690	0.327732
52	1	5.184658	-1.660546	-1.608783
53	1	5.075015	0.316734	2.208900
54	1	6.329354	-0.946781	0.478132
55	6	2.478136	1.100044	2.187511
56	1	2.271666	2.124366	1.851870
57	1	1.515521	0.649976	2.446507
58	1	3.076475	1.169130	3.100492
59	6	2.594911	-1.248141	-2.342602
60	1	1.689609	-1.835705	-2.158208
61	1	2.285926	-0.374190	-2.929719
62	1	3.269920	-1.845393	-2.962045

TS4^{Ar}-5^{Ar} (E = -1101.0013163 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.651473	-0.095726	-0.683199
2	7	-0.596118	1.401148	-0.475323
3	6	2.899307	-1.017834	-0.682197
4	6	2.541722	-0.706801	0.659291
5	6	2.960282	0.204646	-1.422219
6	17	0.246712	-1.349859	-2.645066
7	6	2.351901	0.705939	0.740722
8	6	2.627447	1.268447	-0.544052
9	6	-1.232313	0.239397	-0.454935
10	6	-0.718466	-1.067479	0.958209
11	6	-2.134564	-1.554741	1.149665
12	1	-0.313672	-0.639459	1.881042
13	6	-2.683048	-0.038445	-0.640203
14	6	-3.106532	-1.089631	0.351617
15	1	-3.278440	0.877657	-0.521996
16	1	-2.842105	-0.385566	-1.670805
17	6	-4.559368	-1.494769	0.330694
18	6	-2.309024	-2.593132	2.238102
19	1	-3.348358	-2.909108	2.361949
20	1	-1.958253	-2.201332	3.202968
21	1	-1.707012	-3.486510	2.020814
22	1	-4.801389	-2.248852	1.083300
23	1	-4.830495	-1.902443	-0.653423
24	1	-5.208422	-0.624588	0.503374
25	6	2.528271	-1.669004	1.822091
26	6	3.278475	-2.374565	-1.219777
27	6	3.392760	0.318557	-2.862087
28	6	2.704257	2.746145	-0.840838

29	6	2.128079	1.501145	2.004292
30	1	3.515342	-1.698354	2.304590
31	1	2.289545	-2.689820	1.505822
32	1	1.801466	-1.381075	2.588852
33	1	4.372018	-2.485492	-1.246420
34	1	2.900748	-2.520142	-2.236372
35	1	2.880365	-3.183794	-0.599412
36	1	4.485659	0.233181	-2.944664
37	1	3.103099	1.279287	-3.298922
38	1	2.947738	-0.472333	-3.474165
39	1	3.630711	3.169172	-0.427039
40	1	1.866918	3.298749	-0.403058
41	1	2.709648	2.942934	-1.916829
42	1	3.092321	1.791441	2.446387
43	1	1.586696	0.925666	2.762368
44	1	1.567181	2.421079	1.812231
45	1	-0.098257	-1.943712	0.717937
46	6	-1.091720	2.723712	-0.285301
47	6	-1.053981	3.612168	-1.389002
48	6	-1.621110	3.134536	0.962834
49	6	-1.525348	4.921834	-1.212095
50	6	-2.082240	4.454952	1.091438
51	6	-2.032260	5.347577	0.018516
52	1	-1.501167	5.605914	-2.055112
53	1	-2.482660	4.778139	2.047907
54	1	-2.391770	6.364526	0.138144
55	6	-0.558581	3.157161	-2.743417
56	1	0.490364	2.845412	-2.714101
57	1	-1.128933	2.295771	-3.111141
58	1	-0.652190	3.964664	-3.475736
59	6	-1.696178	2.192811	2.143972
60	1	-2.374152	1.350970	1.958354
61	1	-0.717129	1.764577	2.382761
62	1	-2.058409	2.721828	3.030366

5^{Ar} (E = -1101.0272465 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.914597	-0.073371	-0.149232
2	7	0.988982	-0.009699	0.097060
3	6	-2.976173	-1.319243	-0.042191
4	6	-2.596208	-0.928294	1.270634
5	6	-1.987003	-2.224258	-0.541383
6	17	-1.642548	0.743731	-2.227294
7	6	-1.358524	-1.576271	1.573677
8	6	-0.994067	-2.395031	0.458706
9	6	0.647740	1.322389	-0.014456
10	6	-0.251800	1.980172	0.974997
11	6	-0.336984	3.415372	0.505355
12	1	0.006997	1.852191	2.032433
13	6	1.174549	2.356366	-0.982353
14	6	0.456364	3.619185	-0.559655
15	1	2.266033	2.474466	-0.905687
16	1	0.958740	2.099122	-2.026656
17	6	0.671214	4.896854	-1.324463
18	6	-1.229471	4.391639	1.223345
19	1	-1.157312	5.399542	0.804842
20	1	-0.972629	4.450655	2.290373
21	1	-2.281566	4.078829	1.162988
22	1	0.121987	5.739704	-0.894841
23	1	0.349887	4.780362	-2.368476
24	1	1.737440	5.161757	-1.345997
25	6	-3.423458	-0.101519	2.227872
26	6	-4.256262	-0.953232	-0.748543
27	6	-2.067584	-2.926062	-1.873848

28	6	0.144773	-3.383969	0.454150
29	6	-0.657487	-1.563685	2.911154
30	1	-4.127868	-0.742183	2.777429
31	1	-4.012082	0.660109	1.706026
32	1	-2.800606	0.407229	2.971294
33	1	-5.006320	-1.746592	-0.617543
34	1	-4.095946	-0.814825	-1.821731
35	1	-4.684446	-0.025186	-0.356955
36	1	-2.822785	-3.724130	-1.842587
37	1	-1.114477	-3.386116	-2.150700
38	1	-2.349660	-2.233291	-2.673690
39	1	-0.097335	-4.243330	1.095368
40	1	1.073961	-2.943689	0.828048
41	1	0.341548	-3.772195	-0.548953
42	1	-1.077395	-2.337560	3.570147
43	1	-0.769432	-0.603945	3.427450
44	1	0.412171	-1.765705	2.805226
45	1	-1.332006	1.514904	0.959505
46	6	2.315434	-0.515144	0.024062
47	6	2.744142	-1.248049	-1.112130
48	6	3.213271	-0.259080	1.093611
49	6	4.058609	-1.742473	-1.137328
50	6	4.516465	-0.773773	1.026137
51	6	4.940899	-1.517515	-0.077891
52	1	4.390798	-2.299416	-2.008720
53	1	5.199134	-0.585895	1.850054
54	1	5.952132	-1.909852	-0.116575
55	6	1.838532	-1.472010	-2.302444
56	1	1.019679	-2.162592	-2.075439
57	1	1.373985	-0.539153	-2.639215
58	1	2.406564	-1.892893	-3.138162
59	6	2.781615	0.555787	2.290957
60	1	2.615222	1.607881	2.023662
61	1	1.840800	0.184337	2.712514
62	1	3.544857	0.527146	3.074409

TS5^{Ar}-6^{Ar} (E = -1101.0217512 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.394835	-0.217814	-0.352290
2	7	-0.593488	1.316717	0.350661
3	6	2.057718	-1.566061	0.644124
4	6	2.026292	-0.300814	1.306671
5	6	2.484819	-1.338877	-0.694083
6	17	-0.136455	-0.571482	-2.597296
7	6	2.469018	0.701222	0.386704
8	6	2.746421	0.056481	-0.848081
9	6	-1.661673	0.465785	0.204280
10	6	-1.626010	-0.845870	0.746808
11	6	-2.825149	-1.569467	0.228523
12	1	-1.280273	-1.014659	1.764154
13	6	-2.870457	0.599980	-0.699886
14	6	-3.534158	-0.755179	-0.578037
15	1	-3.535446	1.408314	-0.365797
16	1	-2.591411	0.823996	-1.735145
17	6	-4.814607	-1.048101	-1.310051
18	6	-3.098333	-2.997326	0.614205
19	1	-4.035376	-3.366023	0.187373
20	1	-3.158353	-3.107737	1.705797
21	1	-2.288539	-3.654158	0.267365
22	1	-5.191359	-2.053542	-1.099814
23	1	-4.671526	-0.962632	-2.396019
24	1	-5.597495	-0.328361	-1.033002
25	6	1.762884	-0.081998	2.777229
26	6	1.850676	-2.912659	1.294803

27	6	2.727738	-2.394109	-1.742255
28	6	3.306129	0.687668	-2.098093
29	6	2.746946	2.139683	0.744156
30	1	2.686797	-0.224627	3.356371
31	1	1.021552	-0.784713	3.172931
32	1	1.403526	0.931875	2.974519
33	1	2.800624	-3.289471	1.700474
34	1	1.476723	-3.653552	0.581835
35	1	1.138846	-2.859517	2.124893
36	1	3.780896	-2.710386	-1.732708
37	1	2.496957	-2.022342	-2.744728
38	1	2.112439	-3.282889	-1.571049
39	1	4.367849	0.427314	-2.211823
40	1	3.237501	1.778809	-2.070444
41	1	2.781265	0.340350	-2.994065
42	1	3.688009	2.215457	1.307140
43	1	1.954313	2.568247	1.364345
44	1	2.846500	2.769058	-0.144472
45	1	-0.420603	-1.637529	0.178868
46	6	-0.764232	2.722217	0.523041
47	6	-0.413411	3.638465	-0.499767
48	6	-1.299595	3.189662	1.753179
49	6	-0.586300	5.012198	-0.260787
50	6	-1.453431	4.570382	1.947936
51	6	-1.096832	5.482024	0.951166
52	1	-0.324488	5.715473	-1.046042
53	1	-1.854804	4.926608	2.892383
54	1	-1.221115	6.547721	1.115095
55	6	0.111617	3.179068	-1.840965
56	1	1.127410	2.775705	-1.768294
57	1	-0.504962	2.384928	-2.272332
58	1	0.137392	4.015802	-2.546153
59	6	-1.693617	2.224579	2.848517
60	1	-2.565647	1.620751	2.565185
61	1	-0.885191	1.519524	3.071780
62	1	-1.944077	2.764727	3.766458

6^{Ar} (E = -1101.028515 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.971182	0.380292	-0.108269
2	7	0.860113	-0.250174	0.171430
3	6	-2.957832	0.115387	1.153590
4	6	-2.031731	-0.898098	1.542508
5	6	-3.303037	-0.118932	-0.208347
6	17	-1.074176	1.253370	-2.254530
7	6	-1.835524	-1.778900	0.434992
8	6	-2.621298	-1.291473	-0.645660
9	6	1.334475	1.052162	0.174871
10	6	0.872744	2.035265	1.013342
11	6	1.398748	3.340949	0.589780
12	1	0.353041	1.863880	1.945112
13	6	2.251645	1.695609	-0.847849
14	6	2.223870	3.158736	-0.468586
15	1	3.266069	1.278488	-0.807171
16	1	1.878649	1.535159	-1.864272
17	6	3.040635	4.175383	-1.215397
18	6	1.040107	4.618207	1.301665
19	1	1.580222	5.478982	0.896686
20	1	1.267971	4.550722	2.374118
21	1	-0.035335	4.821317	1.211374
22	1	2.928646	5.179893	-0.795933
23	1	2.745675	4.219070	-2.273076
24	1	4.109025	3.917927	-1.192570
25	6	-1.498205	-1.094206	2.940353

26	6	-3.611732	1.111987	2.077873
27	6	-4.295673	0.674977	-1.016705
28	6	-2.811400	-1.939992	-1.993448
29	6	-1.091525	-3.089111	0.483428
30	1	-2.259554	-1.568462	3.576125
31	1	-1.227350	-0.143720	3.413762
32	1	-0.615084	-1.738182	2.947788
33	1	-4.500283	0.663605	2.545548
34	1	-3.930583	2.010342	1.542238
35	1	-2.936511	1.424839	2.879960
36	1	-5.309870	0.271745	-0.882313
37	1	-4.058268	0.642961	-2.083471
38	1	-4.312117	1.726461	-0.713545
39	1	-3.815923	-2.380466	-2.059175
40	1	-2.089942	-2.743635	-2.164355
41	1	-2.711451	-1.215508	-2.808141
42	1	-1.745237	-3.874372	0.888895
43	1	-0.204255	-3.034057	1.119063
44	1	-0.763231	-3.413563	-0.507323
45	1	-1.465887	1.808574	0.600860
46	6	1.790475	-1.334926	0.054098
47	6	1.926928	-2.067585	-1.151167
48	6	2.589591	-1.659194	1.182749
49	6	2.840674	-3.134496	-1.192842
50	6	3.487019	-2.735006	1.097120
51	6	3.612610	-3.475450	-0.080343
52	1	2.949125	-3.693201	-2.117954
53	1	4.089782	-2.987098	1.964898
54	1	4.310928	-4.304691	-0.133324
55	6	1.140077	-1.722909	-2.395299
56	1	0.077157	-1.966212	-2.293148
57	1	1.188112	-0.656238	-2.629676
58	1	1.525137	-2.280899	-3.254600
59	6	2.493190	-0.865081	2.465995
60	1	2.936999	0.133117	2.357645
61	1	1.452585	-0.711070	2.767514
62	1	3.018973	-1.378029	3.277057

7^{Ar} (E = -1504.0864419 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.177594	-1.058617	-0.259717
2	7	-1.543917	0.297207	0.336167
3	6	1.051023	-2.296279	-1.980180
4	6	-0.065264	-1.616784	-2.567357
5	6	0.548604	-3.278326	-1.088093
6	17	0.321337	-2.022658	1.892700
7	6	-1.255612	-2.169905	-2.014512
8	6	-0.869883	-3.191066	-1.083731
9	6	-2.075238	1.367990	-0.377909
10	6	-1.793514	1.794572	-1.644844
11	6	-2.599063	2.971256	-1.978786
12	1	-1.064697	1.357007	-2.308936
13	6	-3.140310	2.304962	0.180961
14	6	-3.397720	3.289658	-0.931135
15	1	-4.048521	1.761606	0.466453
16	1	-2.795580	2.803377	1.094636
17	6	-4.395169	4.406451	-0.788934
18	6	-2.489027	3.662197	-3.314506
19	1	-3.160266	4.523552	-3.388298
20	1	-2.733706	2.973854	-4.135380
21	1	-1.464195	4.018069	-3.489308
22	1	-4.445276	5.023712	-1.692341
23	1	-4.142025	5.069164	0.051934
24	1	-5.407400	4.022246	-0.593711

25	6	0.009963	-0.716073	-3.775135
26	6	2.487750	-2.126935	-2.407190
27	6	1.355781	-4.304812	-0.340302
28	6	-1.769153	-4.142040	-0.332822
29	6	-2.654045	-1.839624	-2.479282
30	1	0.161339	-1.321203	-4.680993
31	1	0.838859	-0.004465	-3.708024
32	1	-0.913293	-0.146936	-3.912381
33	1	2.702637	-2.758962	-3.280731
34	1	3.185437	-2.412987	-1.614256
35	1	2.706360	-1.092305	-2.689762
36	1	1.386391	-5.246751	-0.907531
37	1	0.923796	-4.511602	0.642138
38	1	2.387722	-3.976079	-0.185203
39	1	-1.562487	-5.175814	-0.641013
40	1	-2.825908	-3.947598	-0.533525
41	1	-1.607577	-4.082977	0.749645
42	1	-2.807559	-2.202375	-3.505196
43	1	-2.844330	-0.760130	-2.476797
44	1	-3.410117	-2.310109	-1.846497
45	1	0.337948	0.230607	-1.195586
46	7	2.761784	0.318071	0.163253
47	6	1.729827	-0.216032	0.020602
48	6	3.956449	1.012451	0.308745
49	6	4.190272	2.138025	-0.516734
50	6	4.884147	0.568202	1.280394
51	6	5.399320	2.824223	-0.346203
52	6	6.077682	1.290320	1.409514
53	6	6.334320	2.406039	0.606174
54	1	5.603782	3.691920	-0.964672
55	1	6.806845	0.973034	2.147554
56	1	7.264687	2.951869	0.723485
57	6	-2.043105	0.225572	1.703053
58	6	-3.213892	-0.507557	2.004234
59	6	-1.372998	0.951529	2.718238
60	6	-3.680776	-0.531108	3.329270
61	6	-1.872916	0.906176	4.028488
62	6	-3.015489	0.164890	4.340224
63	1	-4.579109	-1.096876	3.560018
64	1	-1.356475	1.459910	4.807516
65	1	-3.388075	0.137239	5.359524
66	6	-0.129369	1.757131	2.421874
67	1	0.115203	2.409864	3.266031
68	1	0.727298	1.095935	2.247017
69	1	-0.244151	2.378071	1.526705
70	6	-3.976401	-1.255192	0.935460
71	1	-4.175811	-0.628380	0.059509
72	1	-3.416510	-2.126647	0.582796
73	1	-4.934772	-1.611732	1.325981
74	6	4.592306	-0.638217	2.137626
75	1	3.652067	-0.525316	2.689504
76	1	4.490501	-1.546812	1.530996
77	1	5.396241	-0.801776	2.859761
78	6	3.168971	2.574502	-1.537348
79	1	2.987089	1.790906	-2.283757
80	1	2.200975	2.795480	-1.071256
81	1	3.507112	3.471047	-2.063235

TS7^{Ar} -9^{Ar} (E = -1504.0852024 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	22	-0.955952	-0.163079	-0.110686
2	7	0.640647	-1.388290	-0.272444
3	6	-2.423937	1.344549	1.126383
4	6	-1.613001	0.597038	2.044269
5	6	-3.288190	0.433453	0.464459
6	17	-1.876338	-0.468304	-2.283023
7	6	-1.961639	-0.777616	1.921031
8	6	-2.997120	-0.875449	0.931806
9	6	1.757364	-1.462879	0.549588
10	6	2.043986	-0.762014	1.687999
11	6	3.348253	-1.163755	2.219618
12	1	1.418545	-0.010238	2.143244
13	6	2.928304	-2.405343	0.299084
14	6	3.886116	-2.124322	1.428906
15	1	2.606318	-3.453294	0.287045
16	1	3.385403	-2.226028	-0.681054
17	6	5.194806	-2.853718	1.560450
18	6	3.925741	-0.551367	3.470600
19	1	4.904226	-0.973206	3.720315
20	1	3.261061	-0.712260	4.330728
21	1	4.046866	0.534861	3.357526
22	1	5.759378	-2.520644	2.437834
23	1	5.832756	-2.700147	0.677527
24	1	5.044186	-3.939291	1.655610
25	6	-0.787095	1.199911	3.154055
26	6	-2.504411	2.849172	1.057437
27	6	-4.389035	0.793374	-0.496235
28	6	-3.761706	-2.110250	0.523334
29	6	-1.447447	-1.881472	2.814407
30	1	-1.450811	1.567647	3.950029
31	1	-0.183945	2.047343	2.813142
32	1	-0.114936	0.464767	3.604536
33	1	-3.254351	3.222403	1.769491
34	1	-2.793722	3.194850	0.060426
35	1	-1.549328	3.319915	1.309503
36	1	-5.329433	0.954965	0.051015
37	1	-4.553262	0.000587	-1.230125
38	1	-4.161253	1.709851	-1.048362
39	1	-4.818888	-2.007088	0.802998
40	1	-3.380186	-3.008251	1.016017
41	1	-3.722251	-2.270595	-0.560133
42	1	-1.830938	-1.752181	3.836056
43	1	-0.352861	-1.890869	2.869154
44	1	-1.768657	-2.865222	2.464436
45	1	0.254276	0.903254	0.510925
46	7	0.245100	2.628478	-1.144661
47	6	-0.212051	1.616082	-0.715679
48	6	1.067548	3.732745	-1.333000
49	6	2.137744	3.992701	-0.439978
50	6	0.800176	4.566290	-2.447893
51	6	2.940706	5.113566	-0.690628
52	6	1.630143	5.675299	-2.652820
53	6	2.691704	5.948216	-1.784076
54	1	3.766600	5.328635	-0.020111
55	1	1.441985	6.325056	-3.501263
56	1	3.325594	6.811277	-1.959787
57	6	0.698207	-2.306337	-1.401638
58	6	0.193981	-3.621537	-1.277618
59	6	1.314507	-1.885458	-2.605522
60	6	0.289154	-4.493493	-2.375092
61	6	1.392953	-2.787546	-3.677625
62	6	0.879647	-4.082767	-3.571655
63	1	-0.099495	-5.503494	-2.279660
64	1	1.861806	-2.464291	-4.602669

65	1	0.946079	-4.767296	-4.411597
66	6	1.868440	-0.488464	-2.764329
67	1	2.480624	-0.419643	-3.669249
68	1	1.055995	0.242472	-2.848445
69	1	2.484358	-0.188601	-1.909277
70	6	-0.435217	-4.110697	0.006647
71	1	0.179124	-3.872352	0.881548
72	1	-1.416341	-3.652161	0.170141
73	1	-0.578749	-5.195332	-0.025465
74	6	-0.343197	4.258712	-3.383327
75	1	-0.235146	3.266289	-3.836415
76	1	-1.304670	4.257651	-2.855717
77	1	-0.395132	4.998737	-4.186422
78	6	2.400440	3.095354	0.741558
79	1	1.554196	3.095553	1.440524
80	1	2.556125	2.052141	0.440054
81	1	3.287484	3.426920	1.288242

9^{Ar} (E = -1504.1077694 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.418816	-0.894489	-0.131717
2	7	-1.327932	0.005884	0.324275
3	6	1.847728	-2.246554	-1.677164
4	6	0.568391	-1.992628	-2.265222
5	6	1.650762	-3.040800	-0.528563
6	17	1.086841	-1.289724	2.122167
7	6	-0.421142	-2.663780	-1.485275
8	6	0.245581	-3.288410	-0.391946
9	6	-2.136860	0.728251	-0.547220
10	6	-2.044566	0.878900	-1.902464
11	6	-3.111119	1.755734	-2.393867
12	1	-1.309076	0.422741	-2.544781
13	6	-3.342597	1.542654	-0.091089
14	6	-3.882877	2.159329	-1.356270
15	1	-4.089731	0.914483	0.406989
16	1	-3.056286	2.300647	0.647403
17	6	-5.090694	3.055669	-1.349112
18	6	-3.253510	2.099595	-3.855014
19	1	-4.103880	2.763378	-4.039329
20	1	-3.397054	1.193962	-4.460642
21	1	-2.350063	2.598302	-4.232795
22	1	-5.341171	3.407813	-2.355479
23	1	-4.932096	3.942177	-0.717386
24	1	-5.975161	2.537961	-0.949307
25	6	0.364058	-1.428049	-3.648888
26	6	3.157880	-1.836904	-2.298822
27	6	2.707033	-3.657650	0.348411
28	6	-0.336203	-4.222036	0.639771
29	6	-1.861658	-2.833978	-1.905772
30	1	0.639778	-2.183146	-4.399681
31	1	0.984230	-0.545459	-3.837591
32	1	-0.679440	-1.156946	-3.829645
33	1	3.287466	-2.333794	-3.270147
34	1	4.007521	-2.117657	-1.671502
35	1	3.215514	-0.756627	-2.477831
36	1	2.800132	-4.730454	0.126273
37	1	2.452589	-3.551898	1.406893
38	1	3.687411	-3.199590	0.191900
39	1	0.213354	-5.172552	0.635666
40	1	-1.385551	-4.450641	0.435481
41	1	-0.263404	-3.805987	1.651084
42	1	-1.905359	-3.310328	-2.894507
43	1	-2.396544	-1.880467	-1.973450
44	1	-2.408040	-3.473144	-1.209139

