Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Theoretical study on the hypervalent λ3-bromane strategy for Baeyer-Villiger Oxidation of benzaldehyde and acetaldehyde: rearrangement mechanism

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Supporting Information

Table of Contents

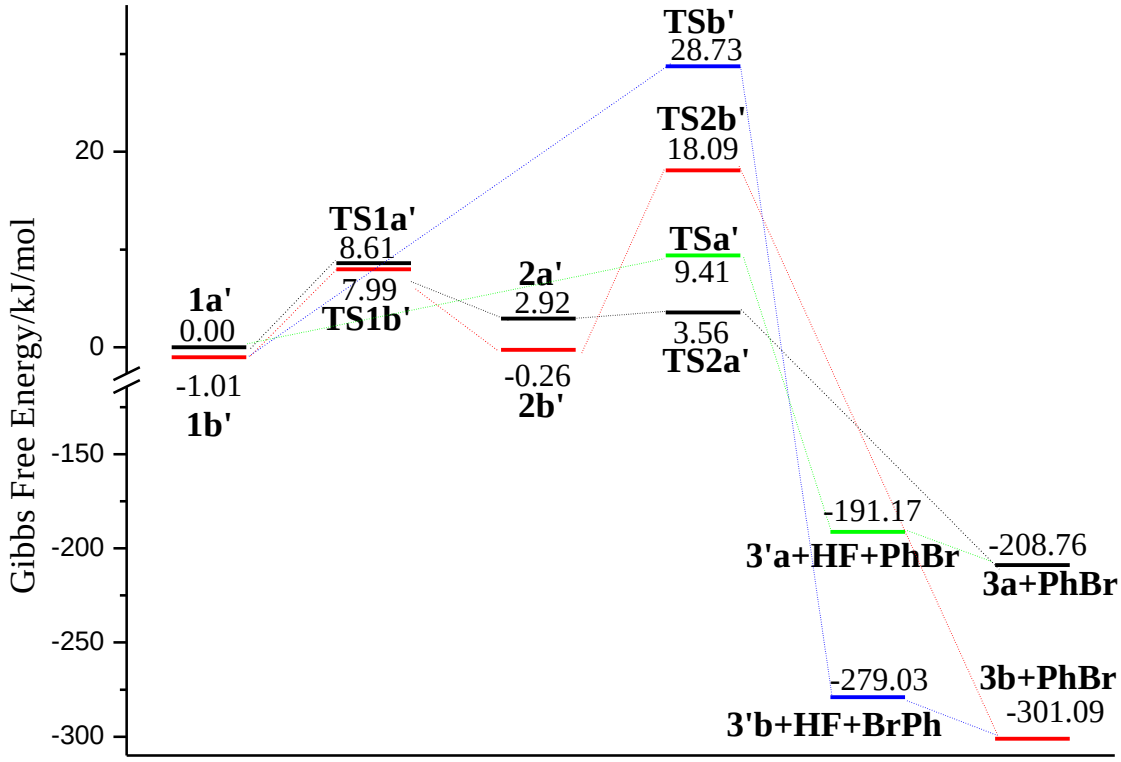

Fig. S1 Reaction profile for the group migration of protonated syn-α-hydroxybenzyloxy-λ^3-bromane: phenyl migration (stepwise mechanism in black line and concerted mechamism in green line) and H migration (stepwise mechanism in red line and concerted mechanism in blue line), using DFT (B3LYP/6-31++G**) method.

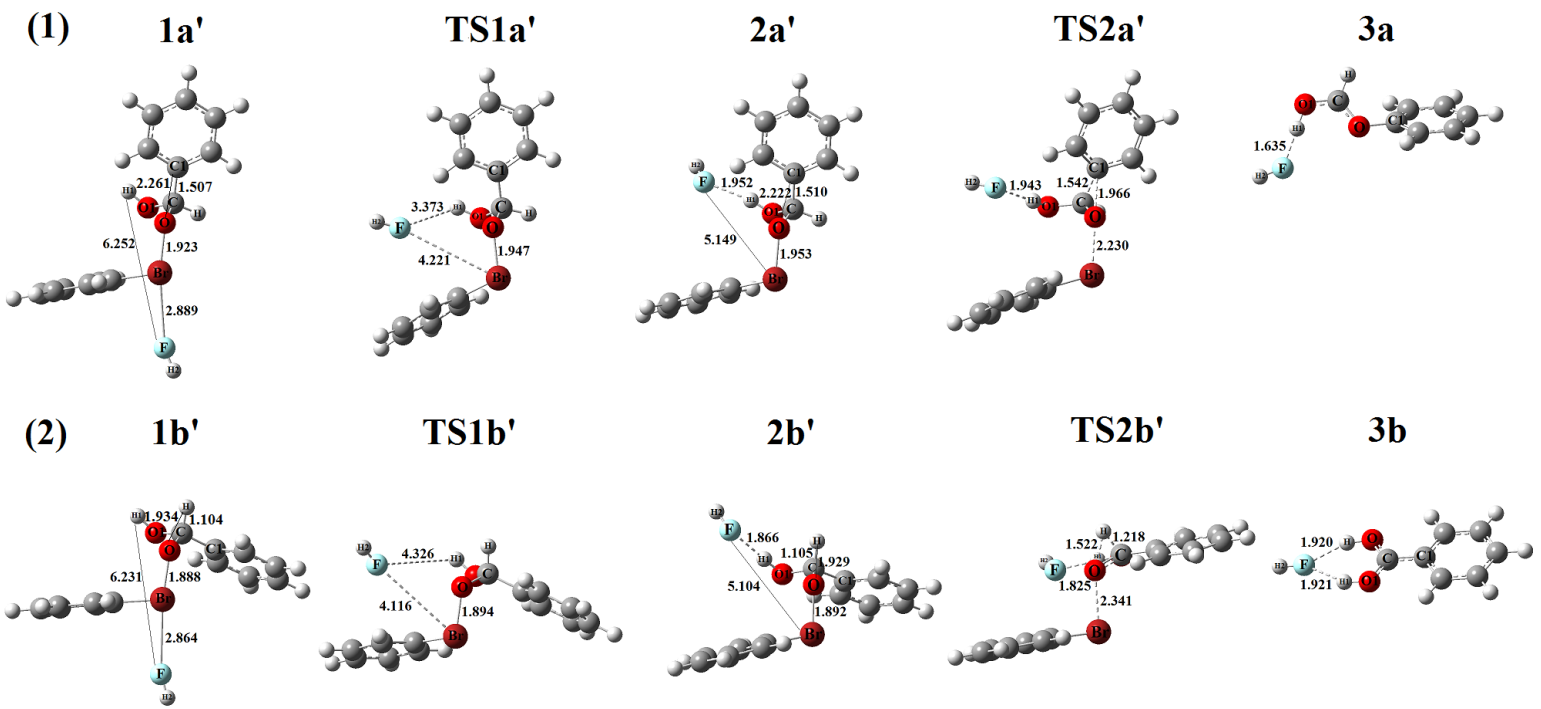

Fig. S2 Structures of intermediates, transition states, and products of stepwise mechanism of protonated syn-α-hydrobenzyloxy-λ^3-bromane, using DFT (B3LYP/6-31++G**) method: phenyl migration (above) and hydrogen migration (below). 1a'(1b'): protonated syn-α-hydroxybenzyloxy-λ^3-bromane, 3a(3b): complex of HF and protonated PhOOCH (PhCOOH). The distances are in Å.

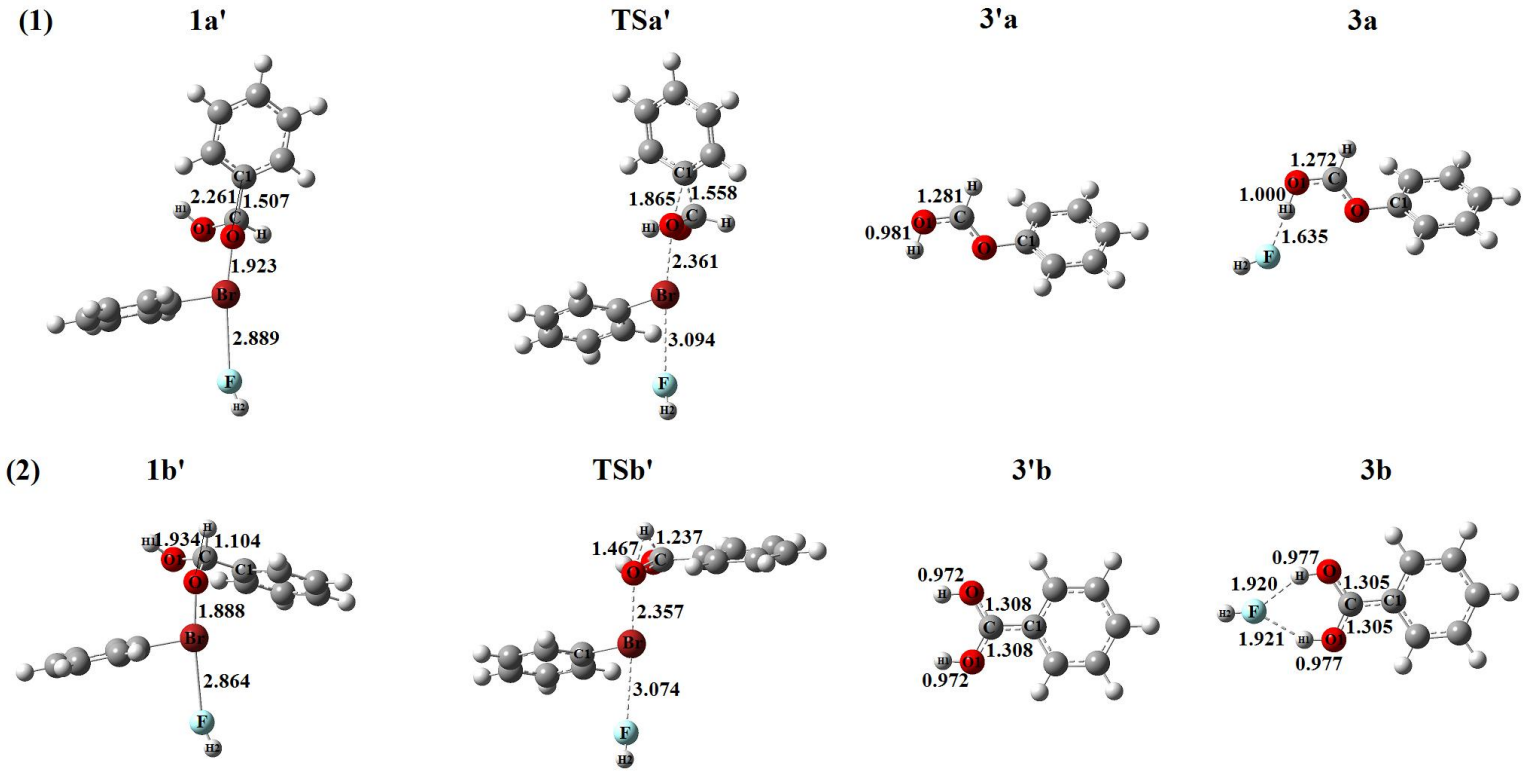

Fig. S3 Structures of intermediates, transition states, and products of concerted mechanism of protonated syn-α-hydroxybenzyloxy-λ^3-bromane, using DFT (B3LYP/6-31++G**) method: phenyl migration (above) and hydrogen migration (below). 1a'(1b'): protonated syn-α-hydroxybenzyloxy-λ^3-bromane, 3a(3b): complex of HF and protonated PhOOCH (PhCOOH).The distances are in Å.

