Supported Information

Computer-Assisted Design of Metal-free Catalysts for Highly Efficient Hydration of Epoxides at Mild Temperature and Atmospheric Pressure via Multiple Hydrogen Bonding Interactions

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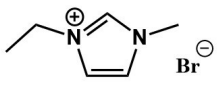
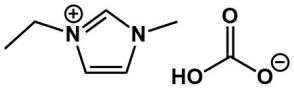
1. General information.

All chemicals used in this work were purchased commercially and used without further purification unless otherwise stated. 1-methylimidazole, 1,2-dimethylimidazole, bromoethane, 2-bromoethanol, bromoacetic acid, 1,3-dibromopropane, 1,3-dibromo-2-propanol, 3-bromo-2-(bromomethyl)propionic acid, tetramethylguanidine, DBU were purchased from Energy-Chemistry Co., Ltd. CO_2 (99.995%) and N_2 (99.999%) were purchased from Hangzhou Jingong Special Gas Co., Ltd. ^1H NMR and ^{13}C NMR spectra were recorded on a Bruker AVANCE III 500. Isotope labeling experiments were recorded on GCTOF-HRMS (Waters GCT Premier).

General procedure for the synthesis of catalyst.



2a



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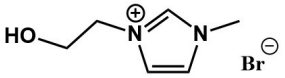

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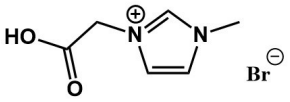

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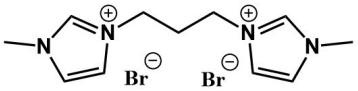

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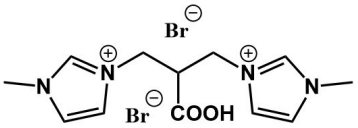

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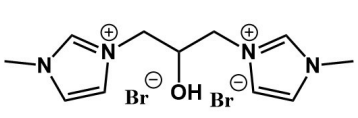
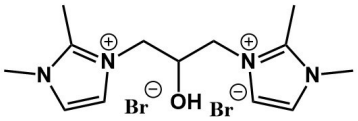


2h'



2i'

Synthesis of 2a: Bromoethane (50 mmol, 2 equiv) was added into the solution of 1-methylimidazole (25 mmol, 1 equiv) in methanol (20 ml). The reaction mixture was stirred at 60℃ for 12 h. After reaction completion, the reaction mixture was concentrated under reduced pressure to afford 2a, which was used without further purification. ^1H NMR (400 MHz, D_2O) 8.69 (s, 1H), 7.45 (dd, 1H), 7.41-7.30 (m, 1H), 4.20 (q, 2H), 3.87 (s, 3H), 1.47 (t, 3H).

Synthesis of 2b: 1-ethylimidazole (60 mmol, 1 equiv) and dimethyl carbonates (102 mmol, 1.7 equiv) were successively added to a 50 mL stainless-steel reactor. The reactor was sealed and stirred at 120 °C for 24 h. Thereafter, the reactor was cooled to room temperature and the mixture was filtered. Residual solids was recrystallized with methanol to afford 1-Ethyl-3-methylimidazolium-2-carboxylate. After adding equal mole of water, 2b was obtained. ^1H NMR (400 MHz, D_2O) 7.48 (d, 1H), 7.41 (d, 1H), 4.22 (q, 2H), 3.88 (s, 3H), 1.49 (t, 3H).

Synthesis of 2d': 1-methylimidazole (14.2 mmol, 1.1 equiv) was added into the solution of 2-bromoethanol (12.9 mmol, 1 equiv) in toluene (25 ml). The reaction mixture was stirred at 70℃ for 12 h. After reaction completion, the toluene was dumped and residual solids was washed by

ethyl acetate to afford 2d. ^{1}H NMR (400 MHz, D_2O) 8.74 (s, 1H), 7.50 (t, 1H), 7.44 (d, 1H), 4.31 (dd, 2H), 3.95-3.90 (m, 2H), 3.89 (s, 3H).

Synthesis of 2e': 1-methylimidazole (14.2 mmol, 1.1 equiv) was added into the solution of bromoacetic acid (12.9 mmol, 1 equiv) in toluene (25 ml). The reaction mixture was stirred at 70℃ for 12 h. After reaction completion, the toluene was dumped. Residual solids was recrystallized with THF and CH_3OH to afford 2e. ^{1}H NMR (400 MHz, D_2O) 8.76 (s, 1H), 7.48-7.44 (m, 2H), 5.05 (s, 2H), 3.91 (s, 3H).

Synthesis of 2f': In the 15ml pressure bottle, 1-methylimidazole (25 mmol, 2.5 equiv) was added into the solution of 1,3-dibromopropane (10 mmol, 1 equiv) in THF (5 ml). The reaction mixture was stirred overnight and heated to 100℃ for 72 h. After cooling to RT, solids were filtered and washed twice with 5ml THF to afford 2f. ^{1}H NMR (400 MHz, D_2O) 8.79 (s, 1H), 7.50 (d, 2H), 7.46 (d, 2H), 4.36-4.25 (m, 4H), 3.89 (s, 6H), 2.58-2.43 (m, 2H).

Synthesis of 2g': In the 25ml pressure bottle, 1-methylimidazole (15.7 mmol, 2.5 equiv) was added into the solution of 3-bromo-2-(bromomethyl)propionic acid (6.27 mmol, 1 equiv) in toulene (10 ml). The reaction mixture was stirred at 135℃ for 72 h. After cooling to RT, solvent in the upper layer was dumped. Residual solids was recrystallized with ethyl acetate and methanol to afford 2g. ^{1}H NMR (400 MHz, D_2O) 8.77 (s, 2H), 7.49 (t, 2H), 7.46 (t, 2H), 4.50 (d, 4H), 3.89 (s, 6H), 3.45 (p, 1H).

Synthesis of 2h': In the 15ml pressure bottle, 1-methylimidazole (25 mmol, 2.5 equiv) was added into the solution of 1,3-dibromo-2-propanol (10 mmol, 1 equiv) in THF (5 ml). The reaction mixture was stirred overnight and heated to 100℃ for 72 h. After cooling to RT, solids were filtered and washed twice with 5ml THF to afford 2f. ^{1}H NMR (400 MHz, D_2O) 8.79 (d, 2H), 7.56-7.50 (m, 2H), 7.48 (dd, 2H), 4.55 (d, 1H), 4.50 (t, 1H), 4.41-4.33 (m, 1H), 4.24 (d, 1H), 4.22-4.17 (m, 1H), 3.91 (s, 6H).

Synthesis of 2i': In the 15ml pressure bottle, 1,2-dimethylimidazole (25 mmol, 2.5 equiv) was added into the solution of 1,3-dibromo-2-propanol (10 mmol, 1 equiv) in THF (5 ml). The reaction mixture was stirred overnight and heated to 100℃ for 72 h. After cooling to RT, solids were filtered and washed twice with 5ml THF to afford 2f. ^{1}H NMR (400 MHz, D_2O) 7.39 (t, 2H), 7.37 (d, 2H), 4.46 (d, 1H), 4.42 (d, 1H), 4.35-4.28 (m, 1H), 4.23 (d, 1H), 4.20 (d, 1H), 3.79 (d, 6H), 2.61 (d, 6H).

Synthesis of 2c-2i: The corresponding equal molar alkali was added to the aqueous solution of 2c'-2i'. After the absorption of CO_2 reaches equilibrium, the catalyst 2c-2i was prepared. Taking the synthesis of guanidine-functionalized and hydroxyl-bridged IL (2h) as an example, 2h' (0.1910 g, 0.5 mmol) and TMG (0.0576 g, 0.5 mmol) were added into the deionized water (0.45 g, 25 mmol). After the absorption of CO_2 reaches equilibrium, the aqueous solution of catalyst

guanidine-functionalized and hydroxyl-bridged IL (2h) were synthesized and could be directly used in the reaction.

General procedure for the hydration of epoxides.

Take catalyst guanidine-functionalized and hydroxyl-bridged IL (2h) and PO as an example. In a typical experiment, catalyst 2h' (0.1910 g, 0.5 mmol), TMG (0.0576 g, 0.5 mmol) and deionized water (0.45 g, 25 mmol) was firstly saturated with CO_2 to get aqueous solution of catalyst 2h, . Then aqueous solution of catalyst 2h, TMG (0.1152 g, 1 mmol) and PO (0.2904 g, 5 mmol) were added into a 30ml stainless steel autoclave equipped with a magnetic stirrer. At room temperature, replaced the air in the reactor using CO_2 and maintained CO_2 pressure at 1 bar. Then the autoclave was heated to 50^{o}C in a water bath. After stirring for 24 h, the autoclave was cooled in an ice-water bath. The reaction mixtures were analyzed by GC, GC-MS, and 2-heptanone was used as the internal standard. For other epoxides, the reaction mixtures were analyzed by ^{1}H NMR and trioxymethylene or acetonitrile was used as the internal standard.

Isotope labeling experiments

Catalyst 2h' (0.1910 g, 0.5 mmol), TMG (0.0576 g, 0.5 mmol) and $H_2{}^{18}O$ (0.5 g, 25 mmol) was firstly saturated with CO_2 to get the solution of catalyst 2h. Then the solution of catalyst 2h, TMG (0.1152 g, 1 mmol) and PO (0.2904 g, 5 mmol) were added into a 30ml stainless steel autoclave equipped with a magnetic stirrer. At room temperature, replaced the air in the reactor using CO_2 and maintained CO_2 pressure at 1 bar. Then the autoclave was heated to 50^{o}C in a water bath. After stirring for 24 h, the autoclave was cooled in an ice-water bath. The reaction mixtures were analyzed by GCTOF-HRMS (Waters GCT Premier).

2. Comparing the effects of various catalysts

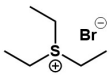
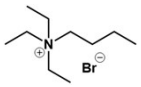
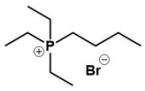
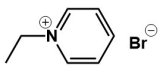
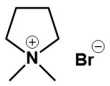
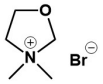
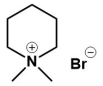
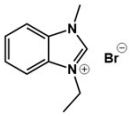
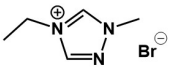
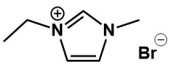
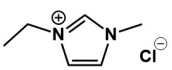
Table S1. The comparison of the hydration of PO catalyzed by metal and metal-free catalyst

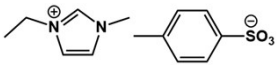
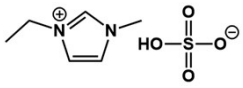
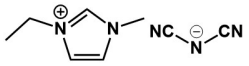
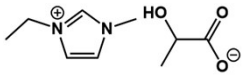
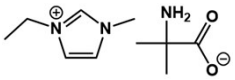
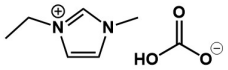
Entry	Catalyst	Reaction condition	Yield (%)	Refs
1	Guanidine-functionalized and hydroxyl-bridged IL (2h)	50 ^{o}C, 1bar CO_2, H_2O/PO = 5 : 1	97	This work
2	VBImBr/VIM	100 ^{o}C, 1.5 MPa CO_2, H_2O/EO = 1.5 : 1	89	[1]
3	DMIC	120 ^{o}C, 2 MPa N_2, H_2O/PO = 5 : 1	89	[2]
4	[Co^{III}(salen)] Encapsulated in Silica-Based Nanoreactors	40 ^{o}C, H_2O/PO = 2 : 1	96	[3]

5	Sn-H-SSZ-13 Zeolite	60 °C, H_2O/PO = 2 : 1	71	[4]
6	Sn-Beta Zeolites	40 °C, H_2O/PO = 2 : 1	36	[5]
7	Co^{III}(salen)-OTs Encapsulated in Silica Nanocages	40 °C, H_2O/PO = 2 : 1	99	[6]
8	Layered niobic acids	110 °C, H_2O/EO = 8 : 1	92	[7]
9	Cobalt–Salen Complexes on Flexible POFs	40 °C, H_2O/PO = 2 : 1	99	[8]
10	Polymorph CIT-13 into Single Crystalline ECNU-21 Zeolite	60 °C, H_2O/PO = 15 : 1	34	[9]

3. Screening of common cations and anions

Table S2. Prediction of the effect of common cations and anions on reaction energy barrier

Entry	Catalyst	Ⅰ	Ⅱ
1		35.38	15.64
2		32.26	14.68
3		32.50	14.53
4		32.50	16.97
5		35.22	18.78
6		33.85	18.50
7		33.20	17.80
8		34.08	18.14
9		30.62	16.98
10		31.10	16.92
11		30.41	16.01
12		29.12	19.70

13		30.65	15.50
14		31.65	15.33
15		28.03	24.30
16		24.53	33.05
17		27.94	18.93
18		25.12	27.24

4. NMR of catalyst 2h

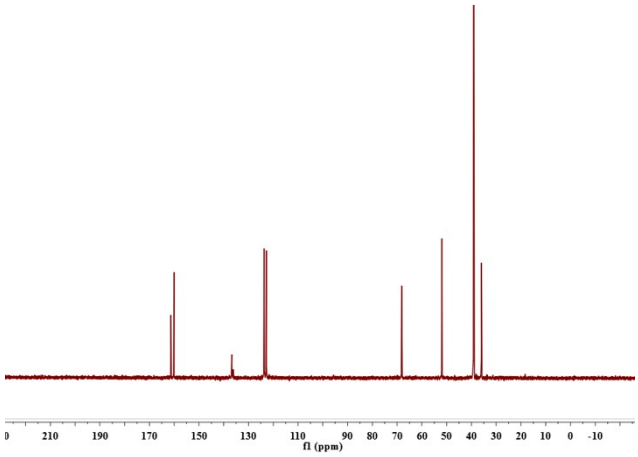
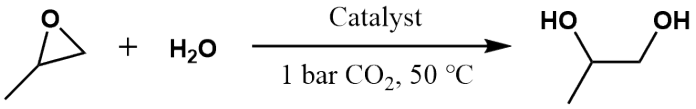


Figure S1. NMR of catalyst 2h

5. Screening of reaction conditions

Table S3. Optimization of the Reaction Conditions



entry	conditions[a]	yield(%)[b]
1	H_2O (1 equiv), catalyst (0.1 equiv)	53
2	H_2O (1.5 equiv), catalyst (0.1 equiv)	56
3	H_2O (2 equiv), catalyst (0.1 equiv)	66
4	H_2O (3 equiv), catalyst (0.1 equiv)	73
5	H_2O (4 equiv), catalyst (0.1 equiv)	91
6	H_2O (5 equiv), catalyst (0.02 equiv)	42

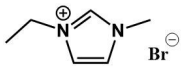
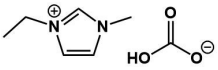
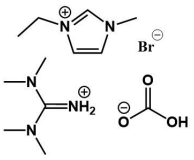
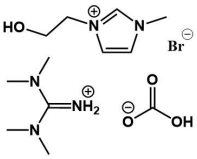
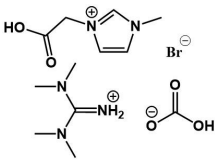
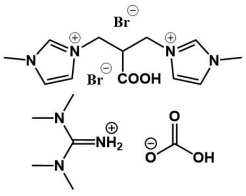
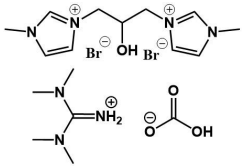
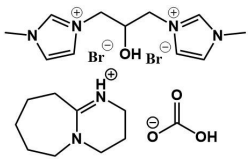
7	H_2O (5 equiv), catalyst (0.05 equiv)	67
8	H_2O (5 equiv), catalyst (0.1 equiv)	97
9	H_2O (5 equiv), catalyst (0.2 equiv)	76

Reaction conditions: PO (5 mmol), catalyst, TMG (1mmol), 50 °C, 24 h and CO_2 (~1 bar).

[b]Determined by GC.

6. Trend of hydrogen bond multiplicity and yield

Table S4. The trend of hydrogen bond multiplicity and yield

entry	multiplicity of hydrogen bonds	catalyst	yield (%)
1	1		25
2	1		30
3	2		68
4	3		76
5	3		65
6	4		88
7	4		97
8	4		88

7. Isotope labeling experiment

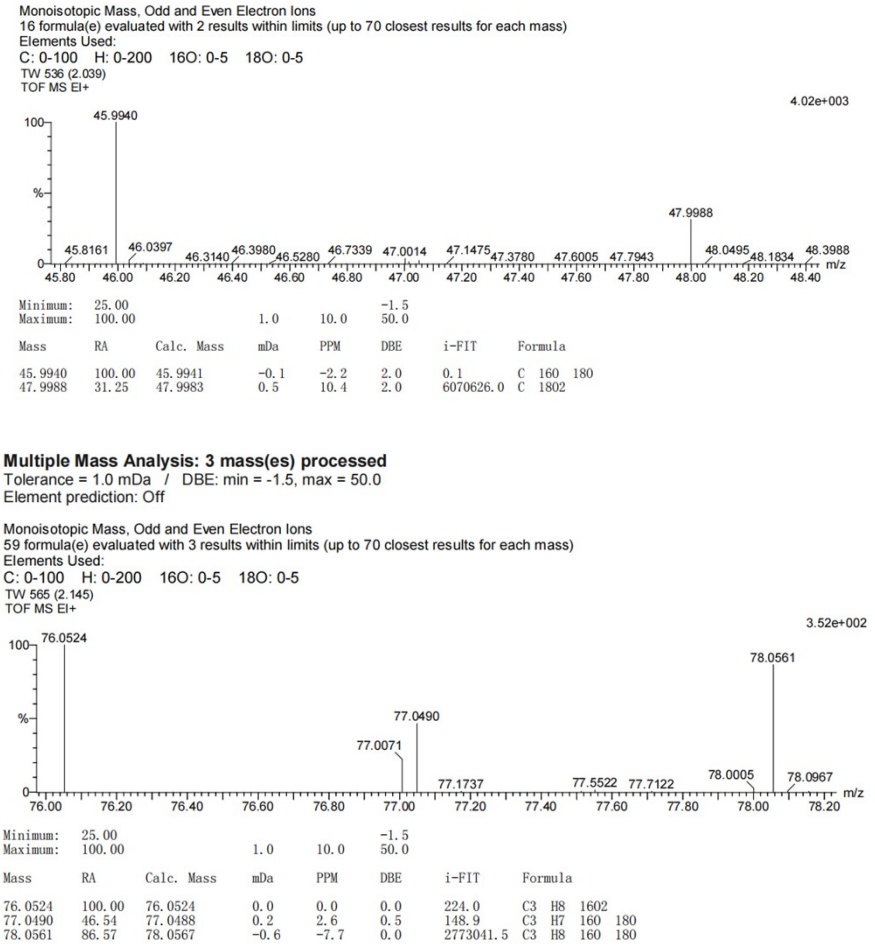


Figure S2. Spectra of the product in isotope labeling experiment

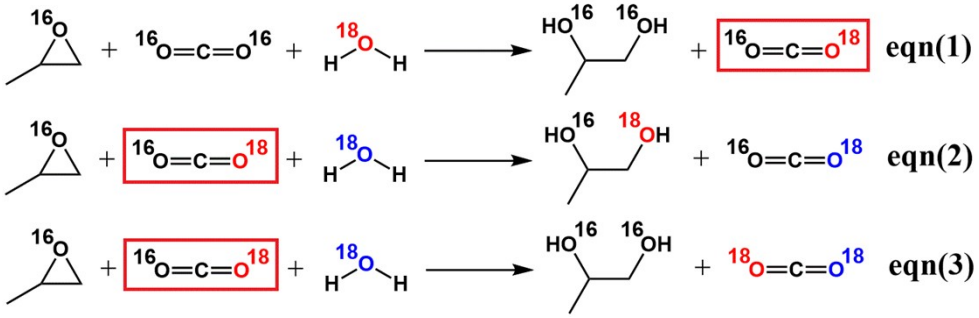


Figure S3. The role of CO_2 as the cocatalyst

When CO_2 first participated in the reaction, one of ^{16}O was replaced by the ^{18}O of $H_2{}^{18}O$, and turned into $C^{16}O^{18}O$ (eqn (1)). Then due to the low amount, CO_2 had to participate in hydration reaction multiple times. In the following reaction, the $C^{16}O^{18}O$ gave its ^{18}O or ^{16}O to the products and generated PG (m/z 78) (eqn (2)), and $C^{18}O^{18}O$ (m/z 48) (eqn (3)), which also proved that CO_2 was a cocatalyst.

8. Interaction between anions and cations[10,11,12]

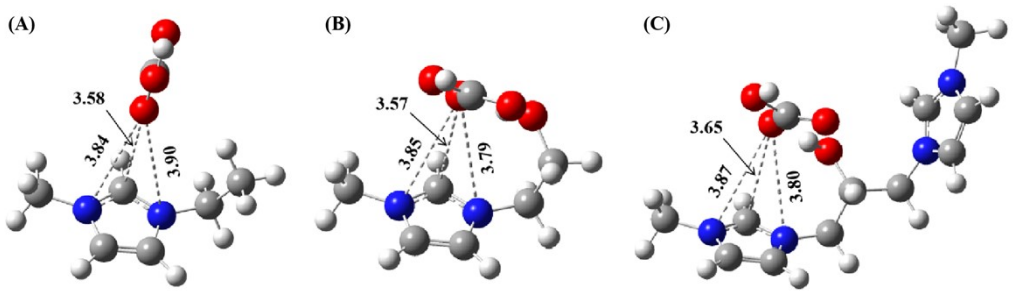


Figure S4. Optimized structures of (A) A-1H, (B) B-2H and (C) C-3H . The dashed lines depict the intermolecular distances in angstroms.

Optimized structures of catalysts with different hydrogen bonds was depicted in Figure S4. From (A) A-1H to (B) B-2H, the addition of hydrogen bond led to the decrease of the distance between anions and cations (3.58A to 3.57A), which may be the reason for the increase of ring-closing barrier of cyclic carbonate (II) in the process catalyzed by B-2H (Table 1, entry 2 and 3). From (B) B-2H to (C) C-3H, the addition of hydrogen bond led to the increase of the distance between anions and cations (3.57A to 3.65A), which may be the reason why the catalyst C-3H had good performance in both ring opening of epoxy (I) and ring closing of cyclic carbonate (II) process.

9. DFT calculation

All calculations were performed with the Gaussian 09 package. B3LYP was chosen as the function and the structures of intermediates and transition states were all optimized at first. The frequency calculations in screening (Table S1) and optimization (Table 1) were carried out at the B3LYP/6-31G(d,p) level. Geometry optimizations and frequency calculations in the effect of catalyst 2h and $[N_{1111}][HCO_3]$ on the reaction (Figure 3 and S5) were carried out at the B3LYP/6-311++G(d,p) level. And the solvation effect of water was included by using solvation model density (SMD). All the relative energies reported in this paper were in the unit of kcal/mol.

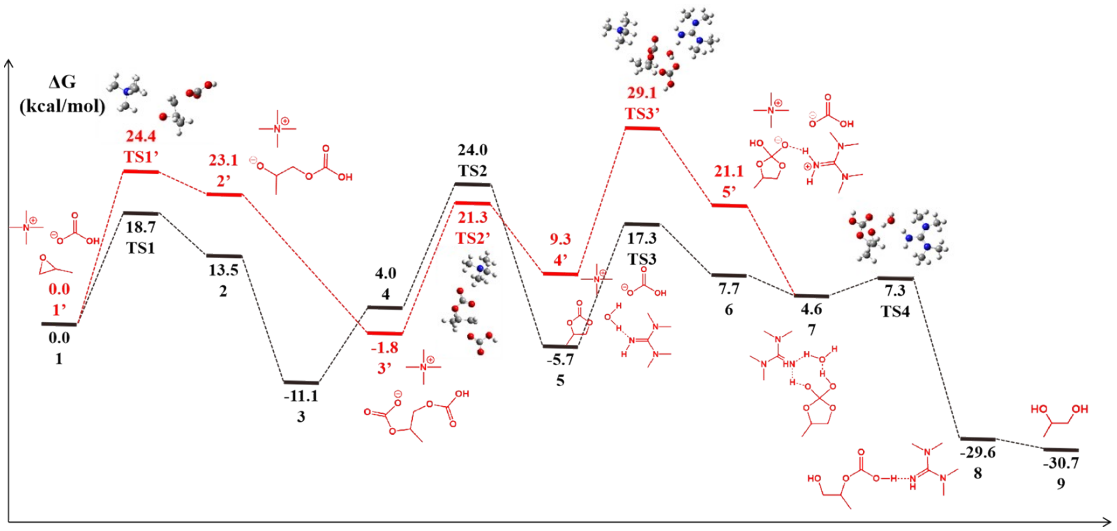
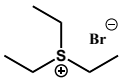
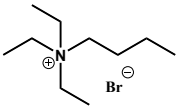
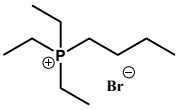
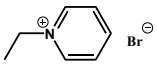
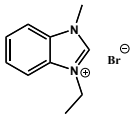
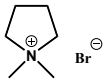
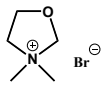
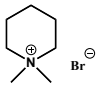
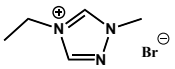
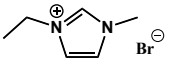
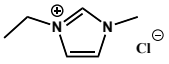
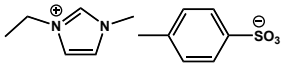
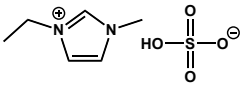
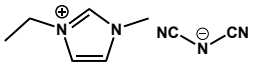
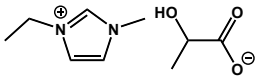
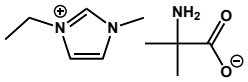
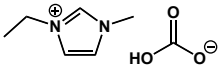
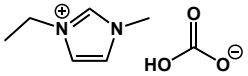
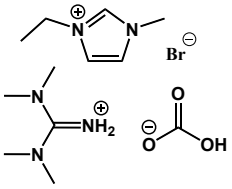
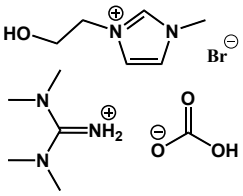
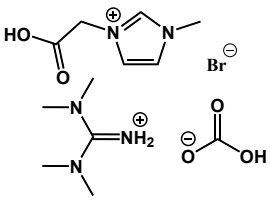
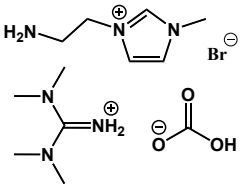


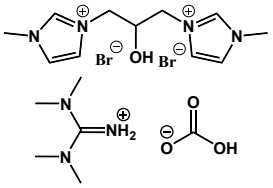
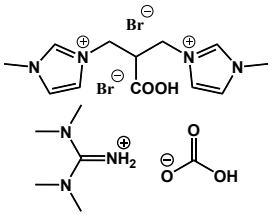
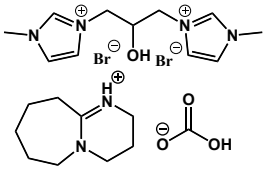
Figure S5. Computational studies of the reaction pathway catalyzed by $[N_{1111}][HCO_3]$ (red pathway) and catalyst 2h (black pathway)

Naming of the intermediates and transition states

Entry	Catalyst	I	II
1		a1 → TSa1	a2 → TSa2
2		b1 → TSb1	b2 → TSb2
3		c1 → TSc1	c2 → TSc2
4		d1 → TSd1	d2 → TSd2
5		e1 → TSe1	e2 → TSe2
6		f1 → TSf1	f2 → TSf2
7		g1 → TSg1	g2 → TSg2
8		h1 → TSh1	h2 → TSh2
9		i1 → TSi1	i2 → TSi2

10		j1 → TSj1	j2 → TSj2
11		k1 → TSk1	k2 → TSk2
12		l1 → TSl1	l2 → TSl2
13		m1 →TSm1	m2 → TSm2
14		n1 → TSn1	n2 → TSn2
15		o1 → TSo1	o2 → TSo2
16		p1 → TSp1	p2 → TSp2
17		q1 → TSq1	q2 → TSq2
18		s1 → TSs1	s2 → TSs2

entry	catalyst	I	II	III	IV
1		s1 → TSs1	s2 → TSs2	s3 → TSs3	s4 → TSs4
2		s1 → TSs1	t2 → TSt2	t3 → TSt3	t4 → TSt4
3		u1 → TSu1	u2 → TSu2	u3 → TSu3	t4 → TSt4
4		v1 → TSv1	v2→ TSv2	v3 → TSv3	t4 → TSt4
5		w1 → TSw1	w2 → TSw2	w3 → TSw3	t4 → TSt4

6		x1 → TSx1	x2 → TSx2	x3 → TSx3	t4 → TSt4
7		y1 → TSy1	y2 → TSy2	y3 → TSy3	t4 → TSt4
8		x1 → TSx1	z2 → TSz2	z3 → TSz3	z4 → TSz4

9. Cartesian coordinates of geometric structures in DFT calculations

1

Charge = 0 Multiplicity = 1

C	4.49384	-2.81376	0.50801
C	3.29223	-2.96582	1.12316
C	3.40849	-0.89233	0.35887
N	4.54545	-1.51389	0.03686
H	5.30954	-3.50209	0.36708
H	2.85684	-3.81365	1.62384
H	3.19028	0.14577	0.13284
C	1.26336	-1.49332	1.49116
H	1.13599	-2.01951	2.43742
H	1.16779	-0.42253	1.67232
C	0.21354	-1.95913	0.47245
H	0.44904	-2.98312	0.17185
C	-1.16284	-1.94531	1.15132
H	-1.16771	-2.6448	1.98833
H	-1.40144	-0.94972	1.5271
N	-2.23513	-2.32748	0.22613
C	-2.37185	-3.55016	-0.40841
C	-3.21427	-1.5166	-0.18934
C	-3.46474	-3.45958	-1.21072
H	-1.69261	-4.36664	-0.23297
H	-3.39058	-0.50575	0.15276
H	-3.9212	-4.18089	-1.86682
O	0.25094	-1.19034	-0.72021
H	-0.10046	-0.28846	-0.56463
C	-5.1641	-1.65003	-1.73423
H	-4.99919	-1.65602	-2.81099
H	-6.02758	-2.2665	-1.48782
H	-5.32802	-0.63087	-1.39218
C	5.65954	-0.9119	-0.70386
H	6.5762	-1.02287	-0.12596
H	5.76616	-1.41466	-1.66479
H	5.43892	0.14474	-0.85474
N	2.63039	-1.75297	1.02665
N	-3.97667	-2.18362	-1.05803
B	3.8924	2.58846	-0.58972
C	-0.05647	2.53612	-1.10236
C	-1.05334	2.53311	-0.0307
O	-0.88308	1.35576	-0.87675
H	-0.27365	3.05104	-2.03359
H	0.99634	2.4073	-0.8612
H	-1.99295	3.04086	-0.23045
C	-0.6858	2.3831	1.41619
H	-0.57052	3.37374	1.86687
H	-1.47233	1.85645	1.96291
H	0.25482	1.83928	1.52909
C	-4.64229	2.34	0.88719
O	-4.54365	3.40493	1.53958
O	-5.18578	2.43692	-0.40102
H	-5.38804	3.3695	-0.56175
O	-4.32461	1.17805	1.22116

TS1

Charge = 0 Multiplicity = 1

C	-3.34472	1.79283	-1.39285
C	-3.52233	1.65428	0.05155
O	-2.24703	2.59387	-0.98097
H	-3.02966	0.87056	-1.89341
H	-2.87654	0.98035	0.59075
H	-3.96365	2.48294	0.58384
C	-4.40872	2.51753	-2.18917
H	-4.00922	2.80797	-3.16537
H	-5.275	1.87018	-2.35569
H	-4.73957	3.41853	-1.66474
C	-5.04835	-0.68687	0.36937
O	-4.04213	-1.36518	0.11594
O	-6.25554	-1.33603	0.58708

H	-6.09642	-2.28681	0.49277
O	-5.15522	0.57471	0.46899
C	0.94292	-2.60431	0.85379
C	-0.72792	-1.59221	1.89428
C	-0.23591	-2.55022	2.72354
N	0.80627	-3.16891	2.05519
H	1.67046	-2.86487	0.09001
H	-1.53557	-0.89255	2.0242
H	-0.53137	-2.84788	3.71514
C	-0.12737	-0.75452	-0.43205
H	-1.18986	-0.6837	-0.66223
H	0.38888	-1.22431	-1.27108
C	0.42091	0.66733	-0.19558
H	-0.01787	1.0749	0.72326
O	0.06977	1.47188	-1.30632
H	-0.84758	1.86977	-1.1566
N	0.01836	-1.64402	0.72934
C	1.61492	-4.27667	2.57209
H	2.38914	-4.50914	1.84492
H	2.07204	-3.97928	3.51494
H	0.98068	-5.14857	2.72833
C	1.9443	0.65119	-0.05321
H	2.25071	0.00542	0.76894
H	2.40962	0.28397	-0.96856
N	2.48753	1.98942	0.21833
C	2.59018	2.54953	1.42848
C	2.90373	2.9078	-0.72786
H	2.33955	2.07596	2.3632
C	3.27168	4.03237	-0.05801
H	2.91068	2.6769	-1.77876
H	3.65962	4.97216	-0.41163
C	3.34923	4.72489	2.37901
H	4.41077	4.96914	2.37919
H	2.7615	5.63079	2.23678
H	3.079	4.25306	3.32102
N	3.06625	3.78777	1.28772
Br	2.89848	-2.6362	-2.18575

2

Charge = 0 Multiplicity = 1

C	-1.40665	-3.20734	0.74898
C	-0.73196	-2.72306	1.82332
C	0.5324	-2.4147	0.03702
N	-0.59429	-3.0128	-0.35668
H	-2.38583	-3.64363	0.66484
H	-1.00925	-2.67072	2.8616
H	1.3825	-2.11589	-0.5752
C	1.40489	-1.35172	2.0485
H	1.35223	-1.55426	3.11897
H	2.4051	-1.58788	1.67982
C	1.01859	0.14426	1.70253
H	0.48001	0.55689	2.57402
C	2.36328	0.94591	1.54058
H	2.67263	1.40369	2.48386
H	3.15337	0.289	1.17163
N	2.23605	1.99532	0.52127
C	3.0484	2.1097	-0.59224
C	1.21504	2.84699	0.40077
C	2.5131	3.08426	-1.37514
H	3.87227	1.43001	-0.75101
H	0.33586	2.89692	1.03049
H	2.82889	3.47595	-2.32603
O	0.24429	0.199	0.57484
H	-0.61199	0.98979	0.64675
C	0.41732	4.5244	-1.23791
H	0.80612	5.53305	-1.08755
H	0.2464	4.35196	-2.3003
H	-0.52299	4.3994	-0.70337
C	-0.95183	-3.31868	-1.74225
H	-1.11783	-4.39115	-1.85319

H	-1.85516	-2.76571	-1.99965
H	-0.12889	-3.01345	-2.3857
N	0.4863	-2.25555	1.36379
N	1.36457	3.53007	-0.73785
Br	3.83972	-1.45264	-0.76248
C	-2.96221	1.22059	-0.38071
C	-2.71697	1.4039	1.04705
O	-1.48086	1.87861	0.66769
H	-2.26079	0.51388	-0.81052
H	-2.92778	2.17849	-0.88984
H	-2.6725	0.45216	1.60219
C	-3.58496	2.40257	1.79597
H	-4.60224	2.0216	1.92985
H	-3.15692	2.60358	2.7828
H	-3.63776	3.34741	1.24698
C	-4.47621	-0.52809	-1.00625
O	-3.64467	-1.41753	-1.04928
O	-5.79063	-0.74863	-1.25183
H	-5.87335	-1.68929	-1.45355
O	-4.29113	0.73825	-0.73721

3

Charge = 0 Multiplicity = 1

C	-2.00828	-3.60573	1.1332
C	-0.89139	-3.09954	0.54424
C	-2.66379	-2.18782	-0.432
N	-3.10232	-3.01934	0.5156
H	-2.12005	-4.31635	1.9333
H	0.16974	-3.23805	0.71265
H	-3.31563	-1.54143	-1.01312
C	-0.42848	-1.37791	-1.23793
H	0.52994	-1.89515	-1.2646
H	-0.83203	-1.29992	-2.25012
C	-0.21406	0.02043	-0.59816
H	0.66203	0.43912	-1.11804
C	-1.43291	0.91186	-0.86247
H	-1.47404	1.19542	-1.91719
H	-2.38341	0.43039	-0.61898
N	-1.42834	2.14899	-0.05793
C	-2.56802	2.88196	0.22235
C	-0.38903	2.70696	0.56361
C	-2.18529	3.91361	1.02199
H	-3.53593	2.55057	-0.13691
H	0.61376	2.31922	0.58435
H	-2.75912	4.70536	1.47117
O	0.01282	-0.0591	0.77715
H	0.9874	-0.32706	0.91535
C	0.0105	4.65744	2.06004
H	1.03916	4.303	2.02696
H	-0.0307	5.68128	1.6872
H	-0.34531	4.62521	3.09022
C	-4.51724	-3.22963	0.8375
H	-4.87529	-4.15047	0.37455
H	-4.62468	-3.29473	1.91975
H	-5.08107	-2.37081	0.46826
N	-1.32508	-2.22211	-0.43575
N	-0.8185	3.79005	1.22318
Br	-4.99395	0.31982	-0.68083
C	5.13174	-0.89999	0.58702
H	4.64402	-0.10568	1.15297
C	6.33377	-1.44584	1.35157
H	7.06945	-0.65835	1.5384
H	6.00481	-1.84579	2.31214
H	6.81721	-2.25467	0.79647
C	4.15445	1.45294	-1.31775
O	4.73378	2.24592	-0.61464
O	3.06466	1.76941	-2.06213
H	2.94954	2.72251	-1.95884
O	4.45181	0.18313	-1.52762
O	4.20582	-1.9734	0.39345