45	1	0.967618	1.320833	-2.178645
46	7	1.797675	0.747636	-0.331866
47	6	0.993967	0.671989	-1.305181
48	6	2.791214	1.735766	-0.025929
49	6	2.554043	3.110466	-0.306966
50	6	3.988321	1.321491	0.611851
51	6	3.535083	4.042992	0.067646
52	6	4.940882	2.293805	0.949216
53	6	4.721462	3.646151	0.684449
54	1	3.353234	5.095164	-0.129052
55	1	5.859990	1.977095	1.432098
56	1	5.464795	4.385743	0.963866
57	6	-1.819175	0.024906	1.699547
58	6	-2.792881	-0.910021	2.122593
59	6	-1.369713	1.032667	2.587871
60	6	-3.271402	-0.849650	3.442479
61	6	-1.874796	1.061603	3.896944
62	6	-2.813610	0.123404	4.331728
63	1	-4.015412	-1.572954	3.764088
64	1	-1.522447	1.831645	4.577198
65	1	-3.190736	0.156875	5.349130
66	6	-0.358552	2.070417	2.164656
67	1	-0.248584	2.836337	2.938742
68	1	0.622914	1.615615	1.996193
69	1	-0.652934	2.568334	1.234617
70	6	-3.345100	-1.960243	1.189001
71	1	-3.701847	-1.526899	0.248140
72	1	-2.583548	-2.699696	0.929557
73	1	-4.180398	-2.489402	1.658129
74	6	4.285251	-0.130123	0.899044
75	1	3.427192	-0.638511	1.344348
76	1	4.549822	-0.668503	-0.019333
77	1	5.133792	-0.214396	1.584782
78	6	1.297158	3.635317	-0.969644
79	1	1.358381	3.581996	-2.064788
80	1	0.399065	3.087928	-0.670286
81	1	1.151373	4.687748	-0.707962

TS9^{Ar}-10^{Ar} (E = -1504.0893298 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.675567	-0.452366	0.103714
2	7	-1.916620	0.991565	-0.543833
3	6	-2.070694	0.884930	0.756485
4	7	0.800378	1.001596	0.694364
5	6	-2.260009	-2.272720	0.494295
6	6	-1.797835	-1.780945	1.754289
7	6	-1.157956	-2.856716	-0.176341
8	17	0.470989	-0.755227	-1.986592
9	6	-0.404224	-2.074012	1.860695
10	6	-0.004101	-2.723540	0.657978
11	6	0.355198	1.887569	1.567488
12	6	-0.859925	1.749146	2.290645
13	1	-3.016802	1.052258	1.264687
14	6	-1.094708	3.023371	3.008993
15	1	-1.087034	0.828342	2.806773
16	6	0.936448	3.259201	1.855852
17	6	-0.094835	3.897433	2.760686
18	1	1.909019	3.161371	2.357443
19	1	1.131711	3.831877	0.943871
20	6	0.091920	5.301123	3.266835
21	6	-2.296472	3.211896	3.897070
22	1	-2.294092	4.185835	4.395276
23	1	-2.330447	2.435387	4.674098
24	1	-3.230658	3.129995	3.324820

25	1	-0.716482	5.606327	3.938482
26	1	0.127341	6.023080	2.437919
27	1	1.040132	5.402455	3.814424
28	6	-2.694919	-1.370752	2.894502
29	6	-3.711574	-2.304126	0.083233
30	6	-1.188554	-3.621286	-1.472969
31	6	1.345605	-3.310140	0.331415
32	6	0.398768	-1.913072	3.131137
33	1	-3.069212	-2.267491	3.410454
34	1	-3.566685	-0.805543	2.551375
35	1	-2.170663	-0.766556	3.641148
36	1	-4.278936	-2.967860	0.750675
37	1	-3.837256	-2.682195	-0.934637
38	1	-4.180097	-1.314125	0.135443
39	1	-1.206174	-4.701726	-1.269017
40	1	-0.307623	-3.403359	-2.082361
41	1	-2.072847	-3.380713	-2.069848
42	1	1.281195	-4.405392	0.269843
43	1	2.092192	-3.066712	1.092515
44	1	1.714150	-2.942982	-0.632682
45	1	-0.083529	-2.466162	3.948222
46	1	0.490898	-0.869503	3.452499
47	1	1.408813	-2.313536	3.018671
48	6	-2.699039	1.734937	-1.486839
49	6	-3.138972	1.109626	-2.684643
50	6	-3.034609	3.094426	-1.233691
51	6	-3.911685	1.850697	-3.592853
52	6	-3.799350	3.793479	-2.180637
53	6	-4.242918	3.183912	-3.353951
54	1	-4.253253	1.361897	-4.500360
55	1	-4.040389	4.834462	-1.985956
56	1	-4.835523	3.740799	-4.072633
57	6	2.088616	1.295639	0.085640
58	6	2.163342	2.109169	-1.071952
59	6	3.263779	0.795005	0.691286
60	6	3.429826	2.382478	-1.614978
61	6	4.508404	1.090405	0.111304
62	6	4.596318	1.876194	-1.038264
63	1	3.491027	3.000686	-2.505657
64	1	5.409679	0.700789	0.575514
65	1	5.563770	2.096508	-1.478336
66	6	-2.828287	-0.329715	-3.014435
67	1	-1.763766	-0.477854	-3.215956
68	1	-3.084742	-0.998179	-2.188337
69	1	-3.396612	-0.645889	-3.894920
70	6	-2.576850	3.839224	0.000125
71	1	-3.100844	3.512920	0.904884
72	1	-1.510510	3.704494	0.192568
73	1	-2.765256	4.910619	-0.119692
74	6	3.210941	-0.042170	1.947401
75	1	4.221348	-0.265553	2.302698
76	1	2.672294	0.462624	2.758181
77	1	2.698825	-0.991841	1.768824
78	6	0.938704	2.689400	-1.740101
79	1	0.274549	1.896993	-2.093526
80	1	0.354349	3.322631	-1.063489
81	1	1.231788	3.303178	-2.597316

10^{Ar} (E = -1504.1214911 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	22	-0.013486	1.082581	0.117338
2	7	-1.625544	0.102597	0.029464
3	6	-1.102815	-0.056044	-1.266636
4	7	1.391381	-0.768264	-0.151973
5	6	-0.329386	3.005155	-1.334037
6	6	0.947284	2.459761	-1.663816
7	6	-0.277593	3.473420	0.006799
8	17	-0.258541	1.193180	2.511988
9	6	1.802770	2.635286	-0.537616
10	6	1.046043	3.249257	0.495427
11	6	0.783680	-1.673475	-0.833613
12	6	-0.427361	-1.363058	-1.661674
13	1	-1.636553	0.408782	-2.098161
14	6	-1.133989	-2.720529	-1.715878
15	1	-0.030191	-1.175293	-2.677407
16	6	1.045753	-3.158834	-0.886722
17	6	-0.311062	-3.702625	-1.310907
18	1	1.823819	-3.401929	-1.624070
19	1	1.402146	-3.546357	0.073012
20	6	-0.557556	-5.186022	-1.268473
21	6	-2.529249	-2.830729	-2.261844
22	1	-2.890872	-3.863028	-2.269165
23	1	-2.573028	-2.448112	-3.291978
24	1	-3.226517	-2.228406	-1.667239
25	1	-1.568510	-5.445763	-1.594873
26	1	-0.421108	-5.575945	-0.249905
27	1	0.154554	-5.721867	-1.912422
28	6	1.333150	2.037424	-3.060148
29	6	-1.410036	3.268764	-2.351090
30	6	-1.359747	4.213341	0.753818
31	6	1.606016	3.760873	1.796356
32	6	3.289155	2.385178	-0.462097
33	1	1.230545	2.885889	-3.751841
34	1	0.694504	1.232067	-3.441393
35	1	2.371605	1.701880	-3.113499
36	1	-1.047918	4.006677	-3.081674
37	1	-2.312592	3.679642	-1.893770
38	1	-1.691858	2.371653	-2.912148
39	1	-1.162675	5.294952	0.742436
40	1	-1.411580	3.892301	1.798627
41	1	-2.346127	4.052291	0.309085
42	1	2.015900	4.772530	1.656224
43	1	2.412781	3.123096	2.171134
44	1	0.839018	3.807327	2.572478
45	1	3.825532	3.342730	-0.407016
46	1	3.658834	1.851476	-1.340017
47	1	3.571492	1.804506	0.422378
48	6	-2.903936	-0.314677	0.515230
49	6	-4.094521	0.287761	0.027333
50	6	-2.993778	-1.352523	1.480906
51	6	-5.339359	-0.158058	0.498901
52	6	-4.259925	-1.768467	1.924388
53	6	-5.430908	-1.182904	1.441148
54	1	-6.241240	0.316986	0.122652
55	1	-4.316973	-2.565724	2.660104
56	1	-6.400227	-1.516720	1.798097
57	6	2.711182	-1.107529	0.370083
58	6	3.796770	-1.086254	-0.543230
59	6	2.919908	-1.449303	1.727984
60	6	5.094001	-1.321196	-0.059660
61	6	4.236330	-1.680686	2.162986
62	6	5.320489	-1.601716	1.288072
63	1	5.926461	-1.287527	-0.756263
64	1	4.398761	-1.937898	3.205047

65	1	6.328854	-1.775079	1.649643
66	6	-4.051887	1.419462	-0.967967
67	1	-3.335165	2.182447	-0.654885
68	1	-3.745291	1.082474	-1.966363
69	1	-5.036425	1.887832	-1.064047
70	6	-1.765551	-2.031723	2.032835
71	1	-1.183112	-2.511028	1.237571
72	1	-1.114229	-1.308620	2.528754
73	1	-2.047538	-2.804108	2.756239
74	6	3.605986	-0.870605	-2.029512
75	1	4.508998	-0.442673	-2.476177
76	1	3.414586	-1.821805	-2.546228
77	1	2.766373	-0.211637	-2.250630
78	6	1.784272	-1.648879	2.699851
79	1	2.173062	-1.929682	3.683084
80	1	1.175962	-0.749103	2.815838
81	1	1.112182	-2.449493	2.367905

11^{Ar} (E = -1504.1147989 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	2.168923	-0.191851	0.518362
2	7	0.631337	0.763416	0.053415
3	6	0.399402	-0.493594	-0.560570
4	7	-2.745751	-0.234007	0.580757
5	6	3.562207	0.804594	-1.090924
6	6	3.504781	-0.594018	-1.392583
7	6	4.204574	0.950145	0.170466
8	17	2.008834	-1.281518	2.572233
9	6	4.158848	-1.294576	-0.327761
10	6	4.587331	-0.345827	0.634420
11	6	-2.131623	-1.067016	-0.154597
12	6	-0.657484	-1.434182	0.067253
13	1	0.412273	-0.544216	-1.647668
14	6	-0.599033	-2.832729	-0.534946
15	1	-0.487342	-1.450432	1.147856
16	6	-2.715449	-2.010110	-1.195406
17	6	-1.699737	-3.128523	-1.245983
18	1	-3.716065	-2.350676	-0.906774
19	1	-2.832794	-1.512680	-2.168883
20	6	-2.017022	-4.385202	-2.011527
21	6	0.593533	-3.713722	-0.285608
22	1	0.512735	-4.677582	-0.796802
23	1	0.711393	-3.904682	0.789511
24	1	1.518085	-3.228266	-0.619200
25	1	-1.204257	-5.116251	-1.974357
26	1	-2.218183	-4.156249	-3.067913
27	1	-2.922651	-4.865320	-1.614622
28	6	3.063836	-1.198656	-2.703001
29	6	3.203311	1.944628	-2.012154
30	6	4.514128	2.262946	0.849671
31	6	5.381404	-0.651348	1.877783
32	6	4.422270	-2.778391	-0.250586
33	1	3.907866	-1.244361	-3.405613
34	1	2.271906	-0.611703	-3.176903
35	1	2.683917	-2.216762	-2.576442
36	1	4.115586	2.462394	-2.338219
37	1	2.553813	2.686225	-1.535933
38	1	2.694705	1.585833	-2.910203
39	1	5.518851	2.608619	0.567669
40	1	4.496487	2.176355	1.941326
41	1	3.806385	3.045590	0.558988
42	1	6.452163	-0.716618	1.637360
43	1	5.078596	-1.602193	2.325494
44	1	5.260377	0.125114	2.639062

45	1	5.487183	-2.982730	-0.428402
46	1	3.853605	-3.332895	-1.001856
47	1	4.170575	-3.186812	0.734344
48	6	0.092175	2.056982	-0.134776
49	6	0.129121	2.933136	0.988778
50	6	-0.436239	2.522611	-1.372343
51	6	-0.364610	4.238117	0.862335
52	6	-0.916747	3.841076	-1.447048
53	6	-0.886884	4.699803	-0.347583
54	1	-0.345768	4.891311	1.729864
55	1	-1.317272	4.191766	-2.393961
56	1	-1.268377	5.712151	-0.431792
57	6	-4.164590	-0.093976	0.515653
58	6	-4.802803	0.719608	-0.449052
59	6	-4.917221	-0.724734	1.539255
60	6	-6.198783	0.867086	-0.387133
61	6	-6.309045	-0.556117	1.559297
62	6	-6.953701	0.232866	0.602236
63	1	-6.690407	1.494882	-1.125271
64	1	-6.885668	-1.042810	2.340948
65	1	-8.031154	0.360652	0.633906
66	6	-4.225279	-1.564156	2.589087
67	1	-3.776312	-2.469939	2.160008
68	1	-3.408237	-1.007615	3.064114
69	1	-4.931625	-1.876619	3.364221
70	6	-4.013097	1.436478	-1.519002
71	1	-3.163776	1.980460	-1.093561
72	1	-3.609499	0.741996	-2.267398
73	1	-4.647458	2.153978	-2.048919
74	6	0.677504	2.473211	2.320054
75	1	0.301519	1.481046	2.588069
76	1	1.776518	2.416508	2.319296
77	1	0.399740	3.174723	3.112865
78	6	-0.494283	1.673877	-2.623693
79	1	0.493506	1.307843	-2.921143
80	1	-1.137910	0.796634	-2.498555
81	1	-0.893383	2.262278	-3.455727

TS11^{Ar}-20^{Ar} (E = -1504.0862955 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	1.060059	0.029256	-0.357112
2	7	0.193741	-0.850320	1.182214
3	6	-0.339934	0.418776	1.259254
4	7	-2.363739	-1.143452	-0.339280
5	6	3.194347	0.281312	0.572039
6	6	2.551950	1.552654	0.681852
7	6	3.400966	0.021490	-0.816672
8	17	0.759414	-1.296636	-2.263811
9	6	2.359768	2.068774	-0.639583
10	6	2.879999	1.119670	-1.557656
11	6	-2.180840	0.092292	-0.541349
12	6	-1.119416	0.921979	0.180321
13	1	-0.086068	1.087956	2.072572
14	6	-1.724611	2.300421	0.228042
15	1	-0.126453	1.117352	-1.018512
16	6	-3.064506	1.075293	-1.285045
17	6	-2.792968	2.383362	-0.586908
18	1	-2.790096	1.125695	-2.347283
19	1	-4.115219	0.772275	-1.245504
20	6	-3.686627	3.562620	-0.849730
21	6	-1.209963	3.380142	1.140529
22	1	-1.811318	4.288967	1.057184
23	1	-0.173928	3.645091	0.912489
24	1	-1.241445	3.060231	2.190171

25	1	-3.379329	4.459861	-0.306196
26	1	-4.724164	3.333359	-0.569639
27	1	-3.695492	3.803147	-1.922200
28	6	2.400552	2.305974	1.981487
29	6	3.747707	-0.512385	1.730592
30	6	4.153747	-1.140435	-1.414267
31	6	2.947630	1.289258	-3.052196
32	6	1.900609	3.457099	-1.020901
33	1	3.358914	2.770781	2.254521
34	1	2.117516	1.644715	2.807012
35	1	1.657009	3.104050	1.920532
36	1	4.686212	-0.062631	2.085168
37	1	3.966484	-1.545770	1.448477
38	1	3.054557	-0.544640	2.576408
39	1	5.169724	-0.823953	-1.689857
40	1	3.661720	-1.517113	-2.315555
41	1	4.249495	-1.972948	-0.711532
42	1	3.915718	1.720355	-3.346514
43	1	2.160893	1.957841	-3.415688
44	1	2.833523	0.331680	-3.567726
45	1	2.732030	4.010346	-1.478342
46	1	1.573698	4.029754	-0.149652
47	1	1.078228	3.443209	-1.743822
48	6	0.343797	-1.745203	2.259989
49	6	1.008061	-2.977876	1.977654
50	6	-0.165159	-1.520368	3.577772
51	6	1.237141	-3.898467	3.005468
52	6	0.088763	-2.483183	4.570779
53	6	0.798653	-3.653747	4.308641
54	1	1.748577	-4.827015	2.769064
55	1	-0.299213	-2.303998	5.569559
56	1	0.979114	-4.376439	5.097678
57	6	-3.503660	-1.841484	-0.826600
58	6	-4.373135	-2.368559	0.166863
59	6	-3.731011	-2.112676	-2.198526
60	6	-5.486420	-3.118360	-0.231671
61	6	-4.852685	-2.886778	-2.548288
62	6	-5.732026	-3.379154	-1.583716
63	1	-6.155134	-3.511432	0.528825
64	1	-5.022925	-3.107176	-3.598603
65	1	-6.590821	-3.973675	-1.879056
66	6	-2.801799	-1.628136	-3.289797
67	1	-3.094442	-0.637850	-3.666890
68	1	-1.767089	-1.556542	-2.946755
69	1	-2.829863	-2.313586	-4.143528
70	6	-4.098767	-2.115727	1.631606
71	1	-3.073288	-2.401864	1.893905
72	1	-4.204235	-1.053550	1.890552
73	1	-4.792626	-2.683244	2.259307
74	6	1.422441	-3.325718	0.571247
75	1	0.577418	-3.256108	-0.120469
76	1	2.194406	-2.651316	0.182406
77	1	1.824609	-4.342898	0.529900
78	6	-1.015615	-0.330737	3.992760
79	1	-0.425361	0.577058	4.170647
80	1	-1.778967	-0.086541	3.247726
81	1	-1.530128	-0.564422	4.930356

20^{Ar} (E = -1504.1074208 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-2.619748	0.560477	0.100363
2	7	-0.744845	0.020213	-0.135771
3	6	-0.140634	1.255175	-0.239677
4	7	2.750471	-0.049657	0.133178

5	6	-3.618735	-1.603631	0.288609
6	6	-3.689041	-1.208218	-1.075349
7	6	-4.404544	-0.687578	1.053339
8	17	-2.755251	2.112108	1.783105
9	6	-4.524013	-0.051935	-1.162036
10	6	-4.974405	0.257469	0.156850
11	6	2.475230	1.162540	-0.162412
12	6	1.128897	1.763939	-0.295180
13	1	-0.893689	2.045392	-0.312053
14	6	1.339571	3.220191	-0.490765
15	1	-2.850342	1.574031	-1.208098
16	6	3.490994	2.284642	-0.367713
17	6	2.654471	3.522079	-0.539138
18	1	4.173968	2.350034	0.487848
19	1	4.125045	2.083824	-1.240866
20	6	3.315374	4.857888	-0.734662
21	6	0.194189	4.191357	-0.620047
22	1	0.551795	5.216050	-0.749122
23	1	-0.448281	4.172513	0.270300
24	1	-0.441295	3.949637	-1.482980
25	1	2.594410	5.671895	-0.852928
26	1	3.961400	4.848103	-1.624858
27	1	3.962318	5.103205	0.120244
28	6	-3.159948	-1.992953	-2.246965
29	6	-3.033076	-2.895416	0.796875
30	6	-4.674512	-0.783102	2.533124
31	6	-5.930036	1.366802	0.512018
32	6	-5.041561	0.570445	-2.434463
33	1	-3.891238	-2.760814	-2.537913
34	1	-2.222349	-2.501687	-2.010025
35	1	-2.989583	-1.355615	-3.119064
36	1	-3.786725	-3.691642	0.712092
37	1	-2.743069	-2.832384	1.848918
38	1	-2.155871	-3.205016	0.225831
39	1	-5.559718	-1.408522	2.715045
40	1	-4.859448	0.199971	2.973633
41	1	-3.835806	-1.235251	3.071326
42	1	-6.965731	1.041943	0.338605
43	1	-5.757473	2.260404	-0.096212
44	1	-5.838958	1.657409	1.561294
45	1	-5.945961	0.042146	-2.768420
46	1	-4.305313	0.517239	-3.241126
47	1	-5.301321	1.622847	-2.291169
48	6	-0.036796	-1.223060	-0.227395
49	6	0.226930	-1.953676	0.952362
50	6	0.339895	-1.716710	-1.496056
51	6	0.839177	-3.210002	0.838703
52	6	0.938285	-2.986071	-1.566925
53	6	1.182976	-3.732854	-0.411751
54	1	1.055886	-3.774752	1.740673
55	1	1.221419	-3.380835	-2.538601
56	1	1.650099	-4.709932	-0.483551
57	6	4.110381	-0.441230	0.282503
58	6	4.849218	-0.900098	-0.835584
59	6	4.681253	-0.458488	1.579294
60	6	6.164172	-1.349409	-0.636808
61	6	5.999348	-0.913971	1.732785
62	6	6.743848	-1.355836	0.635275
63	1	6.732490	-1.701709	-1.493452
64	1	6.438701	-0.924248	2.726606
65	1	7.761540	-1.708397	0.770652
66	6	3.881069	0.004052	2.775806
67	1	3.623290	1.069632	2.713549
68	1	2.933330	-0.541845	2.852626

69	1	4.443721	-0.148874	3.701873
70	6	4.232491	-0.921959	-2.216059
71	1	3.290260	-1.481370	-2.216046
72	1	4.003351	0.086985	-2.583869
73	1	4.912237	-1.389043	-2.935506
74	6	-0.081770	-1.373280	2.312975
75	1	0.454514	-0.429289	2.464470
76	1	-1.147232	-1.152430	2.446371
77	1	0.218758	-2.066383	3.104731
78	6	0.166605	-0.888120	-2.748237
79	1	-0.786971	-0.352535	-2.759258
80	1	0.956024	-0.128765	-2.821098
81	1	0.224335	-1.516045	-3.642872