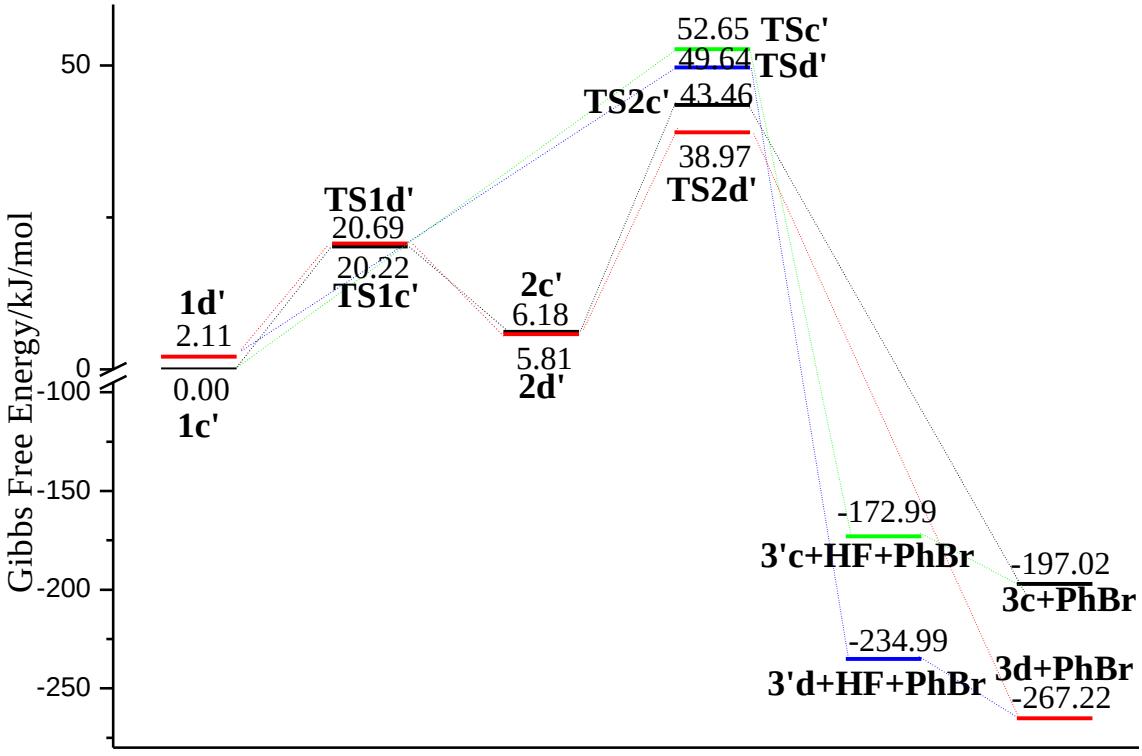

Fig. S4 Reaction profile for the group migration of protonated syn-α-hydroxyethoxy-λ3-bromane: CH_3 migration (stepwise mechanism in black line and concerted mechanism in green line) and H migration (stepwise mechanism in red line and concerted mechanism in blue line), using DFT (B3LYP/6-31++G**) method.

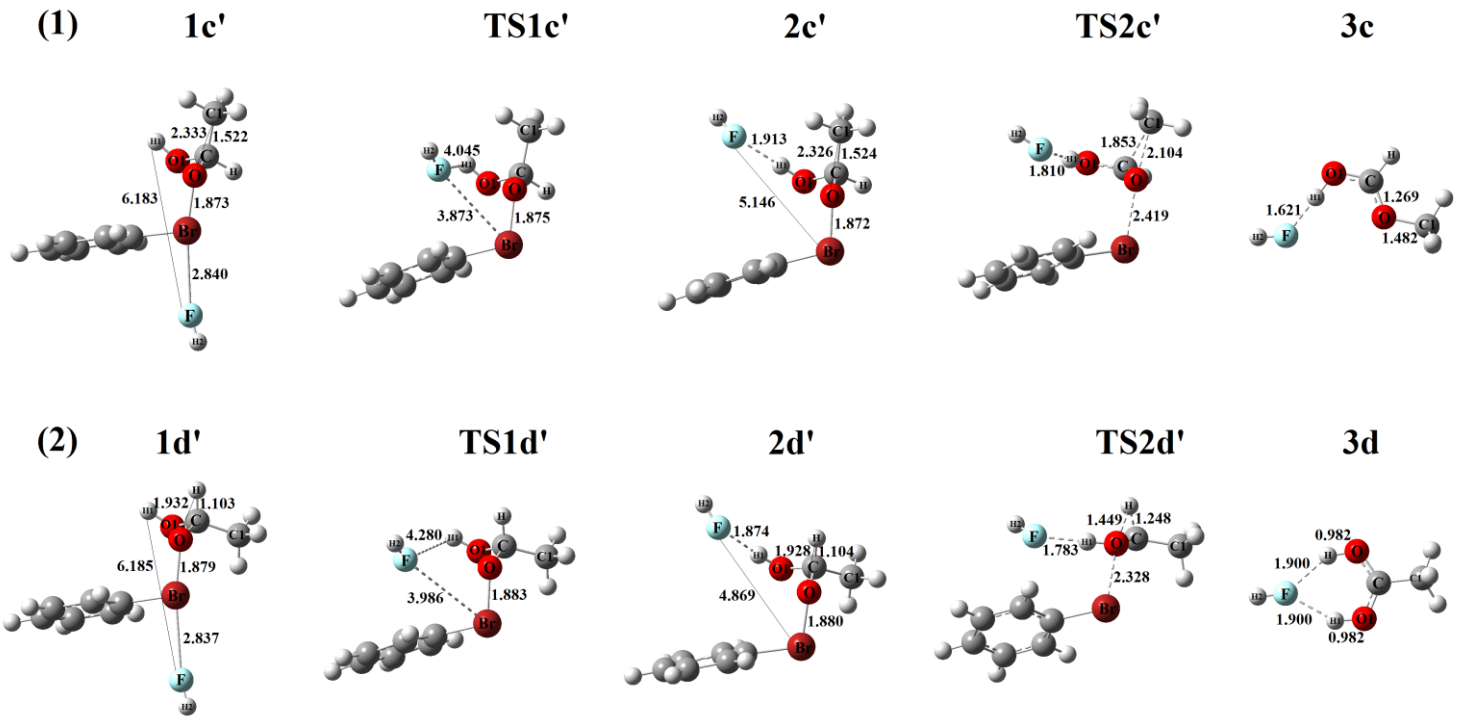

Fig. S5 Structures of intermediates, transition states, and products of stepwise mechanism of protonated syn-α-hydroxyethoxy-λ^3-bromane, using DFT (B3LYP/6-31++G**) method: CH_3 migration (above) and hydrogen migration (below). 1c'(1d'): protonated syn-α-hydroxyethoxy -λ^3-bromane, 3c(3d): complex of HF and protonated $CHOOCH_3$ (CH_3COOH). The distances are in Å.

