Supporting Information

Mechanism of Formation of Chiral Allyl SCF_3 Compounds via Selenium-Catalyzed Sulfenofunctionalization of Allylboronic Acids

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Contents

1. SCF_3 transfer without the participation of acid 4

We considered the mechanism where the transfer of the SCF_3 group from the SCF_3 transfer reagent **2** to Ph_2Se catalyst **3** takes place without the participation of acid **4**. The calculations show that the energy barrier is very high, 50.4 kcal/mol (Figure S1). This result is consistent with the experimental fact that the reaction cannot take place in the absence of acid **4**.

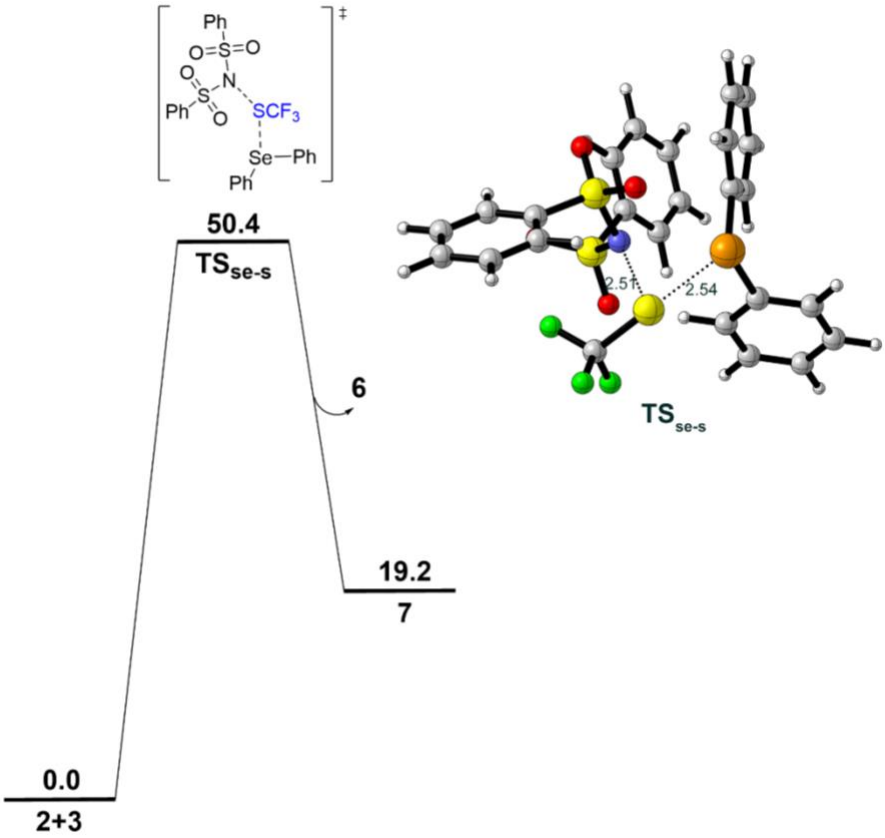

Figure S1. *Calculated free energy profile (kcal/mol) of the pathway for the SCF_3 group transfer without the participation of acid **4**. Optimized transition state structure is also given, where selected bond distances are indicated in Å.*

2. Alternative pathway for the SCF_3 transfer

An alternative pathway was considered, in which a proton is first transferred from acid **4** to $(PhSO_2)_2NSCF_3$, followed by the transfer of the SCF_3 group from the generated $(PhSO_2)_2NHSCF_3$ cation to the Ph_2Se catalyst **3** via **TS'$_{se\text{-}s}$** (Figure S2). The proton transfer step was found to be endergonic by 23.2 kcal/mol, and the barrier for the following transfer of the SCF_3 group is as high as 52.9 kcal/mol. This mechanistic alternative can thus be discarded.

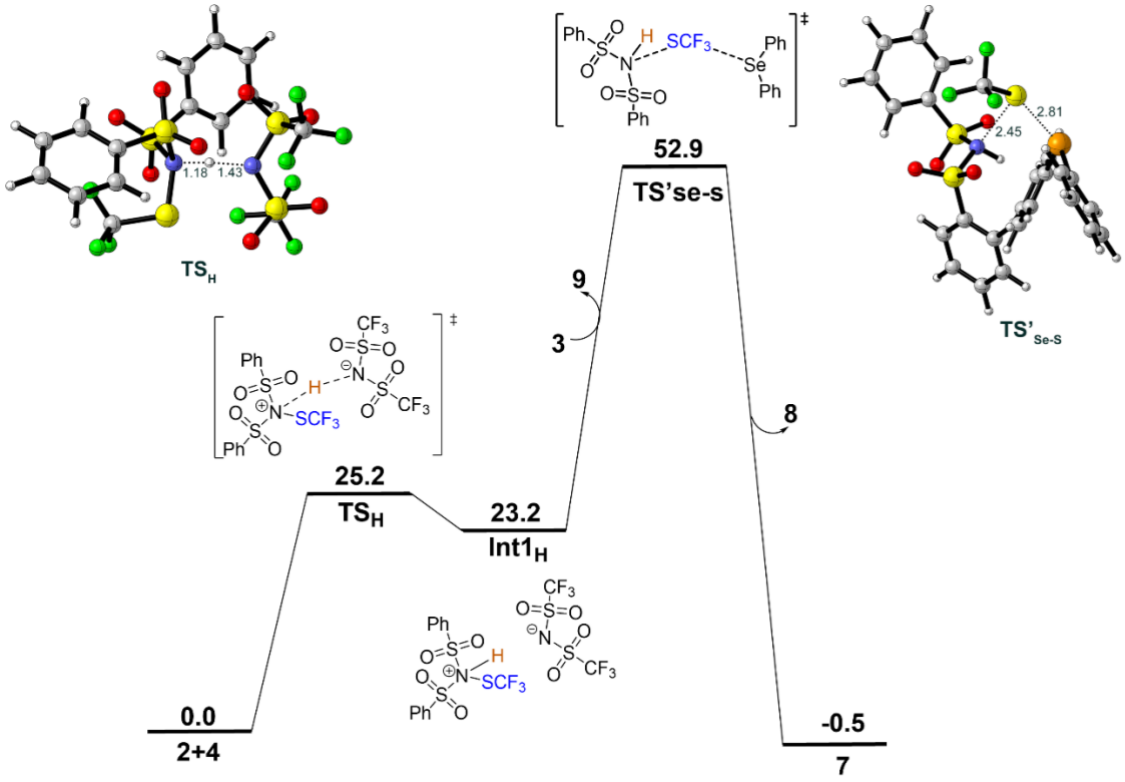

Figure S2. *Calculated free energy profile (kcal/mol) of the alternative pathway. Optimized transition state structure is also given, where selected bond distances are indicated in Å.*

3. Uncatalyzed reaction of model substrate 1a

The uncatalyzed reaction was also investigated, in which the SCF_3 group is transferred directly from reagent **2** to substrate **1a,** generating **Int2a** without the participation of catalyst **3** (Figure S3).

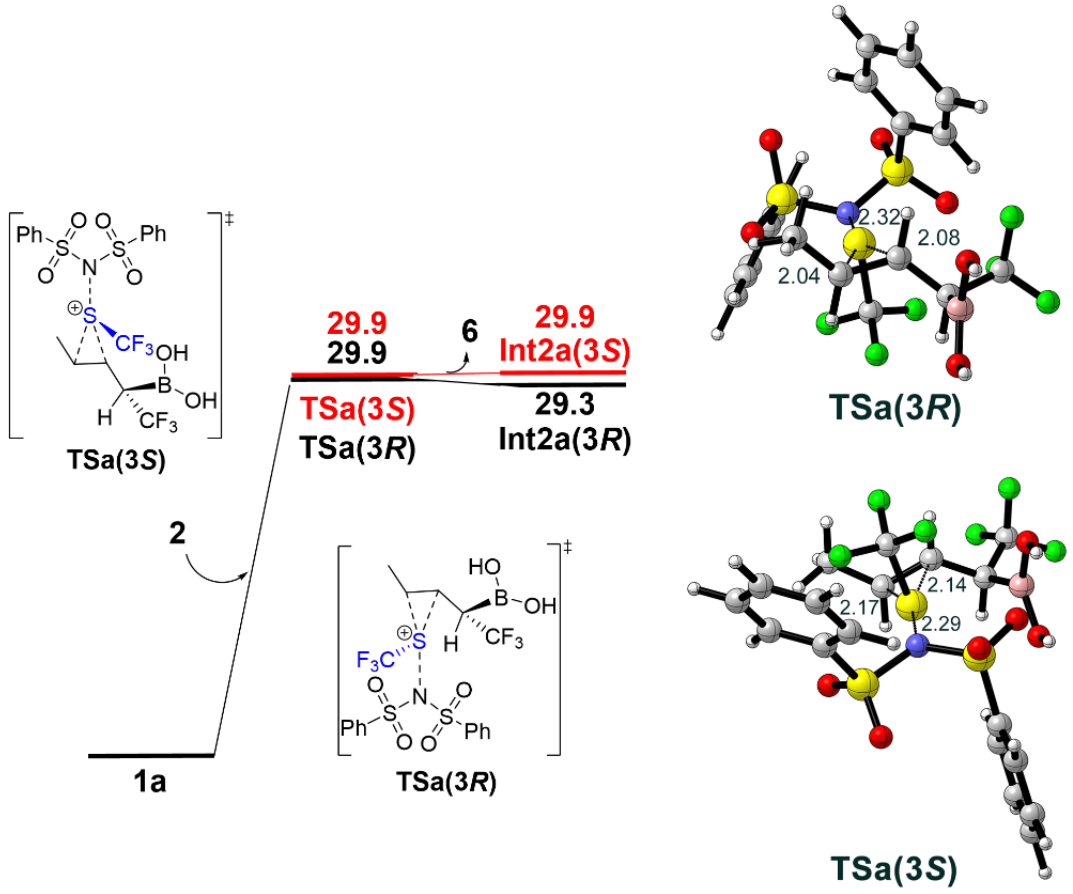

Figure S3. *Calculated free energy profile (kcal/mol) of the uncatalyzed reaction of model substrate* ***1a****. Optimized transition state structures are also given, where selected bond distances are indicated in Å.*

4. Products of model substrate 1a

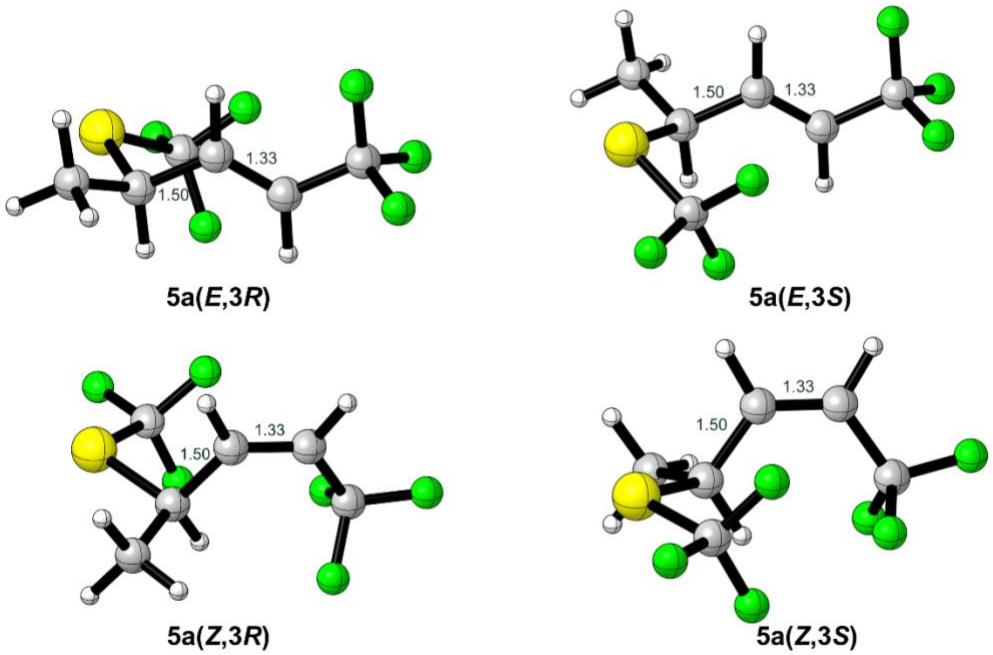

Figure S4. *Optimized structures of the products of model substrate* ***1a***. *Selected bond distances are indicated in Å.*

5. Deborylative elimination with catalyst 3

We considered the mechanism where catalyst **3** takes part in the final deborylative elimination step. The free energy profile of this is scenario shown in Figure S5. The lowest energy barrier in this scenario is 28.3 kcal/mol via **TS4'$_{anti}$(3*R*)** (Figure S6**)** to form the *E*-(3*R*)-configured product. This is 6.6 kcal/mol higher than the case without the participation of catalyst **3**, and this scenario can therefore be ruled out.

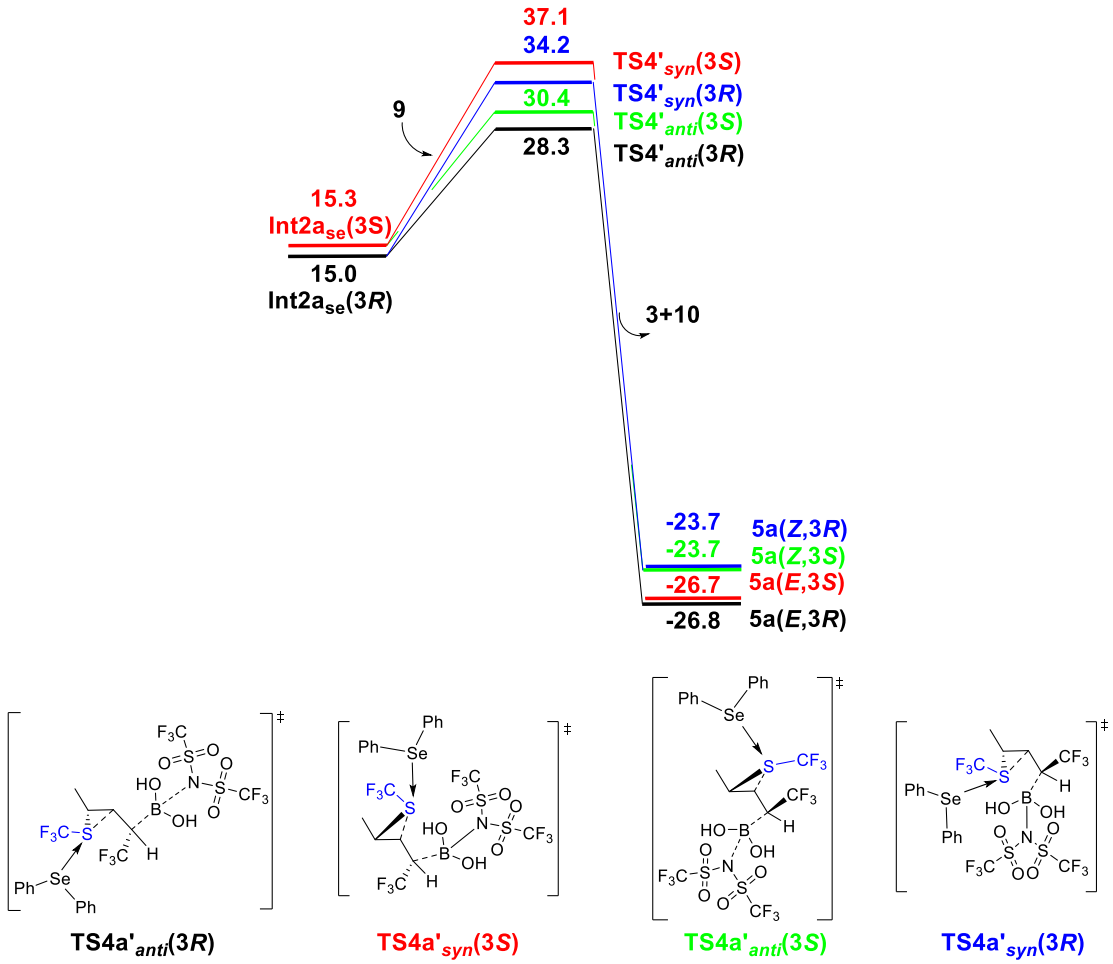

***Figure S5**. Calculated free energy profile (kcal/mol) of the deborylative elimination step with the participation of catalyst **3**.*

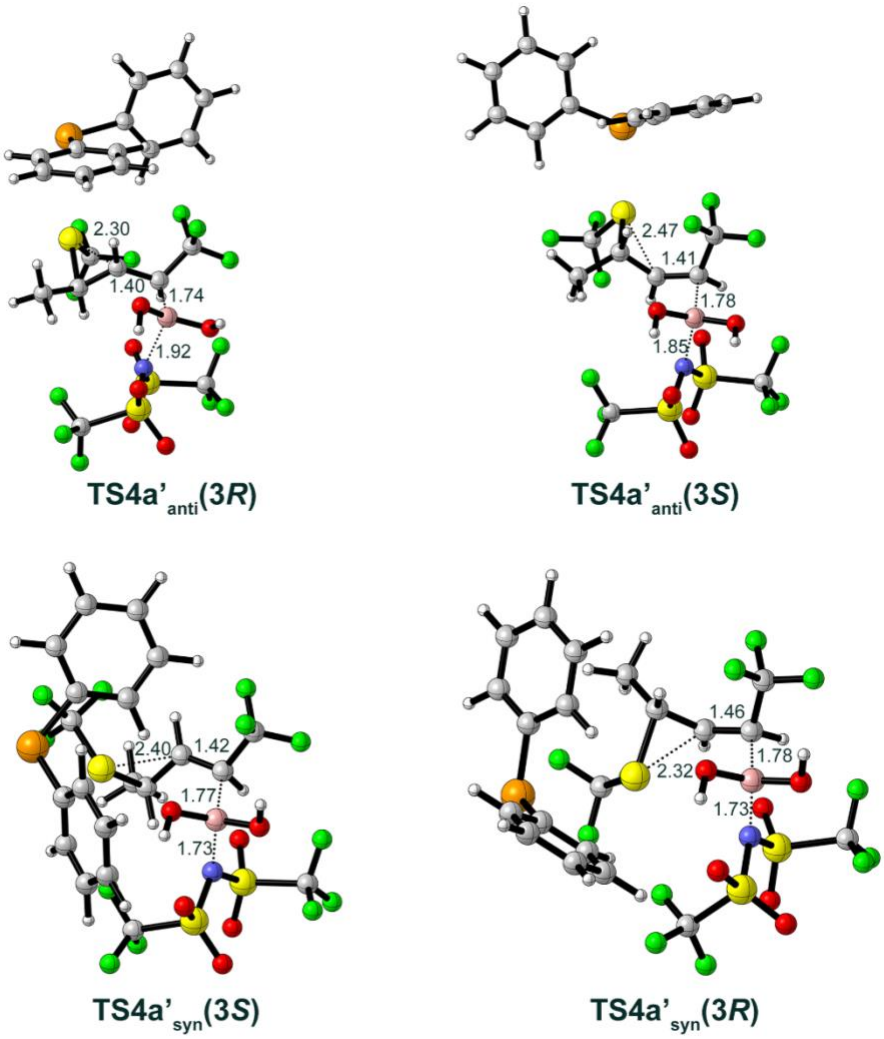

Figure S6. *Optimized structures of the transition states of the deborylative elimination step with the participation of catalyst* ***3***. *Selected bond distances are indicated in Å.*

6. $(PhSO_2)_2NH$ species 8 as the nucleophile

From **Int2a**, we considered the possibility of $(PhSO_2)_2NH$ species **8** attacking the boronate group of **Int2a** to trigger the deborylative opening of the thiiranium ion. The calculated free energy profile is shown in Figure S7 and the optimized structures of the transition states are shown in Figure S8. The energy barriers for this scenario range between 35-42 kcal/mol, which is too high to be accessible.

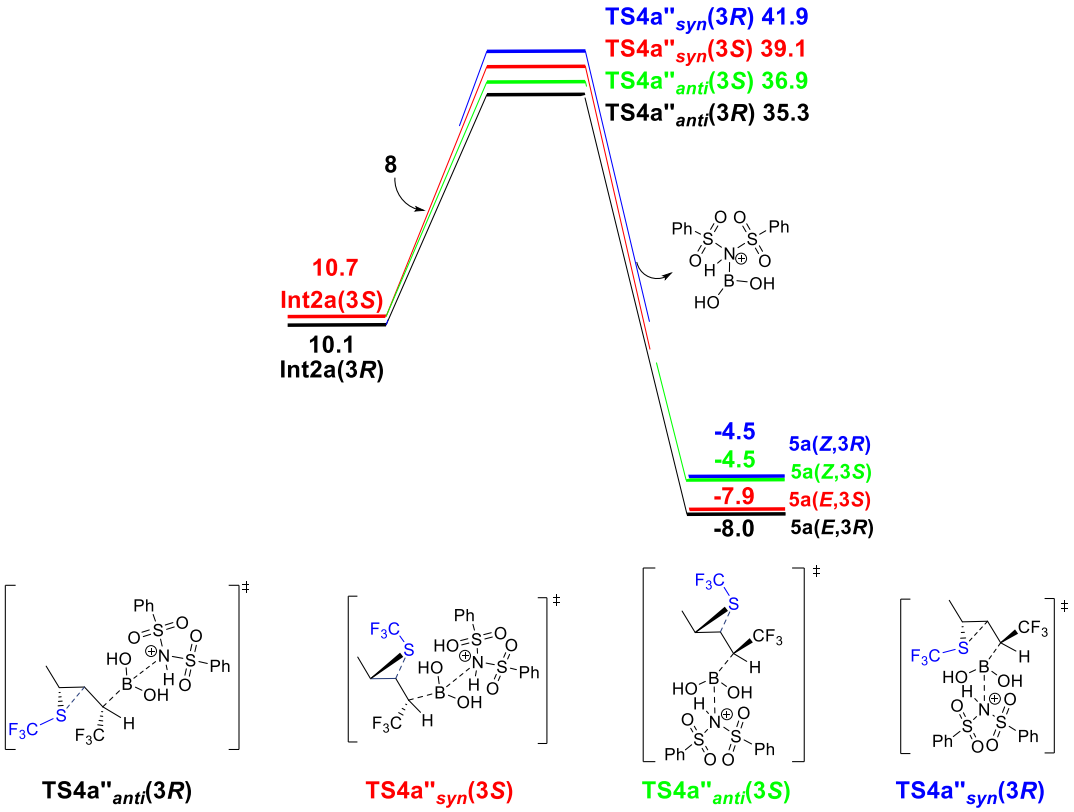

***Figure S7**. Calculated free energy profile (kcal/mol) of $(PhSO_2)_2NH$ species **8** nucleophiles attacking the boronate group of **Int2a**.*

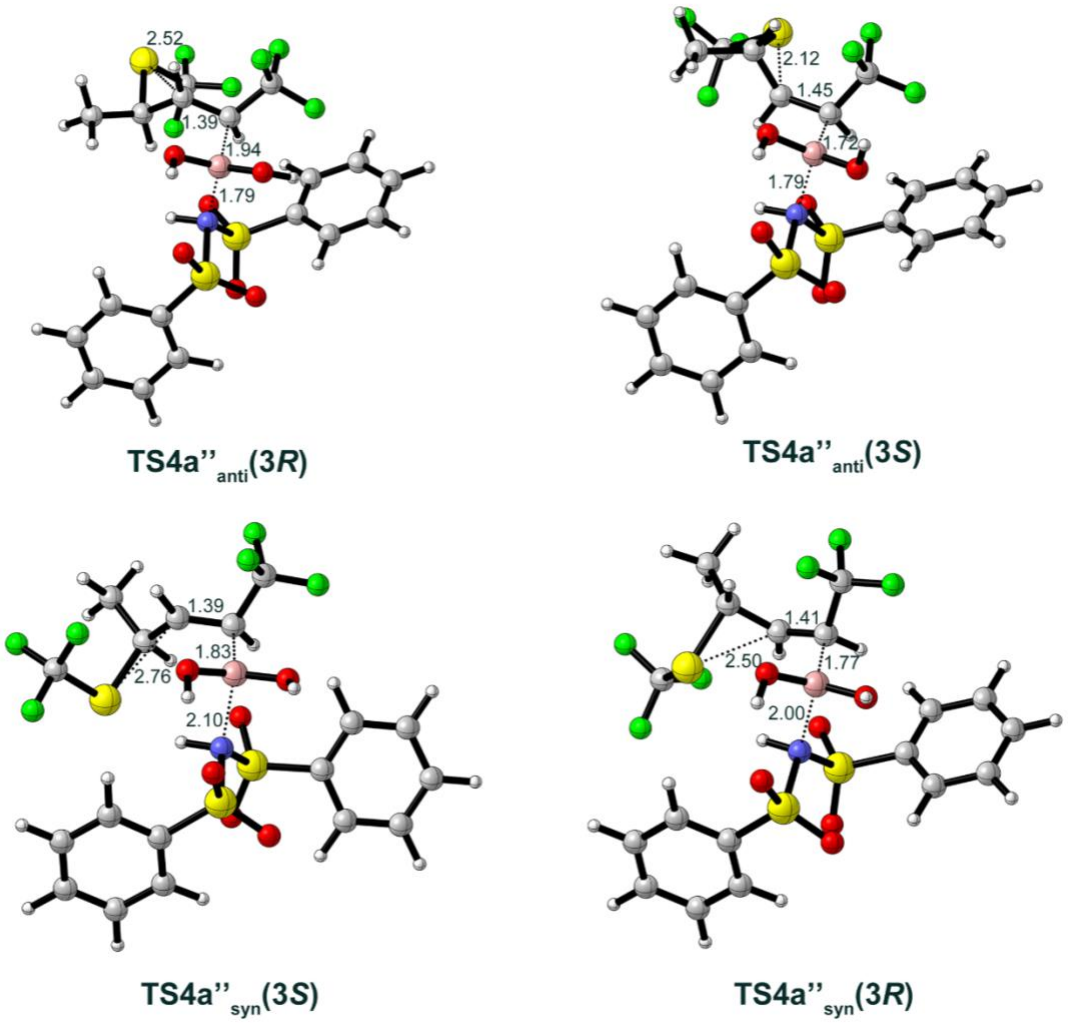

Figure S8. *Optimized structures of the transition states for $(PhSO_2)_2NH$ species* ***8*** *attacking the boronate group of* ***Int2a***. *Selected bond distances are indicated in Å.*

7. Reaction of model substrate 1a with a Bpin substituent

From the $SePh_2SCF_3$ cation **7**, we investigated the reaction to form the *E*-(3*R*)-configured product for the model substrate **1a** having a Bpin group instead of $B(OH)_2$. The calculated free energy profile and the optimized structures of the transition states are shown in Figure S9. The calculations show that the energy barrier in this case is 3.7 kcal/mol higher than that of the substrate with a $B(OH)_2$ group.

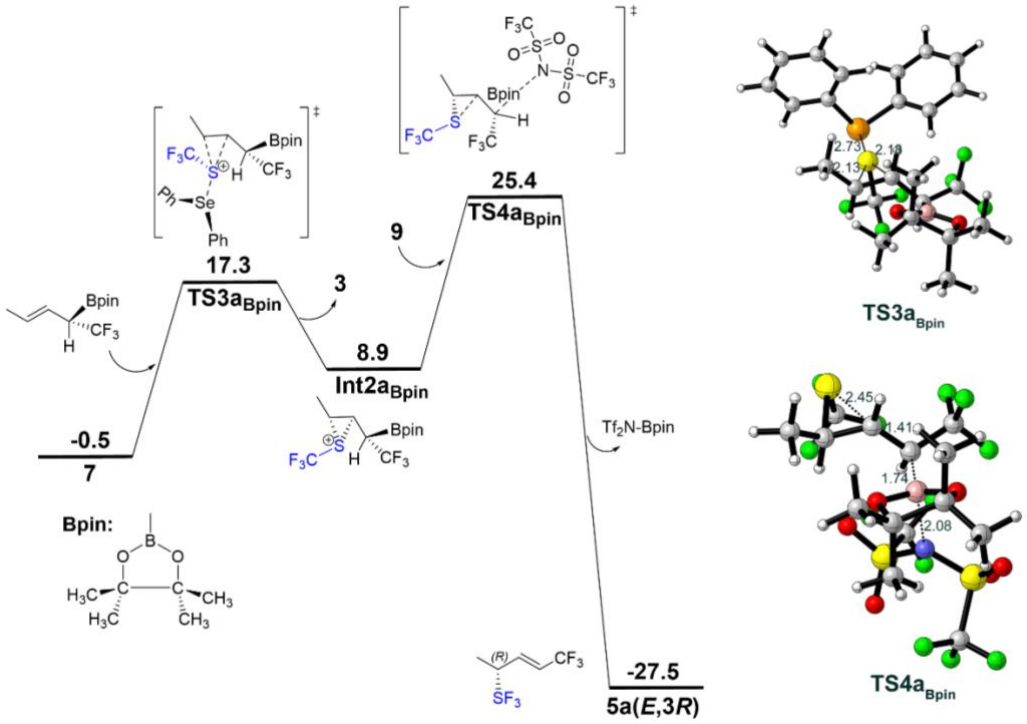

Figure S9. *Calculated free energy profile (kcal/mol) of model substrate* ***1a*** *with Bpin. Optimized transition state structures are also given, where selected bond distances are indicated in Å.*

8. Reaction of substrate 1b

The SCF_3 group of the $SePh_2SCF_3$ cation **7** is transferred to the C=C double bond of the substrate **1b**, generating the thiiranium ion **Int2b**. The optimized structures of the transition states and intermediates are shown in Figure S10.

One small difference compared to substrate **1a** is that the pathway of the *syn*-elimination to form the *Z*-(3*S*)-configured product was found to occur in a stepwise manner. The nucleophilic attack of the Tf_2N^- anion **9** on the boronate group of **Int2b(3*R*)** leads to the formation of a B-N bond at **Int3b(3*R*)**. However, no transition state could be obtained for this step. Linear transit calculations were performed by varying the B-N distance to generate **Int3b(3*R*)** (Figure S11), but the energy increased monotonously. From **Int3b(3*R*)**, the final deborylative opening of the thiiranium ion takes place to form the *Z*-(3*S*)-configured product.

The other three deborylative elimination pathways were found to take place in a concerted manner. The optimized structures of the transition states are shown in Figure S12, and the optimized structures of the products are shown in Figure S13.