21^{Ar} (E = -1504.1202625 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.278638	-0.777308	-0.284537
2	7	-1.238383	0.984873	0.126334
3	6	-0.625167	2.159858	-0.192191
4	7	1.668599	0.236078	0.047700
5	6	-1.664457	-2.437322	0.811048
6	6	-0.446960	-3.051662	0.374208
7	6	-2.436107	-2.113896	-0.341492
8	17	0.280638	-0.204680	-2.572932
9	6	-0.445979	-3.036191	-1.043382
10	6	-1.677714	-2.452790	-1.487448
11	6	1.795177	1.512472	-0.165926
12	6	0.708808	2.419002	-0.399214
13	1	-1.288725	3.021370	-0.242502
14	6	1.285074	3.752338	-0.662423
15	1	0.418923	-1.147588	1.155533
16	6	3.082142	2.316022	-0.171588
17	6	2.629975	3.710603	-0.540039
18	1	3.578124	2.286274	0.806759
19	1	3.799074	1.899472	-0.887826
20	6	3.634423	4.815684	-0.707568
21	6	0.429151	4.945696	-0.993684
22	1	1.033960	5.830574	-1.209617
23	1	-0.243261	5.197612	-0.161794
24	1	-0.201171	4.744296	-1.869997
25	1	3.164984	5.762975	-0.989107
26	1	4.372349	4.563315	-1.482717
27	1	4.197309	4.983866	0.222225
28	6	0.553047	-3.769274	1.246566
29	6	-2.150746	-2.404860	2.237391
30	6	-3.895316	-1.740922	-0.334206
31	6	-2.155890	-2.424032	-2.913300
32	6	0.587265	-3.673869	-1.938541
33	1	0.323367	-4.844416	1.274306
34	1	0.533413	-3.393361	2.273017
35	1	1.576371	-3.657628	0.875087
36	1	-2.627771	-3.361698	2.495816
37	1	-2.889549	-1.615369	2.398499
38	1	-1.327751	-2.247690	2.941555
39	1	-4.499297	-2.660602	-0.334729
40	1	-4.181019	-1.162357	-1.215373
41	1	-4.174111	-1.163863	0.549465
42	1	-2.508360	-3.421206	-3.215262
43	1	-1.355169	-2.123520	-3.594224
44	1	-2.985549	-1.723692	-3.048203
45	1	0.293055	-4.706056	-2.178913
46	1	1.570793	-3.717898	-1.459904
47	1	0.692809	-3.126095	-2.878919
48	6	-2.605533	1.207935	0.552785

49	6	-2.897731	1.235168	1.936486
50	6	-3.608412	1.479875	-0.408102
51	6	-4.223134	1.468253	2.340266
52	6	-4.917366	1.726554	0.039871
53	6	-5.230251	1.709017	1.401182
54	1	-4.455312	1.482375	3.401221
55	1	-5.693865	1.927257	-0.692735
56	1	-6.248445	1.893010	1.729198
57	6	2.831280	-0.475809	0.549538
58	6	3.060299	-0.483607	1.949871
59	6	3.713953	-1.146560	-0.330605
60	6	4.150726	-1.210137	2.452815
61	6	4.792704	-1.862050	0.221180
62	6	5.009887	-1.905732	1.598831
63	1	4.323511	-1.221324	3.524977
64	1	5.470737	-2.379863	-0.450840
65	1	5.847030	-2.466168	2.002823
66	6	-3.295648	1.520164	-1.887749
67	1	-2.788368	2.452729	-2.169302
68	1	-2.626706	0.708537	-2.187661
69	1	-4.215829	1.458632	-2.477110
70	6	-1.804042	1.089111	2.970724
71	1	-1.182916	0.208156	2.790501
72	1	-1.129373	1.955163	2.953706
73	1	-2.230251	1.015670	3.975975
74	6	2.169873	0.279609	2.903257
75	1	2.178425	1.358071	2.700445
76	1	1.129161	-0.049237	2.817066
77	1	2.499272	0.131923	3.936085
78	6	3.574322	-1.077252	-1.834627
79	1	2.570742	-1.334852	-2.177012
80	1	3.766437	-0.063471	-2.209917
81	1	4.294721	-1.748032	-2.312755

TS21^{Ar}-13^{Ar} (E = -1504.1007006 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.872134	0.047758	-0.182025
2	7	0.384077	1.355800	0.978612
3	6	1.315567	0.815600	1.757048
4	7	0.768874	-1.341623	-0.361824
5	6	-3.069102	-0.003902	0.895759
6	6	-2.870611	-1.296253	0.306096
7	6	-3.113168	0.953257	-0.147133
8	17	-0.177501	1.358904	-2.103351
9	6	-2.801119	-1.130281	-1.099440
10	6	-2.938221	0.260253	-1.383761
11	6	1.619616	-1.425226	0.654322
12	6	1.796739	-0.495808	1.714970
13	1	1.820531	1.489800	2.450612
14	6	2.854644	-1.011922	2.610945
15	1	-0.726540	-0.612957	1.327616
16	6	2.647152	-2.528779	0.842637
17	6	3.346877	-2.173505	2.130534
18	1	2.163157	-3.509966	0.884022
19	1	3.340367	-2.571289	-0.006491
20	6	4.429803	-3.055906	2.686219
21	6	3.281499	-0.279872	3.856628
22	1	4.005610	-0.859202	4.436284
23	1	2.419967	-0.068775	4.504188
24	1	3.748166	0.685239	3.615458
25	1	4.824151	-2.677076	3.634132
26	1	5.272821	-3.139933	1.984892
27	1	4.060947	-4.077039	2.861035
28	6	-3.024674	-2.575990	1.086680

29	6	-3.455430	0.181584	2.340269
30	6	-3.401856	2.428965	-0.028410
31	6	-3.177125	0.839047	-2.751413
32	6	-2.745222	-2.204267	-2.157523
33	1	-4.031260	-2.613042	1.526825
34	1	-2.305963	-2.647849	1.910190
35	1	-2.912224	-3.458291	0.455026
36	1	-4.412254	-0.327548	2.525424
37	1	-3.591004	1.233296	2.597118
38	1	-2.718113	-0.249246	3.025838
39	1	-4.416737	2.646235	-0.389766
40	1	-2.704197	3.025593	-0.625312
41	1	-3.334767	2.774443	1.005662
42	1	-4.237278	0.713643	-3.019988
43	1	-2.570903	0.345001	-3.514918
44	1	-2.938546	1.904058	-2.786446
45	1	-3.692775	-2.228283	-2.713353
46	1	-2.588174	-3.194190	-1.725020
47	1	-1.945678	-2.027160	-2.884758
48	6	0.355105	2.809682	1.016146
49	6	-0.490179	3.465971	1.944983
50	6	1.206583	3.565779	0.172666
51	6	-0.581120	4.866676	1.914952
52	6	1.082552	4.965852	0.173993
53	6	0.179295	5.616365	1.015541
54	1	-1.241241	5.366130	2.618904
55	1	1.719421	5.545760	-0.488350
56	1	0.092114	6.698215	0.993484
57	6	1.014677	-2.252733	-1.472024
58	6	0.449867	-3.550083	-1.475912
59	6	1.871760	-1.845253	-2.529450
60	6	0.644821	-4.375993	-2.597389
61	6	2.039569	-2.702683	-3.627954
62	6	1.413906	-3.951257	-3.679704
63	1	0.196426	-5.365807	-2.603204
64	1	2.683434	-2.385510	-4.442773
65	1	1.549833	-4.595786	-4.542398
66	6	-1.202280	2.706772	3.041194
67	1	-2.176185	3.153021	3.270179
68	1	-1.342131	1.657917	2.786157
69	1	-0.612214	2.736166	3.968750
70	6	2.304797	2.943140	-0.661866
71	1	2.244590	1.857623	-0.675365
72	1	2.256560	3.289785	-1.698919
73	1	3.286977	3.231519	-0.260831
74	6	-0.276020	-4.121315	-0.278919
75	1	0.362879	-4.845374	0.245803
76	1	-0.555695	-3.350213	0.437479
77	1	-1.177562	-4.665031	-0.580879
78	6	2.658863	-0.557368	-2.472573
79	1	2.000006	0.313198	-2.443882
80	1	3.293705	-0.515527	-1.577722
81	1	3.311358	-0.473794	-3.347159

13^{Ar} (E = -1504.1014371 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.881298	0.093134	-0.128938
2	7	0.447413	1.410981	1.044344
3	6	1.382780	0.850284	1.786451
4	7	0.716216	-1.282380	-0.335101
5	6	-3.129901	-0.030174	0.820685
6	6	-2.836314	-1.338123	0.310472
7	6	-3.164881	0.870477	-0.270260
8	17	-0.349938	1.762898	-1.828386

9	6	-2.716757	-1.241183	-1.098897
10	6	-2.894201	0.123272	-1.460811
11	6	1.597727	-1.389268	0.668079
12	6	1.829529	-0.477862	1.721932
13	1	1.929619	1.504300	2.467356
14	6	2.911138	-1.013035	2.578773
15	1	-0.822156	-0.417890	1.443113
16	6	2.617120	-2.508245	0.809931
17	6	3.372563	-2.174654	2.070750
18	1	2.135122	-3.487560	0.864084
19	1	3.273462	-2.543919	-0.069000
20	6	4.464465	-3.075512	2.577497
21	6	3.387664	-0.297193	3.816022
22	1	4.119946	-0.893087	4.368060
23	1	2.550355	-0.078223	4.492064
24	1	3.862447	0.662511	3.569241
25	1	4.898283	-2.709124	3.513036
26	1	5.280055	-3.163156	1.844916
27	1	4.090553	-4.093744	2.758234
28	6	-2.954035	-2.580934	1.154242
29	6	-3.598270	0.212519	2.232605
30	6	-3.533478	2.332226	-0.236060
31	6	-3.079232	0.613033	-2.871786
32	6	-2.622453	-2.364090	-2.100955
33	1	-3.960225	-2.629993	1.593594
34	1	-2.236986	-2.588107	1.982768
35	1	-2.808754	-3.489238	0.568024
36	1	-4.553847	-0.308434	2.389670
37	1	-3.768396	1.271945	2.432147
38	1	-2.890661	-0.168963	2.976033
39	1	-4.559648	2.474094	-0.603496
40	1	-2.864653	2.923039	-0.869279
41	1	-3.483612	2.740725	0.776725
42	1	-4.096870	0.368464	-3.212858
43	1	-2.371546	0.146362	-3.563266
44	1	-2.942544	1.693167	-2.944367
45	1	-3.564477	-2.430983	-2.663184
46	1	-2.453731	-3.328791	-1.620176
47	1	-1.819664	-2.209563	-2.828681
48	6	0.453107	2.863652	1.108180
49	6	-0.472730	3.532313	1.939462
50	6	1.426709	3.598064	0.383176
51	6	-0.491643	4.938135	1.946635
52	6	1.376286	4.999854	0.422874
53	6	0.412339	5.671968	1.179631
54	1	-1.213879	5.450363	2.576572
55	1	2.107259	5.565158	-0.147744
56	1	0.382777	6.757111	1.186986
57	6	0.910909	-2.204067	-1.446971
58	6	0.446236	-3.540391	-1.382548
59	6	1.629416	-1.754345	-2.587436
60	6	0.617818	-4.375449	-2.500998
61	6	1.772218	-2.621254	-3.682418
62	6	1.256763	-3.919417	-3.653190
63	1	0.248236	-5.396189	-2.452627
64	1	2.312233	-2.271798	-4.557193
65	1	1.374562	-4.574587	-4.510450
66	6	-1.364123	2.777827	2.897908
67	1	-2.339324	3.265470	3.004453
68	1	-1.513594	1.745941	2.584549
69	1	-0.910529	2.745392	3.899253
70	6	2.533012	2.916001	-0.389434
71	1	2.131227	2.155731	-1.060871
72	1	3.088526	3.647445	-0.984554

73	1	3.249720	2.422749	0.281159
74	6	-0.176335	-4.138134	-0.140070
75	1	0.507204	-4.861872	0.324189
76	1	-0.418338	-3.382014	0.605763
77	1	-1.090078	-4.691148	-0.383244
78	6	2.299742	-0.401762	-2.624766
79	1	1.573050	0.414177	-2.586338
80	1	2.973691	-0.268203	-1.769227
81	1	2.892052	-0.297617	-3.538959

TS13^{Ar}-14^{Ar} (E = -1504.0819784 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-1.409364	-0.345692	-0.343165
2	7	-0.397690	0.776404	0.860167
3	6	0.149813	-0.137705	1.782873
4	7	0.327683	-1.653024	-0.700447
5	6	-3.619340	-0.496868	0.575613
6	6	-3.272461	-1.828108	0.170271
7	6	-3.734714	0.300049	-0.593438
8	17	-0.896775	1.236723	-2.117210
9	6	-3.177480	-1.844193	-1.249395
10	6	-3.450459	-0.531628	-1.718022
11	6	1.300704	-1.624908	0.196584
12	6	1.201253	-0.987519	1.461474
13	1	-0.036809	0.073242	2.840208
14	6	2.254326	-1.525645	2.335830
15	1	-1.103095	-1.308402	1.065505
16	6	2.583970	-2.433281	0.190511
17	6	3.079446	-2.321780	1.616194
18	1	2.430168	-3.467557	-0.124775
19	1	3.301596	-2.003626	-0.522102
20	6	4.349333	-3.002927	2.042504
21	6	2.366637	-1.139052	3.786725
22	1	3.243985	-1.588106	4.260413
23	1	1.481194	-1.461698	4.351125
24	1	2.439634	-0.048831	3.897581
25	1	4.589609	-2.807089	3.091864
26	1	5.201894	-2.666234	1.435014
27	1	4.279492	-4.092503	1.912684
28	6	-3.367706	-3.022242	1.087155
29	6	-4.048879	-0.159962	1.981902
30	6	-4.183537	1.736188	-0.691317
31	6	-3.623544	-0.141432	-3.160707
32	6	-3.030485	-3.052088	-2.140989
33	1	-4.420659	-3.191833	1.356232
34	1	-2.809081	-2.875330	2.016874
35	1	-3.001644	-3.934567	0.612669
36	1	-4.930126	-0.760166	2.249362
37	1	-4.325271	0.890679	2.086113
38	1	-3.270557	-0.380298	2.720655
39	1	-5.135870	1.797094	-1.235620
40	1	-3.452880	2.347437	-1.231838
41	1	-4.339372	2.183280	0.294135
42	1	-4.659852	-0.336065	-3.476014
43	1	-2.962005	-0.712929	-3.818780
44	1	-3.409537	0.917757	-3.317927
45	1	-4.001554	-3.302775	-2.591588
46	1	-2.686112	-3.928312	-1.588855
47	1	-2.324613	-2.880939	-2.959731
48	6	0.035975	2.144064	1.065191
49	6	-0.722354	3.010535	1.890868
50	6	1.247262	2.601725	0.482933
51	6	-0.283700	4.329472	2.091335
52	6	1.643516	3.931595	0.704200

53	6	0.888901	4.796050	1.497316
54	1	-0.873621	4.987568	2.722859
55	1	2.562517	4.282837	0.243983
56	1	1.214318	5.819470	1.655638
57	6	0.485778	-2.642944	-1.756628
58	6	0.138768	-3.988697	-1.474291
59	6	1.015502	-2.287953	-3.021411
60	6	0.240275	-4.945525	-2.497226
61	6	1.095509	-3.279094	-4.015525
62	6	0.698367	-4.594823	-3.767950
63	1	-0.038772	-5.973520	-2.283883
64	1	1.492504	-3.007187	-4.988935
65	1	0.765253	-5.342590	-4.551775
66	6	-1.996637	2.555279	2.558396
67	1	-2.798363	2.425452	1.826030
68	1	-1.876226	1.596625	3.072604
69	1	-2.330638	3.294567	3.293089
70	6	2.133267	1.711741	-0.355981
71	1	1.543443	1.133369	-1.067568
72	1	2.857600	2.315400	-0.912609
73	1	2.695663	1.005220	0.267431
74	6	-0.273142	-4.436757	-0.088822
75	1	0.600783	-4.750906	0.499816
76	1	-0.763710	-3.640511	0.471753
77	1	-0.945620	-5.299366	-0.142003
78	6	1.564160	-0.910934	-3.309495
79	1	0.808332	-0.131686	-3.186830
80	1	2.388627	-0.662711	-2.628716
81	1	1.952516	-0.863793	-4.331381

14^{Ar} (E = -1504.1338969 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.020726	-0.989919	-0.062485
2	7	-1.625321	-0.146680	0.350938
3	6	-1.354243	0.804917	1.470438
4	7	1.082285	0.734356	-0.130487
5	6	0.094002	-2.654502	1.640654
6	6	1.408998	-2.090276	1.610247
7	6	-0.099610	-3.365304	0.424501
8	17	-0.610010	-1.488871	-2.255678
9	6	2.031866	-2.475751	0.388092
10	6	1.100337	-3.251258	-0.343420
11	6	0.438939	1.931513	0.206505
12	6	-0.690167	2.040463	0.951071
13	1	-2.274847	1.009581	2.021786
14	6	-1.096178	3.448861	1.048411
15	1	-0.671702	0.313569	2.184225
16	6	0.839584	3.316842	-0.254609
17	6	-0.215206	4.213804	0.355816
18	1	1.850773	3.606625	0.046656
19	1	0.824136	3.367439	-1.351691
20	6	-0.186017	5.706315	0.170316
21	6	-2.311249	3.894611	1.820908
22	1	-2.447001	4.979141	1.773124
23	1	-2.234097	3.613776	2.880513
24	1	-3.223446	3.424783	1.428989
25	1	-1.028700	6.194985	0.670445
26	1	-0.227754	5.981094	-0.893638
27	1	0.738674	6.144474	0.574056
28	6	2.106833	-1.526531	2.821095
29	6	-0.760673	-2.707296	2.884212
30	6	-1.281222	-4.212431	0.025066
31	6	1.374069	-3.981518	-1.629578
32	6	3.482225	-2.286475	0.021996

33	1	2.415443	-2.352847	3.479101
34	1	1.458864	-0.871059	3.411651
35	1	3.004239	-0.967199	2.552601
36	1	-0.239181	-3.281465	3.663019
37	1	-1.717274	-3.198185	2.698612
38	1	-0.971524	-1.716559	3.301614
39	1	-0.977992	-5.264308	-0.067676
40	1	-1.691643	-3.900526	-0.941820
41	1	-2.084984	-4.166138	0.764302
42	1	1.715015	-5.004785	-1.412944
43	1	2.154192	-3.490137	-2.218816
44	1	0.478227	-4.047097	-2.252260
45	1	4.058659	-3.177404	0.311137
46	1	3.925473	-1.424675	0.524550
47	1	3.618497	-2.144253	-1.053825
48	6	2.501499	0.913838	-0.364334
49	6	3.345486	1.332510	0.703683
50	6	3.047429	0.726435	-1.659998
51	6	4.724430	1.463706	0.473933
52	6	4.432959	0.881237	-1.845501
53	6	5.274340	1.229375	-0.788702
54	1	5.366239	1.765778	1.297023
55	1	4.844407	0.738285	-2.840585
56	1	6.342069	1.338689	-0.950422
57	6	-2.937484	-0.006667	-0.232706
58	6	-4.034790	-0.673744	0.376078
59	6	-3.157556	0.819724	-1.367343
60	6	-5.319996	-0.531130	-0.168074
61	6	-4.462655	0.923301	-1.882833
62	6	-5.538632	0.258150	-1.298074
63	1	-6.149938	-1.050080	0.302842
64	1	-4.624435	1.545928	-2.758171
65	1	-6.536113	0.355434	-1.715086
66	6	-3.853831	-1.552285	1.591217
67	1	-3.292258	-2.457499	1.341842
68	1	-3.305427	-1.048631	2.394120
69	1	-4.825842	-1.859898	1.988820
70	6	-2.073062	1.633256	-2.038829
71	1	-1.098806	1.155097	-1.964777
72	1	-2.308438	1.767808	-3.100266
73	1	-1.993819	2.630283	-1.585981
74	6	2.185945	0.411867	-2.860767
75	1	1.892809	-0.642457	-2.903341
76	1	1.253918	0.983455	-2.849018
77	1	2.726325	0.646349	-3.783577
78	6	2.809072	1.703707	2.071128
79	1	3.564484	1.524102	2.843561
80	1	2.547749	2.769699	2.115408
81	1	1.907837	1.148539	2.328347

TS14^{Ar}-15^{Ar} (E = -1504.1080366 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.481938	-0.378405	-0.027814
2	7	0.505372	-0.505931	1.740608
3	6	-0.218825	1.460336	1.768782
4	7	-1.591839	0.295540	-0.440715
5	6	2.534522	0.794876	-0.459631
6	6	1.636101	1.350530	-1.421399
7	6	2.752962	-0.569669	-0.800928
8	17	0.263550	-2.727755	-0.287180
9	6	1.319111	0.336741	-2.370703
10	6	2.010239	-0.839139	-1.991927
11	6	-2.234462	0.925787	0.540849
12	6	-1.608164	1.397496	1.709368

13	1	0.295705	1.745828	2.676474
14	6	-2.640467	1.678209	2.716906
15	1	0.297160	1.784277	0.866603
16	6	-3.730058	1.101293	0.708212
17	6	-3.865024	1.534964	2.155632
18	1	-4.136295	1.854812	0.023105
19	1	-4.264791	0.170664	0.488064
20	6	-5.218618	1.788597	2.757248
21	6	-2.297706	2.109732	4.117116
22	1	-3.192068	2.296079	4.718164
23	1	-1.698619	3.031030	4.108195
24	1	-1.701876	1.341855	4.627543
25	1	-5.150085	2.101931	3.803477
26	1	-5.846436	0.886848	2.718852
27	1	-5.758285	2.573459	2.207140
28	6	1.378108	2.832922	-1.552145
29	6	3.328589	1.637366	0.507373
30	6	3.728314	-1.531148	-0.168205
31	6	2.095554	-2.096204	-2.813110
32	6	0.542992	0.492800	-3.654221
33	1	2.329478	3.355935	-1.725618
34	1	0.933713	3.280477	-0.654264
35	1	0.722741	3.056963	-2.395654
36	1	3.995092	2.306862	-0.055923
37	1	3.953307	1.028074	1.161316
38	1	2.698477	2.272741	1.140108
39	1	4.594343	-1.687749	-0.826956
40	1	3.266321	-2.507260	0.013540
41	1	4.104048	-1.157852	0.788027
42	1	2.898841	-1.997559	-3.559018
43	1	1.163454	-2.295939	-3.350429
44	1	2.312405	-2.968491	-2.192638
45	1	1.226780	0.467388	-4.514651
46	1	-0.001438	1.438369	-3.690751
47	1	-0.188093	-0.310312	-3.794319
48	6	0.490926	-1.029182	3.036912
49	6	-0.621742	-1.808218	3.486683
50	6	1.572052	-0.785722	3.937457
51	6	-0.614351	-2.318598	4.793604
52	6	1.529373	-1.314032	5.235029
53	6	0.445397	-2.078326	5.670270
54	1	-1.459864	-2.916768	5.120988
55	1	2.362610	-1.122429	5.905208
56	1	0.427522	-2.483170	6.677183
57	6	-2.362540	0.166681	-1.670502
58	6	-2.960016	-1.066441	-2.037109
59	6	-2.563190	1.318222	-2.478346
60	6	-3.645593	-1.146253	-3.262385
61	6	-3.251660	1.189517	-3.695033
62	6	-3.774857	-0.038819	-4.101017
63	1	-4.099039	-2.092689	-3.541892
64	1	-3.383480	2.069370	-4.318626
65	1	-4.302256	-0.125354	-5.045676
66	6	-2.116392	2.700727	-2.053323
67	1	-2.935310	3.240467	-1.557270
68	1	-1.282976	2.672773	-1.353895
69	1	-1.822763	3.299802	-2.922079
70	6	-2.961714	-2.276976	-1.134675
71	1	-2.043198	-2.862155	-1.231582
72	1	-3.036925	-1.996365	-0.080900
73	1	-3.809781	-2.924577	-1.379868
74	6	2.772649	0.021071	3.516273
75	1	3.295882	-0.458462	2.683174
76	1	2.495835	1.025634	3.179663