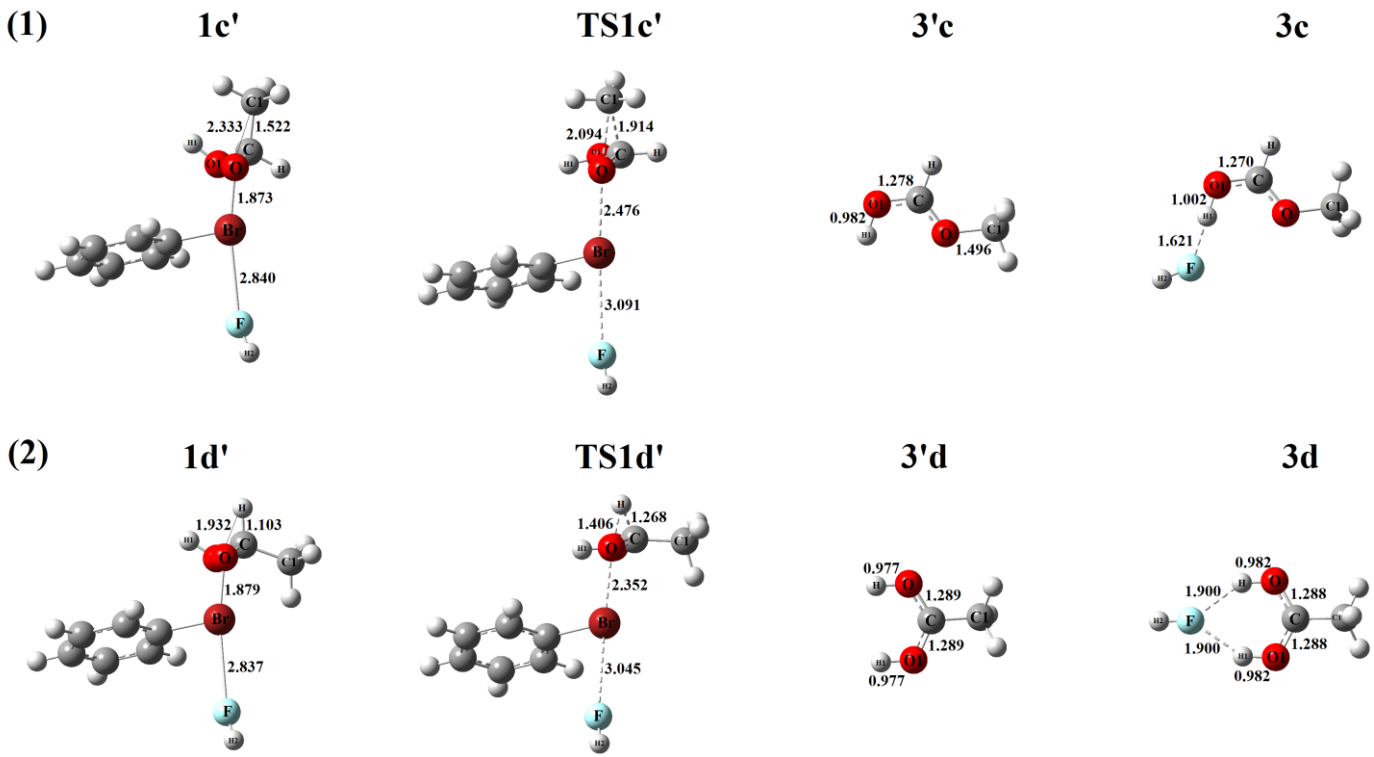

Fig. S6 Structures of intermediates, transition states, and products of concerted mechanism of protonated syn-α-hydroxyethoxy-λ^3-bromane, using DFT (B3LYP/6-31++G**) method: CH_3 migration (above) and hydrogen migration (below). 1c'(1d'): protonated syn-α-hydroxyethoxy -λ^3-bromane, 3c(3d): complex of HF and protonated $CHOOCH_3$ (CH_3COOH). The distances are in Å.

Table S1 Cartesian coordinates of the reported structures.

A. Cartesian coordinates of structures relative to the anti-α-hydrobenzyloxy-λ^3-bromane

1) 1a

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.099656	1.493217	-0.047906
2	6	4.416169	1.725075	-0.440346
3	6	5.313573	0.656224	-0.544643
4	6	4.893508	-0.648226	-0.260678
5	6	3.581563	-0.884268	0.142358
6	6	2.684555	0.191187	0.271409
7	1	2.402837	2.322040	0.037875
8	1	4.744506	2.735622	-0.660975
9	1	6.337588	0.838494	-0.855041
10	1	5.588325	-1.476572	-0.353223
11	1	3.258636	-1.903468	0.338872
12	6	1.269939	-0.037541	0.745905
13	1	0.733390	0.903918	0.888112
14	8	1.075079	-0.780589	1.896559
15	1	1.745136	-1.474984	1.982583
16	8	0.747351	-0.704977	-0.439749
17	6	-2.394162	0.773912	1.175264
18	6	-3.120210	1.956157	1.315013
19	6	-3.487340	2.694405	0.183737
20	6	-3.133169	2.262601	-1.101275
21	6	-2.410196	1.083365	-1.271990
22	6	-2.059359	0.372466	-0.121160
23	1	-2.104450	0.184570	2.038243
24	1	-3.403278	2.295553	2.306145
25	1	-4.054956	3.611750	0.302950
26	1	-3.426998	2.840143	-1.971822
27	1	-2.131847	0.730251	-2.258617
28	35	-1.099811	-1.255049	-0.312731
29	9	-3.700489	-2.501282	-0.272211
30	1	-4.397698	-3.115977	-0.328227

2) TS1a

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.875476	-1.729343	-0.219757
2	6	-4.189766	-1.980518	-0.605505
3	6	-5.143574	-0.957414	-0.547330
4	6	-4.781198	0.321838	-0.109734
5	6	-3.471780	0.575322	0.289566
6	6	-2.518027	-0.457960	0.256923
7	1	-2.134673	-2.522667	-0.259526
8	1	-4.473579	-2.971392	-0.945108
9	1	-6.166131	-1.154141	-0.853654
10	1	-5.520192	1.115753	-0.077398
11	1	-3.195398	1.576563	0.609583
12	6	-1.101923	-0.220111	0.728070
13	1	-0.526152	-1.148994	0.751042
14	8	-0.906715	0.389386	1.955223
15	1	-1.569617	1.077667	2.114523
16	8	-0.653847	0.597179	-0.381305
17	6	2.585656	-0.823585	1.157127
18	6	3.405824	-1.948791	1.231241
19	6	3.836807	-2.584332	0.060556
20	6	3.455997	-2.104242	-1.199492

21	6	2.633394	-0.984483	-1.303853
22	6	2.218628	-0.371808	-0.116063
23	1	2.243454	-0.315523	2.052064
24	1	3.711203	-2.324579	2.202336
25	1	4.479765	-3.456002	0.129534
26	1	3.801239	-2.600600	-2.100608
27	1	2.332416	-0.595836	-2.270421
28	35	1.187591	1.218839	-0.228302
29	9	1.345926	4.144458	-0.361494
30	1	1.495764	5.060310	-0.430174

3) 2a

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.345028	-2.069657	0.261425
2	6	-3.579989	-2.656025	0.006822
3	6	-4.693601	-1.849442	-0.264306
4	6	-4.570518	-0.454535	-0.282357
5	6	-3.341081	0.140369	-0.017763
6	6	-2.227721	-0.667772	0.284901
7	1	-1.479046	-2.690251	0.472393
8	1	-3.680326	-3.736433	0.020625
9	1	-5.654947	-2.309353	-0.470832
10	1	-5.434311	0.164272	-0.502418
11	1	-3.250016	1.221423	-0.044402
12	6	-0.880253	-0.052732	0.615698
13	1	-0.190430	-0.802887	1.012688
14	8	-0.810355	1.027865	1.464996
15	1	-1.442713	1.727369	1.226592
16	8	-0.550984	0.257724	-0.748461
17	6	2.849398	0.212970	1.126896
18	6	3.835562	-0.611804	1.666451
19	6	4.426493	-1.608941	0.881112
20	6	4.040567	-1.794878	-0.452793
21	6	3.054413	-0.987389	-1.016078
22	6	2.481390	-0.000948	-0.206237
23	1	2.381063	0.992773	1.717345
24	1	4.144666	-0.471027	2.697007
25	1	5.196751	-2.242543	1.309264
26	1	4.508834	-2.566215	-1.055453
27	1	2.744839	-1.114983	-2.047477
28	35	1.209777	1.178054	-0.974752
29	9	-2.327304	3.400602	0.791438
30	1	-2.647927	4.110547	1.303115

4) TS2a

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.279241	-2.051561	0.157723
2	6	-3.487450	-2.674124	-0.112608
3	6	-4.651042	-1.901668	-0.268746
4	6	-4.607479	-0.504379	-0.148984
5	6	-3.405510	0.131692	0.128113
6	6	-2.244525	-0.648496	0.333744
7	1	-1.368517	-2.632228	0.265808
8	1	-3.533761	-3.753569	-0.210672
9	1	-5.592810	-2.391564	-0.496130
10	1	-5.511609	0.080352	-0.281329
11	1	-3.365500	1.212197	0.207435
12	6	-0.919904	0.007878	0.780770
13	1	-0.244317	-0.722236	1.237464
14	8	-0.933436	1.112365	1.587156
15	1	-1.416613	1.854505	1.183073
16	8	-0.706764	0.212619	-0.572760

17	6	2.978398	0.320403	1.052399
18	6	3.952905	-0.503187	1.615500
19	6	4.431765	-1.611838	0.908028
20	6	3.940210	-1.909103	-0.369382
21	6	2.962532	-1.102484	-0.949186
22	6	2.496773	-0.002565	-0.220940
23	1	2.602640	1.187617	1.584123
24	1	4.342396	-0.272878	2.601811
25	1	5.194938	-2.243896	1.350943
26	1	4.321541	-2.764863	-0.916936
27	1	2.577808	-1.314138	-1.940744
28	35	1.244413	1.163098	-1.036858
29	9	-2.328916	3.432781	0.573799
30	1	-2.483403	4.253967	0.987234

5) 3a

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.602907	0.058662	0.008573
2	6	1.263744	-1.069125	0.475646
3	6	2.660567	-1.012688	0.526205
4	6	3.333317	0.146418	0.130515
5	6	2.620858	1.265383	-0.313988
6	6	1.225141	1.235729	-0.376107
7	8	-0.848764	0.061214	-0.037090
8	6	-1.469870	-0.862034	-0.654741
9	8	-2.739953	-0.926552	-0.647681
10	1	-0.937622	-1.631747	-1.215337
11	1	-3.201319	-0.213214	-0.120557
12	9	-3.981190	0.943376	0.731602
13	1	-4.893198	1.083431	0.886446
14	1	0.726734	-1.946766	0.822565
15	1	3.214191	-1.872102	0.889025
16	1	4.416483	0.182344	0.178883
17	1	3.146989	2.165897	-0.612299
18	1	0.648201	2.090406	-0.711582

6) 1b

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.801272	0.043067	0.871591
2	6	3.101084	1.249531	1.509611
3	6	2.879164	2.465337	0.856478
4	6	2.354534	2.478211	-0.441738
5	6	2.046693	1.277730	-1.079639
6	6	2.260250	0.056128	-0.421765
7	1	3.002161	-0.902034	1.363010
8	1	3.523460	1.237887	2.509481
9	1	3.131649	3.399667	1.348582
10	1	2.202175	3.420184	-0.959243
11	1	1.648905	1.287952	-2.091038
12	6	1.926881	-1.217764	-1.147022
13	1	2.312829	-1.208734	-2.180334
14	8	0.501674	-1.322372	-1.499141
15	8	2.328685	-2.327956	-0.429325
16	1	2.351268	-3.110410	-0.999393
17	6	-1.658569	0.191458	-0.137831
18	6	-1.245788	1.329876	0.557056
19	6	-2.055125	2.461076	0.465047
20	6	-3.222217	2.434081	-0.308308
21	6	-3.600108	1.275249	-0.997234
22	6	-2.817385	0.124759	-0.914873
23	1	-0.333360	1.334942	1.141845
24	1	-1.771695	3.364152	0.995735
25	1	-3.842073	3.322529	-0.374197

