SUPPORTING INFORMATION

A Theoretical Study of Reaction Pathways to Borazine

W. Rodger Nutt* and Michael L. McKee

Contributions from the Departments of Chemistry, Martin Chemical
Laboratory, Davidson College, Davidson, North Carolina 28035 and

Auburn University, Auburn, Alabama 36849

ronutt@davidson.edu

Table S1. Total Energies (hartrees), Zero-Point Energies (kcal/mol), Thermal Corrections (kcal/mol) and Entropies (cal/mol-K)

	pg ^a	B3LYP/ 6-31G(d)	B3LYP/ 6-311+G(2d,p) ^b	ZPE ^c (NIF)	TC ^d	S ^e
H ₂	D _{∞h}	-1.17548	-1.17957	6.4(0)	2.0	30.9
NH ₃	C _{3v}	-56.54795	-56.58369	21.7(0)	2.3	46.0
BH ₃	D _{3h}	-26.61301	-26.62230	16.6(0)	2.4	44.9
B ₂ H ₆	D _{2h}	-53.28831	-53.30742	39.9(0)	2.8	55.3
H ₂ BNH ₂	C _{2v}	-82.03932	-82.07610	30.2(0)	2.6	54.7
H ₃ BNH ₃	C _{3v}	-83.21320	-83.25224	44.1(0)	3.0	57.4
TS1	C _s	-109.83473	-109.88225	63.4(1)	4.2	71.4
1	C _s	-109.85640	-109.90283	64.5(0)	4.4	72.8
TS2	C ₁	-109.81316	-109.86363	60.2(1)	3.9	69.4
TS3	C _s	-138.58861	-138.65950	52.7(1)	4.7	80.5
2	C _s	-138.59370	-138.66119	55.4(0)	3.8	68.4
TS4	C _s	-83.14630	-83.19072	39.8(1)	2.8	58.4
TS5	C _s	-166.40047	-166.47990	86.6(1)	6.6	92.9
TS6	C ₂	-166.36103	-166.44086	82.6(1)	5.2	79.5
TS7	C ₂	-166.36580	-166.44331	84.5(1)	5.1	80.7
3	C _s	-166.43166	-166.50686	89.3(0)	5.3	80.8
TS8	C _s	-166.39417	-166.47267	85.1(1)	5.8	80.0
A1	C _{2v}	-108.70300	-108.74466	52.8(0)	3.1	61.4
TSA1	C _s	-165.22087	-165.29537	73.6(1)	5.7	85.5
TSA2	C ₁	-165.22502	-165.30053	73.9(1)	5.7	86.9
A2	C ₁	-165.27677	-165.34553	78.2(0)	4.4	74.5
TSA3	C _s	-165.22629	-165.29865	72.7(1)	4.7	77.8
TSA4	C _s	-165.24052	-165.31295	75.1(1)	5.1	80.5
A3	C _s	-165.25589	-165.32687	77.3(0)	4.9	77.8
TSA5	C ₁	-165.25304	-165.32433	77.4(1)	4.2	72.8
TSB1	C ₁	-164.06430	-164.13496	61.9(1)	4.3	73.1
B1	C ₁	-164.08908	-164.15814	63.2(0)	4.4	75.8
TSB2	C _s	-164.08740	-164.15587	63.2(1)	3.8	70.1
TSB3	C ₁	-164.03663	-164.11037	59.8(1)	4.2	72.1
B2	C _s	-162.92449	-162.98925	50.0(0)	3.9	70.1
TSC1	C ₁	-244.95368	-245.04890	82.3(1)	5.4	82.8
C1	C ₁	-244.98780	-245.07898	85.6(0)	4.7	77.8
TSC2	C ₁	-244.93917	-245.03297	81.5(1)	4.3	75.1
TSC3	C ₁	-244.91483	-245.01185	81.4(1)	4.6	77.1
TSC4	C ₁	-244.90125	-244.99740	80.2(1)	4.8	78.5
C2	C ₁	-243.80453	-243.89406	71.3(0)	4.5	76.1
TSC5	C ₁	-243.75394	-243.84768	67.5(1)	4.2	74.8
C3	D _{3h}	-242.67023	-242.75565	58.6(0)	3.9	68.8
TSC6	C ₁	-244.98399	-245.07481	85.5(1)	4.3	75.1
C4	C ₁	-244.98451	-245.07536	85.6(0)	4.7	78.8
TSD1	C ₁	-244.95071	-245.04927	81.8(1)	5.7	85.5
D1	C ₁	-244.97669	-245.07302	83.9(0)	5.2	81.5
TSD2	C ₁	-244.97579	-245.07140	83.2(1)	5.1	80.8
D2	C ₁	-244.97757	-245.07326	83.5(0)	5.6	85.2
TSD3	C ₁	-244.92034	-245.02080	79.8(1)	5.5	84.9

D3	C ₁	-243.80947	-243.90140	69.9(0)	5.3	82.8
TSD4	C _s	-243.80719	-243.89998	69.5(1)	5.0	80.8
D4	C ₁	-243.80947	-243.90140	69.9(0)	5.3	82.8
TSD5	C ₁	-243.79519	-243.88745	69.1(1)	5.0	80.8
D5	C ₁	-243.80303	-243.89485	70.0(0)	5.3	83.9
TSD6	C ₁	-243.79038	-243.88137	69.5(1)	4.6	76.8
TSD7	C ₁	-243.78132	-243.87248	69.7(1)	4.6	77.8
TSD8	C ₁	-244.91606	-245.01677	80.0(1)	5.5	84.9
D6	C ₁	-243.80303	-243.89485	70.0(0)	5.3	83.9
TSD9	C _s	-243.80190	-243.89385	69.9(1)	4.9	80.5
TSE1	C ₁	-246.11469	-246.21609	94.8(1)	6.3	90.6
E1	C ₁	-246.15098	-246.25000	97.2(0)	6.0	90.2
TSE2	C ₁	-246.14762	-246.24640	97.1(1)	5.5	84.2
E2	C ₁	-246.14959	-246.24790	97.4(0)	5.8	86.9
TSE3	C ₁	-246.14919	-246.24747	97.3(1)	5.2	81.8
E3	C ₁	-246.14928	-246.24765	97.4(0)	5.7	85.5
TSE4	C ₁	-246.10466	-246.20195	97.0(1)	5.3	81.5
E4	C _{3v}	-246.18373	-246.27638	100.2(0)	4.8	76.8
TSE5	C _s	-246.17833	-246.27098	100.1(1)	4.6	78.1
E5	C ₂	-246.18425	-246.27710	100.2(0)	4.9	78.8
TSE6	C ₁	-246.08865	-246.18733	95.3(1)	4.8	79.5
TSE7	C ₁	-246.09186	-246.19097	95.0(1)	4.9	79.5
TSE8	C _s	-246.18362	-246.27626	100.1(1)	4.5	76.5
TSF1	C ₁	-246.15076	-246.24971	97.0(1)	5.6	86.2
F1	C ₁	-246.15456	-246.25262	97.5(0)	5.8	86.9
TSF2	C ₁	-246.07507	-246.17963	92.3(1)	6.2	90.9
TSF3	C ₁	-246.05795	-246.17898	92.3(1)	6.2	91.2
F2,F5	C ₁	-244.96311	-245.05973	82.7(0)	6.0	89.9
TSF4	C ₁	-244.96268	-245.05905	82.6(1)	5.5	85.5
F3	C ₁	-244.96391	-245.06031	82.7(0)	6.0	90.2
TSF5	C ₁	-244.96192	-245.05844	82.6(1)	5.5	85.2
F4	C ₁	-244.96360	-245.05931	82.9(0)	5.8	87.5
TSF6	C ₁	-244.96104	-245.05679	82.8(1)	5.3	85.2
TSF7	C ₁	-244.96085	-245.05613	83.0(1)	5.2	82.5
F6	C ₁	-244.96193	-245.05777	82.8(0)	5.9	88.9
TSF8	C ₁	-244.96027	-245.05609	82.5(1)	5.5	85.2
TSF9	C ₁	-244.95999	-245.05564	82.9(1)	5.2	82.8
F7	C ₁	-244.96122	-245.05654	83.2(0)	5.6	85.5
TSF10	C ₁	-244.93607	-245.03077	83.7(1)	4.5	76.8
TSF11	C ₁	-244.90442	-245.00540	79.3(1)	5.6	85.5
F8	C ₁	-244.96493	-245.06035	82.9(0)	5.9	88.2
TSF12	C ₁	-244.96113	-245.05788	82.6(1)	5.4	84.5
TSF13	C ₁	-244.90596	-245.00709	79.0(1)	5.6	86.2
F9	C _s	-243.81297	-243.90579	69.7(0)	5.4	83.9
TSF14	C ₁	-243.79580	-243.88907	69.0(1)	5.0	81.8
TSG1	C ₁	-328.17462	-328.30667	128.4(1)	8.1	106.7
G1	C ₁	-328.21035	-328.33954	130.8(0)	7.9	107.0

^a Point Group. ^b Based on structure optimized at B3LYP/6-31(d). ^c Zero-point energy and number of imaginary frequencies. ^d Thermal corrections. ^e Entropies.

Table S2. Some Barrier Enthalpies (kcal/mol) and Free Energies^a
(kcal/mol) at B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d) Level and
573.15 K

	ΔH	ΔG
H ₃ BNH ₃	0.0	0.0
TS4	34.0	33.5
TS5	15.5	26.6
A1 + NH ₃	0.0	0.0
TSA1	21.1	32.1
TSA2	18.1	28.4
TSA4	10.6	24.9
A2	0.0	0.0
TSA3	24.8	22.2
2 H ₂ BNH ₂	0.0	0.0
TSB1	11.8	32.0
B1	0.0	0.0
TSB3	26.0	27.9
B2 + H ₂ BNH ₂	0.0	0.0
TSC1	11.5	35.3
C1	0.0	0.0
TSC2	24.1	25.9
TSC3	37.6	38.2
C2	0.0	0.0
TSC5	24.8	25.8
C4	0.0	0.0
TSC4	43.6	43.8
B2 + H ₂ BNH ₂	0.0	0.0
TSD1	11.1	33.3
D2	0.0	0.0
TSD3	28.9	29.2
TSD8	31.6	32.0
D4	0.0	0.0
TSD5	7.2	8.9
D5	0.0	0.0
TSD6	6.7	11.5
TSD7	12.4	16.8
C2	0.0	0.0
TSD6	6.3	5.8
TSD7	12.0	11.1

B1 + H₂BNH₂	0.0	0.0
TSE1	12.3	34.1
E1	0.0	0.0
TSE2	1.1	5.2
E3	0.0	0.0
TSE4	27.3	30.4
E4	0.0	0.0
TSE5	2.5	2.6
E5	0.0	0.0
TSE6	51.2	51.0
TSE7	48.8	48.4
E1	0.0	0.0
TSF3	40.0	39.2
F1	0.0	0.0
TSF2	41.2	38.5
F7	0.0	0.0
TSF10	14.8	21.0
F6	0.0	0.0
TSF11	28.8	31.0
F8	0.0	0.0
TSF13	29.0	30.4
F9	0.0	0.0
TSF14	9.0	10.7
E1 + H₂BNH₂	0.0	0.0
TSG1	13.0	34.4

^a The relative enthalpies and free energies are relative to the preceding zero value.

Table S3. Dihedral Angles (Degrees) for Some Conformers of 1,3.5-Triaza-2,4,6-triborahexa-1,5-diene

Conformer ^a	N(1)B(2)N(3)B(4)	B(2)N(3)B(4)N(5)	N(3)B(4)N(5)B(6)
A (F4)	83.7	-81.3	105.8
B (F3)	76.5	169.1	80.6
D (F8)	-79.1	73.1	83.4
E (F5)	-79.7	-149.2	93.4
F (F6)	-66.1	-53.0	103.2
J (F7)	-7.2	69.4	40.0

^a Gung, B. W.; Zhu, Z.; Fouch, R. A. *J. Am Chem. Soc.* **1995**, *117*, 1873.