77	1	3.478565	0.125591	4.345888
78	6	-1.806199	-2.110645	2.598818
79	1	-2.393140	-1.209728	2.391078
80	1	-1.485180	-2.526630	1.641540
81	1	-2.468647	-2.832374	3.088143

15^{Ar} (E = -1504.123483 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.071420	-1.233694	0.224341
2	7	1.588072	-0.810642	0.350292
3	6	1.457103	1.023498	-2.082662
4	7	-0.978676	1.021792	-0.154229
5	6	-0.042362	-2.864643	-1.554862
6	6	-1.263173	-2.172191	-1.788427
7	6	-0.158520	-3.550819	-0.309440
8	17	-0.512750	-1.539189	2.528325
9	6	-2.151885	-2.456607	-0.707333
10	6	-1.478584	-3.320351	0.188297
11	6	-0.334557	2.035518	-0.628856
12	6	0.949440	2.038517	-1.369558
13	1	2.383173	1.134773	-2.633726
14	6	1.465531	3.419514	-1.318228
15	1	0.973991	0.059995	-2.132630
16	6	-0.737411	3.495113	-0.472969
17	6	0.526247	4.248916	-0.818022
18	1	-1.551947	3.748695	-1.163333
19	1	-1.111695	3.709970	0.531104
20	6	0.588994	5.735181	-0.619543
21	6	2.837470	3.763799	-1.827952
22	1	3.084530	4.814599	-1.656136
23	1	2.915141	3.572696	-2.907128
24	1	3.599461	3.147938	-1.334278
25	1	1.559623	6.152095	-0.900942
26	1	0.398745	5.995219	0.431161
27	1	-0.184057	6.241380	-1.215111
28	6	-1.614440	-1.557535	-3.123150
29	6	0.982812	-3.110678	-2.633464
30	6	0.824757	-4.529521	0.286510
31	6	-2.111177	-4.013092	1.364713
32	6	-3.602390	-2.060995	-0.579936
33	1	-1.537109	-2.322684	-3.909067
34	1	-0.946490	-0.738029	-3.414183
35	1	-2.637885	-1.178953	-3.137800
36	1	0.538020	-3.746267	-3.414278
37	1	1.862274	-3.630646	-2.252670
38	1	1.319778	-2.190836	-3.123515
39	1	0.518437	-5.564275	0.074303
40	1	0.891960	-4.420010	1.374069
41	1	1.830150	-4.390599	-0.119449
42	1	-2.624830	-4.925202	1.024349
43	1	-2.848645	-3.377396	1.863338
44	1	-1.368659	-4.302133	2.112354
45	1	-4.250360	-2.941015	-0.698968
46	1	-3.893538	-1.331143	-1.338472
47	1	-3.824942	-1.623328	0.399668
48	6	2.898153	-0.444356	0.642921
49	6	3.149852	0.532542	1.658487
50	6	4.014475	-1.002571	-0.051523
51	6	4.466912	0.915794	1.944988
52	6	5.315423	-0.589262	0.270553
53	6	5.553609	0.365165	1.261182
54	1	4.635292	1.656060	2.722571
55	1	6.149664	-1.030864	-0.268038

56	1	6.567432	0.671632	1.499002
57	6	-2.327284	1.334279	0.333146
58	6	-2.577750	1.583433	1.706578
59	6	-3.376975	1.426405	-0.614376
60	6	-3.906281	1.786672	2.116319
61	6	-4.688905	1.632911	-0.155418
62	6	-4.962111	1.787085	1.203030
63	1	-4.101074	1.963840	3.169408
64	1	-5.494694	1.683442	-0.882141
65	1	-5.981322	1.935766	1.544553
66	6	-3.138641	1.404050	-2.109091
67	1	-3.106992	2.428088	-2.507855
68	1	-2.201523	0.922180	-2.379940
69	1	-3.954109	0.890304	-2.628862
70	6	-1.473630	1.745863	2.723038
71	1	-0.837295	0.863915	2.785553
72	1	-0.831476	2.603128	2.481759
73	1	-1.899537	1.925194	3.714588
74	6	3.821819	-2.033470	-1.130491
75	1	3.316751	-2.924153	-0.742998
76	1	3.203799	-1.647401	-1.946889
77	1	4.784782	-2.343778	-1.548782
78	6	2.015218	1.159568	2.425282
79	1	1.343661	1.710205	1.757859
80	1	1.407132	0.401478	2.926780
81	1	2.396155	1.859145	3.176841

16^{Ar} (E = -828.2657587 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.064002	0.600820	-0.420696
2	7	1.629342	0.466207	-0.252674
3	6	-0.588906	-1.343681	0.779215
4	6	-0.776589	-1.614349	-0.605828
5	6	-1.544330	-0.353124	1.157682
6	17	-0.703872	2.692510	-1.224387
7	6	-1.885010	-0.826626	-1.067052
8	6	-2.366849	-0.057544	0.021483
9	6	-0.070390	-2.690906	-1.394267
10	6	0.365492	-2.072875	1.690548
11	6	-1.739718	0.211628	2.545452
12	6	-3.558654	0.864269	0.000521
13	6	-2.469704	-0.856150	-2.458094
14	1	-0.624694	-3.637662	-1.324187
15	1	0.939626	-2.870227	-1.014823
16	1	0.008671	-2.439559	-2.457071
17	1	-0.050057	-3.050837	1.970742
18	1	0.547830	-1.517618	2.614936
19	1	1.333730	-2.245200	1.211141
20	1	-2.521604	-0.347704	3.077577
21	1	-2.051285	1.261377	2.520795
22	1	-0.826364	0.146947	3.144421
23	1	-4.487434	0.294557	0.144005
24	1	-3.637756	1.401489	-0.949368
25	1	-3.504236	1.613179	0.796129
26	1	-3.237765	-1.638756	-2.532866
27	1	-1.711070	-1.074428	-3.217264
28	1	-2.941629	0.096136	-2.718340
29	6	2.968859	0.200623	-0.037329
30	6	3.559491	0.499933	1.225169
31	6	3.766427	-0.341674	-1.086843
32	6	4.917964	0.220627	1.421360
33	6	5.120887	-0.602481	-0.842885
34	6	5.698942	-0.333138	0.401813
35	1	5.366838	0.448158	2.384302

36	1	5.728071	-1.015707	-1.643572
37	1	6.750169	-0.542580	0.572200
38	6	3.161979	-0.605413	-2.444681
39	1	2.364709	-1.357426	-2.396993
40	1	2.715056	0.305584	-2.863597
41	1	3.921487	-0.965019	-3.145860
42	6	2.734777	1.129278	2.321437
43	1	2.283117	2.072184	1.986739
44	1	1.910891	0.476449	2.636691
45	1	3.350945	1.340441	3.200897

17^{Ar} (E = -675.8655679 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.297305	0.837606	0.006404
2	6	0.111476	0.378815	0.002419
3	6	-1.113310	1.230516	-0.011293
4	6	-2.267266	0.317981	-0.011666
5	6	-0.346816	-1.072842	0.010098
6	6	-1.854569	-0.969819	0.000288
7	1	0.040081	-1.618135	-0.859368
8	1	0.029361	-1.605788	0.891803
9	6	-2.687949	-2.218766	0.004789
10	6	-3.679313	0.837689	-0.023938
11	1	-4.416303	0.030424	-0.022146
12	1	-3.858101	1.457626	-0.912669
13	1	-3.868515	1.471116	0.853043
14	1	-3.760925	-2.008892	-0.001838
15	1	-2.466045	-2.829166	0.891653
16	1	-2.457579	-2.841383	-0.871358
17	6	-1.117490	2.571956	-0.020604
18	1	-2.039266	3.141298	-0.030320
19	1	-0.183875	3.121441	-0.018547
20	6	2.406678	-0.056993	0.020760
21	6	2.990778	-0.457076	-1.204089
22	6	2.970403	-0.443070	1.259580
23	6	4.126141	-1.281036	-1.166847
24	6	4.106171	-1.267279	1.250468
25	6	4.681326	-1.691523	0.048863
26	1	4.578993	-1.593526	-2.103642
27	1	4.543472	-1.568979	2.198120
28	1	5.561662	-2.326273	0.059750
29	6	2.369855	0.037665	2.561562
30	1	2.270914	1.130171	2.572716
31	1	1.363995	-0.369556	2.730090
32	1	2.993885	-0.259812	3.409537
33	6	2.411498	0.008643	-2.521058
34	1	1.408325	-0.400304	-2.700907
35	1	2.313106	1.100981	-2.546441
36	1	3.048960	-0.298734	-3.355397

18^{Ar} (E = -1076.5594162 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.135137	0.001214	-0.397039
2	7	-0.691344	1.623922	-0.302147
3	6	-1.774412	-0.789316	1.107077
4	6	-0.514134	-0.884469	1.766796
5	6	-1.763648	-1.718456	0.028589
6	17	-0.067433	-0.555790	-2.699682
7	6	0.246731	-1.917953	1.127337
8	6	-0.520461	-2.427183	0.054343
9	6	-0.153010	-0.201314	3.064112
10	6	-2.943945	0.045657	1.563952
11	6	-2.906087	-2.030658	-0.905788
12	6	-0.158527	-3.562843	-0.867240

13	6	1.577673	-2.445084	1.602899
14	1	-0.453113	-0.821934	3.921025
15	1	-0.660344	0.762736	3.165938
16	1	0.924741	-0.027506	3.156669
17	1	-3.489174	-0.466529	2.369624
18	1	-3.652131	0.229524	0.750959
19	1	-2.623452	1.020873	1.941908
20	1	-3.428679	-2.940559	-0.576755
21	1	-2.553424	-2.198215	-1.928218
22	1	-3.641539	-1.221437	-0.934409
23	1	-0.749023	-4.458968	-0.629339
24	1	0.898746	-3.833299	-0.779836
25	1	-0.352070	-3.302434	-1.913581
26	1	1.430861	-3.238092	2.349696
27	1	2.182711	-1.663727	2.074405
28	1	2.165152	-2.872325	0.783745
29	7	2.056371	0.237711	-0.175575
30	6	2.899563	-0.372677	-1.043321
31	6	2.593434	0.997329	0.807900
32	6	4.286425	-0.246088	-0.954897
33	1	2.432694	-0.954778	-1.827852
34	6	3.968699	1.168242	0.962134
35	1	1.892707	1.484647	1.471270
36	6	4.835820	0.536059	0.065030
37	1	4.915916	-0.750203	-1.678105
38	1	4.345602	1.790014	1.765245
39	1	5.909772	0.653584	0.156405
40	6	-1.406692	2.806958	-0.225522
41	6	-1.046063	3.826807	0.705438
42	6	-2.516221	3.024895	-1.100516
43	6	-1.797365	5.008424	0.759626
44	6	-3.237176	4.222190	-1.009457
45	6	-2.891170	5.213274	-0.085687
46	1	-1.513781	5.777180	1.473767
47	1	-4.078641	4.377665	-1.679411
48	1	-3.461807	6.135054	-0.030564
49	6	-2.903987	1.980106	-2.117351
50	1	-2.048567	1.681477	-2.731590
51	1	-3.269810	1.063154	-1.637137
52	1	-3.696601	2.353180	-2.774056
53	6	0.148528	3.654576	1.611145
54	1	0.082896	2.728574	2.194861
55	1	1.080161	3.607556	1.032750
56	1	0.230303	4.492238	2.311299

TS9^{Ar}-26IS^{Ar} (E = -1504.1030172 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.338902	-0.857335	-0.020672
2	7	1.881592	0.761291	-0.145534
3	6	0.891108	0.850367	-0.932172
4	7	-1.463817	0.011529	0.341137
5	6	1.833117	-1.993823	-1.621651
6	6	0.571132	-1.737515	-2.239749
7	6	1.628782	-2.905801	-0.562067
8	17	0.726682	-1.480984	2.225153
9	6	-0.419227	-2.511587	-1.555455
10	6	0.237176	-3.227808	-0.514354
11	6	-2.302031	0.653761	-0.563100
12	6	-2.139999	0.872990	-1.902253
13	1	0.631836	1.657172	-1.606271
14	6	-3.297426	1.585029	-2.449737
15	1	-1.290085	0.580506	-2.495640
16	6	-3.646530	1.261627	-0.175389
17	6	-4.193827	1.824152	-1.462512

18	1	-4.315051	0.512306	0.263780
19	1	-3.529948	2.037344	0.590361
20	6	-5.521437	2.528784	-1.520440
21	6	-3.388422	1.962051	-3.906983
22	1	-4.316362	2.495332	-4.135734
23	1	-3.346671	1.070850	-4.548569
24	1	-2.548838	2.607844	-4.200049
25	1	-5.753331	2.875356	-2.533241
26	1	-5.542092	3.406112	-0.856943
27	1	-6.342827	1.871303	-1.199165
28	6	0.399625	-1.060440	-3.578345
29	6	3.159074	-1.464159	-2.100978
30	6	2.687899	-3.544832	0.296135
31	6	-0.340987	-4.292844	0.380763
32	6	-1.847816	-2.695661	-2.005116
33	1	0.881117	-1.664245	-4.360349
34	1	0.854436	-0.064018	-3.615259
35	1	-0.655093	-0.961376	-3.846759
36	1	3.614848	-2.165837	-2.813979
37	1	3.866558	-1.323280	-1.278331
38	1	3.049102	-0.503183	-2.612305
39	1	2.876222	-4.573798	-0.043037
40	1	2.380173	-3.586312	1.345029
41	1	3.636386	-3.002215	0.242173
42	1	0.143311	-5.256297	0.169262
43	1	-1.413880	-4.424204	0.220424
44	1	-0.174325	-4.064116	1.438898
45	1	-2.448467	-3.189275	-1.237571
46	1	-1.880043	-3.322879	-2.907288
47	1	-2.332359	-1.743145	-2.240081
48	6	3.000790	1.635322	0.067877
49	6	3.876569	1.317573	1.142850
50	6	3.278125	2.763093	-0.763650
51	6	4.985555	2.140019	1.388354
52	6	4.405749	3.548339	-0.473641
53	6	5.252745	3.253294	0.593464
54	1	5.643947	1.891982	2.214723
55	1	4.614430	4.405521	-1.106195
56	1	6.115600	3.879334	0.796037
57	6	-1.928042	0.137552	1.717168
58	6	-1.556152	1.274064	2.475010
59	6	-2.795499	-0.833644	2.267384
60	6	-2.044368	1.408107	3.784478
61	6	-3.261140	-0.665119	3.581442
62	6	-2.888346	0.445180	4.342133
63	1	-1.756021	2.279236	4.366074
64	1	-3.923799	-1.415030	4.004183
65	1	-3.256020	0.561460	5.356919
66	6	3.656581	0.123777	2.036087
67	1	2.736929	0.210940	2.620122
68	1	3.556684	-0.802847	1.464367
69	1	4.495724	0.012347	2.729350
70	6	2.452027	3.179571	-1.962305
71	1	2.319663	2.363926	-2.683854
72	1	1.453794	3.538111	-1.681880
73	1	2.953458	3.998889	-2.485359
74	6	-3.221379	-2.047312	1.477124
75	1	-3.635798	-1.776859	0.499506
76	1	-2.370840	-2.710382	1.292496
77	1	-3.979966	-2.616467	2.023545
78	6	-0.640571	2.337972	1.912497
79	1	-0.937906	2.643718	0.903089
80	1	-0.645215	3.224871	2.553988
81	1	0.392954	1.978247	1.847784

26IS^{Ar} (E = -1504.1044452 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.261662	-0.572513	-0.677851
2	7	-2.015387	0.148084	0.502579
3	6	-1.078154	-0.386917	1.168195
4	7	1.371834	0.435935	-0.059521
5	6	-1.414537	-2.747037	-0.794287
6	6	-0.174568	-2.906496	-0.100855
7	6	-1.132138	-2.381787	-2.128709
8	17	-0.741134	0.756499	-2.579305
9	6	0.880408	-2.644368	-1.030297
10	6	0.285269	-2.314774	-2.281205
11	6	2.243327	0.094533	0.971806
12	6	2.074819	-0.788637	1.996344
13	1	-1.012338	-0.436097	2.254891
14	6	3.289510	-0.861991	2.814517
15	1	1.179951	-1.352008	2.205437
16	6	3.645653	0.675798	1.106459
17	6	4.224096	-0.017781	2.314584
18	1	4.235865	0.493935	0.200200
19	1	3.626840	1.763629	1.238107
20	6	5.609372	0.284614	2.816432
21	6	3.386018	-1.753696	4.026554
22	1	4.358288	-1.669318	4.521702
23	1	3.238382	-2.808101	3.754653
24	1	2.610671	-1.500933	4.763177
25	1	5.854694	-0.299076	3.710038
26	1	5.720424	1.348372	3.073558
27	1	6.372073	0.062604	2.055700
28	6	-0.018359	-3.561119	1.250308
29	6	-2.790645	-3.052097	-0.259867
30	6	-2.147799	-2.223564	-3.228494
31	6	0.984801	-2.131536	-3.601497
32	6	2.347651	-2.902201	-0.795857
33	1	-0.276709	-4.627006	1.175803
34	1	-0.667685	-3.122077	2.015358
35	1	1.011704	-3.498612	1.608564
36	1	-3.263301	-3.836823	-0.864952
37	1	-3.452554	-2.178711	-0.285017
38	1	-2.747335	-3.415716	0.770260
39	1	-2.304994	-3.186426	-3.736961
40	1	-1.820257	-1.494909	-3.973788
41	1	-3.115134	-1.890673	-2.839372
42	1	0.824944	-3.018429	-4.231155
43	1	2.062919	-2.004096	-3.479970
44	1	0.594679	-1.263947	-4.143209
45	1	2.972127	-2.339747	-1.495381
46	1	2.568446	-3.969634	-0.940064
47	1	2.656856	-2.625463	0.215207
48	6	-3.239058	0.723892	0.994352
49	6	-3.763458	1.859649	0.322940
50	6	-3.927595	0.164182	2.108233
51	6	-4.961651	2.424044	0.784102
52	6	-5.135728	0.756222	2.512998
53	6	-5.651373	1.879255	1.867714
54	1	-5.353136	3.299636	0.275924
55	1	-5.671127	0.320892	3.351391
56	1	-6.583409	2.322510	2.203077
57	6	1.635917	1.768066	-0.591332
58	6	1.179253	2.900414	0.132397
59	6	2.398185	1.939303	-1.770345
60	6	1.460324	4.183927	-0.362727
61	6	2.661849	3.240986	-2.228138

62	6	2.191106	4.359961	-1.539591
63	1	1.106247	5.049066	0.190808
64	1	3.245896	3.368636	-3.135225
65	1	2.401640	5.358764	-1.909040
66	6	-3.063370	2.488994	-0.854644
67	1	-2.045342	2.809402	-0.609950
68	1	-2.960938	1.789836	-1.688213
69	1	-3.619924	3.365073	-1.200840
70	6	-3.453491	-1.045130	2.888538
71	1	-2.977163	-1.795981	2.253770
72	1	-2.733664	-0.773041	3.671420
73	1	-4.303801	-1.521053	3.386845
74	6	2.919325	0.765967	-2.563199
75	1	3.253918	-0.049410	-1.915668
76	1	2.133597	0.365531	-3.212260
77	1	3.757655	1.070549	-3.198289
78	6	0.421236	2.765643	1.435789
79	1	0.955521	2.132690	2.153788
80	1	0.274778	3.749330	1.892616
81	1	-0.565769	2.315574	1.289251

TS26IS^{Ar}-26^{Ar} (E = -1504.0863331 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.503581	-0.236841	-0.610296
2	7	-2.006736	0.222814	0.737435
3	6	-1.111308	1.124106	0.787984
4	7	1.401303	0.619638	-0.270282
5	6	-1.726481	-2.170299	-1.470268
6	6	-1.080189	-2.531432	-0.255309
7	6	-0.719153	-1.984517	-2.458236
8	17	-1.322936	1.038700	-2.396275
9	6	0.327941	-2.524534	-0.483097
10	6	0.544880	-2.189602	-1.856734
11	6	1.762577	0.981272	0.997815
12	6	1.305439	0.481342	2.194856
13	1	-1.154572	2.030981	1.392106
14	6	1.905694	1.216905	3.311132
15	1	0.682960	-0.392896	2.320576
16	6	2.733742	2.110948	1.324789
17	6	2.743383	2.170183	2.832850
18	1	3.735097	1.929402	0.918787
19	1	2.391715	3.050074	0.872746
20	6	3.609948	3.146544	3.579761
21	6	1.612838	0.879087	4.751319
22	1	2.218372	1.473165	5.442616
23	1	1.814725	-0.181955	4.953208
24	1	0.556653	1.056427	4.995831
25	1	3.516287	3.028596	4.664541
26	1	3.348912	4.187336	3.336739
27	1	4.672122	3.020064	3.322018
28	6	-1.764115	-3.102553	0.960879
29	6	-3.211119	-2.203079	-1.725668
30	6	-0.947139	-1.753814	-3.926112
31	6	1.829875	-2.276027	-2.641324
32	6	1.345837	-3.049862	0.503734
33	1	-2.009502	-4.159563	0.780394
34	1	-2.698830	-2.587557	1.196978
35	1	-1.121874	-3.067115	1.845159
36	1	-3.514866	-3.199313	-2.079359
37	1	-3.503654	-1.480163	-2.493364
38	1	-3.786206	-1.987131	-0.820610
39	1	-0.958515	-2.716754	-4.458585
40	1	-0.157530	-1.137233	-4.365773
41	1	-1.900166	-1.253527	-4.113831