C	2.84147	-1.72252	0.51672
O	2.50362	-0.56749	0.91065
O	2.11444	-2.67825	0.21995
C	5.56655	-0.36561	-0.7737
H	5.93097	-1.18018	-1.39927
H	6.33171	0.40414	-0.66508

4

Charge = 0 Multiplicity = 1

C	5.28797	-2.43208	-1.48554
C	4.04471	-2.40257	-0.93617
C	5.31093	-0.95539	0.15895
N	6.06058	-1.51727	-0.79058
H	5.69275	-3.01424	-2.29574
H	3.15658	-2.9836	-1.1325
H	5.65647	-0.19319	0.84251
C	2.91532	-1.09708	0.91618
H	2.21634	-1.92988	0.84707
H	3.24536	-1.00465	1.95157
C	2.22242	0.19938	0.4627
H	1.31261	0.26319	1.06899
C	3.11573	1.40378	0.7706
H	3.35951	1.40867	1.83523
H	4.04827	1.35678	0.20917
N	2.52799	2.71338	0.42857
C	3.2946	3.83407	0.14631
C	1.23781	3.06094	0.39559
C	2.43337	4.86414	-0.06254
H	4.37378	3.78158	0.1324
H	0.39626	2.41227	0.56662
H	2.61114	5.8978	-0.30902
O	1.88392	0.12392	-0.91413
H	0.93911	0.38666	-1.03136
C	-0.08826	5.12277	-0.05388
H	-0.92731	4.46586	0.163
H	-0.08317	5.95671	0.64683
H	-0.1667	5.49691	-1.07402
C	7.4805	-1.23533	-1.02241
H	8.08319	-2.07216	-0.66974
H	7.64217	-1.08859	-2.08927
H	7.74334	-0.32484	-0.48521
N	4.0786	-1.47628	0.09363
N	1.15496	4.36036	0.09466
Br	6.87784	2.3673	0.70226
C	-2.5106	-2.06588	-1.08369
H	-3.45252	-1.52966	-0.99112
C	-2.47287	-2.83299	-2.39808
H	-3.29913	-3.54754	-2.44387
H	-2.57401	-2.13915	-3.23576
H	-1.53258	-3.37999	-2.50705
C	-3.61582	-2.0056	1.84989
O	-4.68041	-2.32771	1.35773
O	-3.48119	-1.30587	2.987
H	-4.36814	-1.10894	3.32985
O	-2.40814	-2.27245	1.36856
O	-1.42974	-1.10094	-1.04675
C	-1.69504	0.24033	-1.29837
O	-2.87164	0.61522	-1.47793
O	-0.65744	0.94944	-1.30753
C	-2.32735	-2.99658	0.10109
H	-1.33191	-3.44454	0.1171
H	-3.08655	-3.77859	0.09293
C	-6.65312	1.11859	-0.10818
N	-5.51569	0.41671	-0.04606
H	-5.46548	-0.43104	0.50492
H	-4.69587	0.64935	-0.60099
N	-6.8444	1.99171	-1.11385
N	-7.59778	0.93815	0.8394
C	-7.27064	0.31139	2.12278
H	-7.98442	0.67205	2.86458

H	-7.34228	-0.77988	2.072
H	-6.26991	0.59833	2.44346
C	-9.02997	0.98817	0.5178
H	-9.52934	1.80813	1.03917
H	-9.18026	1.09736	-0.5536
H	-9.48518	0.0452	0.83183
C	-7.63861	3.21445	-0.95286
H	-7.02893	4.06379	-1.27121
H	-8.54273	3.18404	-1.56516
H	-7.91077	3.36306	0.08875
C	-6.04907	1.91997	-2.3428
H	-5.12896	2.5064	-2.26405
H	-5.80298	0.88548	-2.57727
H	-6.65058	2.32186	-3.15864
Br	1.27981	-4.61982	0.15909

TS2

Charge = 0 Multiplicity = 1

C	-3.21528	-2.97855	2.40535
C	-2.29638	-2.22528	1.74583
C	-4.20204	-2.11076	0.62645
N	-4.39682	-2.89291	1.69066
H	-3.13537	-3.56486	3.30468
H	-1.25979	-2.03072	1.95793
H	-4.95865	-1.88542	-0.12024
C	-2.32133	-0.77834	-0.34419
H	-1.28631	-1.09351	-0.49066
H	-2.85047	-0.90689	-1.28806
C	-2.35084	0.69514	0.07477
H	-1.77298	1.22484	-0.69015
C	-3.7748	1.27217	0.07933
H	-4.24649	1.12624	-0.89269
H	-4.39333	0.80524	0.84555
N	-3.76034	2.71425	0.36536
C	-3.93685	3.29835	1.60671
C	-3.4074	3.66742	-0.50529
C	-3.70513	4.62987	1.45877
H	-4.21808	2.72165	2.47085
H	-3.19096	3.51734	-1.54995
H	-3.74484	5.43964	2.16714
O	-1.73106	0.85357	1.34402
H	-1.2106	1.68724	1.34359
C	-3.03822	6.1307	-0.47157
H	-2.22972	6.58692	0.09747
H	-2.71687	5.96077	-1.4966
H	-3.91276	6.78029	-0.46117
C	-5.65796	-3.55919	2.03208
H	-5.49512	-4.63573	2.07226
H	-6.00497	-3.20138	3.00092
H	-6.38848	-3.32216	1.25923
N	-2.92909	-1.69366	0.63461
N	-3.37609	4.83839	0.13197
Br	-7.2278	-2.11073	-1.34757
C	6.01937	1.96151	-0.77226
O	6.97068	1.37616	-1.31007
O	6.25273	3.1199	-0.06665
H	7.20125	3.30942	-0.1219
O	4.7994	1.59533	-0.8028
C	2.27986	2.16438	-0.84496
C	3.34197	2.67313	0.10612
H	2.49255	1.13106	-1.11181
H	3.55673	2.13236	1.0129
H	3.8918	3.57323	-0.10337
C	0.90114	3.04495	0.85232
O	-0.19928	3.147	1.41777
O	1.95539	3.72112	1.07978
O	1.02243	2.08814	-0.11704
C	2.11894	3.02369	-2.08679
H	3.05234	3.02662	-2.65454
H	1.33098	2.61825	-2.72428

H	1.86825	4.05421	-1.82268
C	4.93164	-2.28482	0.3655
N	4.29641	-1.38904	-0.39701
H	4.54199	-0.40318	-0.36452
H	3.44556	-1.6392	-0.91584
N	5.66381	-1.87704	1.4228
N	4.84103	-3.5956	0.05572
C	4.82619	-4.65152	1.07236
H	3.9076	-5.23271	0.95463
H	5.67996	-5.32334	0.95589
H	4.83593	-4.23134	2.07394
C	4.4467	-4.02589	-1.28877
H	4.84996	-3.34288	-2.03517
H	4.87071	-5.01639	-1.46066
H	3.36023	-4.07535	-1.40262
C	6.87859	-2.57565	1.85448
H	7.7033	-1.85816	1.86893
H	6.76263	-2.99142	2.85816
H	7.13254	-3.37246	1.16063
C	5.46127	-0.55808	2.02653
H	6.11313	0.19734	1.5777
H	4.42165	-0.25071	1.92779
H	5.69727	-0.63136	3.0895
Br	1.27261	-1.82365	-1.9078

5

Charge = 0 Multiplicity = 1

C	-3.11173	3.19532	-1.72142
C	-3.19139	2.01773	-1.0478
C	-2.95156	1.56699	-3.2006
N	-2.96919	2.89301	-3.06443
H	-3.1546	4.21269	-1.37277
H	-3.30748	1.81771	0.01097
H	-2.84897	1.03281	-4.13044
C	-3.04925	-0.43495	-1.73279
H	-3.82542	-0.66911	-1.00394
H	-3.28657	-0.94501	-2.66612
C	-1.66598	-0.88067	-1.24338
H	-1.39458	-0.33135	-0.33661
C	-1.62688	-2.38749	-0.97613
H	-2.07142	-2.92808	-1.81342
H	-0.58987	-2.71116	-0.89018
N	-2.32296	-2.83076	0.24748
C	-2.45971	-4.17021	0.57583
C	-2.87956	-2.09461	1.21866
C	-3.11522	-4.2242	1.76463
H	-2.03527	-4.94401	-0.04543
H	-2.93525	-1.01665	1.28679
H	-3.41753	-5.06344	2.36776
O	-0.68269	-0.64479	-2.25031
H	-0.28493	0.23091	-2.09262
C	-4.06718	-2.50663	3.3705
H	-5.08992	-2.88234	3.34602
H	-3.54614	-2.91444	4.23573
H	-4.06947	-1.41743	3.41417
C	-2.84546	3.86566	-4.15411
H	-3.72227	4.51164	-4.16258
H	-1.94684	4.46292	-4.00557
H	-2.77678	3.3255	-5.0961
N	-3.09914	1.0081	-1.99395
N	-3.36843	-2.92089	2.14796
Br	-3.62806	1.33827	2.65754
Br	0.55653	-5.6422	-1.12884
C	5.87541	0.40187	0.56032
N	4.8143	-0.01658	-0.22524
N	7.03763	-0.36732	0.47338
C	8.21582	0.126	1.18467
H	9.07865	-0.46112	0.86686
H	8.40745	1.17083	0.93573
H	8.12367	0.02895	2.2769

C	6.91817	-1.83075	0.56566
H	6.03654	-2.19324	0.04461
H	7.79947	-2.2929	0.1166
H	6.85637	-2.15114	1.61581
C	3.5438	0.69025	-0.07504
H	3.55919	1.68039	-0.54899
H	2.76666	0.0908	-0.55362
H	3.29816	0.80886	0.97924
C	5.05758	-0.42918	-1.61357
H	4.27484	-1.12466	-1.92604
H	5.03386	0.44057	-2.28469
H	6.02025	-0.91916	-1.72343
N	5.75234	1.45663	1.31383
H	6.53794	1.54032	1.95258
C	0.37929	4.13363	0.8639
C	-0.07703	2.81286	1.49022
H	0.50069	2.53291	2.36747
H	-1.14646	2.77657	1.70866
C	0.36339	2.47044	-0.72152
O	0.4766	1.90752	-1.79071
O	0.18949	1.83232	0.44132
O	0.41532	3.79253	-0.57082
H	1.40748	4.36746	1.14058
C	-0.53714	5.30969	1.09134
H	-0.57361	5.52891	2.16209
H	-0.16449	6.19634	0.57499
H	-1.54893	5.08572	0.7457
O	4.37841	3.85951	1.3461
H	4.9207	4.46136	0.82446
H	4.83725	2.976	1.28032

TS3

Charge = 0 Multiplicity = 1

H	4.28267	-0.05941	-0.30626
O	3.10582	-1.04016	-0.77049
C	1.16706	-0.16233	-3.02053
C	0.48568	-1.29671	-2.22663
H	2.03234	-0.54037	-3.56545
H	1.04061	-2.232	-2.28576
H	-0.55186	-1.45774	-2.51746
O	0.49596	-0.83202	-0.86063
O	1.66264	0.72139	-1.97482
C	1.43373	0.17092	-0.74306
O	1.54189	0.82193	0.28755
H	2.99116	-1.63914	-0.01184
C	-1.09524	2.73446	0.93274
N	-2.30156	2.45988	0.42583
N	-1.24309	3.61932	1.92052
C	-3.25561	3.17807	1.12853
C	-2.58912	1.48464	-0.63075
C	-2.58976	3.90743	2.06248
H	-4.30742	3.08911	0.89662
C	-3.01888	0.13085	-0.05637
H	-1.69467	1.38277	-1.24641
H	-3.3916	1.89912	-1.23999
H	-2.94444	4.60493	2.80193
C	-3.5645	-0.73755	-1.19641
H	-3.82298	0.29954	0.66276
H	-4.26526	-0.16117	-1.79934
H	-0.15928	2.30872	0.60298
Br	3.01041	-3.30432	2.0766
C	6.28057	0.69071	-0.18312
N	4.9608	0.71729	-0.01066
H	4.5412	1.57971	0.30467
N	6.98645	1.84958	-0.24348
N	6.91864	-0.49459	-0.30701
C	6.29209	3.12616	-0.42204
H	7.0019	3.84487	-0.83311
H	5.46874	3.01994	-1.12732
H	5.91199	3.52071	0.5273

C	8.32901	1.9703	0.33891
H	8.29836	2.70763	1.14666
H	8.65844	1.02343	0.75729
H	9.05183	2.30443	-0.40865
C	8.11687	-0.66937	-1.13224
H	8.36385	0.24393	-1.66548
H	8.97483	-0.97552	-0.52836
H	7.91857	-1.4522	-1.86985
C	6.29719	-1.74465	0.13517
H	5.7832	-2.25213	-0.68564
H	7.0863	-2.40165	0.5075
H	5.58646	-1.56573	0.93848
O	-1.97543	-0.50912	0.66875
H	-1.19486	-0.60944	0.09338
H	-2.75776	-1.09385	-1.83717
N	-4.2858	-1.91281	-0.6913
C	-5.55383	-1.88891	-0.26125
C	-3.77115	-3.1801	-0.48743
H	-6.19617	-1.01578	-0.27742
C	-4.76375	-3.92717	0.06565
H	-2.76144	-3.43541	-0.75841
H	-4.78834	-4.95933	0.37054
N	-5.86719	-3.10221	0.19623
C	-7.16071	-3.48616	0.77272
H	-7.04056	-3.7006	1.83395
H	-7.85782	-2.66188	0.64108
H	-7.53569	-4.37083	0.26037
C	-0.15574	4.19431	2.71786
H	-0.116	5.27016	2.55116
H	-0.33137	3.98859	3.77281
H	0.78173	3.73996	2.40575
Br	-6.54647	1.68764	-0.26281
C	0.25132	0.61684	-3.94215
H	0.78247	1.46152	-4.38741
H	-0.09106	-0.03341	-4.75199
H	-0.62212	0.99022	-3.40112

6

Charge = 0 Multiplicity = 1

C	-3.49611	3.71282	-0.10885
C	-3.69201	2.45375	-0.5828
C	-1.51278	2.86893	-0.60909
N	-2.13215	3.95194	-0.12846
H	-4.19833	4.44639	0.24671
H	-4.58218	1.84885	-0.71829
H	-0.44372	2.75548	-0.71256
C	-2.22606	0.57958	-1.41429
H	-3.14262	0.04082	-1.16519
H	-2.1545	0.63764	-2.50325
C	-0.94905	-0.07492	-0.87776
H	-0.86018	0.10397	0.2002
C	-0.94718	-1.60016	-1.12403
H	-1.21103	-1.82702	-2.15917
H	0.06055	-1.96858	-0.92656
N	-1.85348	-2.35339	-0.23533
C	-1.45575	-2.99626	0.92766
C	-3.17762	-2.50507	-0.38381
C	-2.57611	-3.53765	1.47609
H	-0.41006	-3.02278	1.22042
H	-3.82081	-2.05987	-1.13684
H	-2.70583	-4.12228	2.37007
O	0.16043	0.46229	-1.56482
H	0.73833	0.98765	-0.94253
C	-5.04918	-3.56709	0.8498
H	-5.23621	-4.58163	0.4946
H	-5.27618	-3.50063	1.91323
H	-5.65958	-2.84672	0.30051
C	-1.46089	5.1751	0.32095
H	-1.97347	5.54712	1.20764
H	-0.42958	4.92943	0.57725

H	-1.49714	5.93125	-0.46545
N	-2.44022	1.94472	-0.88829
N	-3.63889	-3.21659	0.6479
Br	-5.77525	-0.47632	-1.15779
Br	2.08857	-2.93053	0.99411
C	4.48467	-0.32121	-1.08055
N	4.62454	0.47438	-2.17682
N	5.4344	-1.26194	-0.83331
C	5.59825	-1.82251	0.51276
H	6.64397	-2.11751	0.63072
H	5.3593	-1.06336	1.25597
H	4.94596	-2.68486	0.67743
C	6.03103	-2.04928	-1.91103
H	5.6665	-1.70808	-2.87729
H	7.12319	-1.97675	-1.89361
H	5.75032	-3.10017	-1.78842
C	3.46572	1.16447	-2.74948
H	3.29447	2.13812	-2.28106
H	3.64655	1.30228	-3.81816
H	2.56877	0.56115	-2.62011
C	5.92952	0.97183	-2.60386
H	6.14272	0.68853	-3.63963
H	5.94345	2.06512	-2.53694
H	6.71332	0.57888	-1.96018
N	3.45645	-0.17782	-0.27111
H	3.11072	-0.98558	0.27299
C	0.58664	1.79732	3.09742
C	2.09224	2.12316	3.25238
H	2.2415	3.1267	3.66618
H	2.62131	1.39218	3.86608
C	1.5479	2.45364	1.05179
O	1.7098	2.02516	-0.163
O	2.6012	2.04718	1.92948
O	0.34776	1.99114	1.69327
H	-0.01825	2.51955	3.65722
C	0.20854	0.3773	3.49352
H	0.34378	0.23712	4.57097
H	-0.84166	0.18184	3.25991
H	0.82612	-0.35405	2.96515
O	1.44352	3.90851	1.12038
H	2.20359	4.22776	0.6195
H	2.88378	0.6857	-0.24427

7

Charge = 0 Multiplicity = 1

C	3.65354	1.24484	0.02898
C	4.18849	0.18857	-0.92633
H	4.12441	1.17437	1.01491
H	3.73433	2.2607	-0.35398
O	3.35217	-0.9575	-0.59109
O	2.25726	0.90315	0.11593
C	2.16942	-0.50977	0.0149
O	1.16702	-0.83155	-0.74775
H	1.28114	-0.81243	1.7385
H	-0.52257	-0.6023	0.07479
H	-0.71934	-0.44329	1.70889
O	-0.18137	-0.36692	2.54195
H	-0.17781	0.57622	2.75037
H	3.96883	0.46956	-1.96088
O	2.1038	-1.11061	1.27442
C	5.64823	-0.16795	-0.76556
H	5.92764	-0.97345	-1.44833
H	6.26412	0.70402	-1.00305
H	5.86355	-0.47958	0.25946
C	-2.59839	-0.09151	-0.1359
N	-1.50669	-0.77601	0.11127
H	-1.6634	-1.77044	-0.02346
N	-3.84599	-0.67525	-0.31096
N	-2.54114	1.28046	-0.21576
C	-3.59628	2.11285	0.37372

H	-3.25664	2.51854	1.33442
H	-3.83455	2.94968	-0.28719
H	-4.49956	1.53781	0.55139
C	-1.22721	1.92005	-0.19489
H	-0.78028	1.92567	0.80634
H	-0.55126	1.41859	-0.88367
H	-1.34946	2.95403	-0.52263
C	-4.69875	-0.21747	-1.41886
H	-4.43249	-0.73866	-2.34754
H	-5.74205	-0.437	-1.18539
H	-4.60165	0.85056	-1.58641
C	-3.94414	-2.12072	-0.10701
H	-3.45624	-2.69286	-0.90789
H	-3.50962	-2.405	0.85183
H	-5.00024	-2.39198	-0.09246

TS4

Charge = 0 Multiplicity = 1

C	-3.00859	1.25847	0.68082
C	-2.3383	1.161	-0.69838
C	-3.92151	-0.82063	0.10129
H	-2.379	0.78098	1.43839
H	-1.27337	1.42244	-0.60299
H	-2.80386	1.89827	-1.37297
O	-4.21011	0.45798	0.52893
O	-2.52821	-0.15053	-1.16214
O	-4.91454	-1.19874	-0.77276
H	-4.87187	-2.16301	-0.84996
O	-3.33331	-1.65427	0.7988
H	-0.60519	-2.21588	-0.14707
C	-3.40261	2.65181	1.11431
H	-3.87613	2.64364	2.09897
H	-2.50759	3.27753	1.17449
H	-4.09016	3.10421	0.39453
O	-0.42787	-1.61382	-0.87973
H	-1.27426	-1.04176	-0.96663
H	0.97527	-0.49605	-0.40113
C	2.94685	0.069	-0.02877
N	1.63833	0.26855	-0.22212
H	1.28657	1.21007	-0.31126
N	3.3809	-1.13819	0.38508
N	3.81489	1.08024	-0.24677
C	2.46267	-2.11279	0.98011
H	2.02949	-2.77299	0.223
H	3.02709	-2.72065	1.68869
H	1.6656	-1.60501	1.51972
C	4.68985	-1.68033	0.00474
H	5.18931	-1.02717	-0.70535
H	5.3284	-1.82085	0.87992
H	4.53528	-2.65107	-0.47325
C	5.0245	1.26469	0.56513
H	5.9235	1.21674	-0.05322
H	4.97801	2.24924	1.038
H	5.08533	0.51463	1.3484
C	3.40842	2.25976	-1.01571
H	2.8957	2.99739	-0.38863
H	4.30611	2.7214	-1.42751
H	2.76158	1.9729	-1.84372

8

Charge = 0 Multiplicity = 1

C	-5.14905	0.05928	-0.93085
C	-4.06217	-0.6374	-0.11761
H	-4.78075	0.22129	-1.95213
H	-3.72337	-1.52595	-0.6559
O	-2.9624	0.31482	-0.08176
O	-5.58058	1.28368	-0.3519
C	-1.70896	-0.18194	0.00722
O	-0.84943	0.81367	0.05852
H	-4.8034	1.84805	-0.26464

H	1.32941	-1.30484	0.28965
O	-1.44562	-1.3677	0.02986
H	-6.02979	-0.58501	-0.98451
C	-4.48027	-1.00448	1.29941
H	-5.29742	-1.73105	1.26859
H	-3.64444	-1.45599	1.83617
H	-4.82521	-0.12204	1.84101
C	2.78578	-0.04147	0.06688
N	1.53072	-0.31202	0.22908
H	0.09897	0.43191	0.12422
N	3.76168	-0.98398	-0.25229
N	3.23946	1.2586	0.20123
C	3.3213	-2.30135	-0.68948
H	4.15497	-2.79995	-1.18872
H	2.99508	-2.94142	0.14424
H	2.50194	-2.20808	-1.40248
C	5.02357	-0.99995	0.48979
H	4.97831	-1.71562	1.32266
H	5.84544	-1.29337	-0.16971
H	5.23439	-0.01554	0.8995
C	2.32261	2.24341	0.76628
H	2.90632	3.10004	1.11167
H	1.58345	2.59426	0.03494
H	1.78911	1.81177	1.61085
C	4.1804	1.8145	-0.77065
H	3.6475	2.39003	-1.53984
H	4.88697	2.48403	-0.27153
H	4.73443	1.01992	-1.26378

9

Charge = 0 Multiplicity = 1

C	-0.46596	0.04936	-0.33631
H	-0.36402	0.08664	-1.43119
C	0.72217	-0.73128	0.21152
H	0.73516	-1.74392	-0.21106
H	0.64122	-0.79695	1.30366
C	-1.79589	-0.58929	0.02992
H	-1.91183	-0.64067	1.11587
H	-2.61677	0.00837	-0.37042
H	-1.87239	-1.59913	-0.38226
O	-0.46064	1.37782	0.184
H	0.43293	1.7219	0.06233
O	1.90285	-0.01036	-0.16459
H	2.6561	-0.34863	0.32704

a1

Charge = 0 Multiplicity = 1

C	0.77513	-1.02766	-1.54235
H	0.2567	-0.07975	-1.32604
H	1.37164	-0.92422	-2.45485
C	-0.14854	-2.23742	-1.6119
H	-0.71744	-2.1646	-2.54437
H	0.3966	-3.18655	-1.63045
H	-0.86906	-2.23512	-0.79335
C	1.28665	-0.8026	1.38636
H	2.14918	-0.62484	2.03528
H	0.72846	0.13447	1.23072
C	0.4285	-1.94978	1.90734
H	0.20087	-1.74068	2.95748
H	-0.52199	-2.00852	1.37544
H	0.94167	-2.91605	1.86693
C	3.00154	0.40647	-0.56547
H	3.32248	0.31068	-1.60687
H	2.24321	1.20149	-0.48129
C	4.19122	0.59428	0.36774
H	4.72662	1.49662	0.05772
H	3.87846	0.74789	1.40334
H	4.89312	-0.24442	0.32909
C	-2.94637	0.08748	1.27487
C	-3.23473	0.01452	-0.16088
O	-2.53417	-1.06347	0.50462
H	-2.13771	0.7446	1.59054
H	-2.5852	0.62365	-0.79076
Br	-0.15279	2.02526	-0.08581
S	2.08904	-1.17224	-0.24259
C	-4.06637	-0.19369	2.29376
H	-3.67802	-0.09785	3.28618
H	-4.86148	0.50829	2.15255
H	-4.43781	-1.18687	2.15047
H	-4.20544	-0.22501	-0.54199

TSa1

Charge = 0 Multiplicity = 1

C	-1.08993	0.08177	-1.1445
H	-0.1287	0.5608	-0.93281
H	-0.90862	-0.99353	-1.18812
C	-1.70447	0.53368	-2.46462
H	-0.95656	0.33357	-3.23814
H	-2.60296	-0.02629	-2.73666
H	-1.9328	1.59808	-2.50675
C	-1.68579	1.72245	0.69501
H	-2.30337	1.78128	1.59236
H	-0.62709	1.73673	0.97215
C	-1.99918	2.89587	-0.22378
H	-1.90448	3.80256	0.38161
H	-1.28104	2.98443	-1.03995
H	-3.01411	2.88623	-0.63067
C	-1.33066	-0.66962	1.17934
H	-1.42281	-1.66212	0.73707
H	-0.27068	-0.3994	1.23257
C	-1.97454	-0.64588	2.55937
H	-1.48332	-1.42366	3.15167
H	-1.81859	0.29727	3.08663
H	-3.04393	-0.87543	2.54898
C	2.63458	1.12869	0.76603
C	2.46286	-0.17856	0.17302
O	1.22737	0.88575	0.59642
H	2.95067	1.13585	1.81426
H	2.39998	-1.06282	0.78705
Br	5.0078	-1.07233	-0.23587
C	3.25589	2.23736	-0.04719
H	3.09005	3.2194	0.40963
H	4.3294	2.04015	-0.12383
H	2.83622	2.2448	-1.0585
H	2.4628	-0.28921	-0.89959

S	-1.91672	0.30742	0.14024

a2

Charge = 0 Multiplicity = 1

C	-2.76096	-1.49123	0.78121
H	-1.72658	-1.85014	0.79811
H	-2.99955	-1.20925	1.8087
C	-3.76808	-2.53527	0.31063
H	-3.65063	-3.3997	0.97171
H	-4.8064	-2.20401	0.3994
H	-3.60338	-2.88462	-0.70762
C	-1.80275	-0.27924	-1.24411
H	-1.93963	0.66763	-1.77055
H	-0.76485	-0.31262	-0.88103
C	-2.07524	-1.43538	-2.19623
H	-1.42545	-1.27988	-3.06288
H	-1.80069	-2.40026	-1.76641
H	-3.10369	-1.48347	-2.56791
C	-1.98025	0.80787	0.9696
H	-2.66852	0.9453	1.80503
H	-1.10493	0.24317	1.31211
C	-1.55949	2.14372	0.37502
H	-1.21447	2.76747	1.20548
H	-0.71554	2.02393	-0.30564
H	-2.37124	2.68786	-0.11944
Br	5.65259	0.99123	-0.15538
C	3.78779	0.52621	0.37023
O	1.07034	-0.04145	-0.25533
C	3.56694	-0.98739	0.30032
H	3.1367	1.07475	-0.30178
H	3.68324	0.88439	1.39337
H	4.38343	-1.46083	0.85663
O	2.4044	-1.35522	1.05874
C	1.14285	-0.87907	0.68314
O	0.21533	-1.36262	1.37112
C	3.5484	-1.54796	-1.12048
H	4.49113	-1.31967	-1.62593
H	3.42492	-2.6345	-1.08533
H	2.72123	-1.11288	-1.6836
S	-2.69174	-0.16428	0.00575

TSa2

Charge = 0 Multiplicity = 1

C	-2.27972	1.00703	-1.19
H	-1.29552	1.47484	-1.06239
H	-2.24129	0.33963	-2.05292
C	-3.35172	2.06618	-1.42344
H	-3.02849	2.64147	-2.29639
H	-4.33577	1.65063	-1.65601
H	-3.45329	2.77128	-0.59938
C	-1.83933	0.72207	1.29727
H	-2.10332	0.0463	2.1126
H	-0.75994	0.68711	1.13787
C	-2.25971	2.14601	1.63009
H	-1.83122	2.37586	2.61069
H	-1.83364	2.85823	0.92293
H	-3.34171	2.28295	1.71257
C	-1.61058	-1.16568	-0.2773
H	-2.02363	-1.5807	-1.19741
H	-0.60723	-0.78	-0.47635
C	-1.56228	-2.23009	0.8108
H	-0.96841	-3.06146	0.41979
H	-1.06279	-1.8837	1.71718
H	-2.54599	-2.62964	1.07395
Br	5.08713	-1.51162	-0.25653
C	2.87201	-0.27586	-0.10819
O	1.1447	0.44033	0.04391
C	3.52154	1.09718	-0.01378
H	2.7551	-0.89844	0.76106
H	2.69525	-0.72237	-1.07261

H	4.32969	1.16016	-0.74052
O	2.54905	2.10324	-0.42776
C	1.2678	1.69328	-0.29161
O	0.34311	2.48495	-0.48814
C	4.02534	1.42523	1.38397
H	4.8056	0.70867	1.64939
H	4.43283	2.43899	1.41183
H	3.20901	1.35794	2.11176
S	-2.44989	0.08379	0.03601

b1

Charge = 0 Multiplicity = 1

N	-1.29906	-0.23717	0.07379
C	-0.39289	0.54671	-0.90078
H	0.60169	0.10392	-0.76459
H	-0.73882	0.26438	-1.89723
C	-0.37866	2.06534	-0.78767
H	0.30846	2.42105	-1.56124
H	-1.35193	2.52525	-0.98381
H	0.01152	2.42903	0.16003
C	-0.60326	-0.46174	1.4293
H	-1.33084	-1.01138	2.02918
H	0.25649	-1.10644	1.19962
C	-0.1247	0.77343	2.17895
H	0.20315	0.42723	3.16465
H	0.73942	1.22963	1.69355
H	-0.90154	1.52574	2.34774
C	-1.46802	-1.62264	-0.57556
H	-1.92691	-1.43952	-1.54822
H	-0.43998	-1.98138	-0.72903
C	-2.28308	-2.6384	0.21274
H	-2.37074	-3.53101	-0.41402
H	-1.78793	-2.94794	1.13482
H	-3.29926	-2.30486	0.44585
C	-2.63274	0.44232	0.30062
H	-3.13865	-0.13234	1.07819
H	-2.41178	1.42542	0.71842
C	-3.52939	0.58562	-0.9314
H	-3.87978	-0.39829	-1.26281
H	-2.96145	1.01518	-1.7629
C	-4.751	1.48192	-0.65278
H	-5.28068	1.62917	-1.60085
H	-4.40754	2.4771	-0.34065
C	-5.73113	0.92408	0.38599
H	-5.28313	0.84833	1.38234
H	-6.60899	1.57066	0.47618
H	-6.08357	-0.0739	0.10144
C	3.68958	0.97395	1.10861
C	3.7384	1.32132	-0.31455
O	2.67629	1.82815	0.52984
H	3.34833	-0.02726	1.36736
H	3.4089	0.53183	-0.99141
Br	2.07255	-1.94985	-0.30036
H	4.41191	2.05534	-0.70506
C	4.63272	1.68194	2.09898
H	4.17016	1.72567	3.06284
H	5.55106	1.13721	2.16846
H	4.83225	2.67487	1.75374

TSb1

Charge = 0 Multiplicity = 1

N	1.93963	0.25207	-0.14929
C	1.15167	0.13409	1.17335
H	0.16205	0.53814	0.93108
H	1.02787	-0.93733	1.34129
C	1.77102	0.75958	2.41822
H	1.05252	0.60965	3.23008
H	2.70408	0.27922	2.7248
H	1.94365	1.8321	2.33719
C	1.63798	1.58892	-0.84718

H	2.22954	1.57107	-1.76367	H	-2.76893	2.27039	0.8791
H	0.57003	1.53121	-1.08759	H	-2.54597	-0.28355	1.01087
C	1.92825	2.86675	-0.07128				
H	1.78975	3.69675	-0.77098	**b2**			
H	1.22212	3.02156	0.74554	Charge =	0 Multiplicity = 1		
H	2.95015	2.93743	0.3119	N	1.93963	0.25207	-0.14929
C	1.36718	-0.85291	-1.06021	C	1.15167	0.13409	1.17335
H	1.51168	-1.78754	-0.51697	H	0.16205	0.53814	0.93108
H	0.29531	-0.62667	-1.10928	H	1.02787	-0.93733	1.34129
C	1.97529	-0.95462	-2.45277	C	1.77102	0.75958	2.41822
H	1.50337	-1.81134	-2.94315	H	1.05252	0.60965	3.23008
H	1.76569	-0.08161	-3.07385	H	2.70408	0.27922	2.7248
H	3.0537	-1.13858	-2.44961	H	1.94365	1.8321	2.33719
C	3.43396	0.09814	0.04642	C	1.63798	1.58892	-0.84718
H	3.89168	0.31992	-0.91902	H	2.22954	1.57107	-1.76367
H	3.74037	0.88483	0.73733	H	0.57003	1.53121	-1.08759
C	3.89977	-1.26502	0.56384	C	1.92825	2.86675	-0.07128
H	3.72668	-2.03788	-0.19308	H	1.78975	3.69675	-0.77098
H	3.31926	-1.55283	1.4464	H	1.22212	3.02156	0.74554
C	5.395	-1.25756	0.93619	H	2.95015	2.93743	0.3119
H	5.62664	-2.22268	1.40014	C	1.36718	-0.85291	-1.06021
H	5.57314	-0.49964	1.71054	H	1.51168	-1.78754	-0.51697
C	6.34737	-1.02737	-0.24301	H	0.29531	-0.62667	-1.10928
H	6.22883	-0.03352	-0.68763	C	1.97529	-0.95462	-2.45277
H	7.38888	-1.11219	0.08005	H	1.50337	-1.81134	-2.94315
H	6.18568	-1.76921	-1.03323	H	1.76569	-0.08161	-3.07385
C	-2.57313	0.94568	-0.80417	H	3.0537	-1.13858	-2.44961
C	-2.58792	-0.30066	-0.06606	C	3.43396	0.09814	0.04642
O	-1.1965	0.66746	-0.58424	H	3.89168	0.31992	-0.91902
H	-2.87859	0.86123	-1.85494	H	3.74037	0.88483	0.73733
H	-2.49548	-1.24325	-0.57986	C	3.89977	-1.26502	0.56384
Br	-5.12418	-0.9441	0.2846	H	3.72668	-2.03788	-0.19308
C	-3.13822	2.18638	-0.14864	H	3.31926	-1.55283	1.4464
H	-2.85378	3.09203	-0.69653	C	5.395	-1.25756	0.93619
H	-4.22833	2.10321	-0.11719	H	5.62664	-2.22268	1.40014

H	5.57314	-0.49964	1.71054
C	6.34737	-1.02737	-0.24301
H	6.22883	-0.03352	-0.68763
H	7.38888	-1.11219	0.08005
H	6.18568	-1.76921	-1.03323
Br	-6.92818	0.28464	-0.19868
C	-5.20385	0.05169	0.58904
O	-3.07085	-0.31266	-0.91473
C	-4.76792	1.40338	0.05534
H	-5.42923	-0.73833	-0.17259
H	-6.00526	0.05723	1.3718
H	-5.49825	2.13911	0.47279
O	-3.40094	1.77537	0.37357
C	-2.47796	0.71244	-0.23527
O	-1.25322	0.63906	-0.20502
C	-4.99201	1.33679	-1.46682
H	-6.00023	1.03904	-1.66621
H	-4.81316	2.30042	-1.89615
H	-4.31836	0.62463	-1.89569

TSb2

Charge = 0 Multiplicity = 1

N	2.44903	0.08411	-0.03639
C	2.27928	1.00831	1.18884
H	1.29544	1.47655	1.06092
H	2.24029	0.34166	2.05232
C	3.35184	2.06706	1.4217
H	3.02874	2.64325	2.29409
H	4.33551	1.65101	1.65487
H	3.45411	2.7714	0.59707
C	1.83889	0.72181	-1.29812
H	2.10201	0.04505	-2.11287
H	0.75955	0.68812	-1.13863
C	2.26064	2.14503	-1.63239
H	1.83212	2.37443	-2.61308
H	1.8357	2.8585	-0.92584
H	3.34276	2.28065	-1.71531
C	1.60932	-1.16491	0.27772
H	2.0225	-1.57959	1.19792
H	0.60624	-0.779	0.47726
C	1.56025	-2.22993	-0.80973
H	0.96574	-3.0606	-0.41822
H	1.06112	-1.88387	-1.71643
H	2.54372	-2.63032	-1.07247
C	3.89893	-0.27201	-0.30176
H	3.91034	-0.81797	-1.24613
H	4.42221	0.67106	-0.46716
C	4.59641	-1.08235	0.79361
H	4.17689	-2.0935	0.84077
H	4.42491	-0.62366	1.7727
C	6.11508	-1.18441	0.55352
H	6.5566	-1.68188	1.42417
H	6.54756	-0.1754	0.53002
C	6.51247	-1.94821	-0.71503
H	6.18127	-1.44191	-1.6279
H	7.59966	-2.04856	-0.78015
H	6.08709	-2.95813	-0.719
Br	-5.08244	-1.51625	0.25551
C	-2.86227	-0.2708	0.10661
O	-1.1475	0.44421	-0.04241
C	-3.52221	1.09782	0.01712
H	-2.75403	-0.894	-0.76344
H	-2.69305	-0.72326	1.06969
H	-4.32701	1.15513	0.74791
O	-2.55107	2.10778	0.42787
C	-1.2706	1.69896	0.29147
O	-0.34444	2.48901	0.48497
C	-4.03362	1.42652	-1.37751
H	-4.81161	0.7065	-1.64011
H	-4.44602	2.4384	-1.40151