Table S4. Some Enthalpy and Free Energy Barriers (kcal/mol) Arranged in Order of Increasing Magnitude

ΔH (298.15 K)		ΔH (573.15 K)		ΔG (298.15 K)		ΔG (573.15 K)	
3.0	TSE5	2.5	TSE5	2.8	TSE5	2.6	TSE5
7.2	TSD6	6.7	TSD6	8.2	TSD5	8.9	TSD5
7.6	TSD5	7.2	TSD5	9.4	TSD6	10.7	TSF14
9.4	TSF14	9.0	TSF14	10.0	TSF14	11.5	TSD6
10.9	TSD1	11.1	TSD1	14.8	TSD7	16.8	TSD7
11.3	TSC1	11.5	TSC1	18.2	TSF10	21.0	TSF10
11.4	TSB1	11.8	TSB1	22.2	TSB1	25.8	TSC5
12.1	TSE1	12.3	TSE1	22.6	TSD1	25.9	TSC2
12.7	TSG1	12.4	TSD7	23.6	TSE1	27.9	TSB3
13.0	TSD7	13.0	TSG1	23.8	TSC1	29.2	TSD3
15.5	TSF10	14.8	TSF10	24.0	TSG1	30.4	TSE4
24.3	TSC2	24.1	TSC2	25.1	TSC2	30.4	TSF13
25.1	TSC5	24.8	TSC5	25.4	TSC5	31.0	TSF11
26.3	TSB3	26.0	TSB3	27.1	TSB3	32.0	TSB1
27.8	TSE4	27.3	TSE4	29.0	TSE4	32.0	TSD8
29.1	TSD3	28.8	TSF11	29.1	TSD3	33.3	TSD1
29.1	TSF11	28.9	TSD3	29.8	TSF13	34.1	TSE1
29.3	TSF13	29.0	TSF13	30.0	TSF11	34.4	TSG1
31.8	TSD8	31.6	TSD8	31.9	TSD8	35.3	TSC1
37.8	TSC3	37.6	TSC3	38.0	TSC3	38.2	TSC3
39.9	TSF3	40.0	TSF3	39.6	TSF3	38.5	TSF2
41.1	TSF2	41.2	TSF2	39.8	TSF2	39.2	TSF3
43.6	TSC4	43.6	TSC4	43.7	TSC4	43.8	TSC4
48.8	TSE7	48.8	TSE7	48.6	TSE7	48.4	TSE7
51.3	TSE6	51.2	TSE6	51.1	TSE6	51.0	TSE6

Table S5. Cartesian Coordinates of Geometries Optimized at the B3LYP/6-31G(d) Level

TS1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.452538	-0.806082	0.000000
2	5	0	0.000000	0.713961	0.000000
3	5	0	-1.842751	0.338186	0.000000
4	1	0	-2.368791	0.052276	1.038419
5	1	0	-0.750566	-0.365005	0.000000
6	1	0	-1.423941	1.496440	0.000000
7	1	0	-2.368791	0.052276	-1.038419
8	1	0	0.377985	1.135446	-1.048944
9	1	0	0.377985	1.135446	1.048944
10	1	0	1.428510	-1.404926	-0.824545
11	1	0	2.345090	-0.315189	0.000000
12	1	0	1.428510	-1.404926	0.824545

1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.121652	-0.655749	0.818862
2	7	0	1.192702	-0.047640	0.000000
3	1	0	2.105678	0.410139	0.000000
4	5	0	0.000000	1.035456	0.000000
5	1	0	0.050548	1.654731	-1.026779
6	1	0	0.050548	1.654731	1.026779
7	1	0	-0.953990	-1.307209	1.026364
8	5	0	-1.427951	-0.876065	0.000000
9	1	0	-2.618022	-0.718089	0.000000
10	1	0	-0.953990	-1.307209	-1.026364
11	1	0	-1.133238	0.460929	0.000000
12	1	0	1.121652	-0.655749	-0.818862

TS2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.756715	0.883272	-0.007151
2	1	0	0.937615	1.449306	-1.042385
3	1	0	0.699546	1.467623	1.028783
4	7	0	1.055434	-0.568832	0.019333
5	1	0	1.323896	-0.977838	0.909088
6	1	0	1.625995	-0.940975	-0.733715
7	5	0	-1.735179	-0.012581	0.037843
8	1	0	-0.944366	0.880961	-0.300408
9	1	0	-1.762116	-0.217815	1.217320
10	1	0	-2.774785	0.029923	-0.560139
11	1	0	-0.384152	-0.947567	-0.259255
12	1	0	-1.217354	-1.115247	-0.548081

2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.888976	0.154587	0.819000
2	7	0	-1.313232	-0.004698	0.000000
3	1	0	-1.888976	0.154587	-0.819000
4	5	0	0.000000	0.710061	0.000000
5	1	0	0.281877	1.304473	1.022532
6	1	0	0.281877	1.304473	-1.022532
7	7	0	1.173556	-0.559078	0.000000
8	1	0	1.026455	-1.147836	0.820200
9	1	0	2.139023	-0.226322	0.000000
10	1	0	1.026455	-1.147836	-0.820200

TS3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-2.083103	-1.049217	0.000000
2	7	0	-1.166748	-1.493146	0.000000
3	5	0	0.000000	1.027336	0.000000
4	7	0	1.396976	0.939469	0.000000
5	1	0	-1.138675	-2.100587	0.817475
6	1	0	-1.138675	-2.100587	-0.817475
7	1	0	-0.571067	1.147990	1.046447
8	1	0	-0.571067	1.147990	-1.046447
9	1	0	1.945495	0.846736	0.843348
10	1	0	1.945495	0.846736	-0.843348

TS4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.298388	0.988650	0.000000
2	5	0	-0.068622	0.820637	0.000000
3	1	0	-0.394168	1.320952	1.037595
4	1	0	-0.394168	1.320952	-1.037595
5	1	0	-0.382154	-1.224931	-0.841204
6	7	0	-0.068622	-0.758979	0.000000
7	1	0	-0.382154	-1.224931	0.841204
8	1	0	1.077714	0.028977	0.000000

TS5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.698854	-2.056358	0.000000

2	1	0	-0.113282	-1.877168	0.817721
3	1	0	-0.113282	-1.877168	-0.817721
4	1	0	-0.981809	-3.036369	0.000000
5	5	0	-1.979746	-1.046007	0.000000
6	1	0	-2.584256	-1.241515	1.024834
7	1	0	-2.584256	-1.241515	-1.024834
8	1	0	-1.499320	0.096706	0.000000
9	1	0	-0.497724	1.867481	0.000000
10	5	0	0.000000	0.779876	0.000000
11	1	0	0.358533	0.289608	1.038600
12	1	0	0.358533	0.289608	-1.038600
13	7	0	2.175254	2.155447	0.000000
14	1	0	2.032931	2.746079	0.816604
15	1	0	2.032931	2.746079	-0.816604
16	1	0	3.154928	1.875201	0.000000

TS6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.727823	1.421779	0.167889
2	1	0	-0.968868	1.350059	1.151804
3	1	0	-1.371392	2.074986	-0.269975
4	5	0	0.727823	1.725474	-0.100597
5	1	0	1.463987	1.672773	0.846403
6	1	0	0.955852	2.561378	-0.934263
7	1	0	1.249379	0.685925	-0.972558
8	1	0	1.101744	-0.009037	-0.493648
9	7	0	0.727823	-1.421779	0.167889
10	1	0	0.968868	-1.350059	1.151804
11	1	0	1.371392	-2.074986	-0.269975
12	5	0	-0.727823	-1.725474	-0.100597
13	1	0	-1.463987	-1.672773	0.846403
14	1	0	-0.955852	-2.561378	-0.934263
15	1	0	-1.249379	-0.685925	-0.972558
16	1	0	-1.101744	0.009037	-0.493648

TS7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	2.114950	0.399146	0.000000
2	1	0	2.692148	0.394096	1.042180
3	1	0	2.692148	0.394096	-1.042180
4	7	0	0.732961	1.043351	0.000000
5	1	0	0.491058	1.590527	0.826042
6	1	0	0.000000	0.171137	0.000000
7	1	0	0.491058	1.590527	-0.826042
8	1	0	1.802434	-1.109904	0.000000
9	1	0	0.987166	-1.194391	0.000000
10	7	0	-0.796907	-1.103043	0.000000
11	1	0	-0.866101	-1.709213	-0.817260
12	1	0	-0.866101	-1.709213	0.817260
13	5	0	-2.095034	-0.086797	0.000000
14	1	0	-3.110878	-0.750691	0.000000

15	1	0	-1.982444	0.594562	-1.010630
16	1	0	-1.982444	0.594562	1.010630

3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.367206	1.386630	0.000000
2	1	0	1.568531	1.430984	0.000000
3	1	0	-0.181080	2.459252	0.000000
4	7	0	-0.094083	0.543720	1.282808
5	1	0	-1.100247	0.574000	1.458255
6	1	0	0.370575	0.909961	2.115080
7	7	0	-0.094083	0.543720	-1.282808
8	1	0	-1.100247	0.574000	-1.458255
9	1	0	0.149249	-0.482023	1.188214
10	1	0	0.149249	-0.482023	-1.188214
11	1	0	0.370575	0.909961	-2.115080
12	1	0	0.568762	-1.939748	0.998963
13	1	0	0.568762	-1.939748	-0.998963
14	5	0	-0.094083	-2.276079	0.000000
15	1	0	-1.185060	-1.701624	0.000000
16	1	0	-0.227519	-3.477828	0.000000

TS8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.370748	0.572384	0.000000
2	5	0	2.527279	1.883808	0.000000
3	1	0	2.029646	2.307984	1.020197
4	1	0	3.735742	1.866071	0.000000
5	1	0	2.029646	2.307984	-1.020197
6	5	0	-0.379283	-1.099349	0.000000
7	1	0	-0.050740	-1.654705	-1.019706
8	7	0	0.000000	0.374112	0.000000
9	1	0	-0.050740	-1.654705	1.019706
10	7	0	-2.063188	-1.256224	0.000000
11	1	0	-0.244634	0.920477	0.823941
12	1	0	1.422023	0.585726	0.000000
13	1	0	-0.244634	0.920477	-0.823941
14	1	0	-2.494852	-0.835048	-0.825038
15	1	0	-2.305014	-2.249114	0.000000
16	1	0	-2.494852	-0.835048	0.825038

A1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.000000	0.000000	0.788318
2	1	0	0.834327	0.000000	1.364016
3	1	0	-0.834327	0.000000	1.364016

4	5	0	0.000000	0.963419	-0.442031
5	1	0	-1.038103	1.530821	-0.611598
6	1	0	1.038103	1.530821	-0.611598
7	5	0	0.000000	-0.963419	-0.442031
8	1	0	1.038103	-1.530821	-0.611598
9	1	0	-1.038103	-1.530821	-0.611598
10	1	0	0.000000	0.000000	-1.379553

TSA1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-0.484476	-2.228362	1.042199
2	5	0	-0.789114	-1.729352	0.000000
3	1	0	-0.484476	-2.228362	-1.042199
4	7	0	-1.826286	-0.735279	0.000000
5	1	0	-2.301020	-0.444022	-0.842945
6	1	0	-2.301020	-0.444022	0.842945
7	1	0	-0.231234	0.924032	1.057008
8	5	0	0.000000	0.420007	0.000000
9	1	0	0.637117	-0.619445	0.000000
10	1	0	-0.231234	0.924032	-1.057008
11	7	0	2.114287	1.527292	0.000000
12	1	0	2.668962	1.290655	-0.820247
13	1	0	2.668962	1.290655	0.820247
14	1	0	1.987979	2.537480	0.000000