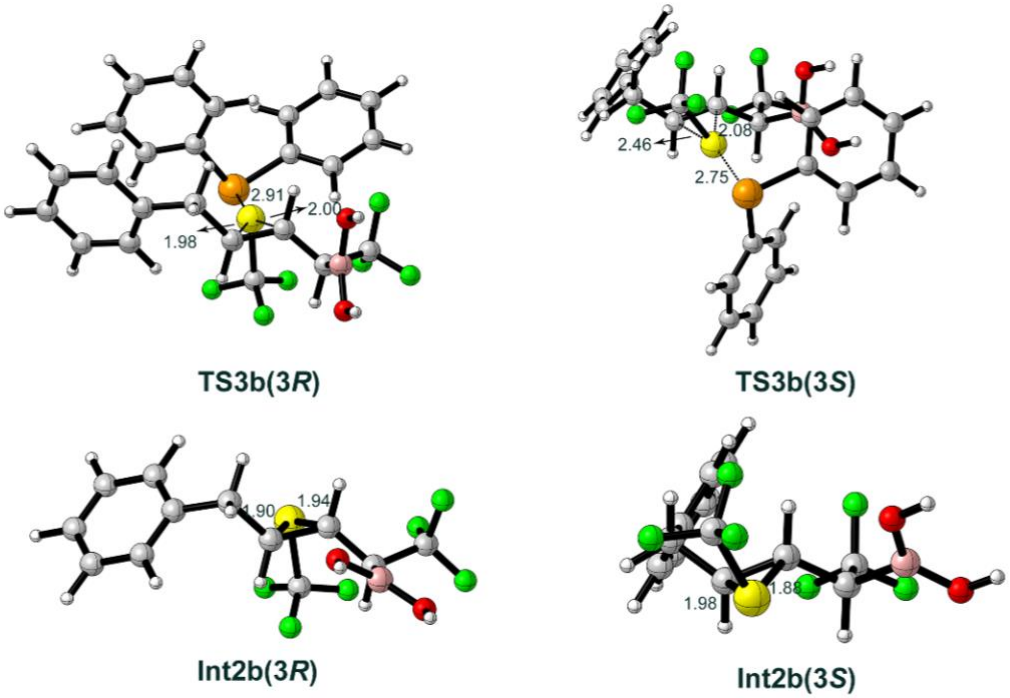

Figure S10. *Optimized structures of the transition states and intermediates for the generation of the thiiranium ion* ***Int2b****. Selected bond distances are indicated in Å.*

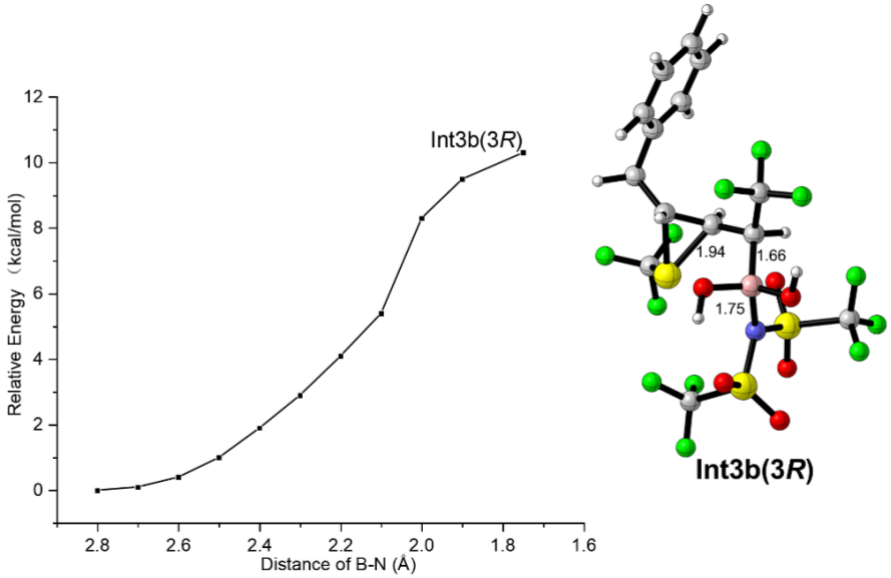

Figure S11. *Energy as a function of the B-N distance to form* ***Int3b(3R)****. Energies are given in kcal/mol at the B3LYP-D3(BJ)/6-31G(d,p) level of theory.*

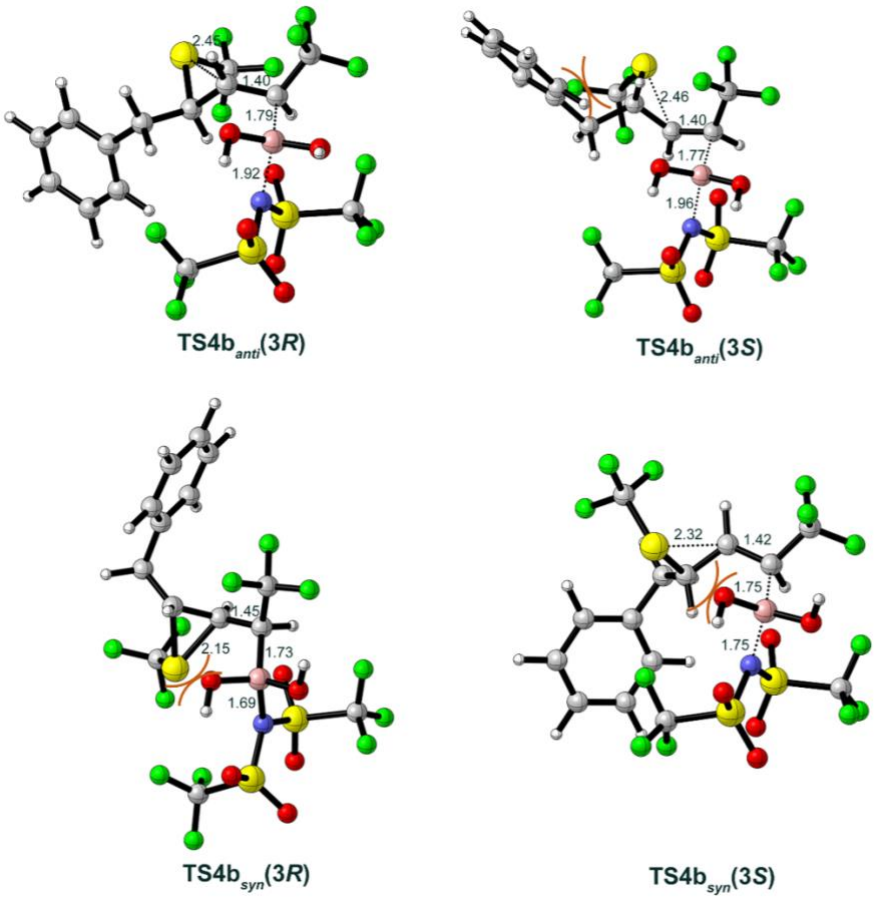

Figure S12. *Optimized structures of the transition states of the deborylative elimination step of substrate* ***1b****. Selected bond distances are shown in Å.*

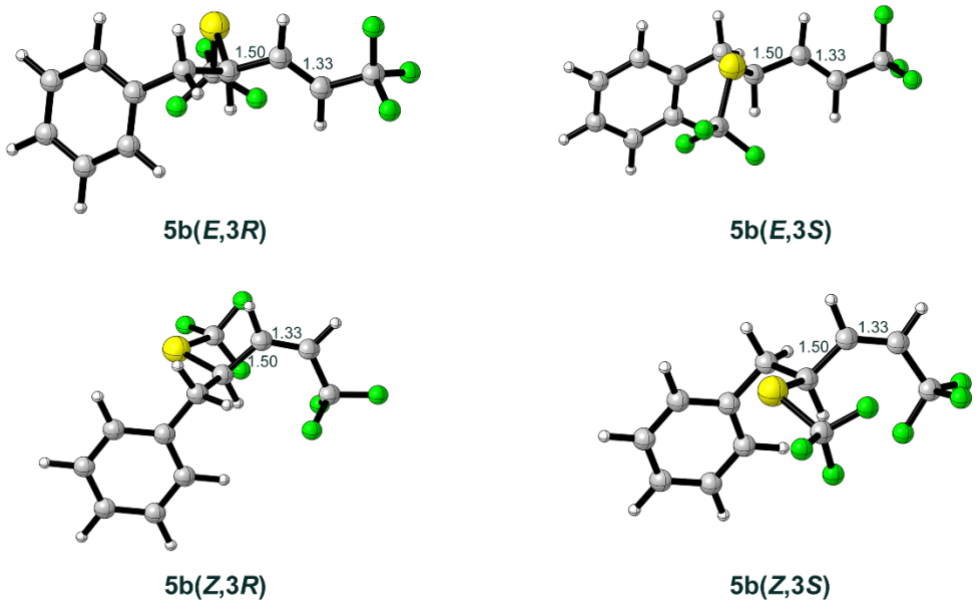

Figure S13. *Optimized structures of the products of substrate* ***1b****. Selected bond distances are indicated in Å.*

9. Reaction of substrate 1c

The calculated free energy profile of substrate **1c** is shown in Figure S14. The optimized structures of the transition states and intermediates for the generation of the thiiranium ion **Int2c** are shown in Figure S15.

In substrate **1c**, both *syn*-elimination steps were found to take place in a stepwise manner, while the *anti*-elimination steps were in a concerted manner. For the *syn*-elimination steps, the Tf_2N^- anion **9** attacks the boronate group of **Int2c**, leading to the formation of a B-N bond at **Int3c**, and no transition state could be located. Linear transit calculations were performed by varying the B-N distance to form **Int3c** (Figure S16), showing monotonous increase of the energy.

The optimized structures of the transition states for the deborylative elimination step are shown in Figure S17, and the optimized structures of the products are shown in Figure S18.

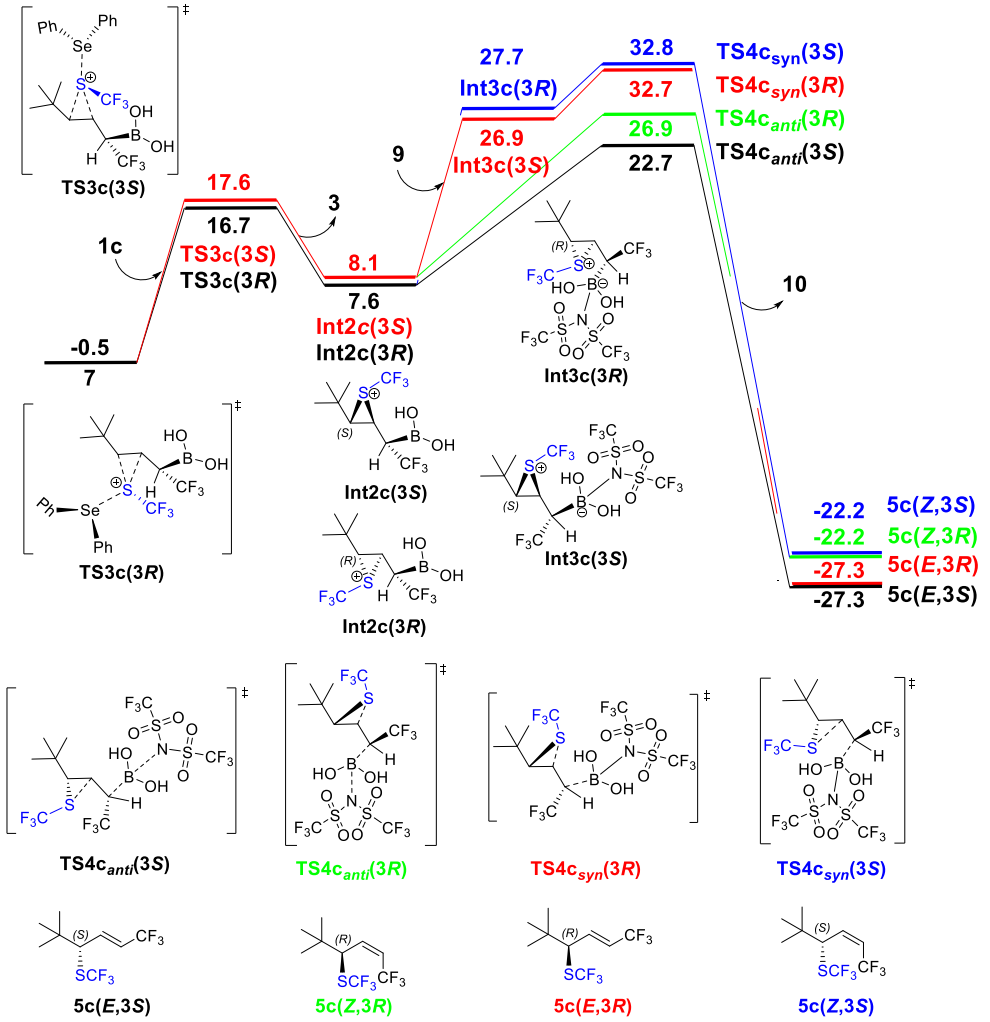

Figure S14. *Calculated free energy profile (kcal/mol) of substrate* ***1c****.*

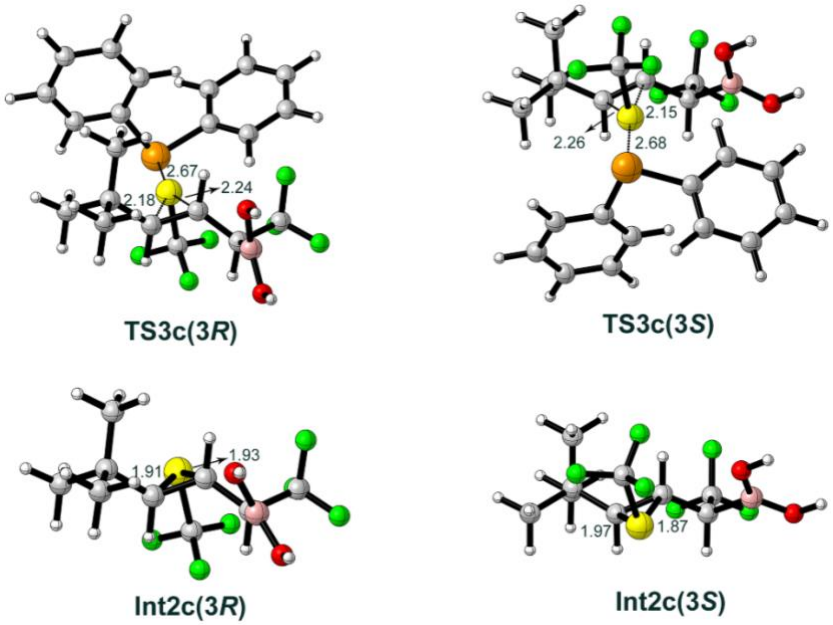

Figure S15. *Optimized structures of the transition states and intermediates for the generation of the thiiranium ion* ***Int2c****. Selected bond distances are indicated in Å.*

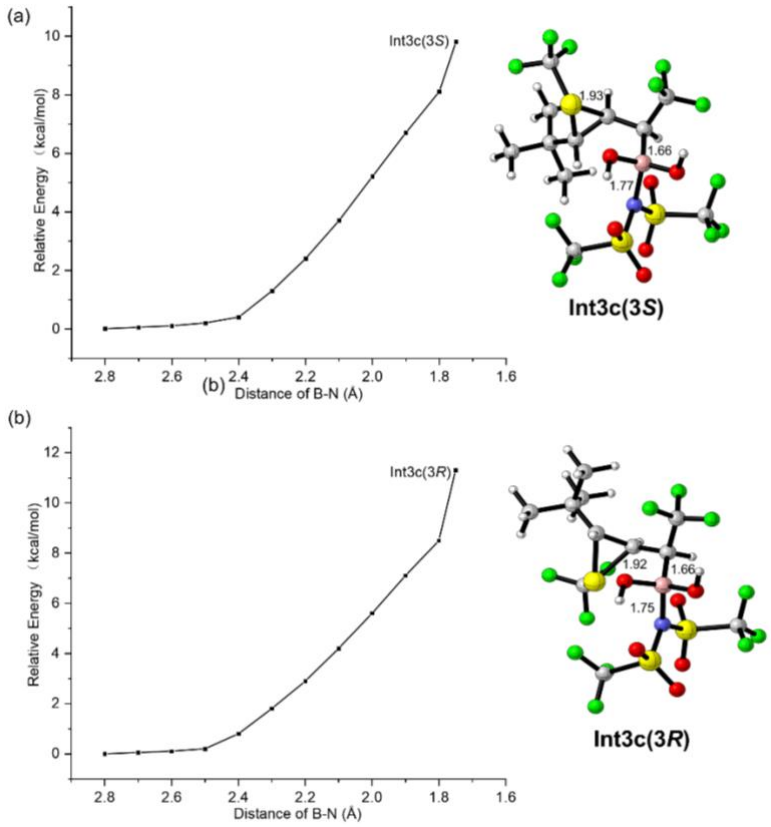

Figure S16. *(a) Energy as a function of B-N distance to form* ***Int3c(3S)****; (b) Energy as a function of B-N distance to form* ***Int3c(3R)****. Energies are given in kcal/mol at the B3LYP-D3(BJ)/6-31G(d,p) level of theory.*

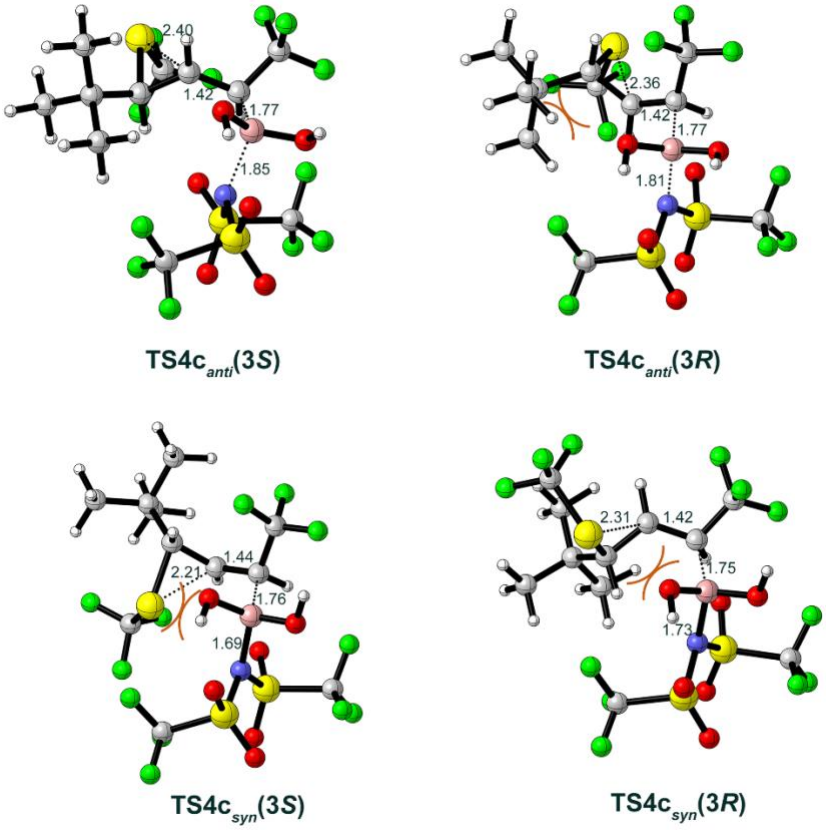

Figure S17. *Optimized structures of the transition states for the deborylative elimination step of substrate* ***1c****. Selected bond distances are shown in Å.*

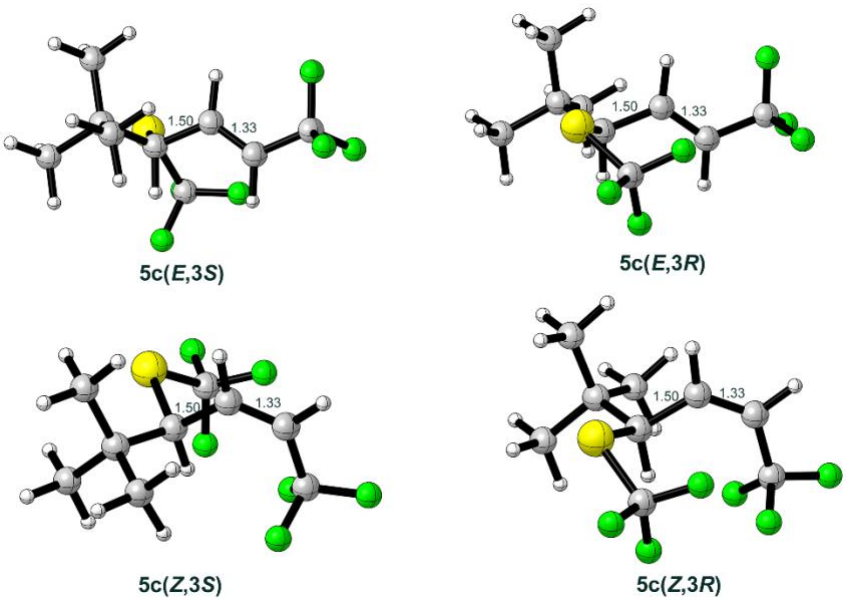

Figure S18. *Optimized structures of the products of substrate* ***1c****. Selected bond distances are indicated in Å.*

9. Intermolecular mechanism of substrate 1d

The optimized structures of the transition states and intermediates for the generation of the thiiranium ion **Int2d** are shown in Figure S19.

In the intermolecular mechanism of substrate **1d**, the *syn*-elimination steps take place in a stepwise manner, while the *anti*-elimination steps are in a concerted manner. No transition state could be located for the formation of the B-N bond at **Int3d**, and linear transit calculations were performed by varying the B-N distance to form **Int3d** showing monotonous increase of the energy (Figure S20).

The optimized structures of the transition states for the final deborylative elimination steps are shown in Figure S21, and the structures of the products are shown in Figure S22.

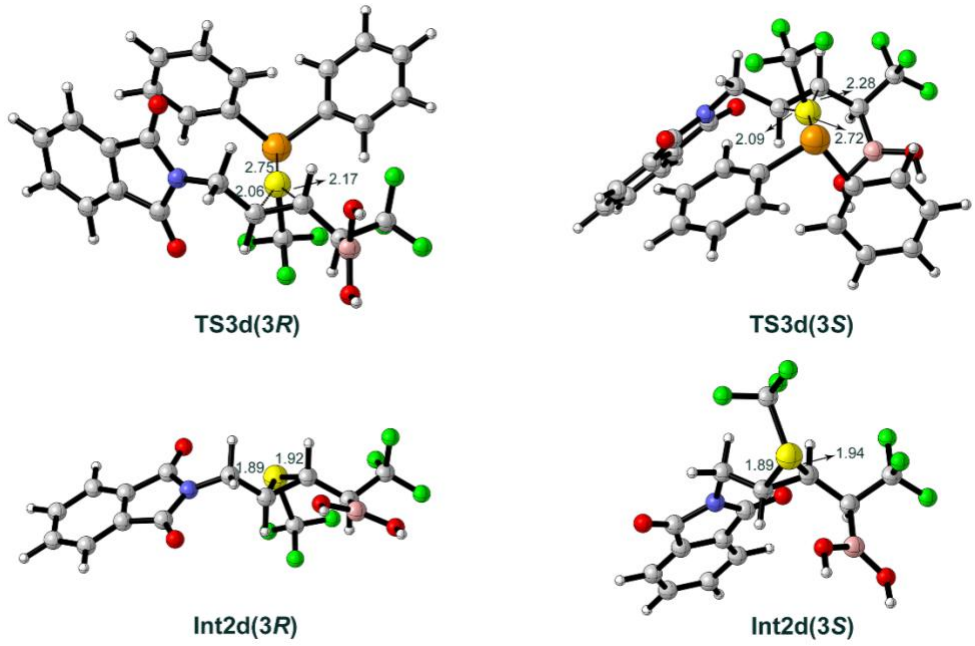

Figure S19. *Optimized structures of the transition states and intermediates for the generation of the thiiranium ion* ***Int2d****. Selected bond distances are indicated in Å.*

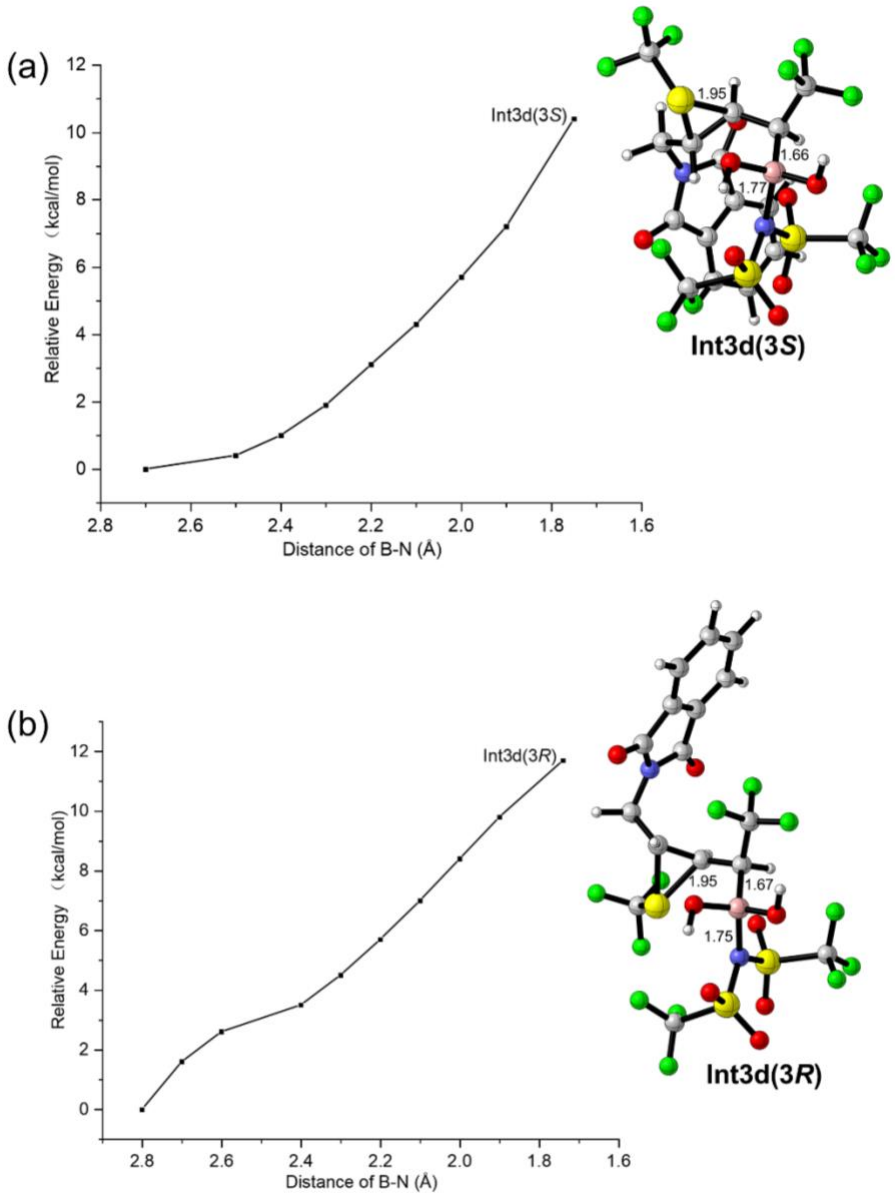

Figure S20. *(a) Energy as a function of B-N distance to form* ***Int3d(3S)****; (b) Energy as a function of B-N distance to form* ***Int3d(3R)****. Energies are given in kcal/mol at the B3LYP-D3(BJ)/6-31G(d,p) level of theory.*

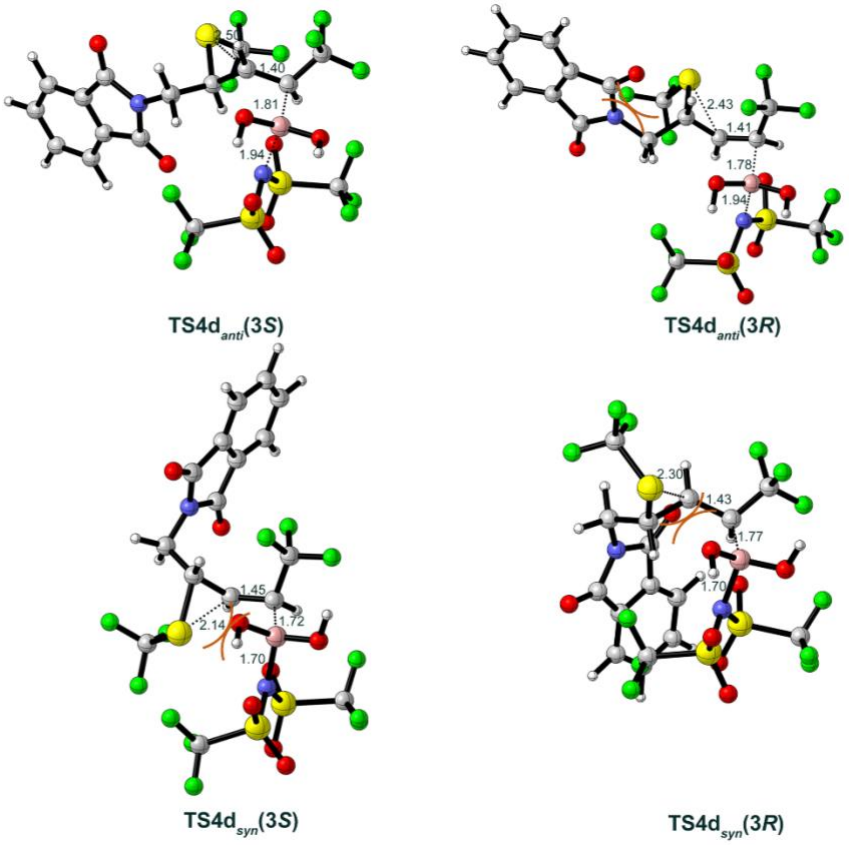

Figure S21. *Optimized structures of the transition state for the deborylative elimination step of the intermolecular mechanism of substrate* ***1d****. Selected bond distances are shown in Å.*

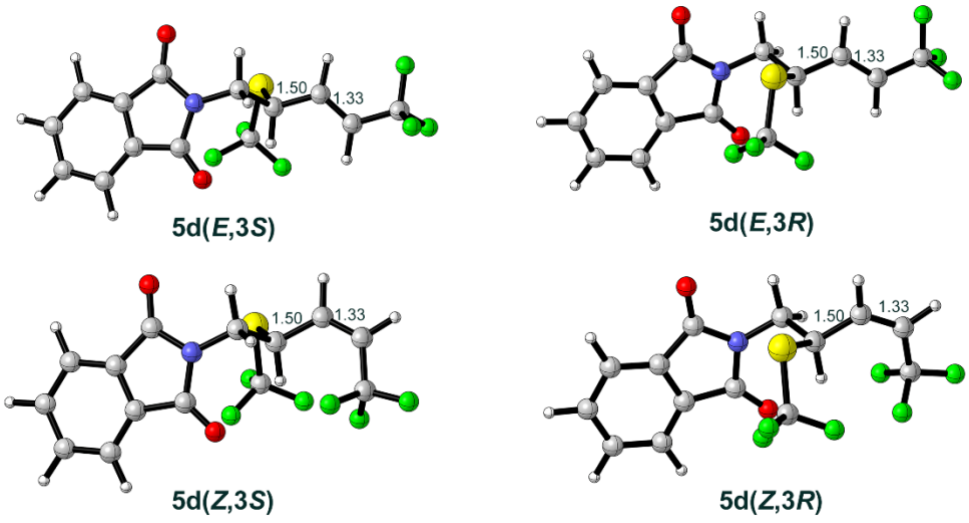

Figure S22. *Optimized structures of the products of substrate* ***1d****. Selected bond distances are indicated in Å.*

10. Intramolecular mechanism of substrate 1d

From **Int2d**, the oxygen atom of NMP performs a nucleophilic attack at the Cβ atom via **TS4d'**, leading to the opening of the thiiranium ion and yielding a six-membered ring intermediate **Int3d'**. The optimized structures of the transition states and intermediates are shown in Figure S23.

Next, the nucleophilic attack of the Tf_2N^- anion **9** on the boronate group of **Int3d'** takes place, triggering the deborylative opening of the six-membered ring to generate the final products. The calculated free energy profile for this step is shown in Figure S24. The calculations show that the *syn*-eliminations take place in a stepwise manner the B-N bond is formed at **Int4d**, and no transition states can be obtained. Linear transit calculations were performed varying the B-N distance, but the energy increases monotonously (Figure S25).

The optimized structures of the transition states for the final deborylative elimination step are shown in Figure S26.