H	-3.22042	1.36451	-2.10932

c1

Charge = 0 Multiplicity = 1

C	-0.00569	1.24939	0.08408
H	0.98246	0.77373	0.02438
H	-0.18007	1.74668	-0.87726
C	-0.0589	2.25266	1.24093
H	-1.00169	2.80845	1.28237
H	0.09559	1.7665	2.20867
C	-0.8025	-1.15808	1.65856
H	0.1749	-1.61073	1.4328
H	-0.64664	-0.42639	2.46036
C	-1.85074	-2.19485	2.08141
H	-1.50647	-2.69002	2.9939
H	-2.82598	-1.74857	2.30086
H	-1.98835	-2.96924	1.32434
C	-1.06506	-1.04605	-1.43224
H	-1.64581	-0.45606	-2.15153
H	0.00187	-1.00355	-1.68462
C	-1.49013	-2.51822	-1.41796
H	-0.76391	-3.09098	-0.83549
H	-2.49946	-2.67972	-1.02576
C	-2.89592	0.47977	0.36904
H	-3.55523	-0.39476	0.35423
H	-2.96173	0.90146	1.37983
C	-3.34822	1.522	-0.66918
H	-3.29481	1.09112	-1.67686
H	-2.6555	2.37141	-0.65805
C	-4.77553	2.04444	-0.42493
H	-4.95902	2.8656	-1.12807
H	-4.83071	2.48639	0.57883
C	-5.87649	0.991	-0.58722
H	-5.79181	0.18693	0.15119
H	-6.86597	1.44084	-0.46196
H	-5.84389	0.53442	-1.58298
P	-1.17566	-0.15129	0.16833
H	0.76135	2.96155	1.10975
H	-1.46812	-2.90363	-2.44134
C	4.01404	1.01385	1.00421
C	4.08529	1.28905	-0.43495
O	3.09396	1.94295	0.39084
H	3.56926	0.06993	1.31576
H	3.66073	0.51509	-1.07576
Br	2.04495	-1.74856	-0.27596
C	5.03977	1.66049	1.95359
H	4.83919	1.35266	2.95853
H	6.0262	1.35229	1.67631
H	4.96662	2.72582	1.88556
H	4.83097	1.92591	-0.86306

TSc1

Charge = 0 Multiplicity = 1

C	1.04449	-1.02053	-1.25482
H	-0.00286	-0.68726	-1.29637
H	1.51953	-0.709	-2.19288
C	1.19346	-2.53432	-1.05627
H	2.24008	-2.84925	-0.99424
H	0.67763	-2.88631	-0.16095
C	0.81802	0.06627	1.60501
H	1.3425	0.77101	2.26116
H	-0.14437	0.50816	1.31047
C	0.62435	-1.28484	2.30629
H	0.14217	-1.11596	3.27287
H	-0.03167	-1.94135	1.73117
H	1.56613	-1.80914	2.49724
C	1.70505	1.77006	-0.63929
H	2.20515	1.74603	-1.61384
H	0.63046	1.9231	-0.81181
C	2.30208	2.85978	0.26031

H	1.76878	2.93718	1.21142
H	3.36374	2.69623	0.47166
C	3.4946	-0.42301	0.3876
H	3.849	0.23646	1.18736
H	3.46118	-1.43366	0.81216
C	4.44468	-0.38357	-0.82377
H	4.48956	0.63706	-1.2246
H	4.04115	-1.01453	-1.62439
C	5.87108	-0.85717	-0.49187
H	6.43303	-0.91469	-1.43143
H	5.82841	-1.88227	-0.10074
C	6.62851	0.04159	0.49108
H	6.15732	0.0662	1.47935
H	7.65242	-0.31638	0.63246
H	6.68677	1.07186	0.1219
P	1.75876	0.06751	0.03396
H	0.74671	-3.04934	-1.91101
H	2.21258	3.82812	-0.23931
C	-2.55177	1.18424	-0.75116
C	-2.68803	-0.09963	-0.09426
O	-1.21138	0.80921	-0.46202
H	-2.79044	1.17996	-1.82246
H	-2.61865	-1.01498	-0.6587
Br	-5.27132	-0.62523	0.04715
C	-3.08854	2.41692	-0.05791
H	-2.71351	3.33348	-0.5275
H	-4.18112	2.401	-0.10577
H	-2.78954	2.4181	0.99573
H	-2.72428	-0.14764	0.98206

c2

Charge = 0 Multiplicity = 1

C	1.15167	0.13409	1.17335
H	0.16205	0.53814	0.93108
H	1.02787	-0.93733	1.34129
C	1.77102	0.75958	2.41822
H	1.05252	0.60965	3.23008
H	2.70408	0.27922	2.7248
H	1.94365	1.8321	2.33719
C	1.63798	1.58892	-0.84718
H	2.22954	1.57107	-1.76367
H	0.57003	1.53121	-1.08759
C	1.92825	2.86675	-0.07128
H	1.78975	3.69675	-0.77098
H	1.22212	3.02156	0.74554
H	2.95015	2.93743	0.3119
C	1.36718	-0.85291	-1.06021
H	1.51168	-1.78754	-0.51697
H	0.29531	-0.62667	-1.10928
C	1.97529	-0.95462	-2.45277
H	1.50337	-1.81134	-2.94315
H	1.76569	-0.08161	-3.07385
H	3.0537	-1.13858	-2.44961
C	3.43396	0.09814	0.04642
H	3.89168	0.31992	-0.91902
H	3.74037	0.88483	0.73733
C	3.89977	-1.26502	0.56384
H	3.72668	-2.03788	-0.19308
H	3.31926	-1.55283	1.4464
C	5.395	-1.25756	0.93619
H	5.62664	-2.22268	1.40014
H	5.57314	-0.49964	1.71054
C	6.34737	-1.02737	-0.24301
H	6.22883	-0.03352	-0.68763
H	7.38888	-1.11219	0.08005
H	6.18568	-1.76921	-1.03323
Br	-6.92818	0.28464	-0.19868
C	-5.20385	0.05169	0.58904
O	-3.07085	-0.31266	-0.91473
C	-4.76792	1.40338	0.05534

H	-5.42923	-0.73833	-0.17259
H	-6.00526	0.05723	1.3718
H	-5.49825	2.13911	0.47279
O	-3.40094	1.77537	0.37357
C	-2.47796	0.71244	-0.23527
O	-1.25322	0.63906	-0.20502
C	-4.99201	1.33679	-1.46682
H	-6.00023	1.03904	-1.66621
H	-4.81316	2.30042	-1.89615
H	-4.31836	0.62463	-1.89569
P	1.93963	0.25207	-0.14929

TSc2

Charge = 0 Multiplicity = 1

C	2.25894	1.13279	1.58086
H	1.20991	1.45546	1.56437
H	2.36904	0.3571	2.34743
C	3.19091	2.31856	1.86449
H	2.99688	2.68894	2.87464
H	4.25086	2.05037	1.81031
H	3.00574	3.14709	1.17724
C	2.03306	1.36245	-1.4435
H	1.81174	0.68553	-2.27616
H	1.08388	1.8175	-1.12947
C	3.07022	2.41068	-1.86918
H	2.66951	2.98298	-2.71017
H	3.29151	3.12221	-1.07028
H	4.01159	1.96019	-2.19809
C	1.3656	-1.16651	-0.02797
H	1.53036	-1.68829	0.92156
H	0.34453	-0.75462	-0.01233
C	1.5372	-2.12399	-1.21569
H	0.80952	-2.93445	-1.12493
H	1.3431	-1.62724	-2.17042
H	2.5336	-2.57503	-1.25677
C	4.22064	-0.26562	-0.21583
H	4.29911	-0.71839	-1.21035
H	4.84455	0.6355	-0.23533
C	4.71611	-1.23365	0.87478
H	4.09276	-2.1366	0.88111
H	4.59494	-0.7652	1.85856
C	6.19009	-1.64079	0.69907
H	6.48749	-2.21452	1.58462
H	6.81581	-0.73844	0.69798
C	6.47618	-2.47222	-0.55572
H	6.27738	-1.9156	-1.47769
H	7.52581	-2.77869	-0.5858
H	5.86576	-3.38214	-0.57558
Br	-5.54795	-1.42036	0.27345
C	-3.23411	-0.39036	-0.02282
O	-1.4799	0.17568	-0.29888
C	-3.75391	1.03535	0.09684
H	-3.28301	-0.92423	-0.95543
H	-3.01144	-0.95819	0.8654
H	-4.46756	1.0894	0.91695
O	-2.64353	1.90025	0.4901
C	-1.43823	1.38087	0.17301
O	-0.41557	2.05589	0.35681
C	-4.36876	1.55941	-1.19219
H	-5.24113	0.94818	-1.43303
H	-4.6733	2.60216	-1.07092
H	-3.6465	1.50006	-2.01389
P	2.47761	0.28567	-0.02836

d1

Charge = 0 Multiplicity = 1

Br	0.14026	-2.13514	0.39989
C	0.63723	1.96296	-0.00665
C	0.79721	2.33658	1.30554
C	1.57238	1.52263	2.15884

C	2.11899	0.35478	1.67218
C	1.89814	-0.01054	0.33501
H	1.72535	1.81052	3.19389
H	0.03052	2.51492	-0.71116
H	0.32665	3.24469	1.66166
H	2.68817	-0.31807	2.30122
H	2.39079	-0.8496	-0.12593
N	1.23484	0.84182	-0.49108
C	1.01249	0.41076	-1.89118
H	0.13103	0.94338	-2.248
H	0.75031	-0.65088	-1.81669
C	2.23277	0.65507	-2.77435
H	3.11144	0.1146	-2.409
H	2.0222	0.29812	-3.78666
H	2.48317	1.71895	-2.83344
C	-2.61973	0.33968	0.16259
C	-2.73772	-0.31347	-1.14469
O	-2.04006	0.94616	-1.0193
H	-1.87307	-0.09303	0.82962
H	-2.10272	-1.17624	-1.33828
H	-3.42938	0.8751	0.6128
C	-4.06506	-0.23454	-1.92157
H	-3.8666	-0.27803	-2.9721
H	-4.69105	-1.05623	-1.64254
H	-4.55979	0.68549	-1.68985

TSd1

Charge = 0 Multiplicity = 1

Br	-4.34001	-0.29986	0.44377
C	2.4157	-0.75751	0.19118
C	3.1821	-1.90583	0.33836
C	4.56877	-1.84039	0.21835
C	5.16817	-0.60555	-0.06312
C	4.37127	0.51228	-0.20443
H	5.17701	-2.73063	0.33747
H	1.31917	-0.71357	0.22215
H	2.67781	-2.84329	0.54278
H	6.24176	-0.50875	-0.17361
H	4.76922	1.49606	-0.42167
N	3.02292	0.4289	-0.07642
C	2.17854	1.65615	-0.20389
H	1.17619	1.30395	-0.5187
H	2.64335	2.27396	-0.97681
C	2.07606	2.39777	1.12668
H	3.05332	2.71157	1.50937
H	1.46248	3.29134	0.98372
H	1.58403	1.77571	1.87916
C	-1.74777	0.18942	0.33285
C	-1.39519	-0.30441	-0.98103
O	-0.21793	0.21274	-0.33404
H	-1.7258	-0.45723	1.19451
H	-1.38994	-1.39322	-1.09342
C	-1.88338	0.41903	-2.21112
H	-1.30933	0.13516	-3.10022
H	-2.93783	0.16914	-2.36029
H	-1.80241	1.50157	-2.07137
H	-2.06131	1.21343	0.45917

d2

Charge = 0 Multiplicity = 1

C	0.63723	1.96296	-0.00665
C	0.79721	2.33658	1.30554
C	1.57238	1.52263	2.15884
C	2.11899	0.35478	1.67218
C	1.89814	-0.01054	0.33501
H	1.72535	1.81052	3.19389
H	0.03052	2.51492	-0.71116
H	0.32665	3.24469	1.66166
H	2.68817	-0.31807	2.30122
H	2.39079	-0.8496	-0.12593

N	1.23484	0.84182	-0.49108
C	1.01249	0.41076	-1.89118
H	0.13103	0.94338	-2.248
H	0.75031	-0.65088	-1.81669
C	2.23277	0.65507	-2.77435
H	3.11144	0.1146	-2.409
H	2.0222	0.29812	-3.78666
H	2.48317	1.71895	-2.83344
C	-2.2444	0.71206	-1.1063
O	-1.56112	0.25073	-2.04322
O	-2.038	1.89529	-0.76739
O	-3.26628	0.09304	-0.3205
C	-4.23562	-0.50612	-1.18438
H	-4.52282	0.1957	-1.93928
C	-3.62819	-1.75535	-1.84926
H	-4.36847	-2.52601	-1.9037
H	-3.29694	-1.50862	-2.83633
C	-5.47359	-0.91224	-0.36335
H	-5.89306	-0.04492	0.10217
H	-6.20069	-1.35657	-1.01048
H	-5.18716	-1.61739	0.38873
Br	-2.14469	-2.36947	-0.81476
C	3.13413	1.67955	1.38873
H	4.06852	1.12324	1.4897
H	3.34696	2.75114	1.35598
H	2.49562	1.47683	2.25549
C	-4.90478	-1.03689	-0.1463
C	-4.53222	-2.35367	0.04302
C	-3.22255	-2.64219	0.44585
C	-2.32591	-1.59725	0.64649
C	-2.74636	-0.28743	0.45289
H	-2.91256	-3.67167	0.59358
H	-5.89847	-0.74443	-0.46257
H	-5.2596	-3.13873	-0.12642
H	-1.29132	-1.74252	0.93452
H	-2.07996	0.58484	0.55726
N	-4.01645	-0.03459	0.06259
C	-4.40605	1.3882	-0.18648
H	-4.04161	1.96539	0.66523
H	-5.49787	1.41856	-0.18554
C	-3.81354	1.9196	-1.48878
H	-4.17938	2.93794	-1.6477
H	-2.72349	1.95979	-1.42008
H	-4.11651	1.30903	-2.34465

TSd2

Charge = 0 Multiplicity = 1

Br	4.39533	-1.03117	-0.49197
C	2.44693	1.23798	0.1056
C	2.05111	-0.23157	0.1128
O	1.24214	2.03932	-0.10088
H	2.22702	-0.85047	0.97493
H	1.78669	-0.72237	-0.80924
C	0.1175	1.38969	0.26262
O	0.28861	0.15204	0.59869
O	-0.96968	1.98923	0.23868
H	3.0764	1.43561	-0.76011

e1

Charge = 0 Multiplicity = 1

Br	-1.15915	-0.86467	1.64287
C	-3.63726	-0.97565	-0.96302
C	-3.76704	0.40922	-0.50079
O	-2.81812	0.0678	-1.54562
H	-3.09476	-1.67026	-0.32418
H	-3.27988	0.62383	0.45078
C	2.21208	0.73342	-0.38688
C	2.33304	-0.65406	-0.58873
C	3.57016	-1.2911	-0.51345
C	4.68048	-0.4946	-0.23613

C	4.55993	0.89118	-0.04204
C	3.32261	1.52984	-0.1138
C	0.18435	-0.1036	-0.7589
H	3.67043	-2.36079	-0.65902
H	5.65922	-0.95789	-0.16629
H	5.44733	1.47753	0.17268
H	3.23009	2.5988	0.04182
H	-0.87371	-0.14573	-0.99411
C	0.6209	-2.52294	-0.87992
H	1.48368	-3.16485	-1.05577
H	0.14961	-2.73083	0.08786
H	-0.10376	-2.67578	-1.68203
C	0.21911	2.33285	-0.26999
H	0.7828	3.10199	-0.80827
H	-0.77624	2.28018	-0.71665
C	0.12778	2.62543	1.22866
H	1.12005	2.74624	1.673
H	-0.43118	3.55308	1.38584
H	-0.38297	1.79701	1.72883
N	1.0523	-1.12899	-0.87181
N	0.86042	1.04016	-0.54303
C	-4.68903	-1.56302	-1.92237
H	-4.43309	-2.57543	-2.15566
H	-5.65153	-1.53693	-1.45566
H	-4.71326	-0.98481	-2.82236
H	-4.57763	1.04143	-0.79771

TSe1

Charge = 0 Multiplicity = 1

Br	-2.92726	-0.72752	-0.23412
C	-0.67071	1.66291	-0.07643
C	-1.2794	0.92084	1.00792
O	0.12495	2.00542	1.05302
H	-0.15754	1.03928	-0.82696
H	-0.88738	-0.02887	1.32664
H	-2.04248	1.38222	1.61805
C	-1.4495	2.78297	-0.73143
H	-0.79288	3.41792	-1.33855
H	-2.22576	2.34992	-1.37076
H	-1.92454	3.40951	0.03096
C	3.45241	-1.50956	-0.43546
C	4.0701	-0.32359	-0.62835
C	5.33406	-0.2272	-1.28728
C	5.88397	-1.39203	-1.7108
C	5.22362	-2.65871	-1.50446
C	4.0239	-2.74037	-0.8779
C	2.04929	0.09853	0.49049
H	5.8314	0.74138	-1.44104
H	6.85546	-1.40588	-2.22724
H	5.73196	-3.56099	-1.87618
H	3.51508	-3.70184	-0.71725
H	1.18909	0.57605	1.00442
C	3.53834	2.30459	-0.04852
H	4.44628	2.49303	0.48537
H	3.63213	2.66721	-1.05082
H	2.72791	2.80613	0.43785
C	1.10374	-2.30511	0.71907
H	1.55008	-3.00212	1.3972
H	0.29346	-1.80329	1.2054
C	0.57437	-3.05758	-0.51591
H	1.18251	-3.91928	-0.69631
H	-0.4357	-3.36419	-0.34088
H	0.6085	-2.41209	-1.36859
N	3.26302	0.78962	-0.07439
N	2.15693	-1.2717	0.27808

e2

Charge = 0 Multiplicity = 1

Br	-1.17931	-1.44522	-1.06082

C	-2.9241	0.62424	0.06196
C	-2.92991	-0.84993	-0.32474
O	-2.04514	0.80812	1.16285
H	-2.57152	1.22813	-0.77849
H	-3.65035	-1.07149	-1.11223
H	-3.0985	-1.49022	0.54085
C	-0.82949	1.47563	0.92087
O	-0.64065	1.98571	-0.20295
O	-0.05704	1.4419	1.9133
C	-4.33014	1.05856	0.48688
H	-4.30765	2.11328	0.7728
H	-5.05179	0.93532	-0.32778
H	-4.67405	0.48103	1.35124
C	3.51085	-0.8128	-0.56629
C	3.44058	0.2018	-1.46937
C	4.15921	0.15179	-2.71365
C	4.90983	-0.95361	-2.94442
C	4.9844	-2.03026	-1.9861
C	4.30717	-1.98435	-0.81229
C	2.10542	0.76839	0.36162
H	4.09771	0.97582	-3.43913
H	5.48751	-1.06292	-3.87449
H	5.61439	-2.89472	-2.24403
H	4.35931	-2.80082	-0.07758
H	1.40022	1.34854	0.99642
C	2.18274	2.60328	-1.63996
H	3.06239	3.18785	-1.81142
H	1.69175	2.4159	-2.57201
H	1.52143	3.1364	-0.98931
C	2.43392	-1.30068	1.86958
H	3.3657	-1.46873	2.36802
H	1.77259	-0.76733	2.52002
C	1.80228	-2.65356	1.49227
H	2.57584	-3.37106	1.31421
H	1.1793	-2.99218	2.2936
H	1.21285	-2.53742	0.60685
N	2.6763	-0.47358	0.59335
N	2.57516	1.26432	-0.9882

TSe2

Charge = 0 Multiplicity = 1

Br	-4.40818	0.77173	-0.19034
C	-2.26938	-1.37993	0.12327
C	-1.95538	0.07586	-0.19101
O	-1.13058	-2.19908	-0.28925
H	-1.90902	0.81517	0.58891
H	-1.9855	0.42457	-1.21009
C	0.01841	-1.4995	-0.35351
O	-0.11121	-0.22164	-0.17827
O	1.08581	-2.08936	-0.57878
H	-3.10116	-1.70888	-0.49693
C	-2.55856	-1.62834	1.59593
H	-3.45467	-1.06875	1.87222
H	-2.72081	-2.69407	1.77607
H	-1.71769	-1.29437	2.21401
C	5.41549	0.55694	0.09308
C	4.70824	1.7027	0.004
C	5.31874	2.98394	0.16769
C	6.65132	2.98963	0.41829
C	7.40779	1.76415	0.51356
C	6.81961	0.55252	0.35673
C	3.18023	-0.01032	-0.34859
H	4.73613	3.91358	0.09377
H	7.19832	3.93419	0.55717
H	8.48535	1.84919	0.71928
H	7.38962	-0.38511	0.42798
H	2.19926	-0.66923	-0.51965
C	4.87501	-2.12494	-0.11101
H	5.59709	-2.33256	-0.87284
H	5.27467	-2.39817	0.8432

H	3.98532	-2.68862	-0.29972
C	2.08802	2.32904	-0.46437
H	2.28132	2.97806	-1.2928
H	1.19849	1.76509	-0.65306
C	1.90217	3.16872	0.81312
H	2.48732	4.06165	0.7413
H	0.86962	3.42683	0.92321
H	2.22043	2.60109	1.66248
N	3.27594	1.3669	-0.27796
N	4.54103	-0.6216	-0.11628
C	-3.61279	-1.38344	0.36518
C	-3.28716	-0.89293	-0.98221
O	-2.50576	-1.94447	-0.36859
H	-2.76564	0.05997	-1.08054
H	-3.89111	-1.21489	-1.8316
H	-3.38053	-0.82054	1.24501
C	-4.7938	-2.3636	0.49199
H	-4.645	-2.993	1.34441
H	-5.70346	-1.81267	0.60988
H	-4.85353	-2.96616	-0.39019

f1

Charge = 0 Multiplicity = 1

Br	-0.8882	1.8888	-0.14195
C	3.44408	0.4677	1.04609
C	1.94302	0.1765	0.97281
C	2.97999	-1.58803	-0.22541
C	4.13319	-0.718	0.30606
H	1.62122	-0.46308	1.7991
H	1.25331	1.02713	0.89499
H	3.68278	1.42006	0.56622
H	3.76419	0.547	2.08713
H	2.72423	-2.38746	0.47431
H	3.14821	-2.02625	-1.21081
H	4.77067	-1.30697	0.96931
H	4.76565	-0.35983	-0.50992
C	1.83015	0.19958	-1.52015
H	1.74246	-0.45179	-2.3913
H	0.98558	0.90027	-1.45439
H	2.77964	0.73331	-1.55054
C	0.46755	-1.4034	-0.27564
H	-0.32283	-0.64865	-0.25292
H	0.39685	-2.01597	-1.175
H	0.42321	-2.03403	0.61259
N	1.78199	-0.67032	-0.28596

TSf1

Charge = 0 Multiplicity = 1

Br	-4.52484	-0.54795	-0.24932
C	3.86297	0.80122	-0.95886
C	2.6398	0.95937	0.05364
C	3.9138	-1.05492	0.7299
C	4.65013	-0.43126	-0.5444
H	2.98054	1.50337	0.93801
H	1.62379	1.27495	-0.20882
H	3.51554	0.33963	-1.89471
H	3.99042	1.87	-1.1459
H	4.28475	-0.5646	1.63299
H	3.81734	-2.12713	0.91978
H	5.65514	-0.75202	-0.25805
H	4.36529	-0.99621	-1.44493
C	1.78795	-1.30426	-0.5678
H	1.66046	-2.32007	-0.19151
H	0.82307	-0.81436	-0.72144
H	2.36641	-1.32467	-1.48875
C	1.71561	-0.5577	1.75849
H	0.74315	-0.10325	1.53981
H	1.61349	-1.60221	2.05709
H	2.24978	-0.00013	2.52901
N	2.5239	-0.50326	0.48335

C	-1.78772	-0.14972	-0.07651
C	-1.6733	1.28435	-0.20117
O	-0.37103	0.6896	0.01223
H	-1.80544	-0.78188	-0.95126
H	-1.79892	1.68721	-1.21
C	-2.22472	2.17755	0.87969
H	-1.83952	3.20025	0.80331
H	-3.31464	2.18102	0.78058
H	-1.97384	1.77821	1.86761
H	-2.00856	-0.5933	0.88189

f2

Charge = 0 Multiplicity = 1

C	3.44408	0.4677	1.04609
C	1.94302	0.1765	0.97281
C	2.97999	-1.58803	-0.22541
C	4.13319	-0.718	0.30606
H	1.62122	-0.46308	1.7991
H	1.25331	1.02713	0.89499
H	3.68278	1.42006	0.56622
H	3.76419	0.547	2.08713
H	2.72423	-2.38746	0.47431
H	3.14821	-2.02625	-1.21081
H	4.77067	-1.30697	0.96931
H	4.76565	-0.35983	-0.50992
C	1.83015	0.19958	-1.52015
H	1.74246	-0.45179	-2.3913
H	0.98558	0.90027	-1.45439
H	2.77964	0.73331	-1.55054
C	0.46755	-1.4034	-0.27564
H	-0.32283	-0.64865	-0.25292
H	0.39685	-2.01597	-1.175
H	0.42321	-2.03403	0.61259
N	1.78199	-0.67032	-0.28596
C	-1.40265	1.53085	-1.02715
O	-0.534	2.11276	-0.34574
O	-2.58855	2.16476	-1.2094
O	-1.36782	0.41954	-1.59397
C	-2.58917	3.43169	-0.54625
H	-2.43175	3.28566	0.50199
C	-3.94476	4.12741	-0.76974
H	-3.94594	5.07454	-0.27189
H	-4.10128	4.27522	-1.81786
H	-4.72892	3.51588	-0.37476
C	-1.46082	4.31053	-1.11725
H	-0.64052	4.32857	-0.43045
H	-1.13374	3.90762	-2.05298
Br	-2.10946	6.08754	-1.38111

TSf2

Charge = 0 Multiplicity = 1

Br	4.58679	-0.97221	0.08076
C	2.43767	1.16389	-0.21876
C	2.13468	-0.28736	0.12768
O	1.23597	1.76781	-0.79056
H	2.20059	-0.645	1.13993
H	2.04164	-1.02087	-0.65605
C	0.10472	1.12544	-0.42995
O	0.28527	0.03526	0.24417
O	-0.99778	1.57737	-0.76818
H	3.18121	1.19349	-1.01316
C	2.88998	1.98541	0.97887
H	3.82502	1.56609	1.35601
H	3.04787	3.02649	0.68566
H	2.13396	1.95742	1.77131
C	-5.5311	-0.67002	0.97148
C	-4.89306	-1.21383	-0.31975
C	-3.81206	0.85609	0.10083
C	-4.7889	0.6698	1.26343
H	-6.60389	-0.52668	0.82678

H	-5.41022	-1.37502	1.79694
H	-5.44405	-0.89205	-1.2065
H	-4.7744	-2.29798	-0.35398
H	-2.85155	1.33341	0.30153
H	-4.28382	1.37437	-0.73808
H	-4.26059	0.62461	2.21869
H	-5.4739	1.51819	1.32097
C	-2.54795	-1.25501	0.5168
H	-2.45265	-2.29037	0.18514
H	-1.57752	-0.7425	0.45439
H	-2.93293	-1.23619	1.53586
C	-2.96925	-0.54815	-1.7944
H	-2.08105	0.08695	-1.77825
H	-2.72862	-1.57204	-2.0844
H	-3.72331	-0.13877	-2.46815
N	-3.52936	-0.55961	-0.39744

g1

Charge = 0 Multiplicity = 1

Br	-0.8842	1.90288	-0.04049
C	1.87632	0.1195	0.92286
C	2.99503	-1.47927	-0.41759
C	3.8783	-0.89294	0.71589
H	1.46355	-0.60455	1.63916
H	1.28484	1.04224	0.91026
H	2.64824	-2.48829	-0.19276
H	3.47482	-1.47658	-1.39605
H	3.92048	-1.58351	1.56816
H	4.89481	-0.66114	0.39429
C	1.9479	0.49414	-1.53019
H	1.98299	-0.0125	-2.49592
H	1.07879	1.1611	-1.45023
H	2.87537	1.03535	-1.34413
C	0.4834	-1.27661	-0.63723
H	-0.30622	-0.52408	-0.55552
H	0.4796	-1.75349	-1.61785
H	0.37665	-2.0264	0.14621
N	1.79364	-0.55742	-0.45598
C	-3.48835	-1.48106	0.37527
C	-3.33051	-0.83264	-0.93482
O	-2.45879	-1.91612	-0.53592
H	-2.84739	0.14393	-0.98088
H	-4.01912	-1.0801	-1.74356
O	3.24176	0.3288	1.08801
H	-3.17055	-1.01107	1.28247
C	-4.62309	-2.51218	0.51931
H	-4.3625	-3.22648	1.27215
H	-5.52628	-2.01173	0.79985
H	-4.76892	-3.01476	-0.41399

TSg1

Charge = 0 Multiplicity = 1

Br	-4.2262	-0.55822	-0.14829
C	2.93161	0.93963	-0.27682
C	4.2768	-0.78239	0.65931
C	4.98461	-0.36685	-0.64161
H	3.1858	1.68922	0.47696
H	1.94168	1.16231	-0.68263
H	4.64581	-0.21544	1.51711
H	4.32901	-1.84691	0.89415
H	5.9882	0.00111	-0.41846
H	5.09997	-1.21721	-1.31756
C	2.09829	-1.39931	-0.37861
H	2.03681	-2.33326	0.18146
H	1.10654	-0.98988	-0.58253
H	2.65362	-1.55953	-1.302
C	2.09023	-0.2184	1.77081
H	1.09189	0.15707	1.52024
H	2.0426	-1.18642	2.27201
H	2.63729	0.49496	2.3892

N	2.8282	-0.38548	0.47093
C	-1.50221	-0.18091	-0.07329
C	-1.35966	1.2269	-0.36263
O	-0.05887	0.65412	-0.11146
H	-1.53242	-0.90957	-0.86854
H	-1.50822	1.51434	-1.40788
C	-1.87942	2.24786	0.61753
H	-1.47605	3.24715	0.41973
H	-2.97048	2.26371	0.53506
H	-1.61935	1.9588	1.64102
H	-1.69061	-0.50969	0.93655
O	4.07839	0.73285	-1.27188
O	1.2682	1.7758	-0.08478
O	-0.89618	1.94971	-0.52643
C	2.35535	0.99368	0.42724
H	2.00283	0.384	1.26428
C	3.43231	1.97357	0.87206
H	4.30842	1.43818	1.24632
H	3.74021	2.60801	0.03425
H	3.04503	2.62107	1.66328
C	2.79796	0.05485	-0.69404
H	1.97275	-0.58833	-0.98756
H	3.20661	0.59796	-1.54627
Br	4.23799	-1.18167	-0.10168
O	-3.44684	-2.02027	0.67492

g2

Charge = 0 Multiplicity = 1

C	-2.96808	-0.58154	0.90649
C	-5.1362	-0.39549	-0.05202
C	-4.86484	-1.90392	0.04078
H	-3.25982	-0.21877	1.89597
H	-1.89189	-0.40238	0.73544
H	-5.63249	-0.02174	0.84734
H	-5.70964	-0.08023	-0.92584
H	-5.63536	-2.38853	0.64467
H	-4.89431	-2.36861	-0.94789
C	-3.15407	0.15607	-1.46554
H	-3.83284	0.63815	-2.17189
H	-2.19386	0.68476	-1.41507
H	-3.02427	-0.89256	-1.72929
C	-3.80249	1.70021	0.30881
H	-2.7703	2.06753	0.25365
H	-4.44009	2.2382	-0.39571
H	-4.21488	1.77472	1.31644
N	-3.77112	0.25201	-0.08936
C	-0.00009	1.17897	-0.10582
O	-0.09214	-0.01456	0.2731

TSg2

Charge = 0 Multiplicity = 1

Br	-4.54264	-0.99522	-0.01043
C	-2.41421	1.18221	0.0821
C	-2.09332	-0.30211	-0.02253
O	-1.24561	1.8743	0.62108
H	-2.10585	-0.80991	-0.97068
H	-2.04351	-0.90712	0.86762
C	-0.09562	1.19703	0.41778
O	-0.2493	0.01757	-0.09376
O	0.98464	1.7179	0.72947
H	-3.20102	1.32736	0.82015
C	-2.79981	1.80656	-1.25057
H	-3.71686	1.33037	-1.60403
H	-2.9659	2.88043	-1.13257
H	-2.0051	1.65537	-1.98945
C	5.30167	-0.91684	-1.11775
C	4.96304	-1.01836	0.38006
C	3.62743	0.75508	-0.45725
H	6.36106	-0.6841	-1.24429
H	5.11977	-1.86465	-1.62939

H	5.63277	-0.40412	0.98629
H	4.95472	-2.03209	0.78398
H	2.60839	1.11879	-0.59772
H	4.20032	1.53724	0.04793
C	2.52501	-1.41226	0.10039
H	2.5457	-2.24037	0.81069
H	1.5445	-0.9221	0.09768
H	2.75991	-1.78334	-0.8966
C	3.28091	0.05557	1.91322
H	2.32942	0.59406	1.87355
H	3.23353	-0.81174	2.57345
H	4.08187	0.7245	2.23206
N	3.58023	-0.41607	0.51845
O	4.37923	0.20921	-1.6738

h1

Charge = 0 Multiplicity = 1

Br	-1.099	1.89907	-0.17295
C	3.30431	0.99594	0.58577
C	1.92685	0.38613	0.82146
C	2.68599	-1.76255	-0.18777
C	4.07767	-1.18095	-0.43536
C	4.41008	-0.06874	0.56906
H	1.88794	-0.10091	1.80126
H	1.10408	1.11269	0.74773
H	3.31101	1.57586	-0.34395
H	3.47521	1.71934	1.38992
H	2.6451	-2.24226	0.7951
H	2.41208	-2.50692	-0.94015
H	4.79558	-2.00476	-0.35776
H	4.15469	-0.80401	-1.46134
H	4.50914	-0.50568	1.57191
H	5.37739	0.38188	0.32519
C	1.3813	-0.13601	-1.56415
H	1.12366	-0.95646	-2.23632
H	0.55849	0.59037	-1.48741
H	2.29431	0.34685	-1.90513
C	0.28599	-1.35216	0.23781
H	-0.48211	-0.5736	0.24203
H	0.03295	-2.13652	-0.47625
H	0.41241	-1.77943	1.2332
N	1.59119	-0.7174	-0.18531
C	-3.62408	-0.77217	-0.13792
C	-3.44589	-0.51298	1.29475
O	-2.71635	-1.5789	0.64873
H	-3.1098	-0.07453	-0.80083
H	-2.84287	0.3474	1.58137
H	-4.48113	-1.28028	-0.52804
C	-4.51929	-0.98471	2.29318
H	-4.0617	-1.18961	3.23845
H	-5.2567	-0.21862	2.41249
H	-4.98528	-1.87365	1.92233

TSh1

Charge = 0 Multiplicity = 1

Br	-4.59885	-0.42259	-0.24537
C	3.57906	1.39331	-0.80165
C	2.60559	0.9208	0.27341
C	3.94544	-1.16355	0.59066
C	4.93917	-0.71017	-0.47838
C	4.98721	0.81998	-0.59111
H	2.92759	1.27267	1.25881
H	1.5668	1.22619	0.10083
H	3.2031	1.13708	-1.79846
H	3.5964	2.48737	-0.7596
H	4.26738	-0.81682	1.57738
H	3.84808	-2.25177	0.62703
H	5.91972	-1.11211	-0.20169
H	4.68883	-1.15802	-1.44645
H	5.4171	1.23814	0.32886

H	5.64915	1.11606	-1.4105
C	1.88848	-1.19657	-0.83531
H	1.81167	-2.2751	-0.68837
H	0.89922	-0.72942	-0.91213
H	2.49344	-0.98959	-1.71505
C	1.6919	-0.9457	1.58354
H	0.70856	-0.49375	1.40769
H	1.62617	-2.03214	1.66268
H	2.16621	-0.53652	2.477
N	2.55044	-0.60502	0.38891
C	-1.96912	-0.27495	-0.06567
C	-1.63043	1.12991	-0.15707
O	-0.37062	0.49259	0.01332
H	-1.94629	-0.90228	-0.94152
H	-1.76913	1.57156	-1.15206
C	-2.08498	2.06143	0.9445
H	-1.57017	3.02739	0.8879
H	-3.16403	2.21455	0.85293
H	-1.8817	1.61505	1.92371
H	-2.10033	-0.73043	0.90251

h2

Charge = 0 Multiplicity = 1

Br	-0.18885	0.74176	0.78668
C	-1.89705	-0.87045	1.68616
C	-0.43696	-1.0784	1.30971
O	-2.5703	-2.16852	1.66503
H	0.35432	-0.82559	1.9931
H	-0.16882	-1.27831	0.28544
C	-2.03084	-3.04889	2.5293
O	-0.94794	-2.64442	3.11524
O	-2.56925	-4.15333	2.69912
H	-2.38562	-0.27963	0.91356
C	-2.07995	-0.23257	3.05492
H	-1.63713	0.76542	3.03363
H	-3.1425	-0.1579	3.29979
H	-1.58541	-0.83228	3.82715
C	-6.42844	-7.79688	2.19731
C	-5.74276	-8.40856	3.40198
C	-4.2411	-8.47076	3.20983
C	-4.35676	-6.49232	1.68336
C	-5.85853	-6.4309	1.87408
H	-3.75938	-8.8693	4.14013
H	-5.97663	-7.79813	4.31359
H	-6.14193	-9.4414	3.57675
H	-6.29984	-8.47347	1.31183
H	-7.52799	-7.70761	2.3961
H	-3.95797	-5.45934	1.50885
H	-4.1217	-7.1027	0.77196
H	-6.09991	-5.71958	2.70721
H	-6.33948	-6.03427	0.94244
H	-4.00091	-9.18034	2.37498
C	-2.16062	-7.22466	2.6168
H	-1.75667	-6.25564	2.41009
H	-1.67552	-7.6373	3.47663
H	-1.99982	-7.86513	1.77486
C	-3.85057	-6.17595	4.10467
H	-3.35273	-6.59883	4.95216
H	-3.43033	-5.21648	3.88626
H	-4.89299	-6.06799	4.32058
N	-3.67161	-7.10364	2.88854