TSA2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.435545	-1.146648	-0.045642
2	7	0	-2.426842	0.001942	0.008307
3	1	0	-2.788716	0.276328	-0.903823
4	1	0	-1.914170	0.808803	0.359132
5	1	0	-3.236051	-0.124093	0.615237
6	1	0	-0.096653	-1.462726	0.964984
7	1	0	0.135353	-1.551177	-1.120359
8	7	0	1.646162	-0.313159	0.055911
9	1	0	2.295220	-0.363892	-0.724627
10	1	0	2.155847	-0.336192	0.934888
11	5	0	0.891016	1.229644	-0.031898
12	1	0	0.018274	1.107478	-0.864273
13	1	0	1.776483	1.959505	-0.406670
14	1	0	0.486369	1.449503	1.083686

A2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.745567	0.871356	0.115120

2	7	0	1.374052	-0.621687	-0.051484
3	1	0	1.345503	-0.964483	-1.012409
4	1	0	0.787091	-1.262651	0.499612
5	1	0	2.337443	-0.653272	0.280910
6	1	0	0.980332	1.193968	1.253799
7	1	0	1.262458	1.576102	-0.718879
8	7	0	-0.811159	0.712896	-0.100718
9	1	0	-1.087617	1.063344	-1.017284
10	1	0	-1.282760	1.320591	0.567885
11	5	0	-1.452359	-0.784002	0.064924
12	1	0	-1.057371	-1.437427	-0.888755
13	1	0	-2.657996	-0.676879	0.074443
14	1	0	-1.033378	-1.234527	1.125870

TSA3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.000000	1.202216	0.000000
2	5	0	1.469127	1.073858	0.000000
3	5	0	-1.250893	-0.404540	0.000000
4	7	0	-0.443406	-1.622251	0.000000
5	1	0	-1.796038	-0.126348	1.034850
6	1	0	-1.796038	-0.126348	-1.034850
7	1	0	-0.375727	1.656313	0.825797
8	1	0	-0.375727	1.656313	-0.825797
9	1	0	-0.425730	-2.196679	0.833819
10	1	0	-0.425730	-2.196679	-0.833819
11	1	0	2.038418	1.219338	-1.040977
12	1	0	1.907212	-0.554456	0.000000
13	1	0	2.038418	1.219338	1.040977
14	1	0	1.223615	-0.957141	0.000000

TSA4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.831101	1.286277	0.000000
2	5	0	2.157430	0.093908	0.000000
3	7	0	0.686629	-0.655046	0.000000
4	1	0	2.721409	-0.184962	1.028592
5	1	0	2.721409	-0.184962	-1.028592
6	1	0	0.546863	-1.225439	-0.827497
7	5	0	0.000000	0.682673	0.000000
8	1	0	0.546863	-1.225439	0.827497
9	1	0	-0.190508	1.204338	1.052112
10	1	0	-0.190508	1.204338	-1.052112
11	1	0	-2.666881	0.913550	0.000000
12	7	0	-2.243342	-0.012788	0.000000
13	1	0	-2.604955	-0.497883	-0.820482
14	1	0	-2.604955	-0.497883	0.820482

A3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.798108	2.081922	0.000000
2	7	0	1.663077	1.069188	0.000000
3	1	0	2.140324	0.701547	0.826086
4	1	0	2.140324	0.701547	-0.826086
5	5	0	0.000000	0.778378	0.000000
6	1	0	-0.373027	1.291236	-1.021508
7	1	0	-0.373027	1.291236	1.021508
8	7	0	-0.230986	-0.746775	0.000000
9	1	0	0.162454	-1.212909	0.818135
10	1	0	0.162454	-1.212909	-0.818135
11	5	0	-1.844644	-1.187866	0.000000
12	1	0	-2.317465	-0.722619	1.015001
13	1	0	-1.824094	-2.405884	0.000000
14	1	0	-2.317465	-0.722619	-1.015001

TSA5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.521059	0.674692	-0.215662
2	7	0	1.865614	-0.211048	0.227376
3	1	0	2.168120	-0.899164	-0.465758
4	1	0	1.722533	-0.696296	1.116278
5	1	0	2.637140	0.443844	0.365511
6	1	0	0.361857	1.412873	0.716480
7	1	0	0.840526	1.212136	-1.248314
8	7	0	-0.661654	-0.328922	-0.416366
9	1	0	-0.455030	-1.278908	-0.105569
10	1	0	-0.881398	-0.418143	-1.407757
11	5	0	-2.074409	0.053318	0.369229
12	1	0	-1.803011	-0.014448	1.554116
13	1	0	-2.875946	-0.794546	0.016825
14	1	0	-2.375762	1.172395	0.013288

TSB1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	0.048440	1.200193	0.750456
2	5	0	-1.347077	0.710211	-0.142474
3	1	0	-2.080435	1.133724	0.700201
4	7	0	-1.097475	-0.715776	-0.179281
5	1	0	-1.098110	1.350655	-1.121025
6	5	0	0.617494	0.114138	0.677031
7	1	0	-0.732096	-1.174778	-1.002776
8	1	0	-1.530407	-1.354502	0.474377
9	1	0	0.593728	-0.538667	1.677637
10	7	0	1.699457	0.038448	-0.241777
11	1	0	2.367371	-0.717451	-0.237619
12	1	0	1.865551	0.720382	-0.966631

B1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-2.499331	0.535084	0.370862
2	7	0	-1.633387	0.372971	-0.122438
3	5	0	-0.675439	-0.513120	0.355279
4	1	0	-0.879712	-1.204339	1.303384
5	7	0	0.644875	-0.624864	-0.338759
6	1	0	0.604158	-0.544071	-1.353444
7	1	0	1.127499	-1.492528	-0.116342
8	5	0	1.608369	0.658052	0.222099
9	1	0	2.733958	0.370867	-0.117588
10	1	0	1.452684	0.673347	1.424156
11	1	0	1.155125	1.635895	-0.333559
12	1	0	-1.439448	1.064337	-0.835980

TSB2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.678821	-1.409642	0.000000
2	5	0	1.077278	-0.092437	0.000000
3	7	0	0.000000	0.985568	0.000000
4	5	0	-1.592047	0.514945	0.000000
5	1	0	-0.307822	-1.648753	0.000000
6	1	0	1.320184	-2.189648	0.000000
7	1	0	0.150756	1.598605	0.805588
8	1	0	0.150756	1.598605	-0.805588
9	1	0	2.228344	0.229486	0.000000
10	1	0	-1.742317	-0.136779	-1.014130
11	1	0	-1.742317	-0.136779	1.014130
12	1	0	-2.235488	1.541239	0.000000

TSB3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.127366	-1.456138	-0.015842
2	7	0	-1.559713	-0.542794	0.017194
3	1	0	-2.567403	-0.561244	-0.012761
4	7	0	0.612595	0.674020	-0.004337
5	1	0	1.051506	1.579404	-0.120843
6	5	0	-0.833045	0.656854	-0.033065
7	1	0	1.241924	0.012935	1.023269
8	5	0	1.603150	-0.568917	-0.153514
9	1	0	-1.420484	1.700248	-0.078769
10	1	0	1.885880	-0.768635	1.147985
11	1	0	1.054159	-1.585357	-0.470140
12	1	0	2.661090	-0.279471	-0.630004

B2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.604389	-2.336943	0.000000
2	5	0	-0.691071	-1.562717	0.000000
3	1	0	0.440909	-1.959330	0.000000
4	7	0	-0.942506	-0.179712	0.000000
5	1	0	-1.917355	0.100557	0.000000
6	5	0	0.000000	0.932433	0.000000
7	1	0	-0.432875	2.049541	0.000000
8	7	0	1.386531	0.743437	0.000000
9	1	0	1.828104	-0.165967	0.000000
10	1	0	2.032787	1.517490	0.000000

TSC1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	0.049111	1.055549	1.662417
2	5	0	0.264087	1.504396	0.570035
3	1	0	-0.046263	2.642275	0.346656
4	5	0	1.416868	-0.532573	-0.380247
5	1	0	2.087269	-1.020347	-1.244301
6	7	0	1.258708	0.876573	-0.266674
7	7	0	0.642648	-1.387786	0.470779
8	1	0	1.665825	1.432341	-1.008892
9	1	0	0.343556	-1.058422	1.381172
10	1	0	0.783536	-2.389019	0.450336
11	5	0	-1.559507	-0.920836	-0.284118
12	1	0	-1.991526	-1.567909	0.625272
13	7	0	-1.645198	0.521345	-0.187263
14	1	0	-1.704690	1.060359	-1.042882
15	1	0	-2.220572	0.927928	0.540897
16	1	0	-1.366585	-1.408618	-1.356914

C1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	0.208839	1.166881	1.651799
2	5	0	0.364798	1.377321	0.458099
3	1	0	0.600459	2.540628	0.220635
4	5	0	1.186682	-0.922602	-0.262533
5	1	0	1.866641	-1.747003	-0.796064
6	7	0	1.408327	0.426983	-0.174178
7	7	0	-0.130547	-1.355968	0.397212
8	1	0	2.245776	0.823212	-0.580614
9	1	0	-0.103285	-1.096292	1.387511
10	1	0	-0.295088	-2.359802	0.349486
11	5	0	-1.418932	-0.580913	-0.247793
12	1	0	-2.368086	-0.800199	0.467016
13	7	0	-1.054259	0.969632	-0.237996

14	1	0	-1.044831	1.318459	-1.196011
15	1	0	-1.790244	1.489373	0.238562
16	1	0	-1.547565	-0.988813	-1.376446

TSC2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-0.019012	-0.590348	1.705590
2	5	0	-0.196349	-1.308635	0.370559
3	1	0	-0.264520	-2.445152	0.741205
4	5	0	-1.290783	0.797051	-0.232842
5	1	0	-2.250344	1.468715	-0.478554
6	7	0	-1.315683	-0.630311	-0.268399
7	7	0	-0.054870	1.315726	0.300773
8	1	0	-2.192012	-1.115835	-0.400804
9	1	0	-0.014060	0.253418	1.426078
10	1	0	-0.041314	2.298868	0.551911
11	5	0	1.344913	0.799482	-0.203639
12	1	0	2.209460	1.050797	0.606777
13	7	0	1.162084	-0.841334	-0.244317
14	1	0	1.174535	-1.142482	-1.218508
15	1	0	1.957904	-1.291894	0.205599
16	1	0	1.609746	1.165854	-1.326091

TSC3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.573825	-0.602366	1.382536
2	5	0	1.449233	-0.369340	0.043223
3	1	0	2.558128	-0.573061	-0.362479
4	5	0	-0.454841	1.469123	-0.136654
5	1	0	-0.702893	2.611949	-0.403678
6	7	0	0.961050	1.099689	0.037142
7	7	0	-1.416769	0.475032	-0.007309
8	1	0	1.666515	1.803547	-0.139550
9	1	0	-1.956317	-1.746599	-0.205173
10	1	0	-2.382205	0.740189	-0.150350
11	5	0	-1.154845	-0.999173	0.316945
12	1	0	-0.990455	-1.244537	1.499465
13	7	0	0.315835	-1.325656	-0.369584
14	1	0	0.200537	-1.254122	-1.383880
15	1	0	0.563063	-2.296866	-0.179015
16	1	0	1.251253	0.315368	1.202804

TSC4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.057285	-1.054519	-1.579160

2	5	0	-0.854296	-1.235386	-0.392441
3	1	0	-1.493787	-2.163559	0.057659
4	5	0	-0.651217	1.373071	-0.106067
5	1	0	-1.254206	2.364249	-0.390390
6	7	0	-1.428754	0.139680	0.338153
7	7	0	0.725836	1.259103	-0.150542
8	1	0	-1.342982	-0.001514	1.348079
9	1	0	1.848679	-0.066770	1.458569
10	1	0	1.253205	2.085073	-0.406074
11	5	0	1.505543	-0.008170	0.006724
12	1	0	2.607956	-0.037434	-0.467438
13	7	0	0.631529	-1.270898	0.013572
14	1	0	1.243892	-0.798764	1.194310
15	1	0	1.119542	-2.099617	-0.310918
16	1	0	-2.425443	0.230083	0.145995