26	1	-4.507308	1.263107	-1.592521
27	1	-3.098138	-0.785115	-1.433515
28	35	-0.614347	-1.391720	0.022376
29	9	-2.196463	-1.933723	2.331206
30	1	-2.616554	-2.320230	3.067062

7) TS1b

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.519962	-1.031463	-0.763047
2	6	2.467723	-2.319954	-1.301593
3	6	1.869289	-3.359079	-0.583095
4	6	1.317746	-3.111873	0.680170
5	6	1.360601	-1.826998	1.218046
6	6	1.949966	-0.779311	0.492987
7	1	3.010590	-0.230120	-1.303573
8	1	2.913231	-2.514968	-2.272075
9	1	1.849111	-4.362940	-0.996328
10	1	0.872278	-3.922046	1.248885
11	1	0.944288	-1.638129	2.204061
12	6	1.991787	0.588471	1.114083
13	1	2.328539	0.543730	2.165278
14	8	0.657334	1.133894	1.402700
15	8	2.725694	1.468139	0.347904
16	1	2.914857	2.277068	0.845574
17	6	-1.754967	0.141265	-0.083708
18	6	-1.609154	-1.032044	-0.830165
19	6	-2.680563	-1.923454	-0.838431
20	6	-3.845443	-1.635621	-0.116594
21	6	-3.958876	-0.448979	0.618224
22	6	-2.905979	0.463593	0.642948
23	1	-0.695095	-1.245115	-1.372631
24	1	-2.603855	-2.843758	-1.408149
25	1	-4.672730	-2.337905	-0.131769
26	1	-4.867750	-0.231888	1.169910
27	1	-2.978614	1.390278	1.201341
28	35	-0.369172	1.442531	-0.156427
29	9	0.633006	4.063541	-1.099446
30	1	0.812305	4.891747	-1.484351

8)2b

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.679129	1.993905	-0.868640
2	6	-1.115787	3.262664	-1.029392
3	6	-0.344570	3.824188	-0.007533
4	6	-0.129547	3.114070	1.180270
5	6	-0.679174	1.843422	1.339984
6	6	-1.448621	1.274610	0.312453
7	1	-2.307278	1.569124	-1.643389
8	1	-1.298269	3.820227	-1.942739
9	1	0.073332	4.819150	-0.127167
10	1	0.450862	3.557490	1.983318
11	1	-0.522129	1.296638	2.266070
12	6	-2.048165	-0.085685	0.529976
13	1	-2.522175	-0.168408	1.524145
14	8	-1.020379	-1.120897	0.770756
15	8	-2.881089	-0.455835	-0.496193
16	1	-3.478134	-1.166550	-0.203689
17	6	1.810273	-0.836479	-0.196594
18	6	2.231416	0.447870	-0.551804
19	6	3.540072	0.801402	-0.225953
20	6	4.375728	-0.108768	0.433088
21	6	3.919414	-1.388791	0.770177
22	6	2.616699	-1.772951	0.456452

23	1	1.566627	1.143345	-1.051103
24	1	3.905319	1.789489	-0.486068
25	1	5.392340	0.179799	0.680246
26	1	4.576001	-2.089074	1.275997
27	1	2.246422	-2.761195	0.705183
28	35	0.074256	-1.404548	-0.740002
29	9	-4.487317	-2.415290	0.785627
30	1	-5.375928	-2.696136	0.797212

9)TS2b

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.947232	0.713710	0.055750
2	6	-5.060610	-0.094649	0.257502
3	6	-4.993096	-1.467118	-0.019482
4	6	-3.809076	-2.037900	-0.504667
5	6	-2.690105	-1.240069	-0.715231
6	6	-2.748197	0.134239	-0.404200
7	1	-3.988225	1.775847	0.266779
8	1	-5.982786	0.340174	0.628556
9	1	-5.868017	-2.091213	0.133910
10	1	-3.766281	-3.099459	-0.724492
11	1	-1.770496	-1.668431	-1.099561
12	6	-1.549213	0.977643	-0.628050
13	1	-1.379928	0.959603	-1.833698
14	8	-0.343459	0.431967	-0.851026
15	8	-1.607005	2.204417	-0.083255
16	1	-0.766556	2.689722	-0.210839
17	6	2.451198	-0.508821	0.252651
18	6	2.836949	-1.716803	-0.332151
19	6	4.126195	-1.810780	-0.855889
20	6	4.997547	-0.718319	-0.779692
21	6	4.588203	0.477308	-0.177852
22	6	3.303869	0.592403	0.353689
23	1	2.153924	-2.557648	-0.376087
24	1	4.449880	-2.738549	-1.316234
25	1	6.000562	-0.800437	-1.186148
26	1	5.270397	1.318792	-0.114188
27	1	2.975184	1.508964	0.830335
28	35	0.726590	-0.403065	1.056513
29	9	0.770355	3.664929	-0.344725
30	1	0.873609	4.589405	-0.413780

10) 3b

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.174877	1.229739	-0.000011
2	6	0.472352	0.000082	-0.000121
3	6	1.174576	-1.229748	-0.000022
4	6	2.561512	-1.220127	0.000095
5	6	3.252877	-0.000259	0.000159
6	6	2.561810	1.219779	0.000106
7	1	0.631479	2.167524	-0.000057
8	1	0.630947	-2.167399	-0.000077
9	1	3.109020	-2.156299	0.000138
10	1	4.338580	-0.000392	0.000260
11	1	3.109547	2.155816	0.000157
12	6	-0.958342	0.000243	-0.000289
13	8	-1.595023	1.139295	-0.000055
14	1	-2.569610	1.069304	0.000101
15	8	-1.595309	-1.138628	-0.000050
16	1	-2.569882	-1.068289	0.000090
17	9	-4.165873	-0.000399	0.000059
18	1	-5.102545	-0.000258	0.000188

11) TSa

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.018259	1.268076	-0.624325
2	6	4.314153	1.436731	-1.080925
3	6	5.309346	0.514766	-0.711786
4	6	5.011806	-0.575919	0.122318
5	6	3.720821	-0.754955	0.592347
6	6	2.728072	0.199405	0.261056
7	1	2.228933	1.952308	-0.918743
8	1	4.558815	2.270223	-1.730576
9	1	6.320670	0.640826	-1.086012
10	1	5.790404	-1.280566	0.394128
11	1	3.486088	-1.595196	1.236045
12	6	1.329002	0.154393	0.947119
13	1	0.846720	1.135991	0.976015
14	8	1.181438	-0.428571	2.175445
15	1	1.364716	-1.379811	2.127678
16	8	1.088774	-0.609714	-0.159653
17	6	-2.508472	0.646456	1.209780
18	6	-3.205750	1.839789	1.396229
19	6	-3.456398	2.687099	0.310821
20	6	-3.007877	2.347627	-0.971773
21	6	-2.305422	1.161463	-1.179531
22	6	-2.066286	0.332106	-0.079120
23	1	-2.316793	-0.024256	2.039834
24	1	-3.560655	2.101812	2.387872
25	1	-4.005659	3.610773	0.463084
26	1	-3.211554	3.002880	-1.812735
27	1	-1.961795	0.879951	-2.168807
28	35	-1.152234	-1.303221	-0.352028
29	9	-3.987054	-2.447262	-0.671391
30	1	-4.777427	-2.912754	-0.823891

12) 3'a

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.035997	-0.164474	-0.164996
2	6	0.514926	1.137855	-0.190960
3	6	1.894105	1.306891	-0.030086
4	6	2.725628	0.195549	0.134119
5	6	2.194047	-1.098672	0.131005
6	6	0.819967	-1.298288	-0.026881
7	8	-1.390938	-0.400708	-0.351751
8	6	-2.247227	0.222944	0.343052
9	8	-3.502061	0.079744	0.131508
10	1	-1.965612	0.903235	1.147631
11	1	-3.713580	-0.532598	-0.604943
12	1	-0.135549	1.989490	-0.366166
13	1	2.311842	2.307794	-0.048618
14	1	3.794664	0.337526	0.251823
15	1	2.845153	-1.958183	0.249122
16	1	0.382413	-2.290383	-0.038418

13) TSb

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-4.095507	-0.681095	-0.636905
2	6	-5.179672	0.121183	-0.299510
3	6	-5.098881	0.987588	0.799494
4	6	-3.929841	1.055356	1.569022
5	6	-2.838880	0.257716	1.244604
6	6	-2.910902	-0.594386	0.122377

7	1	-4.148999	-1.354941	-1.484017
8	1	-6.090063	0.072313	-0.887596
9	1	-5.951988	1.605688	1.061513
10	1	-3.876637	1.724426	2.421365
11	1	-1.930905	0.296002	1.836968
12	6	-1.746696	-1.437144	-0.213945
13	1	-1.601025	-2.206794	0.739571
14	8	-0.545182	-1.253130	0.352274
15	8	-1.794923	-2.024745	-1.424989
16	1	-0.970782	-2.509459	-1.598048
17	6	2.389878	-0.067011	0.114596
18	6	2.819300	0.321237	1.384670
19	6	4.066529	-0.125117	1.820662
20	6	4.853179	-0.936036	0.994641
21	6	4.399203	-1.305547	-0.276982
22	6	3.154087	-0.872219	-0.732053
23	1	2.203973	0.957946	2.010000
24	1	4.424479	0.164727	2.803314
25	1	5.823989	-1.276688	1.340101
26	1	5.015766	-1.927536	-0.917944
27	1	2.797021	-1.138762	-1.720490
28	35	0.708679	0.574345	-0.501772
29	9	2.253266	3.060240	-1.445695
30	1	2.652068	3.824710	-1.793777

14) 3'b

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.517743	1.231703	-0.000026
2	6	-0.185693	0.000000	-0.000225
3	6	0.517743	-1.231703	-0.000038
4	6	1.903734	-1.221108	0.000146
5	6	2.594536	0.000000	0.000243
6	6	1.903733	1.221108	0.000158
7	1	-0.024624	2.170151	-0.000100
8	1	-0.024624	-2.170151	-0.000123
9	1	2.451959	-2.156856	0.000216
10	1	3.680321	0.000000	0.000406
11	1	2.451958	2.156856	0.000238
12	6	-1.611652	0.000000	-0.000512
13	8	-2.246250	1.143428	-0.000001
14	1	-3.217927	1.102900	0.000385
15	8	-2.246250	-1.143427	0.000017
16	1	-3.217928	-1.102900	0.000376