TSh2

Charge = 0 Multiplicity = 1

Br	4.51252	0.90301	-0.28181
C	1.78397	-0.07096	0.54966
C	2.70709	-0.89723	-0.33216
O	0.41119	-0.50854	0.30344
H	3.48974	-1.50271	0.09035
H	2.73389	-0.72596	-1.39585

C	0.35934	-1.80284	-0.17055
O	1.49565	-2.31537	-0.43267
O	-0.76432	-2.31101	-0.30602
H	1.82157	0.96946	0.23261
C	2.10548	-0.19852	2.03132
H	3.111	0.19336	2.19903
H	1.38933	0.3711	2.63106
H	2.0679	-1.24763	2.34318
C	-3.46898	2.55457	-0.33198
C	-4.48865	1.8222	0.55253
C	-4.74644	0.39961	0.05619
C	-2.47881	0.31305	-0.97193
C	-2.18587	1.72825	-0.48937
H	-5.41646	-0.1535	0.7198
H	-4.15141	1.80451	1.59462
H	-5.45138	2.34449	0.55296
H	-3.91186	2.73301	-1.32106
H	-3.24282	3.5372	0.09239
H	-1.58969	-0.31618	-0.99502
H	-2.94461	0.33051	-1.9626
H	-1.61387	1.69554	0.44318
H	-1.51899	2.18391	-1.22834
H	-5.19377	0.42068	-0.94227
C	-3.79802	-1.74561	-0.72326
H	-2.86313	-2.30135	-0.81433
H	-4.5098	-2.27928	-0.09109
H	-4.24075	-1.55712	-1.70241
C	-2.87078	-0.71804	1.27708
H	-3.62352	-1.2333	1.87628
H	-1.99599	-1.34806	1.09811
H	-2.58172	0.21003	1.76252
N	-3.47886	-0.4231	-0.07474

Br	-1.20288	-1.88277	0.22294
C	3.0931	-0.89227	-0.95367
C	1.70097	-0.28806	-0.8808
C	2.70483	1.61306	0.33297
C	4.05492	0.91009	0.1934
H	1.53138	0.34582	-1.75497
H	0.89239	-1.03295	-0.80241
H	3.27359	-1.60089	-0.13231
H	3.18115	-1.44586	-1.8913
H	2.54945	2.2777	-0.5205
H	2.64437	2.19821	1.25464
H	4.83426	1.67129	0.09844
H	4.28377	0.31066	1.08798
C	1.49467	-0.16047	1.6138
H	1.36299	0.54537	2.43556
H	0.63639	-0.84368	1.53142
H	2.4203	-0.71582	1.74948
C	0.24	1.37432	0.19767
H	-0.55553	0.62503	0.17739
H	0.12667	2.03949	1.05411
H	0.25372	1.95167	-0.72676
N	1.55262	0.63493	0.32901
O	4.10356	0.11529	-0.97454
C	-3.81986	1.44197	-0.45713
C	-3.50451	1.01551	0.91434
O	-2.68972	2.00331	0.24091
H	-3.01542	0.05215	1.06355
H	-4.09227	1.4047	1.74671
C	-4.96606	2.4552	-0.63376
H	-4.76605	3.07563	-1.48227
H	-5.8861	1.93019	-0.78475
H	-5.04241	3.06377	0.243
H	-3.61208	0.82374	-1.30537

i1

Charge = 0 Multiplicity = 1

TSi1

Charge = 0 Multiplicity = 1

Br	-4.57414	-0.42829	-0.23442
C	3.61403	1.32682	-0.82768
C	2.59341	0.91487	0.22216
C	3.95308	-1.12365	0.57924
C	4.90881	-0.59423	-0.48988
H	2.8927	1.31079	1.19593
H	1.56246	1.2181	-0.00428
H	3.30763	1.01837	-1.83788
H	3.69238	2.41649	-0.8252
H	4.28076	-0.77796	1.56258
H	3.90869	-2.21599	0.5814
H	5.92314	-0.91204	-0.23448
H	4.66974	-1.01066	-1.48023
C	1.86897	-1.24388	-0.80519
H	1.79715	-2.31591	-0.61569
H	0.87857	-0.78007	-0.88702
H	2.46222	-1.06975	-1.70032
C	1.70847	-0.91295	1.60908
H	0.72074	-0.47072	1.43271
H	1.65242	-1.99692	1.72226
H	2.19468	-0.47184	2.48041
N	2.54372	-0.60413	0.38917
O	4.90895	0.81938	-0.52114
C	-1.94448	-0.27043	-0.06244
C	-1.61033	1.13393	-0.17168
O	-0.34774	0.50191	0.00484
H	-1.92208	-0.90822	-0.93081
H	-1.75105	1.5621	-1.17208
C	-2.06537	2.07805	0.91866
H	-1.55426	3.04498	0.84856
H	-3.14508	2.22616	0.82684
H	-1.85916	1.64512	1.90323
H	-2.07194	-0.71464	0.91149

i2

Charge = 0 Multiplicity = 1

Br	5.00379	-0.80443	-0.09389
C	2.78656	1.07193	-0.2663
C	3.06393	-0.43176	-0.34966
O	1.51524	1.37722	-0.86174
H	2.54245	-0.99649	0.41558
H	2.82968	-0.813	-1.34256
C	0.34287	0.85126	-0.31208
O	0.4368	0.03282	0.63618
O	-0.69225	1.28228	-0.87813
H	3.49622	1.57075	-0.93534
C	2.93838	1.65436	1.13756
H	3.95112	1.474	1.50932
H	2.76381	2.73398	1.1091
H	2.21728	1.19452	1.81517
C	-5.81076	-0.22167	0.20423
C	-4.6942	-0.7042	1.12964
C	-3.04928	-0.62068	-0.75265
C	-4.14949	-0.1327	-1.68983
H	-4.83943	-0.36492	2.15888
H	-5.93634	0.86341	0.29095
H	-6.74552	-0.66635	0.56301
H	-2.07485	-0.1745	-0.9927
H	-2.98916	-1.71355	-0.76369
H	-4.12224	0.96009	-1.76426
H	-3.90463	-0.50602	-2.68967
H	-4.65594	-1.79789	1.13452
C	-2.27783	-0.93336	1.56343
H	-1.27277	-0.59134	1.25628
H	-2.47788	-0.67937	2.60656
H	-2.38272	-2.01084	1.42241
C	-3.14315	1.24587	0.89455
H	-3.18968	1.45912	1.96363
H	-2.17237	1.51328	0.45589

H	-3.94492	1.77168	0.38004
N	-3.31327	-0.24427	0.70849
O	-5.53996	-0.61245	-1.25491

TSi2

Charge = 0 Multiplicity = 1

Br	-5.42995	-0.14022	-0.42307
C	-2.53425	-0.6731	0.28931
C	-3.05842	0.71668	-0.04293
O	-1.08673	-0.68173	0.07476
H	-3.54953	1.31983	0.70028
H	-3.13826	1.03258	-1.06999
C	-0.5567	0.56318	0.13838
O	-1.39435	1.51867	0.23367
O	0.68827	0.66796	0.08835
H	-2.93784	-1.38999	-0.42323
C	-2.83211	-1.10074	1.71864
H	-3.91552	-1.15905	1.84187
H	-2.38657	-2.07776	1.92535
H	-2.4259	-0.37255	2.42936
C	5.91888	-0.67769	0.19915
C	5.32972	0.7029	-0.08817
C	3.26548	-0.44998	-0.82834
C	3.96608	-1.75916	-0.49814
H	5.71065	1.4604	0.602
H	5.77664	-0.96014	1.25346
H	6.99508	-0.63914	0.01064
H	2.18434	-0.46611	-0.64561
H	3.46406	-0.18235	-1.86918
H	3.72272	-2.10807	0.5161
H	3.61812	-2.52081	-1.19964
H	5.57457	0.99726	-1.11146
C	3.27735	2.00519	-0.55054
H	2.18747	1.96534	-0.4653
H	3.69456	2.82793	0.03283
H	3.59163	2.09095	-1.59149
C	3.35137	0.60118	1.44155
H	3.74199	1.46079	1.98825
H	2.25895	0.60645	1.42137
H	3.72801	-0.31751	1.88605
N	3.81741	0.70938	0.00732
O	5.37618	-1.6545	-0.66541

j1

Charge = 0 Multiplicity = 1

C	0.93477	0.00245	-0.87873
C	2.93297	0.84095	-0.64208
N	1.59691	1.16224	-0.674
H	-0.13499	-0.09121	-1.04412
H	3.71589	1.56076	-0.45984
N	1.87228	-0.92959	-1.07519
C	0.97426	2.44432	-0.30198
C	0.98443	2.66215	1.21076
H	-0.04685	2.40836	-0.68696
H	1.50582	3.2349	-0.84027
H	0.516	1.80604	1.70651
H	2.00628	2.77298	1.58703
Br	-0.1624	-0.86432	1.60271
C	-2.97681	0.27122	-0.33525
C	-2.79798	-1.09164	-0.84421
O	-2.0767	0.01206	-1.44645
H	-2.17753	-1.76951	-0.26079
H	-2.44252	0.48958	0.58988
C	1.63995	-2.36724	-1.08544
H	2.60525	-2.85587	-1.20472
H	1.16889	-2.6228	-0.12868
H	0.98061	-2.63052	-1.9149
H	0.43363	3.57674	1.45002
N	3.13236	-0.42491	-0.88047
C	-3.87149	-1.71511	-1.75551

H	-3.57314	-2.70457	-2.03273
H	-4.80347	-1.75722	-1.23155
H	-3.98372	-1.11673	-2.63542
H	-3.83828	0.86285	-0.56488

TSj1

Charge = 0 Multiplicity = 1

Br	-3.00204	-0.63041	-0.22543
C	-0.7312	1.7469	-0.08153
C	-1.33656	1.00953	1.00725
O	0.07442	2.08166	1.04531
H	-0.22832	1.12012	-0.83534
H	-0.95536	0.05253	1.31587
H	-2.09531	1.47388	1.61992
C	1.91811	0.069	0.48897
C	3.16417	-1.509	-0.4407
N	2.03638	-1.25482	0.32218
H	1.13006	0.68238	0.98272
H	3.45964	-2.51113	-0.70642
N	2.93959	0.66178	-0.14613
C	1.09027	-2.28577	0.81196
C	0.12418	-2.77486	-0.26523
H	0.55124	-1.84378	1.65224
H	1.70785	-3.09846	1.20564
H	-0.63498	-2.02235	-0.51321
H	0.66223	-3.08495	-1.16696
C	3.12153	2.11726	-0.19409
H	4.01912	2.39851	0.36116
H	3.2161	2.43597	-1.2339
H	2.23538	2.57192	0.25683
H	-0.41208	-3.64574	0.12289
C	-1.50502	2.87383	-0.72845
H	-0.85067	3.50074	-1.34414
H	-2.29251	2.44733	-1.35666
H	-1.96393	3.50496	0.03846
N	3.73374	-0.30638	-0.73294

j2

Charge = 0 Multiplicity = 1

C	2.11375	0.86101	0.35009
C	3.53277	-0.725	-0.27912
N	2.66766	-0.30152	0.71671
H	1.34652	1.38475	0.96481
H	4.09038	-1.64459	-0.2104
N	2.59639	1.19195	-0.85282
C	2.28182	-1.01837	1.94996
C	1.62411	-2.362	1.646
H	1.57662	-0.35777	2.46054
H	3.17801	-1.13475	2.56753
H	0.73521	-2.21895	1.02618
H	2.30719	-3.04875	1.13538
Br	-1.17931	-1.44522	-1.06082
C	-2.9241	0.62424	0.06196
C	-2.92991	-0.84993	-0.32474
O	-2.04514	0.80812	1.16285
H	-2.57152	1.22813	-0.77849
H	-3.65035	-1.07149	-1.11223
H	-3.0985	-1.49022	0.54085
C	-0.82949	1.47563	0.92087
O	-0.64065	1.98571	-0.20295
O	-0.05704	1.4419	1.9133
C	2.15001	2.37199	-1.6017
H	2.86115	3.19187	-1.47351
H	2.07777	2.10975	-2.65846
H	1.15942	2.63336	-1.21564
H	1.31949	-2.83106	2.58592
C	-4.33014	1.05856	0.48688
H	-4.30765	2.11328	0.7728
H	-5.05179	0.93532	-0.32778
H	-4.67405	0.48103	1.35124

N	3.48938	0.21619	-1.26397

TSj2

Charge = 0 Multiplicity = 1

Br	-4.40818	0.77173	-0.19034
C	-2.26938	-1.37993	0.12327
C	-1.95538	0.07586	-0.19101
O	-1.13058	-2.19908	-0.28925
H	-1.90902	0.81517	0.58891
H	-1.9855	0.42457	-1.21009
C	0.01841	-1.4995	-0.35351
O	-0.11121	-0.22164	-0.17827
O	1.08581	-2.08936	-0.57878
H	-3.10116	-1.70888	-0.49693
C	3.0825	-0.09164	-0.31179
C	4.44633	1.5988	0.1214
N	3.15976	1.24234	-0.24809
H	2.20479	-0.72211	-0.54488
H	4.74567	2.62797	0.23725
N	4.28237	-0.59621	0.00493
C	2.01888	2.15986	-0.46501
C	1.45626	2.69146	0.84957
H	1.25732	1.58006	-0.98713
H	2.3738	2.96419	-1.1152
H	1.05481	1.86777	1.444
H	2.21044	3.22822	1.43352
C	4.56845	-2.0339	0.04708
H	5.28123	-2.29584	-0.73782
H	4.98204	-2.29504	1.02304
H	3.62952	-2.56664	-0.10932
H	0.6375	3.38318	0.63353
C	-2.55856	-1.62834	1.59593
H	-3.45467	-1.06875	1.87222
H	-2.72081	-2.69407	1.77607
H	-1.71769	-1.29437	2.21401

N	5.15377	0.4445	0.27773

k1

Charge = 0 Multiplicity = 1

C	1.01537	0.15507	-0.88499
C	3.20174	-0.20426	-0.81936
C	2.98196	1.08252	-0.44094
N	1.61366	1.29817	-0.51726
H	-0.05208	0.03683	-1.03763
H	4.11653	-0.76723	-0.90663
H	3.66818	1.8567	-0.13944
N	1.96949	-0.75933	-1.12484
C	0.88875	2.47876	-0.02149
C	0.81752	2.48919	1.5057
H	-0.11049	2.42984	-0.45957
H	1.3876	3.36679	-0.4221
H	0.39699	1.5409	1.8577
H	1.81093	2.62015	1.94631
Br	-0.22291	-1.15766	1.47674
C	-2.95385	0.31587	-0.33948
C	-2.75853	-0.94448	-1.06122
O	-2.03096	0.24436	-1.45897
H	-2.14698	-1.70587	-0.57997
H	-2.44031	0.37697	0.62063
C	1.67955	-2.17846	-1.32236
H	2.62062	-2.71753	-1.43298
H	1.12543	-2.5145	-0.43616
H	1.07662	-2.31516	-2.22232
H	0.18652	3.31929	1.83767
C	-3.8106	-1.41222	-2.08394
H	-3.50178	-2.34238	-2.51328
H	-4.75254	-1.54127	-1.59302
H	-3.90847	-0.67801	-2.85611
H	-3.81335	0.93607	-0.48615

TSk1

Charge = 0 Multiplicity = 1

Br	-2.99293	-0.63932	-0.23112
C	-0.73638	1.75111	-0.07343
C	-1.34507	1.00904	1.01092
O	0.05929	2.09362	1.05602
H	-0.2232	1.12748	-0.82396
H	-0.95305	0.05933	1.32964
H	-2.10814	1.47042	1.62105
C	1.91738	0.06953	0.49326
C	3.72372	-0.2894	-0.74468
C	3.16587	-1.49694	-0.44952
N	2.04284	-1.2529	0.32391
H	1.13077	0.67	0.99654
H	4.60384	-0.03625	-1.31477
H	3.46536	-2.49758	-0.71913
N	2.92783	0.67228	-0.14928
C	1.1078	-2.29104	0.82006
C	0.14185	-2.7911	-0.25306
H	0.56755	-1.85064	1.66104
H	1.73466	-3.09732	1.21373
H	-0.62595	-2.04536	-0.49834
H	0.67892	-3.0955	-1.15861
C	3.09766	2.12949	-0.19716
H	3.99741	2.41666	0.35305
H	3.18293	2.44881	-1.23839
H	2.21014	2.57667	0.26008
H	-0.38368	-3.66838	0.1384
C	-1.51516	2.87117	-0.72843
H	-0.85854	3.50612	-1.33555
H	-2.29142	2.43812	-1.36776
H	-1.9902	3.49771	0.03396

k2

Charge = 0 Multiplicity = 1

TSk2

C	-2.24981	0.81818	-0.32806
C	-3.59973	0.15322	1.29845
C	-3.60197	-0.81072	0.33486
N	-2.75305	-0.37431	-0.66969
H	-1.49881	1.35522	-0.94437
H	-4.11711	0.20881	2.2434
H	-4.12063	-1.75481	0.28408
N	-2.74716	1.15604	0.86682
C	-2.33454	-1.10546	-1.88383
C	-1.59001	-2.39548	-1.54685
H	-1.67764	-0.42039	-2.42554
H	-3.22948	-1.29756	-2.48497
H	-0.68831	-2.17945	-0.96576
H	-2.21672	-3.09776	-0.9853
Br	1.45845	-1.55601	0.96069
C	2.86892	0.80449	-0.04704
C	3.0943	-0.67308	0.24947
O	1.96604	0.91894	-1.13738
H	2.43469	1.29976	0.8253
H	3.85238	-0.83252	1.01714
H	3.34275	-1.23012	-0.6542
C	0.70111	1.48315	-0.88654
O	0.46604	1.94346	0.25117
O	-0.05764	1.42427	-1.88741
C	-2.34539	2.36682	1.59156
H	-3.06512	3.17055	1.41266
H	-2.30559	2.13876	2.65866
H	-1.34669	2.63201	1.22915
H	-1.28888	-2.88603	-2.47823
C	4.19433	1.46841	-0.43685
H	4.01443	2.52496	-0.65734
H	4.93034	1.40367	0.37335
H	4.61729	1.00244	-1.3342

Charge = 0 Multiplicity = 1

Br	-4.40138	0.77964	-0.19971
C	-2.27213	-1.38276	0.13128
C	-1.95267	0.07019	-0.19181
O	-1.13854	-2.20909	-0.27926
H	-1.89776	0.81385	0.58349
H	-1.974	0.41161	-1.21373
C	0.01515	-1.51589	-0.34533
O	-0.10926	-0.23668	-0.17364
O	1.07903	-2.11134	-0.56863
H	-3.10531	-1.71483	-0.48527
C	3.07769	-0.08524	-0.31119
C	5.15333	0.44442	0.26445
C	4.44772	1.6008	0.11437
N	3.15751	1.24832	-0.24683
H	2.19833	-0.70979	-0.53943
H	6.18479	0.27398	0.53057
H	4.74909	2.63026	0.22896
N	4.27772	-0.59422	-0.0036
C	2.0172	2.1689	-0.45413
C	1.45876	2.69224	0.86617
H	1.25395	1.59467	-0.98031
H	2.37249	2.97738	-1.09982
H	1.05794	1.86439	1.45713
H	2.2163	3.22436	1.452
C	4.56071	-2.0329	0.03465
H	5.26933	-2.29402	-0.75533
H	4.97935	-2.29566	1.00888
H	3.61909	-2.5634	-0.11778
H	0.63945	3.38704	0.65676
C	-2.5589	-1.62219	1.60661
H	-3.45291	-1.05824	1.88427
H	-2.72489	-2.68754	1.79242
H	-1.71448	-1.28868	2.22201

I1

Charge = 0 Multiplicity = 1

C	0.96893	-0.21889	-0.61818
C	3.16949	-0.41435	-0.45017
C	2.87232	0.91151	-0.4749
N	1.4954	1.01397	-0.61131
H	-0.08704	-0.43398	-0.73545
H	4.11513	-0.92385	-0.36338
H	3.50905	1.77904	-0.41975
N	1.97519	-1.10577	-0.57498
C	0.69863	2.24623	-0.50981
C	0.61022	2.74081	0.93371
H	-0.29114	2.00385	-0.90247
H	1.15099	2.98876	-1.1748
H	0.22283	1.94278	1.57515
H	1.59296	3.04498	1.30749
C	-2.97281	-0.0061	-0.03509
C	-2.75212	-1.40828	-0.39941
O	-2.09139	-0.35103	-1.13743
H	-2.0934	-1.99909	0.23414
H	-2.42841	0.33467	0.84575
C	1.77123	-2.53469	-0.34339
H	2.74302	-3.02836	-0.32165
H	1.2502	-2.63473	0.61575
H	1.1694	-2.96009	-1.14902
H	-0.05404	3.60926	0.98153
Cl	-0.12002	-0.79135	1.95564
C	-3.82386	-2.16508	-1.20578
H	-3.49468	-3.16753	-1.38364
H	-4.73966	-2.18324	-0.6527
H	-3.98191	-1.6703	-2.14125
H	-3.86361	0.52278	-0.3028

TSI1

Charge = 0 Multiplicity = 1

C	-0.73638	1.75111	-0.07343
C	-1.34507	1.00904	1.01092
O	0.05929	2.09362	1.05602
H	-0.2232	1.12748	-0.82396
H	-0.95305	0.05933	1.32964
H	-2.10814	1.47042	1.62105
C	1.91738	0.06953	0.49326
C	3.72372	-0.2894	-0.74468
C	3.16587	-1.49694	-0.44952
N	2.04284	-1.2529	0.32391
H	1.13077	0.67	0.99654
H	4.60384	-0.03625	-1.31477
H	3.46536	-2.49758	-0.71913
N	2.92783	0.67228	-0.14928
C	1.1078	-2.29104	0.82006
C	0.14185	-2.7911	-0.25306
H	0.56755	-1.85064	1.66104
H	1.73466	-3.09732	1.21373
H	-0.62595	-2.04536	-0.49834
H	0.67892	-3.0955	-1.15861
C	3.09766	2.12949	-0.19716
H	3.99741	2.41666	0.35305
H	3.18293	2.44881	-1.23839
H	2.21014	2.57667	0.26008
H	-0.38368	-3.66838	0.1384
C	-1.51516	2.87117	-0.72843
H	-0.85854	3.50612	-1.33555
H	-2.29142	2.43812	-1.36776
H	-1.9902	3.49771	0.03396
Cl	-2.90866	-0.56958	-0.14183

I2

Charge = 0 Multiplicity = 1

C	-2.24981	0.81818	-0.32806
C	-3.59973	0.15322	1.29845
C	-3.60197	-0.81072	0.33486
N	-2.75305	-0.37431	-0.66969
H	-1.49881	1.35522	-0.94437
H	-4.11711	0.20881	2.2434
H	-4.12063	-1.75481	0.28408
N	-2.74716	1.15604	0.86682
C	-2.33454	-1.10546	-1.88383
C	-1.59001	-2.39548	-1.54685
H	-1.67764	-0.42039	-2.42554
H	-3.22948	-1.29756	-2.48497
H	-0.68831	-2.17945	-0.96576
H	-2.21672	-3.09776	-0.9853
C	2.86892	0.80449	-0.04704
C	3.0943	-0.67308	0.24947
O	1.96604	0.91894	-1.13738
H	2.43469	1.29976	0.8253
H	3.85238	-0.83252	1.01714
H	3.34275	-1.23012	-0.6542
C	0.70111	1.48315	-0.88654
O	0.46604	1.94346	0.25117
O	-0.05764	1.42427	-1.88741
C	-2.34539	2.36682	1.59156
H	-3.06512	3.17055	1.41266
H	-2.30559	2.13876	2.65866
H	-1.34669	2.63201	1.22915
H	-1.28888	-2.88603	-2.47823
C	4.19433	1.46841	-0.43685
H	4.01443	2.52496	-0.65734
H	4.93034	1.40367	0.37335
H	4.61729	1.00244	-1.3342
Cl	1.64776	-1.45383	0.87839

TSI2

Charge = 0 Multiplicity = 1

C	-2.27213	-1.38276	0.13128

C	-1.95267	0.07019	-0.19181
O	-1.13854	-2.20909	-0.27926
H	-1.89776	0.81385	0.58349
H	-1.974	0.41161	-1.21373
C	0.01515	-1.51589	-0.34533
O	-0.10926	-0.23668	-0.17364
O	1.07903	-2.11134	-0.56863
H	-3.10531	-1.71483	-0.48527
C	3.07769	-0.08524	-0.31119
C	5.15333	0.44442	0.26445
C	4.44772	1.6008	0.11437
N	3.15751	1.24832	-0.24683
H	2.19833	-0.70979	-0.53943
H	6.18479	0.27398	0.53057
H	4.74909	2.63026	0.22896
N	4.27772	-0.59422	-0.0036
C	2.0172	2.1689	-0.45413
C	1.45876	2.69224	0.86617
H	1.25395	1.59467	-0.98031
H	2.37249	2.97738	-1.09982
H	1.05794	1.86439	1.45713
H	2.2163	3.22436	1.452
C	4.56071	-2.0329	0.03465
H	5.26933	-2.29402	-0.75533
H	4.97935	-2.29566	1.00888
H	3.61909	-2.5634	-0.11778
H	0.63945	3.38704	0.65676
C	-2.5589	-1.62219	1.60661
H	-3.45291	-1.05824	1.88427
H	-2.72489	-2.68754	1.79242
H	-1.71448	-1.28868	2.22201
Cl	-4.2424	0.73507	-0.19605

m1

Charge = 0 Multiplicity = 1

C	2.51301	-0.89802	-0.46269
C	3.31163	-2.94447	-0.23178
C	3.94455	-2.14413	0.67044
N	3.43745	-0.86797	0.504
H	1.92224	-0.05398	-0.79488
H	3.4105	-3.99876	-0.4323
H	4.70097	-2.36727	1.40504
N	2.42678	-2.14643	-0.93146
C	3.74572	0.31289	1.33619
C	2.87527	0.36242	2.59097
H	3.58061	1.18438	0.70095
H	4.81141	0.25601	1.57672
H	1.81648	0.41727	2.32003
H	3.03831	-0.51664	3.22244
C	1.42129	3.11967	-0.43797
C	1.36891	2.69442	-1.84219
O	2.44294	2.24354	-0.98162
H	0.66267	1.91778	-2.12775
H	0.75283	2.60401	0.25153
C	1.45708	-2.60166	-1.93361
H	1.98873	-2.97957	-2.81009
H	0.83782	-3.3784	-1.48482
H	0.81031	-1.75876	-2.18111
H	3.1384	1.25134	3.17289
S	-0.68498	-0.36382	0.09895
O	-0.33519	-1.76255	0.46914
O	-0.1833	0.66829	1.05506
O	-0.3052	-0.04065	-1.32253
C	-2.48257	-0.25903	0.16646
C	-3.10444	0.98809	0.25175
C	-3.25036	-1.42029	0.09799
C	-4.49481	1.06624	0.26065
H	-2.49806	1.88452	0.32393
C	-4.64235	-1.32958	0.10852
H	-2.74989	-2.3811	0.04963

C	-5.28684	-0.08908	0.18948
H	-4.97567	2.03942	0.32799
H	-5.23796	-2.238	0.05613
C	-6.79401	0.00334	0.23389
H	-7.26278	-0.86669	-0.23534
H	-7.15892	0.0522	1.26772
H	-7.15584	0.90045	-0.2783
H	1.75322	4.09707	-0.15617
C	1.81446	3.67695	-2.94116
H	2.20105	3.12847	-3.77459
H	0.97648	4.26242	-3.25725
H	2.57541	4.32261	-2.55519

TSm1

Charge = 0 Multiplicity = 1

C	-1.67212	2.23017	0.23937
C	-0.94345	2.02496	-1.00485
O	-2.70337	2.23028	-0.7421
H	-1.67893	1.36521	0.91852
H	-0.89189	1.05389	-1.46853
H	-0.64089	2.88533	-1.58434
C	-3.59542	-0.42638	-0.36072
C	-5.35838	-1.50298	0.44871
C	-4.35033	-2.40401	0.27978
N	-3.26075	-1.71523	-0.22523
H	-3.01604	0.44663	-0.71342
H	-6.36479	-1.62798	0.81436
H	-4.314	-3.46315	0.47591
N	-4.86554	-0.27578	0.04602
C	-1.93488	-2.31228	-0.52492
C	-1.21725	-2.79378	0.73145
H	-1.32116	-1.55233	-1.01382
H	-2.11586	-3.12908	-1.23033
H	-0.94025	-1.94821	1.36509
H	-1.81119	-3.51872	1.29877
C	-5.57019	1.01146	0.05061
H	-6.3857	0.98966	-0.67592
H	-5.97184	1.19965	1.04839
H	-4.84361	1.78447	-0.21475
H	-0.28626	-3.2751	0.4229
C	-1.4816	3.52647	0.99806
H	-2.30284	3.6814	1.70669
H	-0.5396	3.50105	1.55378
H	-1.46443	4.37368	0.3055
S	1.20944	0.22807	-0.06826
O	0.68411	-0.70506	-1.11347
O	0.69227	-0.03876	1.2992
O	1.05284	1.67446	-0.48946
C	2.98702	-0.04135	-0.00657
C	3.66742	0.10884	1.20117
C	3.68064	-0.37447	-1.17083
C	5.05008	-0.06746	1.23701
H	3.10724	0.34351	2.09966
C	5.06197	-0.54836	-1.1208
H	3.13285	-0.51265	-2.0967
C	5.76961	-0.3921	0.07959
H	5.57899	0.04349	2.18063
H	5.60073	-0.81504	-2.02703
C	7.27146	-0.55003	0.11793
H	7.77535	0.39213	-0.13254
H	7.61801	-0.84908	1.11164
H	7.61462	-1.30045	-0.60103

m2

Charge = 0 Multiplicity = 1

C	2.36991	-0.01792	0.91582
C	2.47429	2.17619	0.6311
C	3.33369	1.59557	-0.25234
N	3.25289	0.22576	-0.05887
H	1.99822	-0.98614	1.25475

H	2.21906	3.21015	0.79483
H	3.97703	2.03253	-0.99839
N	1.88547	1.15159	1.34963
C	3.90573	-0.81856	-0.87451
C	3.34214	-0.86606	-2.29187
H	3.69844	-1.76323	-0.37248
H	4.98172	-0.61786	-0.85999
H	2.29159	-1.1598	-2.24462
H	3.44753	0.09284	-2.80982
C	-2.10815	-2.06418	0.39841
C	-2.70281	-0.78637	-0.18419
O	-0.92433	-2.38136	-0.3131
H	-1.86051	-1.90149	1.45166
H	-3.68708	-0.56264	0.23796
H	-2.75452	-0.85022	-1.27373
C	0.31816	-2.18248	0.33977
O	0.29484	-1.83709	1.55096
O	1.29669	-2.36545	-0.40476
C	0.85087	1.27147	2.38353
H	1.30604	1.55595	3.33558
H	0.12988	2.02257	2.06277
H	0.35923	0.29958	2.46062
H	3.88726	-1.62171	-2.86537
C	-3.10011	-3.21853	0.24602
H	-2.64847	-4.12993	0.64435
H	-4.03096	-3.0265	0.79066
H	-3.33887	-3.39498	-0.80803
O	-1.80777	0.3259	0.173
S	-2.00041	1.72218	-0.56973
O	-0.98265	2.59551	-0.01735
O	-2.17641	1.56658	-2.00638
C	-3.5792	2.217	0.08676
C	-3.69038	2.5978	1.42398
C	-4.70544	2.22411	-0.73663
C	-4.92825	2.98564	1.93825
H	-2.80274	2.593	2.0731
C	-5.94286	2.6113	-0.22242
H	-4.61751	1.92405	-1.79084
C	-6.05423	2.99175	1.11524
H	-5.01584	3.28611	2.99246
H	-6.83064	2.61661	-0.87124
C	-7.42044	3.42019	1.68227
H	-7.5452	4.47504	1.5533
H	-8.20011	2.90275	1.16337
H	-7.46525	3.18048	2.72411

TSm2

Charge = 0 Multiplicity = 1

C	0.59104	2.92437	0.04813
C	0.69756	1.51385	-0.50184
O	1.81807	3.19172	0.77275
H	0.54891	1.30881	-1.54843
H	0.71373	0.68881	0.19216
C	2.86794	2.45103	0.31954
O	2.53222	1.61555	-0.63669
O	3.97968	2.57292	0.81019
H	-0.20401	2.95332	0.79309
C	3.57996	-1.06303	0.05662
C	4.92146	-2.56657	0.96999
C	3.81214	-3.21182	0.5078
N	2.9876	-2.25928	-0.05781
H	3.1891	-0.10131	-0.28792
H	5.79757	-2.93946	1.47516
H	3.53847	-4.25388	0.54003
N	4.75562	-1.22574	0.67957
C	1.65053	-2.50053	-0.66643
C	1.59986	-2.10668	-2.13871
H	0.90002	-1.95024	-0.08833
H	1.45461	-3.56694	-0.53391
H	1.89572	-1.06299	-2.27895

H	2.24711	-2.73998	-2.75309
C	5.70002	-0.14077	0.98464
H	6.00193	-0.22111	2.03045
H	6.57807	-0.2317	0.34105
H	5.20355	0.82235	0.82204
H	0.5644	-2.18829	-2.47747
C	0.36535	3.97494	-1.02841
H	-0.59868	3.79594	-1.51225
H	0.36168	4.97483	-0.58739
H	1.15608	3.92796	-1.78365
S	-1.65189	-0.25661	-0.44494
O	-1.5181	-0.83805	-1.80187
O	-0.89121	-0.97758	0.61983
O	-1.33822	1.23478	-0.41755
C	-3.38628	-0.35763	0.00746
C	-4.35863	-0.37432	-0.99183
C	-3.75189	-0.38641	1.35369
C	-5.70563	-0.41418	-0.63521
H	-4.05306	-0.36644	-2.03235
C	-5.10189	-0.42662	1.695
H	-2.98145	-0.38891	2.11698
C	-6.09912	-0.44097	0.70938
H	-6.46425	-0.42674	-1.41392
H	-5.38754	-0.44917	2.74387
C	-7.55918	-0.51647	1.08838
H	-8.19598	-0.0679	0.32029
H	-7.88275	-1.55768	1.21239
H	-7.75458	-0.00225	2.03428

n1

Charge = 0 Multiplicity = 1

C	1.1995	0.77669	-0.61417
C	3.39198	0.97614	-0.43803
C	2.82121	1.96716	0.30202
N	1.45099	1.82993	0.17192
H	0.21355	0.40562	-0.8679
H	4.42698	0.72715	-0.60625
H	3.26369	2.74777	0.8991
N	2.36304	0.24835	-1.00428
C	0.41831	2.60937	0.88497
C	0.10322	2.00986	2.25477
H	-0.46302	2.61317	0.2415
H	0.79716	3.63252	0.96252
H	-0.26924	0.98565	2.15443
H	0.98836	2.00216	2.89848
C	-2.95711	0.699	-0.44319
C	-2.63624	0.42046	-1.84801
O	-1.84989	1.3758	-1.09701
H	-2.1142	-0.50184	-2.08995
H	-2.626	-0.03399	0.29196
C	2.50537	-0.98307	-1.78912
H	3.04714	-0.76573	-2.71236
H	3.03469	-1.71817	-1.18291
H	1.507	-1.3725	-1.98809
H	-0.66563	2.61769	2.7418
S	-0.18495	-1.99242	0.52385
O	1.25335	-1.92709	0.86982
O	-1.0591	-1.23434	1.45545
O	-0.45952	-1.74056	-0.91704
O	-0.64424	-3.58114	0.68953
H	-0.68425	-3.74386	1.64541
C	-3.50088	1.04719	-2.95761
H	-3.13036	0.74181	-3.91383
H	-4.51408	0.72147	-2.84708
H	-3.45894	2.11376	-2.88288
H	-3.7806	1.32384	-0.16688