C2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.110730	-1.467834	0.109237
2	1	0	0.062432	-2.629873	0.381421
3	5	0	1.295026	0.759449	-0.126635
4	1	0	2.344812	1.288267	-0.359915
5	7	0	1.271088	-0.707434	0.100169
6	7	0	0.079336	1.423116	-0.057039
7	1	0	2.149974	-1.175060	0.284356
8	1	0	-2.218175	1.309894	-0.109181
9	1	0	0.069720	2.421690	-0.217900
10	5	0	-1.242270	0.769750	0.365166
11	1	0	-1.343971	0.565419	1.561261
12	7	0	-1.165930	-0.744346	-0.310511
13	1	0	-1.169646	-0.609691	-1.325740
14	1	0	-2.004031	-1.276823	-0.081471

TSC5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.751248	-1.290531	-0.091895
2	1	0	1.295373	-2.337603	-0.293204
3	5	0	0.868955	1.220793	-0.017092
4	1	0	1.569809	2.190387	-0.087506
5	7	0	1.474307	-0.092111	0.136531
6	7	0	-0.533078	1.317919	-0.117768
7	1	0	-2.544597	0.198970	-0.524864
8	1	0	-0.932877	2.235659	-0.260522
9	5	0	-1.477414	0.189837	0.022117
10	1	0	-1.825168	0.030193	1.347088
11	7	0	-0.697370	-1.220752	-0.087216
12	1	0	-1.219813	-2.008696	-0.453271
13	1	0	-1.247165	-0.800886	1.016448
14	1	0	2.483481	-0.143916	0.169357

C3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.000000	1.410979	0.000000
2	5	0	1.256920	0.725683	0.000000
3	7	0	1.221943	-0.705489	0.000000
4	5	0	0.000000	-1.451367	0.000000
5	7	0	-1.221943	-0.705489	0.000000
6	5	0	-1.256920	0.725683	0.000000
7	1	0	-2.293345	1.324063	0.000000
8	1	0	2.293345	1.324063	0.000000
9	1	0	0.000000	-2.648127	0.000000
10	1	0	2.097807	-1.211169	0.000000
11	1	0	-2.097807	-1.211169	0.000000
12	1	0	0.000000	2.422339	0.000000

C4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.841672	-1.129549	-0.268342
2	5	0	-1.585153	0.247031	0.125833
3	7	0	-0.521322	1.374067	0.041593
4	5	0	0.838063	1.313061	-0.032819
5	7	0	1.500552	-0.090438	-0.103248
6	5	0	0.601435	-1.365607	0.330456
7	1	0	-0.834609	-1.235655	-1.284720
8	1	0	-1.432965	-1.889492	0.068573
9	1	0	-2.476199	0.439809	-0.680089
10	1	0	-2.010881	0.117484	1.255138
11	1	0	-0.916389	2.308189	0.073694
12	1	0	1.581531	2.250865	-0.075320
13	1	0	1.875173	-0.221645	-1.047179
14	1	0	2.331254	-0.092050	0.491772
15	1	0	1.110699	-2.358465	-0.142620
16	1	0	0.537757	-1.370026	1.533378

TSC6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.733510	-1.183474	-0.320844
2	5	0	-1.555586	0.058528	0.295042
3	7	0	-0.691184	1.312655	-0.008757
4	5	0	0.662532	1.395572	-0.146878
5	7	0	1.498144	0.106706	0.078511
6	5	0	0.764720	-1.355805	0.144961
7	1	0	-0.795303	-1.144773	-1.340034
8	1	0	-1.225804	-2.036390	-0.053984
9	1	0	-2.624491	0.134224	-0.278096

10	1	0	-1.679334	-0.149552	1.484405
11	1	0	-1.210072	2.173840	-0.139041
12	1	0	1.283833	2.381424	-0.423206
13	1	0	2.246588	0.081712	-0.615723
14	1	0	1.989393	0.223854	0.967726
15	1	0	1.366514	-2.091634	-0.605335
16	1	0	0.776193	-1.715385	1.295293

TSD1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.512274	-0.923097	-0.556974
2	1	0	1.215529	-1.848360	-0.827591
3	7	0	-0.783233	-1.130950	0.019371
4	1	0	-0.979162	-2.100392	0.243739
5	5	0	-1.942696	-0.274800	0.118052
6	1	0	-3.024007	-0.777000	0.265790
7	7	0	-1.861695	1.126286	0.056569
8	1	0	-2.682510	1.711251	0.089878
9	1	0	-0.994970	1.637889	-0.038699
10	5	0	1.820212	0.905349	-0.461630
11	1	0	2.585647	0.825402	-1.376256
12	1	0	1.167409	1.899908	-0.314788
13	7	0	2.019823	0.045647	0.692484
14	1	0	2.831474	-0.555940	0.749792
15	1	0	1.674235	0.314177	1.604999
16	1	0	0.633136	0.068922	-1.273075

D1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.817613	0.951496	-0.029323
2	1	0	-1.550956	1.892640	0.054347
3	7	0	0.619248	1.184153	-0.163616
4	1	0	0.859524	2.159621	-0.283193
5	5	0	1.737863	0.311291	-0.012098
6	1	0	2.832207	0.781755	0.137988
7	7	0	1.605364	-1.107101	0.020643
8	1	0	2.433297	-1.682720	0.077366
9	1	0	0.832498	-1.586776	-0.424632
10	5	0	-1.751095	-0.701689	-0.668135
11	1	0	-2.943270	-0.710551	-0.781770
12	1	0	-1.124669	-1.625551	-1.111850
13	7	0	-1.271888	-0.281882	0.786891
14	1	0	-2.004031	-0.127634	1.470693
15	1	0	-0.508831	-0.827640	1.183449
16	1	0	-1.340617	0.355168	-1.282043

TSD2

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
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Number	Number	Type	X	Y	Z
1	7	0	1.556590	-1.144289	0.047588
2	5	0	1.756942	0.254963	-0.026224
3	7	0	0.664314	1.177644	-0.193135
4	5	0	-0.744974	1.028008	0.019058
5	7	0	-1.267820	-0.174350	0.773542
6	5	0	-1.793021	-0.742158	-0.668755
7	1	0	2.348412	-1.765820	0.129367
8	1	0	0.736682	-1.598146	-0.339765
9	1	0	2.870257	0.686411	0.084924
10	1	0	0.941392	2.117866	-0.446816
11	1	0	-1.479176	1.964134	-0.051746
12	1	0	-1.429268	0.178956	-1.421843
13	1	0	-0.552269	-0.748581	1.216171
14	1	0	-2.022912	0.011525	1.425161
15	1	0	-1.186973	-1.749740	-0.943547
16	1	0	-2.992466	-0.813704	-0.668267

D2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.504648	1.240127	0.013313
2	1	0	-1.103522	2.245318	-0.213398
3	7	0	0.869021	1.128358	-0.252419
4	1	0	1.293592	1.987940	-0.582649
5	5	0	1.821417	0.046488	-0.016326
6	1	0	2.977620	0.325922	0.119823
7	7	0	1.408105	-1.289361	0.079652
8	1	0	2.079499	-2.029982	0.224417
9	1	0	0.513232	-1.612053	-0.279494
10	5	0	-2.031033	-0.814606	-0.541675
11	1	0	-2.780823	-1.536811	0.074576
12	1	0	-1.142472	-1.419444	-1.108668
13	7	0	-1.270641	0.122642	0.646569
14	1	0	-2.028245	0.474980	1.228482
15	1	0	-0.691943	-0.497559	1.215129
16	1	0	-2.591013	-0.029833	-1.271396

TSD3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.441860	1.052202	-0.114751
2	1	0	-1.074238	2.026503	-0.405939
3	7	0	0.982218	1.131081	-0.046261
4	1	0	1.344513	2.076176	-0.095332
5	5	0	2.001522	0.120808	0.111360
6	1	0	3.106114	0.455402	0.435637
7	7	0	1.757375	-1.253158	-0.102311
8	1	0	2.501215	-1.930888	-0.024049
9	1	0	0.943047	-1.609070	-0.584353
10	5	0	-2.684631	-0.512485	-0.193980
11	1	0	-3.297109	-0.077653	0.911072

12	1	0	-2.878415	-1.692812	-0.179752
13	7	0	-1.164685	-0.147209	0.208879
14	1	0	-2.279799	0.078082	0.959168
15	1	0	-0.642076	-0.918548	0.612940
16	1	0	-3.122768	0.175188	-1.064686

D3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.629311	0.997652	0.101078
2	1	0	1.302434	1.950680	0.360930
3	7	0	-0.785149	1.140373	0.010550
4	1	0	-1.100045	2.103689	0.021237
5	5	0	-1.856407	0.181299	-0.142308
6	1	0	-2.928245	0.563567	-0.518428
7	7	0	-1.702779	-1.191986	0.140052
8	1	0	-2.477571	-1.832266	0.047961
9	1	0	-0.922277	-1.581068	0.651094
10	5	0	2.675859	-0.525032	0.001824
11	1	0	3.099272	-1.611921	-0.272745
12	7	0	1.297323	-0.261245	-0.147638
13	1	0	0.722569	-1.012114	-0.520515
14	1	0	3.394285	0.339838	0.406751

TSD4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.299050	0.537977	0.000000
2	5	0	0.000000	1.171182	0.000000
3	7	0	-1.243028	0.475461	0.000000
4	5	0	-1.690011	-0.900513	0.000000
5	7	0	-0.867319	-2.042223	0.000000
6	5	0	2.545007	1.202689	0.000000
7	1	0	2.568274	2.396773	0.000000
8	1	0	3.553687	0.556014	0.000000
9	1	0	1.339905	-0.474967	0.000000
10	1	0	-0.017667	2.366639	0.000000
11	1	0	-2.028490	1.116326	0.000000
12	1	0	-2.873323	-1.093772	0.000000
13	1	0	-1.279393	-2.963455	0.000000
14	1	0	0.141109	-2.068847	0.000000

D4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	0.922114	-1.581045	0.650767
2	7	0	1.702706	-1.191993	0.139843
3	1	0	2.477489	-1.832320	0.047944
4	5	0	1.856514	0.181391	-0.142053

5	1	0	2.928402	0.563762	-0.517887
6	7	0	0.785116	1.140313	0.010636
7	1	0	1.100026	2.103638	0.021553
8	5	0	-0.629389	0.997669	0.100762
9	1	0	-1.302588	1.950647	0.360542
10	7	0	-1.297285	-0.261305	-0.147701
11	1	0	-0.722514	-1.012296	-0.520266
12	5	0	-2.675787	-0.524990	0.001984
13	1	0	-3.394138	0.340198	0.406366
14	1	0	-3.099238	-1.612045	-0.271927

TSD5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	0.442075	-1.592351	-0.267156
2	7	0	1.397796	-1.305951	-0.108429
3	1	0	2.068869	-2.058488	-0.078730
4	5	0	1.764971	0.021126	0.134696
5	1	0	2.915099	0.273898	0.355772
6	7	0	0.815583	1.130644	0.119771
7	1	0	1.244819	2.028140	0.317784
8	5	0	-0.568915	1.207141	-0.121999
9	1	0	-1.089438	2.289057	-0.093902
10	7	0	-1.391774	0.010253	-0.431092
11	1	0	-1.509307	-0.199917	-1.419353
12	5	0	-2.166908	-0.728054	0.470920
13	1	0	-2.111927	-0.464497	1.638566
14	1	0	-2.857167	-1.621536	0.067181

D5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-2.481938	1.714532	-0.264373
2	7	0	-1.652246	1.143514	-0.206333
3	1	0	-0.790851	1.659485	-0.304867
4	5	0	-1.739907	-0.223977	0.079955
5	1	0	-2.835926	-0.686858	0.235273
6	7	0	-0.626166	-1.154335	0.167512
7	1	0	-0.976059	-2.095931	0.308111
8	5	0	0.771855	-1.192576	-0.075773
9	1	0	1.267495	-2.281187	-0.194063
10	7	0	1.696617	-0.076234	-0.207563
11	1	0	2.579307	-0.379563	-0.608973
12	5	0	1.728631	1.236913	0.299381
13	1	0	0.790465	1.681958	0.889410
14	1	0	2.717180	1.895151	0.146355