42	1	1.729338	-3.038683	-3.425912
43	1	2.673235	-2.561356	-2.010641
44	1	2.089228	-1.333149	-3.131818
45	1	2.273113	-3.330542	-0.003005
46	1	0.960146	-3.949208	0.999474
47	1	1.605866	-2.329260	1.288198
48	6	-3.266360	0.127093	1.439505
49	6	-4.459512	0.473266	0.763564
50	6	-3.282055	-0.293080	2.790794
51	6	-5.676842	0.323921	1.448736
52	6	-4.524049	-0.425112	3.432147
53	6	-5.716348	-0.132692	2.766905
54	1	-6.597698	0.583072	0.935331
55	1	-4.545137	-0.755728	4.466018
56	1	-6.667316	-0.246766	3.276873
57	6	2.349148	1.018993	-1.292009
58	6	2.115709	2.181249	-2.075413
59	6	3.567341	0.302606	-1.460648
60	6	3.012068	2.496644	-3.113034
61	6	4.436288	0.652945	-2.504957
62	6	4.150226	1.727063	-3.351376
63	1	2.816642	3.376662	-3.720178
64	1	5.351212	0.082562	-2.641291
65	1	4.825039	1.981126	-4.163018
66	6	-4.449701	1.065563	-0.625493
67	1	-4.119033	2.112625	-0.601318
68	1	-3.766862	0.548729	-1.300919
69	1	-5.454773	1.046285	-1.057403
70	6	-2.011186	-0.564328	3.561954
71	1	-1.354198	-1.266895	3.042133
72	1	-1.433176	0.353852	3.718968
73	1	-2.243884	-0.983566	4.544980
74	6	4.000976	-0.770120	-0.487620
75	1	4.583959	-0.331283	0.334961
76	1	3.152066	-1.276160	-0.034393
77	1	4.642777	-1.511361	-0.975895
78	6	1.016267	3.175305	-1.768625
79	1	0.411617	2.860919	-0.918933
80	1	1.461047	4.153925	-1.540841
81	1	0.340791	3.308653	-2.619038

26^{Ar} (E = -1504.0959021 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.141191	-0.718291	-0.513068
2	7	-1.908600	0.303932	-0.104522
3	6	-1.208181	0.954212	-0.939923
4	7	1.350069	0.429190	0.092672
5	6	-0.875096	-2.987454	-0.773142
6	6	-1.190283	-2.590106	0.555679
7	6	0.546406	-3.115882	-0.871299
8	17	0.029826	-0.703497	-2.931716
9	6	0.035739	-2.417616	1.260140
10	6	1.104766	-2.781521	0.383474
11	6	1.208182	1.819666	-0.212952
12	6	0.561740	2.790652	0.476101
13	1	-1.494428	1.864868	-1.464500
14	6	0.660500	4.074627	-0.235704
15	1	0.024439	2.658006	1.404634
16	6	1.801188	2.452789	-1.456231
17	6	1.379491	3.899057	-1.370405
18	1	2.893030	2.355573	-1.476212
19	1	1.426708	1.950974	-2.356159
20	6	1.771048	4.906415	-2.416612
21	6	0.035801	5.338409	0.298643

22	1	0.209923	6.192617	-0.362839
23	1	0.443098	5.590979	1.287411
24	1	-1.050279	5.222688	0.418981
25	1	1.373520	5.902148	-2.193875
26	1	1.403339	4.614206	-3.410442
27	1	2.864175	4.994567	-2.496560
28	6	-2.563604	-2.595324	1.177358
29	6	-1.854527	-3.416619	-1.836895
30	6	1.278851	-3.686373	-2.055658
31	6	2.519342	-3.066372	0.816864
32	6	0.168287	-2.224487	2.750390
33	1	-2.784029	-3.598083	1.571379
34	1	-3.347491	-2.346128	0.457531
35	1	-2.644794	-1.891742	2.009589
36	1	-1.940521	-4.513057	-1.850649
37	1	-1.532047	-3.091844	-2.830298
38	1	-2.855865	-3.013524	-1.657071
39	1	1.149251	-4.777916	-2.091697
40	1	2.351851	-3.480161	-2.006704
41	1	0.901347	-3.269250	-2.993897
42	1	2.575744	-4.095564	1.202459
43	1	2.858514	-2.397118	1.609653
44	1	3.228443	-2.986769	-0.009638
45	1	1.128828	-1.778576	3.018465
46	1	0.102439	-3.196961	3.260824
47	1	-0.625192	-1.592329	3.160106
48	6	-3.255627	0.548622	0.340273
49	6	-4.319272	0.427165	-0.585744
50	6	-3.486977	0.882917	1.692051
51	6	-5.627065	0.632549	-0.118238
52	6	-4.811537	1.084374	2.111181
53	6	-5.876778	0.957488	1.217404
54	1	-6.453160	0.533617	-0.815772
55	1	-4.999926	1.341688	3.149151
56	1	-6.895489	1.109125	1.558966
57	6	2.674226	0.179539	0.634006
58	6	3.740452	-0.238093	-0.205075
59	6	2.915690	0.410078	2.016788
60	6	5.013053	-0.441198	0.358669
61	6	4.198622	0.178960	2.538672
62	6	5.247950	-0.242244	1.718765
63	1	5.823651	-0.766470	-0.288104
64	1	4.371033	0.343168	3.598912
65	1	6.235676	-0.411971	2.135923
66	6	-4.084934	0.088205	-2.042211
67	1	-3.693193	0.946096	-2.603330
68	1	-3.362786	-0.723666	-2.170204
69	1	-5.023429	-0.211135	-2.517637
70	6	-2.349337	1.066451	2.669164
71	1	-1.544426	0.346903	2.498855
72	1	-1.905761	2.066698	2.577657
73	1	-2.700907	0.957078	3.699619
74	6	1.842273	0.932468	2.944866
75	1	1.834806	2.030260	2.953283
76	1	0.848280	0.608169	2.633288
77	1	2.019334	0.596218	3.972234
78	6	3.575495	-0.468536	-1.692272
79	1	3.934049	0.395236	-2.269098
80	1	4.168767	-1.331910	-2.015549
81	1	2.537041	-0.633611	-1.977824

TS26^{Ar}-27^{Ar} (E = -1504.0836899 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	22	-0.069757	-0.595960	-0.221080
2	7	-1.671441	0.572934	-0.116289
3	6	-0.738377	1.252263	-0.736172
4	7	1.760259	0.520172	0.134322
5	6	-0.279462	-1.931678	1.756955
6	6	0.892073	-2.455326	1.122707
7	6	-1.403234	-2.254675	0.936423
8	17	-0.037472	-0.987891	-2.576643
9	6	0.504531	-3.020300	-0.112970
10	6	-0.917965	-2.900402	-0.227702
11	6	1.607377	1.855228	0.213570
12	6	0.427748	2.534923	0.545907
13	1	-0.903036	2.016992	-1.489687
14	6	0.626886	3.972754	0.274894
15	1	-0.237001	2.200072	1.324762
16	6	2.633172	2.880203	-0.245325
17	6	1.872739	4.188456	-0.204005
18	1	3.510704	2.905768	0.412304
19	1	3.012681	2.628774	-1.242710
20	6	2.524566	5.476176	-0.627025
21	6	-0.462241	4.982265	0.529345
22	1	-0.145356	6.001379	0.288246
23	1	-0.770114	4.966636	1.584384
24	1	-1.356424	4.755709	-0.066965
25	1	1.853523	6.332728	-0.506726
26	1	2.834535	5.441996	-1.681616
27	1	3.431296	5.675858	-0.037166
28	6	2.228371	-2.644017	1.790881
29	6	-0.340074	-1.440150	3.185015
30	6	-2.854711	-2.139459	1.325534
31	6	-1.755154	-3.537717	-1.304894
32	6	1.387997	-3.772322	-1.073084
33	1	2.248764	-3.631958	2.275132
34	1	2.411443	-1.897336	2.565145
35	1	3.061456	-2.605353	1.085601
36	1	-0.099092	-2.260282	3.876319
37	1	-1.338995	-1.080594	3.444157
38	1	0.369298	-0.630973	3.387883
39	1	-3.184018	-3.075535	1.799084
40	1	-3.501125	-1.961967	0.461961
41	1	-3.032159	-1.329645	2.036225
42	1	-1.898645	-4.606183	-1.086441
43	1	-1.276585	-3.452827	-2.284045
44	1	-2.746284	-3.079493	-1.376042
45	1	1.261357	-4.856852	-0.942598
46	1	2.445597	-3.541099	-0.914193
47	1	1.139242	-3.529363	-2.111142
48	6	-3.063127	0.887530	0.054959
49	6	-3.530402	1.371001	1.299258
50	6	-3.953112	0.710813	-1.034434
51	6	-4.898888	1.655355	1.442261
52	6	-5.311541	1.009165	-0.845390
53	6	-5.788048	1.476043	0.382094
54	1	-5.260855	2.020604	2.399097
55	1	-5.997099	0.869680	-1.675985
56	1	-6.842941	1.696578	0.510236
57	6	3.142537	0.093420	0.250889
58	6	3.788072	0.222587	1.511735
59	6	3.864040	-0.398345	-0.864295
60	6	5.116731	-0.205342	1.650633
61	6	5.195076	-0.816727	-0.679327
62	6	5.819306	-0.735357	0.565742
63	1	5.598994	-0.119084	2.620212
64	1	5.746001	-1.191258	-1.537328

65	1	6.846617	-1.064519	0.686092
66	6	-2.603002	1.616329	2.468636
67	1	-1.755868	0.927103	2.469317
68	1	-2.195201	2.635861	2.446188
69	1	-3.137408	1.504244	3.417904
70	6	-3.473232	0.219398	-2.380444
71	1	-2.846110	0.964660	-2.885251
72	1	-2.859125	-0.681489	-2.297791
73	1	-4.324502	0.004652	-3.033376
74	6	3.085072	0.822608	2.710886
75	1	3.610027	0.560127	3.634750
76	1	3.047877	1.918953	2.655657
77	1	2.049676	0.481870	2.789730
78	6	3.277666	-0.441623	-2.255081
79	1	4.078670	-0.465563	-3.001272
80	1	2.645081	-1.320473	-2.412390
81	1	2.639672	0.422716	-2.455273

27^{Ar} (E = -1504.125476 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.266651	-0.740094	-0.475386
2	7	-1.691565	0.397899	-0.009650
3	6	-0.886302	1.240877	-0.795982
4	7	1.605458	0.537755	0.143168
5	6	-0.507887	-2.310281	1.340604
6	6	0.727127	-2.669771	0.716390
7	6	-1.561953	-2.586762	0.421082
8	17	-0.130509	-0.840732	-2.871032
9	6	0.441178	-3.119023	-0.596721
10	6	-0.974435	-3.072797	-0.777429
11	6	1.353154	1.798546	0.104394
12	6	-0.046761	2.301567	-0.095436
13	1	-1.245647	1.520609	-1.785744
14	6	0.199211	3.661689	-0.740343
15	1	-0.472024	2.478816	0.907260
16	6	2.316916	2.959306	0.064613
17	6	1.488792	4.025653	-0.635077
18	1	2.606980	3.275379	1.076926
19	1	3.246302	2.703614	-0.453755
20	6	2.150386	5.304361	-1.070992
21	6	-0.946899	4.447594	-1.314336
22	1	-0.634592	5.433364	-1.670810
23	1	-1.733429	4.589687	-0.560020
24	1	-1.408858	3.913838	-2.154053
25	1	1.449078	5.988520	-1.556873
26	1	2.966772	5.100272	-1.777977
27	1	2.595820	5.828699	-0.213308
28	6	2.045028	-2.834570	1.430538
29	6	-0.683992	-2.017238	2.811178
30	6	-3.036239	-2.602638	0.736692
31	6	-1.720527	-3.622307	-1.965650
32	6	1.427235	-3.692731	-1.581828
33	1	2.122099	-3.862932	1.814217
34	1	2.138245	-2.161901	2.285658
35	1	2.903840	-2.663387	0.776848
36	1	-0.614731	-2.948901	3.392127
37	1	-1.659765	-1.572581	3.019791
38	1	0.082230	-1.338821	3.200204
39	1	-3.331354	-3.603611	1.084198
40	1	-3.646634	-2.366218	-0.139245
41	1	-3.299414	-1.887272	1.518923
42	1	-1.890475	-4.701601	-1.836615
43	1	-1.161178	-3.473644	-2.892672
44	1	-2.698808	-3.147302	-2.089356

45	1	1.400737	-4.791920	-1.560207
46	1	2.452255	-3.383837	-1.353482
47	1	1.198347	-3.371784	-2.602878
48	6	-3.031512	0.665240	0.397976
49	6	-3.311314	1.051655	1.733530
50	6	-4.089501	0.562225	-0.547050
51	6	-4.644233	1.294795	2.109488
52	6	-5.403479	0.818176	-0.129167
53	6	-5.687915	1.177942	1.191548
54	1	-4.855245	1.583617	3.135862
55	1	-6.209963	0.728261	-0.851669
56	1	-6.711900	1.365788	1.499045
57	6	2.982233	0.164122	0.409866
58	6	3.451727	0.203383	1.743303
59	6	3.826753	-0.224148	-0.654768
60	6	4.774813	-0.191355	1.999359
61	6	5.142986	-0.611583	-0.351106
62	6	5.616289	-0.603457	0.963219
63	1	5.139504	-0.175955	3.022135
64	1	5.798942	-0.912310	-1.162385
65	1	6.634958	-0.910051	1.177591
66	6	-2.218494	1.252811	2.762706
67	1	-1.293915	0.755967	2.466697
68	1	-1.995683	2.320953	2.895639
69	1	-2.523623	0.867050	3.742466
70	6	-3.823668	0.188218	-1.986901
71	1	-3.396294	1.029072	-2.548909
72	1	-3.104476	-0.631064	-2.073203
73	1	-4.752052	-0.104960	-2.487377
74	6	2.571387	0.659524	2.887438
75	1	2.995732	0.346890	3.846085
76	1	2.473675	1.753050	2.917577
77	1	1.557955	0.254216	2.812238
78	6	3.365023	-0.175999	-2.091828
79	1	4.130430	-0.591918	-2.753579
80	1	2.433174	-0.723990	-2.255586
81	1	3.169941	0.855082	-2.416218

TS27^{Ar}-25^{Ar} (E = -1504.1062454 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.211640	-0.487077	-0.291943
2	7	-1.539642	0.795975	0.137915
3	6	-0.669988	1.704884	-0.460446
4	7	1.604536	0.350057	0.326013
5	6	-0.699950	-2.077234	1.435919
6	6	0.500948	-2.565174	0.832079
7	6	-1.753122	-2.189273	0.481357
8	17	-0.082806	-0.424671	-2.688469
9	6	0.205134	-2.915227	-0.506331
10	6	-1.189189	-2.680684	-0.724262
11	6	1.446596	1.616251	-0.076346
12	6	0.326544	2.504030	0.355162
13	1	-0.863713	2.075977	-1.465291
14	6	0.686924	3.863033	-0.192569
15	1	0.115433	2.478764	1.426173
16	6	2.388812	2.407534	-0.961835
17	6	1.812954	3.809039	-0.923113
18	1	3.415882	2.349454	-0.576775
19	1	2.419327	1.994557	-1.977041
20	6	2.502148	4.915449	-1.673282
21	6	-0.207798	5.042506	0.075807
22	1	0.139029	5.950467	-0.426071
23	1	-0.266023	5.252254	1.153050
24	1	-1.231618	4.836374	-0.264379

25	1	1.986126	5.873927	-1.566865
26	1	2.562584	4.680342	-2.745241
27	1	3.534257	5.044136	-1.317555
28	6	1.760172	-2.900611	1.588866
29	6	-0.865772	-1.794335	2.908885
30	6	-3.228181	-2.058937	0.763204
31	6	-1.951656	-3.090422	-1.957234
32	6	1.126320	-3.581354	-1.495205
33	1	1.651488	-3.894990	2.046985
34	1	1.960070	-2.190808	2.394886
35	1	2.642032	-2.927133	0.945139
36	1	-0.864250	-2.736657	3.476255
37	1	-1.809412	-1.285767	3.118968
38	1	-0.054863	-1.176398	3.309010
39	1	-3.636073	-3.041223	1.043107
40	1	-3.786292	-1.707304	-0.108385
41	1	-3.434710	-1.367083	1.582458
42	1	-2.200006	-4.160977	-1.905670
43	1	-1.366535	-2.920474	-2.864742
44	1	-2.891047	-2.538737	-2.058779
45	1	0.884333	-4.650523	-1.580682
46	1	2.173275	-3.502505	-1.189840
47	1	1.029077	-3.138276	-2.491831
48	6	-2.892468	1.147431	0.461041
49	6	-3.228289	1.510365	1.789445
50	6	-3.886789	1.155359	-0.552779
51	6	-4.564462	1.825867	2.092209
52	6	-5.206211	1.485565	-0.207517
53	6	-5.551903	1.811732	1.106764
54	1	-4.821902	2.091433	3.114019
55	1	-5.966853	1.482092	-0.983125
56	1	-6.579334	2.056392	1.357428
57	6	2.965262	-0.098454	0.560071
58	6	3.451963	0.097269	1.881152
59	6	3.792014	-0.685156	-0.425245
60	6	4.740403	-0.346609	2.209699
61	6	5.077353	-1.121843	-0.047953
62	6	5.551308	-0.964410	1.253495
63	1	5.104692	-0.205067	3.222909
64	1	5.709237	-1.583172	-0.801626
65	1	6.544722	-1.311066	1.519767
66	6	-2.190212	1.610589	2.886519
67	1	-1.313270	1.000467	2.667262
68	1	-1.848035	2.647880	3.007796
69	1	-2.605372	1.295504	3.850527
70	6	-3.551536	0.829004	-1.989343
71	1	-2.986915	1.641278	-2.465418
72	1	-2.926169	-0.063166	-2.075065
73	1	-4.464903	0.676189	-2.572816
74	6	2.606905	0.782393	2.932798
75	1	3.095678	0.734425	3.910328
76	1	2.444610	1.841761	2.694569
77	1	1.614966	0.326544	3.016784
78	6	3.391767	-0.816246	-1.876436
79	1	3.842597	-1.709526	-2.321634
80	1	2.313316	-0.867278	-2.018511
81	1	3.750359	0.045081	-2.457590

25^{Ar} (E = -1504.1351264 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	22	-0.110491	-0.868920	-0.417226
2	7	-1.493232	0.379517	-0.039651
3	6	-0.752145	1.489694	-0.573863
4	7	1.385691	0.224855	0.043873
5	6	-0.076255	-2.409587	1.420183
6	6	0.934775	-2.860812	0.519130
7	6	-1.342706	-2.564697	0.779468
8	17	-0.063758	-0.838804	-2.794841
9	6	0.298376	-3.257177	-0.686020
10	6	-1.108501	-3.061906	-0.529654
11	6	0.812435	1.442678	-0.468551
12	6	-0.001481	2.453320	0.334797
13	1	-1.119854	1.903958	-1.511430
14	6	0.280106	3.791274	-0.268600
15	1	-0.155910	2.344386	1.397489
16	6	1.538498	2.249625	-1.551276
17	6	1.094872	3.681871	-1.332682
18	1	2.623809	2.159764	-1.423365
19	1	1.300304	1.879162	-2.553406
20	6	1.577648	4.763496	-2.260967
21	6	-0.372478	5.025647	0.296745
22	1	-0.069961	5.933095	-0.234454
23	1	-0.112906	5.153707	1.356905
24	1	-1.467492	4.949367	0.243480
25	1	1.217990	5.754383	-1.967210
26	1	1.245148	4.576517	-3.291703
27	1	2.676490	4.794890	-2.283292
28	6	2.380310	-3.089595	0.881265
29	6	0.145641	-2.102195	2.879642
30	6	-2.688848	-2.449090	1.446125
31	6	-2.157525	-3.450906	-1.539723
32	6	0.950044	-3.927093	-1.867314
33	1	2.485108	-4.066262	1.375635
34	1	2.760443	-2.328860	1.567025
35	1	3.029798	-3.095962	0.002593
36	1	0.116771	-3.032780	3.465278
37	1	-0.623843	-1.439734	3.284391
38	1	1.119675	-1.637276	3.053946
39	1	-2.980931	-3.429716	1.848866
40	1	-3.470623	-2.129648	0.752482
41	1	-2.677077	-1.741501	2.277564
42	1	-2.349610	-4.532575	-1.493188
43	1	-1.837979	-3.210560	-2.558144
44	1	-3.106633	-2.939012	-1.355245
45	1	0.812131	-5.016009	-1.801679
46	1	2.025743	-3.733129	-1.906058
47	1	0.515894	-3.586533	-2.811163
48	6	-2.864927	0.634371	0.296176
49	6	-3.230128	0.950239	1.629594
50	6	-3.860459	0.580593	-0.717173
51	6	-4.583368	1.176612	1.933177
52	6	-5.200302	0.813904	-0.368615
53	6	-5.566943	1.108566	0.946634
54	1	-4.859095	1.406726	2.958750
55	1	-5.958894	0.763266	-1.144449
56	1	-6.608400	1.282251	1.198557
57	6	2.749245	0.244768	0.488414
58	6	3.073430	0.690703	1.796347
59	6	3.781094	-0.200506	-0.382727
60	6	4.414987	0.669086	2.214765
61	6	5.108784	-0.196010	0.075021
62	6	5.431040	0.232936	1.364271
63	1	4.655069	1.001334	3.220893
64	1	5.893626	-0.536573	-0.594029

65	1	6.462464	0.224340	1.702282
66	6	-2.214045	1.057851	2.745575
67	1	-1.281161	0.558205	2.483400
68	1	-1.977650	2.107400	2.966767
69	1	-2.601032	0.616088	3.671259
70	6	-3.513857	0.303730	-2.162417
71	1	-3.122918	1.202379	-2.659248
72	1	-2.742697	-0.461742	-2.265764
73	1	-4.403520	-0.011644	-2.716911
74	6	2.024735	1.200655	2.759068
75	1	2.339473	1.036872	3.795141
76	1	1.862406	2.278809	2.633313
77	1	1.063790	0.707003	2.604209
78	6	3.494231	-0.681709	-1.787405
79	1	4.410654	-1.057206	-2.253421
80	1	2.746650	-1.478434	-1.807281
81	1	3.094501	0.114536	-2.423512

$1^{1\text{-Ad}}$ (E = -1180.8042688 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	1.665260	0.293218	0.132788
2	7	-1.619514	0.066213	-0.106170
3	6	3.612759	-1.132837	-0.201479
4	6	2.739307	-1.457365	-1.276079
5	6	2.965983	-1.524659	1.012832
6	17	1.312672	0.670788	2.528517
7	6	1.543027	-1.998203	-0.730233
8	6	1.691641	-2.060549	0.687904
9	6	-0.456336	0.131855	-0.057647
10	6	1.522916	1.232527	-1.926681
11	6	2.566708	1.915951	-1.208429
12	1	0.568962	1.728452	-2.081926
13	6	0.806044	2.667298	0.265440
14	6	2.159057	2.648908	-0.056421
15	1	0.491953	3.032489	1.233314
16	1	0.044943	2.623740	-0.498229
17	6	3.172704	3.298164	0.868866
18	6	3.965289	2.074399	-1.774217
19	1	4.749514	2.059715	-1.011733
20	1	4.035236	3.040371	-2.298241
21	1	4.185876	1.296788	-2.509097
22	1	3.499456	4.259658	0.447055
23	1	4.066621	2.683377	1.018525
24	1	2.725162	3.491872	1.847082
25	6	3.103263	-1.501279	-2.737762
26	6	5.075244	-0.770169	-0.301180
27	6	3.637024	-1.567374	2.361774
28	6	0.723260	-2.679548	1.662173
29	6	0.412505	-2.583589	-1.540689
30	1	3.560520	-2.474312	-2.971140
31	1	3.825398	-0.729783	-3.017581
32	1	2.226536	-1.391825	-3.383391
33	1	5.696439	-1.658129	-0.112285
34	1	5.366347	-0.012234	0.434631
35	1	5.337176	-0.392285	-1.291968
36	1	4.290112	-2.451118	2.422856
37	1	2.907953	-1.621840	3.172175
38	1	4.257457	-0.683272	2.539949
39	1	0.998851	-3.723649	1.869719
40	1	-0.299460	-2.679737	1.271955
41	1	0.716753	-2.133843	2.609923
42	1	0.686662	-3.580023	-1.916283
43	1	0.167889	-1.960204	-2.407394
44	1	-0.496865	-2.696703	-0.943865