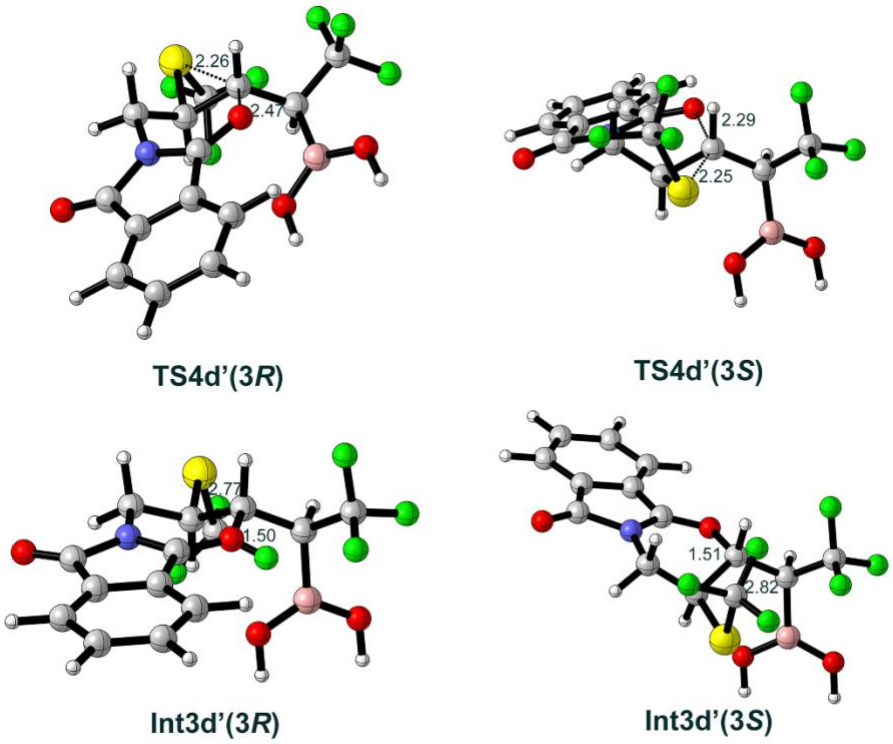

Figure S23. *Optimized structures of the transition states and intermediates for the opening of the thiiranium ion via an intermolecular mechanism of substrate* ***1d****. Selected bond distances are shown in Å.*

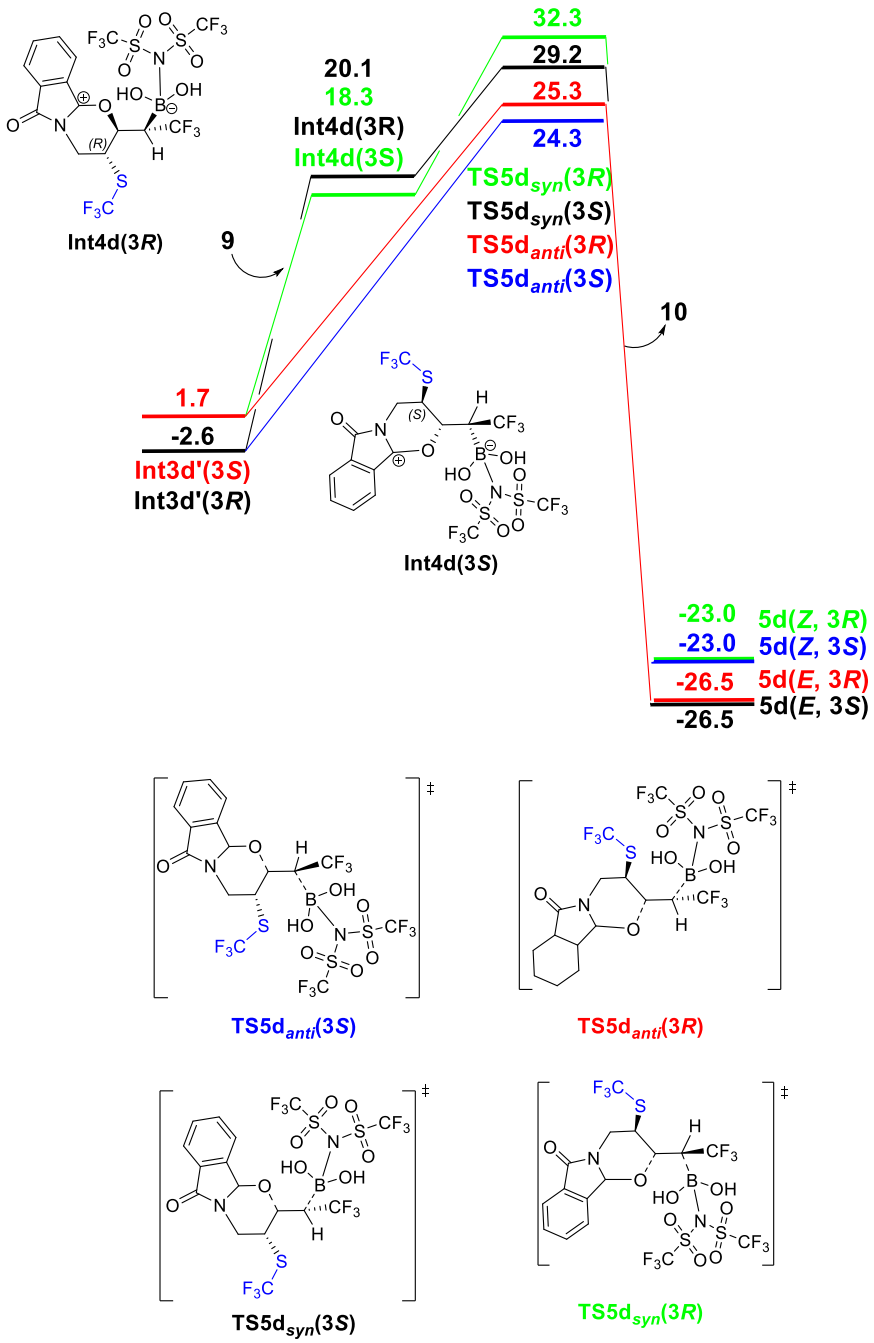

Figure S24. *Calculated free energy profile (kcal/mol) of the intramolecular mechanism from* ***Int3d****' to the products.*

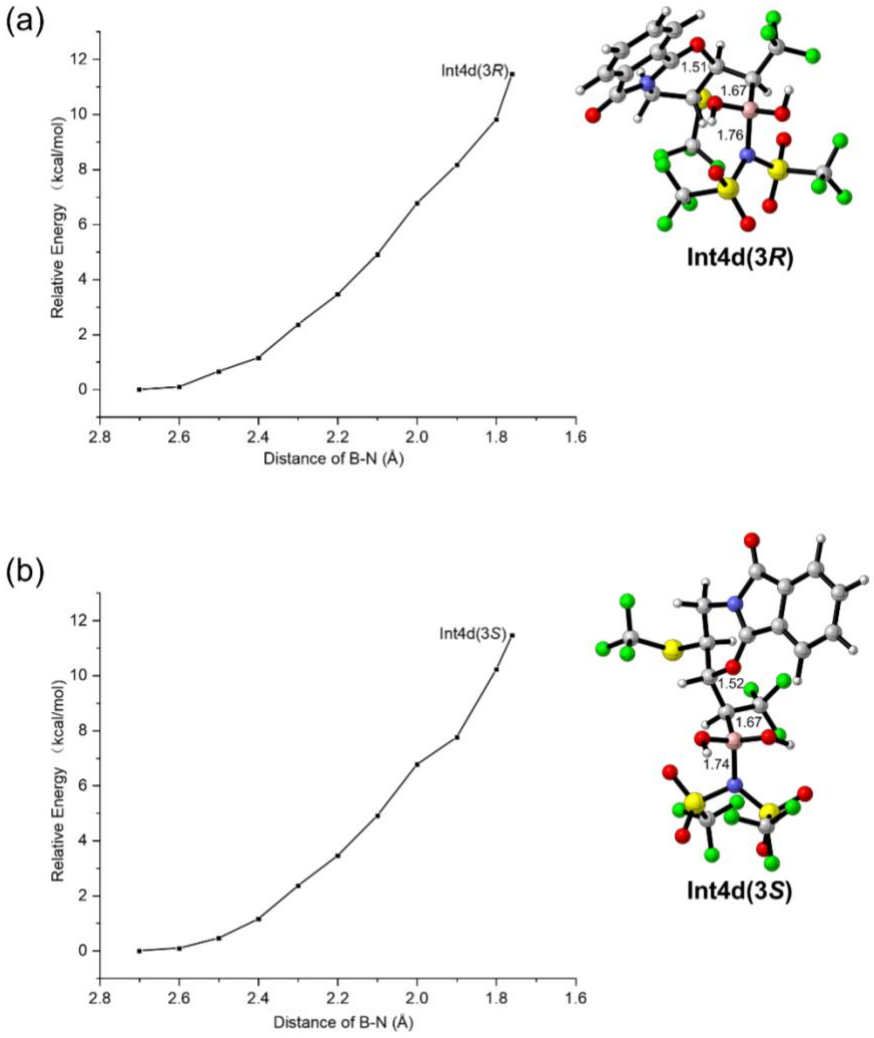

Figure S25. *(a) Energy as a function of B-N distance to form* ***Int4d(3R)****; (b) Energy as a function of B-N distance to form* ***Int4d(3S)****. Energies are given in kcal/mol at the B3LYP-D3(BJ)/6-31G(d,p) level of theory.*

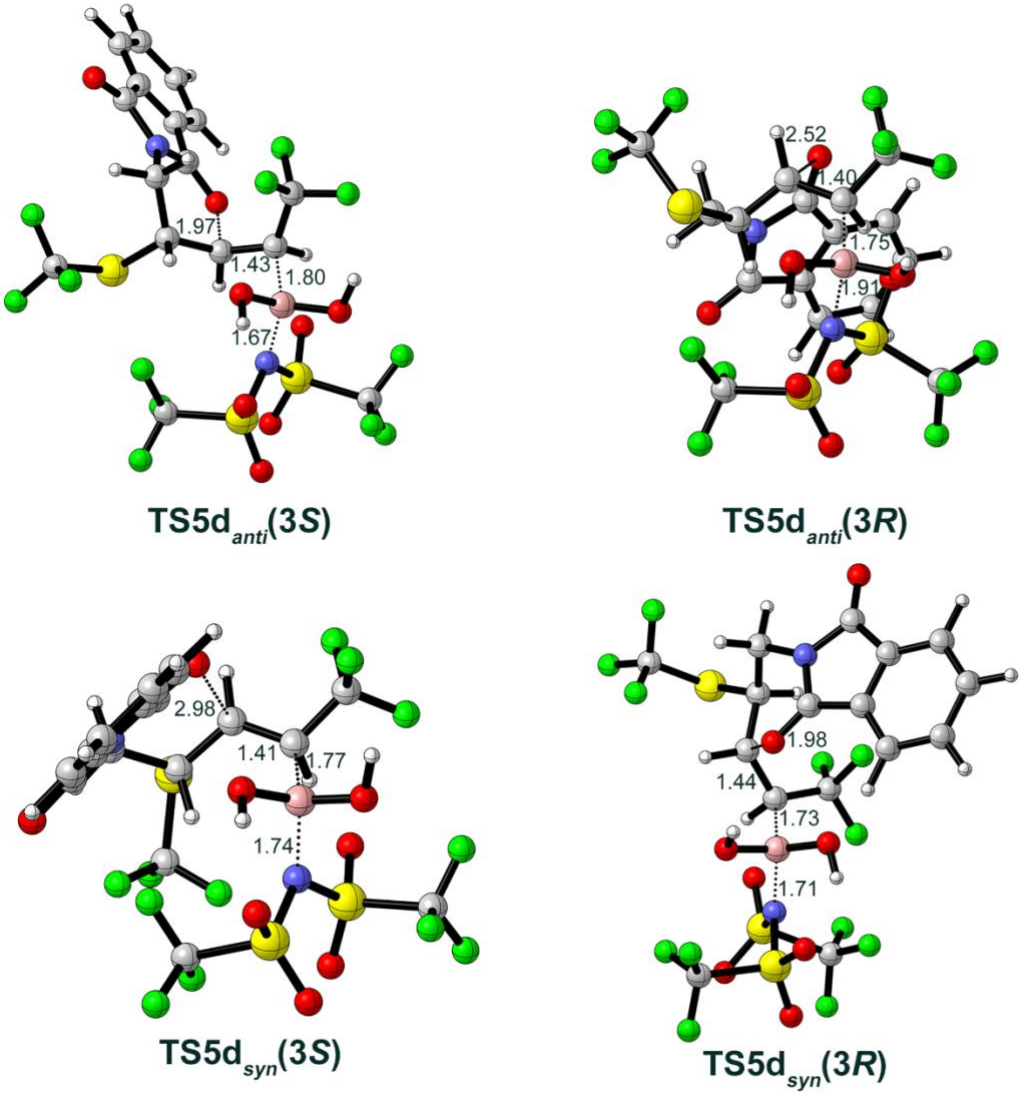

Figure S26. *Optimized structures of the transition states for the deborylative elimination step of the intramolecular mechanism of substrate* ***1d****. Selected bond distances are shown in Å.*

11. Geometry optimization with large basis set and in solvent

To evaluate the influence of the basis set and solvation effects on the geometries, we have performed two sets of calculations in which the geometries for one of the steps (Step 1: **2**+**3**+**4** → **Int1**) were re-optimized both in implicit DCM solvent and with a large basis set, 6-311+G(2d,2p). The calculations show that the geometries are very similar (Figure S27, left), and, importantly, the differences in the final energies are small (Figure S27, right).

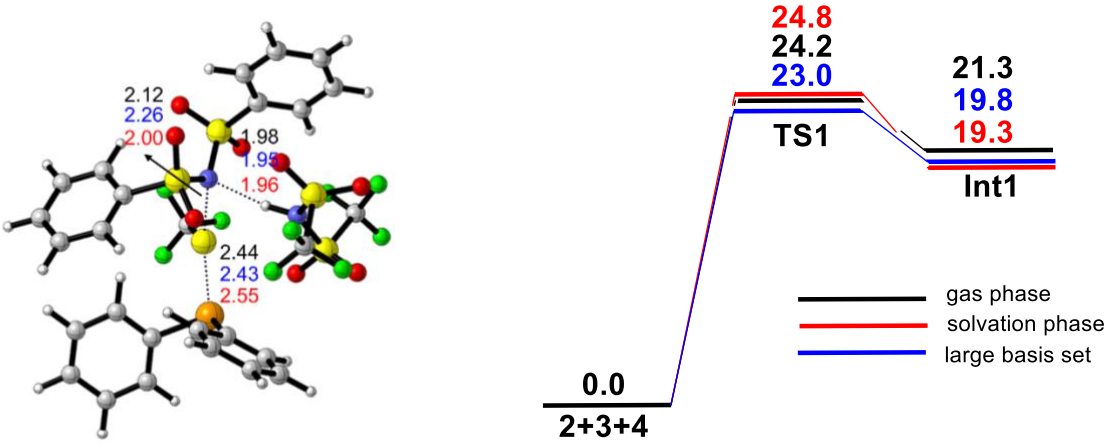

Figure S27. *Optimized structures of* ***TS1*** *with different protocols and resulting energy profiles. Selected bond distances are indicated in Å. Black numbers correspond to geometry optimization with the smaller basis set, 6-31G(d,p), in gas phase. Blue numbers correspond to geometry optimization with the larger basis set, 6-311+G(2d,2p), in the gas phase. Red numbers correspond to geometry optimization with the smaller basis set, 6-31G(d,p), in DCM solvation.*

12. Calculated absolute energies and energy corrections

Table S1*. Calculated absolute energies and energy corrections (a.u.) related to substrate* ***1a****.*

Stationary point	B3LYP-D3(BJ)/ 6-31g(d,p)	B3LYP-D3(BJ)/ 6-311+G(2d,2p)	B3LYP-D3(BJ)/ 6-31g(d,p)-SMD	Gibbs free energy correction
1a	-670.3153156	-670.5491121	-670.3300835	0.098877
2	-2351.085596	-2351.579278	-2351.107457	0.170695
3	-2862.748342	-2865.028775	-2862.764518	0.14135
4	-1827.737809	-1828.21077	-1827.745288	0.020554
TS1	-7041.631367	-7044.841294	-7041.669819	0.386563
Int1	-7041.631625	-7044.840845	-7041.674644	0.386051
TS2	-7041.627261	-7044.836167	-7041.675145	0.382383
7	-3598.336523	-3600.743971	-3598.415199	0.151496
8	-1615.880362	-1616.227641	-1615.904846	0.17136
9	-1827.239352	-1827.729759	-1827.300328	0.009974
$TS_{se\text{-}s}$	-5213.80349	-5216.55634	-5213.840584	0.339761
TS_{H}	-4178.820435	-4179.779624	-4178.845901	0.214390
$Int1_{H}$	-4178.818493	-4179.779736	-4178.845117	0.215236
$TS'_{se\text{-}s}$	-5214.189632	-5216.93448	-5214.272696	0.350867
TS3a(3*R*)	-4268.67053	-4271.301841	-4268.751915	0.275661
Int2a(3*R*)	-1405.87766	-1406.24575	-1405.959598	0.111362
TS3a(3*S*)	-4268.672342	-4271.305553	-4268.75208	0.277992
Int2a(3*S*)	-1405.875125	-1406.244765	-1405.956673	0.110909
$TS4a_{anti}$(3*R*)	-3233.270629	-3234.109064	-3233.284673	0.145371
5a(*E*,3*R*)	-1229.510924	-1229.829338	-1229.519257	0.078000
$TS4a_{anti}$(3*S*)	-3233.269748	-3234.108525	-3233.283557	0.145025
5a(*Z*,3*S*)	-1229.507573	-1229.824154	-1229.514465	0.078720
$TS4a_{syn}$(3*R*)	-3233.264893	-3234.102833	-3233.279932	0.149802

***Table S1 (continued)**. Calculated absolute energies and energy corrections (a.u.) related to substrate **1a**.*

Stationary point	B3LYP-D3(BJ)/ 6-31g(d,p)	B3LYP-D3(BJ)/ 6-311+G(2d,2p)	B3LYP-D3(BJ)/ 6-31g(d,p)-SMD	Gibbs free energy correction
5a(*Z*,3*R*)	-1229.506176	-1229.823383	-1229.513607	0.076692
TS4a$_{syn}$(3*S*)	-3233.260241	-3234.099102	-3233.274292	0.147102
5a(*E*,3*S*)	-1229.510924	-1229.829339	-1229.519451	0.077996
10	-2003.801728	-2004.333491	-2003.806821	0.043209
Int2a$_{se}$(3*R*)	-4268.674342	-4271.304255	-4268.756508	0.278047
Int2a$_{se}$(3*S*)	-4268.674089	-4271.308603	-4268.754869	0.277692
TS4a'$_{anti}$(3*R*)	-6096.05162	-6099.156525	-6096.077101	0.310221
TS4a'$_{syn}$(3*R*)	-6096.053219	-6099.15502	-6096.07636	0.315797
TS4a'$_{anti}$(3*S*)	-6096.045543	-6099.149587	-6096.072156	0.307798
TS4a'$_{syn}$(3*S*)	-6069.048297	-6099.148136	-6096.071938	0.313976
TS4a''$_{anti}$(3*R*)	-3021.780399	-3022.483876	-3021.862244	0.30867
TS4a''$_{syn}$(3*R*)	-3021.776227	-3022.480201	-3021.854579	0.307088
TS4a''$_{anti}$(3*S*)	-3021.779464	-3022.484076	-3021.858982	0.309085
TS4a''$_{syn}$(3*S*)	-3021.774017	-3022.477703	-3021.854134	0.306892
TS3a$_{Bpin}$	-4503.393441	-3468.884664	-3468.017676	0.287307
Int2a$_{Bpin}$	-1640.60231	-1641.018261	-1640.679781	0.251581
TS4a$_{Bpin}$	-3467.974648	-3468.86139	-3468.000529	0.288642
10'	-2238.5117543	-2239.093057	-2238.5219393	0.181143

***Table S2**. Calculated absolute energies and energy corrections (a.u.) related to substrate **1b**.*

Stationary point	B3LYP-D3(BJ)/ 6-31g(d,p)	B3LYP-D3(BJ)/ 6-311+G(2d,2p)	B3LYP-D3(BJ)/ 6-31g(d,p)-SMD	Gibbs free energy correction
1b	-901.3971968	-901.6879563	-901.4197074	0.173229
TS3b(3*R*)	-4499.759853	-4502.446321	-4499.84482	0.35088
Int2b(3*R*)	-1636.964524	-1637.390292	-1637.049384	0.184844
TS3b(3*S*)	-4499.760609	-4502.449864	-4499.843011	0.352755
Int2b(3*S*)	-1636.962764	-1637.389439	-1637.046786	0.184821
Int3b(3*R*)	-3464.350132	-3465.244704	-3464.373911	0.22401
TS4b$_{anti}$(3*R*)	-3464.357499	-3465.252652	-3464.378086	0.220217
5b(*E*,3*R*)	-1460.589955	-1460.966542	-1460.606085	0.150306
TS4b$_{anti}$(3*S*)	-3464.353299	-3465.247911	-3464.372514	0.219962
5b(*Z*,3*S*)	-1460.589488	-1460.963858	-1460.605731	0.152308
TS4b$_{syn}$(3*R*)	-3464.348862	-3465.242791	-3464.370887	0.22527
5b(*Z*,3*R*)	-1460.589488	-1460.963858	-1460.605731	0.152308
TS4b$_{syn}$(3*S*)	-3464.347527	-3465.241312	-3464.366202	0.223597
5b(*E*,3*S*)	-1460.58995	-1460.966235	-1460.606063	0.151254

***Table S3**. Calculated absolute energies and energy corrections (a.u.) related to substrate **1c**.*

Stationary point	B3LYP-D3(BJ)/ 6-31g(d,p)	B3LYP-D3(BJ)/ 6-311+G(2d,2p)	B3LYP-D3(BJ)/ 6-31g(d,p)-SMD	Gibbs free energy correction
1c	-788.2825807	-788.5445794	-788.2990727	0.178518
TS3c(3*S*)	-4386.64774	-4389.304346	-4386.726126	0.356655
Int2c(3*S*)	-1523.852784	-1524.248824	-1523.931771	0.190769
TS3c(3*R*)	-4386.645456	-4389.302853	-4386.724649	0.357418
Int2c(3*R*)	-1523.852437	-1524.248705	-1523.930751	0.190716
Int3c(3*S*)	-3351.234753	-3352.098334	-3351.252573	0.230415
Int3c(3*R*)	-3351.235594	-3352.100145	-3351.252485	0.22998
TS4c$_{anti}$(3S)	-3351.234465	-3352.098656	-3351.248678	0.227101
5c(*E*,3*S*)	-1347.477874	-1347.824484	-1347.487241	0.155687
TS4c$_{anti}$(3*R*)	-3351.231279	-3352.094113	-3351.245298	0.226118
5c(*Z*,3*R*)	-1347.47716	-1347.820169	-1347.486217	0.159603
TS4c$_{syn}$(3*S*)	-3351.231412	-3352.093697	-3351.246904	0.231474
5c(*Z*,3*S*)	-1347.477141	-1347.820385	-1347.486072	0.159335
TS4c$_{syn}$(3*R*)	-3351.228828	-3352.092416	-3351.243584	0.229393
5c(*E*,3*R*)	-1347.47819	-1347.824357	-1347.487549	0.155697

***Table S4**. Calculated absolute energies and energy corrections (a.u.) related to substrate **1d**.*

Stationary point	B3LYP-D3(BJ)/ 6-31g(d,p)	B3LYP-D3(BJ)/ 6-311+G(2d,2p)	B3LYP-D3(BJ)/ 6-31g(d,p)-SMD	Gibbs free energy correction
1d	-1182.249847	-1182.627273	-1182.278482	0.181999
TS3d(3*R*)	-4780.615147	-4783.387514	-4780.703621	0.361291
Int2d(3*R*)	-1917.818683	-1918.329709	-1917.906489	0.195252
TS3d(3*S*)	-4780.613858	-4783.385984	-4780.700622	0.362637
Int2d(3*S*)	-1917.821613	-1918.331689	-1917.905708	0.197352
Int3d(3*R*)	-3745.205866	-3746.18493	-3745.23228	0.23517
Int3d(3*S*)	-3745.203655	-3746.182605	-3745.228502	0.231742
TS4d$_{anti}$(3*S*)	-3745.211003	-3746.191454	-3745.236784	0.231556
5d(*E*,3*S*)	-1741.448068	-1741.909641	-1741.468997	0.162358
TS4d$_{anti}$(3*R*)	-3745.206632	-3746.186867	-3745.23174	0.230216
5d(*Z*,3*R*)	-1741.445948	-1741.905192	-1741.466764	0.163359
TS4d$_{syn}$(3*S*)	-3745.204933	-3746.183748	-3745.230228	0.235704
5d(*Z*,3*S*)	-1741.445948	-1741.905193	-1741.466764	0.163356
TS4d$_{syn}$(3*R*)	-3745.209384	-3746.188285	-3745.232467	0.236238
5d(*E*,3*R*)	-1741.448068	-1741.909649	-1741.468993	0.16227
TS4d'(3*R*)	-1917.819228	-1918.32935	-1917.905647	0.197319
Int3d'(3*R*)	-1917.85247	-1918.360161	-1917.938384	0.201352
TS4d'(3S)	-1917.818349	-1918.327828	-1917.901045	0.198164
Int3d'(3S)	-1917.845664	-1918.352826	-1917.932056	0.201447
Int4d(3*R*)	-3745.22316	-3746.198301	-3745.25412	0.239981
Int4d(3*S*)	-3745.210772	-3746.190969	-3745.248486	0.236512
TS5d$_{anti}$(3*S*)	-3745.213407	-3746.191782	-3745.241407	0.237263
TS5d$_{anti}$(3*R*)	-3745.209495	-3746.190179	-3745.232479	0.232044
TS5d$_{syn}$(3*S*)	-3745.206625	-3746.185323	-3745.230168	0.234268
TS5d$_{syn}$(3*R*)	-3745.195408	-3746.174447	-3745.225812	0.235117

13. Cartesian coordinates

1a			
C	3.80800	-0.13387	0.21424
H	4.40920	0.76684	0.03721
H	4.37565	-0.97608	-0.20029
H	3.72433	-0.27938	1.29510
C	2.45878	-0.02223	-0.43040
H	2.44827	0.11877	-1.51183
C	1.29612	-0.08332	0.22094
H	1.28677	-0.21773	1.30096
C	-0.05546	0.08030	-0.43080
B	-0.66795	1.49528	-0.03184
O	-0.79032	2.41724	-1.03350
H	-1.12131	3.28025	-0.75674
O	-0.98280	1.71084	1.27941
H	-1.33552	2.58489	1.48284
C	-0.99160	-1.05414	-0.07274
F	-2.23860	-0.82367	-0.56155
F	-0.58139	-2.23741	-0.58312
F	-1.11445	-1.22261	1.26209
H	0.05225	0.05416	-1.51956

2			
N	0.22320	0.32765	-0.37640
S	-0.24413	-1.29869	-0.83493
O	-0.31805	-1.31784	-2.29126
O	0.67291	-2.16801	-0.10524
C	-1.89276	-1.42788	-0.17536
C	-2.08094	-1.32359	1.20394
C	-2.94933	-1.61771	-1.06368
C	-3.37917	-1.40948	1.69844
H	-1.23485	-1.16154	1.86227
C	-4.24128	-1.70769	-0.54839
H	-2.75323	-1.68016	-2.12715
C	-4.45412	-1.60116	0.82629
H	-3.55200	-1.32352	2.76602
H	-5.07951	-1.85369	-1.22155
H	-5.46308	-1.66399	1.22159
S	1.31131	0.61920	1.00671
O	0.85803	-0.22836	2.10566
O	1.34340	2.07284	1.11615
C	2.89223	0.05364	0.41822
C	3.34911	-1.21001	0.78664
C	3.63651	0.91352	-0.39087
C	4.59557	-1.62279	0.32056
H	2.73197	-1.84638	1.40658
C	4.87723	0.48128	-0.85213
H	3.25403	1.89743	-0.63603
C	5.35351	-0.78303	-0.49736
H	4.97159	-2.60292	0.59395
H	5.47319	1.13271	-1.48256
H	6.32178	-1.11410	-0.85923
S	-0.41371	1.63863	-1.22931
C	-1.85943	2.10290	-0.17506
F	-2.06841	3.41535	-0.36038
F	-1.63714	1.86156	1.11941
F	-2.98565	1.45858	-0.52330

3			
Se	-0.00004	1.56470	0.00025
C	-1.44409	0.29472	0.08136
C	-2.42680	0.30277	-0.91025
C	-1.52164	-0.61643	1.13859
C	-3.49174	-0.59742	-0.84066
H	-2.35055	1.00578	-1.73303
C	-2.57467	-1.52667	1.19273
H	-0.75399	-0.61214	1.90485
C	-3.56423	-1.51546	0.20644
H	-4.25591	-0.58776	-1.61201
H	-2.62894	-2.23914	2.01039
H	-4.38787	-2.22098	0.25524
C	1.44410	0.29488	-0.08129
C	1.52219	-0.61529	-1.13931
C	2.42628	0.30208	0.91084
C	2.57525	-1.52548	-1.19372
H	0.75493	-0.61029	-1.90596
C	3.49125	-0.59804	0.84101
H	2.34956	1.00438	1.73419
C	3.56429	-1.51514	-0.20690
H	2.62998	-2.23723	-2.01198
H	4.25502	-0.58909	1.61276
H	4.38796	-2.22060	-0.25592

4

N	-0.00015	-0.00027	-0.85305
H	-0.00012	-0.00043	-1.87024
S	1.24080	-0.89942	-0.11960
O	0.80078	-1.33942	1.18872
O	1.72902	-1.78462	-1.16462
C	2.54811	0.42016	0.12985
F	2.09793	1.35426	0.95509
F	2.83716	0.96008	-1.05381
F	3.62713	-0.16502	0.63895
S	-1.24070	0.89931	-0.11964
O	-1.72872	1.78481	-1.16447
O	-0.80042	1.33901	1.18872
C	-2.54827	-0.41998	0.12985
F	-2.83793	-0.95941	-1.05391
F	-2.09784	-1.35450	0.95451
F	-3.62696	0.16513	0.63964

TS1

N	0.48027	1.66412	-0.04859
S	0.08301	2.05110	1.55244
O	-0.08792	0.74953	2.21513
O	1.01614	3.04380	2.08544
C	-1.55406	2.78542	1.45914
C	-1.79286	3.86520	0.60888
C	-2.54813	2.26548	2.28670
C	-3.07172	4.41920	0.58133
H	-0.99909	4.24926	-0.02241
C	-3.81750	2.84232	2.26154
H	-2.31826	1.42350	2.92857
C	-4.08022	3.91350	1.40581
H	-3.27861	5.25209	-0.08276
H	-4.59941	2.45015	2.90395
H	-5.07013	4.35924	1.38366
S	1.44953	2.68329	-1.03177
O	1.03602	4.08427	-0.89314
O	1.40372	2.00502	-2.33059
C	3.11829	2.51848	-0.41847
C	3.93534	1.56090	-1.01961
C	3.57035	3.33140	0.61828
C	5.23128	1.38875	-0.54135
H	3.55764	0.97666	-1.84626
C	4.87204	3.15166	1.08030
H	2.90858	4.06239	1.06138
C	5.69514	2.17844	0.51173
H	5.86967	0.63222	-0.98457
H	5.23975	3.76819	1.89388
H	6.70285	2.03594	0.88922
S	-1.03761	0.33923	-0.70095
C	-1.49557	1.21836	-2.27863
F	-0.81874	0.75325	-3.32450
F	-1.32122	2.53293	-2.16664
F	-2.81253	1.02151	-2.55927
N	1.95412	-0.95798	-0.03159
H	1.35114	-0.11586	-0.10372
S	3.02801	-0.94822	1.29599
S	1.72825	-2.25778	-1.06230
O	2.97489	0.40316	1.81817
O	4.25946	-1.62616	0.93261
O	2.21435	-3.45510	-0.39661
O	0.39940	-2.18884	-1.65768
C	2.12730	-2.04308	2.54337
C	2.90525	-1.85633	-2.46079
F	2.56546	-3.29272	2.45474
F	0.82091	-2.00312	2.30982
F	2.39040	-1.55993	3.75429
F	4.13200	-1.65761	-1.98790
F	2.47840	-0.75875	-3.08172
F	2.90524	-2.88442	-3.30694
Se	-2.52228	-1.51156	-1.28895
C	-4.26440	-0.93180	-0.68124
C	-4.49751	0.35054	-0.19203
C	-5.28365	-1.88382	-0.73685
C	-5.78235	0.68150	0.24065
H	-3.70297	1.08331	-0.14178
C	-6.56111	-1.54364	-0.29784
H	-5.07927	-2.88148	-1.11202
C	-6.81082	-0.25876	0.18849
H	-5.96794	1.67942	0.62199
H	-7.35798	-2.27926	-0.33768
H	-7.80740	0.00766	0.52596
C	-2.08639	-2.45921	0.31906
C	-2.31726	-1.87453	1.56418
C	-1.55605	-3.74282	0.20304
C	-2.02795	-2.60563	2.71333
H	-2.71622	-0.87048	1.63554
C	-1.25981	-4.46037	1.36103
H	-1.36636	-4.16706	-0.77569

C	-1.50525	-3.89621	2.61304	O	3.01647	0.27232	1.79922
H	-2.19577	-2.15861	3.68746	O	4.22240	-1.74628	0.79870
H	-0.83860	-5.45689	1.28139	O	2.17860	-3.46507	-0.51665
H	-1.27618	-4.45774	3.51307	O	0.24773	-2.23047	-1.60833
				C	2.11697	-2.18746	2.44263
Int1				C	2.67099	-1.78155	-2.58133
N	0.63868	1.62677	-0.01732	F	2.63141	-3.41042	2.38299
S	0.21707	1.92418	1.57877	F	0.81897	-2.23230	2.15659
O	-0.01194	0.58280	2.14794	F	2.29613	-1.68419	3.65960
O	1.13926	2.85624	2.23089	F	3.93452	-1.61377	-2.20113
C	-1.41198	2.69348	1.50772	F	2.19810	-0.64659	-3.09107
C	-1.66395	3.75926	0.64443	F	2.59500	-2.75424	-3.48813
C	-2.39265	2.20388	2.37058	Se	-2.60123	-1.43544	-1.21979
C	-2.93610	4.33141	0.64306	C	-4.31234	-0.71211	-0.67954
H	-0.88256	4.12553	-0.01230	C	-4.48299	0.62101	-0.32234
C	-3.65601	2.79382	2.36839	C	-5.37412	-1.61802	-0.66730
H	-2.15604	1.37249	3.02395	C	-5.75627	1.05153	0.05462
C	-3.92824	3.85581	1.50392	H	-3.65158	1.31459	-0.32164
H	-3.14853	5.15719	-0.02842	C	-6.63813	-1.17573	-0.28579
H	-4.42617	2.42157	3.03657	H	-5.21461	-2.65625	-0.94131
H	-4.91114	4.31785	1.50468	C	-6.82860	0.16079	0.07274
S	1.58112	2.70277	-0.92886	H	-5.89583	2.08766	0.34095
O	1.18436	4.09748	-0.68885	H	-7.47017	-1.87207	-0.26979
O	1.52067	2.13564	-2.28057	H	-7.81470	0.50577	0.36664
C	3.25474	2.47852	-0.34745	C	-2.23724	-2.33874	0.42835
C	4.04601	1.52977	-0.99521	C	-2.43544	-1.68606	1.64425
C	3.72357	3.21662	0.73643	C	-1.77601	-3.65183	0.36044
C	5.33476	1.29552	-0.52351	C	-2.17198	-2.38003	2.82179
H	3.65271	0.99686	-1.84980	H	-2.7801	-0.65996	1.67217
C	5.01837	2.97695	1.19106	C	-1.52208	-4.33580	1.54811
H	3.07687	3.93574	1.22045	H	-1.60294	-4.12265	-0.60002
C	5.81701	2.01483	0.57114	C	-1.72526	-3.70202	2.77434
H	5.95388	0.54546	-1.00387	H	-2.30424	-1.88227	3.77635
H	5.39920	3.53594	2.03958	H	-1.15837	-5.35706	1.51187
H	6.81905	1.82392	0.94250	H	-1.52031	-4.23488	3.69720
S	-1.12698	0.29900	-0.72388				
C	-1.37684	1.10484	-2.37980	**TS2**			
F	-0.54264	0.63977	-3.30204	N	-0.88481	1.52476	-0.04560
F	-1.25841	2.42429	-2.27245	S	-0.48733	1.96565	-1.63277
F	-2.63947	0.85426	-2.83363	O	-0.17223	0.6856	-2.28536
N	1.90137	-0.98717	-0.07148	O	-1.45550	2.89642	-2.21236
H	1.35073	-0.09381	-0.11870	C	1.09583	2.82055	-1.48477
S	3.01616	-1.05582	1.21937	C	1.25242	3.91275	-0.63231
S	1.62053	-2.26128	-1.11156	C	2.14807	2.34851	-2.26974

