

## Electronic Supplementary Information

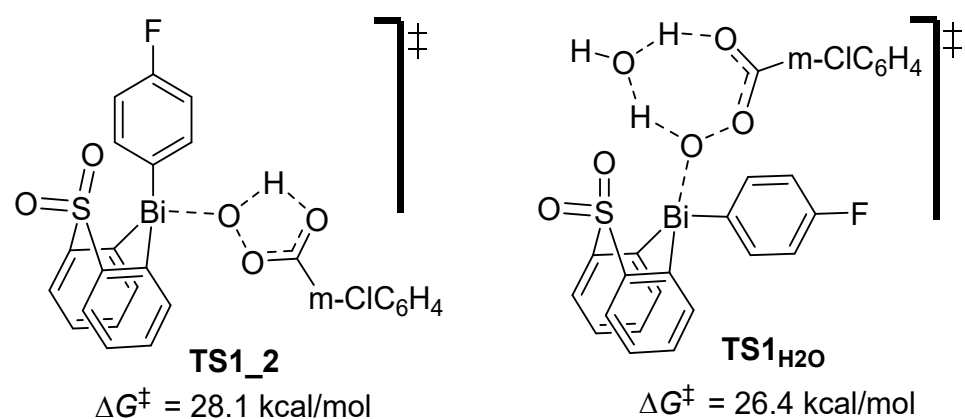
For

### Unveiling the Origin of Chemoselectivity of Bismacrocycles-Mediated C–H Arylation of Phenols: From Mechanism Concept to New Coupling Design