45	1	1.836548	0.676337	-2.801481
46	6	-3.066727	0.061069	-0.101889
47	6	-3.574685	1.339232	0.622026
48	6	-3.586897	0.049088	-1.565380
49	6	-3.579514	-1.200219	0.645438
50	6	-5.123353	1.336370	0.626886
51	1	-3.182048	1.356478	1.645857
52	1	-3.191526	2.226477	0.102518
53	6	-5.135764	0.051666	-1.552797
54	1	-3.202990	0.930364	-2.094458
55	1	-3.206416	-0.842054	-2.080389
56	6	-5.128256	-1.193384	0.649919
57	1	-3.199730	-2.099652	0.143947
58	1	-3.188774	-1.197886	1.670372
59	6	-5.636542	0.079199	1.372067
60	6	-5.644768	1.324621	-0.831587
61	1	-5.474997	2.240580	1.139352
62	6	-5.649078	-1.206316	-0.808786
63	1	-5.496599	0.042968	-2.589060
64	1	-5.483580	-2.086771	1.178724
65	1	-6.734262	0.081456	1.397858
66	1	-5.287269	0.088027	2.413437
67	1	-6.742596	1.343710	-0.837119
68	1	-5.302245	2.223061	-1.362976
69	1	-6.746937	-1.221928	-0.814172
70	1	-5.309490	-2.115500	-1.323789

TS1$^{1\text{-Ad}}$-3$^{1\text{-Ad}}$ (E = -1180.7948007 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-1.117491	-0.597113	-0.560009
2	7	-3.250909	1.258129	-2.065919
3	6	1.265343	-0.862212	-0.997561
4	6	1.130554	-0.263042	0.280698
5	6	0.731012	0.037348	-1.966417
6	17	-1.413838	-2.286902	-2.277530
7	6	0.517483	1.019860	0.105749
8	6	0.275143	1.202460	-1.285083
9	6	-2.672248	0.445002	-1.376710
10	6	-1.763481	-0.146891	1.536768
11	6	-2.003785	-1.555777	1.415285
12	1	-2.602471	0.540530	1.450191
13	6	-3.572063	-0.890039	-0.344203
14	6	-2.856884	-1.947077	0.384706
15	1	-4.206455	-1.283202	-1.131403
16	1	-4.084029	-0.175308	0.297829
17	6	-3.228905	-3.391032	0.129764
18	6	-1.331541	-2.560659	2.332646
19	1	-0.917423	-3.420067	1.795080
20	1	-2.063266	-2.948037	3.055875
21	1	-0.526242	-2.090141	2.902165
22	1	-4.053067	-3.684857	0.797738
23	1	-2.394480	-4.075874	0.305615
24	1	-3.558675	-3.530022	-0.902217
25	6	1.715221	-0.793630	1.566014
26	6	1.936169	-2.178178	-1.298755
27	6	0.791520	-0.127093	-3.461828
28	6	-0.175835	2.485346	-1.936067
29	6	0.400361	2.110972	1.141147
30	1	2.753084	-0.448970	1.680525
31	1	1.730873	-1.887684	1.588429
32	1	1.161859	-0.448294	2.444545
33	1	2.987918	-2.015880	-1.575328
34	1	1.443763	-2.694728	-2.127151
35	1	1.923488	-2.848493	-0.433129

36	1	1.711272	0.330730	-3.855230
37	1	-0.058279	0.354753	-3.955571
38	1	0.783861	-1.180480	-3.750043
39	1	0.696288	3.106967	-2.186553
40	1	-0.822610	3.069062	-1.274536
41	1	-0.734634	2.300140	-2.856823
42	1	1.189329	2.861194	0.987050
43	1	0.513017	1.724140	2.157572
44	1	-0.562605	2.630413	1.086332
45	1	-1.052494	0.159678	2.293007
46	6	-4.614517	1.647003	-2.471725
47	6	-5.586760	1.780124	-1.268175
48	6	-4.512333	3.019139	-3.189893
49	6	-5.169085	0.595117	-3.473829
50	6	-6.982497	2.228479	-1.775148
51	1	-5.678804	0.820282	-0.748795
52	1	-5.184372	2.510759	-0.553587
53	6	-5.904110	3.466083	-3.694881
54	1	-4.099618	3.759765	-2.492021
55	1	-3.807592	2.929336	-4.026227
56	6	-6.567080	1.042042	-3.971484
57	1	-4.472810	0.495630	-4.315729
58	1	-5.235051	-0.384846	-2.985337
59	6	-7.530239	1.170353	-2.765256
60	6	-6.867977	3.596316	-2.490161
61	1	-7.659537	2.315162	-0.915124
62	6	-6.452095	2.410639	-4.687040
63	1	-5.809839	4.435810	-4.200752
64	1	-6.949838	0.288573	-4.672132
65	1	-8.529655	1.464609	-3.113045
66	1	-7.636375	0.199596	-2.260785
67	1	-7.858758	3.924417	-2.832616
68	1	-6.497703	4.358711	-1.790709
69	1	-7.436657	2.721259	-5.062247
70	1	-5.785049	2.327429	-5.556017

3$^{1\text{-Ad}}$ (E = -1180.8329783 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-1.343024	-0.047816	-0.274137
2	7	0.617081	-0.009212	0.347564
3	6	-2.161643	-2.294593	-0.111258
4	6	-3.245209	-1.477417	-0.552430
5	6	-1.810982	-1.887513	1.205811
6	17	-0.881326	-0.064272	-2.576833
7	6	-3.561409	-0.563927	0.491661
8	6	-2.658887	-0.804283	1.575201
9	6	-0.048064	0.877016	0.955207
10	6	-2.091106	2.007578	-0.174527
11	6	-1.072618	3.100297	-0.319653
12	1	-2.568991	2.069607	0.806889
13	6	0.209070	2.181758	1.624740
14	6	-0.041213	3.246033	0.543940
15	1	1.223930	2.282066	2.021946
16	1	-0.486191	2.297092	2.465983
17	6	0.953039	4.387743	0.574737
18	6	-1.309518	4.028269	-1.497554
19	1	-0.495109	4.734143	-1.678082
20	1	-2.236886	4.601728	-1.358701
21	1	-1.440148	3.426814	-2.406878
22	1	0.932983	4.889998	1.553650
23	1	0.751022	5.145840	-0.184907
24	1	1.983082	4.029980	0.426187
25	6	-3.990602	-1.634269	-1.853937
26	6	-1.559032	-3.436974	-0.890869

27	6	-0.787030	-2.541010	2.099270
28	6	-2.725033	-0.152505	2.934084
29	6	-4.755824	0.354697	0.523772
30	1	-4.763342	-2.411223	-1.762814
31	1	-3.319961	-1.919823	-2.669405
32	1	-4.488530	-0.705313	-2.148684
33	1	-2.167931	-4.344959	-0.774292
34	1	-0.546551	-3.673454	-0.549692
35	1	-1.504549	-3.207958	-1.959581
36	1	-1.268264	-3.282445	2.752600
37	1	-0.283611	-1.813133	2.743741
38	1	-0.017670	-3.061744	1.521853
39	1	-3.493102	-0.633317	3.556779
40	1	-2.979494	0.910502	2.865735
41	1	-1.772484	-0.233107	3.467402
42	1	-5.641720	-0.190701	0.879013
43	1	-4.991881	0.755733	-0.467080
44	1	-4.602027	1.203949	1.195710
45	1	-2.871728	2.097165	-0.936971
46	6	2.072679	-0.274285	0.168246
47	6	2.704935	0.864877	-0.678644
48	6	2.795270	-0.365312	1.538511
49	6	2.239364	-1.615556	-0.585748
50	6	4.209962	0.569724	-0.900075
51	1	2.177330	0.936762	-1.636916
52	1	2.580604	1.823240	-0.160253
53	6	4.301066	-0.657436	1.311453
54	1	2.676368	0.575528	2.089998
55	1	2.338326	-1.162416	2.139981
56	6	3.741811	-1.912401	-0.811191
57	1	1.778550	-2.421204	0.001311
58	1	1.706792	-1.558149	-1.542346
59	6	4.369475	-0.773898	-1.652796
60	6	4.926393	0.483499	0.470517
61	1	4.647101	1.381820	-1.495760
62	6	4.460586	-2.000812	0.557979
63	1	4.803464	-0.716986	2.286007
64	1	3.844053	-2.866102	-1.345215
65	1	5.433624	-0.980261	-1.831048
66	1	3.879986	-0.716553	-2.634416
67	1	5.998380	0.294789	0.323044
68	1	4.837255	1.439920	1.005029
69	1	5.526160	-2.223370	0.410893
70	1	4.037773	-2.821214	1.154834

4$^{\mathbf{1\text{-}Ad}}$ (E = -1180.8215966 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-1.243098	-0.154284	-0.202031
2	7	0.795296	0.245024	-0.178282
3	6	-3.246037	-1.521881	0.243430
4	6	-2.429965	-1.523619	1.408952
5	6	-2.532150	-2.187654	-0.791150
6	17	-1.994055	0.553897	-2.320213
7	6	-1.195100	-2.158729	1.082650
8	6	-1.261928	-2.573363	-0.282406
9	6	0.097163	1.300307	-0.265108
10	6	-1.974408	1.428343	1.147296
11	6	-2.030363	2.858062	0.662926
12	1	-1.298280	1.333339	2.010324
13	6	0.282102	2.768296	-0.278171
14	6	-1.005472	3.497402	0.066219
15	1	1.106813	3.073852	0.382695
16	1	0.597305	3.058303	-1.291016
17	6	-0.971731	4.954798	-0.345367

18	6	-3.375098	3.520134	0.918612
19	1	-3.459995	4.527586	0.505167
20	1	-3.583377	3.573383	1.996698
21	1	-4.171853	2.909993	0.471109
22	1	-1.847675	5.519511	-0.021184
23	1	-0.894231	5.049836	-1.439430
24	1	-0.086010	5.453329	0.076996
25	6	-2.851622	-1.145875	2.806579
26	6	-4.653551	-0.992507	0.131064
27	6	-3.074055	-2.545086	-2.149639
28	6	-0.275318	-3.439022	-1.030455
29	6	-0.144384	-2.526083	2.104235
30	1	-3.118146	-2.050542	3.372025
31	1	-3.727068	-0.490748	2.809690
32	1	-2.054159	-0.637603	3.359621
33	1	-5.389109	-1.792838	0.295959
34	1	-4.841541	-0.569666	-0.861483
35	1	-4.852327	-0.207974	0.868329
36	1	-3.614841	-3.501829	-2.100654
37	1	-2.274751	-2.650211	-2.889428
38	1	-3.765740	-1.784789	-2.522161
39	1	-0.707756	-4.432572	-1.213400
40	1	0.648864	-3.582521	-0.466333
41	1	-0.008159	-3.016818	-2.006238
42	1	-0.527587	-3.307435	2.776208
43	1	0.142393	-1.673747	2.731193
44	1	0.762549	-2.915112	1.635416
45	1	-2.962610	1.140871	1.507321
46	6	2.282527	0.076791	-0.082000
47	6	2.657770	-1.386284	-0.407590
48	6	3.007778	1.010310	-1.089679
49	6	2.745371	0.414882	1.361673
50	6	4.189199	-1.585355	-0.291581
51	1	2.141796	-2.055434	0.287850
52	1	2.313624	-1.632884	-1.420135
53	6	4.541644	0.817672	-0.972849
54	1	2.667652	0.779583	-2.108077
55	1	2.756935	2.056768	-0.886244
56	6	4.279771	0.223789	1.473460
57	1	2.473710	1.450100	1.606240
58	1	2.225839	-0.239282	2.073784
59	6	4.642274	-1.246788	1.150495
60	6	4.908319	-0.650777	-1.293585
61	1	4.432902	-2.631289	-0.519490
62	6	4.992705	1.162422	0.468614
63	1	5.038466	1.488551	-1.685797
64	1	4.595734	0.467552	2.496275
65	1	5.725945	-1.395966	1.248988
66	1	4.156121	-1.922201	1.868412
67	1	5.995697	-0.790766	-1.226959
68	1	4.611442	-0.898600	-2.322010
69	1	6.081427	1.048770	0.558209
70	1	4.757376	2.211235	0.698063

TS4$^{1\text{-Ad}}$-5$^{1\text{-Ad}}$ (E = -1180.804138a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.733719	0.011694	-0.757308
2	7	-0.474291	1.546448	-0.466235
3	6	2.815680	-1.241918	-0.725139
4	6	2.497445	-0.860652	0.606581
5	6	3.079931	-0.054711	-1.471945
6	17	0.237302	-1.101138	-2.795440
7	6	2.551732	0.565644	0.680593
8	6	2.930446	1.060847	-0.606047

9	6	-1.141421	0.412212	-0.585351
10	6	-0.775089	-0.960714	0.769796
11	6	-2.195640	-1.460562	0.823973
12	1	-0.449005	-0.528578	1.722236
13	6	-2.553174	0.096857	-0.971382
14	6	-3.076460	-0.985820	-0.067079
15	1	-3.202607	0.976542	-0.916918
16	1	-2.554675	-0.229604	-2.020882
17	6	-4.512248	-1.404857	-0.262103
18	6	-2.471792	-2.520689	1.868664
19	1	-3.518712	-2.836222	1.886015
20	1	-2.215521	-2.148213	2.870221
21	1	-1.852002	-3.411198	1.693077
22	1	-4.822619	-2.189888	0.431796
23	1	-4.667627	-1.778629	-1.283994
24	1	-5.190499	-0.549807	-0.130208
25	6	2.337236	-1.784689	1.789299
26	6	2.966266	-2.649543	-1.244762
27	6	3.553754	-0.007733	-2.902207
28	6	3.317447	2.476954	-0.961844
29	6	2.469171	1.346159	1.972229
30	1	3.301891	-1.918513	2.299694
31	1	1.987111	-2.778150	1.490428
32	1	1.631516	-1.391561	2.528991
33	1	4.020966	-2.959216	-1.217564
34	1	2.617719	-2.730249	-2.278568
35	1	2.396844	-3.368147	-0.646194
36	1	4.631782	-0.217827	-2.959019
37	1	3.384949	0.976981	-3.349907
38	1	3.033673	-0.746671	-3.519272
39	1	4.406250	2.547563	-1.094337
40	1	3.035454	3.183963	-0.178667
41	1	2.853622	2.812179	-1.896233
42	1	3.327038	1.104109	2.615549
43	1	1.562190	1.117986	2.544463
44	1	2.486645	2.424256	1.795754
45	1	-0.131261	-1.830482	0.580560
46	6	-0.985641	2.905250	-0.149237
47	6	-1.917399	2.866918	1.094981
48	6	0.198746	3.853764	0.149362
49	6	-1.766846	3.484343	-1.367130
50	6	-2.438496	4.291452	1.412303
51	1	-2.761638	2.190697	0.914043
52	1	-1.357172	2.466640	1.951106
53	6	-0.310078	5.279180	0.478066
54	1	0.773257	3.457139	0.993770
55	1	0.862616	3.880866	-0.722206
56	6	-2.289859	4.905522	-1.039540
57	1	-1.097212	3.510273	-2.236962
58	1	-2.607051	2.830015	-1.624485
59	6	-3.224018	4.838909	0.194573
60	6	-1.240043	5.223343	1.714727
61	1	-3.100494	4.243814	2.287319
62	6	-1.094619	5.839125	-0.732543
63	1	0.550729	5.926806	0.692415
64	1	-2.847519	5.289380	-1.904160
65	1	-3.617774	5.839011	0.421808
66	1	-4.087424	4.193005	-0.019404
67	1	-1.599385	6.231655	1.961925
68	1	-0.685862	4.853498	2.588991
69	1	-1.454152	6.853828	-0.513123
70	1	-0.436516	5.910400	-1.609687

$5^{1\text{-Ad}}$ (E = -1180.8279474 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		

		X	Y	Z
1	22	-1.255046	-0.190850	-0.146231
2	7	0.614732	0.187632	0.169316
3	6	-3.282175	-1.479840	0.024849
4	6	-2.629205	-1.466693	1.289376
5	6	-2.450168	-2.189224	-0.886754
6	17	-2.069851	0.771133	-2.138044
7	6	-1.398810	-2.182619	1.158833
8	6	-1.288475	-2.633065	-0.191283
9	6	0.025838	1.434815	0.133372
10	6	-0.959742	1.819943	1.190936
11	6	-1.355755	3.238293	0.857011
12	1	-0.641756	1.650594	2.226212
13	6	0.294614	2.649135	-0.738809
14	6	-0.665851	3.687330	-0.203366
15	1	1.327573	3.014444	-0.651316
16	1	0.120723	2.444716	-1.801353
17	6	-0.754022	5.036213	-0.864074
18	6	-2.404979	3.943426	1.673914
19	1	-2.557707	4.975532	1.345378
20	1	-2.127898	3.965667	2.737293
21	1	-3.371501	3.424050	1.604863
22	1	-1.448963	5.708548	-0.352339
23	1	-1.087664	4.933617	-1.905702
24	1	0.231306	5.522269	-0.890262
25	6	-3.199284	-0.954643	2.592401
26	6	-4.644181	-0.912206	-0.287147
27	6	-2.799094	-2.539702	-2.310127
28	6	-0.298019	-3.627104	-0.751885
29	6	-0.525827	-2.572775	2.327941
30	1	-3.708319	-1.765694	3.133100
31	1	-3.932883	-0.157976	2.431810
32	1	-2.419251	-0.564180	3.255729
33	1	-5.413908	-1.694128	-0.216754
34	1	-4.680491	-0.495899	-1.298346
35	1	-4.921597	-0.114745	0.410139
36	1	-3.383661	-3.471010	-2.341439
37	1	-1.902006	-2.690751	-2.919078
38	1	-3.391132	-1.752290	-2.784299
39	1	-0.804184	-4.577900	-0.971279
40	1	0.505475	-3.842050	-0.043484
41	1	0.161479	-3.282078	-1.684941
42	1	-1.074291	-3.253803	2.994120
43	1	-0.215875	-1.709370	2.927381
44	1	0.379161	-3.089062	2.000925
45	1	-1.923100	1.152684	1.147138
46	6	2.075633	-0.038361	0.080048
47	6	2.603213	0.254238	-1.358785
48	6	2.824445	0.875395	1.093428
49	6	2.409606	-1.509549	0.420809
50	6	4.132169	0.015698	-1.432377
51	1	2.076018	-0.400275	-2.065791
52	1	2.375593	1.287698	-1.640693
53	6	4.352655	0.635896	1.011415
54	1	2.598394	1.928145	0.883670
55	1	2.458179	0.658940	2.106786
56	6	3.936120	-1.762310	0.345732
57	1	2.042895	-1.734440	1.428829
58	1	1.886319	-2.166711	-0.280294
59	6	4.442640	-1.459545	-1.085025
60	6	4.848854	0.946504	-0.422678
61	1	4.481116	0.237770	-2.449985
62	6	4.662645	-0.841030	1.355225
63	1	4.859039	1.296832	1.727991

64	1	4.137801	-2.813301	0.594266
65	1	5.523797	-1.644834	-1.149995
66	1	3.954710	-2.127718	-1.808573
67	1	5.936256	0.800788	-0.483208
68	1	4.649474	1.998494	-0.671784
69	1	5.746311	-1.018587	1.316927
70	1	4.332847	-1.067311	2.379114

$10^{1\text{-Ad}}$ (E = -1663.7445409 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.033284	1.198864	0.225779
2	7	1.513427	0.145074	0.126369
3	6	1.152852	0.005169	1.468072
4	7	-1.467463	-0.628873	0.559375
5	6	0.909280	3.158859	1.191516
6	6	-0.026345	2.640016	2.138866
7	6	0.175897	3.607281	0.059087
8	17	-0.392790	1.207524	-2.177904
9	6	-1.335537	2.787588	1.590073
10	6	-1.210927	3.387622	0.307322
11	6	-0.845722	-1.539733	1.219353
12	6	0.384171	-1.192712	2.029391
13	1	1.818903	0.441656	2.215839
14	6	1.040047	-2.544035	2.294091
15	1	0.005521	-0.832418	3.003322
16	6	-1.055192	-3.044431	1.324051
17	6	0.252938	-3.551619	1.892671
18	1	-1.872147	-3.277652	2.018429
19	1	-1.320054	-3.503006	0.368881
20	6	0.475177	-5.035804	2.006666
21	6	2.340790	-2.633009	3.042823
22	1	2.625250	-3.668340	3.252715
23	1	2.266167	-2.101131	4.002515
24	1	3.160142	-2.164556	2.486440
25	1	1.439385	-5.276927	2.463239
26	1	0.443951	-5.511909	1.016356
27	1	-0.313255	-5.507221	2.611148
28	6	0.254851	2.288616	3.578397
29	6	2.382127	3.370421	1.439229
30	6	0.736645	4.321250	-1.144436
31	6	-2.316522	3.838867	-0.612535
32	6	-2.604815	2.527067	2.367507
33	1	0.045665	3.153149	4.226368
34	1	1.300053	2.007956	3.734554
35	1	-0.371022	1.460489	3.928976
36	1	2.549573	4.326586	1.956422
37	1	2.951099	3.397288	0.505319
38	1	2.808139	2.580526	2.065445
39	1	0.661882	5.410510	-1.009757
40	1	0.195054	4.052573	-2.055380
41	1	1.792107	4.079739	-1.304469
42	1	-2.346752	4.936369	-0.662389
43	1	-3.297621	3.496374	-0.271670
44	1	-2.162483	3.465122	-1.631196
45	1	-2.642279	3.173732	3.255353
46	1	-2.677594	1.490587	2.717572
47	1	-3.495279	2.742037	1.770804
48	6	2.777888	-0.249238	-0.531788
49	6	3.004224	0.589176	-1.817131
50	6	4.005401	-0.044204	0.400916
51	6	2.695796	-1.751534	-0.937819
52	6	4.307281	0.151585	-2.530786
53	1	2.144636	0.471591	-2.482194
54	1	3.058596	1.653384	-1.548093