C	2.50376	4.5239	-0.55304	C	4.44114	-0.52089	0.63636
H	0.41832	4.25861	-0.03236	C	4.61196	0.80482	0.25707
C	3.38885	2.97987	-2.19330	C	5.49933	-1.43021	0.64908
H	1.98383	1.49287	-2.91370	C	5.88512	1.22661	-0.12945
C	3.56891	4.0631	-1.33057	H	3.78012	1.49736	0.24623
H	2.64330	5.36752	0.11532	C	6.76396	-0.99498	0.26058
H	4.21382	2.62236	-2.80170	H	5.33933	-2.46344	0.94179
H	4.53569	4.55429	-1.26949	C	6.95584	0.33338	-0.12803
S	-1.86599	2.50235	0.95188	H	6.02757	2.25736	-0.43566
O	-1.54148	3.91940	0.74766	H	7.59582	-1.69150	0.26063
O	-1.70712	1.87748	2.26864	H	7.94250	0.66962	-0.42962
C	-3.54094	2.20948	0.41848	C	2.37457	-2.25051	-0.38385
C	-4.25880	1.19382	1.04956	C	2.69874	-1.73943	-1.64037
C	-4.06954	2.94548	-0.63980	C	1.79546	-3.50573	-0.21424
C	-5.53680	0.89201	0.58770	C	2.44166	-2.52689	-2.75841
H	-3.81767	0.65846	1.87837	H	3.13676	-0.75369	-1.74309
C	-5.35326	2.63738	-1.08280	C	1.54565	-4.28102	-1.34533
H	-3.47486	3.71361	-1.11550	H	1.51517	-3.85500	0.77167
C	-6.07960	1.60956	-0.47910	C	1.87501	-3.79531	-2.61014
H	-6.09872	0.08940	1.05303	H	2.67273	-2.14492	-3.74694
H	-5.78089	3.19251	-1.91125	H	1.07839	-5.25294	-1.23343
H	-7.07234	1.36452	-0.84363	H	1.67189	-4.39902	-3.48854
S	1.30332	0.43129	0.62774				
C	1.39749	1.21407	2.30327	**7**			
F	0.63853	0.59969	3.19870	S	1.13156	-1.25179	1.02744
F	1.06714	2.49609	2.21148	C	2.73636	-1.34696	0.10280
F	2.68080	1.15001	2.76485	F	2.63233	-2.15991	-0.94823
N	-1.77536	-0.91685	0.07109	F	3.66189	-1.78910	0.93848
H	-1.30023	0.22293	0.05162	F	3.06887	-0.12918	-0.35786
S	-2.85984	-1.17679	-1.19921	Se	0.06996	-0.29691	-0.67843
S	-1.38118	-2.16139	1.08226	C	0.08212	1.58357	-0.23467
O	-3.08218	0.13287	-1.78953	C	0.83058	2.10378	0.81350
O	-3.96245	-2.04420	-0.80972	C	-0.67640	2.37846	-1.09614
O	-1.62236	-3.45083	0.44037	C	0.79929	3.48517	1.01528
O	-0.08850	-1.91320	1.73008	H	1.42518	1.46546	1.45539
C	-1.82111	-2.15640	-2.44568	C	-0.69520	3.75373	-0.87545
C	-2.60261	-1.99661	2.49010	H	-1.24920	1.94308	-1.90940
F	-2.20444	-3.43081	-2.44883	C	0.04076	4.30329	0.17742
F	-0.52673	-2.08764	-2.13712	H	1.37172	3.91659	1.82906
F	-2.02167	-1.63174	-3.65150	H	-1.28190	4.39162	-1.52726
F	-3.85365	-1.99435	2.03785	H	0.02501	5.37522	0.34183
F	-2.36501	-0.85999	3.14478	C	-1.70498	-0.76432	-0.13109
F	-2.42601	-3.03137	3.31512	C	-2.33345	-0.07572	0.90681
Se	2.72159	-1.21927	1.19310	C	-2.30181	-1.82873	-0.80887

C	-3.61554	-0.47812	1.27168
H	-1.84628	0.75296	1.40723
C	-3.58628	-2.21342	-0.42856
H	-1.78193	-2.34464	-1.60958
C	-4.23729	-1.53976	0.60686
H	-4.13020	0.03712	2.07530
H	-4.07511	-3.03387	-0.94199
H	-5.23753	-1.84208	0.89787

8

N	-0.01851	0.57592	0.25212
S	-0.0539	-1.31305	0.15465
O	0.59725	-1.57104	-1.11787
O	0.51047	-1.65948	1.45038
C	-1.77966	-1.63053	0.08608
C	-2.49769	-1.66351	1.28788
C	-2.38070	-1.79752	-1.16625
C	-3.87161	-1.86782	1.22044
H	-1.98994	-1.55618	2.24000
C	-3.75631	-2.00516	-1.20588
H	-1.78252	-1.77661	-2.06902
C	-4.49558	-2.03342	-0.02046
H	-4.45439	-1.90690	2.13390
H	-4.25024	-2.14702	-2.16059
H	-5.56783	-2.19294	-0.06215
S	1.88618	1.35915	0.82841
O	1.72133	1.22567	2.26325
O	1.82984	2.60669	0.09181
C	2.99856	0.21141	0.13026
C	3.43181	-0.86305	0.91807
C	3.37439	0.39243	-1.20827
C	4.29382	-1.78188	0.33084
H	3.09953	-0.96841	1.94258
C	4.23208	-0.54566	-1.76753
H	3.01923	1.24435	-1.77564
C	4.68480	-1.62627	-1.00232
H	4.65792	-2.62054	0.91319
H	4.55093	-0.43397	-2.79756
H	5.35215	-2.35445	-1.45104
S	-0.69679	1.40713	-1.13178
C	-2.21378	2.07204	-0.30378
F	-2.61298	3.11490	-1.01454
F	-1.91830	2.44608	0.95365
F	-3.19509	1.17198	-0.23884
H	-0.52751	0.85184	1.10345

9

N	-0.00003	-0.00008	0.89651
S	1.13386	0.85747	0.12417
O	0.82942	1.27848	-1.24920
O	1.67943	1.84203	1.06512
C	2.51681	-0.38298	-0.06892
F	2.11549	-1.46093	-0.75246
F	2.97121	-0.78529	1.12757
F	3.54165	0.18228	-0.73429
S	-1.13386	-0.85749	0.12394
O	-1.67948	-1.84224	1.06466
O	-0.82934	-1.27823	-1.24950
C	-2.51681	0.38299	-0.06900
F	-2.97127	0.78508	1.12754
F	-2.11546	1.46107	-0.75232
F	-3.54161	-0.18215	-0.73453

TSse-s

N	-0.64938	-0.26694	0.14030
S	-1.52272	-1.12358	-1.01252
O	-1.21016	-0.45043	-2.28866
O	-1.24548	-2.56306	-0.89287
C	-3.26675	-0.86456	-0.71625
C	-3.93633	-1.68070	0.19492
C	-3.91715	0.15949	-1.40541
C	-5.28871	-1.44544	0.43201
H	-3.40003	-2.46204	0.71538
C	-5.26994	0.38202	-1.15685
H	-3.36615	0.75583	-2.12049
C	-5.95245	-0.41493	-0.23647
H	-5.82331	-2.06743	1.14256
H	-5.78977	1.17583	-1.68362
H	-7.00557	-0.23553	-0.04274
S	-0.50026	-0.88306	1.69948
O	-1.63375	-1.71997	2.11120
O	-0.12511	0.28377	2.51495
C	0.95848	-1.93742	1.66673
C	0.89036	-3.22375	1.13149
C	2.10799	-1.4729	2.30698
C	2.0038	-4.05337	1.23895
H	-0.01217	-3.55268	0.63426
C	3.21039	-2.31919	2.42010

H	2.11628	-0.47505	2.72678
C	3.15797	-3.60811	1.88802
H	1.96494	-5.05553	0.82420
H	4.10446	-1.97324	2.92951
H	4.01583	-4.26755	1.98027
S	-1.11368	2.10850	-0.51928
C	-2.05179	2.24274	1.06482
F	-1.3254	2.70642	2.08269
F	-2.71584	1.16163	1.46606
F	-2.96299	3.19568	0.74277
Se	1.03257	1.38721	-1.66957
C	2.19965	2.23410	-0.39898
C	1.94325	2.13235	0.96760
C	3.31169	2.92079	-0.88635
C	2.82772	2.73698	1.86028
H	1.08124	1.59227	1.33875
C	4.18770	3.52119	0.01797
H	3.49224	2.98491	-1.95434
C	3.94556	3.42829	1.38956
H	2.63557	2.66393	2.92596
H	5.05340	4.06231	-0.35018
H	4.62786	3.89823	2.09096
C	1.90787	-0.30829	-1.75216
C	2.89129	-0.68637	-0.83418
C	1.57866	-1.13284	-2.83690
C	3.55419	-1.89628	-1.01396
H	3.14516	-0.04730	-0.00086
C	2.23594	-2.34791	-2.99121
H	0.79671	-0.83764	-3.52343
C	3.22393	-2.73107	-2.08173
H	4.31362	-2.19479	-0.30192
H	1.97431	-2.99482	-3.82183
H	3.73425	-3.68116	-2.20354

TS_H

N	0.92699	-0.19802	0.14960
S	1.55861	1.58389	-0.10452
O	0.87772	1.96263	-1.33290
O	1.34998	2.22886	1.18068
C	3.28958	1.39828	-0.41635
C	4.17193	1.45078	0.66466
C	3.7166	1.22595	-1.73483
C	5.53195	1.31373	0.40625
H	3.79154	1.57576	1.67012
C	5.08196	1.08601	-1.96958
H	2.99567	1.21081	-2.54276
C	5.98232	1.12701	-0.90340
H	6.24005	1.34952	1.22694
H	5.44043	0.94574	-2.98340
H	7.04480	1.01513	-1.09428
S	0.99540	-0.84158	1.99407
O	2.16034	-0.19264	2.57732
O	0.91302	-2.27864	1.77457
C	-0.48573	-0.21849	2.70624
C	-1.66494	-0.94381	2.52123
C	-0.42913	0.97829	3.42291
C	-2.83479	-0.43583	3.07313
H	-1.66119	-1.86721	1.96098
C	-1.60912	1.45310	3.98404
H	0.50290	1.51928	3.51109
C	-2.80427	0.75598	3.80051
H	-3.76950	-0.95955	2.91405
H	-1.59894	2.38236	4.54249
H	-3.72516	1.15107	4.21623
S	1.39976	-1.35603	-1.08405
C	3.0407	-2.02585	-0.52313
F	2.91773	-3.31713	-0.21719
F	3.55869	-1.38257	0.52367
F	3.89338	-1.93186	-1.55669
N	-1.57153	-0.02454	-0.60993
H	-0.21794	-0.09529	-0.14705
S	-2.43846	1.29573	-0.09084
S	-2.22200	-1.06294	-1.71141
O	-1.52234	1.98758	0.81566
O	-3.80382	0.97848	0.31407
O	-3.41329	-0.51794	-2.35266
O	-1.12484	-1.63020	-2.49465
C	-2.57905	2.41054	-1.62055
C	-2.80408	-2.47746	-0.64179
F	-3.81736	2.36923	-2.09535
F	-1.71975	2.03227	-2.56538
F	-2.29203	3.65511	-1.23534
F	-3.67916	-2.05334	0.27367
F	-1.74689	-3.01742	-0.00896
F	-3.37480	-3.40641	-1.40475

$Int1_H$

N	-1.06055	0.23463	-0.12830
S	-2.20303	0.38894	1.43478

O	-1.64890	-0.64470	2.29407	F	1.08345	-1.90143	2.57784
O	-2.11702	1.81517	1.70621	F	4.4656	0.28937	-1.16904
C	-3.83455	-0.06440	0.93437	F	3.03375	-0.28942	-2.70266
C	-4.66628	0.90558	0.37003	F	4.78278	-1.52837	-2.32665
C	-4.24511	-1.37986	1.16011				
C	-5.95462	0.52740	0.00750	**TS'$_{se-s}$**			
H	-4.30262	1.91141	0.21089	N	0.71137	-0.02094	0.32335
C	-5.53962	-1.73405	0.79046	S	1.43961	1.5607	-0.20040
H	-3.56737	-2.09337	1.61118	O	1.01951	1.61488	-1.59875
C	-6.38627	-0.78599	0.21346	O	0.99564	2.55716	0.76801
H	-6.62195	1.25817	-0.43598	C	3.17389	1.28319	-0.08099
H	-5.88413	-2.74942	0.95244	C	3.81615	1.51759	1.13724
H	-7.39261	-1.07117	-0.07581	C	3.84949	0.83474	-1.22032
S	-1.18460	1.67240	-1.47629	C	5.18315	1.26800	1.21337
O	-2.45538	2.33078	-1.20702	H	3.25853	1.86810	1.99489
O	-0.90385	0.96186	-2.71290	C	5.21606	0.59392	-1.12006
C	0.18807	2.64566	-0.97321	H	3.31535	0.68994	-2.15009
C	-0.01435	3.65490	-0.02971	C	5.87652	0.80312	0.09327
C	1.45209	2.26686	-1.43407	H	5.70637	1.43707	2.14785
C	1.10587	4.32763	0.44580	H	5.76526	0.24744	-1.98848
H	-1.01027	3.87951	0.32987	H	6.94163	0.60902	0.16441
C	2.55583	2.94675	-0.93252	S	0.49397	-0.40494	2.07783
H	1.56527	1.44892	-2.13234	O	1.60811	0.22004	2.77092
C	2.38105	3.96789	0.00395	O	0.26133	-1.84202	2.06200
H	0.98500	5.11543	1.18097	C	-1.04273	0.40944	2.45350
H	3.54903	2.64952	-1.24458	C	-1.04091	1.75692	2.82124
H	3.25077	4.47498	0.40784	C	-2.21594	-0.34970	2.38697
S	-0.69172	-1.34628	-0.77488	C	-2.26175	2.36048	3.11331
C	-2.26513	-1.70290	-1.69610	H	-0.11324	2.31072	2.86869
F	-1.94147	-2.12501	-2.91878	C	-3.42648	0.27485	2.67782
F	-3.07591	-0.63972	-1.80000	H	-2.17461	-1.39918	2.12834
F	-2.95229	-2.69142	-1.09594	C	-3.44865	1.62569	3.03606
N	1.84995	-0.63809	0.07925	H	-2.28429	3.40358	3.40945
H	-0.16133	0.50922	0.42436	H	-4.34628	-0.29782	2.63410
S	2.10678	0.23351	1.40775	H	-4.39393	2.10503	3.26935
S	2.90661	-1.74612	-0.49202	S	1.29452	-1.57250	-1.48849
O	0.85437	1.04735	1.49937	C	2.41006	-2.38727	-0.26553
O	3.38374	0.92582	1.55187	F	1.81961	-3.40459	0.36222
O	3.89066	-2.18938	0.49442	F	2.95879	-1.58606	0.64916
O	2.13966	-2.71018	-1.27968	F	3.38701	-2.87928	-1.04992
C	1.95770	-0.93645	2.87363	H	-0.22234	-0.02469	-0.09435
C	3.86379	-0.75395	-1.75242	Se	-1.24535	-0.57209	-2.16915
F	1.51152	-0.23780	3.91931	C	-2.37979	-1.60527	-1.01732
F	3.13513	-1.47091	3.16777	C	-1.84226	-2.66799	-0.28361

C	-3.75626	-1.33534	-1.00097
C	-2.69467	-3.45145	0.49273
H	-0.78082	-2.87633	-0.29076
C	-4.59146	-2.12110	-0.21276
H	-4.16589	-0.52713	-1.59500
C	-4.06331	-3.17675	0.53613
H	-2.28056	-4.26809	1.07393
H	-5.65704	-1.91812	-0.19656
H	-4.71913	-3.78796	1.14712
C	-1.89774	1.18506	-1.86879
C	-2.49052	1.58858	-0.66407
C	-1.66114	2.10231	-2.90521
C	-2.85177	2.92130	-0.50654
H	-2.66706	0.88067	0.13464
C	-2.03408	3.42893	-2.73515
H	-1.17977	1.77797	-3.82147
C	-2.62408	3.84035	-1.53583
H	-3.30311	3.24264	0.42480
H	-1.85983	4.14364	-3.53175
H	-2.90256	4.88019	-1.40181

TS3a(3*R*)

C	-1.08426	-3.27263	-0.92064
H	-1.89774	-3.87281	-1.34462
H	-0.43759	-3.93288	-0.33983
H	-0.50509	-2.84921	-1.74517
C	-1.68342	-2.20321	-0.05082
H	-2.13495	-2.52281	0.88515
C	-2.10089	-0.94061	-0.57153
H	-1.77308	-0.70970	-1.58329
C	-3.27025	-0.13859	-0.11070
B	-4.53117	-0.54325	-1.04387
O	-5.66678	-0.85085	-0.38022
H	-6.44602	-1.06102	-0.91033
O	-4.29502	-0.55732	-2.38057
H	-5.04424	-0.75242	-2.95719
C	-3.01696	1.35936	-0.22695
F	-4.16833	2.04595	-0.15411
F	-2.21519	1.80260	0.77360
F	-2.40849	1.67781	-1.38766
H	-3.54170	-0.34800	0.92282
Se	2.29969	0.14207	1.13424
C	2.25651	1.76377	0.10901
C	1.05752	2.42905	-0.14697
C	3.47723	2.27852	-0.33650
C	1.08393	3.61684	-0.87975
H	0.11417	2.04691	0.21873
C	3.49052	3.45914	-1.07508
H	4.40028	1.75377	-0.11534
C	2.29442	4.12766	-1.34745
H	0.15411	4.13741	-1.08415
H	4.43408	3.86049	-1.42957
H	2.30872	5.05017	-1.91829
C	2.80490	-1.10156	-0.23512
C	2.56526	-0.84902	-1.58741
C	3.31475	-2.33143	0.18709
C	2.85781	-1.84117	-2.52500
H	2.17509	0.11121	-1.90525
C	3.59586	-3.31702	-0.75802
H	3.49789	-2.51292	1.24167
C	3.36999	-3.07284	-2.11430
H	2.69136	-1.64549	-3.57964
H	4.00258	-4.26967	-0.43475
H	3.60053	-3.83726	-2.84879
S	-0.23419	-0.82355	0.38156
C	-0.67519	-0.53066	2.18154
F	-1.95246	-0.82260	2.45827
F	-0.44022	0.73597	2.50410
F	0.10504	-1.32100	2.91870

Int2a(3*R*)

C	-0.96489	3.15243	-0.81125
H	-0.14907	3.78831	-0.45085
H	-1.91618	3.62369	-0.55964
H	-0.87519	3.06773	-1.89679
C	-0.80603	1.82951	-0.11835
H	-0.99518	1.81618	0.95207
C	0.09949	0.79692	-0.62174
H	0.49585	0.97511	-1.62139
C	0.97671	-0.05640	0.24556
B	2.19220	0.87044	0.78861
O	3.19178	0.23102	1.41931
H	3.93634	0.75020	1.74753
O	2.03731	2.20840	0.57064
H	2.74527	2.78146	0.89295
C	1.49587	-1.25648	-0.54248
F	2.15493	-2.11053	0.23575
F	0.47865	-1.92554	-1.13762

F	2.31766	-0.83294	-1.53075
H	0.44941	-0.43161	1.12654
S	-1.76185	0.37199	-0.92091
C	-2.24909	-0.68885	0.56810
F	-1.83995	-0.14008	1.71359
F	-1.72139	-1.89108	0.44064
F	-3.56853	-0.75020	0.54086

TS3a(3*S*)

C	2.98846	-3.02605	-0.54092
H	3.20420	-2.75063	-1.57190
H	2.39582	-3.94324	-0.51289
C	2.35166	-1.92983	0.23854
H	2.06811	-2.16575	1.26267
C	2.32565	-0.56360	-0.12614
H	2.74543	-0.27899	-1.08569
C	2.21977	0.55105	0.89023
H	1.69338	0.20197	1.78450
B	1.43218	1.80612	0.27424
O	0.46296	2.35283	1.05217
H	-0.07163	3.04950	0.64433
O	1.75194	2.14773	-1.00002
H	1.21509	2.85546	-1.37956
C	3.62963	0.90833	1.34880
F	4.22678	-0.15173	1.94253
F	3.59824	1.91746	2.23242
F	4.40544	1.27628	0.31114
Se	-2.37371	-0.66562	-0.71496
C	-2.14030	1.23853	-0.85221
C	-2.79093	2.09321	0.04060
C	-1.37805	1.75179	-1.90399
C	-2.61973	3.47227	-0.08146
H	-3.40667	1.68815	0.83480
C	-1.23821	3.13535	-2.03830
H	-0.89453	1.08845	-2.61006
C	-1.84114	3.99747	-1.11799
H	-3.11331	4.13666	0.62003
H	-0.67269	3.53812	-2.87408
H	-1.72975	5.07155	-1.22352
C	-2.37024	-0.91358	1.18614
C	-1.55566	-0.14554	2.02513
C	-3.13632	-1.96793	1.68930
C	-1.52377	-0.43979	3.38849
H	-0.97790	0.68469	1.63728
C	-3.08544	-2.25595	3.05267
H	-3.76921	-2.55156	1.02869
C	-2.28221	-1.49306	3.90223
H	-0.90795	0.16258	4.04885
H	-3.68290	-3.06937	3.45042
H	-2.25389	-1.71488	4.96375
S	0.36044	-1.15557	-0.46156
C	0.54489	-1.71962	-2.24283
F	-0.43404	-1.19198	-2.98571
F	0.45712	-3.04639	-2.30495
F	1.71181	-1.34037	-2.77590
H	3.94113	-3.24524	-0.03789

Int2a(3*S*)

C	1.36569	-2.53525	0.15870
H	2.14001	-3.01495	-0.44192
H	0.63225	-3.30008	0.44236
H	1.79985	-2.12798	1.07134
C	0.59941	-1.51737	-0.63171
H	0.17314	-1.87239	-1.56950
C	-0.06825	-0.35737	-0.03256
H	0.15840	-0.16343	1.01295
C	-1.41453	0.15138	-0.49850
B	-1.64654	1.69896	-0.12031
O	-2.82670	2.23540	-0.48555
H	-3.00008	3.15625	-0.25446
O	-0.59959	2.29734	0.51704
H	-0.71891	3.22179	0.76991
C	-2.46780	-0.74993	0.15291
F	-3.68415	-0.51867	-0.32933
F	-2.16938	-2.05968	-0.05887
F	-2.48001	-0.55925	1.49016
H	-1.52982	0.01551	-1.58020
S	1.39864	0.18635	-1.08426
C	2.78399	0.39538	0.18648
F	2.34194	0.25009	1.43041
F	3.25051	1.61766	0.00417
F	3.72097	-0.50504	-0.06594

TS4a$_{anti}$(3*R*)

C	-0.84250	-3.14255	0.79863
H	0.19684	-2.93348	1.05248
H	-0.88071	-3.92413	0.03736
H	-1.35085	-3.49971	1.69912

C	-1.47114	-1.86499	0.26548
H	-1.02395	-1.51947	-0.66551
C	-1.65639	-0.78054	1.24483
H	-1.98502	-1.08449	2.23604
C	-1.39321	0.57816	1.02172
B	0.30676	0.54122	1.60416
O	0.68947	1.83122	1.87609
H	1.34463	1.87125	2.58384
O	0.46481	-0.54563	2.46178
H	1.39320	-0.62863	2.73179
C	-2.21030	1.54094	1.85913
F	-1.88840	2.81456	1.61548
F	-3.52826	1.39344	1.56691
F	-2.07699	1.30205	3.18276
H	-1.33769	0.88967	-0.01603
S	-3.30482	-2.11772	-0.02115
C	-3.60772	-0.98945	-1.44375
F	-3.48150	0.30305	-1.12545
F	-4.87182	-1.21418	-1.82387
F	-2.79039	-1.25318	-2.46377
N	1.32961	0.07883	0.04504
S	0.99677	0.56669	-1.51977
S	2.94149	-0.15333	0.45220
C	1.04647	2.44383	-1.42003
C	3.15353	-1.98522	0.10946
F	-0.03855	2.87769	-0.77321
F	2.13841	2.84515	-0.78146
F	1.04271	2.92319	-2.66217
F	4.44989	-2.27547	0.13287
F	2.52900	-2.68470	1.07097
F	2.63343	-2.31161	-1.06957
O	-0.41630	0.24643	-1.76490
O	2.01060	0.15322	-2.47689
O	3.04404	-0.04091	1.91661
O	3.89452	0.55066	-0.38944

5a(*E*,3*R*)

S	-1.45242	0.36893	-1.10897
C	-2.58571	-0.43134	0.06483
F	-1.95828	-1.32910	0.84875
F	-3.53426	-1.06634	-0.63878
F	-3.20562	0.43692	0.89148
C	-0.38285	1.80309	1.09862
H	-0.65514	2.75397	0.63250
H	0.49486	1.95791	1.73341
H	-1.21394	1.47593	1.72422
C	-0.03919	0.74965	0.04110
H	0.22291	-0.19431	0.51579
C	1.07700	1.22422	-0.84747
H	0.83903	2.05822	-1.50570
C	2.32304	0.75089	-0.85167
C	2.79246	-0.36637	0.03430
F	2.61726	-0.07823	1.34913
F	4.10394	-0.60725	-0.15482
F	2.12794	-1.52364	-0.19534
H	3.08373	1.17334	-1.49870

TS4a$_{anti}$(3*S*)

S	3.94992	0.12043	0.31174
C	3.91837	-1.41653	1.31654
F	4.44444	-2.46041	0.66213
F	2.67973	-1.76269	1.70512
F	4.66089	-1.17700	2.40028
C	2.47813	-1.68236	-1.44795
H	2.13564	-2.32494	-0.63684
H	3.41359	-2.07564	-1.84915
H	1.71474	-1.67805	-2.22689
C	2.65216	-0.23954	-1.00258
H	2.94133	0.40366	-1.83198
C	1.57462	0.34319	-0.18525
H	1.16190	-0.28350	0.59955
C	0.96317	1.59653	-0.35263
B	-0.44350	1.02510	-1.28099
O	-1.27261	2.10613	-1.46196
H	-1.94485	1.93217	-2.13407
O	0.00885	0.16130	-2.26805
H	-0.73756	-0.17459	-2.78863
C	1.67932	2.67620	-1.14099
F	1.02192	3.83611	-1.07504
F	2.92562	2.88356	-0.62689
F	1.85956	2.36255	-2.44309
H	0.51053	1.99464	0.55304
N	-1.42367	-0.12132	-0.06179
S	-2.59237	-1.00897	-0.85738
S	-1.61023	0.15632	1.57350
C	-1.81984	-2.71263	-0.83473
C	-2.62780	1.73649	1.62926
O	-2.56523	-0.59327	-2.27140

O	-3.86782	-1.10893	-0.16722
O	-0.28569	0.54286	2.07369
O	-2.37772	-0.87574	2.25241
F	-1.58161	-3.08894	0.41785
F	-0.66284	-2.68706	-1.51215
F	-2.65141	-3.57182	-1.41835
F	-3.13879	1.86328	2.85172
F	-1.83704	2.77984	1.36825
F	-3.60895	1.68687	0.73206

5a(*Z*,3*S*)

S	1.97716	0.97621	-0.12455
C	1.87309	-0.83419	0.02791
F	1.16125	-1.41112	-0.95495
F	1.31954	-1.21620	1.19296
F	3.12477	-1.31816	-0.02422
C	0.12174	2.90158	0.45719
H	0.48816	3.50839	-0.37672
H	0.71499	3.13387	1.34481
H	-0.91924	3.17576	0.64762
C	0.18809	1.40522	0.13181
H	-0.14685	0.82803	0.99237
C	-0.60692	1.07754	-1.09759
H	-0.26475	1.55804	-2.01166
C	-1.67632	0.28326	-1.15767
C	-2.24232	-0.45009	0.02147
F	-3.39696	-1.06290	-0.30546
F	-1.39764	-1.39705	0.49256
F	-2.50625	0.37971	1.06488
H	-2.19336	0.10801	-2.09440

Int2a$_{Se}$(3*R*)

C	1.97945	3.16779	1.87331
H	2.97552	3.14384	2.32786
H	1.28035	3.59686	2.59312
H	2.02584	3.80328	0.98947
C	1.62542	1.74448	1.54590
H	1.54076	1.07525	2.40149
C	2.00048	1.09572	0.28637
H	2.33992	1.77371	-0.49288
C	2.53619	-0.30676	0.17283
B	3.99956	-0.38435	0.84632
O	4.67106	-1.54442	0.69509
H	5.55572	-1.60349	1.07606
O	4.39319	0.72779	1.53282
H	5.26571	0.68866	1.94498
C	2.58378	-0.70410	-1.29773
F	2.89806	-1.98814	-1.47113
F	1.39246	-0.47885	-1.91518
F	3.49844	0.05441	-1.94990
H	1.89853	-1.02692	0.69701
Se	-1.64283	-0.62612	-1.25205
C	-0.7796	-1.79244	-0.00363
C	0.04387	-2.80424	-0.50557
C	-0.88189	-1.59286	1.37992
C	0.79353	-3.58879	0.36994
H	0.10472	-2.96648	-1.57563
C	-0.13812	-2.39165	2.25152
H	-1.56432	-0.84594	1.77095
C	0.70963	-3.38115	1.74914
H	1.43796	-4.36612	-0.02653
H	-0.23264	-2.24744	3.32347
H	1.28621	-4.00061	2.42801
C	-3.27015	-0.34451	-0.26645
C	-3.60245	0.91132	0.24391
C	-4.13512	-1.42985	-0.10031
C	-4.80070	1.07588	0.94189
H	-2.94873	1.76179	0.09054
C	-5.32188	-1.26195	0.60856
H	-3.8712	-2.39571	-0.51671
C	-5.65563	-0.00941	1.12976
H	-5.06353	2.05183	1.33700
H	-5.99119	-2.10513	0.74443
H	-6.58496	0.12071	1.67428
S	0.11318	1.26078	0.45199
C	-0.22503	2.86102	-0.48323
F	-0.70908	3.75127	0.37929
F	-1.13478	2.59401	-1.40852
F	0.86690	3.35857	-1.06576

Int2a$_{Se}$(3*S*)

C	3.25412	-2.58528	-0.72543
H	3.33628	-2.32553	-1.77996
H	2.91070	-3.61597	-0.62252
C	2.39214	-1.63333	0.04697
H	2.26091	-1.86307	1.10360
C	2.17138	-0.24709	-0.32466
H	2.52601	0.06547	-1.30269

C	2.02310	0.86894	0.68533
H	1.59080	0.48807	1.61524
B	1.08025	2.02774	0.09462
O	0.23772	2.63344	0.96328
H	-0.40882	3.24492	0.58056
O	1.16037	2.21317	-1.24938
H	0.52408	2.84534	-1.60961
C	3.42426	1.35527	1.03669
F	4.17586	0.33614	1.52321
F	3.37728	2.31872	1.96384
F	4.06168	1.83580	-0.04950
Se	-2.55988	-0.92735	-0.40021
C	-2.49406	0.98444	-0.57013
C	-3.08678	1.80372	0.39583
C	-1.93296	1.54488	-1.72067
C	-3.05538	3.18924	0.24190
H	-3.55408	1.36088	1.26798
C	-1.94452	2.93214	-1.89199
H	-1.49237	0.90765	-2.47828
C	-2.48548	3.75848	-0.90274
H	-3.50337	3.82346	0.99982
H	-1.54723	3.36462	-2.80653
H	-2.49458	4.83531	-1.03674
C	-1.93952	-1.17799	1.39750
C	-1.14986	-0.23773	2.06781
C	-2.20601	-2.42101	1.98099
C	-0.64002	-0.54524	3.33232
H	-0.95374	0.73441	1.63444
C	-1.68097	-2.72078	3.23722
H	-2.82609	-3.14554	1.46212
C	-0.89756	-1.78518	3.91695
H	-0.05125	0.19788	3.86204
H	-1.89654	-3.68307	3.68992
H	-0.50265	-2.01793	4.90008
S	0.53754	-1.23683	-0.53097
C	0.62484	-1.69938	-2.35808
F	-0.51726	-1.31956	-2.91975
F	0.75286	-3.01763	-2.45682
F	1.64033	-1.10862	-2.98942
H	4.25432	-2.51748	-0.27967

TS4a'$_{anti}$(3*R*)

C	-0.59490	-2.82229	0.85053
H	-0.68280	-3.23173	1.85886
H	0.18731	-3.36157	0.30934
C	-0.30431	-1.33637	0.90681
H	-1.01409	-0.75517	1.49166
C	0.10873	-0.69169	-0.34040
H	0.70915	-1.29574	-1.01531
C	-0.33342	0.58814	-0.78730
H	-0.65663	1.25857	0.00129
B	-1.74625	0.05038	-1.65153
O	-2.23584	1.01259	-2.51863
H	-2.30578	0.66748	-3.41596
O	-1.54020	-1.27990	-2.02606
H	-2.38054	-1.68194	-2.30458
C	0.61918	1.30471	-1.71425
F	1.82665	1.49865	-1.11392
F	0.15625	2.51212	-2.06151
F	0.86750	0.60490	-2.84846
S	1.44655	-0.99914	1.50897
C	1.20523	0.53255	2.50060
F	0.99706	1.61877	1.74370
F	2.34955	0.71335	3.17673
F	0.19954	0.42046	3.36728
N	-3.10290	0.01121	-0.29487
S	-3.27045	1.13309	0.92209
S	-4.51888	-0.74868	-0.78930
O	-1.97870	1.23457	1.61444
O	-4.49012	0.91297	1.69014
O	-4.15595	-1.60316	-1.93041
O	-5.68212	0.11944	-0.88652
C	-3.45619	2.77978	0.03610
C	-4.86591	-1.97949	0.61349
F	-2.28357	3.12212	-0.50446
F	-4.38155	2.70068	-0.90795
F	-3.80609	3.69303	0.94291
F	-3.75462	-2.18499	1.33628
F	-5.23492	-3.13225	0.05425
F	-5.83311	-1.53655	1.39751
Se	4.74873	-1.00334	1.11607
C	5.19282	0.65368	0.25776
C	6.33046	0.71815	-0.55195
C	4.39011	1.78019	0.44254
C	6.65640	1.91314	-1.19042
H	6.94402	-0.16658	-0.68224
C	4.72374	2.97478	-0.19625
H	3.50766	1.72519	1.06519