B. Cartesian coordinates of structures relative to the syn-α-hydrobenzyloxy-λ^3-bromane

1) 1a'

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.919104	-0.921602	0.369781
2	6	-5.179503	-0.497267	-0.045661
3	6	-5.352313	0.798467	-0.545571
4	6	-4.264529	1.675495	-0.625312
5	6	-3.004045	1.258681	-0.205052
6	6	-2.831387	-0.036075	0.317833
7	1	-3.784359	-1.925959	0.760703
8	1	-6.025487	-1.173909	0.017767
9	1	-6.334360	1.124913	-0.873120
10	1	-4.399365	2.676106	-1.022927
11	1	-2.158991	1.936235	-0.297797
12	6	-1.485021	-0.486435	0.822383
13	1	-1.522992	-1.481055	1.271774

14	8	-0.830914	0.335199	1.726630
15	1	-1.064306	1.263423	1.577560
16	8	-0.773429	-0.566931	-0.454516
17	6	2.552994	0.962800	-1.299705
18	6	3.398293	2.061089	-1.147740
19	6	3.786993	2.478181	0.131280
20	6	3.338619	1.804017	1.274309
21	6	2.495571	0.701332	1.150920
22	6	2.123232	0.315965	-0.138376
23	1	2.243619	0.622417	-2.281758
24	1	3.755145	2.587064	-2.027203
25	1	4.446460	3.333733	0.237789
26	1	3.650813	2.130751	2.260812
27	1	2.134826	0.166394	2.021455
28	35	1.028940	-1.226337	-0.329588
29	9	3.529748	-2.648192	-0.061960
30	1	4.154289	-3.338623	-0.083259

2) TS1a’

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.806175	-1.006496	0.374784
2	6	-5.054401	-0.434829	0.144438
3	6	-5.160980	0.941793	-0.092335
4	6	-4.017724	1.749436	-0.100064
5	6	-2.766650	1.185578	0.134528
6	6	-2.661211	-0.192747	0.401681
7	1	-3.720837	-2.072720	0.562950
8	1	-5.943832	-1.056429	0.151382
9	1	-6.135436	1.383442	-0.276094
10	1	-4.105137	2.812799	-0.297983
11	1	-1.875404	1.805544	0.092052
12	6	-1.320302	-0.811050	0.707204
13	1	-1.404761	-1.870896	0.957966
14	8	-0.549797	-0.230651	1.701321
15	1	-0.653704	0.732870	1.697601
16	8	-0.720614	-0.662987	-0.607550
17	6	2.952456	0.627466	-0.980395
18	6	4.027406	1.381136	-0.514284
19	6	4.489574	1.207345	0.795972
20	6	3.882504	0.285272	1.658746
21	6	2.810574	-0.485420	1.214591
22	6	2.368980	-0.285782	-0.097359
23	1	2.577333	0.747249	-1.990107
24	1	4.507374	2.095307	-1.175110
25	1	5.329853	1.796856	1.149379
26	1	4.251102	0.156506	2.670975
27	1	2.329046	-1.206423	1.864710
28	35	1.045741	-1.461306	-0.787933
29	9	0.391943	2.709049	-0.827545
30	1	0.414973	3.619039	-1.017364

3) 2a’

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.736361	-0.862120	-0.554446
2	6	4.969260	-0.490669	-0.026777
3	6	5.065045	0.635160	0.801408
4	6	3.926189	1.392488	1.099868
5	6	2.691073	1.032795	0.567728
6	6	2.596059	-0.085306	-0.283499
7	1	3.659035	-1.734580	-1.196620
8	1	5.854874	-1.073577	-0.258028
9	1	6.026675	0.918239	1.218005
10	1	4.003406	2.256436	1.751990

11	1	1.808807	1.614008	0.816406
12	6	1.276855	-0.485668	-0.899887
13	1	1.395009	-1.317292	-1.598208
14	8	0.519687	0.468246	-1.544615
15	1	0.558038	1.333923	-1.103083
16	8	0.650216	-0.967275	0.325889
17	6	-2.912852	-0.011207	1.413713
18	6	-3.936591	0.933812	1.451675
19	6	-4.420845	1.490570	0.261567
20	6	-3.890936	1.112241	-0.978570
21	6	-2.870317	0.165832	-1.043641
22	6	-2.399749	-0.363528	0.161542
23	1	-2.528705	-0.459016	2.323654
24	1	-4.358225	1.228213	2.406991
25	1	-5.220129	2.224042	0.300858
26	1	-4.278139	1.545057	-1.895022
27	1	-2.443313	-0.137396	-1.992509
28	35	-1.117560	-1.763192	0.087378
29	9	0.207626	3.171937	-0.548529
30	1	0.432081	3.972044	-0.970195

4) TS2a’

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.681782	-1.014327	0.336822
2	6	-4.915438	-0.707845	-0.213622
3	6	-5.127454	0.556645	-0.789450
4	6	-4.105342	1.518627	-0.811267
5	6	-2.866661	1.227187	-0.259008
6	6	-2.667089	-0.026311	0.367009
7	1	-3.496077	-1.991334	0.771883
8	1	-5.712692	-1.443468	-0.207242
9	1	-6.090729	0.787989	-1.233669
10	1	-4.280938	2.486631	-1.268411
11	1	-2.070819	1.962860	-0.287350
12	6	-1.356298	-0.341644	1.115391
13	1	-1.482597	-1.150586	1.839491
14	8	-0.656271	0.655630	1.735315
15	1	-0.444552	1.390111	1.133354
16	8	-0.911363	-0.755136	-0.134238
17	6	2.835942	0.145736	-1.416204
18	6	3.909477	1.034918	-1.429977
19	6	4.575727	1.349381	-0.239517
20	6	4.176301	0.776634	0.974211
21	6	3.112651	-0.123888	1.006429
22	6	2.449995	-0.408021	-0.191643
23	1	2.314936	-0.114371	-2.331056
24	1	4.229061	1.473427	-2.369652
25	1	5.412680	2.040463	-0.258290
26	1	4.703789	1.014080	1.892310
27	1	2.799566	-0.584256	1.936859
28	35	1.091884	-1.733020	-0.188493
29	9	0.018027	3.085770	0.305193
30	1	0.241068	3.885710	0.728612

5) 1b’

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.775612	-0.723915	1.235883
2	6	3.859746	0.068876	1.618163
3	6	4.606385	0.751809	0.653868
4	6	4.273285	0.639993	-0.700822
5	6	3.192827	-0.150512	-1.089015
6	6	2.434206	-0.829881	-0.119309
7	1	2.208127	-1.272910	1.978528

8	1	4.125190	0.146368	2.667723
9	1	5.454603	1.359156	0.954179
10	1	4.861654	1.157235	-1.451983
11	1	2.944137	-0.249378	-2.142298
12	6	1.272866	-1.671723	-0.572426
13	1	1.573290	-2.393046	-1.351932
14	8	0.326577	-0.915074	-1.401109
15	8	0.631919	-2.273031	0.493891
16	1	0.094411	-3.017121	0.186961
17	6	-2.114799	0.074808	-0.078878
18	6	-3.109031	0.191085	-1.051899
19	6	-4.403235	-0.183937	-0.692209
20	6	-4.667397	-0.650037	0.601267
21	6	-3.644236	-0.749481	1.552426
22	6	-2.341291	-0.381886	1.220374
23	1	-2.886547	0.561478	-2.046509
24	1	-5.203941	-0.106284	-1.420424
25	1	-5.679120	-0.936136	0.870886
26	1	-3.860206	-1.106647	2.554064
27	1	-1.533533	-0.453582	1.939729
28	35	-0.347092	0.622303	-0.535538
29	9	-1.042559	3.082504	0.755445
30	1	-1.044398	3.981347	0.999125

6) TS1b’

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.912166	-1.131266	0.857430
2	6	-4.054317	-1.599496	0.204733
3	6	-4.766688	-0.760087	-0.656671
4	6	-4.340450	0.556634	-0.865059
5	6	-3.201591	1.030452	-0.216045
6	6	-2.475158	0.182566	0.639016
7	1	-2.370093	-1.772771	1.542636
8	1	-4.391588	-2.616972	0.375027
9	1	-5.659061	-1.125379	-1.155317
10	1	-4.901024	1.214277	-1.521690
11	1	-2.880008	2.057637	-0.365776
12	6	-1.252472	0.725809	1.325374
13	1	-1.487125	1.638980	1.902462
14	8	-0.316017	1.361482	0.400422
15	8	-0.624502	-0.239820	2.087977
16	1	-0.007438	0.173489	2.709088
17	6	1.944963	-0.458543	-0.433297
18	6	3.079139	0.293555	-0.749764
19	6	4.319733	-0.258221	-0.432823
20	6	4.397759	-1.515634	0.176673
21	6	3.237646	-2.241701	0.477524
22	6	1.983165	-1.718527	0.172063
23	1	2.997957	1.268645	-1.214890
24	1	5.223910	0.295545	-0.663405
25	1	5.369210	-1.935454	0.417270
26	1	3.309469	-3.217740	0.946490
27	1	1.073345	-2.260946	0.401822
28	35	0.253255	0.212946	-0.994028
29	9	2.628250	3.040000	0.824475
30	1	2.971034	3.861032	1.094880

7) 2b’

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.875870	0.608644	1.171776
2	6	-4.025661	-0.068921	1.582220
3	6	-4.738376	-0.859257	0.675612
4	6	-4.301581	-0.975436	-0.649004

5	6	-3.151441	-0.306314	-1.063730
6	6	-2.427447	0.481641	-0.150518
7	1	-2.332006	1.239473	1.865411
8	1	-4.369822	0.027985	2.607054
9	1	-5.637921	-1.375561	0.996142
10	1	-4.861540	-1.577610	-1.357361
11	1	-2.820072	-0.385672	-2.095564
12	6	-1.191123	1.194237	-0.628217
13	1	-1.401000	1.825186	-1.511277
14	8	-0.266229	0.277923	-1.312782
15	8	-0.564071	1.879824	0.383379
16	1	0.016098	2.570600	0.018536
17	6	2.116784	-0.728432	0.118549
18	6	3.052629	-1.199717	-0.805696
19	6	4.398378	-0.948325	-0.542215
20	6	4.768039	-0.241564	0.608433
21	6	3.802845	0.218289	1.513394
22	6	2.450311	-0.022111	1.276561
23	1	2.745973	-1.750141	-1.688238
24	1	5.154353	-1.303770	-1.234489
25	1	5.818624	-0.051824	0.804664
26	1	4.101805	0.760198	2.404480
27	1	1.684898	0.329871	1.959185
28	35	0.282476	-1.143099	-0.189878
29	9	1.136394	3.858998	-0.735613
30	1	1.163891	4.790371	-0.710062