TSD6

Standard orientation:

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

1	5	0	-0.740788	-1.341201	0.576022
2	7	0	1.254643	-0.902865	-0.449305
3	5	0	1.414441	0.384549	0.191803
4	7	0	0.363145	1.350901	0.144314
5	5	0	-1.013104	1.075370	-0.199595
6	7	0	-1.452861	-0.274871	-0.121103
7	1	0	-2.281547	-0.530696	-0.644905
8	1	0	-1.740110	1.957323	-0.563092
9	1	0	0.602388	2.299658	0.404233
10	1	0	2.436814	0.615209	0.771801
11	1	0	2.021234	-1.562526	-0.415153
12	1	0	0.721160	-0.985586	-1.305845
13	1	0	-0.276098	-1.123976	1.656903
14	1	0	-0.941074	-2.475158	0.237570

TSD7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.592154	-1.918352	-0.557855
2	7	0	1.057214	-1.215977	-0.055422
3	1	0	0.918385	-1.525685	0.899336
4	5	0	1.528145	0.158027	-0.183282
5	1	0	2.583085	0.384621	-0.709560
6	7	0	0.701308	1.230288	0.251308
7	1	0	1.149972	2.139257	0.247956
8	5	0	-0.732689	1.294392	0.020817
9	1	0	-1.219916	2.378781	-0.143227
10	7	0	-1.502365	0.123953	-0.166408
11	1	0	-2.326790	0.253713	-0.743223
12	5	0	-1.183424	-1.256406	0.168048
13	1	0	-0.959635	-1.529081	1.318364
14	1	0	-1.590524	-2.131176	-0.546048

TSD8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.579438	1.347776	0.002049
2	1	0	-0.967963	2.484922	0.027372
3	7	0	0.828599	1.162981	-0.120023
4	1	0	1.279553	2.067829	-0.197680
5	5	0	1.835873	0.124739	-0.005108
6	1	0	2.977805	0.491862	0.040354
7	7	0	1.600513	-1.254358	0.084908
8	1	0	2.372656	-1.900539	0.151051
9	1	0	0.707247	-1.701403	-0.063029
10	5	0	-1.789746	-1.177685	-0.277234
11	1	0	-2.934812	-1.468246	-0.457657
12	1	0	-1.513456	-1.755631	0.905075
13	7	0	-1.619035	0.357718	0.140247
14	1	0	-2.524670	0.779236	0.312136
15	1	0	-1.450566	-0.743280	0.964589
16	1	0	-0.949782	-1.593285	-1.016674

D6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.771955	-1.192550	-0.075984
2	1	0	-1.267620	-2.281063	-0.195051
3	7	0	0.626016	-1.154384	0.167284
4	1	0	0.975988	-2.096030	0.307318
5	5	0	1.740054	-0.224073	0.080082
6	1	0	2.835712	-0.687619	0.236037
7	7	0	1.652912	1.143378	-0.206107
8	1	0	2.482858	1.714030	-0.264303
9	1	0	0.791757	1.659585	-0.305618
10	5	0	-1.728872	1.237289	0.298991
11	1	0	-2.717190	1.895685	0.145107
12	7	0	-1.697144	-0.076324	-0.206709
13	1	0	-2.579987	-0.379851	-0.607638
14	1	0	-0.790137	1.683241	0.887428

TSD9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	2.077990	-0.157487	0.000000
2	5	0	1.435829	1.083634	0.000000
3	7	0	0.000000	1.317161	0.000000
4	5	0	-1.258129	0.658152	0.000000
5	7	0	-1.595270	-0.758812	0.000000
6	5	0	-0.945755	-2.007776	0.000000
7	1	0	3.085086	-0.217644	0.000000
8	1	0	1.608832	-1.051335	0.000000
9	1	0	2.128512	2.063687	0.000000
10	1	0	-0.166434	2.317877	0.000000
11	1	0	-2.218177	1.381642	0.000000
12	1	0	-2.606431	-0.856965	0.000000
13	1	0	-1.612072	-3.002443	0.000000
14	1	0	0.241925	-2.110905	0.000000

TSE1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.326916	-1.029982	-1.039095
2	7	0	1.561354	-0.771333	-0.081363
3	5	0	0.469350	-0.095803	0.670022
4	1	0	1.904285	-1.603849	0.392694
5	5	0	2.783230	0.398610	-0.108945
6	1	0	2.480151	1.132091	-1.026752
7	1	0	2.714488	0.950095	0.972070
8	1	0	3.814663	-0.207150	-0.271131

9	7	0	-0.310418	0.898391	-0.035403
10	1	0	0.346437	-0.281487	1.834112
11	1	0	-0.842607	1.563127	0.517183
12	1	0	0.104477	1.333872	-0.855066
13	1	0	-1.397725	-0.488051	-1.639326
14	5	0	-1.562660	-0.432191	-0.446159
15	7	0	-2.834447	-0.002747	0.122134
16	1	0	-1.021624	-1.358162	0.151827
17	1	0	-3.552149	0.320384	-0.513336
18	1	0	-3.242341	-0.554138	0.864660

E1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.980991	-1.480519	0.841072
2	5	0	-1.776498	-0.430140	0.468080
3	7	0	-2.831903	0.086168	-0.270745
4	1	0	-1.934407	-0.848824	1.570284
5	7	0	-0.397299	-0.459740	-0.119118
6	1	0	0.209669	-1.178684	0.298100
7	5	0	0.382316	0.952840	0.196908
8	1	0	-0.367952	-0.628163	-1.125199
9	1	0	0.144142	1.227436	1.348570
10	1	0	-0.036376	1.767789	-0.592247
11	7	0	1.929168	0.675991	0.003918
12	1	0	2.272207	1.167529	-0.820369
13	5	0	2.442421	-0.873207	-0.119049
14	1	0	2.426427	1.095623	0.788217
15	1	0	-2.733961	0.515252	-1.182264
16	1	0	-3.763152	0.163752	0.112692
17	1	0	2.008059	-1.301874	-1.175945
18	1	0	3.653394	-0.863710	-0.091000

TSE2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.388934	-1.778693	-0.381409
2	5	0	1.464055	-0.726970	-0.046890
3	7	0	2.573386	0.020182	-0.414659
4	1	0	1.317505	-1.846156	-0.418972
5	7	0	0.432698	-0.103155	0.861716
6	1	0	-0.273601	-0.792268	1.152434
7	5	0	-0.461233	1.148234	0.250933
8	1	0	0.866282	0.275800	1.704435
9	1	0	0.273014	1.830340	-0.428373
10	1	0	-0.910433	1.725745	1.210015
11	7	0	-1.635668	0.502616	-0.570781
12	1	0	-2.412370	1.162714	-0.544776
13	5	0	-2.210986	-0.940179	-0.048768
14	1	0	-1.400713	0.409566	-1.559145
15	1	0	2.683788	1.004318	-0.203557
16	1	0	3.286998	-0.348401	-1.027128
17	1	0	-2.310191	-0.857783	1.166891

18	1	0	-3.283438	-1.128109	-0.580727
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E2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-0.588565	-1.744382	0.307661
2	5	0	1.418805	-0.478824	0.501972
3	7	0	2.036664	-0.335843	-0.730753
4	1	0	1.739338	-1.324483	1.274371
5	7	0	0.431962	0.601798	0.943792
6	1	0	-0.183433	0.198042	1.657134
7	5	0	-0.548206	1.266386	-0.170901
8	1	0	0.936963	1.371387	1.389760
9	1	0	0.142133	1.722419	-1.059487
10	1	0	-1.193317	2.113261	0.398750
11	7	0	-1.494563	0.112503	-0.686318
12	1	0	-2.418340	0.512533	-0.846044
13	5	0	-1.680110	-1.185044	0.281225
14	1	0	-1.192154	-0.230799	-1.597385
15	1	0	1.780262	0.387371	-1.391263
16	1	0	2.724118	-0.993455	-1.069093
17	1	0	-1.988723	-0.772481	1.389475
18	1	0	-2.529164	-1.901203	-0.202410

TSE3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-0.133631	-1.474157	0.574969
2	5	0	1.289353	-0.359284	0.547717
3	7	0	1.924735	-0.422939	-0.704282
4	1	0	1.739405	-0.930724	1.492309
5	7	0	0.403674	0.881126	0.797225
6	1	0	-0.096484	0.745700	1.677050
7	5	0	-0.682447	1.244414	-0.346162
8	1	0	0.999056	1.702714	0.921774
9	1	0	-0.078166	1.611787	-1.330888
10	1	0	-1.417981	2.091612	0.100494
11	7	0	-1.487591	-0.093417	-0.633079
12	1	0	-2.475757	0.135394	-0.733082
13	5	0	-1.354818	-1.250773	0.479908
14	1	0	-1.212522	-0.490643	-1.530781
15	1	0	1.615068	0.105766	-1.508658
16	1	0	2.593218	-1.147083	-0.921123
17	1	0	-1.771190	-0.820293	1.536558
18	1	0	-1.907184	-2.255243	0.095012

E3

Standard orientation:

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

1	1	0	0.019892	-1.385375	0.574810
2	5	0	1.237988	-0.340989	0.545624
3	7	0	1.920846	-0.392757	-0.699842
4	1	0	1.749127	-0.816713	1.516680
5	7	0	0.377801	0.938272	0.757882
6	1	0	-0.073423	0.877911	1.671071
7	5	0	-0.746354	1.234204	-0.358548
8	1	0	1.000137	1.747809	0.793785
9	1	0	-0.187201	1.597048	-1.369687
10	1	0	-1.516632	2.053984	0.080770
11	7	0	-1.496245	-0.153123	-0.600858
12	1	0	-2.500105	0.018991	-0.641142
13	5	0	-1.232849	-1.285987	0.498097
14	1	0	-1.252638	-0.531118	-1.515758
15	1	0	1.563531	0.048829	-1.536396
16	1	0	2.588545	-1.125280	-0.890281
17	1	0	-1.655542	-0.913384	1.569292
18	1	0	-1.646429	-2.355587	0.120722

TSE4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	0.929798	-0.275342	1.551591
2	5	0	1.422731	0.177305	0.524093
3	7	0	1.343998	-0.911533	-0.559678
4	1	0	2.508412	0.695771	0.738777
5	7	0	0.440519	1.382783	0.033362
6	1	0	0.590898	2.153423	0.684611
7	5	0	-1.119600	1.151150	-0.063532
8	1	0	0.802079	1.728246	-0.857469
9	1	0	-1.596379	1.772304	-0.987685
10	1	0	-1.635295	1.385446	1.000851
11	7	0	-1.406347	-0.427182	-0.369295
12	1	0	-2.429649	-0.482724	-0.351213
13	5	0	-0.842707	-1.423039	0.626682
14	1	0	-1.088667	-0.678602	-1.305764
15	1	0	1.834745	-0.656159	-1.419056
16	1	0	1.793552	-1.765935	-0.239621
17	1	0	-1.119702	-1.203128	1.761022
18	1	0	-0.539102	-2.508854	0.257019

E4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	0.000000	1.680018	-1.198095
2	7	0	0.000000	1.485513	-0.194035
3	1	0	0.000000	2.409579	0.239553
4	5	0	1.369618	0.790750	0.242766
5	1	0	1.456438	0.840875	1.443324
6	1	0	2.291777	1.323158	-0.340371
7	5	0	-1.369618	0.790750	0.242766
8	1	0	-2.291777	1.323158	-0.340371
9	1	0	-1.456438	0.840875	1.443324
10	7	0	1.286492	-0.742756	-0.194035

11	1	0	2.086757	-1.204790	0.239553
12	1	0	1.454938	-0.840009	-1.198095
13	7	0	-1.286492	-0.742756	-0.194035
14	1	0	-2.086757	-1.204790	0.239553
15	1	0	-1.454938	-0.840009	-1.198095
16	5	0	0.000000	-1.581499	0.242766
17	1	0	0.000000	-2.646316	-0.340371
18	1	0	0.000000	-1.681750	1.443324