C	5.85287	3.04149	-1.01232
H	7.53663	1.96395	-1.82362
H	4.09447	3.84865	-0.06157
H	6.10759	3.97179	-1.51028
C	3.87777	-1.88693	-0.34295
C	3.50815	-1.23379	-1.52124
C	3.51456	-3.22477	-0.14495
C	2.78058	-1.92072	-2.49411
H	3.75665	-0.19099	-1.66923
C	2.77732	-3.90116	-1.11716
H	3.80478	-3.73266	0.77024
C	2.40614	-3.25143	-2.29641
H	2.48337	-1.39945	-3.39753
H	2.50117	-4.93863	-0.95423
H	1.83037	-3.77516	-3.05218
H	-1.54083	-2.95968	0.32341

TS4a'$_{syn}$(3*R*)

C	1.65315	3.25422	1.27599
H	2.71194	3.00260	1.21582
H	1.33603	3.26249	2.31864
C	0.83107	2.30658	0.42395
H	1.13557	2.33209	-0.61846
C	-0.62319	2.26271	0.59711
H	-1.00016	2.22114	1.61227
C	-1.56558	2.27978	-0.47992
H	-2.56649	2.49032	-0.11425
B	-1.67660	0.68740	-1.27728
O	-2.64820	0.72025	-2.29539
H	-2.31175	1.14985	-3.08962
O	-0.32366	0.39887	-1.59113
H	-0.25902	-0.49883	-1.95038
C	-1.24049	3.3113	-1.54932
F	-0.93773	4.51329	-0.98237
F	-2.30048	3.51253	-2.35505
F	-0.18996	3.00575	-2.34519
Se	3.73518	-1.07625	0.90697
C	4.15480	0.59398	0.07058
C	3.56993	0.98406	-1.13830
C	5.01538	1.46533	0.74448
C	3.84900	2.24439	-1.66591
H	2.89243	0.31466	-1.65561
C	5.28477	2.72750	0.21360
H	5.47518	1.15228	1.67656
C	4.70323	3.12099	-0.99289
H	3.38953	2.54258	-2.60355
H	5.95635	3.39837	0.74053
H	4.91650	4.10093	-1.40743
C	3.33110	-2.09114	-0.66990
C	2.02521	-2.51742	-0.91152
C	4.35983	-2.41738	-1.55842
C	1.74153	-3.26730	-2.05471
H	1.23465	-2.27046	-0.21651
C	4.06967	-3.15160	-2.70586
H	5.37171	-2.08627	-1.35145
C	2.76170	-3.57730	-2.95347
H	0.72195	-3.58625	-2.23734
H	4.86483	-3.39874	-3.40252
H	2.54007	-4.15334	-3.84647
S	0.84521	0.47313	0.82546
C	1.20486	0.51389	2.63012
F	2.44600	0.95159	2.91317
F	1.09656	-0.74331	3.07063
F	0.34389	1.28555	3.32272
N	-2.31033	-0.41089	-0.17937
S	-3.46257	-0.04376	0.98274
S	-2.28023	-2.03332	-0.69453
O	-3.02722	1.14382	1.71498
O	-3.82674	-1.26230	1.69281
O	-1.23876	-2.11427	-1.72475
O	-3.59344	-2.60951	-0.92939
C	-4.98769	0.50710	0.02275
C	-1.53365	-2.96946	0.78353
F	-4.79736	1.74370	-0.44461
F	-6.00869	0.51542	0.88067
F	-5.24116	-0.31905	-0.97740
F	-0.86904	-2.13487	1.58848
F	-2.46694	-3.61213	1.45897
F	-0.67057	-3.85526	0.27294
H	1.50726	4.25610	0.86088

TS4a'$_{anti}$(3*S*)

C	-0.10146	-2.15193	1.23770
H	0.25619	-2.74859	0.39796
H	-0.98433	-2.63129	1.66463
C	-0.41337	-0.72125	0.83258
H	-0.73414	-0.12178	1.68244
C	0.57571	-0.03332	0.00486

H	1.04845	-0.61657	-0.77948
C	1.05927	1.28186	0.15786
H	1.48760	1.69842	-0.75088
B	2.48317	0.89714	1.16142
O	3.16148	2.08747	1.35528
H	3.80344	2.01209	2.07325
O	2.04676	0.05423	2.18551
H	2.77120	-0.13325	2.79960
C	0.20593	2.31920	0.86329
F	-0.98229	2.45359	0.21449
F	0.79460	3.51991	0.85676
F	-0.09277	2.00489	2.14443
Se	-4.74115	0.29016	-1.39193
C	-4.33491	1.61890	-0.07150
C	-4.15317	1.28526	1.27399
C	-4.12570	2.92998	-0.50516
C	-3.76809	2.27126	2.18156
H	-4.31632	0.26620	1.60598
C	-3.73537	3.90805	0.40847
H	-4.27196	3.18240	-1.55065
C	-3.55735	3.58234	1.75300
H	-3.62909	2.01168	3.22666
H	-3.57206	4.92540	0.06714
H	-3.25157	4.34450	2.46226
C	-5.78545	-0.89397	-0.30077
C	-5.31551	-2.16794	0.02078
C	-7.04424	-0.47196	0.13732
C	-6.10826	-3.01857	0.79422
H	-4.34201	-2.49415	-0.32229
C	-7.82283	-1.31890	0.92199
H	-7.39689	0.51804	-0.13032
C	-7.35633	-2.59458	1.24906
H	-5.74453	-4.01018	1.04515
H	-8.79631	-0.98790	1.27011
H	-7.96726	-3.25662	1.85461
S	-1.83445	-0.44441	-0.40225
C	-1.66611	-1.92651	-1.47058
F	-2.45704	-1.76856	-2.53489
F	-2.05479	-3.05276	-0.83508
F	-0.40786	-2.13256	-1.89967
N	3.61247	-0.14205	0.11346
S	3.87154	0.07255	-1.52767
S	4.84385	-0.83414	1.01787
O	2.55243	0.27480	-2.13446
O	4.79347	-0.90210	-2.08830
O	6.15052	-0.81483	0.38140
O	4.70372	-0.34369	2.39896
C	4.70851	1.75509	-1.61935
C	4.29000	-2.62183	1.06809
F	5.62576	1.87115	-0.66324
F	3.79087	2.71270	-1.47797
F	5.28534	1.86733	-2.81445
F	3.15864	-2.72272	1.77732
F	5.24102	-3.34575	1.65361
F	4.07374	-3.06839	-0.16555
H	0.68901	-2.10309	1.98767

TS4a'$_{syn}$(3*S*)

C	0.40017	-1.75357	3.37063
H	-0.28710	-2.57170	3.58311
H	0.27574	-0.97771	4.12795
C	0.21498	-1.17178	1.97988
H	0.95917	-0.40820	1.77060
C	0.03014	-2.07831	0.84438
H	-0.75356	-2.82414	0.94239
C	0.82739	-2.02926	-0.32797
H	1.84000	-2.29054	0.01703
B	1.23655	-0.43719	-0.97538
O	1.84715	-0.56630	-2.23218
H	1.18435	-0.65727	-2.92570
O	0.06586	0.32334	-0.79795
H	0.15286	1.20818	-1.18288
C	0.40904	-2.97206	-1.43681
F	-0.35089	-4.00487	-0.99058
F	1.47847	-3.49679	-2.05522
F	-0.33947	-2.35109	-2.39316
S	-1.41059	-0.28471	1.52795
C	-2.55898	-1.23451	2.62079
F	-3.82683	-0.95096	2.30904
F	-2.37653	-0.93343	3.91666
F	-2.39994	-2.57147	2.49346
N	2.50433	0.23673	-0.00262
S	2.77206	1.89027	-0.29994
S	3.78499	-0.63153	0.65981
O	3.20247	-1.83259	1.27615
O	4.67917	0.20988	1.43606
O	1.80897	2.34063	-1.30174
O	4.17742	2.23786	-0.42052

C	4.73557	-1.26212	-0.83772
C	2.15297	2.62477	1.31000
F	4.06160	-2.27215	-1.38546
F	5.91995	-1.69677	-0.40951
F	4.89976	-0.28888	-1.72101
F	2.09131	3.95029	1.16404
F	0.92152	2.15891	1.57259
F	2.95543	2.31720	2.31997
Se	-3.86753	1.41008	0.42739
C	-2.71331	2.40752	-0.72934
C	-1.62469	3.07664	-0.16559
C	-2.98101	2.52094	-2.09559
C	-0.79527	3.85447	-0.97363
H	-1.41317	2.97306	0.89246
C	-2.13079	3.27513	-2.90177
H	-3.83515	2.00764	-2.52283
C	-1.03884	3.94435	-2.34417
H	0.06203	4.35425	-0.53825
H	-2.32753	3.34819	-3.96705
H	-0.37579	4.52729	-2.97460
C	-4.20416	-0.13349	-0.66154
C	-3.18351	-0.78270	-1.36463
C	-5.50643	-0.63870	-0.67339
C	-3.48006	-1.94692	-2.07269
H	-2.17279	-0.39030	-1.35366
C	-5.78918	-1.81132	-1.37372
H	-6.29118	-0.11381	-0.13829
C	-4.77677	-2.46580	-2.07475
H	-2.68795	-2.45680	-2.60842
H	-6.80139	-2.20387	-1.37866
H	-4.99635	-3.37614	-2.62383
H	1.42652	-2.12870	3.41944

TS4a''$_{anti}$(3*R*)

C	-0.83945	-3.57388	1.43697
H	-0.66464	-4.44249	0.79972
H	-1.46857	-3.87814	2.27830
C	-1.48598	-2.45172	0.63277
H	-0.93908	-2.21356	-0.28077
C	-1.85688	-1.24857	1.40677
H	-2.26303	-1.42227	2.40109
C	-1.69691	0.05785	0.97046
H	-1.55458	0.18370	-0.09360
B	0.05760	0.35240	1.74823
O	0.15343	1.64504	2.16056
H	-0.08216	2.34009	1.53446
O	0.31148	-0.69901	2.61267
H	1.03124	-0.46837	3.21941
C	-2.64863	1.08530	1.54839
F	-3.88173	0.90764	1.03384
F	-2.27319	2.34654	1.23258
F	-2.73824	0.98931	2.88363
S	-3.21522	-2.95331	0.12824
C	-3.37785	-2.04413	-1.46232
F	-3.47440	-0.70918	-1.29829
F	-4.49605	-2.48055	-2.03542
F	-2.33903	-2.27259	-2.27170
N	1.18141	0.07966	0.37428
S	0.81963	0.53182	-1.37388
S	2.91717	0.57798	0.99773
O	-0.07232	-0.56755	-1.74886
O	2.10056	0.73729	-2.02750
O	2.88045	0.19538	2.40263
O	3.07534	1.95298	0.55822
C	3.97634	-0.53048	0.12136
C	4.69101	-0.05982	-0.98170
C	4.09053	-1.84083	0.60039
C	5.54566	-0.94697	-1.63089
H	4.57412	0.96255	-1.31536
C	4.94169	-2.71149	-0.07239
H	3.55235	-2.15583	1.48750
C	5.66395	-2.26448	-1.18322
H	6.11818	-0.60747	-2.48668
H	5.05409	-3.73147	0.27796
H	6.33031	-2.94807	-1.69856
C	-0.09998	2.04319	-1.26740
C	0.50457	3.19362	-0.74842
C	-1.39366	2.04235	-1.79811
C	-0.24564	4.36749	-0.72087
H	1.52357	3.17033	-0.38163
C	-2.11406	3.23438	-1.77679
H	-1.82292	1.13461	-2.20530
C	-1.54693	4.38705	-1.23225
H	0.19370	5.27087	-0.31226
H	-3.12005	3.25762	-2.18046
H	-2.11817	5.30887	-1.21021
H	1.22893	-0.94425	0.30660
H	0.10907	-3.21704	1.84530

TS4a''$_{syn}$(3*R*)

C	-0.19694	4.51576	-0.71291
H	-0.90617	5.20388	-0.25020
H	-0.52216	4.29311	-1.72910
C	-0.04793	3.26026	0.14283
H	0.31343	3.49730	1.14227
C	0.70643	2.15128	-0.47009
H	0.33211	1.78309	-1.42191
C	1.80078	1.47473	0.10859
H	2.32121	0.83085	-0.59871
B	1.20687	0.33561	1.33074
O	0.35473	1.00195	2.17095
H	-0.07017	0.40130	2.80624
O	2.19965	-0.54269	1.65802
H	2.32016	-0.65967	2.60831
C	2.82166	2.36416	0.83363
F	3.14061	3.41572	0.04030
F	3.93863	1.67697	1.08027
F	2.36849	2.87463	1.99405
S	-1.60558	2.26059	0.47936
C	-2.57410	2.50837	-1.06911
F	-3.04856	3.74870	-1.18130
F	-3.59865	1.65317	-1.00021
F	-1.85114	2.23442	-2.16858
N	-0.03915	-0.83369	0.28207
O	-0.82074	-1.32201	2.70961
O	-0.15880	-3.28788	1.24257
O	0.32511	-0.24681	-2.15158
O	-0.39761	-2.63229	-1.63354
H	-0.77548	-0.15204	0.04810
C	-2.50147	-2.05684	0.81059
C	-2.88771	-3.09084	-0.04340
C	-3.36672	-1.02571	1.19310
C	-4.19097	-3.07832	-0.53603
H	-2.18580	-3.86793	-0.31531
C	-4.65949	-1.02749	0.67860
H	-3.04216	-0.26371	1.89217
C	-5.06705	-2.04975	-0.18353
H	-4.51943	-3.87245	-1.19711
H	-5.35140	-0.24159	0.96040
H	-6.07788	-2.04727	-0.57742
C	2.13796	-1.92512	-1.18709
C	2.49051	-3.02689	-0.40575
C	3.07672	-1.17842	-1.90590
C	3.83879	-3.36258	-0.32113
H	1.73711	-3.59282	0.12599
C	4.41911	-1.53605	-1.80910
H	2.75649	-0.36214	-2.54262
C	4.79764	-2.61892	-1.01312
H	4.13966	-4.21031	0.28446
H	5.16490	-0.97611	-2.36245
H	5.84516	-2.89148	-0.94004
S	-0.84022	-2.01771	1.41882
S	0.43520	-1.47371	-1.35539
H	0.78311	4.99875	-0.75601

TS4a''$_{anti}$(3*S*)

S	4.37129	-1.36027	-0.30603
C	3.48014	-0.13034	2.20092
H	3.63312	0.87989	1.82187
H	4.37274	-0.45018	2.74053
H	2.62944	-0.11465	2.88605
C	3.13783	-1.11347	1.09681
H	2.97653	-2.11894	1.48176
C	2.15755	-0.70877	0.08088
H	2.21743	0.31788	-0.26026
C	1.06970	-1.47004	-0.42464
B	-0.29815	-0.81311	0.58920
O	0.27786	0.01522	1.57708
H	-0.40758	0.30734	2.19758
O	-1.15887	-1.86124	0.93777
H	-0.76773	-2.46266	1.58193
C	1.13663	-2.97538	-0.28519
F	2.28674	-3.47446	-0.79692
F	0.12004	-3.56648	-0.91881
F	1.10892	-3.37629	1.02263
H	0.82289	-1.20392	-1.45136
C	5.20631	0.2853	-0.38827
F	5.96698	0.26286	-1.47848
F	5.97419	0.50057	0.68142
F	4.33171	1.30263	-0.48188
N	-1.31280	0.06962	-0.43001
H	-1.64341	-0.56313	-1.17040
S	-2.93388	0.51922	0.49080
S	-0.65035	1.50054	-1.43737
O	-2.51369	0.65287	1.88041
O	-3.47375	1.63674	-0.26582

O	-1.58288	1.55946	-2.55098
O	0.75131	1.13951	-1.63401
C	-3.92642	-0.91207	0.20549
C	-4.54143	-1.02945	-1.04547
C	-4.10763	-1.83729	1.23423
C	-5.35834	-2.13416	-1.26899
H	-4.39952	-0.27068	-1.80744
C	-4.94294	-2.92359	0.99245
H	-3.60860	-1.70048	2.18434
C	-5.55748	-3.07372	-0.25370
H	-5.84881	-2.25328	-2.22860
H	-5.11345	-3.65394	1.77559
H	-6.20231	-3.92743	-0.43358
C	-0.76574	2.91930	-0.39382
C	0.10916	3.04215	0.68974
C	-1.68567	3.91043	-0.74422
C	0.03884	4.20150	1.45558
H	0.79811	2.24561	0.93768
C	-1.72553	5.06726	0.02820
H	-2.34761	3.76706	-1.58822
C	-0.87135	5.20894	1.12377
H	0.69834	4.32240	2.30789
H	-2.42714	5.85448	-0.22371
H	-0.91395	6.11168	1.72402

TS4a'' $_{syn}$**(3*S*)**

C	2.67973	-2.86941	-2.22768
H	3.48201	-3.16315	-1.54897
H	3.11940	-2.40889	-3.11501
C	1.71080	-1.87034	-1.57548
H	0.93882	-1.54800	-2.27794
C	1.07584	-2.49519	-0.38780
H	1.74479	-2.99684	0.30904
C	-0.28838	-2.52230	-0.11078
H	-0.94113	-2.18107	-0.91169
B	-0.39183	-1.25300	1.20484
O	-1.64693	-1.28590	1.70047
H	-1.72707	-1.03626	2.63065
O	0.81152	-1.09289	1.81802
H	0.76031	-0.41975	2.51811
C	-0.78986	-3.80283	0.56526
F	-0.46510	-4.86135	-0.20669
F	-2.11965	-3.78347	0.69407
F	-0.22779	-3.99345	1.77132
S	2.48023	-0.23471	-1.15151
C	3.88274	-0.70672	-0.06211
F	4.30087	0.41138	0.54333
F	4.89639	-1.22296	-0.76162
F	3.53555	-1.60275	0.87507
N	-0.46855	0.54754	0.12335
O	-1.01850	-0.41898	-2.13081
O	-1.17212	2.10529	-1.87501
O	-0.13225	1.28727	2.58361
O	-1.85372	2.51303	1.17541
C	0.74699	2.97365	0.73927
C	2.07043	2.64899	1.05299
C	0.40586	4.06958	-0.05395
C	3.08403	3.45529	0.54377
H	2.29984	1.79698	1.68113
C	1.43588	4.87089	-0.54223
H	-0.63131	4.27887	-0.28112
C	2.76550	4.56222	-0.24868
H	4.11836	3.22452	0.77227
H	1.19819	5.73345	-1.15465
H	3.56065	5.18930	-0.63786
S	-0.54116	1.90667	1.31630
C	-3.13064	0.61155	-0.87072
C	-3.65916	-0.64825	-0.57589
C	-3.90473	1.77452	-0.84438
C	-5.00357	-0.73352	-0.22918
H	-3.05163	-1.54131	-0.60552
C	-5.24900	1.66551	-0.50226
H	-3.45864	2.73050	-1.08388
C	-5.79393	0.41794	-0.19262
H	-5.43442	-1.70027	0.00614
H	-5.86887	2.55467	-0.47760
H	-6.84255	0.34058	0.07479
S	-1.44443	0.76561	-1.37111
H	0.50579	0.54460	-0.22436
H	2.13471	-3.76546	-2.53840

TS3a$_{Bpin}$

C	0.79200	2.93083	0.01717
H	1.77976	3.36594	-0.17637
H	0.21245	3.63169	0.62030
H	0.29017	2.78535	-0.94304
C	1.01212	1.63591	0.73712
H	1.32248	1.69184	1.77677

C	1.26547	0.42739	0.05406
H	1.06970	0.42548	-1.01659
C	2.17805	-0.65321	0.52360
B	3.63998	-0.19410	0.02856
O	4.65753	-1.03638	-0.23830
O	3.90682	1.13258	-0.12498
C	1.78177	-2.02303	0.00413
F	2.67303	-2.95802	0.33595
F	0.58114	-2.41050	0.51676
F	1.64689	-2.00788	-1.34134
H	2.21758	-0.71094	1.61323
Se	-3.50443	0.03321	0.88670
C	-3.64926	-1.39429	-0.38866
C	-2.57058	-2.22715	-0.68208
C	-4.90186	-1.59485	-0.97564
C	-2.75069	-3.26829	-1.59480
H	-1.60622	-2.08438	-0.21440
C	-5.06567	-2.62997	-1.89244
H	-5.73118	-0.94234	-0.72477
C	-3.99048	-3.46663	-2.20165
H	-1.91666	-3.92173	-1.82861
H	-6.03309	-2.78758	-2.35743
H	-4.12274	-4.27657	-2.91129
C	-3.66397	1.53654	-0.29099
C	-3.29539	1.45636	-1.63494
C	-4.07079	2.74524	0.27694
C	-3.35274	2.60809	-2.42046
H	-2.98781	0.50975	-2.06461
C	-4.11796	3.89009	-0.51720
H	-4.35580	2.78879	1.32347
C	-3.76178	3.82198	-1.86546
H	-3.08295	2.55362	-3.47033
H	-4.44352	4.83040	-0.08467
H	-3.80947	4.71204	-2.48392
S	-0.82627	0.55082	0.67878
C	-0.74855	-0.17109	2.39922
F	0.49508	-0.19336	2.90118
F	-1.22910	-1.41353	2.39256
F	-1.50261	0.57649	3.20821
C	5.23511	1.20724	-0.76870
C	5.85706	-0.19310	-0.40690
C	4.96724	1.38798	-2.26219
H	4.35972	2.28406	-2.41121
H	5.89951	1.51186	-2.81786
H	4.42900	0.53248	-2.67912
C	5.97685	2.40713	-0.20138
H	6.03503	2.37042	0.88685
H	6.99312	2.44874	-0.60350
H	5.46452	3.32903	-0.48794
C	6.72346	-0.81120	-1.49318
H	6.16919	-0.95529	-2.42106
H	7.58963	-0.17454	-1.69603
H	7.08925	-1.78494	-1.15994
C	6.57797	-0.21092	0.94007
H	7.52147	0.33778	0.89025
H	5.96362	0.22835	1.73087
H	6.79563	-1.24585	1.21233

Int2a$_{Bpin}$

C	-0.93011	2.81485	-1.60077
H	0.14309	3.01676	-1.51348
H	-1.48457	3.72630	-1.37290
H	-1.13742	2.50746	-2.62847
C	-1.21980	1.72826	-0.60714
H	-1.15022	1.99839	0.44304
C	-0.99568	0.31850	-0.91904
H	-0.79636	0.09796	-1.96762
C	-0.38987	-0.65877	0.04138
B	1.15952	-0.24201	0.15848
O	2.12240	-1.05200	0.62955
O	1.54912	1.00604	-0.22281
C	-0.56311	-2.08788	-0.45291
F	-0.08294	-2.96715	0.42411
F	-1.86881	-2.37322	-0.67236
F	0.07874	-2.24681	-1.63384
H	-0.82090	-0.58428	1.04310
S	-2.87429	0.78164	-0.88224
C	-3.41753	0.35265	0.87573
F	-2.57827	0.85485	1.78380
F	-3.47648	-0.95948	1.00773
F	-4.61554	0.89167	1.01978
C	2.96135	1.13540	0.21725
C	3.40413	-0.37076	0.34390
C	3.71502	1.94021	-0.82866
H	3.33610	2.96530	-0.85482
H	4.77826	1.98485	-0.57626
H	3.61397	1.50756	-1.82456
C	2.91762	1.87380	1.55285

H	3.92557	2.06404	1.92836
H	2.41893	2.83684	1.41689
H	2.37166	1.30365	2.30933
C	3.91319	-0.97142	-0.96488
H	4.89550	-0.57126	-1.22658
H	4.00249	-2.05332	-0.84703
H	3.22603	-0.77569	-1.79288
C	4.36337	-0.66181	1.48666
H	5.30074	-0.11643	1.34276
H	3.94129	-0.38422	2.45298
H	4.59313	-1.72932	1.50846

TS4a$_{Bpin}$

C	2.90841	2.24391	-2.37131
H	3.43146	3.09133	-1.91843
H	1.92651	2.58031	-2.71229
C	2.66289	1.12861	-1.38449
H	2.17667	0.24407	-1.79265
C	2.23419	1.45414	-0.03010
H	2.52091	2.43166	0.35567
C	1.26802	0.69415	0.73149
H	1.26169	-0.35286	0.46761
B	-0.14366	1.38468	0.16460
O	-0.90738	2.10568	1.02971
O	-0.07251	1.94034	-1.10455
C	1.41749	0.84345	2.23005
F	2.55519	0.23677	2.65821
F	0.39296	0.29179	2.88362
F	1.51925	2.14526	2.59141
S	4.22112	0.61403	-0.44799
C	4.01048	-1.23480	-0.31172
F	3.24916	-1.59349	0.71648
F	5.24670	-1.70447	-0.12028
F	3.50745	-1.74205	-1.43030
N	-1.23399	-0.48681	-0.09350
S	-0.56678	-1.64299	-1.04058
S	-2.55899	-0.88500	0.83608
O	0.60957	-1.02341	-1.67441
O	-1.52272	-2.38353	-1.85832
O	-3.00971	0.33936	1.48664
O	-2.33524	-2.11415	1.59711
C	0.21572	-2.93837	0.10103
C	-3.96289	-1.30565	-0.36654
F	0.59004	-2.36932	1.25820
F	-0.61075	-3.94216	0.33849
F	1.31462	-3.40707	-0.50985
F	-3.83819	-0.62452	-1.51105
F	-5.10454	-0.94351	0.22727
F	-4.00024	-2.60693	-0.62050
C	-1.15725	2.91923	-1.18175
C	-1.36669	3.29743	0.33402
C	-0.68770	4.06530	-2.06933
H	-0.55922	3.70724	-3.09479
H	-1.43292	4.86604	-2.08555
H	0.26044	4.48419	-1.72700
C	-2.36454	2.22755	-1.81031
H	-3.17194	2.94251	-1.99049
H	-2.06546	1.79064	-2.76627
H	-2.73976	1.42704	-1.17957
C	-0.45896	4.43675	0.80610
H	-0.77986	5.40208	0.40520
H	-0.49353	4.48086	1.89663
H	0.58089	4.26852	0.51048
C	-2.81192	3.56446	0.73165
H	-3.42903	2.68017	0.58177
H	-2.85458	3.82336	1.79244
H	-3.22024	4.40209	0.15685
H	3.48432	1.88439	-3.22595

1b

C	-1.58756	1.66843	-0.36991
H	-1.85526	2.67602	-0.02701
H	-1.37937	1.75174	-1.44476
C	-0.35319	1.18629	0.33605
H	-0.40686	1.14478	1.42395
C	0.74018	0.74001	-0.28279
H	0.79260	0.75912	-1.36974
C	1.94366	0.16831	0.42381
B	3.24089	1.04991	0.14760
O	3.81474	1.65882	1.22749
H	4.57838	2.21384	1.02798
O	3.66476	1.17212	-1.14463
H	4.44487	1.72343	-1.27622
C	2.15281	-1.27661	0.01650
F	3.26746	-1.79017	0.59560
F	1.11481	-2.06384	0.39018
F	2.29411	-1.42318	-1.31836
H	1.76467	0.15256	1.50337

C	-2.77924	0.74671	-0.15349
C	-4.06979	1.27291	-0.03090
C	-2.61120	-0.64270	-0.09744
C	-5.17183	0.43398	0.13222
H	-4.21151	2.35028	-0.06467
C	-3.71167	-1.48317	0.06767
H	-1.61245	-1.06268	-0.16879
C	-4.99570	-0.94904	0.18137
H	-6.16610	0.86077	0.22627
H	-3.56428	-2.55827	0.11114
H	-5.85129	-1.60460	0.31225

TS3b(3*R*)

C	-0.06948	3.39909	-0.24404
H	-0.50650	4.13571	-0.93423
H	-0.30931	3.73285	0.76467
C	-0.78242	2.11671	-0.57347
H	-0.59813	1.74953	-1.58283
C	-1.90945	1.59140	0.08114
H	-2.18476	2.02664	1.03808
C	-2.93292	0.73151	-0.59244
B	-3.87713	1.63973	-1.53899
O	-4.97905	1.04703	-2.04697
H	-5.55840	1.58488	-2.60025
O	-3.43545	2.91027	-1.76408
H	-3.98451	3.45544	-2.34183
C	-3.75755	-0.04335	0.42930
F	-4.49499	-0.99667	-0.15075
F	-2.98231	-0.64065	1.36754
F	-4.58335	0.79798	1.09563
H	-2.44819	-0.00659	-1.24464
Se	1.08461	-1.95050	1.14560
C	2.64673	-1.80468	0.04111
C	3.16277	-0.56461	-0.33585
C	3.27704	-2.99695	-0.32755
C	4.32148	-0.52776	-1.11337
H	2.68937	0.36152	-0.03323
C	4.42568	-2.94563	-1.11306
H	2.86625	-3.95008	-0.01223
C	4.94701	-1.71078	-1.50576
H	4.72534	0.43309	-1.40986
H	4.91566	-3.86694	-1.40973
H	5.84564	-1.67254	-2.11262
C	-0.17131	-2.66248	-0.11649
C	0.01899	-2.55345	-1.49432
C	-1.36585	-3.15245	0.41453
C	-1.00750	-2.95931	-2.34950
H	0.95021	-2.16829	-1.89329
C	-2.38779	-3.54066	-0.44961
H	-1.50318	-3.21154	1.48924
C	-2.20857	-3.44726	-1.83135
H	-0.86508	-2.89368	-3.42349
H	-3.32147	-3.91342	-0.04283
H	-3.00297	-3.75657	-2.50222
S	-0.15130	0.31488	0.42441
C	0.17305	0.87658	2.16806
F	-0.26551	2.12053	2.41057
F	1.48579	0.83423	2.41997
F	-0.44524	0.04578	3.00922
C	1.42804	3.31232	-0.45765
C	2.30009	3.31409	0.63530
C	1.95368	3.19632	-1.74947
C	3.67754	3.20322	0.44035
H	1.90459	3.41068	1.64062
C	3.32900	3.08606	-1.94653
H	1.28791	3.21140	-2.60903
C	4.19448	3.09192	-0.85044
H	4.34496	3.21550	1.29576
H	3.72560	3.01040	-2.95385
H	5.26691	3.02392	-1.00268

Int2b(3*R*)

C	-1.55363	-1.52904	0.78664
H	-1.35657	-2.54988	0.43450
H	-1.37789	-1.52705	1.86714
C	-0.51287	-0.68282	0.08601
H	-0.63035	-0.59966	-0.99153
C	0.83364	-0.47089	0.61393
H	0.99193	-0.81326	1.63646
C	2.07632	-0.43432	-0.22475
B	2.41157	-1.95321	-0.68159
O	3.60000	-2.14816	-1.27955
H	3.83392	-3.04340	-1.55407
O	1.42311	-2.86081	-0.43502
H	1.59919	-3.77219	-0.70259
C	3.23036	0.18282	0.56008
F	4.30643	0.36318	-0.20198
F	2.87833	1.38215	1.08322

F	3.55608	-0.61866	1.60126
H	1.93937	0.14849	-1.13947
S	-0.32541	1.06780	0.80991
C	0.02879	2.12318	-0.71509
F	1.20113	2.71518	-0.57697
F	-0.94331	3.01747	-0.76181
F	0.02922	1.39068	-1.83073
C	-2.95705	-1.08379	0.45156
C	-3.53136	-1.42266	-0.77884
C	-3.66869	-0.27417	1.34317
C	-4.80177	-0.95715	-1.11316
H	-2.99178	-2.06435	-1.47144
C	-4.94097	0.19045	1.00924
H	-3.23686	-0.02057	2.30804
C	-5.50690	-0.14847	-0.21978
H	-5.24449	-1.23181	-2.06481
H	-5.49078	0.80901	1.71075
H	-6.49814	0.20883	-0.47794

TS3b(3*S*)

C	3.06431	-1.40701	-1.30214
H	2.93666	-0.8861	-2.25069
H	2.96280	-2.48276	-1.45760
C	2.14483	-0.90349	-0.25202
H	2.08587	-1.48171	0.66746
C	1.47932	0.3416	-0.28730
H	1.65420	0.97403	-1.15124
C	1.11721	1.10665	0.97346
H	0.80125	0.41760	1.76367
B	-0.07088	2.14048	0.67154
O	-1.11675	2.14360	1.54020
H	-1.86695	2.70704	1.30186
O	0.04187	2.87285	-0.46698
H	-0.72170	3.42808	-0.67120
C	2.36679	1.80056	1.50051
F	3.27880	0.90818	1.94482
F	2.06041	2.62018	2.52202
F	2.96398	2.53835	0.53900
Se	-2.99120	-1.12057	-0.82694
C	-3.37225	0.74706	-0.57999
C	-4.18495	1.17579	0.47112
C	-2.87181	1.65678	-1.51425
C	-4.44331	2.53849	0.62484
H	-4.59303	0.46009	1.17474
C	-3.15919	3.01562	-1.36936
H	-2.26035	1.31675	-2.34113
C	-3.92846	3.46188	-0.29066
H	-5.06372	2.87549	1.44868
H	-2.79418	3.72212	-2.10947
H	-4.14860	4.51839	-0.17872
C	-2.85649	-1.73332	0.98285
C	-2.26161	-0.95229	1.97900
C	-3.29092	-3.03515	1.24505
C	-2.11263	-1.49043	3.25683
H	-1.94052	0.06251	1.77755
C	-3.12602	-3.56187	2.52541
H	-3.75666	-3.62716	0.46395
C	-2.53954	-2.79122	3.53067
H	-1.66426	-0.88689	4.03958
H	-3.46594	-4.56996	2.73755
H	-2.42128	-3.20225	4.52767
S	-0.27442	-0.70955	-0.70529
C	-0.02999	-0.86080	-2.54883
F	-1.19707	-0.68979	-3.18675
F	0.44527	-2.06797	-2.86267
F	0.82375	0.05967	-3.02129
C	4.40765	-1.07049	-0.65329
C	5.08373	-2.02936	0.11302
C	4.92455	0.22908	-0.75427
C	6.28556	-1.70249	0.73505
H	4.67939	-3.03371	0.20201
C	6.12519	0.55288	-0.12980
H	4.38988	0.98378	-1.32257
C	6.80647	-0.41177	0.61503
H	6.81699	-2.45289	1.31068
H	6.52699	1.55626	-0.22080
H	7.74140	-0.15812	1.10351