TSn1

Charge = 0 Multiplicity = 1

C	0.39815	2.06362	0.30803

C	1.05492	1.71615	-0.94539
O	-0.61125	2.31074	-0.66461
H	0.19365	1.21281	0.97471
H	0.89151	0.75666	-1.40701
H	1.53621	2.49622	-1.51762
C	-2.17752	-0.01615	-0.37736
C	-4.19638	-0.6269	0.31221
C	-3.44172	-1.75113	0.15863
N	-2.18839	-1.35063	-0.27197
H	-1.37486	0.68732	-0.67264
H	-5.22035	-0.49991	0.6246
H	-3.68566	-2.78897	0.31752
N	-3.38801	0.44313	-0.02435
C	-1.03632	-2.25038	-0.52418
C	-0.48126	-2.85805	0.75958
H	-0.25318	-1.66484	-1.00777
H	-1.38657	-3.01887	-1.21946
H	-0.07351	-2.08202	1.41081
H	-1.23282	-3.44186	1.30176
C	-3.74449	1.86674	-0.01185
H	-4.49658	2.06694	-0.77832
H	-4.14136	2.13129	0.97036
H	-2.83351	2.43564	-0.2157
H	0.3481	-3.51638	0.49187
C	0.87546	3.27295	1.08415
H	0.11044	3.59862	1.79769
H	1.78849	3.03104	1.63675
H	1.08333	4.10399	0.40347
S	2.88777	-0.54303	-0.14339
O	4.20626	-1.17275	-0.03793
O	1.84576	-1.26047	-0.91204
O	2.93335	0.92265	-0.46991
O	2.25652	-0.6049	1.41844
H	3.02699	-0.52981	2.00298

n2

Charge = 0 Multiplicity = 1

C	-1.95031	-0.07951	-0.99302
C	-3.03726	1.74328	-0.358
C	-3.6605	0.66758	0.19849
N	-2.9654	-0.46007	-0.20901
H	-1.15958	-0.70292	-1.43433
H	-3.24625	2.79782	-0.28304
H	-4.52167	0.6096	0.84384
N	-1.97691	1.25344	-1.09852
C	-3.18266	-1.84547	0.2514
C	-2.86616	-2.00251	1.73601
H	-2.49627	-2.46341	-0.32708
H	-4.21707	-2.11502	0.01536
H	-1.80468	-1.8012	1.89245
H	-3.47576	-1.34054	2.35994
C	3.01126	-0.55079	-0.59848
C	3.32882	0.72294	0.18367
O	1.99413	-1.25695	0.10299
H	2.62961	-0.27969	-1.58675
H	4.09175	1.31526	-0.32835
H	3.66169	0.49376	1.19685
C	0.73924	-1.43009	-0.5279
O	0.60632	-0.98514	-1.70122
O	-0.10241	-1.98982	0.19554
C	-0.94584	2.03385	-1.79041
H	-1.39132	2.58734	-2.62027
H	-0.47941	2.70305	-1.06715
H	-0.19296	1.33093	-2.14988
H	-3.07122	-3.0341	2.03723
C	4.24925	-1.43752	-0.72409
H	3.99872	-2.33377	-1.29695
H	5.06489	-0.91723	-1.23911
H	4.60416	-1.75443	0.26216
O	2.15938	1.58276	0.2279

S	1.1186	1.80232	1.3151
O	-0.17605	1.53792	0.86506
O	1.64587	1.05981	2.37304
O	1.30034	3.4354	1.61328
H	0.65802	3.7147	2.2698

TSn2

Charge = 0 Multiplicity = 1

C	1.21132	2.29736	0.48485
C	1.06815	1.33689	-0.69054
O	0.10998	3.24026	0.43964
H	0.91442	0.28332	-0.5372
H	1.35758	1.66188	-1.678
C	-0.99235	2.73433	-0.17986
O	-0.73046	1.67285	-0.9065
O	-2.09245	3.24372	-0.03891
H	2.11855	2.88759	0.35006
C	-2.47079	-0.60085	-0.36407
C	-4.40238	-1.54564	0.1539
C	-3.44331	-2.51447	0.16213
N	-2.24516	-1.90569	-0.1654
H	-1.73757	0.16652	-0.63137
H	-5.46137	-1.59867	0.34853
H	-3.50996	-3.56974	0.37161
N	-3.77454	-0.35774	-0.17353
C	-0.91705	-2.56477	-0.22076
C	-0.37872	-2.90778	1.16398
H	-0.22781	-1.88837	-0.72733
H	-1.03206	-3.45691	-0.84227
H	-0.31003	-2.0118	1.78623
H	-0.99923	-3.65016	1.6759
C	-4.41325	0.96048	-0.31619
H	-5.00505	0.97996	-1.2341
H	-5.06407	1.12845	0.54357
H	-3.64225	1.73868	-0.34467
H	0.63354	-3.29932	1.04686
C	1.21824	1.60878	1.84346
H	2.0916	0.96083	1.9372
H	1.23744	2.35986	2.63724
H	0.31355	1.00297	1.97091
S	3.28989	-0.73962	-0.38508
O	2.03535	-1.52327	-0.44198
O	4.42743	-1.21605	-1.17299
O	3.0332	0.74171	-0.5367
O	3.74647	-0.91709	1.20987
H	4.70714	-0.78005	1.21979

o1

Charge = 0 Multiplicity = 1

C	-1.29917	0.12001	-0.54302
C	-3.49159	0.39761	-0.46446
C	-3.23374	-0.93544	-0.35913
N	-1.86119	-1.08776	-0.41953
H	-0.23204	0.29587	-0.61258
H	-4.42298	0.93986	-0.46469
H	-3.8982	-1.77572	-0.24141
N	-2.27233	1.04015	-0.57882
C	-1.11785	-2.3552	-0.24744
C	-1.0741	-2.78803	1.2166
H	-0.11604	-2.17403	-0.64124
H	-1.61079	-3.09705	-0.88313
H	-0.61657	-2.0044	1.82892
H	-2.07702	-3.00216	1.60017
C	2.82431	-0.81362	-0.25653
C	2.85077	-0.26466	-1.61735
O	1.6016	-0.70806	-1.02804
H	2.93294	0.81305	-1.74008
H	2.87371	-0.09468	0.55881
C	-2.06683	2.49002	-0.70672
H	-1.96806	2.76119	-1.76035

H	-2.93269	2.99502	-0.27788
H	-1.16555	2.75574	-0.14506
H	-0.48112	-3.70414	1.29825
N	0.59105	2.26637	1.11359
C	0.4293	1.15266	1.79582
N	0.14634	0.1738	2.38815
C	1.70194	2.47357	0.42797
N	2.6306	2.74274	-0.24208
H	3.15087	-1.80681	-0.02886
C	3.35053	-1.14812	-2.7755
H	2.85994	-0.85959	-3.68157
H	4.40753	-1.02514	-2.88746
H	3.13138	-2.17348	-2.56217

TSo1

Charge = 0 Multiplicity = 1

C	-1.11824	-1.44052	0.67846
C	-1.68795	-0.99062	-0.58612
O	-0.24827	-2.01162	-0.28052
H	-0.66432	-0.64359	1.29108
H	-1.22297	-0.18436	-1.13091
H	-2.35432	-1.65233	-1.12253
C	1.94922	-0.281	-0.31733
C	4.16492	-0.20659	-0.19479
C	3.69654	1.07324	-0.1853
N	2.31539	1.00622	-0.26346
H	0.94543	-0.7631	-0.38451
H	5.17141	-0.59086	-0.15429
H	4.22114	2.0133	-0.12998
N	3.05911	-1.03326	-0.27488
C	1.38934	2.16344	-0.2289
C	1.3585	2.84604	1.13382
H	0.38922	1.80426	-0.47649
H	1.70554	2.85132	-1.018
H	1.09622	2.13115	1.91832
H	2.31469	3.31552	1.38625
C	3.03963	-2.50023	-0.30957
H	3.50305	-2.85609	-1.23232
H	3.58575	-2.89147	0.55113
H	1.99495	-2.81706	-0.26658
H	0.57604	3.60712	1.11012
C	-1.89483	-2.41907	1.53492
H	-1.22668	-2.90875	2.25143
H	-2.68364	-1.90254	2.09039
H	-2.35072	-3.19219	0.90958
N	-3.1707	0.4077	-0.16277
C	-4.45491	0.2816	-0.47171
N	-5.56714	0.03165	-0.74483
C	-2.55953	1.56549	-0.03146
N	-1.82392	2.47655	0.09157

o2

Charge = 0 Multiplicity = 1

C	-1.95031	-0.07951	-0.99302
C	-3.03726	1.74328	-0.358
C	-3.6605	0.66758	0.19849
N	-2.9654	-0.46007	-0.20901
H	-1.15958	-0.70292	-1.43433
H	-3.24625	2.79782	-0.28304
H	-4.52167	0.6096	0.84384
N	-1.97691	1.25344	-1.09852
C	-3.18266	-1.84547	0.2514
C	-2.86616	-2.00251	1.73601
H	-2.49627	-2.46341	-0.32708
H	-4.21707	-2.11502	0.01536
H	-1.80468	-1.8012	1.89245
H	-3.47576	-1.34054	2.35994
C	3.01126	-0.55079	-0.59848
C	3.32882	0.72294	0.18367
O	1.99413	-1.25695	0.10299

H	2.62961	-0.27969	-1.58675
H	4.09175	1.31526	-0.32835
H	3.66169	0.49376	1.19685
C	0.73924	-1.43009	-0.5279
O	0.60632	-0.98514	-1.70122
O	-0.10241	-1.98982	0.19554
C	-0.94584	2.03385	-1.79041
H	-1.39132	2.58734	-2.62027
H	-0.47941	2.70305	-1.06715
H	-0.19296	1.33093	-2.14988
H	-3.07122	-3.0341	2.03723
C	4.24925	-1.43752	-0.72409
H	3.99872	-2.33377	-1.29695
H	5.06489	-0.91723	-1.23911
H	4.60416	-1.75443	0.26216
N	2.14504	1.59331	0.22845
C	1.96375	2.10402	1.5949
N	1.82069	2.50703	2.6732
C	2.33099	2.72133	-0.69561
N	2.47772	3.61147	-1.4248

TSo2

Charge = 0 Multiplicity = 1

C	-2.26125	-1.59582	-0.34812
C	-1.73136	-0.24289	0.10908
O	-1.1474	-2.31829	-0.93784
H	-1.83298	0.07762	1.13301
H	-1.36456	0.46343	-0.61772
C	0.04743	-1.91093	-0.44059
O	-0.03633	-0.91	0.38542
O	1.09266	-2.44688	-0.81578
H	-2.97135	-1.4506	-1.16274
C	2.77089	-0.05234	-0.32643
C	4.608	0.62167	0.70722
C	3.86614	1.72335	0.40111
N	2.72403	1.28108	-0.24552
H	2.02946	-0.73365	-0.73624
H	5.55947	0.52702	1.20503
H	4.04975	2.76894	0.58778
N	3.90287	-0.47657	0.24593
C	1.57836	2.11575	-0.67795
C	0.79305	2.68052	0.50138
H	0.94824	1.47073	-1.29133
H	1.97457	2.90627	-1.32102
H	0.48372	1.87216	1.1685
H	1.38414	3.40456	1.07062
C	4.26996	-1.8928	0.36191
H	5.11617	-2.11433	-0.292
H	4.53593	-2.11105	1.39763
H	3.40023	-2.48439	0.07018
H	-0.10934	3.17416	0.12667
C	-2.87968	-2.41482	0.7762
H	-3.77823	-1.91952	1.15467
H	-3.15571	-3.40475	0.40479
H	-2.16686	-2.5358	1.59812
N	-3.47226	0.85157	-0.22346
C	-3.05147	2.07252	-0.51566
N	-2.48628	3.05354	-0.82992
C	-4.58098	0.63627	0.47763
N	-5.51816	0.2972	1.09511

p1

Charge = 0 Multiplicity = 1

C	1.66054	0.22395	-0.49407
C	3.84582	-0.09986	-0.35443
C	3.51951	0.9218	0.48278
N	2.15212	1.12376	0.36432
H	0.62862	0.1003	-0.79672
H	4.79603	-0.56053	-0.57003
H	4.13029	1.5205	1.13857

N	2.67314	-0.51126	-0.96608
C	1.31812	2.01714	1.18846
C	0.89883	1.34924	2.49834
H	0.45047	2.27308	0.5772
H	1.90025	2.92771	1.36005
H	0.36198	0.41797	2.29763
H	1.76916	1.12151	3.12234
C	-2.48034	1.63187	-0.63104
C	-1.97313	1.19369	-1.93786
O	-1.1353	1.96821	-1.04694
H	-1.66603	0.15646	-2.05869
H	-2.51212	0.881	0.15928
C	2.48066	-1.66998	-1.8392
H	2.85581	-1.4555	-2.84326
H	3.01643	-2.52246	-1.41751
H	1.4065	-1.88283	-1.85129
H	0.248	2.02975	3.05632
C	-0.50789	-1.7585	0.23697
O	0.52674	-1.62299	0.93727
O	-0.60797	-1.5522	-1.01176
C	-1.79712	-2.16585	1.00385
H	-1.49036	-2.86178	1.79788
O	-2.27651	-0.94607	1.61087
H	-3.06287	-1.17466	2.12436
C	-2.86402	-2.79812	0.12244
H	-2.50138	-3.73725	-0.30777
H	-3.7723	-3.02108	0.69844
H	-3.11265	-2.12633	-0.70143
C	-2.41512	1.95131	-3.20366
H	-1.95866	1.50657	-4.06317
H	-3.47967	1.89833	-3.29759
H	-2.11412	2.97544	-3.12972
H	-3.15364	2.45763	-0.53259

TSp1

Charge = 0 Multiplicity = 1

C	1.03287	1.84042	0.44868
C	1.58218	1.40086	-0.82187
O	0.0084	2.18277	-0.47497
H	0.76818	1.02214	1.13794
H	1.28762	0.45011	-1.23184
H	2.09467	2.11742	-1.44657
C	-1.80034	0.11341	-0.28239
C	-3.93531	-0.37725	0.09421
C	-3.23752	-1.54569	0.02253
N	-1.91194	-1.21918	-0.21245
H	-0.91549	0.7845	-0.45708
H	-4.9839	-0.18913	0.25999
H	-3.56721	-2.56746	0.11824
N	-3.01991	0.64233	-0.09565
C	-0.78433	-2.17342	-0.32471
C	-0.51115	-2.90317	0.986
H	0.11221	-1.61126	-0.60062
H	-1.03229	-2.87066	-1.13063
H	-0.29461	-2.18826	1.78389
H	-1.34187	-3.54576	1.2968
C	-3.27518	2.08653	-0.09943
H	-3.90723	2.35106	-0.95022
H	-3.77239	2.37202	0.83005
H	-2.30775	2.58907	-0.17801
H	0.38138	-3.51706	0.84901
C	1.67603	2.99897	1.18078
H	0.99327	3.40835	1.93384
H	2.59276	2.66768	1.6783
H	1.92665	3.79782	0.47634
C	3.1907	-0.78936	-0.21554
O	2.12274	-1.44783	-0.28688
O	3.39259	0.44018	-0.41686
C	4.45991	-1.57151	0.17038
H	4.87509	-1.15825	1.06578

O	4.12555	-2.9445	0.3895
H	4.91625	-3.43221	0.63144
C	5.49167	-1.46986	-0.96837
H	5.88194	-0.47438	-1.00824
H	6.29017	-2.15908	-0.78875
H	5.01975	-1.7055	-1.89932

p2

Charge = 0 Multiplicity = 1

C	-1.95031	-0.07951	-0.99302
C	-3.03726	1.74328	-0.358
C	-3.6605	0.66758	0.19849
N	-2.9654	-0.46007	-0.20901
H	-1.15958	-0.70292	-1.43433
H	-3.24625	2.79782	-0.28304
H	-4.52167	0.6096	0.84384
N	-1.97691	1.25344	-1.09852
C	-3.18266	-1.84547	0.2514
C	-2.86616	-2.00251	1.73601
H	-2.49627	-2.46341	-0.32708
H	-4.21707	-2.11502	0.01536
H	-1.80468	-1.8012	1.89245
H	-3.47576	-1.34054	2.35994
C	3.0181	-0.55223	-0.60563
C	3.33567	0.72149	0.17652
O	2.00097	-1.2584	0.09584
H	2.63645	-0.28113	-1.5939
H	4.09859	1.31382	-0.3355
H	3.66854	0.49231	1.1897
C	0.74609	-1.43153	-0.53505
O	0.61317	-0.98659	-1.70837
O	-0.09557	-1.99126	0.18839
C	-0.94584	2.03385	-1.79041
H	-1.39132	2.58734	-2.62027
H	-0.47941	2.70305	-1.06715
H	-0.19296	1.33093	-2.14988
H	-3.07122	-3.0341	2.03723
C	4.25609	-1.43896	-0.73124
H	4.00556	-2.33521	-1.3041
H	5.07173	-0.91868	-1.24626
H	4.61101	-1.75588	0.25501
C	1.30432	1.52576	1.23235
O	0.19694	2.02215	1.17062
O	2.16622	1.58132	0.22076
C	1.86255	0.84934	2.49822
H	1.72541	-0.20944	2.42684
C	1.11651	1.3813	3.73597
H	1.57345	0.99286	4.6221
H	1.16433	2.45015	3.74918
H	0.0934	1.07051	3.69663
O	3.25695	1.14226	2.61972
H	3.49087	1.2079	3.54847

TSp2

Charge = 0 Multiplicity = 1

C	1.51275	2.35049	0.04846
C	1.44859	0.83926	-0.10691
O	0.24622	2.91929	-0.39557
H	1.5543	0.17619	0.73153
H	1.50289	0.4126	-1.09588
C	-0.76257	2.02387	-0.3554
O	-0.39315	0.81421	-0.06371
O	-1.9231	2.37404	-0.60366
H	2.27029	2.73601	-0.6322
C	-3.25316	-0.19987	-0.36023
C	-5.04328	-1.34982	0.26716
C	-4.01459	-2.22731	0.09458
N	-2.90952	-1.49161	-0.29864
H	-2.61889	0.66474	-0.60005
H	-6.06781	-1.51099	0.56129

H	-3.97634	-3.29793	0.2148
N	-4.54404	-0.09094	-0.02006
C	-1.54052	-2.01038	-0.53015
C	-0.80963	-2.30667	0.77575
H	-1.01433	-1.23104	-1.07886
H	-1.63708	-2.89712	-1.16268
H	-0.80657	-1.41488	1.40559
H	-1.26275	-3.14067	1.32118
C	-5.25983	1.1876	0.03295
H	-6.02434	1.22103	-0.74629
H	-5.72658	1.30354	1.01291
H	-4.53204	1.98486	-0.12405
H	0.23447	-2.54674	0.55514
C	1.80064	2.78774	1.47574
H	2.78432	2.40967	1.76136
H	1.79537	3.87829	1.55074
H	1.04779	2.38668	2.16322
C	4.30782	-0.15087	-0.27367
O	5.4161	-0.10807	-0.81729
O	3.48332	0.83025	-0.1755
C	3.98147	-1.53311	0.36826
H	4.77525	-1.68121	1.1144
C	4.0685	-2.64815	-0.6741
H	3.96966	-3.63864	-0.21134
H	3.26929	-2.53768	-1.4156
H	5.03	-2.58794	-1.18647
O	2.70399	-1.56289	1.04081
H	2.72377	-2.32223	1.63681

q1

Charge = 0 Multiplicity = 1

C	1.82461	0.07372	-0.46242
C	3.81892	-0.89058	-0.49003
C	3.80927	0.02156	0.51927
N	2.56203	0.62804	0.50693
H	0.79906	0.30624	-0.71929
H	4.59094	-1.56209	-0.82865
H	4.56953	0.29361	1.23315
N	2.57493	-0.83404	-1.09747
C	2.02967	1.56305	1.51408
C	1.49808	0.81779	2.73847
H	1.23787	2.1272	1.0178
H	2.83809	2.25438	1.77097
H	0.75418	0.07784	2.42941
H	2.30359	0.30173	3.27114
C	-1.84936	2.45345	-0.53339
C	-1.10883	2.31154	-1.7939
O	-0.40057	2.44874	-0.54301
H	-1.03637	1.32398	-2.24472
H	-2.29273	1.54388	-0.12446
C	2.0668	-1.69706	-2.16529
H	2.48825	-1.3962	-3.12809
H	2.34599	-2.72977	-1.94755
H	0.97569	-1.59801	-2.16028
H	1.03824	1.53257	3.42786
C	-0.91509	-1.2938	-0.05823
O	0.05101	-1.4714	0.72593
O	-0.83696	-0.87509	-1.25928
C	-2.34673	-1.66943	0.44049
C	-2.59951	-3.13021	-0.00051
H	-1.87586	-3.81355	0.45725
H	-3.60603	-3.45515	0.29387
H	-2.51184	-3.21701	-1.08849
C	-2.45945	-1.54955	1.96263
H	-3.45878	-1.85129	2.3019
H	-1.71469	-2.17956	2.45259
H	-2.29661	-0.51418	2.27468
N	-3.28879	-0.72512	-0.19094
H	-3.01807	-0.66699	-1.1716
H	-4.2344	-1.10373	-0.15081

H	-2.30544	3.37808	-0.24712
C	-0.97988	3.52182	-2.73739
H	-0.07016	3.44382	-3.29527
H	-1.81102	3.53905	-3.41104
H	-0.96886	4.4235	-2.16141

TSq1

Charge = 0 Multiplicity = 1

C	-0.15603	2.17258	0.46545
C	0.57271	1.99027	-0.78009
O	-1.18707	2.31932	-0.49266
H	-0.23568	1.26279	1.08731
H	0.55125	1.04196	-1.28991
H	0.92612	2.86652	-1.30504
C	-2.31931	-0.22296	-0.35902
C	-4.20609	-1.27832	0.15159
C	-3.20937	-2.20463	0.06665
N	-2.04444	-1.52915	-0.25333
H	-1.66945	0.6589	-0.57683
H	-5.25603	-1.38687	0.37095
H	-3.22862	-3.27349	0.20562
N	-3.62767	-0.05021	-0.113
C	-0.69125	-2.12504	-0.37379
C	-0.07922	-2.46511	0.98177
H	-0.04527	-1.39939	-0.87296
H	-0.78875	-3.00838	-1.01117
H	-0.11626	-1.59542	1.6443
H	-0.58223	-3.30429	1.47433
C	-4.27838	1.26408	-0.12765
H	-4.96111	1.33453	-0.97767
H	-4.83427	1.40355	0.80183
H	-3.48969	2.01702	-0.21116
H	0.97669	-2.70046	0.82669
C	0.12802	3.3893	1.3233
H	-0.68207	3.55203	2.04321
H	1.06575	3.25589	1.87192
H	0.21012	4.28205	0.69575
C	2.59663	0.13267	-0.31615
O	1.81601	-0.64435	-0.90656
O	2.51752	1.40342	-0.23178
C	3.84808	-0.46182	0.37176
C	5.0548	-0.35586	-0.56485
H	5.23139	0.68828	-0.83792
H	5.9641	-0.7438	-0.08737
H	4.86733	-0.93421	-1.47475
N	3.5727	-1.85909	0.73605
H	4.39278	-2.4109	0.58451
H	3.31217	-1.90702	1.70033
C	4.10752	0.38203	1.63359
H	3.20172	0.46991	2.19635
H	4.85524	-0.09362	2.23323
H	4.44586	1.3561	1.34791

q2

Charge = 0 Multiplicity = 1

C	2.19586	-0.98117	0.53259
C	3.13518	0.64763	1.7036
C	3.7384	0.60696	0.48306
N	3.13611	-0.41549	-0.23298
H	1.47817	-1.76879	0.25531
H	3.29053	1.30027	2.5469
H	4.52781	1.21216	0.06851
N	2.18171	-0.35391	1.71365
C	3.37328	-0.7655	-1.64647
C	2.97449	0.36648	-2.58844
H	2.74821	-1.63546	-1.84711
H	4.42894	-1.0367	-1.74914
H	1.89938	0.53548	-2.50416
H	3.52134	1.29136	-2.37799
C	-2.747	-1.45274	0.10519

C	-3.15039	-0.11723	0.72908
O	-1.84197	-1.18073	-0.96334
H	-2.23047	-2.06557	0.84881
H	-3.85905	-0.27739	1.54695
H	-3.6045	0.55197	-0.0021
C	-0.49105	-1.58788	-0.82594
O	-0.21256	-2.3696	0.12154
O	0.26072	-1.0756	-1.67452
C	1.20852	-0.63417	2.7751
H	1.73062	-0.93654	3.68567
H	0.60611	0.2614	2.93253
H	0.55818	-1.43386	2.41938
H	3.19895	0.06977	-3.61731
C	-3.96489	-2.19302	-0.44389
H	-3.64715	-3.13983	-0.88737
H	-4.69081	-2.40926	0.34775
H	-4.46358	-1.60456	-1.22144
C	-1.20766	1.41104	0.74233
O	-0.19247	1.75755	1.31711
O	-2.01372	0.52579	1.35623
C	-1.57752	1.95485	-0.64657
C	-0.52465	2.93176	-1.15206
H	-0.81667	3.30844	-2.13869
H	-0.4182	3.77458	-0.46564
H	0.44308	2.4348	-1.2495
N	-2.88994	2.60257	-0.50907
H	-2.77803	3.49155	-0.06501
H	-3.29485	2.73081	-1.41439
C	-1.66052	0.73648	-1.58481
H	-0.88785	0.04002	-1.33419
H	-2.61488	0.26547	-1.47416
H	-1.53651	1.05744	-2.59798

TSq2

Charge = 0 Multiplicity = 1

C	1.52619	2.33967	0.06284
C	1.4969	0.8283	-0.10082
O	0.26677	2.89606	-0.40811
H	1.56716	0.16065	0.73712
H	1.53481	0.40568	-1.09219
C	-0.74229	1.99627	-0.37689
O	-0.3773	0.79236	-0.07447
O	-1.89827	2.35227	-0.64535
H	2.29432	2.7409	-0.597
C	-3.25317	-0.18928	-0.36428
C	-5.05377	-1.31415	0.28017
C	-4.03325	-2.20336	0.11974
N	-2.92172	-1.48324	-0.28428
H	-2.61086	0.66797	-0.61639
H	-6.07955	-1.46172	0.57705
H	-4.00478	-3.27245	0.25526
N	-4.54296	-0.06412	-0.02512
C	-1.55752	-2.01672	-0.50862
C	-0.8316	-2.30686	0.80138
H	-1.02285	-1.24632	-1.06182
H	-1.66081	-2.90849	-1.13304
H	-0.81825	-1.40749	1.42013
H	-1.29444	-3.12924	1.35624
C	-5.24642	1.22174	0.01011
H	-6.01007	1.25231	-0.77012
H	-5.71277	1.35545	0.98802
H	-4.51062	2.00958	-0.15696
H	0.20956	-2.56185	0.58397
C	1.77567	2.77121	1.49971
H	2.75706	2.40533	1.80863
H	1.75379	3.86111	1.58093
H	1.01176	2.35586	2.16608
C	4.32035	-0.15417	-0.24576
O	5.4405	-0.09992	-0.76056
O	3.50176	0.83509	-0.14262

C	3.96846	-1.55487	0.33592
C	3.99372	-2.6156	-0.76572
H	3.87448	-3.62489	-0.35142
H	3.18032	-2.44242	-1.4792
H	4.94408	-2.56027	-1.29944
C	5.10495	-1.84642	1.3334
H	5.21563	-1.01708	2.00036
H	4.86987	-2.72657	1.89463
H	6.019	-1.9982	0.79825
N	2.68784	-1.58346	1.0571
H	2.01119	-2.08198	0.51523
H	2.81151	-2.04022	1.93804

s1

Charge = 0 Multiplicity = 1

C	1.34126	0.08379	-0.5518
C	3.54869	0.22565	-0.44808
C	3.03507	1.44144	-0.11814
N	1.65512	1.33777	-0.20692
H	0.35185	-0.33409	-0.68649
H	4.56843	-0.11718	-0.51288
H	3.52132	2.36049	0.16567
N	2.47495	-0.60481	-0.72455
C	0.67262	2.3485	0.22628
C	0.44973	2.29657	1.73787
H	-0.25028	2.13187	-0.31445
H	1.04815	3.3222	-0.103
H	0.14631	1.28825	2.0351
H	1.36057	2.56383	2.28358
C	-3.06996	0.31386	-0.38798
C	-2.63026	-0.32417	-1.63705
O	-1.91199	0.80794	-1.09679
H	-2.08688	-1.26518	-1.57968
H	-2.82282	-0.20249	0.54004
C	2.51576	-2.03794	-1.02635
H	2.8223	-2.19698	-2.06357
H	3.22874	-2.51819	-0.35366
H	1.50917	-2.42963	-0.84284
H	-0.33224	3.01132	2.01263
C	-0.50445	-1.73017	1.03966
O	0.33647	-1.01857	1.61942
O	-0.49347	-2.16767	-0.15297
O	-1.63398	-2.07124	1.78824
H	-2.13237	-2.65912	1.20187
H	-3.9104	0.97509	-0.3513
C	-3.39755	-0.02774	-2.93897
H	-2.73353	-0.11913	-3.77301
H	-4.20206	-0.72511	-3.0455
H	-3.79018	0.96697	-2.90298

TSs1

Charge = 0 Multiplicity = 1

C	1.05473	1.83717	0.45171
C	1.59972	1.40254	-0.82302
O	0.03458	2.20271	-0.46485
H	0.78019	1.01513	1.1336
H	1.28571	0.46457	-1.24739
H	2.11858	2.11968	-1.44228
C	-1.79426	0.11433	-0.28512
C	-3.9355	-0.34038	0.08867
C	-3.25689	-1.52029	0.01756
N	-1.92564	-1.216	-0.21606
H	-0.90145	0.76303	-0.45889
H	-4.98147	-0.13339	0.25313
H	-3.60189	-2.53776	0.11289
N	-3.00389	0.66475	-0.09989
C	-0.81256	-2.18834	-0.32194
C	-0.54858	-2.90838	0.99656
H	0.09126	-1.64132	-0.60536
H	-1.07448	-2.88936	-1.12087

H	-0.30853	-2.18799	1.784
H	-1.39431	-3.52617	1.32066
C	-3.23544	2.11345	-0.10348
H	-3.86108	2.38745	-0.95698
H	-3.73158	2.40483	0.82563
H	-2.25873	2.60006	-0.17849
H	0.32751	-3.54793	0.86225
C	1.71591	2.9783	1.19719
H	1.03747	3.38996	1.95462
H	2.62776	2.62757	1.69289
H	1.97985	3.78237	0.50182
C	3.17248	-0.80874	-0.22115
O	2.09438	-1.45172	-0.27003
O	4.30816	-1.52555	0.11887
H	3.98375	-2.43321	0.2397
O	3.39169	0.41497	-0.43915

s2

Charge = 0 Multiplicity = 1

C	-1.95661	0.08144	0.99552
C	-3.01229	-1.75928	0.36149
C	-3.65037	-0.6948	-0.19966
N	-2.97465	0.44483	0.20754
H	-1.17901	0.7194	1.43583
H	-3.20305	-2.81816	0.28907
H	-4.51022	-0.65022	-0.84898
N	-1.96237	-1.25136	1.10503
C	-3.21448	1.82546	-0.2554
C	-2.91039	1.98339	-1.74293
H	-2.5358	2.45593	0.31897
H	-4.25175	2.08019	-0.01293
H	-1.84797	1.79003	-1.90845
H	-3.51974	1.31475	-2.36189
C	3.00849	0.57717	0.60345
C	3.3463	-0.7082	-0.15158
O	1.98685	1.25437	-0.11826
H	2.62392	0.32205	1.59475
H	4.10568	-1.28786	0.38063
H	3.69034	-0.49646	-1.16504
C	0.73158	1.44332	0.51024
O	0.60463	1.04019	1.6987
O	-0.11397	1.97224	-0.23149
C	-0.92766	-2.01502	1.8099
H	-1.37241	-2.55832	2.64794
H	-0.45696	-2.69404	1.0981
H	-0.17897	-1.30264	2.1608
H	-3.12725	3.01386	-2.04368
C	4.23525	1.48155	0.72014
H	3.96907	2.38621	1.27459
H	5.05448	0.981	1.25127
H	4.59345	1.78415	-0.27055
C	1.3307	-1.539	-1.21561
O	0.22143	-2.03104	-1.15538
O	1.833	-0.97149	-2.33218
H	1.09927	-0.95147	-2.96913
O	2.18344	-1.57661	-0.19547

TSs2

Charge = 0 Multiplicity = 1

C	-2.25687	-1.66151	0.01915
C	-2.0249	-0.25734	-0.5148
O	-1.06677	-2.45884	-0.25159
H	-2.05748	0.59822	0.13841
H	-2.01028	-0.09214	-1.58061
C	0.03661	-1.69332	-0.37857
O	-0.19468	-0.41691	-0.39585
O	1.15107	-2.22427	-0.47592
H	-3.05651	-2.13025	-0.55174
C	2.96438	-0.01608	-0.28798
C	4.93846	0.72097	0.40339

C	4.16619	1.80192	0.09856
N	2.94086	1.32039	-0.33251
H	2.15608	-0.72379	-0.52876
H	5.95281	0.65492	0.76466
H	4.38086	2.85795	0.14811
N	4.16705	-0.40214	0.15717
C	1.75767	2.12801	-0.70569
C	1.05464	2.70967	0.51762
H	1.08541	1.45432	-1.23787
H	2.10604	2.90765	-1.38953
H	0.67035	1.90368	1.14834
H	1.71908	3.34931	1.10892
C	4.54886	-1.80613	0.34357
H	5.33312	-2.07639	-0.36798
H	4.9092	-1.95215	1.36445
H	3.66208	-2.41948	0.17391
H	0.20394	3.31373	0.18727
C	-2.55552	-1.69519	1.51105
H	-3.46428	-1.12394	1.71279
H	-2.69095	-2.72724	1.84858
H	-1.73005	-1.24815	2.07743
C	-4.64581	0.91793	-0.13135
O	-5.78514	1.33954	-0.29967
O	-3.86871	1.5215	0.88346
H	-4.46797	2.19466	1.24611
O	-4.03067	-0.0188	-0.74605

s3

Charge = 0 Multiplicity = 1

H	-0.36989	1.88331	1.19763
O	0.06511	1.42744	1.97019
C	2.68519	0.46846	-0.6735
C	2.95972	0.42699	0.83628
H	1.925	1.19217	-0.97167
H	2.08888	0.7939	1.39094
O	3.0456	-1.01017	1.0903
O	2.15831	-0.84766	-0.94596
C	2.44986	-1.67743	0.08618
O	2.19116	-2.85516	0.08668
H	0.13944	2.13296	2.63026
H	3.60164	0.59788	-1.26286
C	-1.62454	-0.67141	-0.5702
N	-1.39374	-1.92037	-1.00127
N	-2.62495	-0.71725	0.32142
C	-2.25855	-2.78677	-0.35892
C	-0.38118	-2.29978	-1.99381
C	-3.03158	-2.03146	0.46919
H	-2.2442	-3.84929	-0.54407
H	0.41995	-2.85912	-1.5054
H	0.03486	-1.38888	-2.42131
H	-3.82787	-2.31121	1.14028
H	-1.07415	0.2242	-0.91157
H	-0.85923	-2.89774	-2.77373
C	-3.21709	0.45018	1.0137
H	-4.28022	0.4659	0.75048
H	-2.73183	1.33672	0.59395
C	-3.0075	0.38551	2.52425
H	-1.93852	0.44658	2.74743
H	-3.50856	1.24435	2.98367
H	-3.43145	-0.52427	2.96522
C	4.241	1.10111	1.28276
H	4.18033	2.17766	1.08522
H	4.39848	0.96176	2.35655
H	5.10682	0.6962	0.74726
C	-0.71854	2.62754	-1.15865
O	-0.18793	1.61471	-1.69729
O	-0.7588	3.77773	-1.91715
H	-0.35115	3.52706	-2.76284
O	-1.22948	2.72507	-0.0143

TSs3

Charge = 0 Multiplicity = 1

H	0.63303	1.78775	1.01229
O	1.67058	1.29254	1.3324
C	2.51993	0.38035	-1.18241
C	3.67133	0.05674	-0.18486
H	2.44096	1.4491	-1.40162
H	4.13461	0.98991	0.16111
O	3.0063	-0.56988	0.91528
O	1.33827	-0.06374	-0.51745
C	1.64257	-0.21757	0.86867
O	0.83467	-0.87088	1.56931
H	1.65386	1.21977	2.30352
H	2.61439	-0.17868	-2.12097
C	-1.79096	-0.75195	0.38531
N	-1.84004	-1.75155	-0.507
N	-2.99921	-0.17434	0.43103
C	-3.11252	-1.81167	-1.0438
C	-0.69838	-2.62718	-0.85699
C	-3.84027	-0.82144	-0.456
H	-3.38008	-2.53436	-1.79841
H	0.15768	-1.96987	-1.02464
H	-0.97074	-3.10939	-1.80024
H	-4.86433	-0.51422	-0.59729
H	-0.88886	-0.51186	0.96472
C	4.73573	-0.88429	-0.7281
H	5.27093	-0.41772	-1.56403
H	5.46522	-1.13304	0.0496
H	4.27834	-1.81534	-1.0811
C	-3.35862	0.96655	1.28114
H	-4.04731	1.60592	0.7275
H	-3.83001	0.6079	2.20047
H	-2.44822	1.53426	1.48232
C	-0.39009	-3.64621	0.23713
H	-1.27023	-4.24762	0.49102
H	0.39605	-4.32127	-0.11802
H	-0.01502	-3.12803	1.12371
C	-0.59852	2.75457	-0.44529
O	0.33225	3.06351	-1.17838
O	-1.90269	2.98685	-0.85007
H	-1.80465	3.41348	-1.71772
O	-0.57088	2.2075	0.72777

s4

Charge = -1 Multiplicity = 1

C	-1.68211	-1.35778	0.56992
C	-2.8017	-0.93719	-0.43154
H	-2.08155	-1.83204	1.47499
H	-0.96181	-2.03909	0.09859
O	-2.59229	0.45883	-0.61134
O	-1.0725	-0.13574	0.93954
C	-1.27792	0.74455	-0.1867
O	-0.41009	0.42339	-1.21156
H	-0.28554	2.32788	0.24199
H	0.51978	0.32031	-0.85776
H	1.77537	1.77368	0.2128
O	1.3877	2.61545	0.60072
H	1.37101	2.41078	1.54877
H	-2.66315	-1.45781	-1.38955
O	-1.23844	2.03926	0.22553
C	-4.21941	-1.15866	0.08046
H	-4.95093	-0.73106	-0.61432
H	-4.4321	-2.23021	0.18821
H	-4.34804	-0.67384	1.05471
C	3.18302	-0.27445	0.83059
O	3.83672	0.41973	1.608
O	3.39127	-1.61511	0.85663
H	4.06192	-1.84402	1.5207
O	2.19999	0.10317	-0.13685