TSE5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-0.342316	-1.196860	2.092456
2	7	0	0.113601	-0.813928	1.264272
3	1	0	1.067438	-1.178433	1.306794
4	5	0	-0.640023	-1.417493	0.000000
5	1	0	-0.528971	-2.625708	0.000000
6	1	0	-1.782584	-1.029539	0.000000
7	5	0	0.113601	0.773664	1.442509
8	1	0	1.119190	1.101744	2.033597
9	1	0	-0.901244	1.073205	2.025273
10	7	0	0.105128	1.506524	0.000000
11	1	0	-0.723340	2.097456	0.000000
12	1	0	0.886544	2.158634	0.000000
13	7	0	0.113601	-0.813928	-1.264272
14	1	0	-0.342316	-1.196860	-2.092456
15	1	0	1.067438	-1.178433	-1.306794
16	5	0	0.113601	0.773664	-1.442509
17	1	0	1.119190	1.101744	-2.033597
18	1	0	-0.901244	1.073205	-2.025273

E5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.147514	1.672274	0.463618
2	5	0	0.000000	1.371408	0.701385
3	1	0	-0.603559	2.223627	1.315003
4	7	0	0.000000	0.000000	1.537352
5	1	0	-0.806530	-0.028575	2.160599
6	1	0	0.806530	0.028575	2.160599
7	7	0	-0.727429	1.060694	-0.678483
8	1	0	-0.796732	1.940116	-1.189938
9	1	0	-1.692667	0.772349	-0.510617
10	5	0	0.000000	-1.371408	0.701385
11	1	0	-1.147514	-1.672274	0.463618
12	1	0	0.603559	-2.223627	1.315003
13	5	0	0.000000	0.000000	-1.633612
14	1	0	0.827317	0.586120	-2.292908
15	1	0	-0.827317	-0.586120	-2.292908
16	7	0	0.727429	-1.060694	-0.678483
17	1	0	0.796732	-1.940116	-1.189938
18	1	0	1.692667	-0.772349	-0.510617

TSE6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	0.562195	1.085594	-1.664295
2	5	0	0.541152	1.355415	-0.467897
3	1	0	0.999342	2.456036	-0.246229
4	7	0	1.485578	0.236127	0.232599
5	1	0	1.672781	0.528810	1.191475
6	1	0	2.386596	0.264019	-0.242807
7	7	0	-0.857513	1.179182	0.177146
8	1	0	-1.471880	1.982959	0.126549
9	1	0	-1.157937	0.327191	1.340820
10	5	0	0.930229	-1.258824	0.228649
11	1	0	0.783449	-1.656631	1.361171
12	1	0	1.627870	-1.971246	-0.453966
13	5	0	-1.538088	-0.165877	0.107659
14	1	0	-2.694361	-0.285413	-0.194883
15	1	0	-1.574182	-0.527272	1.496912
16	7	0	-0.546079	-1.225994	-0.442371
17	1	0	-0.936391	-2.167156	-0.389830
18	1	0	-0.437846	-1.015668	-1.438590

TSE7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-2.103541	0.777291	-1.147895
2	5	0	-1.444765	0.327465	-0.257420
3	1	0	-2.443416	0.176405	0.799148
4	7	0	-0.416375	1.293988	0.388371
5	1	0	-0.297085	1.088135	1.381308
6	1	0	-0.714457	2.266676	0.321175
7	7	0	-0.927988	-1.082375	-0.320713
8	1	0	-1.155758	-1.612067	-1.152856
9	1	0	-2.025691	-0.656465	0.539102
10	5	0	1.034108	1.148983	-0.332874
11	1	0	1.784827	1.935896	0.196892
12	1	0	0.868142	1.357574	-1.510430
13	5	0	0.361068	-1.394777	0.448458
14	1	0	0.754436	-2.525669	0.273239
15	1	0	0.231175	-1.121677	1.635477
16	7	0	1.512032	-0.354025	-0.096595
17	1	0	2.296802	-0.384639	0.554114
18	1	0	1.878826	-0.712924	-0.977537

TSE8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	0.465141	1.445570	0.000000
2	1	0	1.643347	1.166920	0.000000
3	7	0	-0.215117	0.777755	1.277543

4	1	0	-1.173253	1.115124	1.374006
5	1	0	0.272009	1.147000	2.093145
6	7	0	-0.215117	0.777755	-1.277543
7	1	0	-1.173253	1.115124	-1.374006
8	1	0	0.272009	1.147000	-2.093145
9	5	0	-0.215117	-0.833770	1.363646
10	1	0	0.488654	-1.176382	2.287714
11	1	0	-1.354666	-1.226044	1.449928
12	5	0	-0.215117	-0.833770	-1.363646
13	1	0	-1.354666	-1.226044	-1.449928
14	1	0	0.488654	-1.176382	-2.287714
15	1	0	0.260313	2.639942	0.000000
16	7	0	0.399130	-1.381024	0.000000
17	1	0	0.262886	-2.392205	0.000000
18	1	0	1.411168	-1.245613	0.000000

TSF1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.034310	-1.521147	0.772269
2	5	0	-1.816067	-0.338082	0.526493
3	7	0	-2.796556	0.045581	-0.376857
4	1	0	-2.071648	-0.553114	1.668712
5	7	0	-0.395550	-0.478364	0.068338
6	1	0	0.163373	-1.111314	0.651354
7	5	0	0.382232	0.970307	0.123842
8	1	0	-0.281753	-0.839726	-0.880283
9	1	0	0.105346	1.477838	1.185035
10	1	0	-0.006385	1.601317	-0.830986
11	7	0	1.932770	0.663992	0.020656
12	1	0	2.324363	1.206774	-0.747634
13	5	0	2.426277	-0.881040	-0.197626
14	1	0	2.401873	1.011926	0.855804
15	1	0	-2.613257	0.305017	-1.338026
16	1	0	-3.754847	0.194372	-0.094485
17	1	0	1.915308	-1.274090	-1.234922
18	1	0	3.636464	-0.872240	-0.255341

F1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.114157	1.178417	1.464712
2	5	0	1.814105	-0.373847	0.055565
3	7	0	1.984717	0.953955	-0.290704
4	1	0	2.664494	-1.194719	-0.097371
5	7	0	0.502505	-0.804349	0.667991
6	1	0	0.615490	-1.608975	1.280504
7	5	0	-0.615216	-1.171474	-0.494574
8	1	0	0.071126	-0.039257	1.211517
9	1	0	-0.966399	-2.312286	-0.307591
10	1	0	-0.110468	-0.990984	-1.574165
11	7	0	-1.818911	-0.155792	-0.294542
12	1	0	-2.244299	-0.016767	-1.210836

13	5	0	-1.548117	1.326318	0.323645
14	1	0	-2.552496	-0.588177	0.268021
15	1	0	1.225164	1.627977	-0.241467
16	1	0	2.815488	1.287250	-0.757934
17	1	0	-0.731313	1.879416	-0.393613
18	1	0	-2.604667	1.916422	0.355825

TSF2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.773573	1.612100	-0.777501
2	5	0	-2.018214	-0.400007	-0.340043
3	7	0	-2.653605	0.671531	0.276914
4	1	0	-2.608800	-1.404559	-0.593246
5	7	0	-0.569868	-0.312824	-0.669844
6	1	0	-0.269139	-1.016096	-1.341409
7	5	0	0.451734	-0.527990	0.758311
8	1	0	-0.254651	0.594022	-1.016804
9	1	0	0.108845	-1.593035	1.215654
10	1	0	0.124809	0.439423	1.415516
11	7	0	1.861505	-0.485306	0.266953
12	1	0	2.656380	0.512134	0.928729
13	5	0	2.532065	0.750966	-0.403860
14	1	0	2.359364	-1.359494	0.153093
15	1	0	-2.163290	1.492688	0.608324
16	1	0	-3.615524	0.623011	0.579596
17	1	0	3.096569	1.357870	0.712284
18	1	0	3.497714	0.513283	-1.074429

TSF3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.773573	1.612100	-0.777501
2	5	0	-2.018214	-0.400007	-0.340043
3	7	0	-2.653605	0.671531	0.276914
4	1	0	-2.608800	-1.404559	-0.593246
5	7	0	-0.569868	-0.312824	-0.669844
6	1	0	-0.269139	-1.016096	-1.341409
7	5	0	0.451734	-0.527990	0.758311
8	1	0	-0.254651	0.594022	-1.016804
9	1	0	0.108845	-1.593035	1.215654
10	1	0	0.124809	0.439423	1.415516
11	7	0	1.861505	-0.485306	0.266953
12	1	0	2.656380	0.512134	0.928729
13	5	0	2.532065	0.750966	-0.403860
14	1	0	2.359364	-1.359494	0.153093
15	1	0	-2.163290	1.492688	0.608324
16	1	0	-3.615524	0.623011	0.579596
17	1	0	3.096569	1.357870	0.712284
18	1	0	3.497714	0.513283	-1.074429

F2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-2.765138	-0.319933	-0.104418
2	5	0	-1.784702	0.664357	-0.100614
3	7	0	-0.484415	0.411383	0.591151
4	5	0	0.537134	-0.562556	-0.439730
5	7	0	1.930359	-0.472180	0.128268
6	5	0	2.958051	0.408113	-0.213385
7	1	0	-2.616879	-1.258414	0.244504
8	1	0	-3.624206	-0.213605	-0.624454
9	1	0	-1.951153	1.709123	-0.647340
10	1	0	0.045697	1.264282	0.763189
11	1	0	-0.562756	-0.085084	1.477899
12	1	0	0.410861	-0.043542	-1.521287
13	1	0	0.027229	-1.658901	-0.337548
14	1	0	2.167437	-1.181228	0.816386
15	1	0	4.029882	0.320807	0.325660
16	1	0	2.755836	1.262104	-1.033374

TSF4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	2.732708	-0.296573	-0.129625
2	5	0	1.758910	0.627969	0.222200
3	7	0	0.382022	0.503624	-0.354765
4	5	0	-0.509786	-0.697532	0.462408
5	7	0	-1.939906	-0.567487	-0.047655
6	5	0	-2.783902	0.535147	-0.002831
7	1	0	2.542526	-1.128227	-0.674645
8	1	0	3.654016	-0.285540	0.283749
9	1	0	1.990377	1.519075	0.977224
10	1	0	-0.168303	1.355899	-0.244879
11	1	0	0.356630	0.255149	-1.343885
12	1	0	-0.349343	-0.424744	1.631100
13	1	0	0.014594	-1.740602	0.131803
14	1	0	-2.321768	-1.412941	-0.458497
15	1	0	-3.902097	0.482718	-0.438250
16	1	0	-2.366507	1.574348	0.451707

F3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.457821	-0.370972	-0.627542
2	1	0	-0.102482	-1.185011	-1.126087
3	1	0	-0.246668	0.447319	-1.198375
4	5	0	0.544309	-0.162708	0.779755
5	1	0	0.187050	-1.041081	1.532004
6	1	0	0.242664	0.954830	1.130193
7	7	0	1.970900	-0.308143	0.303702
8	1	0	2.404377	-1.205434	0.498106

9	5	0	2.773520	0.642502	-0.324408
10	1	0	2.311313	1.725380	-0.576283
11	1	0	3.904957	0.379744	-0.634208
12	5	0	-1.892284	-0.508715	-0.231637
13	1	0	-2.387503	-1.592564	-0.230801
14	7	0	-2.611671	0.617988	0.143217
15	1	0	-3.560071	0.558662	0.484781
16	1	0	-2.191221	1.530652	0.266483