Int2b(3*S*)

C	1.55233	-1.49149	0.79329
H	1.34168	-2.51276	0.44527
H	1.39702	-1.48894	1.87688
C	0.50464	-0.64519	0.11015
H	0.60303	-0.55426	-0.96901
C	-0.82369	-0.38411	0.66999
H	-0.98602	-0.73286	1.68966
C	-2.08352	-0.31127	-0.16235
H	-1.87150	0.06448	-1.16638

B	-3.24060	0.57235	0.52154
O	-4.35297	0.76695	-0.21489
H	-5.07625	1.26696	0.18280
O	-2.95338	1.03434	1.76957
H	-3.64111	1.54579	2.21412
C	-2.54253	-1.76044	-0.35610
F	-1.51319	-2.53171	-0.79533
F	-3.53195	-1.84599	-1.24095
F	-2.95775	-2.28534	0.81676
S	0.32229	1.11771	0.84769
C	-0.09553	2.18179	-0.65013
F	0.79374	3.15854	-0.65295
F	-1.32071	2.67420	-0.50326
F	-0.02860	1.49384	-1.78662
C	2.95393	-1.06213	0.42862
C	3.68720	-0.25155	1.30155
C	3.50358	-1.41819	-0.80793
C	4.95796	0.19800	0.94233
H	3.27450	0.01305	2.27196
C	4.77266	-0.96739	-1.16704
H	2.94725	-2.06189	-1.48505
C	5.49993	-0.15735	-0.29292
H	5.52572	0.81663	1.62936
H	5.19699	-1.25547	-2.12304
H	6.49028	0.18767	-0.57048

Int3b(3*R*)

S	-0.34404	1.74576	-0.23013
C	-0.55114	2.88130	1.24133
F	-1.20857	3.98600	0.86242
F	0.68067	3.21574	1.61761
F	-1.19724	2.34824	2.28526
C	-3.32445	1.89634	-0.03211
H	-3.17889	2.29761	0.97042
H	-3.50347	2.73477	-0.71105
C	-2.10853	1.12287	-0.50302
H	-2.11762	0.82390	-1.54674
C	-1.36174	0.20519	0.37122
H	-1.49988	0.35400	1.43577
C	-0.85805	-1.14332	-0.05650
B	0.42510	-1.07092	-1.12057
O	0.03038	-0.06745	-2.07452
H	0.74335	0.05321	-2.72109
O	0.93338	-2.30915	-1.56152
H	0.24967	-2.86347	-1.95078
C	-2.00679	-1.94057	-0.64548
F	-3.06841	-1.98985	0.19981
F	-1.63726	-3.22178	-0.87932
F	-2.47732	-1.45008	-1.81766
H	-0.56947	-1.68608	0.83959
N	1.81186	-0.41509	-0.27586
S	2.12422	-0.70063	1.34618
S	3.11858	0.00891	-1.26033
C	2.36747	-2.56311	1.44149
C	3.23760	1.86839	-0.96169
F	1.19376	-3.19025	1.32020
F	3.19406	-2.96295	0.48813
F	2.88445	-2.83842	2.64014
F	2.99509	2.19688	0.30809
F	2.33079	2.48752	-1.73408
F	4.45512	2.27289	-1.30660
O	2.68137	-0.08354	-2.65398
O	4.38218	-0.57084	-0.83854
O	3.38112	-0.10810	1.77696
O	0.88849	-0.41140	2.08101
C	-4.48407	0.91964	-0.03159
C	-4.93258	0.36592	1.17097
C	-5.05994	0.49914	-1.23522
C	-5.94693	-0.59000	1.17266
H	-4.48565	0.68364	2.10914
C	-6.07121	-0.45862	-1.23529
H	-4.71353	0.91943	-2.17558
C	-6.51527	-1.00614	-0.03093
H	-6.28950	-1.01153	2.11223
H	-6.51035	-0.77918	-2.17451
H	-7.30126	-1.75447	-0.03125

TS4b$_{anti}$(3*R*)

C	2.23554	-0.64884	-1.50832
H	2.68190	-0.28390	-2.43978
H	1.36108	-1.24252	-1.78461
C	1.69131	0.52872	-0.69196
H	1.31880	0.21968	0.28362
C	0.77874	1.44658	-1.38686
H	1.03879	1.70178	-2.41145
C	-0.42291	1.94736	-0.85903
B	-1.47896	0.63860	-1.47454
O	-2.78207	1.07623	-1.45101

H	-3.27298	0.79017	-2.23062
O	-0.85899	0.03511	-2.56609
H	-1.37090	-0.73923	-2.85155
C	-0.86541	3.28229	-1.42067
F	-2.02034	3.69351	-0.88806
F	0.06790	4.22844	-1.14355
F	-0.99572	3.24799	-2.76666
H	-0.51069	1.91799	0.22198
S	3.01066	1.82237	-0.43004
C	2.56129	2.44479	1.24182
F	1.40408	3.11617	1.25678
F	3.54425	3.28158	1.59810
F	2.48433	1.45509	2.13094
N	-1.44371	-0.69931	-0.08697
S	-1.39338	-0.37024	1.55428
S	-2.30435	-2.06012	-0.56970
C	-2.91161	0.69925	1.85953
C	-0.98342	-3.38837	-0.55554
F	-2.70324	1.91580	1.34904
F	-3.98476	0.15688	1.30086
F	-3.08251	0.79643	3.17672
F	-1.55571	-4.55109	-0.85169
F	-0.05981	-3.10226	-1.48511
F	-0.39161	-3.46708	0.63428
O	-0.25395	0.53408	1.75916
O	-1.53326	-1.56102	2.37812
O	-2.61970	-1.89614	-1.99786
O	-3.34389	-2.48697	0.35242
C	3.22608	-1.46385	-0.71530
C	2.78491	-2.25110	0.35562
C	4.59267	-1.41588	-1.00533
C	3.69537	-2.97663	1.12036
H	1.72694	-2.30250	0.58880
C	5.50558	-2.14531	-0.24317
H	4.94331	-0.80673	-1.83402
C	5.05847	-2.92569	0.82234
H	3.33967	-3.58392	1.94667
H	6.56378	-2.10175	-0.48132
H	5.76740	-3.49269	1.41742

TS4b$_{anti}$(3*S*)

S	-2.82123	-2.05578	0.75295
C	-2.77312	-1.52126	2.50886
F	-3.74127	-0.63979	2.80682
F	-1.60311	-0.96226	2.85938
F	-2.96963	-2.61716	3.24582
C	-2.39918	0.81476	0.32536
H	-2.38754	0.88012	1.41302
H	-1.58156	1.43770	-0.04436
C	-2.05956	-0.60486	-0.15546
H	-2.40368	-0.74697	-1.17871
C	-0.67894	-1.07540	0.03212
H	-0.20370	-0.86671	0.98615
C	0.13826	-1.69119	-0.93264
B	0.95056	-0.23110	-1.53157
O	1.92033	-0.64081	-2.41141
H	2.31231	0.11045	-2.87772
O	-0.00100	0.75442	-1.75155
H	0.42140	1.55234	-2.10568
C	-0.49819	-2.40342	-2.11476
F	0.42255	-3.04576	-2.83730
F	-1.39356	-3.33131	-1.67836
F	-1.18278	-1.57683	-2.93660
H	0.95527	-2.27400	-0.51203
N	1.97676	0.46488	-0.01119
S	2.60322	1.97059	-0.35982
S	2.73517	-0.46514	1.14554
C	1.51647	3.07612	0.68941
C	4.05886	-1.37499	0.16791
O	2.22924	2.27911	-1.75318
O	3.97243	2.18825	0.07804
O	1.77451	-1.50823	1.52499
O	3.41152	0.31688	2.16846
F	1.50683	2.64662	1.94740
F	0.26423	3.06040	0.20851
F	1.98851	4.31823	0.63516
F	4.93810	-1.88710	1.02572
F	3.49041	-2.36380	-0.52797
F	4.67462	-0.54372	-0.66856
C	-3.71074	1.28609	-0.25513
C	-4.86764	1.38855	0.52163
C	-3.77314	1.60525	-1.61859
C	-6.06820	1.80839	-0.05345
H	-4.82944	1.14085	1.57649
C	-4.97169	2.01975	-2.19376
H	-2.87220	1.53021	-2.22275
C	-6.12349	2.12267	-1.41051
H	-6.95978	1.88835	0.56072

H	-5.00682	2.26820	-3.24992
H	-7.05776	2.44869	-1.85671

TS4b$_{syn}$(3*R*)

S	-0.38383	1.90825	-0.40696
C	-0.55284	3.04755	1.04756
F	-1.37604	4.06942	0.76704
F	0.66660	3.53439	1.28031
F	-1.00180	2.45468	2.16580
C	-3.30838	1.86701	0.09009
H	-3.11957	2.24426	1.09478
H	-3.52997	2.72151	-0.55543
C	-2.09237	1.13414	-0.46161
H	-2.20610	0.82302	-1.49575
C	-1.37211	0.15169	0.35681
H	-1.28852	0.36683	1.41517
C	-0.91235	-1.14973	-0.10867
B	0.47806	-1.04316	-1.13591
O	0.07394	-0.07886	-2.11153
H	0.80658	0.0733	-2.72824
O	0.95824	-2.30392	-1.53777
H	0.34987	-2.74663	-2.13845
C	-2.01240	-1.91007	-0.83674
F	-3.11348	-2.03873	-0.05449
F	-1.61354	-3.16318	-1.14614
F	-2.42839	-1.33447	-1.98873
H	-0.63648	-1.75692	0.74929
N	1.78161	-0.42852	-0.24020
S	2.05266	-0.79322	1.37952
S	3.13078	0.01549	-1.16918
C	2.31869	-2.65690	1.40241
C	3.27251	1.86103	-0.79316
F	1.14910	-3.28594	1.26119
F	3.14784	-3.01687	0.43622
F	2.83902	-2.96737	2.59070
F	2.94927	2.14737	0.46626
F	2.44294	2.52970	-1.60673
F	4.52307	2.23753	-1.03653
O	2.73672	-0.02375	-2.57844
O	4.36767	-0.60504	-0.72796
O	3.28972	-0.19824	1.85888
O	0.79653	-0.56158	2.09604
C	-4.45295	0.87545	0.11919
C	-4.82520	0.26980	1.32275
C	-5.09336	0.49290	-1.06431
C	-5.82501	-0.70153	1.34544
H	-4.33004	0.55937	2.24582
C	-6.09052	-0.47927	-1.04398
H	-4.80775	0.95463	-2.00581
C	-6.45679	-1.07989	0.16137
H	-6.10710	-1.16370	2.28606
H	-6.57987	-0.76960	-1.96816
H	-7.23183	-1.83943	0.17678

TS4b$_{syn}$(3*S*)

C	-2.32554	-0.17562	-1.73038
H	-1.72670	0.11306	-2.60058
H	-3.33129	0.21314	-1.88827
C	-1.62727	0.48188	-0.53312
H	-0.83333	-0.16325	-0.16914
C	-1.19398	1.88440	-0.55737
H	-1.91661	2.63378	-0.86550
C	0.15246	2.24206	-0.26645
H	0.71855	1.80977	-1.10928
B	0.93564	1.36892	1.03193
O	2.16550	1.95459	1.36911
H	2.03731	2.69907	1.96792
O	-0.06921	1.16797	1.99434
H	0.29304	0.67810	2.74845
C	0.41625	3.73064	-0.18904
F	-0.46499	4.44889	-0.93685
F	1.64864	4.02763	-0.63153
F	0.30980	4.20439	1.07622
S	-2.57265	0.89636	1.03186
C	-4.21251	1.38230	0.34447
F	-4.87172	1.99604	1.33145
F	-4.94886	0.33169	-0.05560
F	-4.12704	2.22642	-0.70343
N	1.42293	-0.20419	0.42415
S	1.87937	-1.31139	1.63776
S	2.03490	-0.48182	-1.11180
O	1.13953	0.21028	-2.05388
O	2.35427	-1.88294	-1.33392
O	1.56315	-0.71066	2.93513
O	3.18011	-1.91512	1.40354
C	3.64344	0.49643	-1.17243
C	0.58311	-2.66195	1.44314
F	3.35687	1.79082	-1.30094

F	4.32228	0.08204	-2.24195
F	4.35205	0.28973	-0.07436
F	0.57438	-3.36734	2.57301
F	-0.62144	-2.10262	1.26488
F	0.86468	-3.45522	0.42188
C	-2.29976	-1.68031	-1.58207
C	-3.30677	-2.36506	-0.89362
C	-1.19675	-2.39453	-2.06618
C	-3.21079	-3.74233	-0.69391
H	-4.16406	-1.82317	-0.51164
C	-1.10166	-3.76984	-1.86608
H	-0.40398	-1.86854	-2.58833
C	-2.10827	-4.44710	-1.17713
H	-3.99869	-4.26393	-0.15925
H	-0.23537	-4.30615	-2.23889
H	-2.03399	-5.51828	-1.01775

5b(*E*,3*R*)

C	0.57176	-1.55649	-0.74391
H	0.49717	-1.67471	-1.83023
H	0.09343	-2.43571	-0.29587
C	-0.25104	-0.32560	-0.30548
H	-0.06341	-0.12948	0.75170
C	-1.71926	-0.50259	-0.53708
H	-2.03328	-0.73806	-1.55125
C	-2.63423	-0.39765	0.42372
C	-4.09525	-0.59111	0.18275
F	-4.79519	0.51866	0.50946
F	-4.37577	-0.88513	-1.10433
F	-4.58305	-1.59847	0.94473
H	-2.37322	-0.15349	1.44930
S	0.31975	1.20233	-1.21252
C	0.84652	2.16736	0.23003
F	-0.15230	2.34583	1.12012
F	1.25405	3.37145	-0.19525
F	1.85796	1.58961	0.90250
C	2.01501	-1.47412	-0.31149
C	2.36217	-1.74342	1.01761
C	3.01684	-1.07703	-1.20181
C	3.68027	-1.61490	1.44989
H	1.59225	-2.05690	1.71873
C	4.33821	-0.94933	-0.77386
H	2.75781	-0.86011	-2.23355
C	4.67279	-1.21559	0.55337
H	3.93363	-1.82865	2.48374
H	5.10496	-0.63969	-1.47734
H	5.70070	-1.11523	0.88767

5b(*Z*,3*R*)

S	-0.17077	1.84486	0.55887
C	1.28085	2.31326	-0.43037
F	2.43115	2.30202	0.27242
F	1.08988	3.56416	-0.87887
F	1.46167	1.50163	-1.48737
C	-1.03060	-0.61609	1.44942
H	-0.73922	-1.65390	1.63983
H	-1.17728	-0.13733	2.42344
C	0.17024	0.03281	0.72171
H	0.21513	-0.36024	-0.29245
C	1.45329	-0.22410	1.45472
H	1.60979	0.34813	2.36553
C	2.37085	-1.12068	1.08917
C	2.25087	-1.97688	-0.13662
F	1.09032	-2.69234	-0.15007
F	3.26295	-2.86184	-0.20523
F	2.26170	-1.25459	-1.28118
H	3.26794	-1.28371	1.67563
C	-2.29839	-0.57772	0.63106
C	-2.40669	-1.37944	-0.51248
C	-3.36049	0.26368	0.97190
C	-3.55469	-1.33751	-1.29985
H	-1.58414	-2.03764	-0.78050
C	-4.51230	0.30676	0.18523
H	-3.28446	0.88940	1.85704
C	-4.61137	-0.49297	-0.95243
H	-3.62721	-1.96529	-2.18267
H	-5.32994	0.9654	0.46151
H	-5.50684	-0.46068	-1.56524

5b(*E*,3*S*)

C	0.47788	-1.52821	0.74030
H	-0.02042	-2.39692	0.29352
H	0.38584	-1.63303	1.82650
C	-0.30703	-0.27811	0.28337
H	-0.12248	-0.10036	-0.77785
C	-1.77838	-0.41628	0.52619
H	-2.09340	-0.59172	1.55226
C	-2.69501	-0.35732	-0.43680

H	-2.43519	-0.17876	-1.47616
C	-4.15740	-0.52045	-0.18082
F	-4.43667	-0.73522	1.12202
F	-4.65822	-1.56542	-0.88104
F	-4.84632	0.57580	-0.57038
S	0.29032	1.25328	1.16690
C	1.03696	2.11152	-0.24797
F	1.46006	3.31233	0.17355
F	0.15681	2.29977	-1.25389
F	2.08398	1.45478	-0.77419
C	1.92781	-1.49271	0.32660
C	2.92539	-1.09015	1.21931
C	2.28673	-1.80718	-0.98925
C	4.25397	-0.99792	0.80518
H	2.65700	-0.83945	2.24087
C	3.61227	-1.71437	-1.40756
H	1.51985	-2.12578	-1.69138
C	4.60023	-1.30664	-0.50979
H	5.01747	-0.68261	1.50969
H	3.87496	-1.96190	-2.43151
H	5.63383	-1.23337	-0.83341

5b(*Z*,3*S*)

S	-0.29777	1.50492	-0.88963
C	0.92426	2.04618	0.34298
F	2.19757	1.79870	-0.01553
F	0.73591	1.46170	1.54000
F	0.78661	3.37327	0.49367
C	-1.24964	-1.03622	-1.38343
H	-1.42446	-0.69614	-2.41069
H	-0.99975	-2.10202	-1.44601
C	-0.00263	-0.32915	-0.81017
H	0.09947	-0.57660	0.24260
C	1.22237	-0.67952	-1.60020
H	1.10298	-0.56261	-2.67624
C	2.41314	-1.10374	-1.17333
C	2.88859	-1.31567	0.22849
F	3.33547	-2.58496	0.38489
F	3.92762	-0.49770	0.50329
F	1.95372	-1.10634	1.18169
H	3.19503	-1.31293	-1.89716
C	-2.48992	-0.84324	-0.54446
C	-3.54342	-0.03887	-0.98763
C	-2.58961	-1.45457	0.71116
C	-4.67430	0.15416	-0.19402
H	-3.47554	0.44228	-1.95945
C	-3.71625	-1.26258	1.50780
H	-1.77940	-2.08707	1.06562
C	-4.76280	-0.45638	1.05634
H	-5.48375	0.78261	-0.55245
H	-3.77933	-1.74387	2.47891
H	-5.64173	-0.30691	1.67563

1c

C	2.88433	-0.02678	-0.00326
C	1.47288	0.04904	-0.54567
H	1.41313	0.20989	-1.62406
C	0.33549	-0.05605	0.14245
H	0.34908	-0.20911	1.21756
C	-1.03695	0.08583	-0.47161
B	-1.65136	1.49342	-0.05219
O	-1.80223	2.41944	-1.04631
H	-2.12947	3.27983	-0.75727
O	-1.93664	1.70174	1.26717
H	-2.29045	2.57261	1.48199
C	-1.94333	-1.06253	-0.08512
F	-3.20731	-0.85538	-0.53874
F	-1.52680	-2.24016	-0.60411
F	-2.02514	-1.23022	1.25332
H	-0.96120	0.06143	-1.56303
C	3.59875	1.30241	-0.32836
H	3.58879	1.50297	-1.40506
H	3.10885	2.14161	0.17536
H	4.64405	1.26869	-0.00203
C	2.91878	-0.26688	1.51204
H	2.42050	0.54201	2.05566
H	2.42776	-1.20830	1.77723
H	3.95459	-0.31799	1.86219
C	3.61534	-1.18073	-0.72184
H	4.66024	-1.23691	-0.39742
H	3.13581	-2.14017	-0.50546
H	3.60748	-1.03722	-1.80764

TS3c(3*R*)

C	1.67863	2.89995	-0.21199
C	2.00219	1.53624	0.37222
H	2.42849	1.55885	1.37313
C	2.20828	0.36606	-0.37590

H	1.86683	0.36922	-1.40656
C	3.16556	-0.72583	-0.04622
B	4.53623	-0.41126	-0.84771
O	5.67635	-0.60604	-0.14902
H	6.50978	-0.45269	-0.61154
O	4.39417	0.05319	-2.11833
H	5.20598	0.21117	-2.61616
C	2.63631	-2.09701	-0.44276
F	3.61995	-3.01078	-0.45691
F	1.69080	-2.53456	0.42778
F	2.06460	-2.07938	-1.66577
H	3.41039	-0.76413	1.01455
Se	-2.40372	-0.13087	1.10516
C	-2.68873	-1.66474	-0.01356
C	-1.63537	-2.46895	-0.44634
C	-4.01443	-1.96361	-0.34093
C	-1.92090	-3.58349	-1.23688
H	-0.61110	-2.25050	-0.17798
C	-4.28434	-3.07307	-1.13818
H	-4.82028	-1.33070	0.01508
C	-3.23772	-3.88252	-1.58580
H	-1.10775	-4.21524	-1.57858
H	-5.31000	-3.30808	-1.40206
H	-3.45095	-4.74981	-2.20174
C	-2.75253	1.26956	-0.15676
C	-2.69613	1.05812	-1.53394
C	-2.96051	2.54471	0.37376
C	-2.85913	2.14862	-2.38987
H	-2.53356	0.06380	-1.93288
C	-3.11324	3.62672	-0.49155
H	-3.00538	2.68906	1.44896
C	-3.06356	3.42916	-1.87312
H	-2.82594	1.99435	-3.46349
H	-3.28076	4.61909	-0.08625
H	-3.19096	4.27088	-2.54552
S	0.15787	0.38373	0.53714
C	0.48907	-0.28756	2.24618
F	1.79231	-0.33982	2.54890
F	-0.02277	-1.51557	2.35999
F	-0.11204	0.50352	3.14110
C	3.06932	3.53378	-0.47341
H	3.65480	3.61851	0.44728
H	3.63974	2.94381	-1.19753
H	2.93673	4.54033	-0.88043
C	0.89063	2.83121	-1.52824
H	1.43968	2.30128	-2.31244
H	-0.08651	2.35755	-1.39904
H	0.70965	3.84655	-1.88978
C	0.90927	3.73634	0.82290
H	0.80020	4.76333	0.46481
H	-0.09146	3.32967	0.99036
H	1.43612	3.76969	1.78203

Int2c(3*R*)

C	-2.38876	-1.52298	0.12166
C	-1.28628	-0.54065	-0.25169
H	-1.30398	-0.22201	-1.29339
C	0.03025	-0.46797	0.39169
H	0.11411	-0.98604	1.34460
C	1.33212	-0.31872	-0.33385
B	1.86393	-1.80122	-0.71505
O	2.70478	-1.85989	-1.76499
H	3.08446	-2.71689	-1.99625
O	1.38165	-2.81784	0.05194
H	1.71908	-3.70373	-0.13300
C	2.36428	0.38972	0.53943
F	3.54875	0.46122	-0.07137
F	1.96778	1.65144	0.83351
F	2.52112	-0.26274	1.71151
H	1.23409	0.25365	-1.25661
S	-1.11829	1.02401	0.82765
C	-0.84459	2.36758	-0.47096
F	-0.33816	1.87690	-1.60260
F	-0.03738	3.27700	0.03499
F	-2.03872	2.88958	-0.71125
C	-2.35649	-1.91072	1.60621
H	-1.43232	-2.42908	1.87797
H	-2.48295	-1.04197	2.26261
H	-3.18368	-2.59167	1.81867
C	-2.11005	-2.76679	-0.75640
H	-2.16025	-2.52648	-1.82289
H	-1.12942	-3.19585	-0.53563
H	-2.87083	-3.52395	-0.54954
C	-3.74572	-0.90418	-0.24839
H	-4.54226	-1.63450	-0.08826
H	-3.96728	-0.02854	0.36971
H	-3.77638	-0.60159	-1.29995

TS3c(3*S*)

C	-2.19228	3.04047	-0.33021
C	-2.32694	1.67323	0.27128
H	-2.77769	1.63750	1.25939
C	-2.11919	0.45623	-0.38843
H	-1.76649	0.50888	-1.41577
C	-2.77601	-0.86121	-0.06044
H	-3.06555	-0.91291	0.98946
B	-1.75349	-2.04634	-0.41000
O	-1.41555	-2.87575	0.60796
H	-0.71640	-3.51259	0.40477
O	-1.24300	-2.03883	-1.66873
H	-0.54516	-2.68531	-1.84218
C	-4.07024	-0.93152	-0.86270
F	-4.92597	0.04915	-0.48172
F	-4.68115	-2.11152	-0.67621
F	-3.85331	-0.77108	-2.18368
Se	2.34436	-0.10984	1.13604
C	3.25165	1.00599	-0.13623
C	4.52347	0.60284	-0.55328
C	2.69831	2.21178	-0.56641
C	5.23118	1.40383	-1.44571
H	4.94705	-0.32913	-0.19460
C	3.42297	3.01253	-1.45117
H	1.72448	2.53254	-0.21698
C	4.68138	2.60713	-1.89490
H	6.21514	1.09369	-1.78092
H	3.00110	3.95241	-1.79125
H	5.23910	3.23178	-2.58447
C	2.10619	-1.68443	0.06666
C	2.05563	-1.62910	-1.32571
C	1.95793	-2.89742	0.74496
C	1.86519	-2.80956	-2.04761
H	2.17477	-0.68473	-1.84332
C	1.74857	-4.06987	0.01713
H	2.01133	-2.92720	1.82795
C	1.70544	-4.02823	-1.38096
H	1.84731	-2.77562	-3.13240
H	1.65338	-5.01677	0.53923
H	1.56936	-4.94382	-1.94710
S	-0.16924	0.66020	0.52921
C	-0.49712	0.12508	2.29163
F	0.15858	0.94623	3.11459
F	-0.04451	-1.11888	2.49465
F	-1.79428	0.14857	2.61327
C	-1.40921	3.06265	-1.64983
H	-0.38240	2.70452	-1.52047
H	-1.89154	2.46261	-2.42667
H	-1.35363	4.08931	-2.01967
C	-1.56363	4.00735	0.69059
H	-1.59923	5.02970	0.30567
H	-2.10152	3.98805	1.64337
H	-0.51887	3.74774	0.88407
C	-3.67180	3.45723	-0.59434
H	-4.24509	3.51246	0.33498
H	-3.67601	4.44865	-1.05644
H	-4.17113	2.75539	-1.26716

Int2c(3*S*)

C	2.5744	-1.09057	0.20835
C	1.34036	-0.31423	-0.21093
H	1.27516	-0.08574	-1.27259
C	0.06885	-0.29234	0.51593
H	0.07022	-0.76232	1.49678
C	-1.28907	-0.30576	-0.15679
H	-1.28356	0.26507	-1.08807
B	-2.45348	0.24896	0.80435
O	-3.64621	0.48428	0.22146
H	-4.36898	0.79290	0.78154
O	-2.08738	0.44295	2.10133
H	-2.77047	0.75839	2.70628
C	-1.54102	-1.75495	-0.58019
F	-0.58908	-2.16785	-1.45555
F	-2.72804	-1.90099	-1.16337
F	-1.47682	-2.57956	0.49045
S	0.99666	1.33527	0.76673
C	0.26616	2.47530	-0.53904
F	1.00233	3.57288	-0.50744
F	-0.99131	2.75535	-0.21154
F	0.29632	1.93736	-1.75609
C	2.36636	-2.49337	-0.42165
H	1.48005	-2.98909	-0.01931
H	2.26942	-2.44121	-1.50909
H	3.24081	-3.10636	-0.18835
C	2.71780	-1.22105	1.73138
H	3.62277	-1.78932	1.95728
H	2.82410	-0.24621	2.22102
H	1.88118	-1.75772	2.18799

C	3.81590	-0.41475	-0.39433
H	3.97854	0.57759	0.03830
H	4.70313	-1.01770	-0.18790
H	3.72822	-0.30959	-1.48010

Int3c(3*R*)

S	1.25652	-1.25512	-0.12478
C	1.60853	-2.20017	1.45229
F	2.60004	-3.08526	1.26692
F	0.48198	-2.86928	1.69223
F	1.90306	-1.44602	2.50913
C	4.21171	-0.38981	-0.23040
C	2.73921	-0.11248	-0.50916
H	2.53235	0.09095	-1.55827
C	1.75932	0.52513	0.38503
H	1.98409	0.46586	1.44380
C	0.83628	1.63844	-0.03590
B	-0.34144	1.18333	-1.12363
O	0.34164	0.36370	-2.08514
H	-0.29862	0.04400	-2.73943
O	-1.20036	2.21781	-1.55454
H	-0.73734	2.86911	-2.09123
C	1.67736	2.76800	-0.58982
F	2.69020	3.10177	0.26879
F	0.95028	3.88466	-0.78101
F	2.27881	2.47751	-1.77038
H	0.37886	2.04430	0.86234
N	-1.47807	0.12940	-0.30029
S	-1.87241	0.26813	1.32205
S	-2.58700	-0.64548	-1.31469
C	-2.67043	1.96601	1.45150
C	-2.12649	-2.45579	-1.07397
F	-1.74398	2.92306	1.34775
F	-3.57934	2.11280	0.50020
F	-3.24693	2.04787	2.65175
F	-1.89373	-2.75626	0.20317
F	-1.01253	-2.71569	-1.77717
F	-3.12105	-3.20570	-1.53879
O	-2.19618	-0.38289	-2.70055
O	-3.96922	-0.49621	-0.89260
O	-2.89135	-0.68715	1.72869
O	-0.61027	0.35082	2.06535
C	4.93215	0.83383	-0.85542
H	4.71981	0.92314	-1.92410
H	4.63220	1.76432	-0.37015
H	6.01123	0.70770	-0.72983
C	4.63741	-1.66635	-0.97334
H	4.37315	-1.61234	-2.03411
H	5.72117	-1.79403	-0.90238
H	4.16276	-2.55207	-0.54520
C	4.58621	-0.46719	1.25519
H	4.25818	0.42209	1.80119
H	4.18405	-1.35087	1.74772
H	5.67520	-0.51658	1.33976

Int3c(3*S*)

C	1.99621	-1.83448	1.59092
C	1.59357	-0.86223	0.49168
H	0.74019	-1.20552	-0.08453
C	1.76030	0.59212	0.46830
H	2.51918	0.98835	1.13687
C	0.67814	1.55000	0.05534
H	0.15974	1.77400	0.99160
B	-0.39202	0.96557	-1.06832
O	-1.27639	1.90643	-1.64451
H	-0.82302	2.46820	-2.28206
O	0.37934	0.12633	-1.93107
H	-0.18171	-0.25520	-2.62300
C	1.29045	2.86158	-0.38412
F	2.32175	3.24379	0.42406
F	0.39036	3.85811	-0.37050
F	1.80605	2.79964	-1.64018
S	2.72612	-0.25454	-0.97559
C	4.48478	-0.17955	-0.34409
F	5.17894	0.31519	-1.37394
F	4.96853	-1.39531	-0.05827
F	4.66761	0.61409	0.71441
N	-1.54604	-0.09921	-0.23422
S	-2.48108	-1.06318	-1.26405
S	-2.22324	0.29607	1.25754
O	-1.11635	0.67176	2.14454
O	-3.19300	-0.69485	1.69814
O	-1.96099	-0.94305	-2.62782
O	-3.91095	-0.98729	-1.01704
C	-3.16161	1.89908	0.94651
C	-1.92361	-2.77809	-0.75193
F	-2.29743	2.90930	0.86772
F	-3.96936	2.09099	1.99165

F	-3.87523	1.81500	-0.16535
F	-2.56501	-3.67251	-1.49741
F	-0.59767	-2.89278	-0.97935
F	-2.15174	-3.02055	0.53638
C	3.07603	-1.32970	2.55616
H	4.06150	-1.26395	2.09946
H	2.81585	-0.35549	2.98053
H	3.15265	-2.03326	3.38935
C	2.39202	-3.17912	0.95746
H	2.53286	-3.92802	1.74166
H	1.60797	-3.53763	0.28466
H	3.32379	-3.09836	0.39374
C	0.67811	-2.02420	2.39028
H	-0.11860	-2.43124	1.76570
H	0.86920	-2.73401	3.20030
H	0.32320	-1.08657	2.82040

TS4c$_{anti}$(3*S*)