8) TS2b’

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.947152	0.714457	0.055991
2	6	-5.060820	-0.093496	0.257758
3	6	-4.993871	-1.465956	-0.019413
4	6	-3.810119	-2.037139	-0.504781
5	6	-2.690857	-1.239719	-0.715350
6	6	-2.748383	0.134576	-0.404144
7	1	-3.987715	1.776584	0.267151
8	1	-5.982791	0.341640	0.628955
9	1	-5.869019	-2.089730	0.133991
10	1	-3.767758	-3.098687	-0.724743
11	1	-1.771452	-1.668390	-1.099823
12	6	-1.549089	0.977545	-0.628007
13	1	-1.379943	0.959538	-1.833669
14	8	-0.343556	0.431448	-0.851142
15	8	-1.606455	2.204281	-0.083096
16	1	-0.765919	2.689394	-0.210822
17	6	2.451250	-0.508952	0.252624
18	6	2.837194	-1.716349	-0.333262
19	6	4.126515	-1.809720	-0.856919
20	6	4.997778	-0.717270	-0.779533
21	6	4.588258	0.477744	-0.176598
22	6	3.303827	0.592238	0.354838
23	1	2.154246	-2.557209	-0.378085
24	1	4.450340	-2.737021	-1.318108
25	1	6.000860	-0.798923	-1.185915
26	1	5.270388	1.319210	-0.112003
27	1	2.975000	1.508319	0.832311
28	35	0.726540	-0.404104	1.056367
29	9	0.771419	3.664094	-0.344764
30	1	0.874975	4.588481	-0.414531

9) TSa’

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.785278	-1.049618	0.058528

2	6	-5.006060	-0.737289	-0.514026
3	6	-5.306150	0.599693	-0.828563
4	6	-4.388049	1.630829	-0.563901
5	6	-3.164199	1.335092	0.012624
6	6	-2.878920	-0.004726	0.376219
7	1	-3.521844	-2.077345	0.287072
8	1	-5.723158	-1.521725	-0.730806
9	1	-6.258114	0.838916	-1.292612
10	1	-4.636179	2.656360	-0.815599
11	1	-2.451308	2.126169	0.216344
12	6	-1.621012	-0.341743	1.230717
13	1	-1.751480	-1.247210	1.828530
14	8	-1.049592	0.613751	2.023070
15	1	-0.697913	1.340214	1.485028
16	8	-1.130383	-0.504270	-0.036746
17	6	2.350551	0.968562	-1.362551
18	6	3.150860	2.110843	-1.348098
19	6	3.720283	2.558269	-0.150183
20	6	3.498825	1.860381	1.043270
21	6	2.707378	0.712166	1.048430
22	6	2.139979	0.292653	-0.157758
23	1	1.908880	0.606891	-2.284587
24	1	3.331992	2.648379	-2.273462
25	1	4.342349	3.447714	-0.147613
26	1	3.951182	2.201904	1.968884
27	1	2.538425	0.154332	1.962742
28	35	1.092960	-1.287969	-0.170225
29	9	3.888735	-2.605036	-0.311044
30	1	4.645513	-3.136895	-0.405483

10) TSb'

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.693420	-1.207497	0.732177
2	6	4.888808	-0.570629	1.045913
3	6	5.233158	0.630878	0.411648
4	6	4.384434	1.198945	-0.547855
5	6	3.187250	0.572170	-0.872641
6	6	2.827104	-0.622280	-0.213349
7	1	3.418959	-2.137270	1.216612
8	1	5.554736	-1.006620	1.783117
9	1	6.171011	1.119481	0.657000
10	1	4.662004	2.124333	-1.041349
11	1	2.528919	0.997255	-1.623203
12	6	1.556328	-1.281191	-0.566621
13	1	1.645755	-1.591635	-1.760362
14	8	0.610441	-0.663512	-1.293289
15	8	1.174743	-2.275414	0.256941
16	1	0.313160	-2.631155	-0.018456
17	6	-2.313838	-0.051750	-0.007612
18	6	-3.175353	-0.012436	-1.105145
19	6	-4.381022	-0.709357	-1.020133
20	6	-4.703644	-1.421329	0.140584
21	6	-3.823414	-1.439075	1.229069
22	6	-2.612273	-0.749445	1.164700
23	1	-2.916534	0.550594	-1.994920
24	1	-5.068643	-0.691162	-1.859570
25	1	-5.645064	-1.958156	0.199944
26	1	-4.082177	-1.981830	2.132710
27	1	-1.928883	-0.740681	2.006856
28	35	-0.677646	0.913265	-0.105594
29	9	-2.330307	3.273141	0.965047
30	1	-2.810095	4.013676	1.258356

C. Cartesian coordinates of structures relative to the anti-α-hydroxyethoxy-λ^3-bromane

1) 1c

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	-0.450423	0.979302	-0.260522
2	6	1.081291	-0.132109	-0.072477
3	6	1.399512	-0.589665	1.209232
4	6	1.820351	-0.440171	-1.217534
5	6	2.525593	-1.401254	1.340248
6	6	2.936472	-1.259051	-1.057733
7	6	3.285855	-1.734758	0.212913
8	1	0.803590	-0.311902	2.071846
9	1	1.537823	-0.056756	-2.191802
10	1	2.808624	-1.769109	2.321025
11	1	3.536807	-1.519171	-1.923397
12	1	4.160822	-2.367199	0.325171
13	8	-1.779895	-0.216896	-0.812400
14	6	-2.414753	-0.956433	0.287673
15	1	-1.646128	-1.550767	0.789086
16	6	-3.431774	-1.819595	-0.447889
17	1	-2.942773	-2.467922	-1.177183
18	1	-3.943187	-2.442210	0.292279
19	1	-4.168338	-1.197122	-0.965397
20	8	-2.931283	-0.097775	1.237924
21	1	-3.772565	0.280693	0.937594
22	9	1.354059	3.077813	0.357445
23	1	1.677755	3.941148	0.491251

2) TS1c

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	-0.497687	0.810903	-0.080858
2	6	1.307001	0.219758	-0.005579
3	6	1.801165	-0.228935	1.224996
4	6	2.087663	0.322072	-1.162518
5	6	3.143627	-0.600416	1.285408
6	6	3.425434	-0.055811	-1.073849
7	6	3.947433	-0.516574	0.142218
8	1	1.165309	-0.280921	2.102375
9	1	1.667958	0.687847	-2.093381
10	1	3.560121	-0.950724	2.224076
11	1	4.060280	0.012968	-1.951057
12	1	4.991914	-0.806221	0.200216
13	8	-1.415562	-0.641511	-0.832727
14	6	-1.740799	-1.703322	0.127264
15	1	-0.805827	-2.110104	0.522439
16	6	-2.488200	-2.704669	-0.746043
17	1	-1.867125	-3.042173	-1.577733
18	1	-2.744434	-3.566152	-0.122088
19	1	-3.406321	-2.263017	-1.145515
20	8	-2.441331	-1.208891	1.208648
21	1	-3.363633	-1.028535	0.967419
22	9	-2.337144	3.060262	0.186839
23	1	-2.849687	3.833667	0.262982

3) 2c

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	-0.109932	-1.109491	-0.051815
2	6	1.604795	-0.289184	-0.057621

3	6	1.984888	0.424658	-1.199563
4	6	2.440675	-0.492277	1.045452
5	6	3.269563	0.965769	-1.223312
6	6	3.717994	0.061745	0.995652
7	6	4.126838	0.787653	-0.130821
8	1	1.309298	0.546150	-2.039595
9	1	2.108707	-1.062516	1.906223
10	1	3.599246	1.522347	-2.094375
11	1	4.394018	-0.077243	1.832841
12	1	5.125530	1.211916	-0.159792
13	8	-1.199661	0.061153	0.919498
14	6	-1.716689	1.194409	0.122066
15	1	-0.862458	1.803369	-0.187024
16	6	-2.598721	1.904176	1.144441
17	1	-2.022964	2.201107	2.022890
18	1	-3.000440	2.802162	0.665021
19	1	-3.426368	1.260998	1.455526
20	8	-2.338287	0.761596	-1.022341
21	1	-3.213959	0.380712	-0.826621
22	9	-4.797328	-0.560270	-0.377103
23	1	-5.659506	-0.638058	-0.722658

4) TS2c

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	0.061535	-1.359827	-0.510812
2	6	-1.483057	-0.364696	-0.047269
3	6	-1.817980	-0.228590	1.305073
4	6	-2.304892	0.121963	-1.070499
5	6	-2.993517	0.445159	1.636006
6	6	-3.478782	0.787894	-0.721476
7	6	-3.821502	0.949796	0.626839
8	1	-1.174537	-0.635884	2.077511
9	1	-2.035692	-0.024497	-2.110987
10	1	-3.267362	0.562187	2.679452
11	1	-4.129429	1.169681	-1.501484
12	1	-4.739349	1.465633	0.890842
13	8	1.604727	0.473684	-0.894709
14	6	1.577758	1.348875	0.056702
15	1	0.734738	2.045527	0.147295
16	6	2.662753	2.269390	-1.135215
17	1	2.020711	2.625753	-1.933036
18	1	2.927030	3.006943	-0.374992
19	1	3.489481	1.640985	-1.450171
20	8	2.152819	1.130370	1.236944
21	1	2.802400	0.395202	1.198350
22	9	4.043190	-0.917887	1.104910
23	1	4.724537	-1.207794	1.672613

5) 3c

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.484317	0.887647	-0.000189
2	1	-1.195782	1.716243	0.000163
3	8	0.746047	1.200934	0.000103
4	1	1.389088	0.432946	0.000079
5	9	2.434270	-0.805938	0.000046
6	1	3.370121	-0.816772	0.000170
7	8	-0.863530	-0.323735	-0.000140
8	6	-2.301247	-0.682439	0.000056
9	1	-2.454910	-1.275541	-0.899520
10	1	-2.454706	-1.275575	0.899645
11	1	-2.908992	0.223308	0.000141