55	6	5.307846	-0.493836	-0.307355
56	1	4.075744	1.015695	0.677573
57	1	3.870391	-0.613537	1.328107
58	6	3.999640	-2.194555	-1.645978
59	1	2.518694	-2.363513	-0.044263
60	1	1.832475	-1.883875	-1.603057
61	6	4.205361	-1.343354	-2.922613
62	6	5.516324	0.352489	-1.586266
63	1	4.440358	0.760007	-3.435731
64	6	5.201299	-1.990463	-0.690817
65	1	6.156672	-0.348137	0.375304
66	1	3.921153	-3.256388	-1.918135
67	1	5.119191	-1.660094	-3.445017
68	1	3.365293	-1.494222	-3.614568
69	1	6.446415	0.053353	-2.089890
70	1	5.617626	1.415014	-1.322591
71	1	6.130167	-2.320427	-1.176854
72	1	5.074019	-2.603745	0.213087
73	6	-2.764747	-0.911087	-0.183913
74	6	-2.488356	-1.676677	-1.510117
75	6	-3.799655	-1.699626	0.672999
76	6	-3.415926	0.455083	-0.526497
77	6	-3.813596	-1.877536	-2.289766
78	1	-1.773765	-1.103317	-2.108291
79	1	-2.037277	-2.653892	-1.301290
80	6	-5.118191	-1.897961	-0.122539
81	1	-3.425041	-2.686735	0.947925
82	1	-3.994077	-1.147521	1.603582
83	6	-4.726266	0.268577	-1.329051
84	1	-3.628648	0.986020	0.407453
85	1	-2.712926	1.053969	-1.108315
86	6	-4.424522	-0.499127	-2.638300
87	6	-4.814235	-2.681499	-1.424079
88	1	-3.597380	-2.430048	-3.213909
89	6	-5.739594	-0.529245	-0.478161
90	1	-5.816641	-2.473640	0.499993
91	1	-5.138059	1.258433	-1.568416
92	1	-5.347924	-0.631893	-3.219073
93	1	-3.725455	0.075262	-3.259806
94	1	-5.744427	-2.852215	-1.983166
95	1	-4.397212	-3.670096	-1.182426
96	1	-6.677113	-0.672644	-1.032891
97	1	-5.986078	0.025086	0.438637

11$^{\text{1-Ad}}$ (E = -1663.7257759 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-2.781991	-0.224206	-0.491218
2	7	-1.195161	0.666707	-0.220999
3	6	-0.852542	-0.633804	0.217567
4	7	2.434871	-0.681209	-0.642769
5	6	-3.798318	0.007434	1.624758
6	6	-3.757096	-1.395606	1.339542
7	6	-4.674010	0.618441	0.683563
8	17	-3.024647	-0.669790	-2.771996
9	6	-4.632168	-1.642250	0.236711
10	6	-5.184128	-0.401941	-0.175923
11	6	1.586911	-1.431151	-0.073696
12	6	0.134680	-1.528522	-0.581131
13	1	-0.713060	-0.757242	1.298069
14	6	-0.133752	-3.014238	-0.352964
15	1	0.088408	-1.246806	-1.635879
16	6	1.728561	-2.504145	1.010102
17	6	0.706142	-3.528448	0.560715
18	1	2.731288	-2.927229	1.076064

19	1	1.495899	-2.093683	2.003172
20	6	0.760904	-4.926911	1.115116
21	6	-1.196928	-3.746398	-1.124738
22	1	-1.161688	-4.825306	-0.943321
23	1	-1.068636	-3.576470	-2.201675
24	1	-2.207052	-3.402337	-0.876361
25	1	-0.009397	-5.576494	0.689130
26	1	0.627209	-4.918754	2.206624
27	1	1.739602	-5.388264	0.920130
28	6	-3.098102	-2.440840	2.205185
29	6	-3.164078	0.659969	2.827676
30	6	-5.107440	2.065539	0.645744
31	6	-6.210256	-0.214448	-1.263967
32	6	-4.987498	-2.980941	-0.362267
33	1	-3.779538	-2.754842	3.009151
34	1	-2.186270	-2.060053	2.673980
35	1	-2.823818	-3.332916	1.634891
36	1	-3.776394	0.482672	3.723293
37	1	-3.067880	1.741943	2.702361
38	1	-2.165774	0.259134	3.029740
39	1	-6.160024	2.148834	0.949138
40	1	-5.026388	2.502258	-0.356892
41	1	-4.518742	2.684022	1.327796
42	1	-7.219413	-0.419034	-0.877869
43	1	-6.029465	-0.888687	-2.106246
44	1	-6.207057	0.808889	-1.652317
45	1	-6.028495	-3.239055	-0.123410
46	1	-4.354380	-3.782302	0.028791
47	1	-4.892956	-2.975464	-1.454057
48	6	3.882235	-0.613408	-0.309548
49	6	4.625528	-1.901912	-0.772854
50	6	4.456875	0.576195	-1.131990
51	6	4.180535	-0.346136	1.193647
52	6	6.149898	-1.757944	-0.532929
53	1	4.249641	-2.779001	-0.233432
54	1	4.418895	-2.064324	-1.839171
55	6	5.978573	0.731244	-0.908956
56	1	4.236213	0.403171	-2.193406
57	1	3.932826	1.495418	-0.841328
58	6	5.708282	-0.206139	1.419432
59	1	3.665458	0.574464	1.501861
60	1	3.794180	-1.159280	1.817770
61	6	6.414974	-1.510823	0.973382
62	6	6.696905	-0.565526	-1.353934
63	1	6.650415	-2.683810	-0.847627
64	6	6.253331	0.983680	0.593541
65	1	6.348304	1.580048	-1.500071
66	1	5.897705	-0.032059	2.487581
67	1	7.495666	-1.433351	1.156276
68	1	6.047594	-2.360945	1.566426
69	1	7.781240	-0.469648	-1.202766
70	1	6.532324	-0.739207	-2.426340
71	1	7.332186	1.100097	0.767513
72	1	5.770524	1.917599	0.914085
73	6	-0.521170	1.972420	-0.073786
74	6	-1.597582	3.086742	-0.166926
75	6	0.214922	2.099100	1.286421
76	6	0.501092	2.183075	-1.227463
77	6	-0.947747	4.486269	-0.048898
78	1	-2.127876	2.994993	-1.126013
79	1	-2.331296	2.947210	0.636744
80	6	0.867673	3.500358	1.407593
81	1	-0.498438	1.943731	2.106626
82	1	0.981179	1.317366	1.359449

83	6	1.160004	3.580799	-1.103743
84	1	1.256194	1.390715	-1.193544
85	1	-0.028365	2.095288	-2.185805
86	6	0.073430	4.679765	-1.196335
87	6	-0.223844	4.594934	1.315954
88	1	-1.729817	5.255034	-0.114917
89	6	1.886720	3.697038	0.259221
90	1	1.382256	3.573880	2.375605
91	1	1.884456	3.708331	-1.919428
92	1	0.532961	5.675607	-1.126242
93	1	-0.436944	4.624684	-2.168069
94	1	0.231236	5.589257	1.422879
95	1	-0.946086	4.479475	2.137057
96	1	2.366403	4.681990	0.348042
97	1	2.680732	2.942090	0.330106

TS11$^{1\text{-}Ad}$-12$^{1\text{-}Ad}$ (E = -1663.7021739 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	1.091059	0.021358	-0.255810
2	7	0.387211	-0.767374	1.344820
3	6	-0.217056	0.464631	1.457617
4	7	-2.408225	-1.027493	-0.077578
5	6	3.350594	0.437099	0.237323
6	6	2.669120	1.680454	0.400875
7	6	3.305977	0.098428	-1.149203
8	17	0.652003	-1.613062	-1.887619
9	6	2.203175	2.101414	-0.884301
10	6	2.600478	1.122932	-1.837104
11	6	-2.151186	0.179766	-0.326402
12	6	-1.043917	0.963455	0.402668
13	1	0.025886	1.131066	2.285701
14	6	-1.598877	2.364010	0.462141
15	1	-0.198418	1.055249	-0.826668
16	6	-2.853570	1.230970	-1.188117
17	6	-2.590367	2.513558	-0.434664
18	1	-2.415276	1.259090	-2.195984
19	1	-3.919409	1.039462	-1.309683
20	6	-3.417908	3.733288	-0.729760
21	6	-1.134242	3.380043	1.471378
22	1	-1.591965	4.357175	1.294410
23	1	-0.048485	3.509516	1.458299
24	1	-1.404729	3.067338	2.489263
25	1	-3.108627	4.605529	-0.147378
26	1	-4.479905	3.544619	-0.518251
27	1	-3.349784	3.995405	-1.795024
28	6	2.700772	2.501500	1.668379
29	6	4.226473	-0.229230	1.270100
30	6	4.005429	-1.075077	-1.786254
31	6	2.356499	1.182297	-3.322620
32	6	1.568783	3.428276	-1.225668
33	1	3.712048	2.901911	1.829132
34	1	2.439675	1.912427	2.553969
35	1	2.020229	3.355204	1.621426
36	1	5.252080	0.164137	1.204022
37	1	4.283965	-1.312199	1.124669
38	1	3.870577	-0.046413	2.287343
39	1	5.037490	-0.801426	-2.050242
40	1	3.495710	-1.399841	-2.696568
41	1	4.053489	-1.935708	-1.111541
42	1	3.226071	1.609197	-3.842880
43	1	1.488576	1.804832	-3.562730
44	1	2.172919	0.185489	-3.734499
45	1	2.329530	4.122136	-1.610779
46	1	1.106751	3.900246	-0.355712

47	1	0.796728	3.325719	-1.994802
48	6	-3.496657	-1.820273	-0.702251
49	6	-3.532192	-1.739447	-2.256176
50	6	-3.222701	-3.301006	-0.309890
51	6	-4.885209	-1.421651	-0.122057
52	6	-4.640352	-2.670314	-2.812625
53	1	-3.726950	-0.715017	-2.590251
54	1	-2.549803	-2.030792	-2.648710
55	6	-4.317989	-4.239454	-0.865284
56	1	-2.233758	-3.586503	-0.690546
57	1	-3.181210	-3.368700	0.784716
58	6	-5.987048	-2.351452	-0.691666
59	1	-4.848818	-1.496797	0.973286
60	1	-5.117782	-0.378046	-0.368682
61	6	-6.012104	-2.237816	-2.236529
62	6	-4.349181	-4.134996	-2.408867
63	1	-4.658625	-2.585954	-3.907822
64	6	-5.692149	-3.817322	-0.290041
65	1	-4.095575	-5.273494	-0.568671
66	1	-6.959943	-2.045003	-0.283413
67	1	-6.809384	-2.873731	-2.645708
68	1	-6.238474	-1.204001	-2.535884
69	1	-5.121963	-4.800262	-2.819115
70	1	-3.386083	-4.456714	-2.828313
71	1	-6.483031	-4.477609	-0.672624
72	1	-5.689023	-3.914720	0.804666
73	6	0.539150	-1.699725	2.474783
74	6	1.418497	-2.889928	2.020690
75	6	1.187113	-1.030607	3.722001
76	6	-0.860169	-2.243323	2.886915
77	6	1.562462	-3.921434	3.165719
78	1	0.959799	-3.351691	1.137946
79	1	2.406635	-2.519499	1.719231
80	6	1.332209	-2.065090	4.867605
81	1	2.171043	-0.627902	3.452168
82	1	0.566163	-0.190541	4.062326
83	6	-0.721606	-3.274450	4.032245
84	1	-1.491810	-1.401281	3.202123
85	1	-1.336466	-2.687474	2.008140
86	6	0.163031	-4.454640	3.559923
87	6	2.219354	-3.242261	4.393041
88	1	2.191807	-4.754332	2.824204
89	6	-0.066378	-2.599723	5.261720
90	1	1.798956	-1.577135	5.734365
91	1	-1.718861	-3.647061	4.303695
92	1	0.255952	-5.201413	4.360932
93	1	-0.304170	-4.954997	2.700592
94	1	2.342562	-3.970497	5.206719
95	1	3.222756	-2.877374	4.130861
96	1	0.025977	-3.320646	6.085975
97	1	-0.698101	-1.775082	5.621627

12$^{1\text{-Ad}}$ (E = -1663.7160899 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-1.284270	-0.994575	-0.693488
2	7	-1.176775	0.558252	0.443464
3	6	-0.928650	-0.153030	1.608885
4	7	1.948891	0.109448	0.538424
5	6	-3.581654	-1.256529	-1.184760
6	6	-3.319961	-1.978064	0.014947
7	6	-2.905157	-1.925632	-2.252606
8	17	-0.186489	-0.321866	-2.618576
9	6	-2.454762	-3.065472	-0.305776
10	6	-2.210326	-3.034004	-1.711805

11	6	1.523360	-0.909689	1.159416
12	6	0.176709	-0.933314	1.834041
13	1	-1.704737	-0.157983	2.376968
14	6	0.282289	-1.911590	2.928074
15	1	-0.161520	-2.193781	-0.370357
16	6	2.214227	-2.205066	1.595034
17	6	1.416918	-2.636417	2.800734
18	1	2.154585	-2.957591	0.797723
19	1	3.271073	-2.067369	1.829202
20	6	1.916439	-3.758862	3.663733
21	6	-0.754132	-2.033215	4.015225
22	1	-0.477250	-2.789243	4.754662
23	1	-1.736820	-2.305882	3.610759
24	1	-0.879256	-1.078548	4.543105
25	1	1.240956	-3.990250	4.491895
26	1	2.901155	-3.514605	4.086932
27	1	2.048980	-4.673147	3.067684
28	6	-4.008814	-1.752407	1.338254
29	6	-4.614271	-0.171159	-1.362653
30	6	-3.026354	-1.582676	-3.713763
31	6	-1.372482	-4.012477	-2.492434
32	6	-2.017325	-4.153971	0.641236
33	1	-4.999941	-2.228494	1.330918
34	1	-4.157131	-0.689696	1.552092
35	1	-3.446270	-2.186773	2.169067
36	1	-5.582220	-0.616965	-1.635446
37	1	-4.342884	0.527905	-2.159727
38	1	-4.765859	0.405709	-0.446672
39	1	-3.904036	-2.085355	-4.145627
40	1	-2.144136	-1.899113	-4.275965
41	1	-3.145215	-0.506693	-3.871107
42	1	-1.998057	-4.808038	-2.921762
43	1	-0.616460	-4.486341	-1.859271
44	1	-0.849294	-3.518217	-3.317128
45	1	-2.791433	-4.931736	0.712376
46	1	-1.837287	-3.771600	1.649877
47	1	-1.093377	-4.630546	0.302222
48	6	3.297113	0.255637	-0.056182
49	6	3.747335	-0.940244	-0.944720
50	6	3.220865	1.520963	-0.959707
51	6	4.365748	0.520147	1.045883
52	6	5.125041	-0.635629	-1.588329
53	1	3.827620	-1.858056	-0.352733
54	1	2.988915	-1.112656	-1.719010
55	6	4.588648	1.829078	-1.609153
56	1	2.452190	1.357260	-1.724765
57	1	2.889172	2.366127	-0.342154
58	6	5.741765	0.812860	0.395139
59	1	4.041588	1.372742	1.657954
60	1	4.448802	-0.347074	1.713264
61	6	6.171875	-0.397365	-0.471291
62	6	5.024660	0.625441	-2.478924
63	1	5.429936	-1.495937	-2.199945
64	6	5.639468	2.072981	-0.498724
65	1	4.500005	2.726121	-2.237054
66	1	6.483849	0.981264	1.187774
67	1	7.159217	-0.208078	-0.915041
68	1	6.266727	-1.296133	0.155562
69	1	5.995245	0.830511	-2.952391
70	1	4.296976	0.460076	-3.285195
71	1	6.618803	2.297215	-0.944436
72	1	5.351947	2.942995	0.108182
73	6	-1.587182	1.982870	0.531672
74	6	-1.866649	2.515660	-0.894523

75	6	-2.852241	2.200781	1.412233
76	6	-0.414700	2.805026	1.144583
77	6	-2.234285	4.018812	-0.847910
78	1	-0.978132	2.352690	-1.514392
79	1	-2.686854	1.944274	-1.346982
80	6	-3.218466	3.707016	1.458583
81	1	-3.689784	1.624391	0.999671
82	1	-2.671698	1.838300	2.433234
83	6	-0.778494	4.308307	1.195791
84	1	-0.201860	2.430929	2.155890
85	1	0.484983	2.633167	0.544619
86	6	-1.058048	4.820212	-0.238573
87	6	-3.498722	4.216312	0.023603
88	1	-2.430995	4.371497	-1.869334
89	6	-2.041416	4.506559	2.068964
90	1	-4.115557	3.838544	2.079222
91	1	0.061661	4.867259	1.630028
92	1	-1.302608	5.891493	-0.216777
93	1	-0.160803	4.703311	-0.861654
94	1	-3.777652	5.278874	0.050397
95	1	-4.347606	3.670219	-0.412252
96	1	-2.301068	5.572940	2.123457
97	1	-1.847372	4.167435	3.096591

TS12$^{1\text{-}Ad}$-13$^{1\text{-}Ad}$ (E = -1663.7051386 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.103314	-0.848376	0.726967
2	7	-1.530240	0.473177	0.370116
3	6	-1.203377	1.645288	1.001443
4	7	1.556529	0.730180	0.011223
5	6	-1.434265	-2.143900	2.259031
6	6	-0.247749	-1.744999	2.936855
7	6	-1.063109	-3.035285	1.216025
8	17	0.004020	-1.709476	-1.594362
9	6	0.855172	-2.456721	2.359299
10	6	0.357905	-3.235185	1.296786
11	6	1.284323	1.918625	0.457560
12	6	0.012926	2.275591	1.088498
13	1	-2.028705	2.197713	1.441944
14	6	0.155591	3.606212	1.708712
15	1	0.726620	-0.056545	1.904054
16	6	2.151112	3.181467	0.547901
17	6	1.349466	4.140917	1.387423
18	1	3.113396	2.976823	1.016776
19	1	2.360820	3.599212	-0.444210
20	6	1.916038	5.488870	1.734049
21	6	-0.937612	4.245758	2.524566
22	1	-0.608814	5.191194	2.964724
23	1	-1.258365	3.586136	3.341563
24	1	-1.824760	4.457471	1.911904
25	1	1.248983	6.066889	2.380321
26	1	2.101147	6.083483	0.827455
27	1	2.882415	5.389655	2.249172
28	6	-0.206058	-0.946523	4.215117
29	6	-2.823768	-1.816102	2.749757
30	6	-1.962614	-3.872970	0.344895
31	6	1.118775	-4.227604	0.457952
32	6	2.262003	-2.422926	2.898692
33	1	-0.426965	-1.593680	5.077248
34	1	-0.944570	-0.138260	4.210432
35	1	0.777831	-0.495766	4.374089
36	1	-2.983009	-2.268984	3.738543
37	1	-3.595630	-2.207892	2.083297
38	1	-2.985238	-0.738053	2.853781

39	1	-1.845541	-4.936140	0.598288
40	1	-1.713034	-3.753321	-0.714901
41	1	-3.016786	-3.617483	0.477910
42	1	0.860584	-5.252986	0.759681
43	1	2.200968	-4.112453	0.569949
44	1	0.873434	-4.116323	-0.602716
45	1	2.308672	-2.937477	3.868857
46	1	2.611877	-1.395984	3.054525
47	1	2.966783	-2.921445	2.227865
48	6	-2.835921	0.525173	-0.399995
49	6	-3.305106	-0.896757	-0.784795
50	6	-4.000808	1.219364	0.370973
51	6	-2.559485	1.326839	-1.708133
52	6	-4.570105	-0.841311	-1.677132
53	1	-2.497591	-1.413829	-1.307166
54	1	-3.531083	-1.458532	0.125588
55	6	-5.275098	1.273895	-0.514344
56	1	-4.206292	0.671914	1.300785
57	1	-3.740838	2.248875	0.642914
58	6	-3.832524	1.393089	-2.586458
59	1	-2.225794	2.340838	-1.446678
60	1	-1.740961	0.838325	-2.249329
61	6	-4.266272	-0.042935	-2.967410
62	6	-5.717350	-0.155924	-0.900349
63	1	-4.860686	-1.867699	-1.939720
64	6	-4.971482	2.084542	-1.798622
65	1	-6.074325	1.769487	0.053659
66	1	-3.610696	1.967016	-3.496535
67	1	-5.157012	-0.011165	-3.610441
68	1	-3.468788	-0.538070	-3.537427
69	1	-6.626669	-0.115464	-1.516082
70	1	-5.962466	-0.733642	0.002400
71	1	-5.874858	2.152333	-2.420456
72	1	-4.680903	3.112152	-1.537003
73	6	2.822690	0.383727	-0.749641
74	6	4.116675	1.192405	-0.413597
75	6	3.151333	-1.104198	-0.443847
76	6	2.533781	0.569209	-2.269339
77	6	5.320188	0.679154	-1.254337
78	1	3.994549	2.248160	-0.657370
79	1	4.345272	1.110147	0.658091
80	6	4.324017	-1.617432	-1.312144
81	1	3.410995	-1.189095	0.619287
82	1	2.269269	-1.716316	-0.633155
83	6	3.730927	0.059872	-3.111235
84	1	1.623017	0.025754	-2.528960
85	1	2.358536	1.636729	-2.469291
86	6	5.002199	0.866903	-2.757875
87	6	5.595624	-0.812006	-0.969152
88	1	6.201932	1.277836	-0.986563
89	6	3.975053	-1.440039	-2.810770
90	1	4.486086	-2.682637	-1.096505
91	1	3.494035	0.187532	-4.176265
92	1	5.851427	0.526388	-3.366508
93	1	4.849375	1.932358	-2.982567
94	1	6.447896	-1.159867	-1.569352
95	1	5.861743	-0.955723	0.087913
96	1	4.797776	-1.818069	-3.433978
97	1	3.078921	-2.022770	-3.058810

13$^{1\text{-Ad}}$ (E = -1663.7110075 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.046051	-0.820856	0.536807
2	7	-1.602211	0.642184	0.100389