C	1.47559	3.01686	0.05102
C	1.75840	1.51047	-0.09041
H	1.30727	1.08593	-0.98687
C	1.69262	0.60125	1.05932
H	1.99563	1.00616	2.02039
C	1.18478	-0.73081	1.04490
B	-0.45708	-0.49310	1.60794
O	-0.97633	-1.69885	2.06124
H	-1.38799	-1.60592	2.92746
O	-0.48853	0.68165	2.37486
H	-1.39987	0.86224	2.65364
C	1.91184	-1.65668	2.00357
F	1.47816	-2.91726	1.91227
F	3.24470	-1.67726	1.72375
F	1.80103	-1.25059	3.28905
H	1.14271	-1.18064	0.06059
S	3.59762	1.10608	-0.11689
C	3.66092	-0.14891	-1.47129
F	3.20680	-1.34733	-1.10525
F	4.95535	-0.26112	-1.79204
F	2.97682	0.25876	-2.54088
N	-1.47990	-0.15467	0.08929
S	-1.20591	-0.83321	-1.41508
S	-3.09386	0.12528	0.50762
C	-1.25842	-2.69417	-1.12869
C	-3.43669	1.83197	-0.22001
F	-0.17166	-3.07495	-0.45000
F	-2.34651	-3.03618	-0.45702
F	-1.25586	-3.28247	-2.32499
F	-4.75253	1.95437	-0.36546
F	-2.99890	2.76434	0.63312
F	-2.83621	2.00323	-1.39583
O	0.19556	-0.55277	-1.75908
O	-2.26224	-0.52989	-2.36866
O	-3.13434	0.34963	1.95925
O	-4.04081	-0.78648	-0.11396
C	2.10927	3.61133	1.31732
H	1.67862	3.18077	2.22607
H	3.19641	3.47166	1.34146
H	1.92212	4.68806	1.34704
C	-0.05465	3.15706	0.12039
H	-0.32184	4.21366	0.21588
H	-0.52822	2.76941	-0.78417
H	-0.45738	2.61500	0.97601
C	2.00358	3.73394	-1.20108
H	1.60011	3.28194	-2.11276
H	1.69564	4.78295	-1.18044
H	3.09521	3.70478	-1.25935

TS4c$_{anti}$(3*R*)

S	-3.54795	-0.89465	0.56018
C	-3.39053	-0.09537	2.21350
F	-4.16452	0.99344	2.35070
F	-2.13931	0.24870	2.53487
F	-3.82274	-1.01951	3.07817
C	-2.91415	1.71895	-0.79879
C	-2.67725	0.19276	-0.72539
H	-3.05450	-0.27129	-1.63724
C	-1.39825	-0.39575	-0.29314
H	-0.95356	0.02216	0.60150
C	-0.65350	-1.43000	-0.90578
B	0.79298	-0.59939	-1.50156
O	1.64550	-1.58832	-1.97861
H	2.19026	-1.26754	-2.70689
O	0.35917	0.48270	-2.27243
H	1.11316	0.94262	-2.66881
C	-1.31597	-2.21063	-2.02172
F	-0.57288	-3.24358	-2.42334
F	-2.51436	-2.72387	-1.60266
F	-1.60117	-1.44408	-3.09835

H	-0.19393	-2.09660	-0.17638
N	1.62457	0.10944	-0.05323
S	2.81645	1.22099	-0.48609
S	1.77883	-0.63814	1.44355
C	1.97278	2.83366	-0.03887
C	2.89915	-2.10994	1.09312
O	2.91804	1.23118	-1.95227
O	4.02446	1.14163	0.31749
O	0.47209	-1.22844	1.74987
O	2.44597	0.20206	2.42445
F	1.44992	2.75686	1.18412
F	0.99396	3.08598	-0.91687
F	2.87124	3.81264	-0.08712
F	3.37487	-2.55079	2.25621
F	2.18376	-3.07308	0.51143
F	3.90336	-1.75544	0.29888
C	-2.38252	2.14182	-2.18738
H	-2.53042	3.21865	-2.31124
H	-1.32243	1.91124	-2.29257
H	-2.92527	1.63234	-2.99031
C	-4.42312	2.00156	-0.73807
H	-4.96479	1.41946	-1.49107
H	-4.84549	1.77271	0.24122
H	-4.60145	3.06056	-0.94450
C	-2.16174	2.51168	0.28012
H	-1.08737	2.32238	0.24667
H	-2.30541	3.57950	0.09278
H	-2.52321	2.30896	1.28682

TS4c$_{syn}$(3*S*)

S	1.40759	-1.39445	-0.37916
C	1.65082	-2.40383	1.15462
F	2.74515	-3.18281	1.09432
F	0.57962	-3.20013	1.20765
F	1.71319	-1.69318	2.28652
C	4.20655	-0.27425	-0.00029
C	2.73276	-0.06229	-0.39428
H	2.66022	0.24807	-1.43527
C	1.73503	0.63338	0.43237
H	1.68542	0.35727	1.47780
C	0.88026	1.71407	-0.00906
B	-0.40922	1.17601	-1.08480
O	0.30389	0.47728	-2.09724
H	-0.32864	0.12742	-2.74304
O	-1.27268	2.23720	-1.41211
H	-0.86417	2.85809	-2.02406
C	1.65713	2.81794	-0.70774
F	2.61369	3.32567	0.12300
F	0.86517	3.85626	-1.04131
F	2.30169	2.43207	-1.83136
H	0.39123	2.16719	0.84915
N	-1.43433	0.12053	-0.25293
S	-1.82777	0.29689	1.37431
S	-2.57774	-0.64933	-1.25085
C	-2.69040	1.96841	1.48500
C	-2.15614	-2.46921	-1.01613
F	-1.78885	2.95165	1.41280
F	-3.58147	2.09810	0.51607
F	-3.29527	2.02005	2.67248
F	-1.94574	-2.78036	0.25774
F	-1.04990	-2.75062	-1.71879
F	-3.17129	-3.18264	-1.49576
O	-2.20426	-0.38810	-2.64207
O	-3.94745	-0.46864	-0.80204
O	-2.80447	-0.69386	1.79512
O	-0.57020	0.45322	2.10788
C	4.91628	1.02738	-0.44394
H	4.79578	1.20637	-1.51579
H	4.52918	1.89833	0.08828
H	5.98535	0.94138	-0.23013
C	4.77496	-1.45503	-0.80146
H	4.61156	-1.31725	-1.87517
H	5.85307	-1.52974	-0.63327
H	4.32036	-2.40134	-0.50350
C	4.44494	-0.46356	1.50459
H	4.00729	0.35179	2.08869
H	4.05851	-1.40808	1.88134
H	5.52227	-0.45423	1.69224

TS4c$_{syn}$(3*R*)

C	2.30906	-1.06328	1.87494
C	1.85053	-0.40172	0.55866
H	0.94904	-0.90065	0.21307
C	1.72787	1.05260	0.38880
H	2.60237	1.65346	0.61884
C	0.50757	1.68062	0.02117
H	-0.15337	1.54058	0.90248
B	-0.53415	0.86403	-1.12319

O	-1.49836	1.73290	-1.66233
H	-1.09898	2.35341	-2.28267
O	0.34096	0.14255	-1.95873
H	-0.15853	-0.33445	-2.63789
C	0.62656	3.16153	-0.26431
F	1.65091	3.74219	0.41719
F	-0.49594	3.81592	0.06896
F	0.86699	3.40544	-1.57982
S	2.82490	-0.37894	-1.05743
C	4.57674	-0.05451	-0.59025
F	5.21636	0.13809	-1.75044
F	5.17051	-1.08174	0.04005
F	4.74443	1.04230	0.17092
N	-1.50635	-0.26796	-0.24158
S	-2.14263	-1.55717	-1.14581
S	-2.38071	0.16594	1.14104
O	-1.50559	1.04589	1.93066
O	-2.98711	-0.98908	1.78097
O	-1.73384	-1.41823	-2.54377
O	-3.52527	-1.85614	-0.81527
C	-3.76827	1.29571	0.51972
C	-1.11901	-2.98488	-0.49445
F	-3.31428	2.54023	0.45628
F	-4.75574	1.22218	1.41139
F	-4.20068	0.90129	-0.66902
F	-1.57479	-4.11130	-1.03040
F	0.16590	-2.81432	-0.85251
F	-1.18427	-3.05692	0.83441
C	3.42650	-0.31721	2.61730
H	4.38450	-0.36223	2.10397
H	3.16863	0.73318	2.78618
H	3.56074	-0.77755	3.60013
C	2.70053	-2.52205	1.59681
H	2.88164	-3.04065	2.54261
H	1.89825	-3.04730	1.07133
H	3.60819	-2.58929	0.99473
C	1.03723	-1.04197	2.75777
H	0.22215	-1.60912	2.30277
H	1.26526	-1.49762	3.72548
H	0.67758	-0.02589	2.93929

5c(*E*,3*S*)

C	-1.22053	2.12666	0.11138
C	-0.69921	0.65806	0.15658
H	-0.81341	0.29383	1.18096
C	0.72073	0.49357	-0.28732
H	0.96980	0.83512	-1.28750
C	1.66906	-0.05633	0.46768
C	3.08151	-0.21448	0.01212
F	3.45596	-1.51383	0.01538
F	3.28317	0.26324	-1.23454
F	3.93342	0.43860	0.83833
H	1.47115	-0.43478	1.46592
S	-1.78211	-0.45130	-0.88742
C	-1.62103	-1.96694	0.09839
F	-0.36367	-2.44168	0.14766
F	-2.40222	-2.90533	-0.45631
F	-2.01614	-1.79235	1.37789
C	-1.30326	2.65442	-1.33081
H	-0.33089	2.6334	-1.83146
H	-2.01092	2.07656	-1.93425
H	-1.64888	3.69253	-1.32685
C	-0.23634	2.99315	0.91974
H	-0.60320	4.02281	0.96985
H	-0.13303	2.62203	1.94495
H	0.75882	3.00907	0.46792
C	-2.60637	2.20266	0.77249
H	-2.56973	1.83309	1.80282
H	-2.94981	3.24131	0.80013
H	-3.34813	1.61327	0.22909

5c(*Z*,3*S*)

S	1.83373	-0.73223	0.44502
C	0.87262	-2.18044	-0.08607
F	-0.20212	-2.41977	0.68401
F	1.68393	-3.24911	-0.01065
F	0.43529	-2.07340	-1.35438
C	1.29427	1.96251	-0.14762
C	0.57125	0.60328	0.12092
H	0.05944	0.31168	-0.79595
C	-0.38183	0.63781	1.27832
H	0.06709	0.82368	2.25045
C	-1.70287	0.45485	1.23101
C	-2.49509	0.20008	-0.01645
F	-2.54208	1.29043	-0.82702
F	-3.76793	-0.12007	0.29012
F	-1.99417	-0.80859	-0.76829
H	-2.30157	0.50602	2.13379

C	0.21134	3.04623	-0.30616
H	-0.50981	2.77648	-1.08196
H	-0.34398	3.20223	0.62242
H	0.67894	3.99531	-0.58546
C	2.08956	1.86375	-1.45993
H	1.43203	1.60264	-2.29571
H	2.55471	2.82811	-1.68640
H	2.87868	1.11068	-1.40278
C	2.23723	2.34723	1.00476
H	1.70454	2.43647	1.95620
H	3.04462	1.61907	1.13282
H	2.70067	3.31604	0.79538

5c(*E*,3*R*)

S	-1.28611	1.50501	-0.37885
C	0.29183	2.28599	0.07695
F	1.27276	2.06832	-0.81519
F	0.74611	1.86920	1.27376
F	0.08177	3.61136	0.14317
C	-2.10938	-1.13321	0.13761
C	-0.82204	-0.27902	-0.09581
H	-0.24500	-0.29036	0.82725
C	0.01382	-0.73535	-1.25435
H	-0.46362	-0.67400	-2.22885
C	1.27160	-1.17977	-1.21135
C	2.11839	-1.29551	0.02008
F	3.16766	-2.11260	-0.20791
F	2.61582	-0.10235	0.41574
F	1.44410	-1.80255	1.08677
H	1.79108	-1.45077	-2.12416
C	-1.67661	-2.60687	0.25705
H	-2.54201	-3.22535	0.51390
H	-1.25922	-2.98178	-0.68130
H	-0.91829	-2.73610	1.03351
C	-2.77188	-0.70338	1.45699
H	-2.07712	-0.81299	2.29619
H	-3.10362	0.33703	1.42690
H	-3.64431	-1.33274	1.65807
C	-3.11223	-0.98881	-1.01942
H	-2.67734	-1.28987	-1.97710
H	-3.98107	-1.62854	-0.83725
H	-3.47677	0.03855	-1.11908

5c(*Z*,3*R*)

C	-1.77480	1.85123	-0.07742
C	-0.95107	0.53970	-0.26273
H	-0.94812	0.29365	-1.32736
C	0.45445	0.61856	0.24176
H	0.59486	0.88106	1.28571
C	1.51705	0.35385	-0.51535
H	1.42866	0.05608	-1.55564
C	2.91730	0.41898	-0.00279
F	2.98003	0.78406	1.29531
F	3.65165	1.31074	-0.71014
F	3.53736	-0.77667	-0.12030
S	-1.82548	-0.87930	0.57881
C	-0.83140	-2.25727	-0.07185
F	-1.54125	-3.38582	0.08561
F	0.34104	-2.42167	0.56305
F	-0.54993	-2.11290	-1.38442
C	-1.96202	2.21209	1.40604
H	-2.51968	1.44130	1.94634
H	-1.00521	2.35695	1.91549
H	-2.52376	3.14734	1.48948
C	-3.14920	1.70021	-0.75139
H	-3.69226	2.64911	-0.70507
H	-3.04168	1.42475	-1.80578
H	-3.76305	0.93726	-0.26650
C	-0.99831	2.97872	-0.78385
H	-0.83208	2.74303	-1.84035
H	-1.56903	3.91086	-0.73246
H	-0.02303	3.15140	-0.32148

1d

C	3.41064	-0.66115	-0.39895
C	3.47077	0.47390	0.41329
C	4.52797	1.36611	0.33454
C	5.53921	1.08665	-0.59396
C	5.47885	-0.05072	-1.40777
C	4.40556	-0.94689	-1.31995
C	2.15847	-1.40578	-0.07082
C	2.25578	0.49186	1.28140
H	4.56336	2.24358	0.97117
H	6.38422	1.76164	-0.68551
H	6.27769	-0.23937	-2.11788
H	4.34684	-1.83154	-1.94473
O	1.72574	-2.43166	-0.55484
O	1.90905	1.31884	2.10214

N	1.54579	-0.67112	0.95700
C	0.23803	-1.00693	1.51523
H	0.10929	-2.08335	1.38696
H	0.27351	-0.77207	2.58280
C	-0.86549	-0.24435	0.83543
H	-0.89291	0.82461	1.02940
C	-1.75908	-0.82025	0.03158
H	-1.70552	-1.89617	-0.12901
C	-2.87705	-0.10575	-0.69699
H	-2.89556	-0.47016	-1.73137
B	-2.70772	1.47612	-0.76803
O	-2.89210	2.20874	0.36923
H	-2.78268	3.16225	0.27304
O	-2.36058	1.99251	-1.98480
H	-2.23517	2.94896	-2.00315
C	-4.22652	-0.50158	-0.12651
F	-4.45388	-1.83225	-0.25023
F	-5.22975	0.13322	-0.78685
F	-4.35243	-0.19978	1.17891

TS3d(3*R*)

C	5.05704	-0.20931	-0.46124
C	4.34122	-0.99023	0.45193
C	4.97637	-1.67859	1.47309
C	6.37019	-1.56491	1.55456
C	7.08733	-0.78397	0.64031
C	6.43569	-0.08946	-0.38699
C	4.09165	0.40503	-1.41503
C	2.89399	-0.90217	0.11336
H	4.40859	-2.27720	2.17694
H	6.90474	-2.08899	2.34012
H	8.16645	-0.71533	0.73174
H	6.98045	0.52101	-1.09879
O	4.28561	1.16872	-2.33788
O	1.93240	-1.38870	0.67130
N	2.82789	-0.08289	-1.02824
C	1.59224	0.31228	-1.65521
H	1.84623	0.81526	-2.59105
H	0.97900	-0.56132	-1.87317
C	0.77143	1.21168	-0.72557
H	0.57559	0.71550	0.22474
C	-0.43422	1.80968	-1.31796
H	-0.33127	2.22453	-2.31834
C	-1.69452	1.82733	-0.71212
H	-1.70978	1.67545	0.36260
B	-2.23210	0.25271	-1.41329
O	-3.59971	0.21989	-1.35068
H	-3.97311	-0.3957	-1.99498
O	-1.46011	-0.03542	-2.53707
H	-1.68313	-0.92087	-2.86906
C	-2.61485	2.94747	-1.15027
F	-2.07435	4.14013	-0.79128
F	-3.81805	2.86542	-0.57652
F	-2.77080	2.97789	-2.49236
S	1.66464	2.81044	-0.39695
C	1.15848	3.09438	1.34726
F	-0.15383	3.31608	1.47879
F	1.82089	4.18491	1.75377
F	1.49216	2.06476	2.12754
N	-1.67558	-1.07659	-0.10998
S	-1.63429	-0.84416	1.54552
S	-2.05776	-2.61223	-0.66294
O	-2.48647	-2.45732	-2.06647
O	-2.86569	-3.41001	0.24586
O	-0.88147	0.39647	1.77312
O	-1.31247	-2.05286	2.28588
C	-0.39567	-3.46749	-0.79388
C	-3.40799	-0.38579	1.98062
F	0.39910	-2.77270	-1.62376
F	-0.60942	-4.67488	-1.31890
F	0.18127	-3.58431	0.38808
F	-3.66192	0.85518	1.55122
F	-3.52765	-0.42479	3.30686
F	-4.26605	-1.23059	1.42361

Int2d(3*R*)

C	-4.08933	0.27036	0.54802
C	-4.20072	-0.86681	-0.26581
C	-5.38713	-1.18323	-0.90862
C	-6.47455	-0.32114	-0.71254
C	-6.36335	0.81357	0.09946
C	-5.16027	1.12836	0.74518
C	-2.70802	0.33375	1.08460
C	-2.89612	-1.57617	-0.27418
H	-5.46561	-2.06519	-1.53449
H	-7.42081	-0.53675	-1.19709
H	-7.22510	1.45903	0.23141
H	-5.06632	2.00392	1.37793

O	-2.16814	1.14544	1.81298
O	-2.53884	-2.59119	-0.83070
N	-2.05014	-0.79279	0.55206
C	-0.71750	-1.17606	0.91620
H	-0.56229	-1.01098	1.98638
H	-0.59284	-2.24238	0.69646
C	0.34632	-0.46993	0.10180
H	0.22978	-0.53903	-0.97629
C	1.70302	-0.30506	0.62125
H	1.82197	-0.52996	1.68121
C	2.94713	-0.50561	-0.19223
H	2.88043	-0.03265	-1.17520
B	3.11600	-2.09724	-0.45058
O	4.26905	-2.49022	-1.01973
H	4.40325	-3.43290	-1.17765
O	2.04071	-2.85576	-0.09043
H	2.10317	-3.80542	-0.25606
C	4.15460	0.08072	0.53229
F	3.92642	1.36522	0.89802
F	5.24798	0.05262	-0.22621
F	4.38907	-0.61528	1.66952
S	0.68123	1.32907	0.59748
C	1.16237	2.12139	-1.04901
F	2.38826	2.60512	-0.96286
F	0.28900	3.09577	-1.24095
F	1.09759	1.24898	-2.05790

TS3d(3*S*)

C	-5.10632	-0.65363	0.58670
C	-4.87812	0.69428	0.27432
C	-5.73080	1.69376	0.71547
C	-6.83461	1.30472	1.48624
C	-7.06128	-0.04041	1.79915
C	-6.19270	-1.04553	1.35236
C	-4.01833	-1.46589	-0.01807
C	-3.63974	0.78730	-0.54226
H	-5.54897	2.73366	0.46765
H	-7.52709	2.05802	1.84655
H	-7.92557	-0.30837	2.39748
H	-6.36078	-2.09010	1.58994
O	-3.76976	-2.65165	0.04986
O	-3.04859	1.75793	-0.97731
N	-3.21790	-0.54203	-0.72370
C	-2.03144	-0.91809	-1.44573
H	-2.25660	-1.74909	-2.11722
H	-1.74948	-0.05034	-2.04260
C	-0.94174	-1.32755	-0.45750
H	-1.12744	-1.01083	0.56572
C	-0.07472	-2.42585	-0.61595
H	0.02558	-2.84683	-1.61175
C	0.54307	-3.19727	0.51303
H	-0.29069	-3.65557	1.06625
B	1.34213	-2.26079	1.55443
O	2.65739	-2.47955	1.74174
H	3.11735	-1.84980	2.31546
O	0.58845	-1.26834	2.11966
H	1.08960	-0.62884	2.64874
C	1.38247	-4.33168	-0.05474
F	0.64256	-5.10209	-0.88872
F	1.86245	-5.11792	0.91545
F	2.41419	-3.85122	-0.78044
Se	2.60406	1.75566	-0.80856
C	3.05686	1.25165	0.98913
C	2.24893	1.58391	2.07992
C	4.20971	0.48394	1.16124
C	2.61014	1.14414	3.35621
H	1.35932	2.18668	1.93825
C	4.56616	0.04987	2.44073
H	4.83008	0.23005	0.30768
C	3.76703	0.37760	3.54005
H	2.00049	1.42114	4.21093
H	5.47419	-0.52885	2.57651
H	4.05258	0.05493	4.53578
C	1.36083	3.17157	-0.42938
C	-0.01767	3.01181	-0.56585
C	1.91364	4.39355	-0.03368
C	-0.85616	4.09232	-0.28702
H	-0.45754	2.07848	-0.88749
C	1.06693	5.46265	0.24910
H	2.98918	4.50229	0.05660
C	-0.31615	5.31159	0.12212
H	-1.92662	3.96023	-0.39650
H	1.48825	6.41290	0.55968
H	-0.97148	6.14937	0.33658
S	0.89288	-0.36158	-0.72490
C	0.97285	-0.28578	-2.58803
F	2.22916	-0.48517	-2.97732
F	0.58208	0.92584	-3.00535

F	0.19102	-1.20089	-3.17675

Int2d(3*S*)

C	-3.52030	-0.57709	-0.59085
C	-4.11979	0.37307	0.24852
C	-5.46851	0.31466	0.56150
C	-6.21247	-0.73394	0.00320
C	-5.61427	-1.68252	-0.83450
C	-4.24926	-1.61839	-1.14455
C	-2.08270	-0.24570	-0.72615
C	-3.08785	1.35101	0.67486
H	-5.92439	1.05415	1.21033
H	-7.27195	-0.81203	0.22235
H	-6.21977	-2.47993	-1.25172
H	-3.77902	-2.34764	-1.79479
O	-1.18908	-0.82132	-1.32775
O	-3.15204	2.32040	1.39355
N	-1.88780	0.91495	0.03758
C	-0.64495	1.64274	0.11036
H	-0.34850	1.99556	-0.87975
H	-0.81706	2.49955	0.76572
C	0.39894	0.70128	0.69425
H	0.15122	0.29987	1.67334
C	1.22464	-0.13885	-0.17310
H	1.24082	0.15703	-1.21654
C	1.58686	-1.57835	0.07861
H	0.73929	-2.12984	-0.35337
B	1.78826	-2.04783	1.59862
O	1.85647	-3.37364	1.81799
H	2.02096	-3.68136	2.71770
O	1.86823	-1.04324	2.52758
H	2.04380	-1.29831	3.44267
C	2.81166	-1.94965	-0.75841
F	2.72429	-1.45621	-2.01264
F	2.97077	-3.27018	-0.83704
F	3.92876	-1.41722	-0.19850
S	2.22257	1.21038	0.81001
C	2.35564	2.59965	-0.45485
F	3.63795	2.92347	-0.48672
F	1.62895	3.63137	-0.03856
F	1.94731	2.23391	-1.66837

Int3d(3*R*)

C	-5.42849	0.13169	-0.68564
C	-5.25422	-0.14182	0.67542
C	-6.06630	-1.04399	1.34308
C	-7.07524	-1.67211	0.60185
C	-7.25017	-1.39836	-0.75976
C	-6.42224	-0.48676	-1.42716
C	-4.39578	1.11674	-1.10685
C	-4.09831	0.65155	1.17221
H	-5.91677	-1.25350	2.39645
H	-7.73089	-2.38649	1.08887
H	-8.03880	-1.90462	-1.30672
H	-6.54440	-0.27099	-2.48284
O	-4.16191	1.59722	-2.19545
O	-3.57525	0.68192	2.26677
N	-3.67419	1.41686	0.06673
C	-2.49186	2.24760	0.09292
H	-2.64495	3.11465	-0.55086
H	-2.34031	2.56389	1.12361
C	-1.34846	1.39268	-0.42835
H	-1.41672	1.13950	-1.48201
C	-0.70921	0.37112	0.41932
H	-0.83842	0.50345	1.48764
C	-0.34850	-1.00155	-0.06062
H	-0.10104	-1.60403	0.80922
B	0.92055	-1.01990	-1.15010
O	0.60577	0.04614	-2.06362
H	1.31685	0.12663	-2.71847
O	1.28657	-2.28993	-1.64077
H	0.58500	-2.68959	-2.16475
C	-1.58216	-1.65377	-0.65285
F	-2.62228	-1.64820	0.23343
F	-1.35708	-2.94388	-0.97000
F	-2.05249	-1.04643	-1.77048
S	0.44421	1.83534	-0.14918
C	0.34754	2.94390	1.35626
F	-0.23831	4.10094	1.01444
F	1.60816	3.18014	1.70933
F	-0.31409	2.42913	2.39437
N	2.36997	-0.54286	-0.31259
S	2.68133	-0.90886	1.29531
S	3.69594	-0.21258	-1.30883
O	3.22960	-0.21312	-2.69620
O	4.90385	-0.92590	-0.93210
O	1.49511	-0.51926	2.06315
O	4.00003	-0.45857	1.71298

C	3.99550	1.61617	-0.94726
C	2.73723	-2.78838	1.32686
F	1.50444	-3.28940	1.20817
F	3.24388	-3.15438	2.50509
F	3.50324	-3.23550	0.34410
F	3.78341	1.92326	0.33383
F	3.15309	2.34556	-1.69566
F	5.24662	1.91255	-1.27997

Int3d(3*S*)

C	-1.58236	3.15716	-1.26512
C	-2.14471	3.05721	0.01233
C	-3.51341	3.12898	0.21057
C	-4.31692	3.32154	-0.91956
C	-3.75396	3.43263	-2.19609
C	-2.36940	3.34597	-2.38826
C	-0.11695	2.93442	-1.15401
C	-1.05750	2.80669	0.99211
H	-3.93766	3.01979	1.20213
H	-5.39474	3.37398	-0.80709
H	-4.40472	3.57367	-3.05294
H	-1.92510	3.40495	-3.37550
O	0.74818	2.88354	-2.00502
O	-1.09291	2.65922	2.19574
N	0.12593	2.76730	0.22398
C	1.41848	2.42818	0.76166
H	2.17819	2.96667	0.19739
H	1.44145	2.72465	1.81103
C	1.57053	0.91874	0.63615
H	0.83831	0.34671	1.19577
C	2.08192	0.28586	-0.58179
H	2.61097	0.94585	-1.26282
C	1.52885	-0.98360	-1.14881
H	0.77374	-0.62712	-1.85579
B	0.85227	-2.01441	-0.03942
O	0.49242	-3.29782	-0.50897
H	1.26703	-3.85741	-0.62901
O	1.68325	-1.90926	1.12086
H	1.33849	-2.46376	1.83804
C	2.57473	-1.67467	-1.99689
F	3.27150	-0.79594	-2.77011
F	2.02176	-2.57744	-2.82398
F	3.49947	-2.32793	-1.24548
S	3.23138	0.07992	0.99086
C	4.41482	1.50963	0.74208
F	5.63609	0.98498	0.85721
F	4.24228	2.42257	1.70591
F	4.31690	2.12296	-0.44291
N	-0.74094	-1.38036	0.42645
S	-1.43143	-2.13291	1.78271
S	-1.79502	-0.71334	-0.69354
O	-1.02719	0.28742	-1.44247
O	-3.07380	-0.34339	-0.10481
O	-0.40005	-2.95253	2.42409
O	-2.75941	-2.67347	1.54307
C	-2.13521	-2.08826	-1.93302
C	-1.61270	-0.68016	2.95651
F	-1.07469	-2.24638	-2.72399
F	-3.17930	-1.70198	-2.67106
F	-2.41786	-3.22054	-1.30968
F	-1.98398	-1.15851	4.14279
F	-0.41653	-0.07972	3.08338
F	-2.50477	0.19850	2.52629

TS4d$_{anti}$(3*S*)

C	5.05711	-0.20966	-0.46121
C	4.34128	-0.99066	0.45188
C	4.97641	-1.67909	1.47301
C	6.37023	-1.56540	1.55453
C	7.08739	-0.78439	0.64035
C	6.43576	-0.08980	-0.38692
C	4.09174	0.40474	-1.41498
C	2.89406	-0.90259	0.11328
H	4.40862	-2.27775	2.17680
H	6.90476	-2.08953	2.34006
H	8.16650	-0.71574	0.73181
H	6.98054	0.52072	-1.09866
O	4.28571	1.16850	-2.33777
O	1.93244	-1.38917	0.67115
N	2.82798	-0.08322	-1.02825
C	1.59233	0.31196	-1.65521
H	1.84628	0.81482	-2.59112
H	0.97902	-0.56162	-1.87301
C	0.77163	1.21152	-0.72561
H	0.57573	0.71541	0.22472
C	-0.43396	1.80963	-1.31803
H	-0.33097	2.22442	-2.31843
C	-1.69426	1.82747	-0.71216

H	-1.70951	1.67564	0.36256
B	-2.23207	0.25288	-1.41328
O	-3.59969	0.22038	-1.35084
H	-3.97312	-0.39578	-1.99458
O	-1.45998	-0.03548	-2.53693
H	-1.68337	-0.92075	-2.86914
C	-2.61443	2.94773	-1.15034
F	-2.07377	4.14032	-0.79140
F	-3.81764	2.86585	-0.57656
F	-2.77040	2.97812	-2.49242
S	1.66497	2.81022	-0.39706
C	1.15897	3.09416	1.34720
F	-0.15333	3.31593	1.47883
F	1.82147	4.18464	1.75366
F	1.49265	2.06451	2.12743
N	-1.67592	-1.07648	-0.10987
S	-1.63437	-0.84399	1.54560
S	-2.05839	-2.61204	-0.66280
O	-0.88134	0.39653	1.77307
O	-1.31264	-2.05271	2.28598
O	-2.48741	-2.45701	-2.06622
O	-2.86619	-3.40977	0.24615
C	-3.40795	-0.38532	1.98085
C	-0.39642	-3.46747	-0.79412
F	-3.66182	0.85555	1.55112
F	-4.26618	-1.23020	1.42422
F	-3.52741	-0.42393	3.30713
F	0.39825	-2.77276	-1.62415
F	-0.61039	-4.67485	-1.31909
F	0.18074	-3.58434	0.38774

TS4d$_{syn}$(3*S*)

C	5.46566	0.14671	0.56687
C	5.22229	-0.20820	-0.76440
C	6.00672	-1.14272	-1.42038
C	7.06074	-1.71795	-0.69902
C	7.30500	-1.36256	0.63262
C	6.50379	-0.41940	1.28895
C	4.44578	1.14770	0.98378
C	4.03202	0.54528	-1.24238
H	5.80346	-1.41557	-2.45002
H	7.69734	-2.45472	-1.17793
H	8.12725	-1.82928	1.16510
H	6.67966	-0.14066	2.32208
O	4.26397	1.68720	2.05480
O	3.44561	0.50110	-2.30422
N	3.66204	1.37443	-0.16516
C	2.48257	2.20834	-0.18560
H	2.65999	3.09629	0.42231
H	2.30024	2.49006	-1.22102
C	1.33778	1.38935	0.40142
H	1.49321	1.14064	1.44720
C	0.72001	0.31613	-0.38851
H	0.64900	0.47716	-1.45714
C	0.38777	-1.00490	0.13424
H	0.16728	-1.67039	-0.69586
B	-0.98671	-0.98831	1.18178
O	-0.66811	0.06278	2.09994
H	-1.40308	0.17654	2.72222
O	-1.32702	-2.26785	1.66098
H	-0.69389	-2.58901	2.31134
C	1.56738	-1.61789	0.87102
F	2.67719	-1.64551	0.07410
F	1.31980	-2.89439	1.21946
F	1.94064	-0.96230	1.99387
S	-0.42218	1.98714	0.30247
C	-0.34348	3.08271	-1.19732
F	0.39234	4.17757	-0.94624
F	-1.59876	3.45673	-1.44314
F	0.15859	2.49137	-2.28906
N	-2.35499	-0.55320	0.28271
S	-2.60774	-1.00630	-1.31819
S	-3.72806	-0.19056	1.21082
O	-3.31578	-0.12769	2.61400
O	-4.90841	-0.94005	0.81824
O	-1.39014	-0.67910	-2.06216
O	-3.90478	-0.55748	-1.79798
C	-4.03839	1.61596	0.75055
C	-2.68658	-2.88579	-1.25758
F	-1.45919	-3.38816	-1.09919
F	-3.18025	-3.30076	-2.42470
F	-3.46980	-3.28132	-0.26680
F	-3.73102	1.87509	-0.51966
F	-3.27945	2.39383	1.53566
F	-5.31963	1.88669	0.97058

TS4d$_{syn}$(3*R*)