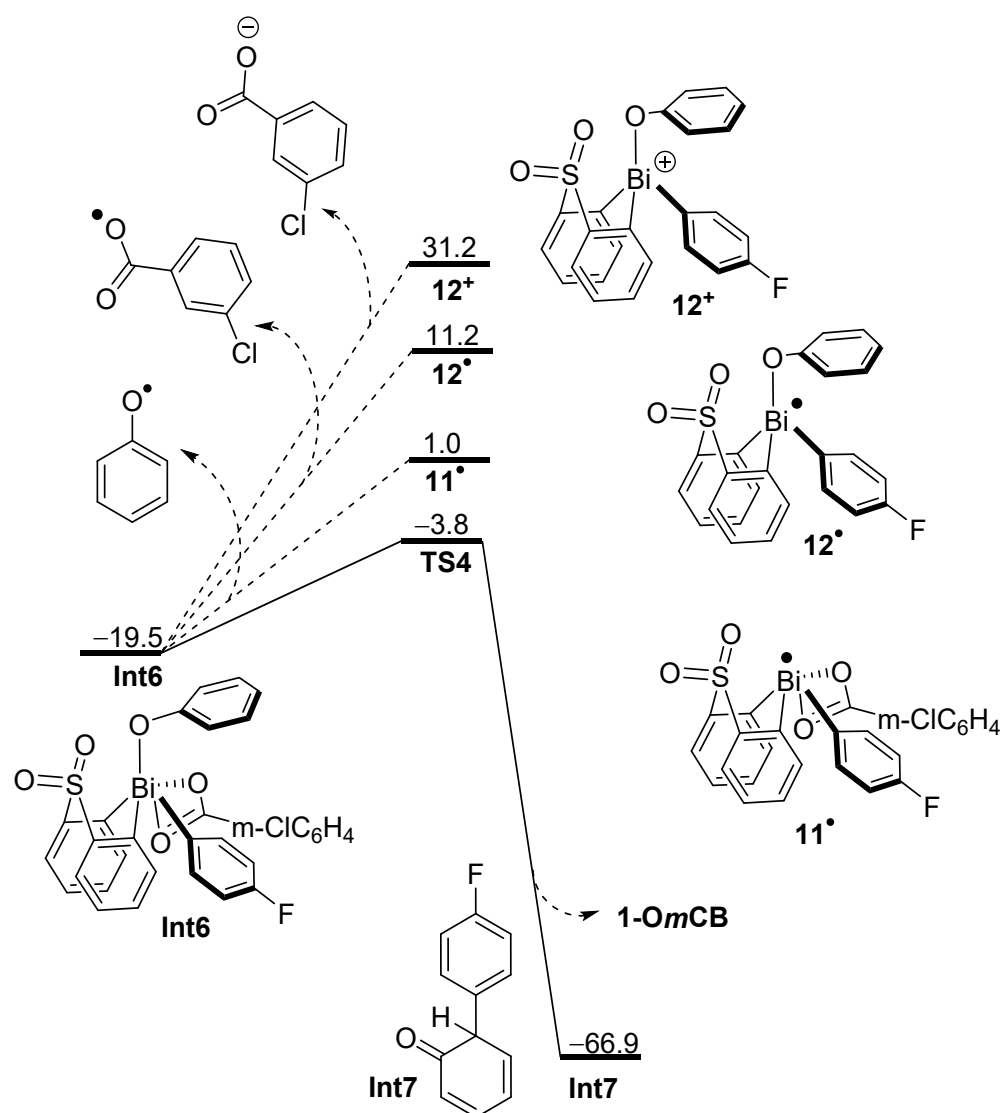
Yumiao Ma and Aqeel A. Hussein\*

**Yumiao Ma** - BSJ Institute, Haidian, Beijing, 100084, People's Republic of China; Hangzhou Yanqu Information Technology Co., Ltd. Xixi Legu Creative Pioneering Park, No. 712 Wen'er West Road, Xihu District, Hangzhou City, Zhejiang Province, 310003, People's Republic of China.

**Aqeel A. Hussein** – Department of Biomedical Sciences, College of Science, Komar University for Science and Technology, Chaq Chaq-Qularaisi, 46001 Sulaymaniyah, Iraq; Email: [aqeel.alaa@komar.edu.iq](mailto:aqeel.alaa@komar.edu.iq)

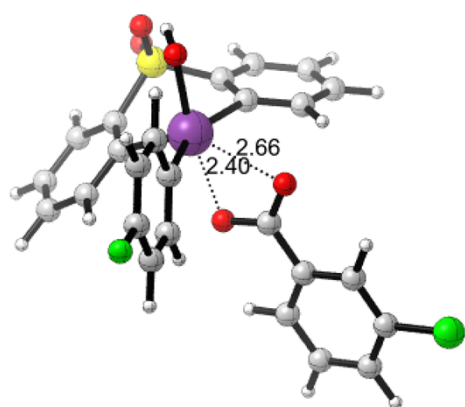


**Figure SI1.** Disfavorable alternative TSs for the oxidative addition step.



**Figure SI2.** Alternative pathways for **Int6** rather than reductive elimination.

Although the release of phenol radical is not competitive at room temperature, it might be a source of by-reactions at elevated temperature, at which its release is promoted because of the gain in entropy.