TSs4

Charge = -1 Multiplicity = 1

C	0.88799	1.40068	-0.22504
C	0.66909	0.83568	1.17922
C	2.02901	-0.57721	-0.26957
H	0.07076	1.05137	-0.86722
H	-0.39543	0.77792	1.41727
H	1.23197	1.39949	1.934
O	2.1174	0.7779	-0.6119
O	1.22322	-0.48872	1.08787
O	3.30615	-0.99943	0.05457
H	3.31493	-1.90966	-0.27298
O	1.38972	-1.37644	-1.09486
H	0.41064	-1.84905	-0.5559
C	1.02581	2.9069	-0.30642
H	1.24187	3.21947	-1.33262
H	0.08843	3.37711	0.00704
H	1.83748	3.25929	0.33951
O	-0.41596	-2.12569	0.36645
H	0.33315	-1.28679	0.94746
H	-1.3875	-1.66691	0.14373
C	-2.94215	-0.04622	-0.04333
O	-2.31298	0.95899	0.3493
O	-4.26814	0.17634	-0.43661
H	-4.36937	1.12845	-0.295
O	-2.58883	-1.25041	-0.14913

t2

Charge = 0 Multiplicity = 1

C	-2.81789	-3.63711	-0.76233
H	-2.10904	-2.85101	-1.04788
C	-4.14993	-2.99803	-0.35501
H	-4.4962	-2.31005	-1.13626
H	-4.89846	-3.77429	-0.17817
N	-4.05622	-2.21568	0.88476
C	-5.06624	-2.05879	1.81964
C	-3.1046	-1.30658	1.12925
C	-4.68678	-1.05965	2.65909
H	-5.94841	-2.67729	1.81091
H	-2.18139	-1.1996	0.58469
H	-5.17584	-0.63523	3.52034
C	-2.77988	0.6198	2.62023
H	-1.69925	0.47297	2.63432
H	-3.03524	1.37255	1.86601
H	-3.12377	0.91284	3.61305
N	-3.44182	-0.62316	2.23333
C	0.12769	0.6172	-1.41421
H	1.20938	0.47301	-1.43718
C	-0.45435	0.5492	-2.82536
H	-0.02108	1.32955	-3.46094
H	-0.22805	-0.42297	-3.27233
H	-1.53967	0.68934	-2.78411
C	1.3674	2.3241	0.96201
O	2.31177	2.5555	0.21825
O	1.44961	2.36886	2.30388
H	2.36939	2.58759	2.51017
O	0.12672	2.03667	0.62408
O	-0.45936	-0.44178	-0.64771
C	0.29358	-1.16572	0.29814
O	1.50779	-0.85571	0.46461
O	-0.35571	-2.04203	0.88033
C	-0.21337	1.97119	-0.79189
H	-1.29677	2.12692	-0.81811
H	0.30708	2.77664	-1.31618
C	4.85254	-0.37943	-0.20323
N	3.67709	0.13565	-0.51847
H	3.59714	1.12035	-0.73789
H	2.7599	-0.30892	-0.19626
N	4.97431	-1.72076	-0.02554
N	5.95896	0.40991	-0.07299

C	5.82585	1.85647	0.09243
H	6.64576	2.21473	0.72169
H	5.87818	2.38255	-0.87047
H	4.88007	2.10535	0.57471
C	7.28162	-0.04317	-0.50497
H	8.00316	-0.01022	0.31866
H	7.22357	-1.0601	-0.8895
H	7.6454	0.60898	-1.30787
C	5.82151	-2.27545	1.03331
H	5.18938	-2.77382	1.77675
H	6.52649	-3.00945	0.62885
H	6.37672	-1.48375	1.53414
C	3.90751	-2.61828	-0.49434
H	3.05845	-2.6342	0.19654
H	3.55198	-2.28291	-1.4695
H	4.33424	-3.6185	-0.59843
Br	-3.85109	1.55527	-1.29019
H	-3.02713	-4.2239	-1.66912
H	-2.42209	-4.27709	-0.00163

TSt2

Charge = 0 Multiplicity = 1

C	-6.54388	-2.11582	1.07576
H	-7.39268	-2.66493	0.66231
H	-6.58332	-2.14151	2.16625
N	-6.57628	-0.72138	0.62001
C	-7.47043	0.26856	0.99141
C	-5.67495	-0.20403	-0.22482
C	-7.08459	1.40705	0.34893
H	-8.28279	0.08526	1.67603
H	-4.82407	-0.79052	-0.63343
H	-7.49956	2.40184	0.37037
C	-5.16977	2.00145	-1.25194
H	-5.06982	2.94281	-0.70449
H	-4.17961	1.54377	-1.33256
N	-5.9618	1.09109	-0.39864
C	0.9595	1.65939	1.91561
O	1.93813	2.10284	2.51822
O	-0.21995	1.47803	2.61484
H	0.00574	1.72043	3.52459
O	0.88744	1.34288	0.67075
C	-0.27774	-0.81642	-0.28351
C	-0.81473	0.58609	-0.05899
H	0.42313	-1.09769	0.50454
H	-1.29981	0.83898	0.86834
H	-0.71073	1.349	-0.81251
C	-2.55727	-1.21129	-0.56585
O	-3.55857	-1.94573	-0.65366
O	-2.5276	0.05566	-0.81311
O	-1.3894	-1.74374	-0.15225
C	0.38804	-1.0091	-1.6383
H	1.19253	-0.2783	-1.75946
H	0.83666	-2.00337	-1.67402
H	-0.33484	-0.87932	-2.45096
C	4.68799	0.75331	-0.42202
N	3.46015	0.35331	-0.16166
H	2.69712	0.99127	0.08555
H	3.26294	-0.67006	0.05881
N	5.10293	2.02965	-0.1872
N	5.58571	-0.11639	-0.97993
C	6.92978	-0.25227	-0.41902
H	7.01365	-1.20784	0.11284
H	7.68785	-0.22639	-1.21039
H	7.12942	0.55045	0.29011
C	5.10844	-1.28826	-1.72741
H	4.24737	-1.00183	-2.33334
H	5.91792	-1.6079	-2.39119
H	4.79623	-2.10806	-1.06902
C	6.11438	2.67199	-1.01959
H	5.69955	3.59338	-1.44625

H	7.00457	2.93938	-0.43732
H	6.40695	2.01055	-1.83392
C	4.36482	2.93018	0.69666
H	3.73102	3.61526	0.11765
H	3.72707	2.38656	1.39612
H	5.08461	3.5291	1.26484
Br	2.78938	-2.64178	0.59008
H	-5.60665	-2.55636	0.73123
C	-5.81393	2.2179	-2.6189
H	-6.81251	2.65815	-2.53499
H	-5.19168	2.89893	-3.2061
H	-5.89385	1.27518	-3.16704

t3

Charge = 0 Multiplicity = 1

H	0.45646	0.34211	1.56072
O	-0.35737	-0.22313	1.71108
C	1.73157	-3.4221	0.74144
C	0.22323	-3.6542	0.91565
H	2.26599	-3.26966	1.67995
H	-0.13817	-3.17136	1.82972
O	-0.32053	-2.88019	-0.19136
O	1.79207	-2.19987	-0.02212
C	0.59182	-1.97353	-0.5844
O	0.36787	-1.07168	-1.35978
H	-0.33525	-0.44361	2.65439
H	2.21515	-4.21689	0.16339
C	-2.41312	0.55789	-0.46723
N	-2.95364	0.399	-1.6832
N	-3.02912	1.58088	0.14053
C	-3.94509	1.34836	-1.85453
C	-2.57186	-0.62719	-2.66333
C	-3.99215	2.0892	-0.71242
H	-4.51856	1.41611	-2.76591
H	-1.60264	-1.03483	-2.37451
H	-2.49628	-0.16084	-3.64756
H	-4.61331	2.92856	-0.44188
H	-1.61034	-0.0238	-0.02855
H	-3.33054	-1.41352	-2.68477
C	-2.72558	2.06969	1.50423
H	-2.51826	3.14078	1.4221
H	-1.81011	1.55572	1.80686
C	-3.86884	1.79497	2.47885
H	-4.06088	0.72116	2.56726
H	-3.59567	2.17675	3.46752
H	-4.79693	2.29043	2.17566
C	-0.23576	-5.09445	0.8285
H	0.18537	-5.66978	1.66039
H	-1.32571	-5.15873	0.89046
H	0.09004	-5.5511	-0.11143
C	2.86486	2.03297	1.54924
N	1.81754	1.4211	1.09965
H	1.58974	1.38308	0.12668
C	5.36811	2.03647	1.30849
H	6.15597	1.99787	0.58552
H	5.57857	2.80297	2.02479
H	5.2951	1.0926	1.80718
C	3.99694	3.83699	0.21202
H	4.73418	4.02937	-0.53923
H	3.02728	4.08067	-0.16915
H	4.20196	4.43599	1.07461
C	2.94035	3.98469	3.13334
H	2.53996	4.27746	4.08142
H	3.94144	4.35089	3.0405
H	2.33701	4.39331	2.34981
C	4.24121	1.89528	3.64947
H	4.47822	0.95383	3.19958
H	5.04109	2.58463	3.4766
H	4.1055	1.76323	4.70258
N	4.03637	2.34728	0.60036

N	2.94418	2.44816	3.03009
Br	2.41723	1.40271	-2.42889

TSt3

Charge = 0 Multiplicity = 1

C	1.43479	3.25671	-2.05758
C	1.59238	3.98207	-0.91751
C	0.34965	2.21266	-0.43722
N	0.62899	2.1774	-1.74523
H	1.82018	3.41375	-3.05155
H	2.13311	4.89533	-0.7318
H	-0.30506	1.52085	0.10815
C	0.90266	3.62985	1.51647
H	0.59797	4.67362	1.64405
H	0.13097	2.99935	1.96358
C	2.27673	3.3515	2.12779
H	3.01764	4.08105	1.78551
C	0.42156	0.98406	-2.56266
H	0.41893	1.26571	-3.61679
H	1.24211	0.29649	-2.32593
H	-0.53694	0.53836	-2.29147
N	0.88806	3.32448	0.077
Br	2.90696	0.27861	-0.09299
C	0.41511	-2.90985	0.26049
N	1.07618	-2.40654	1.32038
N	1.1216	-3.73167	-0.60805
C	0.38821	-4.7188	-1.38401
H	1.07623	-5.52044	-1.67041
H	-0.41632	-5.14907	-0.78472
H	-0.04188	-4.30805	-2.3135
C	2.34554	-3.23613	-1.25406
H	2.63902	-2.26381	-0.84704
H	3.1666	-3.95381	-1.14046
H	2.16007	-3.09751	-2.32838
C	0.58559	-1.25645	2.07381
H	0.30405	-1.56394	3.09
H	1.38793	-0.51481	2.10755
H	-0.26832	-0.79767	1.58402
C	2.38063	-2.89199	1.75941
H	3.15548	-2.16745	1.48332
H	2.36015	-2.99774	2.85015
H	2.5911	-3.86518	1.31858
N	-0.87768	-2.69474	0.08415
H	-1.19263	-2.90734	-0.85377
C	-4.84695	0.06786	0.05157
C	-4.00328	-0.11876	-1.23025
H	-4.11923	-1.11963	-1.6585
H	-4.24903	0.62813	-1.9964
C	-2.65179	0.38406	0.55996
O	-1.67594	0.92496	1.07761
O	-2.65521	0.08486	-0.80869
O	-3.93394	0.74063	0.92571
H	-5.07627	-0.90984	0.48805
C	-6.10235	0.90255	-0.12155
H	-6.80017	0.40292	-0.80236
H	-6.60715	1.0434	0.83807
H	-5.85845	1.88736	-0.53178
O	-2.70515	-1.40148	1.1612
H	-2.62435	-1.28984	2.11803
H	-1.7129	-2.05591	0.71559
H	2.21416	3.42047	3.21803
H	2.62057	2.35366	1.8346

t4

Charge = 0 Multiplicity = 1

C	-3.74121	-1.0827	0.3544
C	-4.31802	-0.12151	-0.71499
H	-4.00956	-0.75417	1.3678
H	-4.05532	-2.12107	0.21702
O	-3.17771	0.6334	-1.14783

O	-2.33395	-1.00859	0.1517
C	-2.09654	0.33342	-0.32684
O	-0.9578	0.34788	-1.09031
H	-1.53834	0.78433	1.46722
H	-0.18613	0.51839	-0.504
H	0.2912	-0.18819	1.77787
O	-0.50238	-0.42254	2.31541
H	-0.97743	-1.07049	1.76262
H	-4.67255	-0.68314	-1.58855
O	-2.06419	1.21597	0.74546
C	-5.41764	0.79379	-0.19571
H	-5.74901	1.48063	-0.98086
H	-6.28448	0.20682	0.13401
H	-5.04572	1.38408	0.64749
C	2.60701	0.12655	0.0653
N	1.46825	0.60351	0.4887
H	1.49573	1.61928	0.55768
N	3.78466	0.86715	-0.02547
N	2.71167	-1.19721	-0.30631
C	3.88523	-1.98604	0.06717
H	3.6444	-2.65086	0.90979
H	4.21486	-2.60749	-0.77398
H	4.70239	-1.33311	0.3707
C	1.4909	-1.98787	-0.43583
H	1.12085	-2.32886	0.54256
H	0.70493	-1.41167	-0.92283
H	1.71627	-2.86809	-1.04651
C	4.60015	0.79605	-1.23927
H	4.398	1.65669	-1.89482
H	5.66696	0.80043	-0.986
H	4.3695	-0.11356	-1.79247
C	3.8418	2.15499	0.64936
H	3.33689	2.95855	0.08772
H	3.39099	2.07804	1.64181
H	4.89173	2.44021	0.7703

TSt4

Charge = 0 Multiplicity = 1

C	2.28411	1.34842	-0.62789
C	2.5532	1.43027	0.88484
C	3.02235	-0.79961	-0.19629
H	1.23698	1.05139	-0.79434
H	1.71005	1.89694	1.41576
H	3.45441	2.03233	1.07507
O	3.14703	0.29234	-1.04032
O	2.75254	0.09989	1.29796
O	4.26021	-1.35069	-0.04557
H	4.08961	-2.28606	0.13384
O	2.02919	-1.60371	-0.327
H	1.17858	-1.59718	0.79416
C	2.61644	2.59687	-1.42185
H	2.4436	2.43638	-2.48952
H	1.98958	3.43353	-1.09469
H	3.66622	2.86995	-1.27984
O	0.80228	-1.26958	1.73476
H	1.60405	-0.54578	1.77292
H	-0.05673	-0.78226	1.48297
C	-2.64896	-0.109	1.31911
N	-1.3943	0.08966	1.03718
H	-1.28611	0.69796	0.2302
N	-3.02805	-1.10396	2.19323
N	-3.69709	0.65221	0.79651
C	-2.05155	-2.11387	2.58821
H	-1.41395	-1.76764	3.41358
H	-2.59155	-3.00426	2.92397
H	-1.41036	-2.3898	1.7524
C	-4.07849	-0.87278	3.18288
H	-4.64606	0.02175	2.93241
H	-4.76089	-1.72911	3.22954
H	-3.6388	-0.7343	4.18065

C	-4.87269	-0.01644	0.23739
H	-5.78302	0.54412	0.4771
H	-4.79701	-0.09504	-0.85745
H	-4.9593	-1.02241	0.64434
C	-3.37541	1.9171	0.15532
H	-3.01452	1.79843	-0.87988
H	-4.27758	2.53506	0.12206
H	-2.61683	2.44738	0.73464

u1

Charge = 0 Multiplicity = 1

C	0.88813	1.82341	0.18193
O	0.58451	1.81784	-1.05196
O	1.8819	2.73263	0.54352
H	2.09579	3.18738	-0.28804
O	0.43117	1.123	1.10548
C	-3.19448	-0.96902	-0.16704
C	-2.14158	0.94079	-0.54706
C	-3.42301	1.22819	-0.1768
N	-4.06857	0.02345	0.06057
H	-3.40632	-2.02192	-0.06781
H	-1.26362	1.53897	-0.8154
H	-3.92757	2.17306	-0.05076
C	-0.78724	-1.1866	-0.83354
H	-0.06678	-0.43814	-1.16996
H	-0.99639	-1.89809	-1.63784
C	-0.25783	-1.9325	0.40682
H	0.01659	-1.18354	1.15712
H	-1.05387	-2.57238	0.81881
O	0.8074	-2.7645	0.02612
H	1.64547	-2.26031	0.12948
N	-2.0283	-0.43656	-0.54102
C	-5.44986	-0.13822	0.50338
H	-5.68408	-1.20202	0.56536
H	-5.58039	0.31648	1.48878
H	-6.12653	0.337	-0.2113
C	3.41387	-0.22466	1.17532
C	3.61852	-0.17087	-0.27672
O	3.22629	-1.4119	0.36118
H	4.28465	-0.27799	1.82894
H	2.50559	0.1989	1.59818
H	2.82414	0.28279	-0.86969
C	4.9901	-0.16675	-0.8998
H	4.98853	-0.70985	-1.85212
H	5.31255	0.86237	-1.09871
H	5.72048	-0.64006	-0.23556

TSu1

Charge = 0 Multiplicity = 1

C	3.0968	-1.02008	-0.10305
C	2.5229	-0.15841	0.93225
O	2.60741	-2.03301	0.73785
H	2.58147	-0.95287	-1.07613
H	1.45449	-0.02697	0.96081
H	3.07872	-0.05239	1.85276
C	4.60382	-1.00591	-0.29369
H	4.9148	-1.86954	-0.89311
H	4.92433	-0.08798	-0.80013
H	5.10686	-1.068	0.67768
C	1.80408	2.28638	-0.07705
O	0.69838	1.78133	-0.40249
O	2.0107	3.60941	-0.39991
H	1.20339	3.87487	-0.87033
O	2.78038	1.75271	0.51671
C	-3.29784	-0.77107	-0.3377
C	-2.04944	1.01653	0.03125
C	-3.32929	1.30777	0.40609
N	-4.09851	0.18029	0.16899
H	-3.60999	-1.76336	-0.62328
H	-1.12258	1.59148	0.02082

H	-3.75789	2.20936	0.81497
C	-0.86935	-1.05777	-0.87386
H	-0.05323	-0.33719	-0.95563
H	-1.08174	-1.48315	-1.85815
C	-0.52176	-2.1985	0.11495
H	-0.28152	-1.75804	1.096
H	-1.42404	-2.82334	0.25384
O	0.51103	-2.95443	-0.40627
H	1.38239	-2.64551	0.05413
N	-2.05718	-0.28655	-0.43501
C	-5.53029	0.04539	0.42834
H	-5.8544	-0.95252	0.12995
H	-5.72882	0.18403	1.49397
H	-6.08342	0.79076	-0.14837

u2

Charge = 0 Multiplicity = 1

C	2.05116	0.06652	0.56428
H	1.08415	0.04975	1.08547
C	2.96016	1.14017	1.22323
H	2.84943	1.10325	2.31226
H	4.02299	1.01037	0.9995
N	2.65615	2.50572	0.76337
C	3.603	3.49394	0.53665
C	1.45952	2.94866	0.37464
C	2.93563	4.55782	0.00661
H	4.65847	3.29629	0.72009
H	0.53536	2.38261	0.32051
H	3.29247	5.52099	-0.31974
O	1.86932	0.32685	-0.80356
H	0.92603	0.57058	-0.9463
C	0.50345	4.96803	-0.67174
H	-0.3182	4.28042	-0.88011
H	0.177	5.75138	0.01741
H	0.8381	5.42226	-1.60626
N	1.59922	4.19503	-0.09169
C	-2.28111	-1.58193	-0.39061
H	-3.27611	-1.13926	-0.40412
C	-2.06669	-2.42467	-1.6471
H	-2.83178	-3.20597	-1.7216
H	-2.14432	-1.78417	-2.53126
H	-1.08337	-2.90608	-1.61336
C	-3.30208	-1.26612	2.57376
O	-4.41766	-1.43822	2.08824
O	-3.11	-0.63825	3.74953
H	-3.99221	-0.4113	4.07741
O	-2.14318	-1.63741	2.08838
O	-1.30814	-0.52496	-0.34215
C	-1.64979	0.75425	-0.73472
O	-2.85338	1.06066	-0.93477
O	-0.65265	1.50971	-0.85431
C	-2.10758	-2.43438	0.86042
H	-1.1264	-2.91951	0.8685
H	-2.89635	-3.18861	0.91309
C	-6.37538	0.83541	-0.42072
N	-5.21483	0.38522	0.01716
H	-5.16985	-0.31705	0.75632
H	-4.27615	0.67721	-0.38144
N	-6.46461	1.46186	-1.62212
N	-7.50579	0.68428	0.33163
C	-7.39389	0.36199	1.75377
H	-8.30453	0.69824	2.25603
H	-7.26952	-0.71373	1.93125
H	-6.54126	0.88627	2.18668
C	-8.79469	0.35718	-0.28192
H	-9.56572	1.07802	0.01034
H	-8.70421	0.35058	-1.36686
H	-9.11295	-0.64093	0.04153
C	-7.35069	2.60824	-1.82745
H	-6.74888	3.49196	-2.06818

H	-8.04596	2.42876	-2.65462
H	-7.91808	2.81654	-0.92147
C	-5.39608	1.30802	-2.61785
H	-4.56074	1.99068	-2.43588
H	-5.00504	0.2915	-2.58816
H	-5.82701	1.49616	-3.60424
Br	0.83054	-4.23714	-0.23073
H	2.47329	-0.90653	0.70523

TSu2

Charge = 0 Multiplicity = 1

C	-7.42274	-1.34772	0.15491
H	-8.19696	-1.6383	-0.56256
H	-7.86076	-1.32052	1.15663
N	-7.01218	0.03734	-0.1711
C	-7.86101	1.1311	-0.16135
C	-5.77896	0.45344	-0.49098
C	-7.1157	2.22194	-0.49012
H	-8.9081	1.03887	0.07801
H	-4.87766	-0.16608	-0.56962
H	-7.38889	3.25958	-0.59367
O	-5.34472	-2.05309	1.14814
H	-4.46637	-1.9296	0.71527
C	-4.66356	2.60214	-1.06266
H	-4.8329	3.04322	-2.04745
H	-4.53693	3.39423	-0.3218
H	-3.77487	1.96421	-1.07917
N	-5.82161	1.77732	-0.69299
C	1.45877	2.05453	1.68871
O	2.4851	2.45451	2.23879
O	0.27063	2.09129	2.39335
H	0.52323	2.41321	3.27083
O	1.3453	1.59979	0.48938
C	-0.04903	-0.51368	-0.21838
C	-0.43726	0.95292	-0.1508
H	0.62312	-0.78178	0.59873
H	-0.88533	1.3553	0.742
H	-0.26547	1.61197	-0.98556
C	-2.35622	-0.69224	-0.45936
O	-3.43304	-1.32978	-0.47867
O	-2.20316	0.52297	-0.84182
O	-1.25445	-1.30103	0.00811
C	0.57947	-0.922	-1.54197
H	1.45708	-0.29902	-1.73564
H	0.91924	-1.95651	-1.4691
H	-0.13073	-0.80096	-2.36718
C	5.06621	0.48481	-0.51541
N	3.80685	0.24729	-0.20874
H	3.12035	0.98804	-0.0397
H	3.4995	-0.71826	0.11846
N	5.61185	1.7305	-0.42826
N	5.8619	-0.53018	-0.97031
C	7.20415	-0.7241	-0.42295
H	7.2197	-1.62151	0.20728
H	7.93997	-0.84999	-1.22571
H	7.49126	0.12846	0.19155
C	5.26051	-1.72848	-1.57154
H	4.4162	-1.43324	-2.19637
H	6.02153	-2.19811	-2.2026
H	4.8866	-2.43373	-0.81976
C	6.66179	2.17209	-1.34042
H	6.3311	3.08028	-1.85881
H	7.58948	2.4069	-0.80454
H	6.86456	1.40124	-2.08272
C	4.98426	2.79395	0.35438
H	4.41262	3.47222	-0.29316
H	4.30709	2.39906	1.11358
H	5.77065	3.37481	0.84814
Br	2.78954	-2.56292	0.82703
C	-6.26826	-2.35206	0.13906

H	-5.80064	-2.37496	-0.85467
H	-6.72897	-3.33972	0.29804

u3

Charge = 0 Multiplicity = 1

C	4.77586	1.08155	1.35326
C	4.2081	-0.1136	1.03079
C	3.25383	0.62988	2.88693
N	4.1743	1.52614	2.51907
H	5.53843	1.65654	0.85282
H	4.32499	-0.76944	0.1713
H	2.57767	0.72117	3.71991
C	2.27222	-1.46915	1.98957
H	2.63801	-2.21185	1.27659
H	2.23672	-1.90785	2.99114
C	0.87292	-0.92693	1.59853
H	0.91758	-0.59425	0.55794
O	0.55529	0.1578	2.45191
H	0.67997	0.98583	1.93832
C	4.325	2.85858	3.10053
H	5.37535	3.15267	3.06043
H	3.70926	3.56123	2.53317
H	3.99768	2.83642	4.14125
N	3.25961	-0.37843	2.0064
Br	-3.65539	-1.24896	2.3372
C	-3.70492	1.90633	-1.05859
N	-3.55809	1.98221	0.29635
N	-4.92228	1.3572	-1.4886
C	-5.3516	1.63513	-2.84539
H	-6.43144	1.46293	-2.91845
H	-5.1475	2.67938	-3.09622
H	-4.86362	0.99024	-3.59986
C	-5.3106	0.03046	-0.99851
H	-4.78581	-0.22401	-0.07327
H	-6.3915	-0.00729	-0.81458
H	-5.06697	-0.74031	-1.7493
C	-2.2438	2.05551	0.91123
H	-2.05776	3.05256	1.34034
H	-2.19559	1.30151	1.70593
H	-1.47954	1.85668	0.16195
C	-4.67575	2.11892	1.22432
H	-4.71006	1.26083	1.90565
H	-4.54339	3.0398	1.8121
H	-5.61114	2.19403	0.66976
N	-2.77851	2.35198	-1.86544
H	-2.95101	2.03312	-2.81702
C	2.18324	2.28623	-2.4621
C	1.15661	1.1504	-2.26335
H	0.22277	1.32642	-2.79635
H	1.5744	0.1607	-2.46946
C	1.63603	2.10201	-0.24704
O	1.61373	2.30449	0.95634
O	0.86384	1.19262	-0.84775
O	2.47753	2.69633	-1.08934
H	1.7156	3.15297	-2.93059
C	3.46463	1.85769	-3.15288
H	3.25447	1.65046	-4.20882
H	4.21458	2.65418	-3.10935
H	3.86253	0.94085	-2.70487
O	-0.36626	3.73891	-1.69623
H	-0.52873	4.53462	-1.17015
H	-1.25123	3.27534	-1.7129
H	0.11397	-1.67396	1.70269

TSu3

Charge = 0 Multiplicity = 1

C	0.27328	-1.18525	2.41952
C	1.12777	-1.63242	1.45683
C	-0.77469	-2.7526	1.27482
N	-0.90536	-1.90342	2.29875

H	0.39915	-0.42968	3.17726
H	2.1352	-1.3403	1.14932
H	-1.53724	-3.40272	0.88249
C	0.93469	-3.32093	-0.44448
H	1.98532	-3.03786	-0.57695
H	0.8514	-4.39469	-0.25599
C	0.1149	-2.92637	-1.68328
H	0.34158	-1.88731	-1.93986
O	-1.27317	-3.12351	-1.50274
H	-1.6596	-2.24892	-1.28164
C	-2.15603	-1.61696	2.99603
H	-1.93898	-1.38444	4.04005
H	-2.65258	-0.77442	2.50725
H	-2.79717	-2.49867	2.95677
N	0.44974	-2.61567	0.75669
Br	3.8648	-1.06425	-0.49687
C	1.25877	2.39626	-0.01968
N	1.78198	1.87146	-1.14881
N	2.13237	2.99635	0.86813
C	1.6273	3.99118	1.79924
H	2.44454	4.66503	2.07492
H	0.83627	4.5785	1.32928
H	1.23593	3.54944	2.73099
C	3.35181	2.3008	1.30102
H	3.49557	1.36673	0.74921
H	4.23404	2.93813	1.17148
H	3.26793	2.0502	2.36773
C	1.11649	0.79746	-1.87838
H	0.76464	1.15142	-2.85737
H	1.84652	-0.00966	-2.00466
H	0.27124	0.42385	-1.3032
C	3.06206	2.28809	-1.71983
H	3.79628	1.48074	-1.61748
H	2.91137	2.50487	-2.78436
H	3.4146	3.19417	-1.22887
N	-0.04393	2.37372	0.19972
H	-0.30135	2.53489	1.16535
C	-4.78147	1.15417	-0.88865
C	-4.33971	1.53881	0.54857
H	-4.12939	2.6089	0.6344
H	-5.08097	1.25322	1.30372
C	-2.75969	0.19601	-0.42516
O	-1.9008	-0.68785	-0.42458
O	-3.14954	0.78382	0.78076
O	-3.86949	0.10485	-1.23893
H	-4.60938	1.99719	-1.5655
C	-6.20771	0.64583	-1.00556
H	-6.91649	1.43922	-0.74483
H	-6.4196	0.32294	-2.02843
H	-6.37086	-0.20318	-0.33453
O	-2.02658	1.74213	-1.16635
H	-1.78096	1.45614	-2.05663
H	-1.00216	2.04555	-0.55201
H	0.46379	-3.55729	-2.51028

v1

Charge = 0 Multiplicity = 1

C	0.66336	2.03749	0.16029
O	-0.06764	2.74976	-0.58768
O	1.95933	2.51833	0.36733
H	1.98604	3.34393	-0.14479
O	0.39072	0.95696	0.72348
C	-2.94978	-0.95244	-0.36278
C	-2.47282	1.18006	0.01464
C	-3.50322	0.82584	0.83174
N	-3.78729	-0.51312	0.58532
H	-2.8911	-1.96207	-0.73278
H	-1.85516	2.07322	-0.10201
H	-4.04248	1.38922	1.57639
C	-1.03375	-0.03023	-1.65914

H	-0.60715	0.97214	-1.73935
H	-1.3918	-0.36499	-2.63922
O	1.19283	-0.77241	-1.6432
H	1.90317	-1.25519	-1.11608
N	-2.16429	0.05945	-0.7359
C	-4.79811	-1.31394	1.26703
H	-4.77228	-2.33134	0.87412
H	-4.58744	-1.33979	2.33918
H	-5.7904	-0.88706	1.09866
C	2.84831	-1.08186	1.28624
C	3.83593	-0.41177	0.43529
O	3.13296	-1.5943	-0.04927
H	3.1868	-1.74877	2.07821
H	1.87175	-0.61417	1.39998
H	3.49986	0.51091	-0.0366
C	5.32085	-0.57805	0.61612
H	5.83837	-0.54831	-0.34981
H	5.71692	0.23553	1.23549
H	5.5514	-1.53213	1.10123
C	0.00342	-1.02166	-1.12155
O	-0.28827	-1.94411	-0.38514

TSv1

Charge = 0 Multiplicity = 1

C	-3.32153	-1.01756	-0.00317
C	-2.41768	-0.40131	-0.94981
O	-2.53832	-2.04309	-0.73564
H	-3.01498	-0.97209	1.04023
H	-1.43256	-0.08662	-0.63979
H	-2.74883	-0.20398	-1.95861
C	-4.8026	-1.07422	-0.24465
H	-5.26431	-1.88874	0.32295
H	-5.24185	-0.12369	0.07617
H	-5.0204	-1.21547	-1.30757
C	-1.81813	2.33695	0.03799
O	-0.72143	1.80283	0.38938
O	-1.98004	3.67162	0.37722
H	-1.1696	3.90015	0.86023
O	-2.77925	1.82785	-0.57466
C	3.20873	-0.65661	0.32542
C	2.11493	1.26498	0.2058
C	3.29372	1.40911	-0.46248
N	3.96875	0.19835	-0.37406
H	3.43454	-1.69222	0.51336
H	1.24297	1.90309	0.33137
H	3.70559	2.24922	-0.99891
C	0.9519	-0.66741	1.36334
H	0.16962	0.0889	1.445
H	1.248	-1.00396	2.36172
O	-0.7493	-2.21355	0.89109
H	-1.68785	-2.29339	-0.07423
N	2.09544	-0.027	0.70455
C	5.26683	-0.1059	-0.96772
H	5.51299	-1.14955	-0.76765
H	5.22437	0.04919	-2.04869
H	6.0378	0.53697	-0.5347
C	0.43271	-1.87671	0.52847
O	1.1561	-2.36632	-0.33908

v2

Charge = 0 Multiplicity = 1

C	-4.29531	-2.20181	-0.69284
H	-4.69443	-1.52553	-1.45894
H	-5.00526	-3.00897	-0.49638
N	-4.19404	-1.42129	0.54749
C	-5.17912	-1.30994	1.51495
C	-3.2732	-0.47474	0.76636
C	-4.81425	-0.29942	2.34722
H	-6.03497	-1.96424	1.53106
H	-2.37312	-0.3276	0.19319

H	-5.29241	0.10099	3.22591
O	-2.36652	-3.60578	-0.16896
H	-1.64965	-3.08601	0.25715
C	-2.98015	1.45733	2.25653
H	-1.8945	1.35511	2.23534
H	-3.29028	2.20196	1.5149
H	-3.30372	1.73193	3.26139
N	-3.60257	0.18972	1.88429
C	0.12769	0.6172	-1.41421
H	1.20938	0.47301	-1.43718
C	-0.45435	0.5492	-2.82536
H	-0.02108	1.32955	-3.46094
H	-0.22805	-0.42297	-3.27233
H	-1.53967	0.68934	-2.78411
C	1.3674	2.3241	0.96201
O	2.31177	2.5555	0.21825
O	1.44961	2.36886	2.30388
H	2.36939	2.58759	2.51017
O	0.12672	2.03667	0.62408
O	-0.45936	-0.44178	-0.64771
C	0.29358	-1.16572	0.29814
O	1.50779	-0.85571	0.46461
O	-0.35571	-2.04203	0.88033
C	-0.21337	1.97119	-0.79189
H	-1.29677	2.12692	-0.81811
H	0.30708	2.77664	-1.31618
C	4.85254	-0.37943	-0.20323
N	3.67709	0.13565	-0.51847
H	3.59714	1.12035	-0.73789
H	2.7599	-0.30892	-0.19626
N	4.97431	-1.72076	-0.02554
N	5.95896	0.40991	-0.07299
C	5.82585	1.85647	0.09243
H	6.64576	2.21473	0.72169
H	5.87818	2.38255	-0.87047
H	4.88007	2.10535	0.57471
C	7.28162	-0.04317	-0.50497
H	8.00316	-0.01022	0.31866
H	7.22357	-1.0601	-0.8895
H	7.6454	0.60898	-1.30787
C	5.82151	-2.27545	1.03331
H	5.18938	-2.77382	1.77675
H	6.52649	-3.00945	0.62885
H	6.37672	-1.48375	1.53414
C	3.90751	-2.61828	-0.49434
H	3.05845	-2.6342	0.19654
H	3.55198	-2.28291	-1.4695
H	4.33424	-3.6185	-0.59843
Br	-3.85109	1.55527	-1.29019
C	-2.95191	-2.7838	-1.14589
O	-2.38331	-2.60382	-2.21855

TSv2

Charge = 0 Multiplicity = 1

N	5.65226	0.07328	0.57527
C	4.70162	1.02989	0.8806
C	6.85333	0.6554	0.51357
C	5.3634	2.21208	1.02328
H	3.6547	0.76585	0.91155
H	7.76396	0.15799	0.22532
H	5.00073	3.19964	1.25745
C	7.78448	2.94696	0.82558
H	7.57726	3.74168	0.1063
H	7.86975	3.3707	1.82843
H	8.72164	2.45924	0.55843
N	6.70732	1.95869	0.79121
C	-1.12348	2.62142	0.0526
O	-2.07673	3.39794	0.03488
O	0.1275	3.10044	0.39418
H	-0.02704	4.03993	0.57282

O	-1.1547	1.36144	-0.22037
C	-0.11418	-0.98008	0.16213
C	0.51653	0.34628	-0.22215
H	-1.10236	-1.08735	-0.28805
H	0.66574	0.59317	-1.26181
H	0.91649	1.01789	0.51613
C	1.97434	-1.76515	-0.52509
O	2.74526	-2.69464	-0.86015
O	2.30717	-0.55774	-0.25269
O	0.66488	-2.05128	-0.43412
C	-0.22839	-1.18201	1.66496
H	-0.79665	-0.3521	2.09525
H	-0.7841	-2.10067	1.86023
H	0.76127	-1.21672	2.13388
C	-5.06815	0.78623	-0.21151
N	-3.85932	0.37458	0.11497
H	-3.02198	0.91628	-0.11225
H	-3.70061	-0.63947	0.39328
N	-5.26584	1.76752	-1.13741
N	-6.15956	0.22879	0.38465
C	-7.35455	-0.10574	-0.3878
H	-7.46657	-1.19532	-0.4351
H	-8.25402	0.31696	0.07489
H	-7.26512	0.27419	-1.40485
C	-6.01438	-0.49541	1.65472
H	-5.29967	0.03172	2.28878
H	-6.99059	-0.503	2.1487
H	-5.64481	-1.5169	1.50378
C	-6.30372	2.78035	-0.96677
H	-5.83813	3.76538	-0.84068
H	-6.96678	2.81974	-1.83903
H	-6.89635	2.56197	-0.07934
C	-4.20518	2.11507	-2.08532
H	-3.52421	2.8638	-1.66664
H	-3.63474	1.22047	-2.33919
H	-4.67329	2.50025	-2.99648
Br	-3.36454	-2.68814	0.59918
C	5.36593	-1.32256	0.23072
H	4.3084	-1.49547	0.40794
H	5.95795	-1.9787	0.87467
O	4.9535	-2.30171	-1.9431
H	4.02005	-2.45122	-1.47718
C	5.77961	-1.58648	-1.24061
O	6.85071	-1.14852	-1.6315

v3

Charge = 0 Multiplicity = 1

C	-5.08552	0.01819	0.86192
C	-3.92969	-0.39848	0.27189
C	-4.11326	1.79429	-0.02826
N	-5.1821	1.38964	0.66934
H	-5.84146	-0.53433	1.39593
H	-3.45261	-1.37933	0.12807
H	-3.88442	2.81116	-0.29797
C	-2.07384	0.711	-1.03303
H	-1.67684	-0.31569	-0.95944
H	-2.29252	0.87993	-2.0925
O	-1.52792	2.80472	0.01445
H	-0.75625	3.40532	0.24828
C	-6.27364	2.24691	1.1262
H	-7.19264	2.00247	0.58819
H	-6.42786	2.10317	2.19738
H	-6.01148	3.28863	0.94127
N	-3.34163	0.73088	-0.27925
Br	-1.93521	-2.73948	-1.05018
C	2.33612	-2.39739	0.61404
N	1.77593	-2.64185	-0.60826
N	1.96927	-3.2982	1.61926
C	2.79164	-3.37017	2.81208
H	2.61324	-4.32897	3.30978