C	-0.93808	2.47789	-2.12577

C	-1.19153	3.27378	-1.00256
C	-2.43793	3.83608	-0.78041
C	-3.43481	3.58344	-1.72995
C	-3.17945	2.79093	-2.85484
C	-1.92007	2.21930	-3.06778
C	0.44372	1.94867	-2.01819
C	0.02783	3.30044	-0.15281
H	-2.63020	4.42998	0.10593
H	-4.42768	3.99602	-1.58512
H	-3.97864	2.60233	-3.56389
H	-1.71995	1.57495	-3.91562
O	1.05144	1.15817	-2.72030
O	0.23788	3.83984	0.91154
N	0.97484	2.50765	-0.84630
C	2.23921	2.0889	-0.28687
H	3.02371	2.17767	-1.03804
H	2.45584	2.74287	0.55828
C	2.05469	0.64719	0.18762
H	1.20936	0.56836	0.86180
C	2.12578	-0.45499	-0.77914
H	2.92218	-0.40912	-1.51365
C	1.16216	-1.51670	-0.81816
H	0.33051	-1.04265	-1.38524
B	0.37282	-1.94443	0.62648
O	-0.25688	-3.20418	0.58913
H	0.39302	-3.91561	0.56354
O	1.28258	-1.63962	1.66841
H	0.89009	-1.83521	2.53257
C	1.61257	-2.71380	-1.62852
F	2.47282	-2.38059	-2.62453
F	0.57143	-3.34532	-2.19098
F	2.26648	-3.62028	-0.85166
S	3.43030	-0.23880	1.09116
C	4.89332	0.62074	0.36372
F	5.97374	-0.02790	0.80606
F	4.97275	1.90095	0.75992
F	4.91084	0.61505	-0.98359
N	-1.02763	-0.87438	0.79451
S	-1.64279	-0.67331	2.36288
S	-2.14664	-0.69865	-0.45818
O	-1.36762	-0.58376	-1.70001
O	-3.14962	0.31232	-0.16079
O	-0.79058	-1.39816	3.30713
O	-3.08886	-0.80687	2.43366
C	-3.03415	-2.36620	-0.60730
C	-1.25960	1.13376	2.67349
F	-2.33577	-3.15888	-1.40927
F	-4.22514	-2.11578	-1.15543
F	-3.19421	-2.93221	0.57876
F	-1.68124	1.44834	3.89410
F	0.06795	1.32631	2.60450
F	-1.86025	1.90512	1.77329

TS4d$_{anti}$(3*R*)

C	1.78821	-0.35170	-0.39795
H	1.45496	-1.07008	0.35132
C	1.25439	1.05760	-0.13539
H	1.53384	1.71807	-0.95438
C	-0.16301	1.15566	0.25072
H	-0.51991	0.46405	1.00690
C	-1.13238	2.00230	-0.30807
H	-1.96407	2.22739	0.35637
B	-1.83467	0.79667	-1.41121
O	-0.80317	0.13603	-2.06067
H	-1.16036	-0.55226	-2.64496
O	-2.93281	1.37303	-1.99878
H	-3.22250	0.88347	-2.77978
C	-0.69430	3.22010	-1.09896
F	0.14215	3.98939	-0.34750
F	-1.74418	3.97666	-1.43212
F	-0.01725	2.91184	-2.22477
S	1.84676	1.98018	1.37481
C	1.98812	0.67231	2.66363
F	1.91342	1.28850	3.84584
F	3.16247	0.03430	2.59898
F	1.01414	-0.24877	2.58819
N	-2.59465	-0.56890	-0.23588
S	-3.37817	-0.25810	1.20428
S	-2.97766	-1.96306	-1.06740
O	-2.67833	-1.71750	-2.49007
O	-4.24566	-2.57285	-0.70196
O	-2.55167	0.72799	1.91053
O	-3.83473	-1.45726	1.88898
C	-1.62230	-3.10906	-0.47467
C	-4.90856	0.69083	0.66418
F	-0.42975	-2.61259	-0.83956
F	-1.66121	-3.21558	0.84912
F	-1.78921	-4.30388	-1.03479

F	-4.57045	1.95081	0.38147
F	-5.78356	0.68210	1.66733
F	-5.44867	0.12292	-0.41125
H	1.35985	-0.64141	-1.36071
N	3.23256	-0.40844	-0.42757
C	4.05916	0.45256	-1.16613
C	3.96431	-1.43478	0.21218
C	5.44736	-0.03792	-0.94225
C	5.39044	-1.16508	-0.11806
O	3.67266	1.39600	-1.82945
O	3.47449	-2.32543	0.87104
C	6.65304	0.45495	-1.41535
C	7.81809	-0.22316	-1.03466
C	7.76116	-1.35254	-0.20918
C	6.53721	-1.84304	0.26360
H	6.68404	1.33032	-2.05476
H	8.78215	0.13114	-1.38478
H	8.68202	-1.85555	0.06742
H	6.48012	-2.71701	0.90310

5d(*E*,3*S*)

C	-3.37201	-0.83917	0.51607
C	-3.09893	-0.7095	-0.84841
C	-4.08881	-0.37146	-1.75695
C	-5.37985	-0.16397	-1.25476
C	-5.65379	-0.29464	0.11186
C	-4.64591	-0.63716	1.02236
C	-2.10729	-1.19921	1.21857
C	-1.64945	-0.97759	-1.06332
H	-3.86331	-0.27096	-2.81298
H	-6.18222	0.10425	-1.93450
H	-6.66426	-0.12588	0.46997
H	-4.84480	-0.73932	2.08359
O	-1.90821	-1.40552	2.39675
O	-0.99861	-0.95667	-2.08962
N	-1.13042	-1.27320	0.20609
C	0.27347	-1.49750	0.45660
H	0.36271	-1.84627	1.48792
H	0.64193	-2.27786	-0.21614
C	1.11194	-0.22765	0.21842
H	0.94070	0.11033	-0.80430
C	2.57038	-0.48168	0.43997
H	2.87381	-0.79435	1.43629
C	3.48724	-0.35663	-0.51637
H	3.23471	-0.04295	-1.52497
C	4.93959	-0.62734	-0.29183
F	5.68439	0.46945	-0.55552
F	5.38092	-1.60806	-1.11271
F	5.20732	-1.00718	0.97505
S	0.54365	1.14691	1.33801
C	-0.01721	2.31185	0.06565
F	0.92238	2.55753	-0.86632
F	-0.33449	3.46582	0.66776
F	-1.11011	1.8749	-0.59712

5d(Z,3*S*)

C	-2.65684	-0.94146	-0.64038
C	-3.18264	-0.48440	0.57110
C	-4.51096	-0.10742	0.68816
C	-5.31004	-0.20018	-0.45849
C	-4.78285	-0.65716	-1.67227
C	-3.43900	-1.03708	-1.78005
C	-1.21402	-1.25420	-0.43756
C	-2.09379	-0.48948	1.58941
H	-4.90664	0.24746	1.63353
H	-6.35509	0.08815	-0.40784
H	-5.42749	-0.71562	-2.54339
H	-3.01767	-1.39035	-2.71486
O	-0.38803	-1.65837	-1.23037
O	-2.12542	-0.16253	2.75735
N	-0.95867	-0.97873	0.91605
C	0.35922	-1.02749	1.50203
H	0.23446	-0.91464	2.58112
H	0.81843	-1.99651	1.28928
C	1.28853	0.05711	0.91961
H	1.35597	-0.10974	-0.15376
C	2.64553	0.00896	1.55930
H	2.71046	0.39125	2.57548
C	3.74583	-0.48636	0.99223
H	4.69422	-0.49909	1.51761
C	3.77781	-1.05889	-0.39589
F	2.87112	-2.05414	-0.55395
F	4.99376	-1.56928	-0.67289
F	3.50003	-0.13010	-1.34066
S	0.55201	1.74537	1.14399
C	0.55018	2.25127	-0.59970
F	1.76604	2.17596	-1.16513
F	0.12507	3.52164	-0.66330

F	-0.27626	1.49505	-1.35231

5d(*Z*,3*R*)

C	2.65643	-0.94183	-0.64021
C	3.18221	-0.48471	0.57126
C	4.51055	-0.10776	0.68831
C	5.30964	-0.20062	-0.45832
C	4.78246	-0.65766	-1.67208
C	3.4386	-1.03755	-1.77986
C	1.21358	-1.25445	-0.43742
C	2.09333	-0.48964	1.58953
H	4.90623	0.24716	1.63366
H	6.35469	0.08768	-0.40767
H	5.42711	-0.71618	-2.54318
H	3.01726	-1.39087	-2.71464
O	0.38759	-1.65855	-1.23028
O	2.12489	-0.16254	2.75742
N	0.95821	-0.97895	0.91615
C	-0.35973	-1.02744	1.50206
H	-0.81912	-1.99638	1.28936
H	-0.23499	-0.91455	2.58115
C	-1.28877	0.05730	0.91955
H	-1.35625	-0.10954	-0.15383
C	-2.64580	0.00956	1.55919
H	-2.71075	0.39194	2.57534
C	-3.74619	-0.48558	0.99210
H	-4.69460	-0.49810	1.51746
C	-3.77824	-1.05823	-0.39596
F	-3.49988	-0.12967	-1.34079
F	-4.99442	-1.56803	-0.67308
F	-2.87204	-2.05394	-0.55379
S	-0.55197	1.74548	1.14396
C	-0.54872	2.25096	-0.59987
F	-0.12384	3.52141	-0.66337
F	-1.76407	2.17523	-1.16634
F	0.27855	1.49482	-1.35161

5d(*E*,3*R*)

C	-3.10036	-0.70544	0.84986
C	-3.37367	-0.84060	-0.51405
C	-4.64754	-0.64009	-1.02101
C	-5.65513	-0.29330	-0.11181
C	-5.38096	-0.15710	1.25423
C	-4.08997	-0.36316	1.75712
C	-1.65102	-0.97343	1.06577
C	-2.10913	-1.20384	-1.21520
H	-4.84661	-0.74646	-2.08179
H	-6.66554	-0.12548	-0.47050
H	-6.18311	0.11431	1.93295
H	-3.86429	-0.25843	2.81271
O	-1.00013	-0.94849	2.09194
O	-1.91027	-1.41507	-2.39255
N	-1.13219	-1.27436	-0.20251
C	0.27157	-1.49994	-0.45261
H	0.63993	-2.27871	0.22201
H	0.36054	-1.85137	-1.48304
C	1.11043	-0.22958	-0.21780
H	0.93923	0.11077	0.80415
C	2.56879	-0.48438	-0.43883
H	2.87201	-0.79952	-1.43446
C	3.48584	-0.35695	0.51697
H	3.23355	-0.04059	1.52480
C	4.93813	-0.62830	0.29278
F	5.37988	-1.60593	1.11710
F	5.68297	0.46950	0.55205
F	5.20536	-1.01282	-0.97282
S	0.54160	1.14184	-1.34074
C	-0.01151	2.31297	-0.07059
F	-0.32845	3.46549	-0.67569
F	0.93235	2.55985	0.85677
F	-1.10273	1.88099	0.59799

TS4d'(3*R*)

C	-3.94866	-0.85228	0.01359
C	-3.40865	0.40612	-0.28821
C	-4.15700	1.56685	-0.16469
C	-5.48048	1.43282	0.27730
C	-6.01805	0.17704	0.58223
C	-5.25445	-0.99243	0.45400
C	-2.90676	-1.88328	-0.22687
C	-2.00630	0.21625	-0.71906
H	-3.73725	2.53497	-0.41567
H	-6.10195	2.31590	0.37982
H	-7.04649	0.10774	0.91992
H	-5.66513	-1.96886	0.68551
O	-2.92027	-3.08144	-0.09011
O	-1.16073	1.05784	-1.02013
N	-1.76675	-1.14855	-0.68774

C	-0.52682	-1.77054	-1.08628
H	-0.62036	-2.83783	-0.87302
H	-0.36118	-1.63995	-2.16192
C	0.62873	-1.16980	-0.28872
H	0.54603	-1.33399	0.78329
C	1.11147	0.15358	-0.67226
H	1.03211	0.43322	-1.71706
C	1.65371	1.13607	0.26484
H	2.16566	0.65410	1.10237
B	0.37986	1.85112	1.00784
O	-0.29683	0.99320	1.82158
H	-1.02585	1.37093	2.32882
O	0.22251	3.16971	0.82309
H	-0.48338	3.61572	1.30577
C	2.61483	2.10312	-0.41654
F	3.67791	1.42988	-0.91312
F	3.06924	3.01382	0.44939
F	2.01751	2.72580	-1.44740
S	2.27637	-1.77348	-0.92785
C	3.30649	-1.82525	0.63597
F	2.53577	-1.81535	1.72850
F	4.13005	-0.78395	0.68724
F	4.00709	-2.94755	0.58601

Int3d'(3*R*)

C	-3.78922	-0.97795	0.05507
C	-3.09042	0.24292	0.02439
C	-3.69885	1.45050	0.33156
C	-5.05774	1.40359	0.67685
C	-5.75583	0.19229	0.70904
C	-5.12780	-1.02660	0.39769
C	-2.85059	-2.06639	-0.31796
C	-1.72370	-0.06684	-0.37117
H	-3.14845	2.38431	0.30339
H	-5.57638	2.32368	0.92219
H	-6.80614	0.19304	0.97953
H	-5.66785	-1.96639	0.42271
O	-2.96817	-3.25438	-0.41118
O	-0.78715	0.79753	-0.50392
N	-1.58317	-1.37523	-0.57932
C	-0.32216	-2.00338	-0.96798
H	-0.27597	-2.99132	-0.50777
H	-0.30124	-2.13044	-2.05515
C	0.81660	-1.10642	-0.47071
H	0.87049	-1.17399	0.61549
C	0.60131	0.35830	-0.87615
H	0.61659	0.46325	-1.96349
C	1.53388	1.37118	-0.22539
H	2.54844	1.09913	-0.53390
B	1.51775	1.40064	1.37936
O	0.60309	0.60108	2.01533
H	0.64109	0.61871	2.98010
O	2.42318	2.21221	1.96533
H	2.42769	2.26374	2.92846
C	1.30049	2.77187	-0.79016
F	1.06792	2.73921	-2.12480
F	2.35692	3.56092	-0.57676
F	0.21987	3.35755	-0.21658
S	2.39830	-1.73150	-1.16505
C	3.31282	-1.89947	0.40976
F	3.52030	-0.70605	1.00804
F	4.48885	-2.45142	0.13744
F	2.64970	-2.66348	1.29201

TS4d'(3*S*)

C	-3.41438	-0.63915	-0.47319
C	-4.09310	0.39460	0.18940
C	-5.46255	0.34724	0.38979
C	-6.14489	-0.77606	-0.10033
C	-5.46739	-1.80650	-0.76151
C	-4.08042	-1.75429	-0.95764
C	-1.97959	-0.28903	-0.51613
C	-3.10764	1.43299	0.58312
H	-5.98086	1.14923	0.90338
H	-7.21881	-0.84764	0.03414
H	-6.02646	-2.65981	-1.12980
H	-3.54963	-2.54817	-1.47107
O	-1.03070	-0.93249	-0.97494
O	-3.23342	2.47848	1.17010
N	-1.84823	0.93789	0.10709
C	-0.60737	1.67731	0.19464
H	-0.33893	2.07897	-0.78476
H	-0.77248	2.50845	0.88283
C	0.46724	0.72856	0.72056
H	0.23342	0.33614	1.70733
C	1.02246	-0.25043	-0.21415
H	1.14895	0.08814	-1.23519
C	1.51076	-1.62529	0.09870

H	0.68197	-2.27227	-0.22464
B	1.84893	-2.02038	1.62085
O	2.03462	-3.33435	1.85140
H	2.28950	-3.60986	2.74039
O	1.91134	-1.00153	2.53055
H	2.16112	-1.23456	3.43410
C	2.68628	-1.99016	-0.81939
F	2.49355	-1.53618	-2.07688
F	2.85956	-3.31124	-0.87572
F	3.82847	-1.42951	-0.35936
S	2.23555	1.31882	0.84289
C	2.31005	2.63068	-0.47297
F	3.58201	2.99680	-0.54415
F	1.55622	3.67830	-0.13619
F	1.90296	2.18887	-1.67204

TS4d'(3*S*)

C	-3.41438	-0.63915	-0.47319
C	-4.09310	0.39460	0.18940
C	-5.46255	0.34724	0.38979
C	-6.14489	-0.77606	-0.10033
C	-5.46739	-1.80650	-0.76151
C	-4.08042	-1.75429	-0.95764
C	-1.97959	-0.28903	-0.51613
C	-3.10764	1.43299	0.58312
H	-5.98086	1.14923	0.90338
H	-7.21881	-0.84764	0.03414
H	-6.02646	-2.65981	-1.12980
H	-3.54963	-2.54817	-1.47107
O	-1.03070	-0.93249	-0.97494
O	-3.23342	2.47848	1.17010
N	-1.84823	0.93789	0.10709
C	-0.60737	1.67731	0.19464
H	-0.33893	2.07897	-0.78476
H	-0.77248	2.50845	0.88283
C	0.46724	0.72856	0.72056
H	0.23342	0.33614	1.70733
C	1.02246	-0.25043	-0.21415
H	1.14895	0.08814	-1.23519
C	1.51076	-1.62529	0.09870
H	0.68197	-2.27227	-0.22464
B	1.84893	-2.02038	1.62085
O	2.03462	-3.33435	1.85140
H	2.28950	-3.60986	2.74039
O	1.91134	-1.00153	2.53055
H	2.16112	-1.23456	3.43410
C	2.68628	-1.99016	-0.81939
F	2.49355	-1.53618	-2.07688
F	2.85956	-3.31124	-0.87572
F	3.82847	-1.42951	-0.35936
S	2.23555	1.31882	0.84289
C	2.31005	2.63068	-0.47297
F	3.58201	2.99680	-0.54415
F	1.55622	3.67830	-0.13619
F	1.90296	2.18887	-1.67204

Int3d'(3*S*)

C	-3.32768	-0.67752	-0.18970
C	-4.09483	0.48671	0.00211
C	-5.47604	0.45113	-0.04100
C	-6.07966	-0.79507	-0.28421
C	-5.31576	-1.95028	-0.47527
C	-3.91414	-1.91109	-0.43171
C	-1.92897	-0.27796	-0.09089
C	-3.17197	1.62455	0.23625
H	-6.06550	1.34914	0.10602
H	-7.16139	-0.86153	-0.32552
H	-5.81530	-2.89439	-0.66179
H	-3.31922	-2.80481	-0.58139
O	-0.92433	-1.07454	-0.20540
O	-3.34547	2.78498	0.47414
N	-1.83292	1.03093	0.13763
C	-0.57047	1.73913	0.36647
H	-0.28012	2.25794	-0.54871
H	-0.73707	2.48557	1.14464
C	0.45618	0.68935	0.79976
H	0.17813	0.29766	1.78120
C	0.46888	-0.49079	-0.18474
H	0.60659	-0.12941	-1.20302
C	1.39995	-1.68505	0.07669
H	0.78020	-2.57494	-0.09262
B	1.97978	-1.86043	1.56282
O	3.22533	-2.36118	1.69965
H	3.55850	-2.49989	2.59405
O	1.11294	-1.54495	2.57839
H	1.43921	-1.71076	3.47195
C	2.47140	-1.77940	-1.00999
F	1.92047	-1.60359	-2.24071

F	3.05033	-2.98532	-0.99975
F	3.42959	-0.84343	-0.87372
S	2.11625	1.37150	1.13766
C	2.47420	2.26568	-0.42074
F	3.77204	2.54168	-0.43933
F	1.78424	3.41862	-0.50442
F	2.15369	1.54496	-1.51511

Int4d(3*R*)

C	-4.36052	0.47654	-0.72748
C	-3.92404	-0.60281	0.05493
C	-4.44508	-1.87712	-0.08283
C	-5.46504	-2.04202	-1.02977
C	-5.91241	-0.96850	-1.80793
C	-5.35713	0.31326	-1.67370
C	-3.55803	1.67904	-0.36235
C	-2.83053	-0.09817	0.88276
H	-4.05736	-2.70343	0.50183
H	-5.90774	-3.02202	-1.17129
H	-6.69749	-1.13387	-2.53802
H	-5.68635	1.14380	-2.28797
O	-3.59091	2.81504	-0.75457
O	-2.23442	-0.72181	1.82912
N	-2.66445	1.21038	0.66673
C	-1.69924	1.97437	1.44200
H	-1.43550	2.86684	0.87958
H	-2.15362	2.27209	2.39231
C	-0.46266	1.09276	1.67980
H	0.11469	1.02875	0.76002
C	-0.80618	-0.33769	2.14917
H	-0.82049	-0.40742	3.23721
C	0.07824	-1.40116	1.51613
H	1.09296	-1.16984	1.84679
B	0.05018	-1.46556	-0.15151
O	0.49716	-2.67700	-0.73677
H	-0.03266	-3.42528	-0.44273
O	-1.23073	-0.96696	-0.57177
H	-1.28544	-0.99074	-1.54000
C	-0.22507	-2.76264	2.10331
F	-0.51447	-2.71666	3.43226
F	0.81234	-3.60570	1.95580
F	-1.30213	-3.36906	1.51265
S	0.60547	1.82381	2.98559
C	1.54985	3.01104	1.97191
F	2.43199	2.43036	1.15834
F	2.20789	3.81510	2.81580
F	0.73960	3.77155	1.20044
N	1.24509	-0.34722	-0.81339
S	2.85978	-0.37899	-0.28655
S	0.98991	0.18517	-2.39614
O	2.83083	-0.51344	1.16922
O	3.64146	0.68021	-0.90470
O	2.18998	0.20700	-3.21528
O	-0.23639	-0.41391	-2.93596
C	3.54844	-2.02041	-0.92215
C	0.51760	1.97007	-2.08943
F	3.25834	-2.98837	-0.06071
F	4.87438	-1.87902	-0.99633
F	3.06352	-2.31004	-2.12256
F	1.44279	2.6013	-1.37651
F	0.35038	2.57859	-3.26011
F	-0.64842	2.00911	-1.41021

Int4d(3*S*)

C	3.46266	2.37178	-0.23458
C	4.82810	2.37407	0.09158
C	5.50219	3.56628	0.28540
C	4.76055	4.75189	0.14118
C	3.39480	4.73477	-0.16397
C	2.70691	3.52664	-0.35288
C	3.05723	0.97871	-0.31988
C	5.28247	0.95752	0.22174
H	6.55464	3.58295	0.54526
H	5.25776	5.70562	0.28315
H	2.85715	5.67301	-0.24667
H	1.64057	3.46859	-0.55487
O	1.89783	0.57970	-0.61748
O	6.35004	0.47518	0.48901
N	4.09342	0.17274	-0.04775
C	3.94036	-1.28073	-0.08419
H	4.07105	-1.63137	-1.10957
H	4.71594	-1.72414	0.54062
C	2.53346	-1.57404	0.46428
H	2.53370	-1.26690	1.50990
C	1.41334	-0.82464	-0.28520
H	1.21940	-1.24482	-1.26823
C	0.08517	-0.58699	0.41079
H	-0.46610	-1.52806	0.36114

B	-0.77054	0.53357	-0.48990
O	-0.52628	1.91233	-0.20229
H	-0.87159	2.18929	0.65715
O	-0.57893	0.21267	-1.85592
H	-0.96025	0.91210	-2.39881
C	0.24031	-0.22493	1.86200
F	0.65241	-1.28189	2.63644
F	-0.88992	0.22490	2.41790
F	1.19611	0.74315	2.04909
S	2.11987	-3.35482	0.60066
C	2.64705	-3.97061	-1.03128
F	2.16435	-5.20502	-1.17609
F	3.99255	-4.03111	-1.15284
F	2.20955	-3.20522	-2.05174
N	-2.44387	0.24416	-0.08165
S	-3.19057	-1.15094	-0.65865
S	-3.41964	1.50239	0.39409
O	-2.71162	2.30135	1.39765
O	-4.77730	1.03670	0.64911
O	-2.12386	-2.11150	-0.93465
O	-4.22950	-0.87240	-1.64318
C	-3.52853	2.60451	-1.14722
C	-4.04660	-1.86992	0.87730
F	-2.75149	3.67605	-1.00233
F	-3.14504	1.92836	-2.23724
F	-4.79173	2.99527	-1.29774
F	-3.48996	-1.37758	1.98788
F	-5.34726	-1.62428	0.86801
F	-3.85301	-3.19226	0.84645

TS5d$_{anti}$(3*S*)

C	5.44873	-0.71270	-0.36657
C	4.41708	-1.39615	-1.01999
C	4.66876	-2.31233	-2.02780
C	6.01086	-2.53273	-2.36722
C	7.04411	-1.85090	-1.71549
C	6.77579	-0.92274	-0.69881
C	4.83769	0.19343	0.64415
C	3.13973	-0.93302	-0.43818
H	3.86018	-2.83314	-2.52818
H	6.25312	-3.24373	-3.14986
H	8.07207	-2.04398	-2.00373
H	7.56982	-0.38702	-0.19064
O	5.34248	0.97041	1.41602
O	1.99888	-1.28156	-0.79108
N	3.42980	-0.02711	0.53870
C	2.44158	0.67731	1.33820
H	2.24965	0.13077	2.25980
H	2.86733	1.64510	1.59843
C	1.13467	0.85449	0.55365
H	0.38459	1.31384	1.20918
C	0.48980	-0.42419	0.08503
H	-0.00087	-0.36113	-0.87918
C	-0.14077	-1.39620	0.92516
H	-0.44105	-2.25539	0.33079
B	-1.72276	-0.66197	1.37435
O	-1.34740	0.46904	2.13249
H	-2.13421	0.91213	2.48031
O	-2.55372	-1.66310	1.91391
H	-2.20304	-2.01900	2.73752
C	0.55503	-1.90811	2.16013
F	-0.12334	-2.95595	2.67961
F	0.70252	-1.01086	3.16195
F	1.81346	-2.36089	1.87956
S	1.35506	1.92871	-0.93995
C	1.68591	3.51035	-0.10402
F	0.87601	3.71662	0.94779
F	1.50664	4.49351	-0.99270
F	2.95284	3.59994	0.35874
N	-2.52882	-0.18648	-0.01392
S	-2.78227	-1.23447	-1.32021
S	-3.61442	1.11302	0.14572
O	-3.76081	1.45537	1.56081
O	-4.79263	0.95565	-0.68986
O	-1.57252	-2.04955	-1.44506
O	-3.29655	-0.52332	-2.47898
C	-2.59776	2.49524	-0.60777
C	-4.13669	-2.41844	-0.73096
F	-4.80207	-2.82387	-1.81288
F	-4.96620	-1.80781	0.10531
F	-3.57780	-3.46661	-0.13742
F	-1.62080	2.84180	0.23732
F	-3.39558	3.54119	-0.80990
F	-2.06497	2.10260	-1.76203

TS5d$_{syn}$(3*S*)

C	-3.97697	-1.56530	-0.02635
C	-3.63653	-1.00526	1.20980

C	-3.93368	-1.64019	2.40363
C	-4.60134	-2.86961	2.32634
C	-4.94470	-3.43067	1.09091
C	-4.63294	-2.78232	-0.11168
C	-3.49588	-0.65800	-1.10535
C	-2.91022	0.25931	0.94925
H	-3.65039	-1.20150	3.35375
H	-4.85218	-3.40008	3.23900
H	-5.45610	-4.38726	1.06544
H	-4.88512	-3.21269	-1.07451
O	-3.58798	-0.75140	-2.30778
O	-2.41948	1.06066	1.73972
N	-2.88074	0.42160	-0.42474
C	-2.23054	1.54341	-1.06217
H	-2.32612	1.40229	-2.13938
H	-2.73923	2.46467	-0.77441
C	-0.74124	1.60176	-0.67208
H	-0.25205	0.68560	-1.00168
C	-0.48718	1.83453	0.77907
H	-0.96021	2.69980	1.22272
C	0.53425	1.13594	1.45692
H	1.45990	1.33223	0.87979
B	0.62583	-0.62283	1.24721
O	1.44769	-1.19000	2.23358
H	1.00836	-1.18348	3.09180
O	-0.69126	-1.06898	1.05461
H	-0.68808	-2.03531	0.98341
C	0.73976	1.55609	2.89687
F	0.34707	2.83344	3.12840
F	2.03305	1.46526	3.25160
F	0.02955	0.77950	3.75707
S	0.22658	2.93403	-1.53217
C	-0.94277	4.33540	-1.48649
F	-1.97203	4.19467	-2.34212
F	-0.26110	5.43021	-1.83463
F	-1.47938	4.53181	-0.26213
N	1.51962	-0.95285	-0.21149
S	2.95162	-0.16803	-0.63043
S	1.30066	-2.51192	-0.85786
O	2.70992	1.26444	-0.38656
O	3.46704	-0.58993	-1.92060
O	2.54273	-3.13541	-1.28037
O	0.36049	-3.25531	-0.01687
C	4.19980	-0.69694	0.68294
C	0.32555	-2.08477	-2.39831
F	4.02146	0.03304	1.77757
F	5.41450	-0.46800	0.18520
F	4.05731	-1.98590	0.95641
F	1.00700	-1.25413	-3.17896
F	0.05211	-3.20892	-3.05278
F	-0.82147	-1.49203	-2.03302

TS5d$_{anti}$(3*R*)

C	1.11587	3.41886	-0.05562
C	1.46057	3.15388	-1.38575
C	2.69552	3.51385	-1.89749
C	3.58480	4.16442	-1.03293
C	3.23855	4.43048	0.29697
C	1.99152	4.05297	0.80975
C	-0.22646	2.84150	0.19411
C	0.33830	2.42277	-2.03383
H	2.96040	3.28279	-2.92293
H	4.56393	4.45902	-1.39612
H	3.95394	4.92822	0.94335
H	1.72062	4.23336	1.84383
O	-0.89717	2.79490	1.21749
O	0.20198	2.02556	-3.16785
N	-0.63551	2.27826	-1.01076
C	-1.91542	1.62984	-1.16655
H	-2.70801	2.31038	-0.85467
H	-2.03125	1.38898	-2.22395
C	-1.92935	0.33218	-0.34224
H	-1.10644	-0.29170	-0.67913
C	-1.90194	0.48123	1.13712
H	-2.76618	0.96338	1.58177
C	-0.93029	-0.11585	1.94957
H	0.06974	0.29273	1.69491
B	-0.41743	-1.73073	1.49560
O	-1.48041	-2.39496	0.90949
H	-1.19533	-3.25242	0.55356
O	0.40305	-2.26472	2.47437
H	-0.05325	-2.94470	2.98258
C	-1.17005	0.01263	3.44220
F	-0.01488	0.11074	4.11551
F	-1.84543	-1.05573	3.93472
F	-1.91441	1.10428	3.74538
S	-3.41946	-0.75767	-0.55258
C	-4.74156	0.49056	-0.71918

F	-5.90802	-0.15790	-0.64203
F	-4.70843	1.15118	-1.89110
F	-4.70534	1.42595	0.25675
N	0.82305	-1.43060	0.07032
S	2.08649	-0.33406	0.13072
S	1.03547	-2.71282	-0.98425
O	1.68204	0.66769	1.13296
O	2.51144	0.12203	-1.18688
O	0.28965	-3.87262	-0.48605
O	2.42812	-2.85097	-1.39126
C	3.56047	-1.24500	0.92124
C	0.08803	-2.15069	-2.50481
F	0.34896	-0.87476	-2.77863
F	0.43631	-2.91937	-3.53031
F	-1.22550	-2.28229	-2.27414
F	4.04825	-0.45046	1.87234
F	3.16225	-2.39299	1.45506
F	4.48907	-1.45799	0.00159

TS5d$_{syn}$(3*R*)

C	3.08764	2.58557	-0.61193
C	4.33824	2.73696	0.00619
C	4.81287	3.98866	0.35686
C	3.99178	5.09051	0.06973
C	2.73498	4.92962	-0.52370
C	2.25349	3.65973	-0.87132
C	2.86901	1.14650	-0.80123
C	4.92056	1.38294	0.24049
H	5.77409	4.10670	0.84456
H	4.33138	6.08768	0.32955
H	2.11784	5.80273	-0.70659
H	1.26496	3.49874	-1.28448
O	1.90075	0.54647	-1.29464
O	5.95229	1.03969	0.76314
N	3.95268	0.48211	-0.30099
C	3.96471	-0.96765	-0.27361
H	4.02245	-1.35344	-1.29312
H	4.84514	-1.28736	0.28400
C	2.67826	-1.42097	0.43744
H	2.70732	-1.00206	1.44059
C	1.37292	-1.05786	-0.24354
H	1.16035	-1.57461	-1.17118
C	0.20698	-0.59277	0.46224
H	-0.45824	-1.46451	0.55252
B	-0.79834	0.39320	-0.53238
O	-0.42212	1.73361	-0.28174
H	-1.13253	2.31837	-0.58635
O	-0.78627	-0.10064	-1.87158
H	-0.22946	0.48698	-2.39399
C	0.46527	-0.02573	1.83650
F	0.89888	-0.97936	2.71799
F	-0.61083	0.54260	2.38832
F	1.45682	0.91454	1.80305
S	2.56730	-3.22968	0.79112
C	3.10552	-3.93952	-0.80248
F	2.83309	-5.24499	-0.77543
F	4.42776	-3.78905	-1.01439
F	2.48059	-3.3845	-1.86160
N	-2.43821	0.15494	-0.08912
S	-3.15281	-0.95732	0.94564
S	-3.51095	1.05679	-1.01790
O	-2.80826	2.25743	-1.48463
O	-4.79177	1.18192	-0.33462
O	-2.09037	-1.81194	1.48426
O	-4.34327	-1.56472	0.36888
C	-3.80658	0.00460	-2.57203
C	-3.73109	0.11540	2.40655
F	-3.08170	0.48718	-3.57739
F	-3.49237	-1.26486	-2.35400
F	-5.10023	0.10341	-2.87783
F	-3.25063	1.35264	2.30212
F	-5.05613	0.14528	2.42950
F	-3.27684	-0.44197	3.52923