6) 1d

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	-0.595849	0.772452	-0.211698
2	6	1.113492	-0.054227	-0.106050
3	6	1.477858	-0.672912	1.091642
4	6	1.938580	0.015742	-1.230827
5	6	2.742633	-1.254650	1.154620
6	6	3.194613	-0.582366	-1.143016
7	6	3.592906	-1.212022	0.042490
8	1	0.809157	-0.694001	1.944519
9	1	1.615362	0.514726	-2.137801
10	1	3.064039	-1.737759	2.071569
11	1	3.862552	-0.550196	-1.997503
12	1	4.575147	-1.670058	0.101632
13	8	-1.615854	-0.559519	-1.071521
14	6	-2.695533	-1.120833	-0.254094
15	1	-3.100238	-1.793360	-1.029154
16	6	-2.217330	-1.877750	0.962629
17	1	-1.402850	-2.554559	0.696241
18	1	-1.892866	-1.182840	1.743427
19	1	-3.046362	-2.461699	1.369810
20	8	-3.588768	-0.138554	0.132177
21	1	-4.101138	0.182259	-0.625420
22	9	0.706684	3.018759	0.936873
23	1	0.865397	3.881543	1.250635

7) TS1d

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	-0.538915	-0.674381	-0.055009
2	6	1.314725	-0.246505	-0.036927
3	6	1.845346	0.472271	-1.112959
4	6	2.088451	-0.745403	1.016213
5	6	3.218581	0.710569	-1.116805
6	6	3.458253	-0.491081	0.988807
7	6	4.018110	0.233724	-0.070669
8	1	1.215102	0.833490	-1.918110
9	1	1.639638	-1.313510	1.823862
10	1	3.662970	1.263146	-1.938144
11	1	4.087209	-0.863296	1.790765
12	1	5.086614	0.424101	-0.083856
13	8	-1.276494	0.551288	1.174442
14	6	-2.075565	1.628689	0.580590
15	1	-2.389766	2.075975	1.540427
16	6	-1.278405	2.594165	-0.263513
17	1	-0.366218	2.896280	0.254839
18	1	-1.032785	2.141771	-1.229143
19	1	-1.884812	3.481092	-0.462902
20	8	-3.128369	1.127419	-0.155669
21	1	-3.762620	0.666484	0.414440
22	9	-2.710767	-2.568572	-0.608644
23	1	-3.294506	-3.253271	-0.847673

8) 2d

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	-0.268466	-0.505593	-0.695937
2	6	1.540330	-0.240343	-0.171057
3	6	2.178724	0.945271	-0.547130
4	6	2.177960	-1.287056	0.501634
5	6	3.524825	1.084288	-0.213855
6	6	3.523002	-1.119668	0.825658
7	6	4.189956	0.059255	0.470608

8	1	1.650055	1.729472	-1.077373
9	1	1.647213	-2.196784	0.760439
10	1	4.053340	1.990189	-0.491990
11	1	4.049015	-1.910962	1.349420
12	1	5.238382	0.178601	0.724971
13	8	-1.232177	-0.054739	0.861356
14	6	-2.140443	1.089602	0.684735
15	1	-2.607504	1.012896	1.683227
16	6	-1.424284	2.404699	0.489651
17	1	-0.627621	2.520876	1.227434
18	1	-1.014653	2.470286	-0.523338
19	1	-2.138334	3.223897	0.605765
20	8	-3.020459	0.865958	-0.347597
21	1	-3.624861	0.133143	-0.130956
22	9	-4.376033	-1.522424	0.383255
23	1	-5.243742	-1.860070	0.429354

9) TS2d

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	-0.085723	-0.030847	1.104467
2	6	1.610194	0.038075	0.241702
3	6	2.345275	-1.143179	0.116349
4	6	2.093424	1.283591	-0.166259
5	6	3.615055	-1.065372	-0.454389
6	6	3.365350	1.337122	-0.735456
7	6	4.121441	0.168150	-0.881362
8	1	1.943898	-2.090127	0.459308
9	1	1.499655	2.181526	-0.037619
10	1	4.208914	-1.967246	-0.561551
11	1	3.765404	2.291999	-1.060433
12	1	5.111768	0.219318	-1.322389
13	8	-1.332359	-0.262697	-0.859950
14	6	-2.541570	-0.839112	-0.775481
15	1	-2.233175	-0.585168	-1.955356
16	6	-2.679185	-2.326305	-0.582741
17	1	-1.912978	-2.863121	-1.141886
18	1	-2.555068	-2.529348	0.488783
19	1	-3.674885	-2.658704	-0.880556
20	8	-3.565988	-0.134313	-0.300806
21	1	-3.402373	0.834259	-0.329777
22	9	-3.152240	2.601009	-0.355252
23	1	-3.773850	3.295435	-0.405741

10) 3d

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.195139	0.000005	0.010678
2	1	-2.509804	-0.000320	1.064419
3	1	-2.583219	0.904722	-0.459397
4	1	-2.583212	-0.904457	-0.459904
5	6	-0.719953	0.000005	-0.015445
6	8	-0.109750	-1.134694	-0.015434
7	1	0.871477	-1.095230	-0.005050
8	8	-0.109742	1.134698	-0.015434
9	1	0.871485	1.095226	-0.005050
10	9	2.424154	-0.000004	0.014228
11	1	3.362372	-0.000003	0.012471

11) TSc

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	-0.066611	1.342484	-0.160029

2	6	0.945318	-0.255745	-0.091262
3	6	1.211044	-0.832750	1.155558
4	6	1.440352	-0.794088	-1.283933
5	6	1.982865	-1.993991	1.200044
6	6	2.211711	-1.953456	-1.218409
7	6	2.482266	-2.552911	0.018303
8	1	0.835838	-0.378453	2.066065
9	1	1.236477	-0.311278	-2.233509
10	1	2.202794	-2.453471	2.158397
11	1	2.609920	-2.382904	-2.132190
12	1	3.088549	-3.452181	0.060660
13	8	-2.289557	0.278185	-0.522947
14	6	-2.457384	-0.700849	0.289603
15	1	-1.971893	-1.671314	0.133101
16	6	-3.968825	-0.899558	-0.874619
17	1	-3.574035	-1.400027	-1.751703
18	1	-4.455445	-1.530865	-0.129528
19	1	-4.462958	0.049361	-1.054548
20	8	-2.766281	-0.515474	1.571520
21	1	-3.036939	0.406355	1.736234
22	9	2.648682	2.737833	0.307232
23	1	3.383591	3.295755	0.422661

12) 3'c

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.583977	0.388077	-0.000089
2	8	1.793391	-0.023476	0.000087
3	8	-0.385154	-0.424213	-0.000485
4	1	0.453027	1.472535	0.000010
5	6	-1.800465	0.059923	0.000267
6	1	-2.385668	-0.855370	-0.010064
7	1	-1.961884	0.629774	0.914657
8	1	-1.957717	0.647567	-0.903547
9	1	1.885277	-1.000995	0.001061

13) TSd

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	-0.365529	0.834589	-0.033869
2	6	1.237525	-0.183564	0.002748
3	6	1.800711	-0.491763	1.242623
4	6	1.819475	-0.551690	-1.211987
5	6	2.996815	-1.208107	1.257011
6	6	3.015609	-1.267134	-1.173588
7	6	3.601165	-1.595757	0.055007
8	1	1.325578	-0.176682	2.164686
9	1	1.360958	-0.278922	-2.155753
10	1	3.457836	-1.459545	2.206701
11	1	3.491430	-1.563551	-2.102789
12	1	4.533132	-2.151557	0.075698
13	8	-1.776114	-1.075992	-0.017322
14	6	-3.102265	-0.896924	-0.030021
15	1	-2.733116	-2.105053	0.066601
16	6	-3.855210	-0.471435	1.198297
17	1	-3.422409	-0.919214	2.092557
18	1	-3.776528	0.621786	1.267315
19	1	-4.911272	-0.731401	1.108246
20	8	-3.698082	-0.562315	-1.175886
21	1	-3.121130	-0.728779	-1.942759
22	9	1.479372	3.260655	-0.008939
23	1	1.985321	4.041098	-0.009512

14) 3'd

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.046340	-0.000145	-0.010784
2	6	1.428135	-0.001030	-0.005395
3	1	1.809334	-0.911275	-0.470761
4	1	1.809834	0.899240	-0.489864
5	1	1.756068	0.011142	1.044946
6	8	-0.651554	-1.138242	-0.002030
7	1	-1.628482	-1.138061	0.022708
8	8	-0.649802	1.138941	-0.002151
9	1	-1.626684	1.140409	0.023491

D. Cartesian coordinates of structures relative to the syn-α-hydroxyethoxy-λ^3-bromane

1) 1c'

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	0.458010	1.049457	-0.207724
2	6	-1.037607	-0.124576	-0.131638
3	6	-1.740010	-0.360136	-1.315921
4	6	-1.389532	-0.660248	1.108887
5	6	-2.855230	-1.193415	-1.242240
6	6	-2.509370	-1.488361	1.152177
7	6	-3.236866	-1.751370	-0.015844
8	1	-1.432370	0.086957	-2.254839
9	1	-0.807905	-0.449980	1.998883
10	1	-3.428193	-1.400381	-2.140210
11	1	-2.816723	-1.921957	2.098227
12	1	-4.109074	-2.395776	0.030419
13	8	1.882338	-0.031765	-0.763628
14	6	2.700128	-0.560572	0.339264
15	1	3.047710	0.279193	0.946158
16	6	3.833292	-1.258157	-0.399860
17	1	4.381134	-0.556413	-1.031246
18	1	4.518352	-1.671068	0.346893
19	1	3.449479	-2.071027	-1.024650
20	8	1.949842	-1.367303	1.175783
21	1	1.848847	-2.252296	0.791934
22	9	-1.350753	3.037795	0.709018
23	1	-1.771115	3.855151	0.861416

2) TS1c'