H	3.84908	-3.31283	2.54326
H	2.57041	-2.57279	3.54331
C	0.54715	-3.57671	1.8491
H	-0.06054	-3.27319	0.99312
H	0.38954	-4.64634	2.0321
H	0.19082	-3.02511	2.73325
C	1.68981	-1.58603	-1.60326
H	2.60717	-1.48945	-2.20286
H	0.84574	-1.81738	-2.25832
H	1.492	-0.62954	-1.1203
C	1.52535	-3.99168	-1.10567
H	0.47392	-4.09606	-1.39195
H	2.16266	-4.18824	-1.9803
H	1.7702	-4.72116	-0.3345
N	3.16417	-1.40232	0.78555
H	3.32067	-1.23696	1.77719
C	3.3562	2.80483	-0.54303
C	3.16316	2.19883	0.85922
H	3.01545	1.11966	0.83561
H	3.96662	2.46333	1.55361
C	1.52805	3.7376	0.46856
O	0.50446	4.38655	0.63081
O	1.94076	2.81054	1.3368
O	2.35603	3.87675	-0.56413
H	3.06779	2.07636	-1.30027
C	4.73299	3.36505	-0.82353
H	5.43683	2.52927	-0.83017
H	4.75965	3.85341	-1.80153
H	5.02796	4.09302	-0.06047
O	4.70397	0.12564	-0.97427
H	4.94989	-0.42649	-1.72481
H	4.17947	-0.47503	-0.38332
C	-1.03126	1.7294	-0.60066
O	0.14282	1.56628	-0.8668

TSv3

Charge = 0 Multiplicity = 1

C	0.24175	-1.21369	2.41624
C	1.09987	-1.65468	1.45395
C	-0.80349	-2.77003	1.25439
N	-0.93746	-1.92885	2.28447
H	0.36533	-0.46463	3.1808
H	2.10895	-1.3617	1.15346
H	-1.56549	-3.41528	0.85301
C	0.91147	-3.32635	-0.46271
H	1.96423	-3.04765	-0.58674
H	0.82143	-4.40158	-0.28608
O	-1.29007	-3.10333	-1.52844
H	-1.6703	-2.22801	-1.29837
C	-2.19132	-1.64397	2.97666
H	-1.98038	-1.42438	4.02475
H	-2.68	-0.79329	2.49403
H	-2.83661	-2.52186	2.92291
N	0.42361	-2.63138	0.74316
Br	3.85123	-1.08021	-0.48374
C	1.28139	2.39619	-0.01455
N	1.79715	1.8731	-1.1462
N	2.15614	2.98398	0.87782
C	1.65965	3.98282	1.80985
H	2.48188	4.65167	2.08276
H	0.87099	4.57472	1.3418
H	1.2685	3.54345	2.74257
C	3.37465	2.28284	1.30482
H	3.50719	1.34401	0.75801
H	4.26029	2.91311	1.16477
H	3.29636	2.03985	2.37346
C	1.12377	0.80561	-1.87983
H	0.79204	1.16223	-2.86435
H	1.84372	-0.01258	-1.9923
H	0.26382	0.44855	-1.31628

C	3.08387	2.27663	-1.71232
H	3.80942	1.46194	-1.6065
H	2.93857	2.49356	-2.77737
H	3.44339	3.17981	-1.22107
N	-0.02254	2.38598	0.20699
H	-0.28383	2.53513	1.17296
C	-4.76616	1.1814	-0.88518
C	-4.31067	1.57565	0.5456
H	-4.07444	2.64137	0.61397
H	-5.05452	1.31755	1.30788
C	-2.75143	0.21006	-0.4228
O	-1.89395	-0.67494	-0.42647
O	-3.1371	0.79689	0.78383
O	-3.86076	0.12656	-1.23635
H	-4.59665	2.01871	-1.56936
C	-6.19491	0.67619	-0.98595
H	-6.89935	1.47419	-0.72748
H	-6.41577	0.34392	-2.00395
H	-6.35567	-0.16581	-0.30548
O	-2.01007	1.77629	-1.16427
H	-1.78027	1.49451	-2.05994
H	-0.95062	2.07811	-0.53349
C	0.09982	-2.91388	-1.70126
O	0.53262	-2.46337	-2.75769

w1

Charge = 0 Multiplicity = 1

C	-0.33372	-3.18177	0.05151
O	-0.3012	-4.34335	-0.44195
O	-0.29615	-3.13385	1.44572
H	-0.25039	-4.06451	1.70586
O	-0.38371	-2.07215	-0.51655
C	3.39545	1.15839	-0.36307
C	2.39813	-0.79619	-0.01827
C	3.74558	-1.00594	-0.09176
N	4.35525	0.22085	-0.31756
H	3.5553	2.21074	-0.53478
H	1.52732	-1.48256	0.14144
H	4.31668	-1.91811	-0.02764
C	0.90565	1.25649	-0.13507
H	0.20392	0.60686	-0.67331
H	1.0156	2.22389	-0.62982
C	0.38804	1.42244	1.2988
H	0.33334	0.41733	1.75184
H	1.09923	2.01052	1.89299
N	2.21362	0.56844	-0.17802
C	5.78476	0.45494	-0.4938
H	5.96103	1.52329	-0.62092
H	6.33013	0.10502	0.38494
H	6.14332	-0.07507	-1.37938
C	-3.41451	-0.9794	0.75225
C	-3.14844	-0.29145	-0.5112
O	-2.93526	0.38824	0.74961
H	-4.44499	-1.08236	1.1006
H	-2.71568	-1.74359	1.082
H	-2.22512	-0.56829	-1.01623
C	-4.26199	0.28165	-1.35244
H	-3.94063	1.20596	-1.84825
H	-4.55963	-0.42835	-2.13205
H	-5.13575	0.51314	-0.73716
N	-0.87101	2.13339	1.21288
H	-1.61572	1.52894	0.86402
H	-1.15725	2.43722	2.13998

TSw1

Charge = 0 Multiplicity = 1

C	3.10778	-0.96614	-0.10047
C	2.51689	-0.14144	0.95518
O	2.63257	-2.00603	0.71157
H	2.5928	-0.882	-1.07299

H	1.44601	-0.03078	0.98096
H	3.06962	-0.04153	1.87791
C	4.61478	-0.91999	-0.28833
H	4.94188	-1.76267	-0.90691
H	4.92063	0.01385	-0.77217
H	5.11673	-0.99646	0.68154
C	1.7864	2.29239	-0.0752
O	0.71878	1.75251	-0.46836
O	1.97181	3.61978	-0.39425
H	1.19343	3.85305	-0.9203
O	2.73615	1.79025	0.5829
C	-3.30109	-0.77016	-0.2753
C	-2.0168	1.01395	-0.04104
C	-3.28591	1.35231	0.33222
N	-4.07744	0.22603	0.17952
H	-3.63473	-1.77265	-0.48918
H	-1.07802	1.57076	-0.09502
H	-3.69066	2.28513	0.69037
C	-0.88851	-1.12926	-0.86121
H	-0.04415	-0.43797	-0.89788
H	-1.08915	-1.49872	-1.8692
C	-0.6091	-2.31213	0.0869
H	-0.50872	-1.91069	1.1139
H	-1.49442	-2.96757	0.09505
H	1.44362	-2.60925	0.05179
N	-2.05442	-0.31566	-0.41987
C	-5.50616	0.13315	0.47043
H	-5.85373	-0.87355	0.23824
H	-5.6843	0.33887	1.52804
H	-6.05671	0.85204	-0.13994
N	0.55081	-3.01096	-0.41714
H	0.49296	-3.99378	-0.16577

w2

Charge = 0 Multiplicity = 1

C	-2.95191	-2.7838	-1.14589
H	-2.28547	-1.968	-1.44969
C	-4.29531	-2.20181	-0.69284
H	-4.69443	-1.52553	-1.45894
H	-5.00526	-3.00897	-0.49638
N	-4.19404	-1.42129	0.54749
C	-5.17912	-1.30994	1.51495
C	-3.2732	-0.47474	0.76636
C	-4.81425	-0.29942	2.34722
H	-6.03497	-1.96424	1.53106
H	-2.37312	-0.3276	0.19319
H	-5.29241	0.10099	3.22591
H	-1.64965	-3.08601	0.25715
C	-2.98015	1.45733	2.25653
H	-1.8945	1.35511	2.23534
H	-3.29028	2.20196	1.5149
H	-3.30372	1.73193	3.26139
N	-3.60257	0.18972	1.88429
C	0.12769	0.6172	-1.41421
H	1.20938	0.47301	-1.43718
C	-0.45435	0.5492	-2.82536
H	-0.02108	1.32955	-3.46094
H	-0.22805	-0.42297	-3.27233
H	-1.53967	0.68934	-2.78411
C	1.3674	2.3241	0.96201
O	2.31177	2.5555	0.21825
O	1.44961	2.36886	2.30388
H	2.36939	2.58759	2.51017
O	0.12672	2.03667	0.62408
O	-0.45936	-0.44178	-0.64771
C	0.29358	-1.16572	0.29814
O	1.50779	-0.85571	0.46461
O	-0.35571	-2.04203	0.88033
C	-0.21337	1.97119	-0.79189
H	-1.29677	2.12692	-0.81811

H	0.30708	2.77664	-1.31618	C	-5.79031	0.45	-0.48542
C	4.85254	-0.37943	-0.20323	C	-7.16763	2.18885	-0.538
N	3.67709	0.13565	-0.51847	H	-8.96328	0.95642	-0.10083
H	3.59714	1.12035	-0.73789	H	-4.86423	-0.15002	-0.51795
H	2.7599	-0.30892	-0.19626	H	-7.45824	3.22177	-0.64159
N	4.97431	-1.72076	-0.02554	H	-4.52728	-1.93348	0.8266
N	5.95896	0.40991	-0.07299	C	-4.69656	2.6358	-0.95198
C	5.82585	1.85647	0.09243	H	-4.83325	3.11603	-1.92343
H	6.64576	2.21473	0.72169	H	-4.61555	3.39779	-0.17389
H	5.87818	2.38255	-0.87047	H	-3.795	2.0158	-0.96016
H	4.88007	2.10535	0.57471	N	-5.85354	1.77641	-0.66824
C	7.28162	-0.04317	-0.50497	C	1.53832	2.03759	1.73313
H	8.00316	-0.01022	0.31866	O	2.57707	2.42084	2.27129
H	7.22357	-1.0601	-0.8895	O	0.36596	2.05392	2.46322
H	7.6454	0.60898	-1.30787	H	0.63631	2.35196	3.34385
C	5.82151	-2.27545	1.03331	O	1.39849	1.61714	0.52346
H	5.18938	-2.77382	1.77675	C	-0.04628	-0.46799	-0.17147
H	6.52649	-3.00945	0.62885	C	-0.40195	1.00662	-0.09969
H	6.37672	-1.48375	1.53414	H	0.63016	-0.75084	0.637
C	3.90751	-2.61828	-0.49434	H	-0.83376	1.41744	0.79727
H	3.05845	-2.6342	0.19654	H	-0.22505	1.66227	-0.93606
H	3.55198	-2.28291	-1.4695	C	-2.35826	-0.59729	-0.38839
H	4.33424	-3.6185	-0.59843	O	-3.4484	-1.21232	-0.39573
Br	-3.85109	1.55527	-1.29019	O	-2.18342	0.61322	-0.77464
H	-3.16589	-3.37504	-2.04868	O	-1.26567	-1.22913	0.07019
N	-2.33923	-3.64409	-0.12343	C	0.55603	-0.88995	-1.50298
H	-2.67479	-4.58	-0.23058	H	1.4462	-0.28864	-1.70751
				H	0.87162	-1.93237	-1.43514
TSw2				H	-0.16119	-0.75095	-2.31927
Charge =	0 Multiplicity = 1			C	5.06878	0.46081	-0.55296
C	-7.433	-1.39635	0.02289	N	3.81408	0.23438	-0.22055
H	-8.13907	-1.69439	-0.75904	H	3.13609	0.98104	-0.0397
H	-7.95198	-1.3965	0.98558	H	3.50354	-0.72796	0.11219
N	-7.03198	0.0025	-0.24843	N	5.62547	1.70262	-0.48055
C	-7.90587	1.07637	-0.27323	N	5.84754	-0.56169	-1.02054

C	7.19934	-0.76361	-0.50024
H	7.22119	-1.65793	0.13423
H	7.91708	-0.89944	-1.31758
H	7.50603	0.08975	0.10358
C	5.22425	-1.75817	-1.60273
H	4.36937	-1.45942	-2.21125
H	5.96814	-2.23725	-2.24696
H	4.86019	-2.45671	-0.83994
C	6.65864	2.13422	-1.41636
H	6.32254	3.04224	-1.9316
H	7.59866	2.36574	-0.90094
H	6.84148	1.35924	-2.15959
C	5.02013	2.77299	0.31029
H	4.43696	3.45045	-0.3278
H	4.35901	2.38433	1.08689
H	5.8201	3.35277	0.78297
Br	2.77682	-2.56386	0.83093
C	-6.25953	-2.37535	0.08578
H	-5.70614	-2.36779	-0.86223
H	-6.70812	-3.37556	0.18855
N	-5.39158	-2.06409	1.23063
H	-5.76776	-2.48217	2.05749

w3

Charge = 0 Multiplicity = 1

C	1.43624	-1.31425	-2.26107
C	0.9582	-1.88747	-1.11976
C	3.17383	-1.87436	-1.0189
N	2.82087	-1.32149	-2.18547
H	0.9189	-0.91318	-3.11721
H	-0.04647	-2.11087	-0.74307
H	4.17503	-1.96631	-0.63441
C	2.04356	-2.75649	1.01869
H	1.00534	-3.04547	1.23112
H	2.69361	-3.63449	1.05202
C	2.53818	-1.69323	2.00503
H	1.8466	-0.84208	2.00367
H	3.83799	-0.41463	1.29247
C	3.73467	-0.64101	-3.09907
H	3.35699	-0.73256	-4.1182
H	3.81204	0.41019	-2.81302
H	4.71807	-1.10879	-3.04026
N	2.06618	-2.229	-0.36021
Br	-1.55516	-2.9638	0.89585
C	-3.14204	1.00096	-0.41523
N	-2.93032	0.43685	0.8084
N	-4.11652	0.3787	-1.1978
C	-4.72044	1.13371	-2.27953
H	-5.69168	0.69112	-2.52374
H	-4.87947	2.16954	-1.97164
H	-4.11616	1.13053	-3.2037
C	-4.04777	-1.06859	-1.43072
H	-3.35379	-1.55017	-0.73697
H	-5.0378	-1.52681	-1.32153
H	-3.69378	-1.26833	-2.45369
C	-1.67546	0.61977	1.51702
H	-1.78093	1.32181	2.35714
H	-1.3455	-0.36084	1.87728
H	-0.93177	1.01445	0.8264
C	-3.95197	-0.29357	1.55256
H	-3.64128	-1.33407	1.69781
H	-4.08779	0.18069	2.53451
H	-4.90011	-0.25404	1.01788
N	-2.48065	2.0717	-0.78135
H	-2.59573	2.23686	-1.7783
C	1.21644	3.21018	0.99573
C	1.01494	3.1697	-0.52677
H	0.10408	2.6426	-0.81827
H	1.04336	4.15395	-0.99263
C	2.69638	1.74075	0.03786

O	3.57697	0.90941	-0.07918
O	2.1633	2.40595	-0.99715
O	2.14278	2.08999	1.2027
H	0.29192	2.97398	1.51524
C	1.82933	4.49098	1.52789
H	1.09296	5.29157	1.41992
H	2.08414	4.38705	2.58572
H	2.73502	4.76178	0.97462
O	-1.47227	4.26604	0.56345
H	-2.17258	4.65716	1.09798
H	-1.89438	3.47291	0.13221
H	2.50877	-2.14042	3.00571
N	3.91608	-1.2744	1.71034
H	4.55657	-1.87394	2.19026

TSw3

Charge = 0 Multiplicity = 1

C	0.24175	-1.21369	2.41624
C	1.09987	-1.65468	1.45395
C	-0.80349	-2.77003	1.25439
N	-0.93746	-1.92885	2.28447
H	0.36533	-0.46463	3.1808
H	2.10895	-1.3617	1.15346
H	-1.56549	-3.41528	0.85301
C	0.91147	-3.32635	-0.46271
H	1.96423	-3.04765	-0.58674
H	0.82143	-4.40158	-0.28608
C	0.09982	-2.91388	-1.70126
H	0.33437	-1.87373	-1.94592
H	-1.6703	-2.22801	-1.29837
C	-2.19132	-1.64397	2.97666
H	-1.98038	-1.42438	4.02475
H	-2.68	-0.79329	2.49403
H	-2.83661	-2.52186	2.92291
N	0.42361	-2.63138	0.74316
Br	3.85123	-1.08021	-0.48374
C	1.28139	2.39619	-0.01455
N	1.79715	1.8731	-1.1462
N	2.15614	2.98398	0.87782
C	1.65965	3.98282	1.80985
H	2.48188	4.65167	2.08276
H	0.87099	4.57472	1.3418
H	1.2685	3.54345	2.74257
C	3.37465	2.28284	1.30482
H	3.50719	1.34401	0.75801
H	4.26029	2.91311	1.16477
H	3.29636	2.03985	2.37346
C	1.12377	0.80561	-1.87983
H	0.79204	1.16223	-2.86435
H	1.84372	-0.01258	-1.9923
H	0.26382	0.44855	-1.31628
C	3.08387	2.27663	-1.71232
H	3.80942	1.46194	-1.6065
H	2.93857	2.49356	-2.77737
H	3.44339	3.17981	-1.22107
N	-0.02254	2.38598	0.20699
H	-0.28383	2.53513	1.17296
C	-4.76616	1.1814	-0.88518
C	-4.31067	1.57565	0.5456
H	-4.07444	2.64137	0.61397
H	-5.05452	1.31755	1.30788
C	-2.75143	0.21006	-0.4228
O	-1.89395	-0.67494	-0.42647
O	-3.1371	0.79689	0.78383
O	-3.86076	0.12656	-1.23635
H	-4.59665	2.01871	-1.56936
C	-6.19491	0.67619	-0.98595
H	-6.89935	1.47419	-0.72748
H	-6.41577	0.34392	-2.00395
H	-6.35567	-0.16581	-0.30548

O	-2.01007	1.77629	-1.16427
H	-1.78027	1.49451	-2.05994
H	-0.95062	2.07811	-0.53349
H	0.44819	-3.53866	-2.53315
N	-1.34578	-3.11092	-1.52151
H	-1.60025	-4.02328	-1.84221

x1

Charge = 0 Multiplicity = 1

C	-2.57338	-1.6684	0.73882
C	-1.71254	-1.4543	1.7724
C	-0.52246	-2.18689	0.05565
N	-1.80328	-2.13549	-0.3165
H	-3.63186	-1.41031	0.63127
H	-1.8898	-1.07897	2.76774
H	0.34457	-2.46188	-0.5431
C	0.82409	-1.44452	1.96886
H	0.72297	-1.58041	3.04934
H	1.5705	-2.14144	1.57443
C	1.22174	0.03724	1.61376
H	0.91076	0.69597	2.43668
C	2.77336	0.10879	1.45247
H	3.26099	0.41901	2.38063
H	3.16982	-0.86004	1.12512
N	3.15247	1.05384	0.39387
C	3.25457	0.70824	-0.94125
C	3.29593	2.37454	0.51437
C	3.49432	1.86269	-1.62502
H	3.14344	-0.33816	-1.23681
H	3.24573	2.93439	1.43512
H	3.64505	2.04128	-2.67798
O	0.63273	0.47108	0.41701
H	-0.22794	0.89977	0.63707
C	3.74469	4.30826	-0.99848
H	3.65833	4.88705	-0.07782
H	4.74495	4.44301	-1.41769
H	2.9964	4.65809	-1.71354
C	-2.31939	-2.44759	-1.65322
H	-2.90454	-3.37035	-1.61243
H	-2.94496	-1.60065	-1.95921
H	-1.47274	-2.58155	-2.32855
N	-0.43986	-1.79187	1.33568
N	3.51492	2.89634	-0.70061
Br	2.9182	-2.72776	-0.60974
C	-2.87088	2.03239	1.54252
C	-2.15953	3.00718	0.70346
O	-1.42221	1.97775	1.41731
H	-3.20558	2.33011	2.53629
H	-3.4228	1.21534	1.07892
H	-1.98184	3.99616	1.13276
C	-2.16989	2.92888	-0.80028
H	-2.86305	3.6795	-1.19927
H	-1.17275	3.14813	-1.20435
H	-2.50837	1.9454	-1.14605
C	-4.89665	0.17745	-0.86754
O	-5.11011	-0.21081	0.31691
O	-6.00774	0.67699	-1.54423
H	-6.72941	0.58596	-0.90007
O	-3.82624	0.18408	-1.5162

TSx1

Charge = 0 Multiplicity = 1

C	-1.67063	-2.82651	0.86773
C	-0.89765	-2.38379	1.89484
C	0.38581	-2.53205	0.09758
N	-0.8449	-2.92019	-0.24189
H	-2.73109	-2.99732	0.78257
H	-1.14608	-2.16344	2.92096
H	1.26244	-2.42229	-0.54321
C	1.44074	-1.38669	1.97611

H	1.46636	-1.54193	3.05788
H	2.38218	-1.71796	1.5245
C	1.16381	0.11065	1.60714
H	0.59771	0.58418	2.42574
C	2.53284	0.86346	1.442
H	2.85853	1.34311	2.36981
H	3.30404	0.17715	1.07687
N	2.38381	1.88786	0.40194
C	2.65758	1.66799	-0.93702
C	1.67428	3.01445	0.51838
C	2.12146	2.7188	-1.62009
H	3.15078	0.74626	-1.2459
H	1.2453	3.39944	1.42879
H	2.10834	2.94241	-2.67489
O	0.43349	0.15168	0.42219
H	-0.18058	0.95529	0.41357
C	0.61479	4.6704	-0.98539
H	0.83849	5.50772	-0.32053
H	0.77074	4.98343	-2.01824
H	-0.41199	4.32627	-0.83441
C	-1.28837	-3.29563	-1.58693
H	-1.46638	-4.37378	-1.6319
H	-2.20759	-2.74115	-1.79192
H	-0.50485	-3.02695	-2.29675
N	0.38903	-2.22242	1.40236
N	1.51154	3.55051	-0.69419
Br	3.71872	-1.68919	-0.71451
C	-2.52659	1.39965	-0.44196
C	-2.43069	1.90835	0.91268
O	-1.16109	2.21366	0.32418
H	-2.17688	0.40508	-0.67555
H	-2.80552	2.07309	-1.23719
H	-2.3751	1.13898	1.69342
C	-3.26689	3.09439	1.3361
H	-4.29317	2.76951	1.53684
H	-2.85875	3.55987	2.2417
H	-3.29374	3.84743	0.54071
C	-4.56216	-0.63383	-0.76989
O	-3.63014	-1.47879	-0.78894
O	-5.85319	-1.12615	-0.88974
H	-5.7338	-2.0849	-0.98779
O	-4.50417	0.61756	-0.65426

x2

Charge = 0 Multiplicity = 1

C	4.44551	-2.48563	-2.25324
C	3.41327	-2.56034	-1.36474
C	4.93161	-1.16719	-0.54348
N	5.38034	-1.60653	-1.72359
H	4.59923	-2.98072	-3.19945
H	2.49589	-3.1437	-1.33893
H	5.47565	-0.4449	0.0673
C	2.83323	-1.4201	0.81325
H	2.04303	-2.17904	0.77121
H	3.38379	-1.54022	1.75248
C	2.22195	-0.00192	0.69784
H	1.29064	-0.02972	1.27998
C	3.17373	1.05376	1.3334
H	3.09169	1.01658	2.42562
H	4.22648	0.90033	1.08324
N	2.8813	2.42628	0.8851
C	3.83656	3.33978	0.46647
C	1.66642	2.95326	0.70625
C	3.16017	4.4451	0.04137
H	4.89358	3.07839	0.47621
H	0.71619	2.44678	0.82111
H	3.51896	5.38018	-0.35998
O	1.9378	0.30008	-0.64644
H	0.9976	0.60393	-0.70775
C	0.69319	5.04854	-0.19253

H	-0.21068	4.43913	-0.25411
H	0.56177	5.85021	0.54026
H	0.90123	5.47961	-1.17462
C	6.64981	-1.18125	-2.31873
H	7.36794	-2.00589	-2.30206
H	6.47365	-0.86215	-3.34927
H	7.02917	-0.33803	-1.73351
N	3.73866	-1.727	-0.3063
N	1.80598	4.18249	0.19433
Br	6.82212	1.44654	0.59807
C	-2.39634	-1.46142	-0.24981
H	-3.34427	-0.92592	-0.26191
C	-2.28295	-2.35837	-1.48343
H	-3.13295	-3.05126	-1.53504
H	-2.28419	-1.73964	-2.38817
H	-1.35828	-2.94472	-1.44659
C	-3.45133	-1.04283	2.69936
O	-4.56989	-1.18512	2.20802
O	-3.24506	-0.38979	3.86108
H	-4.11718	-0.1046	4.18197
O	-2.30468	-1.47037	2.2335
O	-1.33139	-0.49723	-0.25873
C	-1.59336	0.85235	-0.39738
O	-2.78014	1.26915	-0.46433
O	-0.5441	1.54483	-0.44435
C	-2.28222	-2.2943	1.02133
H	-1.32006	-2.81091	1.0621
H	-3.09887	-3.01838	1.08226
C	-6.43558	0.89183	-0.631
N	-5.33762	0.55256	0.02469
H	-5.35942	-0.1128	0.79868
H	-4.37505	0.8758	-0.23191
N	-6.35528	1.44942	-1.86561
N	-7.66218	0.69009	-0.06751
C	-7.77444	0.44603	1.37169
H	-8.78338	0.7258	1.68849
H	-7.60536	-0.60873	1.62854
H	-7.05527	1.06368	1.913
C	-8.80628	0.23696	-0.86388
H	-9.66374	0.90724	-0.7333
H	-8.54166	0.19434	-1.92012
H	-9.09881	-0.77046	-0.54129
C	-7.27349	2.50577	-2.29684
H	-6.70166	3.42206	-2.48902
H	-7.79369	2.22189	-3.21921
H	-8.00814	2.71486	-1.51908
C	-5.12559	1.32751	-2.66023
H	-4.38823	2.09401	-2.3966
H	-4.67205	0.34828	-2.50288
H	-5.39749	1.42564	-3.71516
Br	0.63965	-4.209	0.0441

TSx2

Charge = 0 Multiplicity = 1

C	-2.17013	-2.79984	2.48273
C	-1.38896	-2.1812	1.5535
C	-3.39185	-2.51456	0.65952
N	-3.41813	-2.99026	1.90782
H	-1.95166	-3.11923	3.48928
H	-0.34555	-1.88863	1.5512
H	-4.27085	-2.50017	0.00988
C	-1.76145	-1.2624	-0.77036
H	-0.66893	-1.21213	-0.73497
H	-2.05354	-1.83118	-1.65927
C	-2.36982	0.16324	-0.78358
H	-1.70796	0.76283	-1.42206
C	-3.78804	0.14554	-1.4082
H	-3.72181	-0.01552	-2.49039
H	-4.43766	-0.63437	-0.99661
N	-4.51772	1.40114	-1.16271

C	-5.87313	1.48407	-0.88165	H	1.77533	0.59071	-1.98564
C	-3.97501	2.61713	-1.05947	H	1.75555	2.36468	-2.2645
C	-6.13678	2.7952	-0.61753	C	5.90677	-1.00125	-0.74096
H	-6.48074	0.58238	-0.83528	N	4.82353	-0.40311	-0.27159
H	-2.92083	2.86719	-1.11289	H	4.82005	0.53293	0.15495
H	-7.05653	3.2897	-0.34806	H	3.92388	-0.91868	-0.19972
O	-2.40395	0.68945	0.51666	N	7.15322	-0.53987	-0.46502
H	-1.92432	1.55234	0.49655	N	5.78356	-2.09425	-1.54909
C	-4.70341	4.90584	-0.47327	C	6.61974	-3.27753	-1.34821
H	-5.08138	5.51039	-1.30244	H	5.99413	-4.11342	-1.01083
H	-5.20986	5.19357	0.45063	H	7.11886	-3.5708	-2.27967
H	-3.62878	5.05832	-0.35618	H	7.37333	-3.08504	-0.58439
C	-4.6099	-3.57636	2.5277	C	4.55078	-2.32475	-2.31194
H	-4.51692	-4.66518	2.56852	H	4.15577	-1.3694	-2.66174
H	-4.71389	-3.17781	3.53938	H	4.80858	-2.94171	-3.17903
H	-5.47685	-3.28789	1.92329	H	3.77003	-2.81281	-1.71733
N	-2.17087	-2.0186	0.42157	C	8.25205	-0.68207	-1.41746
N	-4.93767	3.485	-0.72831	H	8.66426	0.31049	-1.63614
Br	-6.57348	-1.97549	-0.32227	H	9.05791	-1.30432	-1.0093
C	4.45173	2.14699	2.18835	H	7.89323	-1.1235	-2.347
O	5.36023	1.49302	2.69918	C	7.41415	0.38068	0.64266
O	3.73337	3.02464	2.96661	H	7.50175	1.41259	0.27797
H	4.10908	2.92766	3.85757	H	6.62234	0.35525	1.39248
O	4.07901	2.11265	0.95119	H	8.36287	0.09809	1.11225
C	1.8089	1.75207	-0.18416	Br	1.84219	-1.86927	-0.01262
C	2.42014	2.9988	0.42686				
H	2.09299	0.86956	0.3881	**x3**			
H	2.2045	3.27164	1.44625	Charge =	0 Multiplicity = 1		
H	3.00421	3.68536	-0.16397	C	-4.83181	-0.96016	1.27388
C	-0.10227	3.10438	-0.07425	C	-4.2306	0.2132	0.93248
O	-1.34999	3.21287	-0.05175	C	-3.35763	-0.48335	2.84632
O	0.77448	4.01293	-0.10493	N	-4.28063	-1.3753	2.47463
O	0.3764	1.81741	-0.03683	H	-5.58598	-1.53717	0.76469
C	2.16826	1.55517	-1.65232	H	-4.30416	0.84047	0.04731
H	3.25617	1.54369	-1.77741	H	-2.70998	-0.55936	3.70259

C	-2.30217	1.56292	1.91513
H	-2.62551	2.2895	1.16687
H	-2.2889	2.03285	2.90249
C	-0.90448	0.97603	1.58858
H	-0.92567	0.61293	0.55746
C	0.21485	2.02711	1.74196
H	-0.05747	2.81584	2.45231
H	1.12299	1.531	2.11856
N	0.59952	2.66816	0.46781
C	1.89217	3.06194	0.14738
C	-0.21218	2.9511	-0.55845
C	1.83267	3.59411	-1.10683
H	2.71814	2.82484	0.82267
H	-1.2676	2.69795	-0.6786
H	2.60845	4.00538	-1.73199
O	-0.64176	-0.08656	2.48633
H	-0.76295	-0.92656	1.99818
C	-0.03169	3.91514	-2.82915
H	-0.07953	5.00495	-2.89331
H	0.61015	3.5309	-3.62436
H	-1.03357	3.4868	-2.92264
C	-4.47475	-2.68554	3.09253
H	-5.52555	-2.96777	3.01725
H	-3.84566	-3.41383	2.5757
H	-4.19252	-2.63367	4.14452
N	-3.31378	0.49456	1.9331
N	0.51545	3.51002	-1.5321
Br	-3.13858	1.90692	-1.84976
Br	3.60314	1.19894	2.38515
C	3.65451	-1.93101	-1.02655
N	3.5464	-2.01938	0.33109
N	4.84284	-1.34148	-1.48363
C	5.24476	-1.59551	-2.85375
H	6.31487	-1.38671	-2.9551
H	5.06954	-2.6432	-3.10835
H	4.71615	-0.96303	-3.58996
C	5.19751	-0.00487	-0.99438
H	4.6927	0.22403	-0.05229
H	6.28047	0.07216	-0.84294
H	4.90326	0.76178	-1.72992
C	2.25178	-2.11814	0.98533
H	2.12024	-3.10307	1.45785
H	2.19663	-1.337	1.75271
H	1.45945	-1.98093	0.2528
C	4.69343	-2.1197	1.2281
H	4.72401	-1.25879	1.90542
H	4.60259	-3.03992	1.82286
H	5.61409	-2.17324	0.64846
N	2.72297	-2.40132	-1.81306
H	2.86365	-2.07429	-2.76569
C	-2.11154	-2.34669	-2.40657
C	-1.07538	-1.22153	-2.19869
H	-0.12122	-1.43186	-2.68023
H	-1.46699	-0.23359	-2.45748
C	-1.66175	-2.09807	-0.17582
O	-1.69135	-2.26429	1.03319
O	-0.84836	-1.22071	-0.76974
O	-2.47543	-2.70552	-1.03482
H	-1.63599	-3.23589	-2.82215
C	-3.35198	-1.92129	-3.16842
H	-3.08998	-1.75248	-4.21845
H	-4.11559	-2.70358	-3.13503
H	-3.75338	-0.98463	-2.76933
O	0.36827	-3.82496	-1.53744
H	0.52855	-4.56072	-0.93573
H	1.24818	-3.35958	-1.59948

TSx3

Charge = 0 Multiplicity = 1

C	4.54135	-1.29021	-1.19839

C	4.01115	-0.03903	-1.11836	C	-3.26969	-1.82366	1.31676
C	2.90117	-1.16628	-2.66932	N	-3.51204	-2.11571	0.02165
N	3.84266	-1.97659	-2.17756	N	-4.29457	-1.22993	2.03496
H	5.33646	-1.75547	-0.63872	C	-4.31651	-1.36625	3.48151
H	4.20791	0.79823	-0.45232	H	-5.34752	-1.2443	3.83084
H	2.15647	-1.42904	-3.40028	H	-3.96601	-2.3596	3.77146
C	2.01125	1.11254	-2.19935	H	-3.70132	-0.60736	3.99582
H	2.41735	1.96054	-1.64098	C	-4.94711	-0.01908	1.51853
H	1.94473	1.369	-3.26114	H	-4.61399	0.21229	0.50107
C	0.6203	0.6676	-1.67895	H	-6.03838	-0.12909	1.52529
H	0.70257	0.46308	-0.60715	H	-4.68496	0.83521	2.1602
C	-0.46368	1.74104	-1.91397	C	-2.43905	-2.23961	-0.96031
H	-0.23574	2.37559	-2.77847	H	-2.40944	-3.25875	-1.36906
H	-1.42328	1.24115	-2.10307	H	-2.62985	-1.51744	-1.76173
N	-0.68624	2.61966	-0.74625	H	-1.48066	-2.01924	-0.499
C	-1.92441	3.1217	-0.36784	C	-4.85681	-2.26938	-0.53177
C	0.24453	3.06185	0.10837	H	-5.0875	-1.42936	-1.19751
C	-1.70945	3.88487	0.7415	H	-4.88659	-3.2039	-1.10679
H	-2.82835	2.80161	-0.88789	H	-5.58778	-2.33213	0.27435
H	1.30823	2.81196	0.15118	N	-2.12171	-2.13427	1.89452
H	-2.39763	4.4456	1.35426	H	-1.96751	-1.64127	2.76699
O	0.23397	-0.50553	-2.36843	C	2.44311	-2.11877	2.4095
H	0.38414	-1.26854	-1.75292	C	1.63664	-0.81748	2.21472
C	0.35011	4.47158	2.14054	H	0.94386	-0.6333	3.04242
H	0.3585	5.55599	2.00093	H	2.26135	0.07015	2.05445
H	-0.15981	4.22652	3.07556	C	1.25764	-2.2732	0.4708
H	1.37448	4.08586	2.1602	O	1.08758	-2.50791	-0.73764
C	3.89713	-3.41834	-2.41112	O	0.8874	-1.0533	1.01131
H	4.92417	-3.76332	-2.28038	O	2.40424	-2.70653	1.09563
H	3.22922	-3.90713	-1.69735	H	1.91377	-2.79837	3.08644
H	3.5734	-3.63155	-3.4315	C	3.88187	-1.91772	2.84797
N	2.98457	0.01721	-2.04925	H	3.90962	-1.49755	3.85978
N	-0.35326	3.83151	1.0253	H	4.41972	-2.87146	2.86217
Br	3.42907	2.52613	1.12236	H	4.39903	-1.22167	2.18006
Br	-4.00859	0.96019	-2.04989	O	0.00224	-3.32682	1.39151