TSF5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.579773	-0.803883	-0.563097
2	1	0	-0.625150	-1.742088	-0.953762
3	1	0	-0.211341	-0.178680	-1.279532
4	5	0	0.697998	-0.805513	0.670685
5	1	0	0.241688	-0.111360	1.543736
6	1	0	0.800580	-1.977533	0.946233
7	5	0	-1.862480	-0.356237	0.050652
8	1	0	-2.565801	-1.176000	0.553410
9	7	0	-2.221236	0.987357	0.029996
10	1	0	-3.034871	1.323728	0.524656
11	1	0	-1.614175	1.730494	-0.292945
12	7	0	1.912105	-0.211345	-0.002457
13	1	0	2.545088	-0.882427	-0.428224
14	5	0	2.312487	1.123899	-0.058037
15	1	0	3.332886	1.428861	-0.616299
16	1	0	1.613401	1.969353	0.435124

F4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.609139	1.490360	1.271549
2	5	0	1.999104	1.084421	0.212467
3	1	0	2.754121	1.743840	-0.454308
4	7	0	1.556395	-0.152162	-0.262550
5	1	0	1.974703	-0.454007	-1.138939
6	5	0	0.699370	-1.187968	0.423359
7	1	0	1.014984	-2.331141	0.174665
8	1	0	0.493182	-0.959475	1.588958
9	7	0	-0.891751	-1.100575	-0.310624
10	1	0	-0.731226	-1.009380	-1.313213
11	1	0	-1.325657	-2.006343	-0.144835
12	5	0	-1.667045	0.024534	0.295976
13	1	0	-2.420820	-0.223045	1.184490
14	7	0	-1.498224	1.318349	-0.180559
15	1	0	-0.762471	1.574443	-0.826816
16	1	0	-1.928030	2.110536	0.275572

TSF6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.355818	0.645166	-0.245309
2	1	0	-0.096708	0.946824	-1.190203
3	1	0	0.083884	1.349415	0.356601
4	5	0	0.430781	-0.782491	0.059514
5	1	0	-0.033672	-1.591903	-0.720352
6	1	0	0.155155	-1.030711	1.215999
7	7	0	1.913221	-0.517216	-0.203797
8	1	0	2.354561	-1.167604	-0.844962
9	5	0	2.728843	0.467953	0.336271
10	1	0	2.247843	1.279553	1.093618
11	1	0	3.890998	0.549017	0.043437
12	5	0	-1.867845	0.710969	-0.091169
13	1	0	-2.423583	1.760313	-0.220464
14	7	0	-2.557135	-0.450454	0.183456
15	1	0	-3.560093	-0.483295	0.298655
16	1	0	-2.079161	-1.336233	0.304144

F5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.484363	0.411630	0.590182
2	1	0	0.562127	-0.084622	1.477117
3	1	0	-0.045707	1.264658	0.761763
4	5	0	-0.537449	-0.562199	-0.440652
5	1	0	-0.027322	-1.658484	-0.339135
6	1	0	-0.411764	-0.042596	-1.521990
7	7	0	-1.930369	-0.472340	0.128193
8	1	0	-2.166926	-1.181844	0.816031
9	5	0	-2.958448	0.407951	-0.212305
10	1	0	-2.756863	1.262515	-1.031861
11	1	0	-4.029920	0.320100	0.327365
12	5	0	1.785151	0.664271	-0.100748
13	1	0	1.952041	1.708772	-0.647838
14	7	0	2.765468	-0.320144	-0.103495
15	1	0	3.624983	-0.214193	-0.622882
16	1	0	2.616852	-1.258438	0.245801

TSF7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.502403	1.813826	0.654111
2	5	0	2.036722	1.064653	-0.127085
3	1	0	2.911966	1.480163	-0.837743
4	7	0	1.619038	-0.259146	-0.202191
5	1	0	2.139887	-0.835845	-0.857539
6	5	0	0.612104	-1.017554	0.648948
7	1	0	0.913657	-2.184269	0.795366
8	1	0	0.327355	-0.448117	1.674869
9	7	0	-0.846387	-1.114897	-0.214192
10	1	0	-0.598350	-1.335037	-1.183955

11	1	0	-1.335816	-1.950417	0.114660
12	5	0	-1.831033	0.049766	-0.227142
13	1	0	-2.955163	-0.158799	-0.577409
14	7	0	-1.414446	1.306197	0.150109
15	1	0	-0.469353	1.503965	0.465865
16	1	0	-2.032991	2.105130	0.142094

F6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.406606	-0.126945	-0.641307
2	7	0	1.853067	-1.027091	0.313631
3	5	0	-1.990133	-1.207863	-0.057388
4	7	0	-1.645244	0.138179	-0.189665
5	5	0	-0.718375	0.967847	0.658683
6	7	0	0.791515	1.169454	-0.188967
7	1	0	0.645463	1.810444	-0.967066
8	1	0	1.370207	1.659995	0.493660
9	1	0	-1.068634	2.119549	0.806179
10	1	0	-0.367892	0.415137	1.676413
11	1	0	-2.158718	0.650893	-0.901288
12	1	0	-2.805436	-1.694437	-0.796356
13	1	0	-1.464170	-1.875115	0.791259
14	1	0	2.215229	-1.935825	0.062972
15	1	0	1.628417	-0.933951	1.296849
16	1	0	1.519671	-0.345680	-1.807548

TSF8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-1.392271	0.005575	0.530406
2	7	0	-0.842299	1.199564	-0.168106
3	5	0	0.983240	1.206679	-0.244196
4	7	0	1.506522	-0.046593	0.391463
5	5	0	1.827721	-1.263036	-0.214325
6	7	0	-1.765220	-1.129451	-0.183044
7	1	0	-2.059559	-1.974356	0.285703
8	1	0	-1.577353	-1.266528	-1.168151
9	1	0	2.270914	-2.167213	0.443393
10	1	0	1.647157	-1.401718	-1.394299
11	1	0	1.695642	0.016153	1.387478
12	1	0	1.145029	1.257557	-1.437347
13	1	0	1.227711	2.218320	0.370322
14	1	0	-1.126642	1.281252	-1.142172
15	1	0	-1.081591	2.070274	0.299529
16	1	0	-1.527781	0.055526	1.713927

TSF9

Standard orientation:

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

1	5	0	-1.761064	1.313496	0.122817
2	7	0	-1.819181	-0.037796	-0.190800
3	5	0	-0.716736	-1.026644	-0.543368
4	7	0	0.480371	-0.904395	0.641748
5	5	0	1.401879	0.300192	0.599537
6	7	0	2.129539	0.527928	-0.557155
7	1	0	-2.759903	1.941053	0.351252
8	1	0	-0.687162	1.858565	0.194440
9	1	0	-2.747715	-0.446686	-0.212399
10	1	0	-1.094642	-2.176971	-0.463845
11	1	0	-0.122188	-0.811404	-1.583557
12	1	0	0.017264	-0.982231	1.547386
13	1	0	1.029815	-1.757214	0.519960
14	1	0	1.546294	0.963669	1.577756
15	1	0	1.915666	0.055106	-1.427224
16	1	0	2.747077	1.320735	-0.655258

F7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.705374	-1.220915	0.323583
2	7	0	1.675101	-0.031479	-0.384356
3	5	0	0.675385	1.119629	-0.433364
4	7	0	-0.448421	0.843083	0.737862
5	5	0	-1.424240	-0.316553	0.559118
6	7	0	-1.941972	-0.543732	-0.701388
7	1	0	0.808173	-1.485586	1.090369
8	1	0	2.612460	-1.997714	0.200195
9	1	0	2.470816	0.130972	-0.995186
10	1	0	0.052970	1.193064	-1.483284
11	1	0	1.170320	2.195926	-0.157830
12	1	0	0.042021	0.743695	1.628471
13	1	0	-0.975926	1.716588	0.803700
14	1	0	-1.785275	-0.926903	1.516221
15	1	0	-2.599055	-1.285283	-0.895701
16	1	0	-1.572060	-0.070671	-1.518469

TSF10

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-1.491045	0.116560	0.702387
2	5	0	-0.981946	-0.645955	-0.462268
3	7	0	0.405022	-1.313672	-0.225531
4	5	0	1.498629	-0.250104	0.422259
5	7	0	0.987025	1.111003	-0.084350
6	5	0	-0.315908	1.246193	-0.563454
7	1	0	-2.486725	0.236283	0.831745
8	1	0	-0.964077	0.156934	1.565656
9	1	0	-1.770958	-1.241137	-1.144241
10	1	0	0.760939	-1.678718	-1.109311
11	1	0	0.321027	-2.120031	0.393625
12	1	0	2.601654	-0.575186	0.032191

13	1	0	1.390135	-0.378595	1.634477
14	1	0	1.429265	1.931783	0.310073
15	1	0	-0.951999	2.212072	-0.842750
16	1	0	-0.640153	0.308692	-1.401693

TSF11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-1.780100	-0.003867	-0.221616
2	7	0	-1.449154	1.327200	0.072833
3	5	0	1.949728	1.112864	0.123472
4	7	0	1.564743	-0.128541	-0.376926
5	5	0	0.708958	-1.204631	0.196954
6	7	0	-0.877433	-1.120735	-0.011444
7	1	0	-1.284868	-2.029835	-0.198735
8	1	0	-0.211440	-1.036963	1.201368
9	1	0	1.066356	-2.341512	0.064616
10	1	0	0.733377	-1.027194	1.546037
11	1	0	1.964300	-0.388910	-1.274438
12	1	0	2.685737	1.819491	-0.504473
13	1	0	1.521124	1.468882	1.190735
14	1	0	-2.108494	2.075206	-0.080240
15	1	0	-0.545378	1.640067	0.399709
16	1	0	-2.880737	-0.246531	-0.629874

F8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-1.768015	0.154211	0.044200
2	7	0	-0.688052	1.009170	-0.533668
3	5	0	0.669793	1.102305	0.549604
4	7	0	1.363651	-0.244213	0.483756
5	5	0	2.298826	-0.697730	-0.446173
6	7	0	-1.659334	-1.229414	-0.021106
7	1	0	-2.336889	-1.843079	0.407929
8	1	0	-0.832692	-1.700799	-0.366728
9	1	0	2.788277	-1.790606	-0.331669
10	1	0	2.584928	0.000525	-1.382651
11	1	0	1.166256	-0.867452	1.260526
12	1	0	1.302649	2.011404	0.069783
13	1	0	0.176578	1.341333	1.628271
14	1	0	-0.280220	0.654646	-1.398616
15	1	0	-0.989619	1.967455	-0.699177
16	1	0	-2.696141	0.683844	0.571302

TSF12

Standard orientation:

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

1	7	0	-0.496307	0.619699	-0.518481
2	1	0	-0.209723	-0.084054	-1.198171
3	1	0	-0.295050	1.535305	-0.912907
4	5	0	0.668890	0.440309	0.819480
5	1	0	0.007002	-0.031323	1.715961
6	1	0	1.024477	1.577690	0.992878
7	7	0	1.739008	-0.491586	0.307508
8	1	0	1.637319	-1.462846	0.586600
9	5	0	2.890425	-0.182155	-0.419026
10	1	0	3.085458	0.953507	-0.758985
11	1	0	3.666665	-1.050477	-0.718705
12	5	0	-1.879107	0.484000	0.009511
13	1	0	-2.378798	1.431156	0.530210
14	7	0	-2.568508	-0.721628	-0.094524
15	1	0	-3.470906	-0.852837	0.339344
16	1	0	-2.186837	-1.572285	-0.487579

TSF13

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-1.526857	-0.312803	0.302907
2	7	0	-0.693203	0.800609	-0.086744
3	5	0	0.917183	0.905475	0.079683
4	7	0	1.658493	-0.361990	0.215782
5	5	0	2.897480	-0.673547	-0.356832
6	7	0	-2.802991	-0.533856	-0.239690
7	1	0	-3.380282	-1.308267	0.052133
8	1	0	-3.221224	0.025572	-0.970882
9	1	0	3.380789	-1.755528	-0.165318
10	1	0	3.454755	0.142045	-1.034171
11	1	0	1.223802	-1.084337	0.781645
12	1	0	1.361325	1.747729	-0.641033
13	1	0	0.873186	1.534756	1.301355
14	1	0	-1.054820	1.451142	-0.778740
15	1	0	-0.088067	1.380010	0.954146
16	1	0	-1.124584	-1.062086	1.146640