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	0.449299	-0.329353	1.316740
2	6	-1.151123	-0.241938	0.294660
3	6	-1.929346	0.913987	0.414054
4	6	-1.558280	-1.392279	-0.390269
5	6	-3.175550	0.913993	-0.209999
6	6	-2.808023	-1.361877	-1.003495
7	6	-3.610184	-0.216004	-0.912746
8	1	-1.569574	1.781261	0.955116
9	1	-0.920218	-2.266058	-0.453981
10	1	-3.805839	1.794608	-0.143429
11	1	-3.157839	-2.233729	-1.546540
12	1	-4.583910	-0.206164	-1.392259
13	8	1.867833	0.350045	0.295161
14	6	2.504568	-0.638058	-0.582299
15	1	2.810913	-1.497878	0.018848
16	6	3.689732	0.141108	-1.138215
17	1	4.353058	0.472339	-0.337309
18	1	4.244551	-0.526637	-1.804577

19	1	3.350425	1.014724	-1.703381
20	8	1.611956	-1.114757	-1.525254
21	1	1.495619	-0.468630	-2.239471
22	9	0.232744	3.017175	-0.620890
23	1	0.353599	3.913042	-0.840317

3) 2c'

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	-0.171182	-1.633286	0.091202
2	6	1.288486	-0.418758	0.021980
3	6	2.046273	-0.380385	-1.152794
4	6	1.612663	0.292191	1.181370
5	6	3.180311	0.429435	-1.161212
6	6	2.748849	1.097578	1.143590
7	6	3.526332	1.163425	-0.019934
8	1	1.764616	-0.960638	-2.024889
9	1	0.990801	0.234921	2.067455
10	1	3.792891	0.482937	-2.055082
11	1	3.030102	1.666231	2.023780
12	1	4.412423	1.790287	-0.036132
13	8	-1.650060	-0.743926	-0.635318
14	6	-2.480973	-0.040394	0.366285
15	1	-2.805988	-0.771713	1.110483
16	6	-3.630465	0.467460	-0.496044
17	1	-4.149842	-0.358790	-0.984613
18	1	-4.333865	0.985606	0.163352
19	1	-3.268582	1.165742	-1.255850
20	8	-1.754963	0.920050	1.031385
21	1	-1.655567	1.722500	0.487913
22	9	-1.406664	3.323978	-0.527634
23	1	-1.634317	4.219802	-0.407749

4) TS2c'

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	-0.177640	-1.612414	-0.024662
2	6	1.350771	-0.489725	0.001623
3	6	1.964864	-0.167575	-1.212959
4	6	1.872455	-0.085211	1.234993
5	6	3.135691	0.588635	-1.184710
6	6	3.039586	0.676952	1.243316
7	6	3.669537	1.012265	0.038255
8	1	1.545830	-0.510803	-2.152511
9	1	1.382266	-0.361662	2.162110
10	1	3.632611	0.840119	-2.116061
11	1	3.463274	0.996029	2.190080
12	1	4.582894	1.598711	0.053294
13	8	-2.172244	-0.312684	-0.452807
14	6	-2.724468	0.215798	0.592394
15	1	-3.290604	-0.401638	1.298727
16	6	-4.041524	0.635326	-0.642177
17	1	-4.557821	-0.286944	-0.884710
18	1	-4.550675	1.286104	0.071645
19	1	-3.602957	1.157109	-1.486453
20	8	-2.211350	1.287019	1.194672
21	1	-1.596092	1.775272	0.606479
22	9	-0.551080	2.731521	-0.520873
23	1	-0.364305	3.645029	-0.550916

5) 1d'

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	35	0.619630	0.837948	-0.301997
2	6	-1.062233	-0.035265	-0.116573
3	6	-1.913783	-0.052569	-1.223319
4	6	-1.384414	-0.577613	1.128896
5	6	-3.155800	-0.666027	-1.064018
6	6	-2.633387	-1.181903	1.259652
7	6	-3.511970	-1.225125	0.169428
8	1	-1.622273	0.391648	-2.168749
9	1	-0.687384	-0.538432	1.958064
10	1	-3.845687	-0.701086	-1.900870
11	1	-2.921389	-1.612800	2.212991
12	1	-4.483099	-1.696559	0.282700
13	8	1.700197	-0.467125	-1.115361
14	6	2.558065	-1.233778	-0.202308
15	1	3.049970	-1.842068	-0.979569
16	6	3.547013	-0.381609	0.558158
17	1	4.067119	0.298717	-0.119732
18	1	3.044324	0.187214	1.346928
19	1	4.282633	-1.030174	1.040184
20	8	1.810387	-1.989489	0.681400
21	1	1.374404	-2.723437	0.223242
22	9	-0.641227	3.086627	0.882280
23	1	-0.920244	3.935391	1.146382

6) TS1d’

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	-0.648448	-0.004670	-1.157501
2	6	1.048485	-0.304028	-0.353740
3	6	1.988346	0.728886	-0.420581
4	6	1.323348	-1.583431	0.141428
5	6	3.270241	0.456550	0.054584
6	6	2.613076	-1.822976	0.609090
7	6	3.579722	-0.809110	0.566005
8	1	1.726531	1.705957	-0.808999
9	1	0.560749	-2.353073	0.172334
10	1	4.026156	1.234455	0.023454
11	1	2.864600	-2.802838	1.002043
12	1	4.581942	-1.009500	0.931025
13	8	-1.724225	0.826831	0.145444
14	6	-2.515329	-0.078613	0.981424
15	1	-3.003793	0.712060	1.577318
16	6	-3.520435	-0.904217	0.212936
17	1	-4.093749	-0.270959	-0.467527
18	1	-3.023256	-1.701197	-0.349287
19	1	-4.207439	-1.379416	0.917442
20	8	-1.705287	-0.901795	1.740956
21	1	-1.236430	-0.391258	2.418211
22	9	0.520923	3.203119	0.898576
23	1	0.523411	4.092497	1.171267

7) 2d’

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	-0.519414	-1.420716	-0.057381
2	6	1.166755	-0.551462	0.063345
3	6	2.054528	-0.704907	-1.005821
4	6	1.481350	0.123497	1.246308
5	6	3.322183	-0.140382	-0.875413
6	6	2.754585	0.680189	1.348558
7	6	3.667082	0.548476	0.293729
8	1	1.770394	-1.246510	-1.901625
9	1	0.756326	0.224128	2.046305
10	1	4.038192	-0.241656	-1.684294
11	1	3.034609	1.211014	2.252468

12	1	4.657610	0.982877	0.385745
13	8	-1.616627	-0.210970	-0.987510
14	6	-2.479538	0.621468	-0.126156
15	1	-2.928913	1.200891	-0.951713
16	6	-3.509918	-0.183785	0.629901
17	1	-4.016988	-0.883145	-0.038175
18	1	-3.044737	-0.727825	1.458650
19	1	-4.251116	0.494143	1.060654
20	8	-1.738616	1.393299	0.736371
21	1	-1.272522	2.098178	0.252609
22	9	-0.440998	3.386702	-0.825017
23	1	-0.494594	4.315456	-0.884704

8) TS2d'

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	-0.387097	-1.468147	0.014943
2	6	1.273391	-0.544816	0.077936
3	6	2.064092	-0.522979	-1.074066
4	6	1.687354	0.012854	1.290641
5	6	3.316481	0.085645	-1.000828
6	6	2.942463	0.618045	1.342009
7	6	3.752904	0.655574	0.200878
8	1	1.718262	-0.979509	-1.994979
9	1	1.053674	-0.030880	2.169732
10	1	3.951564	0.108029	-1.880444
11	1	3.289714	1.049836	2.275084
12	1	4.731582	1.122369	0.250851
13	8	-1.909416	-0.006105	-0.967713
14	6	-2.755350	0.636872	-0.143955
15	1	-3.007169	0.860302	-1.345693
16	6	-3.905888	-0.086910	0.502516
17	1	-4.328957	-0.828836	-0.174636
18	1	-3.512885	-0.590242	1.395457
19	1	-4.671151	0.623022	0.820628
20	8	-2.319343	1.687432	0.545302
21	1	-1.515320	2.087945	0.148114
22	9	-0.081625	2.848662	-0.589874
23	1	0.151088	3.748796	-0.669751

9) TSc'

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	-0.179966	1.222052	0.068884
2	6	1.062511	-0.209626	0.085112
3	6	1.578465	-0.636251	1.312217
4	6	1.448810	-0.782731	-1.130546
5	6	2.504118	-1.679556	1.314796
6	6	2.374544	-1.825393	-1.106949
7	6	2.900296	-2.274194	0.111147
8	1	1.272656	-0.158791	2.236639
9	1	1.049676	-0.412812	-2.068880
10	1	2.920919	-2.021791	2.256629
11	1	2.693864	-2.278229	-2.040262
12	1	3.624144	-3.082866	0.121016
13	8	-2.323950	0.073026	0.528884
14	6	-2.965347	-0.295326	-0.521539
15	1	-3.587246	0.398706	-1.096855
16	6	-4.211032	-0.775935	0.849200
17	1	-4.685069	0.154360	1.141685
18	1	-4.756317	-1.395550	0.135244
19	1	-3.718939	-1.326305	1.643984
20	8	-2.559917	-1.314853	-1.277158
21	1	-1.879045	-1.840059	-0.818106
22	9	2.360365	2.936861	-0.333247

23	1	3.037624	3.568449	-0.417247

10) TSd'

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	-0.378409	1.065238	0.171608
2	6	1.096189	-0.129474	0.067551
3	6	1.850579	-0.356374	1.220809
4	6	1.393742	-0.723740	-1.161307
5	6	2.939466	-1.224150	1.133513
6	6	2.486771	-1.587499	-1.226218
7	6	3.256105	-1.838657	-0.083295
8	1	1.599931	0.134051	2.154961
9	1	0.800906	-0.507413	-2.043439
10	1	3.542908	-1.413566	2.015437
11	1	2.743241	-2.054811	-2.171669
12	1	4.107449	-2.509124	-0.143429
13	8	-2.041815	-0.357650	1.032466
14	6	-2.886319	-0.915978	0.154672
15	1	-3.136406	-1.172198	1.371264
16	6	-4.010350	-0.138782	-0.466941
17	1	-4.435013	0.567596	0.246176
18	1	-3.589480	0.413464	-1.317975
19	1	-4.779092	-0.814827	-0.845109
20	8	-2.465104	-1.944825	-0.581665
21	1	-1.660647	-2.348018	-0.208328
22	9	1.680850	3.159637	-0.631308
23	1	2.221112	3.892515	-0.821494