H	-0.09572	-4.07305	0.7795
H	-1.09636	-2.77657	1.52937

y1

Charge = 0 Multiplicity = 1

C	-1.51008	-2.28757	0.49389
C	-0.94018	-1.66804	1.56405
C	0.65888	-2.03828	0.07216
N	-0.49098	-2.49878	-0.41841
H	-2.53566	-2.59193	0.23232
H	-1.36923	-1.31187	2.48559
H	1.65714	-2.11041	-0.35334
C	1.39646	-0.83535	2.13414
H	1.1193	-1.0568	3.16566
H	2.37	-1.2893	1.91491
C	1.48367	0.72939	1.96364
H	1.54526	1.122	2.98204
C	2.79548	1.21629	1.25649
H	3.22692	2.03353	1.83833
H	3.51662	0.39162	1.2023
N	2.68089	1.71505	-0.12915
C	2.9508	0.98872	-1.2758
C	2.21123	2.91409	-0.48101
C	2.62806	1.78733	-2.32922
H	3.37192	-0.01733	-1.19498
H	1.89209	3.68968	0.19494
H	2.69407	1.61318	-3.39062
C	1.66654	4.11857	-2.59139
H	1.43742	4.94374	-1.91753
H	2.42293	4.43961	-3.30991
H	0.75738	3.82215	-3.11803
C	-0.71716	-3.07577	-1.74991
H	-0.89334	-4.14895	-1.6536
H	-1.60878	-2.57515	-2.15002
H	0.16561	-2.89713	-2.36419
N	0.41301	-1.51207	1.2856
N	2.17168	2.98974	-1.81353
Br	4.12619	-1.84568	0.11743
C	-3.66205	3.27279	0.84127
C	-4.25096	2.04192	0.29868
O	-3.0968	1.97405	1.1614
H	-3.0439	3.89261	0.19614
H	-4.12233	3.80323	1.6708
H	-4.02391	1.7904	-0.73843
C	-5.52287	1.45221	0.84584
H	-6.37855	1.79299	0.25418
H	-5.49735	0.3581	0.80674
H	-5.67334	1.76341	1.88226
C	-4.14109	-1.90013	-1.34976
O	-4.0893	-2.94472	-0.64535
O	-5.39619	-1.27381	-1.40187
H	-5.96121	-1.86551	-0.88461
O	-3.23196	-1.30732	-1.96922
C	0.17497	1.26131	1.37582
O	-0.01655	1.45456	0.19695
O	-0.7464	1.42885	2.32808
H	-1.62054	1.63162	1.89418

TSy1

Charge = 0 Multiplicity = 1

C	-0.00474	1.46284	-1.68277
C	-0.16985	0.1804	-1.26229
C	1.95257	0.42939	-1.85583
N	1.32426	1.59633	-2.05641
H	-0.72699	2.26261	-1.68548
H	-1.05739	-0.30378	-0.89923
H	3.02811	0.24202	-1.89833
C	1.4225	-1.82996	-0.99089
H	0.91922	-2.50815	-1.6812
H	2.50842	-1.89261	-1.11272

C	1.06896	-2.23363	0.45238
H	1.4759	-3.25346	0.53033
C	1.79744	-1.46734	1.57352
H	1.62599	-1.98359	2.51842
H	2.86743	-1.4323	1.34514
N	1.3776	-0.05749	1.76295
C	2.17172	1.04724	1.49931
C	0.20366	0.36435	2.26174
C	1.43491	2.14456	1.83743
H	3.16241	0.91757	1.06391
H	-0.60924	-0.28452	2.5471
H	1.67499	3.19435	1.79305
C	-0.94521	2.53208	2.65473
H	-1.47912	2.0745	3.48863
H	-0.58532	3.51544	2.95871
H	-1.59593	2.58599	1.77243
C	1.96017	2.8038	-2.57782
H	1.61144	3.00696	-3.59298
H	1.71545	3.65079	-1.93414
H	3.04035	2.65736	-2.58431
N	1.06252	-0.44683	-1.36813
N	0.21538	1.69802	2.31481
Br	4.69345	-0.49369	-0.34854
C	-4.01239	-0.9072	0.3169
C	-4.15334	-1.6124	-0.94839
O	-3.73241	-2.61691	-0.02272
H	-3.05825	-0.51279	0.62682
H	-4.83376	-0.91428	1.01576
H	-3.40251	-1.36573	-1.71198
C	-5.52577	-1.81592	-1.54889
H	-5.86241	-0.89607	-2.03699
H	-5.5067	-2.62399	-2.28752
H	-6.24355	-2.08184	-0.76762
C	-3.64473	1.97374	-0.12775
O	-2.39143	1.81538	0.00998
O	-4.06871	3.26377	-0.41284
H	-3.25518	3.78532	-0.4537
O	-4.56253	1.13376	-0.03701
C	-0.432	-2.40854	0.74399
O	-1.12976	-2.72844	-0.32689
O	-0.88312	-2.27865	1.8721
H	-2.14221	-2.78245	-0.12111

y2

Charge = 0 Multiplicity = 1

C	4.8877	1.65675	1.97128
C	3.93438	2.07248	1.09076
C	5.05078	0.39173	0.16233
N	5.56682	0.60239	1.37743
H	5.144	2.01673	2.95413
H	3.22668	2.89827	1.09213
H	5.37969	-0.4192	-0.48943
C	3.1386	1.31211	-1.17942
H	2.66464	2.30262	-1.14256
H	3.72755	1.23892	-2.09889
C	2.0728	0.19326	-1.10644
H	1.26173	0.51074	-1.77605
C	2.66754	-1.14173	-1.63305
H	2.74979	-1.10693	-2.72467
H	3.66353	-1.36256	-1.23841
N	1.8596	-2.31416	-1.2572
C	2.37709	-3.5513	-0.90199
C	0.53816	-2.32401	-1.07568
C	1.3199	-4.31687	-0.50899
H	3.4534	-3.71937	-0.90887
H	-0.14262	-1.48318	-1.15906
H	1.28108	-5.3323	-0.14994
C	-1.18593	-3.87832	-0.23995
H	-1.75562	-2.95147	-0.15205
H	-1.63942	-4.5327	-0.98912

H	-1.17353	-4.3859	0.72642
C	6.65147	-0.19727	1.95024
H	7.59723	0.34722	1.88869
H	6.41956	-0.40866	2.99582
H	6.71118	-1.1343	1.38666
N	4.05784	1.26957	-0.03199
N	0.18136	-3.53024	-0.61947
Br	5.95111	-2.83975	-0.73588
C	-3.17102	2.07951	0.50594
H	-4.00663	1.479	0.86272
C	-2.6609	2.98397	1.62696
H	-3.46561	3.62989	1.99652
H	-2.30803	2.36668	2.45909
H	-1.84969	3.62013	1.25673
C	-5.12368	1.50907	-1.90058
O	-6.00159	1.50902	-1.04085
O	-5.26697	0.8861	-3.08587
H	-6.15757	0.50651	-3.08119
O	-3.94614	2.08152	-1.85344
O	-2.12052	1.19702	0.07712
C	-2.08158	-0.10852	0.52575
O	-3.06406	-0.60352	1.13587
O	-0.99818	-0.68468	0.25446
C	-3.60294	2.91042	-0.6961
H	-2.78506	3.55066	-1.04151
H	-4.47071	3.52186	-0.43745
C	-6.52022	-0.97959	1.93149
N	-5.68664	-0.35721	1.11966
H	-6.02748	0.31998	0.43643
H	-4.63301	-0.47768	1.14419
N	-6.06609	-1.57529	3.06405
N	-7.85401	-1.04047	1.64166
C	-8.31656	-0.74757	0.28552
H	-9.27802	-1.24494	0.13439
H	-8.44395	0.32799	0.10924
H	-7.60297	-1.13656	-0.44162
C	-8.87057	-0.9125	2.68806
H	-9.56469	-1.75949	2.67033
H	-8.39793	-0.85799	3.66733
H	-9.44411	0.00891	2.53256
C	-6.6164	-2.84563	3.53825
H	-5.83119	-3.60991	3.51817
H	-6.9866	-2.7585	4.56547
H	-7.42919	-3.17238	2.89115
C	-4.75186	-1.21661	3.6127
H	-3.93762	-1.75694	3.12077
H	-4.5714	-0.1508	3.47636
H	-4.76129	-1.44329	4.68162
Br	2.35894	4.62135	-0.47368
C	1.4441	0.10626	0.30356
O	1.06792	-0.97	0.98895
O	1.37211	1.22012	0.88163
H	0.14804	-0.64294	1.23525

TSy2

Charge = 0 Multiplicity = 1

C	2.24233	-3.67131	-2.03685
C	1.38092	-2.7803	-1.47292
C	3.2849	-2.71365	-0.3361
N	3.42412	-3.60957	-1.31456
H	2.11917	-4.33483	-2.87696
H	0.3487	-2.52776	-1.6842
H	4.10124	-2.45807	0.34788
C	1.52774	-1.0769	0.39064
H	0.47468	-0.97456	0.1109
H	1.55762	-1.36988	1.44507
C	2.26215	0.27692	0.21455
H	1.55112	1.02092	0.58134
C	3.53398	0.32987	1.08967
H	3.25099	0.29786	2.14659

H	4.22975	-0.49527	0.90649	H	-1.64553	0.22837	1.74689
N	4.33965	1.54724	0.86638	H	-1.62866	1.87959	2.45739
C	5.70354	1.54933	0.61659	C	-5.8926	-1.2268	0.74609
C	3.88247	2.80535	0.83706	N	-4.88351	-0.49191	0.30722
C	6.06128	2.85198	0.43637	H	-4.95763	0.50909	0.09068
H	6.25788	0.61156	0.59639	H	-3.98927	-0.94034	0.02435
H	2.84448	3.11799	0.92924	N	-7.17371	-0.78096	0.69888
H	7.01897	3.2949	0.21677	N	-5.65279	-2.45478	1.29073
C	4.80057	5.06707	0.41596	C	-6.47731	-3.61035	0.93749
H	5.32973	5.57569	1.22505	H	-5.86901	-4.33736	0.38683
H	5.22649	5.36231	-0.54478	H	-6.87789	-4.10055	1.83217
H	3.74438	5.33669	0.43789	H	-7.30447	-3.30531	0.29755
C	4.66798	-4.34096	-1.57163	C	-4.3403	-2.7747	1.86529
H	4.54587	-5.39415	-1.30728	H	-3.94035	-1.89406	2.36941
H	4.91864	-4.25297	-2.63036	H	-4.48567	-3.56889	2.60366
H	5.45667	-3.88414	-0.96564	H	-3.61131	-3.08608	1.10894
N	2.05211	-2.1955	-0.40973	C	-8.15819	-1.16629	1.70737
N	4.91217	3.61742	0.57355	H	-8.57226	-0.26065	2.16493
Br	6.31748	-1.96052	0.93996	H	-8.98557	-1.73334	1.26541
C	-4.84516	2.52189	-1.59346	H	-7.68911	-1.76593	2.4861
O	-5.79143	1.94923	-2.13113	C	-7.57842	0.32757	-0.16758
O	-4.21919	3.55481	-2.24695	H	-7.65979	1.25975	0.40513
H	-4.67371	3.62051	-3.09954	H	-6.86886	0.49368	-0.97839
O	-4.35118	2.2587	-0.4267	H	-8.56091	0.09647	-0.59165
C	-1.93712	1.79966	0.31282	Br	-1.9653	-1.73497	-0.60106
C	-2.67634	3.10908	0.11673	C	2.61086	0.60345	-1.25288
H	-2.25682	1.06705	-0.42777	O	3.25854	-0.15366	-1.94374
H	-2.6017	3.64607	-0.81404	O	2.22371	1.79693	-1.70745
H	-3.2108	3.57648	0.9272	H	1.71086	2.32013	-1.04254
C	-0.11935	3.27989	0.34913				
O	1.11179	3.48883	0.22176	**y3**			
O	-1.02408	4.07521	0.71774	Charge =	0 Multiplicity = 1		
O	-0.53735	2.01227	0.02009	C	4.79577	0.58097	1.97814
C	-2.0942	1.22371	1.71502	C	4.25874	-0.47425	1.30261
H	-3.15574	1.1221	1.95865	C	3.14923	-0.23313	3.20498

N	4.09463	0.71257	3.16621	H	-7.8119	2.3582	-2.84808
H	5.59419	1.25523	1.71016	H	-6.49547	3.54475	-2.96621
H	4.43442	-0.8626	0.30301	H	-6.44191	2.03964	-3.93021
H	2.41529	-0.36261	3.98412	C	-6.51643	0.44687	-1.60408
C	2.26481	-2.01028	1.71101	H	-5.85281	-0.07551	-0.91156
H	2.73061	-2.6231	0.93571	H	-7.53604	0.43118	-1.19894
H	2.0668	-2.62568	2.59381	H	-6.51635	-0.11056	-2.55563
C	0.95437	-1.35807	1.20749	C	-2.91083	1.82149	0.03106
H	1.18434	-0.82506	0.27907	H	-2.56049	2.77493	0.45721
C	-0.12823	-2.43475	0.95487	H	-2.73953	1.01433	0.74965
H	0.18409	-3.42315	1.3122	H	-2.33884	1.62345	-0.87493
H	-1.05177	-2.16484	1.48508	C	-5.21754	1.76067	0.8712
N	-0.49299	-2.57274	-0.47007	H	-5.20684	0.73974	1.27127
C	-1.78687	-2.72221	-0.94881	H	-4.87085	2.453	1.6526
C	0.36287	-2.61622	-1.49933	H	-6.23362	2.03904	0.58917
C	-1.68596	-2.85595	-2.30277	N	-3.94823	2.78164	-2.38266
H	-2.63292	-2.68279	-0.25853	H	-4.3329	2.77219	-3.32532
H	1.4405	-2.44776	-1.47603	C	1.37567	3.27031	-3.17588
H	-2.4482	-2.98589	-3.05545	C	0.4639	2.03533	-3.32297
C	0.25896	-2.83896	-3.96286	H	-0.49562	2.27874	-3.77805
H	0.14843	-3.84462	-4.37795	H	0.96139	1.19688	-3.81791
H	-0.23643	-2.11477	-4.61458	C	0.93997	2.36234	-1.11485
H	1.31768	-2.58357	-3.87358	O	0.95839	2.17951	0.09215
C	4.25572	1.79324	4.13831	O	0.20742	1.62836	-1.95603
H	5.31596	1.9185	4.36881	O	1.67465	3.28052	-1.74193
H	3.8475	2.71821	3.7225	H	0.81362	4.18605	-3.36734
H	3.71676	1.53537	5.05136	C	2.67061	3.20599	-3.96299
N	3.2366	-0.97479	2.09333	H	2.44434	3.20697	-5.03651
N	-0.33845	-2.78041	-2.62721	H	3.29869	4.07724	-3.74884
Br	3.45916	-1.30066	-1.9748	H	3.22359	2.28968	-3.73138
Br	-3.62691	-2.1646	1.87188	O	-1.5532	4.2028	-2.42357
C	-4.75154	2.17721	-1.54096	H	-1.75779	5.08203	-2.07373
N	-4.329	1.86283	-0.28289	H	-2.41011	3.68893	-2.3356
N	-6.07821	1.83034	-1.82869	C	0.44791	-0.3759	2.28007
C	-6.72767	2.47605	-2.95482	O	0.24886	-0.54898	3.48173

O	0.19664	0.85691	1.77168
H	-0.24957	1.6622	1.36681

TSy3

Charge = 0 Multiplicity = 1

C	4.01892	-2.51746	0.10539
C	3.7475	-1.21198	-0.16611
C	2.93703	-2.44306	-1.81854
N	3.50842	-3.26944	-0.93699
H	4.49912	-2.97274	0.95525
H	3.95774	-0.28573	0.3622
H	2.43974	-2.74081	-2.72746
C	2.45738	0.02095	-1.96762
H	2.88433	0.85774	-1.4055
H	2.75394	0.074	-3.0185
C	0.91398	-0.0022	-1.86324
H	0.62431	-0.09531	-0.81397
C	0.28877	1.28918	-2.44287
H	0.84842	1.65544	-3.30656
H	-0.74455	1.08811	-2.75332
N	0.19877	2.37498	-1.44567
C	-0.96389	2.70035	-0.7607
C	1.19175	3.17051	-1.02179
C	-0.64242	3.72168	0.08054
H	-1.89572	2.17566	-0.98924
H	2.23573	3.11055	-1.28681
H	-1.24911	4.27825	0.77585
C	1.51078	4.95721	0.66731
H	1.74002	5.83445	0.05785
H	0.94032	5.26534	1.54366
H	2.42912	4.44403	0.97326
C	3.41929	-4.72696	-0.9718
H	4.37347	-5.15754	-0.66449
H	2.6244	-5.0503	-0.29604
H	3.18949	-5.04949	-1.98747
N	3.06845	-1.18742	-1.37158
N	0.70333	4.00214	-0.09484
Br	3.7763	2.17795	0.69456
Br	-3.31375	0.78853	-2.34623
C	-3.92543	-0.89757	1.56334
N	-3.97202	-1.58285	0.40371
N	-4.9938	-0.05198	1.84183
C	-5.29631	0.25581	3.22984
H	-6.34128	0.57372	3.29862
H	-5.16261	-0.63146	3.8518
H	-4.6775	1.07301	3.63958
C	-5.32241	1.02343	0.8941
H	-4.77168	0.90925	-0.04447
H	-6.39812	1.04488	0.68556
H	-5.03927	1.99318	1.32812
C	-2.77179	-2.1189	-0.23656
H	-2.95053	-3.15913	-0.53047
H	-2.56407	-1.51404	-1.12593
H	-1.92494	-2.08913	0.44101
C	-5.18305	-1.71734	-0.40477
H	-5.10649	-1.09421	-1.30321
H	-5.27665	-2.767	-0.70636
H	-6.05854	-1.4419	0.18088
N	-2.94572	-1.06436	2.43675
H	-2.93026	-0.34111	3.1449
C	1.46532	-0.59854	3.34194
C	0.80771	0.43292	2.40648
H	0.01668	1.00809	2.89705
H	1.55029	1.10348	1.95835
C	0.64849	-1.68214	1.51852
O	0.68593	-2.45489	0.5452
O	0.23317	-0.36872	1.35847
O	1.65043	-1.72172	2.45783
H	0.76491	-0.91451	4.12335
C	2.79532	-0.1627	3.92949

H	2.6267	0.60608	4.69135
H	3.29603	-1.00695	4.41247
H	3.44645	0.26622	3.16195
O	-0.76966	-2.25025	2.58781
H	-0.80089	-3.19864	2.40547
H	-1.87781	-1.73553	2.42662
C	0.41137	-1.19846	-2.68639
O	0.54002	-1.2128	-3.89527
O	-0.05765	-2.25199	-2.01986
H	0.05978	-2.17543	-1.03245

z2

Charge = 0 Multiplicity = 1

C	4.3711	-2.97372	-2.05909
C	3.32989	-2.78427	-1.20033
C	5.07644	-1.64965	-0.43247
N	5.44859	-2.25049	-1.56695
H	4.44348	-3.55607	-2.9638
H	2.3275	-3.2023	-1.13888
H	5.73505	-0.98604	0.12996
C	2.95099	-1.4079	0.88046
H	2.06616	-2.05678	0.91979
H	3.49084	-1.50136	1.82866
C	2.54986	0.06245	0.60445
H	1.65686	0.24916	1.21759
C	3.68423	1.01196	1.07452
H	3.71528	1.04318	2.16962
H	4.67613	0.70941	0.72606
N	3.52638	2.38708	0.57126
C	4.57365	3.21029	0.18321
C	2.36929	2.99907	0.31379
C	4.01139	4.35018	-0.30881
H	5.60194	2.85604	0.24071
H	1.36842	2.58116	0.39501
H	4.46262	5.23842	-0.72179
O	2.26383	0.2498	-0.75611
H	1.35433	0.63728	-0.82747
C	1.60249	5.11752	-0.69144
H	0.65985	4.56839	-0.73959
H	1.50958	5.96897	-0.0108
H	1.86348	5.47566	-1.69013
C	6.77981	-2.11139	-2.16049
H	7.36622	-3.01895	-1.99048
H	6.67264	-1.94034	-3.2343
H	7.26689	-1.24804	-1.69406
N	3.79585	-1.95656	-0.1914
N	2.63425	4.19623	-0.22329
Br	7.26464	0.88362	0.15001
C	-2.07131	-1.02751	-0.04367
H	-2.97202	-0.41229	-0.09478
C	-2.14138	-2.18204	-1.04124
H	-3.02033	-2.81048	-0.84348
H	-2.22042	-1.78331	-2.05848
H	-1.24892	-2.8128	-0.95511
C	-2.50392	0.29333	2.73942
O	-3.70571	0.23297	2.48715
O	-1.98554	1.211	3.57259
H	-2.73209	1.76721	3.85035
O	-1.54942	-0.50185	2.32163
O	-0.96117	-0.19847	-0.39648
C	-1.08163	1.17832	-0.2314
O	-2.15505	1.66066	0.18604
O	-0.02063	1.78196	-0.55377
C	-1.87922	-1.56433	1.37642
H	-1.0215	-2.24331	1.41288
H	-2.77784	-2.08005	1.72821
Br	0.60328	-4.10694	0.5217
C	-8.02596	0.2041	-1.64079
C	-7.86222	-1.31652	-1.73054
C	-5.99525	-0.76674	0.42164

C	-8.05926	-2.05146	-0.39609
C	-7.38057	-1.33471	0.78008
H	-8.88427	0.46531	-1.00562
H	-5.46627	-1.4501	-0.25595
H	-6.87947	-1.53862	-2.16259
H	-7.6585	-3.06764	-0.49258
H	-8.24913	0.58888	-2.63886
H	-8.59713	-1.68072	-2.45786
H	-5.37292	-0.69485	1.31526
H	-9.13039	-2.15978	-0.18544
H	-7.25855	-2.03139	1.6158
H	-8.01919	-0.52627	1.15887
C	-6.7544	2.33902	-1.76444
H	-7.45199	2.99824	-1.22917
H	-7.0934	2.27658	-2.80215
C	-5.3319	2.88412	-1.69979
H	-4.6795	2.3028	-2.36072
H	-5.32265	3.92062	-2.04997
C	-5.99457	0.61068	-0.21227
N	-5.08026	1.44923	0.2437
H	-4.39856	1.08473	0.92065
N	-6.84005	0.9759	-1.19324
C	-4.81637	2.79706	-0.27261
H	-5.31693	3.52796	0.376
H	-3.73384	2.93207	-0.21146

TSz2

Charge = 0 Multiplicity = 1

C	-2.52008	-3.21989	1.7161
C	-1.7657	-2.47219	0.86273
C	-3.85031	-2.49687	0.10237
N	-3.81909	-3.21458	1.22904
H	-2.25267	-3.75157	2.61533
H	-0.70391	-2.25797	0.81168
H	-4.77139	-2.29602	-0.44915
C	-2.2366	-1.08253	-1.19218
H	-1.14528	-1.13519	-1.26452
H	-2.66337	-1.42502	-2.14045
C	-2.69452	0.35853	-0.85129
H	-2.0556	1.02655	-1.44619
C	-4.16887	0.5676	-1.28542
H	-4.23376	0.62564	-2.37803
H	-4.83648	-0.23631	-0.95877
N	-4.7611	1.78967	-0.71501
C	-6.06769	1.89189	-0.26085
C	-4.12022	2.9333	-0.46124
C	-6.20006	3.14137	0.26747
H	-6.7364	1.03419	-0.31368
H	-3.06449	3.1355	-0.60024
H	-7.04461	3.62541	0.73176
O	-2.52739	0.60796	0.51796
H	-1.98734	1.43305	0.60841
C	-4.60493	5.10703	0.61273
H	-5.022	5.87508	-0.04455
H	-4.98699	5.24547	1.6265
H	-3.51561	5.17608	0.6267
C	-5.00085	-3.84314	1.82561
H	-4.99985	-4.91777	1.62279
H	-4.98379	-3.67258	2.90441
H	-5.88732	-3.3705	1.38827
N	-2.6164	-2.03573	-0.13971
N	-4.97164	3.77359	0.13787
Br	-7.04361	-1.53725	-0.38143
C	5.18473	3.49293	0.78292
O	6.37896	3.19665	0.77241
O	4.79167	4.79479	0.94797
H	5.61884	5.29895	1.03005
O	4.20113	2.66216	0.64727
C	1.87688	1.97178	-0.00846
C	2.42899	3.3428	0.35185

H	2.34705	1.2306	0.63529
H	2.36029	3.7103	1.3634
H	2.79073	4.02545	-0.39821
C	-0.14631	3.12102	0.22353
O	-1.39279	3.09759	0.34389
O	0.60653	4.11491	0.02391
O	0.48193	1.9076	0.33777
C	2.07665	1.59524	-1.47141
H	3.13953	1.65967	-1.72885
H	1.73723	0.56595	-1.62745
H	1.52038	2.28005	-2.12171
Br	1.27709	-2.16485	-0.93134
C	3.89947	-3.52406	1.75145
C	4.83756	-4.0706	0.66929
C	4.79868	-3.26322	-0.63206
C	4.22383	-2.09242	2.19662
C	4.01662	-1.02328	1.10084
C	5.1204	-0.91796	0.08429
H	2.87293	-3.54331	1.3625
H	5.8717	-4.12866	1.03936
H	3.76231	-3.04763	-0.92563
H	5.24627	-2.03287	2.59659
H	3.9291	-0.0396	1.56968
H	3.93465	-4.18663	2.62587
H	4.53336	-5.09553	0.42131
H	5.25527	-3.83966	-1.44094
H	3.55486	-1.82435	3.02278
H	3.06861	-1.22084	0.56832
C	6.69501	-1.88202	-1.52368
H	6.30653	-1.80871	-2.54863
H	7.26026	-2.81702	-1.4534
C	7.59013	-0.68944	-1.19675
H	8.13317	-0.87517	-0.26282
H	8.33091	-0.55999	-1.99171
C	6.73393	0.56292	-1.0498
H	6.3044	0.85782	-2.01688
H	7.28612	1.41614	-0.65198
N	5.55888	-1.98606	-0.5896
N	5.66034	0.27889	-0.10098
H	5.23667	1.08785	0.37049

z3

Charge = 0 Multiplicity = 1

C	4.16259	-2.45273	-1.50037
C	3.92136	-1.11279	-1.53358
C	2.34072	-2.13207	-2.70429
N	3.17125	-3.07207	-2.24339
H	4.93882	-3.01625	-1.0078
H	4.40043	-0.27208	-1.03511
H	1.43823	-2.30428	-3.26557
C	2.03337	0.32399	-2.47076
H	2.71948	1.1317	-2.20585
H	1.7598	0.40939	-3.52655
C	0.7546	0.3232	-1.59207
H	1.05656	0.34773	-0.54208
C	-0.16932	1.51463	-1.89035
H	-0.17102	1.76786	-2.95675
H	-1.20367	1.25712	-1.61566
N	0.162	2.73832	-1.13097
C	-0.73079	3.78326	-0.92954
C	1.31141	3.02109	-0.50572
C	-0.07913	4.70796	-0.16861
H	-1.76486	3.68896	-1.26059
H	2.20496	2.40268	-0.40775
H	-0.41199	5.65579	0.22398
O	0.02513	-0.86219	-1.86512
H	0.19259	-1.48145	-1.11943
C	2.24482	4.84534	0.88644
H	2.5928	5.7543	0.38828
H	1.84827	5.09733	1.87317

H	3.06909	4.13261	0.98569
C	2.92288	-4.51128	-2.29957
H	3.87407	-5.03753	-2.39804
H	2.41087	-4.81711	-1.38346
H	2.29737	-4.73536	-3.16514
N	2.77742	-0.93433	-2.29546
N	1.19038	4.21462	0.08796
Br	4.29403	1.66219	0.4656
Br	-3.58712	2.01782	-1.27407
C	2.65327	-1.59621	3.02111
C	1.88615	-0.3323	2.57763
H	1.11629	-0.04286	3.29048
H	2.54937	0.49315	2.3047
C	1.54743	-2.00153	1.05761
O	1.14969	-2.57466	0.05573
O	1.21705	-0.7469	1.36377
O	2.41235	-2.529	1.92278
H	2.18767	-2.04816	3.89884
C	4.14668	-1.38884	3.19777
H	4.32417	-0.77521	4.08879
H	4.65998	-2.34569	3.33755
H	4.56866	-0.85671	2.3383
O	-0.48359	-1.98421	3.23878
H	-1.02741	-2.51501	3.83888
H	-1.1604	-1.43322	2.7371
C	-5.29346	-1.082	-0.45105
C	-3.25202	-1.16937	1.07826
C	-4.53715	-1.72387	-1.61135
C	-2.64788	-2.41782	0.44293
C	-4.20019	-3.20852	-1.41639
C	-3.63116	-3.50002	-0.01946
H	-6.17141	-1.6917	-0.17888
H	-2.02114	-2.09837	-0.40016
H	-3.64506	-1.11697	-1.79996
H	-3.47159	-3.51035	-2.18199
H	-5.66086	-0.11493	-0.81136
H	-5.16538	-1.60915	-2.50385
H	-1.95275	-2.81084	1.19001
H	-5.09561	-3.82295	-1.5843
H	-3.127	-4.47494	-0.02091
H	-4.44849	-3.58049	0.70898
C	-5.17556	0.305	1.53222
H	-6.21185	-0.00266	1.73494
H	-5.19791	1.19571	0.89088
C	-4.43845	0.61899	2.82774
H	-4.61063	-0.16234	3.57986
H	-4.81426	1.56409	3.23807
C	-2.94704	0.69009	2.4988
H	-2.35003	0.92159	3.38951
H	-2.78231	1.48467	1.75535
N	-2.48556	-0.58048	1.95048
N	-4.5283	-0.77723	0.7717

TSz3

Charge = 0 Multiplicity = 1

C	3.87245	-2.62778	-1.31733
C	3.75855	-1.27326	-1.39491
C	2.10228	-2.17792	-2.55438
N	2.8359	-3.1762	-2.05473
H	4.58619	-3.24603	-0.79711
H	4.31826	-0.46132	-0.93169
H	1.19016	-2.28274	-3.1158
C	2.02089	0.30378	-2.3902
H	2.77491	1.04783	-2.11921
H	1.77868	0.39764	-3.45328
C	0.72731	0.42032	-1.54092
H	1.00479	0.38969	-0.48497
C	-0.06713	1.7061	-1.8202
H	-0.01493	1.99927	-2.87533
H	-1.12159	1.5282	-1.56551

N	0.35338	2.86224	-1.00048
C	-0.47314	3.93963	-0.71066
C	1.53861	3.05085	-0.40588
C	0.25342	4.78854	0.06958
H	-1.52116	3.92147	-0.99783
H	2.40733	2.38834	-0.37856
H	-0.01365	5.7299	0.52324
O	-0.11233	-0.67837	-1.85232
H	-0.00795	-1.34192	-1.12224
C	2.61573	4.7538	1.03891
H	2.9587	5.69339	0.59753
H	2.27998	4.93089	2.06392
H	3.42526	4.01706	1.03044
C	2.42412	-4.57801	-2.03026
H	3.31199	-5.21237	-2.00966
H	1.81068	-4.74055	-1.1402
H	1.84521	-4.80036	-2.92854
N	2.64463	-1.01351	-2.17825
N	1.50277	4.21696	0.25044
Br	4.56962	1.65018	0.24849
Br	-3.43282	2.29309	-0.75698
C	2.5071	-2.1241	2.80817
C	2.19245	-0.67782	2.35394
H	1.64721	-0.12154	3.12102
H	3.06674	-0.10633	2.02247
C	1.07319	-2.17801	1.03233
O	0.58361	-2.59769	-0.02301
O	1.34653	-0.84979	1.20772
O	1.96974	-2.93069	1.73781
H	1.94252	-2.36789	3.71309
C	3.98445	-2.42801	2.98302
H	4.39229	-1.83855	3.81202
H	4.14063	-3.48801	3.20923
H	4.54326	-2.16922	2.0777
O	-0.38888	-2.20501	2.37657
H	-0.65599	-3.13758	2.3995
H	-1.36343	-1.55145	1.95889
C	-5.49565	-0.59725	-0.29119
C	-3.28613	-1.15488	0.82497
C	-4.99968	-1.02679	-1.66911
C	-2.89218	-2.25089	-0.15068
C	-4.78139	-2.53604	-1.83839
C	-4.02552	-3.15442	-0.65221
H	-6.37193	-1.19006	0.0147
H	-2.38027	-1.77191	-0.99478
H	-4.09818	-0.44455	-1.88753
H	-4.21768	-2.7087	-2.76517
H	-5.81007	0.4472	-0.38096
H	-5.75097	-0.68621	-2.39271
H	-2.12003	-2.8364	0.3543
H	-5.74596	-3.04637	-1.96414
H	-3.60883	-4.12637	-0.94381
H	-4.72004	-3.35781	0.17331
C	-4.91976	0.35821	1.8681
H	-5.95627	0.125	2.14548
H	-4.8906	1.35683	1.41473
C	-4.0056	0.30751	3.08575
H	-4.18903	-0.59617	3.68077
H	-4.21011	1.17451	3.724
C	-2.56364	0.30722	2.58321
H	-1.84184	0.22336	3.40173
H	-2.3675	1.23193	2.02351
N	-2.35813	-0.83045	1.69403
N	-4.51979	-0.60173	0.82049

z4

Charge = 0 Multiplicity = 1

C	-4.14727	-0.50585	1.09302
C	-4.57137	-0.91967	-0.33861
H	-4.55763	0.47879	1.35522

H	-4.44032	-1.23205	1.85586
O	-3.38253	-0.72887	-1.11725
O	-2.72617	-0.46613	1.02716
C	-2.4242	-0.08742	-0.33719
O	-1.19031	-0.56224	-0.6731
H	-2.10173	1.70285	0.29061
H	-0.51108	0.13066	-0.49527
H	-0.30264	1.49429	1.39131
O	-1.12545	1.80286	1.8303
H	-1.5909	0.97913	2.05346
H	-4.80601	-1.99106	-0.377
O	-2.55867	1.28916	-0.47902
C	-5.73099	-0.10814	-0.89731
H	-5.95403	-0.41177	-1.92383
H	-6.63334	-0.2585	-0.29277
H	-5.47564	0.95502	-0.89752
C	1.94518	-1.95793	1.21292
C	3.40991	-2.40751	1.27113
C	4.40683	-1.48063	0.5634
C	1.67794	-0.55335	1.79795
C	4.42432	-0.04358	1.11177
C	2.03023	0.58115	0.85554
H	1.5665	-1.98889	0.18485
H	3.71077	-2.49672	2.32525
H	4.20299	-1.44444	-0.5145
H	4.40818	-0.06383	2.2096
H	2.20973	-0.43483	2.75104
H	1.33709	-2.67432	1.77569
H	3.49355	-3.41458	0.84547
H	5.4155	-1.89721	0.67729
H	0.61134	-0.45902	2.00194
H	5.3628	0.43986	0.82918
C	3.74752	1.9046	-0.30817
H	4.68454	2.33697	0.05938
H	3.95011	1.4945	-1.30859
C	1.31418	2.30031	-0.6393
H	1.28813	1.88357	-1.65653
H	0.49809	3.02764	-0.58327
C	2.66085	2.97247	-0.38067
H	2.90234	3.69445	-1.16722
H	2.62117	3.51865	0.56872
N	1.03432	1.23362	0.32368
N	3.35338	0.82631	0.60876

TSz4

Charge = 0 Multiplicity = 1

C	3.31997	0.57784	1.31023
C	2.96838	-0.91251	1.48787
C	3.70731	-0.21912	-0.82167
H	2.41382	1.13993	1.03805
H	1.9914	-1.03244	1.97952
H	3.72947	-1.40416	2.11303
O	4.21427	0.56464	0.20305
O	2.97125	-1.45731	0.19192
O	4.75946	-0.85434	-1.418
H	4.48354	-0.96632	-2.33847
O	2.78064	0.23846	-1.58164
H	1.67868	-0.66539	-1.62953
C	4.00789	1.22849	2.49512
H	4.26251	2.26888	2.27501
H	3.35011	1.2138	3.371
H	4.92934	0.69243	2.74092
O	1.01245	-1.39801	-1.23357
H	1.72984	-1.60141	-0.4575
H	0.22078	-0.84317	-0.85364
C	-3.837	1.17095	1.62725
C	-3.21805	1.45837	3.00624
C	-2.61805	0.22612	3.69623
C	-1.49597	-0.47536	2.91991
C	-1.89086	0.14528	0.46409

C	-1.89614	-0.95379	1.50726	C	-2.23564	1.72617	-1.77399
H	-4.4394	0.25346	1.67466	H	-2.15923	2.57452	-2.46117
H	-2.46164	2.2462	2.89629	H	-2.83869	0.95523	-2.2667
H	-3.42603	-0.49752	3.87631	C	-0.85767	1.15879	-1.44057
H	-0.62113	0.18192	2.83629	H	-0.38033	0.71777	-2.32184
H	-4.52949	1.97634	1.37042	H	-0.19373	1.96545	-1.0949
H	-4.00576	1.86903	3.65011	C	-2.92423	2.16544	-0.48482
H	-2.24367	0.51582	4.68524	H	-3.97541	2.40675	-0.67672
H	-1.16878	-1.34873	3.4952	H	-2.44984	3.07546	-0.08821
H	-1.18577	-1.70577	1.15951	N	-0.93086	0.12317	-0.40917
H	-2.88077	-1.43715	1.54385	N	-2.87942	1.09257	0.5181

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