F9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.247173	2.596736	0.000000
2	7	0	2.411443	1.598741	0.000000
3	1	0	3.390295	1.355090	0.000000
4	5	0	1.399567	0.622309	0.000000
5	1	0	1.732159	-0.528833	0.000000
6	7	0	0.000000	0.960415	0.000000
7	1	0	-0.226587	1.950172	0.000000
8	5	0	-1.142513	0.106104	0.000000
9	1	0	-2.233840	0.594542	0.000000
10	7	0	-1.039854	-1.331999	0.000000
11	1	0	-0.101398	-1.721783	0.000000
12	5	0	-2.114382	-2.245553	0.000000
13	1	0	-3.234720	-1.828050	0.000000

14	1	0	-1.887564	-3.422272	0.000000
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TSF14

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-2.268965	-0.658701	-1.351734
2	7	0	-2.362887	-0.741171	-0.346834
3	1	0	-3.047214	-1.422728	-0.047925
4	5	0	-1.610933	0.026046	0.542405
5	1	0	-1.780722	-0.154606	1.717630
6	7	0	-0.639640	1.014397	0.031649
7	1	0	-1.010417	1.943382	-0.138587
8	5	0	0.755027	0.892818	-0.144304
9	1	0	1.396790	1.834851	-0.506000
10	7	0	1.450082	-0.360938	0.088517
11	1	0	0.885271	-1.153972	0.383285
12	5	0	2.831517	-0.596025	-0.049127
13	1	0	3.543960	0.299208	-0.397095
14	1	0	3.270355	-1.687649	0.182225

TSG1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-3.816504	-0.560952	0.087339
2	5	0	-2.519440	-0.570376	-0.505689
3	7	0	-1.564649	1.131397	-0.059880
4	5	0	-0.748199	0.162867	0.635465
5	7	0	0.553589	-0.237785	-0.011051
6	5	0	1.629987	0.989727	0.070931
7	1	0	-4.018518	-0.986718	0.979319
8	1	0	-4.644794	-0.349950	-0.448734
9	1	0	-1.679541	-1.239994	0.099543
10	1	0	-2.349768	-0.531987	-1.690382
11	1	0	-2.237625	1.681606	0.459241
12	1	0	-1.203498	1.618229	-0.872904
13	1	0	-0.898389	-0.044102	1.795404
14	1	0	0.453147	-0.534188	-0.983348
15	1	0	1.011947	-1.024733	0.467748
16	1	0	1.331923	1.785219	-0.794149
17	1	0	1.552042	1.446235	1.186676
18	7	0	3.063009	0.365976	-0.164438
19	5	0	3.251111	-1.248076	0.039962
20	1	0	3.403331	0.591305	-1.098594
21	1	0	3.711646	0.827893	0.471590
22	1	0	2.664664	-1.784432	-0.886147
23	1	0	2.748890	-1.530187	1.120936
24	1	0	4.439132	-1.485368	0.026669

G1

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
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Number	Number	Type	X	Y	Z
1	7	0	3.596546	0.062873	0.904314
2	5	0	3.057786	-0.260392	-0.328598
3	7	0	1.569572	-0.471158	-0.449988
4	5	0	0.746316	0.959051	-0.388677
5	7	0	-0.785056	0.618559	-0.540481
6	5	0	-1.280044	-0.804159	-0.004734
7	1	0	3.038505	0.257337	1.726816
8	1	0	4.581874	0.248178	1.027561
9	1	0	1.153956	1.645436	-1.293793
10	1	0	3.734019	-0.377642	-1.301159
11	1	0	1.169948	-1.035016	0.306448
12	1	0	1.330198	-0.959892	-1.312778
13	1	0	0.958893	1.407044	0.710153
14	1	0	-1.099707	0.752420	-1.502236
15	1	0	-1.325928	1.307155	-0.004162
16	1	0	-0.938012	-1.657388	-0.806939
17	1	0	-0.777327	-0.979187	1.090224
18	7	0	-2.849291	-0.766032	0.153710
19	5	0	-3.540202	0.676588	0.507518
20	1	0	-3.310757	-1.131766	-0.679203
21	1	0	-3.100773	-1.415216	0.898315
22	1	0	-3.487591	1.344491	-0.513628
23	1	0	-2.882785	1.169531	1.410915
24	1	0	-4.686192	0.459382	0.843029

Table S6. Bimolecular Rate Constants (M-sec⁻¹) Calculated with the Conventional TST Method^a and the TST method^a with Eckart Tunneling Correction^{a,b} and Arranged in Order of Decreasing Magnitude

TST ^c				TST with Tunneling ^c			
298 K	TS	573 K	TS	298 K	TS	573 K	TS
8.9E+02	TS1	6.8E+05	TS1	1.1E+03	TS1	7.5E+05	TS1
1.3E+01	TSA4	1.8E+05	TSA4	1.6E+01	TSA4	2.0E+05	TSA4
6.4E-02	TS5	4.1E+04	TS5	7.5E-02	TS5	4.4E+04	TS5
1.9E-02	TSB1	7.9E+03	TSA2	2.4E-02	TSB1	8.4E+03	TSA2
4.2E-03	TSD1	8.0E+02	TSB1	5.2E-03	TSD1	9.0E+02	TSB1
1.5E-03	TSA2	3.3E+02	TSA1	1.6E-03	TSA2	3.8E+02	TSA1
7.9E-04	TSE1	1.1E+02	TSD1	9.8E-04	TSG1	1.2E+02	TSD1
7.5E-04	TSG1	9.0E+01	TSG1	9.4E-04	TSE1	1.0E+02	TSG1
5.3E-04	TSC1	5.5E+01	TSE1	6.4E-04	TSC1	6.0E+01	TSE1
5.5E-06	TSA1	1.9E+01	TSC1	7.4E-06	TSA1	2.1E+01	TSC1

^a Zhang, S.; Truong, T. N. **Vlab**, version 1.0, University of Utah, 2001. ^b Truong, T. N.; Truhlar, D. G. *J. Chem. Phys.*, **1990**, 93, 1761. ^c Units are M-sec⁻¹.

Table S7. Unimolecular Rate Constants (sec^{-1}) Calculated with the Conventional TST Method^a and the TST method with Eckart Tunneling Correction^{a,b} and Arranged in Order of Decreasing Magnitude

TST ^c				TST with Tunneling ^c			
298 K	TS	573 K	TS	298 K	TS	573 K	TS
6.1E+10	TSE5	1.2E+12	TSE5	6.8E+10	TSE5	1.2E+12	TSE5
5.8E+06	TSD5	4.9E+09	TSD5	6.8E+06	TSD5	5.3E+09	TSD5
6.8E+05	TSD6	9.9E+08	TSF14	8.2E+05	TSD6	1.1E+09	TSF14
2.9E+05	TSF14	3.9E+08	TSD6	3.3E+05	TSF14	4.2E+08	TSD6
7.9E+01	TSD7	4.6E+06	TSD7	1.0E+02	TSD7	5.2E+06	TSD7
2.5E-01	TSF10	1.2E+05	TSF10	3.2E-01	TSF10	1.3E+05	TSF10
3.7E-03	TS2	6.5E+04	TS2	9.1E-03	TS2	8.9E+04	TS2
5.3E-05	TSA3	4.2E+04	TSA3	1.9E-04	TSC5	4.8E+04	TSA3
2.3E-06	TSC2	1.6E+03	TSC5	7.4E-05	TSA3	4.0E+03	TSC5
1.4E-06	TSC5	1.5E+03	TSC2	6.2E-06	TSC2	2.1E+03	TSC2
8.8E-08	TSB3	5.1E+02	TSD3	2.6E-06	TSB3	1.0E+03	TSD3
1.6E-08	TSD3	2.8E+02	TSB3	4.9E-07	TSD3	5.7E+02	TSB3
3.0E-09	TSE4	3.2E+01	TSE4	4.9E-08	TSF13	6.6E+01	TSF13
8.6E-10	TSF13	3.1E+01	TSF13	2.2E-08	TSF11	3.7E+01	TSE4
5.9E-10	TSF11	1.8E+01	TSF11	4.3E-09	TSE4	3.7E+01	TSF11
2.4E-11	TSD8	7.2E+00	TSD8	9.2E-10	TSD8	1.5E+01	TSD8
1.0E-12	TS4	2.0E+00	TS4	5.3E-11	TS4	4.3E+00	TS4
8.5E-16	TSC3	3.1E-02	TSC3	4.7E-14	TSC3	6.7E-02	TSC3
6.0E-17	TSF3	2.5E-02	TSF2	2.8E-15	TSF3	5.3E-02	TSF2
4.4E-17	TSF2	1.3E-02	TSF3	2.1E-15	TSF2	2.7E-02	TSF3
5.2E-20	TSC4	2.3E-04	TSC4	3.4E-17	TSC4	5.7E-04	TSC4
1.5E-23	TSE7	4.3E-06	TSE7	3.3E-21	TSE7	9.8E-06	TSE7
2.1E-25	TSE6	4.4E-07	TSE6	4.2E-23	TSE6	1.0E-06	TSE6

^a Zhang, S.; Truong, T. N. **Vlab**, version 1.0, University of Utah, 2001. ^b Truong, T. N.; Truhlar, D. G. *J. Chem. Phys.*, **1990**, 93, 1761. ^c Units are sec^{-1} .

Table S8. A Comparison of Reaction Enthalpies and Free Energies (kcal/mol) Calculated at B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d) and CCSD(T)/CBS Level and 298.15 K

Reaction	ΔH^a	ΔG^a	ΔH	ΔG
1 $\rightarrow$ H ₂ BNH ₂ + BH ₃ + H ₂	7.0	-10.4	13.2 ^b	-4.5 ^b
H ₃ BNH ₃ $\rightarrow$ H ₂ BNH ₂ + H ₂	-8.0	-16.5	-5.6 ^b	-13.4 ^b
BH ₃ + NH ₃ $\rightarrow$ H ₃ BNH ₃	-25.0	-15.0	-27.6 ^b	-18.2 ^b
A3 $\rightarrow$ A2	-11.2	-10.4	-12.3 ^c	-11.3 ^c
C2 $\rightarrow$ C3 + H ₂	-30.7	-37.8	-27.9 ^c	-35.1 ^c
E4 $\rightarrow$ E5	-0.3	-0.9	-1.1 ^c	-1.9 ^c
E5 $\rightarrow$ C4 + H ₂	7.5	-1.7	11.4 ^c	2.3 ^c

^a Calculated at B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d) level. ^b Obtained from electronic energies calculated at the CCSD(T)/CBS level and ZPE, thermal correction, and entropies calculated at MP2/cc-pVTZ level, ref. 18. ^c Obtained from heats of formation and entropies calculated at MP2/cc-pVTZ level, ref. 21.

Figure S1. Molecular Plots^a

TSA2

A2

TSA3, C_s

TSA4, C_s

A3, C_s

TSA5

TSB1

B1

TSB2, C_s

TSB3

B2, C_s

TSC6

TSC1

C1

TSC2

TSC3

TSC4

C2

TSC5

C3, D_{3h}

C4

TSD1

D1

TSD2

D2

TSD3

D3

TSD4, C_s

D4

TSD5

D5

TSD6

TSD7

TSD8

D6

TSD9, C_s

TSE1

E1

TSE2

E2

TSE3

E3

TSE4

E4, C_{3v}

TSE5, C_s

E5, C_2

TSE6

TSE7

TSF1

F1

TSF2

TSF3

F2

TSF4

F3

TSF5

F4

TSF6

F5

TSF7

F6

TSF8

TSF9

F7

TSF10

TSF11

F8

TSF12

TSF13

F9, C_s

TSF14

TSE8, C_s

TSG1

G1

TS6

TS7

3

TS8

^a Drawn with Molden