3	6	-1.227401	1.880418	0.341628
4	7	1.547296	0.509048	0.161945
5	6	-1.253973	-2.079752	2.239861
6	6	-0.025532	-1.571685	2.777085
7	6	-0.936143	-3.022917	1.231687
8	17	-0.388012	-1.547625	-1.816369
9	6	1.048075	-2.224602	2.100477
10	6	0.483926	-3.100541	1.124594
11	6	1.304491	1.764212	0.594381
12	6	0.033308	2.370208	0.738837
13	1	-1.964894	2.664641	0.195133
14	6	0.200848	3.763085	1.210343
15	1	-0.168991	0.240074	1.767863
16	6	2.323583	2.832403	1.004398
17	6	1.508107	4.039367	1.378549
18	1	2.909131	2.468969	1.856060
19	1	3.038434	3.074539	0.214615
20	6	2.174539	5.304862	1.843158
21	6	-0.964436	4.687831	1.454744
22	1	-0.636678	5.637420	1.887414
23	1	-1.692267	4.236852	2.142549
24	1	-1.499413	4.918978	0.523149
25	1	1.447526	6.078821	2.108294
26	1	2.830786	5.719763	1.063913
27	1	2.805826	5.123560	2.725247
28	6	0.101296	-0.788159	4.060229
29	6	-2.604014	-1.775452	2.841798
30	6	-1.880271	-3.901862	0.454599
31	6	1.199057	-4.101413	0.252897
32	6	2.482203	-2.171362	2.570483
33	1	0.134878	-1.475395	4.918969
34	1	-0.745160	-0.110352	4.202651
35	1	1.015130	-0.187096	4.076851
36	1	-2.619459	-2.085698	3.895716
37	1	-3.407320	-2.313497	2.332272
38	1	-2.839677	-0.705892	2.812732
39	1	-1.725557	-4.953664	0.733435
40	1	-1.706496	-3.813671	-0.623017
41	1	-2.926525	-3.656085	0.652061
42	1	0.908487	-5.122519	0.536598
43	1	2.285151	-4.029513	0.353220
44	1	0.943844	-3.963744	-0.803658
45	1	2.581365	-2.728016	3.513643
46	1	2.816284	-1.146548	2.759042
47	1	3.171563	-2.623236	1.853338
48	6	-2.996700	0.541876	-0.514789
49	6	-3.472979	-0.928487	-0.590066
50	6	-4.055798	1.319353	0.331828
51	6	-2.964522	1.127109	-1.956922
52	6	-4.869353	-1.028340	-1.256030
53	1	-2.751598	-1.516658	-1.157575
54	1	-3.524006	-1.338904	0.422496
55	6	-5.454349	1.233576	-0.332690
56	1	-4.087112	0.894514	1.344602
57	1	-3.789818	2.377447	0.433609
58	6	-4.366426	1.040207	-2.608533
59	1	-2.635628	2.174956	-1.923102
60	1	-2.226808	0.568577	-2.543356
61	6	-4.805956	-0.441535	-2.686650
62	6	-5.904023	-0.242442	-0.419573
63	1	-5.158995	-2.087017	-1.305667
64	6	-5.385209	1.837347	-1.757554
65	1	-6.168652	1.805187	0.275669
66	1	-4.316999	1.465571	-3.620034

67	1	-5.789888	-0.519223	-3.170116
68	1	-4.094763	-1.013017	-3.297793
69	1	-6.899247	-0.308368	-0.880951
70	1	-5.984500	-0.673368	0.588693
71	1	-6.378338	1.803030	-2.226448
72	1	-5.088870	2.895012	-1.705852
73	6	2.855084	0.222436	-0.572170
74	6	4.150889	0.467043	0.266448
75	6	2.887996	-1.269754	-0.997592
76	6	2.895279	1.075468	-1.876492
77	6	5.416019	0.153699	-0.578370
78	1	4.229195	1.497872	0.606279
79	1	4.127868	-0.170477	1.159204
80	6	4.147857	-1.604526	-1.834821
81	1	2.873886	-1.896056	-0.101219
82	1	1.997601	-1.502200	-1.581593
83	6	4.171416	0.761490	-2.697081
84	1	1.996709	0.847203	-2.462734
85	1	2.864935	2.145663	-1.640224
86	6	5.427289	1.053396	-1.839667
87	6	5.418706	-1.330611	-1.002095
88	1	6.303525	0.367750	0.033151
89	6	4.165253	-0.729091	-3.110205
90	1	4.106780	-2.665412	-2.117189
91	1	4.181708	1.394750	-3.594631
92	1	6.336301	0.863053	-2.426853
93	1	5.448752	2.113552	-1.547723
94	1	6.319080	-1.557554	-1.589993
95	1	5.439960	-1.977980	-0.113617
96	1	5.053959	-0.958788	-3.714576
97	1	3.283904	-0.945082	-3.728706

TS13$^{1\text{-Ad}}$-14$^{1\text{-Ad}}$ (E = -1663.6976382 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.793912	0.287945	0.091183
2	7	0.158737	0.033882	-1.672126
3	6	-0.835324	-0.930060	-1.415242
4	7	-1.238393	0.730633	0.946265
5	6	2.758470	-1.023005	-0.274761
6	6	2.051944	-1.618187	0.812591
7	6	3.215341	0.252996	0.149131
8	17	0.999905	2.750314	-0.164075
9	6	2.143998	-0.733095	1.936785
10	6	2.845615	0.420370	1.525732
11	6	-2.247148	0.308252	0.206424
12	6	-2.069102	-0.630376	-0.862882
13	1	-0.744179	-1.876713	-1.951042
14	6	-3.341744	-1.313859	-1.116935
15	1	-0.081316	-1.151283	0.313942
16	6	-3.762004	0.457037	0.366851
17	6	-4.331619	-0.681959	-0.447621
18	1	-4.121695	0.449884	1.392727
19	1	-4.079005	1.415434	-0.066144
20	6	-5.814445	-0.919975	-0.492225
21	6	-3.461410	-2.479642	-2.062887
22	1	-4.495530	-2.824261	-2.151254
23	1	-2.854652	-3.329268	-1.722260
24	1	-3.106562	-2.212169	-3.067316
25	1	-6.079118	-1.751093	-1.152873
26	1	-6.347798	-0.026215	-0.848070
27	1	-6.211385	-1.147529	0.507577
28	6	1.613071	-3.060720	0.879745
29	6	3.109201	-1.751265	-1.549062
30	6	4.119184	1.201528	-0.595149

31	6	3.270771	1.595234	2.366671
32	6	1.709164	-1.115001	3.330739
33	1	2.451844	-3.697776	1.198823
34	1	1.272700	-3.424667	-0.094603
35	1	0.794808	-3.202096	1.592387
36	1	3.821993	-2.559966	-1.333118
37	1	3.578329	-1.088276	-2.279761
38	1	2.231950	-2.203301	-2.023163
39	1	5.118262	1.212224	-0.136124
40	1	3.725564	2.222893	-0.570483
41	1	4.239409	0.912379	-1.642463
42	1	4.364390	1.606474	2.476282
43	1	2.837700	1.560026	3.370218
44	1	2.973610	2.540693	1.899722
45	1	2.293314	-1.977898	3.680230
46	1	0.651881	-1.402053	3.374330
47	1	1.868671	-0.303641	4.046108
48	6	0.272512	0.519255	-3.090280
49	6	1.633529	1.224346	-3.307245
50	6	0.145676	-0.632595	-4.130084
51	6	-0.867601	1.549205	-3.347424
52	6	1.728779	1.794066	-4.744688
53	1	1.744995	2.023836	-2.570108
54	1	2.442051	0.503248	-3.145469
55	6	0.245429	-0.068222	-5.571274
56	1	0.936878	-1.375375	-3.957716
57	1	-0.819012	-1.143834	-4.018007
58	6	-0.774871	2.107914	-4.789283
59	1	-1.839833	1.063388	-3.192217
60	1	-0.777609	2.356164	-2.611806
61	6	0.588956	2.814604	-4.978932
62	6	1.607389	0.638749	-5.766358
63	1	2.700091	2.293203	-4.863854
64	6	-0.900662	0.946710	-5.805286
65	1	0.153714	-0.899330	-6.284014
66	1	-1.589745	2.827545	-4.947814
67	1	0.660316	3.233562	-5.992578
68	1	0.680901	3.650364	-4.272399
69	1	1.686323	1.026481	-6.791582
70	1	2.429198	-0.078130	-5.626663
71	1	-0.853123	1.335156	-6.832138
72	1	-1.874596	0.449178	-5.692117
73	6	-1.524017	1.479997	2.239601
74	6	-2.208055	0.530720	3.275546
75	6	-0.187237	1.935146	2.882450
76	6	-2.374553	2.764153	2.011317
77	6	-2.479793	1.282087	4.603981
78	1	-3.147324	0.123252	2.895075
79	1	-1.542333	-0.324099	3.453868
80	6	-0.418043	2.666123	4.229363
81	1	0.440054	1.055993	3.047579
82	1	0.338829	2.596488	2.193073
83	6	-2.629254	3.485687	3.360549
84	1	-1.829963	3.419227	1.320212
85	1	-3.338346	2.533807	1.553409
86	6	-3.363269	2.525062	4.329670
87	6	-1.138173	1.730546	5.226293
88	1	-3.001788	0.603890	5.292857
89	6	-1.284901	3.922953	3.984707
90	1	0.557736	2.964179	4.636972
91	1	-3.255693	4.368401	3.173539
92	1	-3.583499	3.041187	5.274248
93	1	-4.327515	2.216975	3.899408
94	1	-1.315042	2.251284	6.177709

95	1	-0.513991	0.853300	5.447705
96	1	-1.460036	4.453816	4.930863
97	1	-0.764404	4.616978	3.311269

14$^{1\text{-Ad}}$ (E = -1663.7400535 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	0.086409	-1.036141	0.219812
2	7	-1.570127	-0.211216	0.361093
3	6	-1.194312	0.501305	1.610259
4	7	1.244116	0.670699	0.198509
5	6	-0.765328	-2.929913	1.503399
6	6	0.327771	-2.385034	2.243298
7	6	-0.241356	-3.483541	0.310457
8	17	0.093045	-1.335371	-2.132718
9	6	1.538150	-2.680627	1.538360
10	6	1.188273	-3.338414	0.339625
11	6	0.623179	1.828211	0.656231
12	6	-0.546455	1.811230	1.374624
13	1	-2.009256	0.502461	2.335885
14	6	-0.956882	3.160572	1.766673
15	1	-0.412655	-0.131073	2.096457
16	6	0.967443	3.306335	0.457857
17	6	-0.076353	4.052406	1.255243
18	1	1.979316	3.592258	0.748060
19	1	0.861082	3.570426	-0.600117
20	6	-0.043408	5.551042	1.376847
21	6	-2.155931	3.446286	2.635321
22	1	-2.207898	4.503737	2.911624
23	1	-2.120861	2.860775	3.564263
24	1	-3.095595	3.190851	2.128436
25	1	-0.876325	5.928971	1.979003
26	1	-0.102051	6.037166	0.391769
27	1	0.889415	5.898293	1.845546
28	6	0.279825	-1.905359	3.676343
29	6	-2.179906	-3.044281	2.013308
30	6	-0.990437	-4.272481	-0.731731
31	6	2.109991	-3.927115	-0.695636
32	6	2.907560	-2.528382	2.156473
33	1	0.550078	-2.727599	4.355547
34	1	-0.719921	-1.564707	3.963002
35	1	0.983949	-1.086759	3.863975
36	1	-2.249686	-3.853428	2.754467
37	1	-2.882465	-3.273383	1.208394
38	1	-2.521935	-2.124355	2.497878
39	1	-0.798025	-5.348020	-0.606534
40	1	-0.680128	-3.990402	-1.742648
41	1	-2.070783	-4.118304	-0.660028
42	1	2.033256	-5.023451	-0.696473
43	1	3.155700	-3.667839	-0.507844
44	1	1.849746	-3.577843	-1.701629
45	1	2.980318	-3.165018	3.049845
46	1	3.115597	-1.500618	2.474552
47	1	3.703406	-2.837526	1.473588
48	6	-2.865594	0.091426	-0.306311
49	6	-3.289030	-1.119961	-1.182986
50	6	-4.011997	0.366073	0.710281
51	6	-2.704738	1.338681	-1.229417
52	6	-4.609766	-0.820175	-1.933371
53	1	-2.491361	-1.347357	-1.894410
54	1	-3.419502	-1.998336	-0.538662
55	6	-5.338009	0.666921	-0.035876

56	1	-4.137792	-0.506087	1.366999
57	1	-3.762869	1.225265	1.343597
58	6	-4.031824	1.637141	-1.970322
59	1	-2.404041	2.204193	-0.626398
60	1	-1.898435	1.139999	-1.944950
61	6	-4.422423	0.419246	-2.841796
62	6	-5.735529	-0.545941	-0.909091
63	1	-4.872689	-1.691438	-2.548613
64	6	-5.151092	1.912474	-0.936805
65	1	-6.123951	0.862930	0.706389
66	1	-3.894332	2.520136	-2.609319
67	1	-5.351801	0.628568	-3.389871
68	1	-3.640217	0.224294	-3.587936
69	1	-6.682307	-0.341889	-1.428174
70	1	-5.896266	-1.431047	-0.277072
71	1	-6.093146	2.146360	-1.451876
72	1	-4.891960	2.787441	-0.323499
73	6	2.655624	0.794706	-0.346317
74	6	3.636007	1.339052	0.739071
75	6	3.186917	-0.603912	-0.763178
76	6	2.715882	1.682398	-1.628676
77	6	5.076818	1.445663	0.177120
78	1	3.318533	2.318301	1.105207
79	1	3.616010	0.656710	1.599758
80	6	4.637625	-0.536079	-1.304955
81	1	3.159123	-1.264126	0.102604
82	1	2.536051	-1.026412	-1.531661
83	6	4.168506	1.774069	-2.164766
84	1	2.052629	1.242911	-2.384319
85	1	2.361305	2.693833	-1.430383
86	6	5.085079	2.369199	-1.066640
87	6	5.579601	0.039931	-0.223347
88	1	5.730954	1.867164	0.952875
89	6	4.675618	0.368755	-2.556851
90	1	4.958031	-1.552582	-1.573015
91	1	4.177190	2.430400	-3.045820
92	1	6.110408	2.472957	-1.448061
93	1	4.740111	3.376663	-0.791619
94	1	6.607742	0.097988	-0.607275
95	1	5.598958	-0.618064	0.657066
96	1	5.699159	0.428740	-2.952734
97	1	4.042494	-0.053539	-3.349039

18$^{1\text{-Ad}}$ (E = -1156.3621902 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	22	-0.218821	-0.037681	-0.398422
2	7	-0.753621	1.563763	-0.264842
3	6	-1.921453	-1.031960	0.907801
4	6	-0.725704	-1.050376	1.683824
5	6	-1.736459	-1.918269	-0.190872
6	17	0.048800	-0.453530	-2.720849
7	6	0.169283	-2.000453	1.091942
8	6	-0.451634	-2.530902	-0.064617
9	6	-0.526880	-0.365099	3.015569
10	6	-3.207715	-0.336179	1.277796
11	6	-2.759287	-2.261864	-1.245474
12	6	0.091610	-3.590316	-0.989280
13	6	1.487567	-2.439313	1.680449
14	1	-0.880911	-1.001393	3.839968
15	1	-1.077105	0.579632	3.067316
16	1	0.529332	-0.146101	3.208712
17	1	-3.826359	-0.988288	1.911888
18	1	-3.798698	-0.078311	0.393701
19	1	-3.021817	0.588163	1.831801

20	1	-3.315081	-3.168334	-0.963615
21	1	-2.285324	-2.445999	-2.214377
22	1	-3.488186	-1.456455	-1.380951
23	1	-0.464918	-4.531412	-0.876695
24	1	1.144909	-3.806128	-0.781590
25	1	0.013427	-3.279901	-2.037610
26	1	1.332396	-3.245781	2.411184
27	1	1.995378	-1.621701	2.203071
28	1	2.171862	-2.820299	0.915336
29	7	1.920026	0.329738	0.029270
30	6	2.888054	-0.287749	-0.687645
31	6	2.294467	1.214691	0.983107
32	6	4.246468	-0.048200	-0.475417
33	1	2.548096	-0.970233	-1.456942
34	6	3.631640	1.498748	1.260005
35	1	1.489737	1.707323	1.513555
36	6	4.629458	0.857919	0.517945
37	1	4.982394	-0.561975	-1.082014
38	1	3.879723	2.214803	2.034239
39	1	5.677386	1.063870	0.705415
40	6	-1.282673	2.907071	-0.241812
41	6	-1.433003	3.439617	1.215081
42	6	-0.318809	3.859575	-1.015936
43	6	-2.678608	2.957690	-0.934388
44	6	-1.985421	4.886685	1.211252
45	1	-2.106404	2.776051	1.773644
46	1	-0.452881	3.407626	1.711883
47	6	-0.870024	5.306310	-1.019883
48	1	0.671369	3.827818	-0.540985
49	1	-0.202905	3.484503	-2.040350
50	6	-3.231027	4.404211	-0.937757
51	1	-2.576357	2.579704	-1.959644
52	1	-3.366091	2.287483	-0.402440
53	6	-3.371778	4.907026	0.520612
54	6	-1.011481	5.809839	0.437943
55	1	-2.084726	5.240422	2.247034
56	6	-2.256706	5.328216	-1.709250
57	1	-0.175669	5.957453	-1.568861
58	1	-4.214552	4.415161	-1.427474
59	1	-3.781209	5.926970	0.530239
60	1	-4.076988	4.269559	1.072689
61	1	-1.386503	6.842957	0.445973
62	1	-0.028692	5.818226	0.930918
63	1	-2.649475	6.354563	-1.733186
64	1	-2.164032	4.991027	-2.750975

17$^{\mathbf{1\text{-}Ad}}$ (E = -755.667076 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.249133	0.708974	0.069182
2	6	0.060997	0.263766	0.105792
3	6	-1.117243	1.195434	0.151040
4	6	-2.321304	0.374760	0.338151
5	6	-0.518361	-1.154909	0.156711
6	6	-2.000525	-0.937157	0.356943
7	1	-0.329579	-1.694775	-0.778114
8	1	-0.076366	-1.756771	0.957478
9	6	-2.908848	-2.121888	0.522644
10	6	-3.685590	0.995194	0.476451
11	1	-4.468079	0.245196	0.619548
12	1	-3.938424	1.581850	-0.416946
13	1	-3.714917	1.683760	1.331396
14	1	-3.955928	-1.833982	0.650660
15	1	-2.611809	-2.719273	1.396437
16	1	-2.843823	-2.786706	-0.350641

17	6	-1.044467	2.529572	0.036809
18	1	-1.926406	3.157544	0.079866
19	1	-0.083270	3.009001	-0.102482
20	6	2.488134	-0.100445	0.069081
21	6	2.531622	-1.233552	-0.996165
22	6	3.643115	0.895295	-0.239824
23	6	2.742179	-0.711567	1.479073
24	6	3.908210	-1.947515	-0.961382
25	1	1.746769	-1.973448	-0.808107
26	1	2.348198	-0.802129	-1.990050
27	6	5.016793	0.188577	-0.204479
28	1	3.465781	1.345084	-1.226153
29	1	3.606160	1.708829	0.496016
30	6	4.112985	-1.434015	1.508638
31	1	2.716609	0.092527	2.226318
32	1	1.942948	-1.419759	1.732785
33	6	4.128657	-2.559649	0.444738
34	6	5.038636	-0.936516	-1.266933
35	1	3.913235	-2.746613	-1.715209
36	6	5.242768	-0.421013	1.200975
37	1	5.807999	0.918723	-0.421724
38	1	4.266860	-1.867326	2.506284
39	1	5.089017	-3.092453	0.476191
40	1	3.342835	-3.297300	0.662906
41	1	6.011692	-1.447178	-1.260385
42	1	4.902621	-0.510184	-2.270660
43	1	6.219246	-0.923311	1.243564
44	1	5.253126	0.373925	1.959507

***t*BuNC** (E = -250.6583893 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.737505	-0.430693	1.404646
2	6	0.263125	-0.000022	0.000011
3	1	0.375421	0.266012	2.166704
4	1	0.374586	-1.434410	1.645664
5	1	1.831820	-0.439411	1.431318
6	6	0.736938	-1.001115	-1.075554
7	6	0.737059	1.431851	-0.329658
8	1	0.373669	-0.707783	-2.065118
9	1	1.831264	-1.019829	-1.096823
10	1	0.374878	-2.009443	-0.853247
11	1	1.831374	1.459241	-0.336595
12	1	0.373986	1.743484	-1.313691
13	1	0.374919	2.142414	0.419470
14	7	-1.198682	-0.000043	0.000457
15	6	-2.367404	0.000005	0.000691

MeNC (E = -132.7370076 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	0.318638	0.000007	0.464006
2	6	1.486403	-0.000005	0.463974
3	6	-1.116184	0.000000	0.463782
4	1	-1.483851	0.930378	0.862416
5	1	-1.483826	-0.844873	-0.556668
6	1	-1.484098	-0.085526	1.085397

EtNC (E = -172.0442071 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	0.308823	0.020652	-0.009177
2	6	1.477067	0.032425	-0.014352
3	6	-1.134586	-0.016348	0.007225
4	1	-1.482227	0.839779	0.593959
5	1	-1.482143	0.120335	-1.021650

6	6	-1.662525	-1.332305	0.593204
7	1	-1.322787	-1.464168	1.624684
8	1	-2.756964	-1.318581	0.587035
9	1	-1.322701	-2.187143	0.001147

ArNC (E = -403.0543015 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	0.229094	-0.000343	-0.000107
2	6	1.401398	-0.000401	-0.000233
3	6	-1.167283	-0.000261	-0.000031
4	6	-1.843059	0.086721	1.237835
5	6	-1.843156	-0.087166	-1.237836
6	6	-3.244288	0.084845	1.210076
7	6	-3.244395	-0.085135	-1.209977
8	6	-3.939639	-0.000107	0.000074
9	1	-3.788608	0.150639	2.146375
10	1	-3.788803	-0.150867	-2.146231
11	1	-5.024663	-0.000046	0.000123
12	6	-1.078717	0.177807	2.535320
13	1	-0.430330	-0.694774	2.681748
14	1	-0.430153	1.062159	2.558308
15	1	-1.764396	0.237527	3.384370
16	6	-1.078890	-0.178339	-2.535364
17	1	-0.430390	0.694155	-2.681804
18	1	-0.430440	-1.062772	-2.558382
19	1	-1.764588	-0.237962	-3.384397

1-AdNC (E = -482.8664564 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	0.257579	-0.027219	-0.056585
2	6	1.424721	-0.039054	-0.123086
3	6	-1.188684	-0.011404	0.026632
4	6	-1.773992	-1.022005	-0.997342
5	6	-1.625317	-0.412173	1.462197
6	6	-1.706951	1.416857	-0.295807
7	6	-3.319755	-1.001584	-0.904722
8	1	-1.442956	-0.748718	-2.006900
9	1	-1.386537	-2.024985	-0.779391
10	6	-3.171607	-0.394231	1.546972
11	1	-1.236575	-1.411453	1.694036
12	1	-1.189981	0.290549	2.183433
13	6	-3.252986	1.429068	-0.205253
14	1	-1.271946	2.129810	0.415482
15	1	-1.375794	1.704792	-1.301260
16	6	-3.838432	0.422149	-1.226611
17	6	-3.757177	-1.401859	0.526360
18	1	-3.726547	-1.717205	-1.630480
19	6	-3.690577	1.029646	1.226000
20	1	-3.473143	-0.678343	2.563176
21	1	-3.612239	2.440429	-0.434192
22	1	-4.935556	0.439815	-1.183228
23	1	-3.549662	0.707826	-2.247358
24	1	-4.853169	-1.409952	0.594627
25	1	-3.410494	-2.418458	0.757217
26	1	-4.785667	1.055569	1.303764
27	1	-3.296664	1.749442	1.956541

Pyridine (E = -248.2546674 a.u.)

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	6	-1.149804	-0.722726	-0.000195
2	6	-1.201845	0.675263	-0.000127
3	6	0.000234	1.389949	0.000097
4	6	1.202071	0.674860	0.000208
5	6	1.149561	-0.723113	0.000086
6	7	-0.000241	-1.427760	-0.000089
7	1	0.000410	2.474941	0.000168
8	1	-2.064633	-1.307919	-0.000368
9	1	-2.158930	1.184850	-0.000233
10	1	2.159332	1.184115	0.000383
11	1	2.064191	-1.308614	0.000202