**Figure SI3.** The geometry of **Int4**, in which the distances are in Å.

## Energetics (in Hartree) for the Species

Structure	E_SPC	E	ZPE	H_SPC	T.S	T.qh-S	G(T)_SPC	qh-G(T)_SPC
<b>A</b>	-1300.594957	-1091.048752	0.183499	-1300.395045	0.057184	0.055823	-1300.452229	-1300.450868
<b>B</b>	-2524.803053	-2105.754576	0.344839	-2524.427454	0.092346	0.085752	-2524.5198	-2524.513205
<b>1-p-F-Ar</b>	-1555.456034	-1345.833788	0.253404	-1555.181934	0.068227	0.064855	-1555.250161	-1555.246788
<b>mCPBA</b>	-955.085856	-954.869067	0.11039	-954.965142	0.043216	0.042438	-955.008358	-955.007581
<b>Int1</b>	-2510.551237	-2300.714942	0.364345	-2510.154515	0.098073	0.089052	-2510.252588	-2510.243566
<b>TS1</b>	-2510.521694	-2300.688071	0.361938	-2510.12791	0.098084	0.088804	-2510.225994	-2510.216714
<b>TS1<sub>H2O</sub></b>	-2586.919177	-2377.046566	0.387854	-2586.497177	0.102116	0.092796	-2586.599293	-2586.589973
<b>Int2</b>	-1630.541587	-1420.880577	0.256097	-1630.2633	0.07157	0.067927	-1630.33487	-1630.331228
<b>mCBA</b>	-880.003175	-879.818381	0.107001	-879.886962	0.040448	0.039931	-879.92741	-879.926893
<b>Int3</b>	-2510.562669	-2300.719284	0.363352	-2510.167081	0.098022	0.089065	-2510.265103	-2510.256146
<b>Int3<sub>H2O</sub></b>	-2586.973234	-2377.09342	0.388849	-2586.550359	0.100008	0.091758	-2586.650366	-2586.642117
<b>TS2</b>	-2510.563118	-2300.66024	0.363437	-2510.16842	0.094527	0.086706	-2510.262947	-2510.255126
<b>TS2<sub>H2O</sub></b>	-2586.973161	-2377.092865	0.384941	-2586.554862	0.098248	0.090374	-2586.65311	-2586.645237
<b>Int4</b>	-2510.594099	-2300.757205	0.364065	-2510.198175	0.094504	0.08734	-2510.29268	-2510.285515
<b>PhOH</b>	-307.248224	-307.136977	0.105597	-307.136209	0.032355	0.032362	-307.168564	-307.168571
<b>H<sub>2</sub>O</b>	-76.383584	-76.340813	0.021258	-76.358547	0.019071	0.019071	-76.377618	-76.377618
<b>Int5</b>	-2817.856918	-2607.913813	0.471132	-2817.346905	0.111064	0.100935	-2817.457969	-2817.447840
<b>TS3</b>	-2817.852813	-2607.911893	0.46741	-2817.347291	0.108558	0.099205	-2817.45585	-2817.446497
<b>Int6<sub>H2O</sub></b>	-2817.850833	-2607.911308	0.469832	-2817.341318	0.11273	0.102673	-2817.454048	-2817.443991
<b>Int6</b>	-2741.459996	-2531.556593	0.444978	-2740.978195	0.10755	0.097451	-2741.085745	-2741.075646
<b>TS4</b>	-2741.435278	-2531.539703	0.443578	-2740.955407	0.104364	0.096027	-2741.059771	-2741.051434
<b>TS4<sub>H2O</sub></b>	-2817.809075	-2607.876745	0.46894	-2817.301293	0.10917	0.100629	-2817.410464	-2817.401922
<b>TS4<sub>O</sub></b>	-2741.426759	-2531.530063	0.442787	-2740.947344	0.106892	0.097156	-2741.054236	-2741.044500
<b>TS4<sub>O,H2O</sub></b>	-2817.813568	-2607.878139	0.468413	-2817.306136	0.111237	0.101298	-2817.417373	-2817.407434
<b>TS4<sub>CBA</sub></b>	-2741.418545	-2531.520131	0.442745	-2740.939389	0.105327	0.096303	-2741.044716	-2741.035693
<b>Int7</b>	-637.282261	-637.065004	0.178254	-637.092016	0.04759	0.045741	-637.139606	-637.137758
<b>TS5</b>	-713.644998	-713.383127	0.198524	-713.433085	0.049542	0.04825	-713.482627	-713.481334
<b>5</b>	-637.318807	-637.095987	0.179133	-637.12788	0.045927	0.044968	-637.173807	-637.172848
<b>6</b>	-637.300248	-637.080793	0.178705	-637.109819	0.047526	0.045417	-637.157345	-637.155236
<b>Int8</b>	-1937.829678	-1728.06631	0.362142	-1937.438463	0.087463	0.081236	-1937.525926	-1937.519699
<b>TS6</b>	-1937.795398	-1728.03635	0.361433	-1937.405532	0.084518	0.079698	-1937.49005	-1937.485230
<b>TS6<sub>H2O</sub></b>	-2014.190804	-1804.394946	0.38539	-2013.773551	0.091641	0.086157	-2013.865192	-2013.859708
<b>Int6a</b>	-2734.439941	-2524.546449	0.451971	-2733.950207	0.109514	0.09929	-2734.059722	-2734.049497
<b>Int6b</b>	-2642.267654	-2432.404738	0.453445	-2641.778312	0.10492	0.095364	-2641.883232	-2641.873676
<b>Int6c</b>	-2681.553711	-2471.678001	0.480825	-2681.034991	0.110364	0.099628	-2681.145355	-2681.134619
<b>Int6d</b>	-2756.717785	-2546.810555	0.486449	-2756.192826	0.111164	0.100725	-2756.303991	-2756.293551
<b>Int6e</b>	-2925.79916	-2715.83501	0.441773	-2925.316852	0.115308	0.104718	-2925.43216	-2925.421570
<b>Int6f</b>	-2939.842422	-2729.857471	0.428315	-2939.375558	0.111683	0.101013	-2939.48724	-2939.476571
<b>Int6g</b>	-2820.033417	-2610.104467	0.500105	-2819.492664	0.117165	0.105287	-2819.60983	-2819.597952
<b>Int6h</b>	-2970.361668	-2760.369875	0.511288	-2969.808413	0.118595	0.107442	-2969.927008	-2969.915856
<b>Int6i</b>	-2833.640295	-2623.705838	0.443899	-2833.157846	0.111217	0.100857	-2833.269063	-2833.258702
<b>Int6j</b>	-2840.652695	-2630.70937	0.436881	-2840.178195	0.110053	0.099416	-2840.288248	-2840.277612

Int6k	-2780.744487	-2570.828828	0.472754	-2780.233106	0.111635	0.100941	-2780.34474	-2780.334047
Int6l	-2855.907058	-2645.96075	0.477867	-2855.389793	0.113187	0.102466	-2855.50298	-2855.492259
TS4a	-2734.419501	-2524.533076	0.450406	-2733.931818	0.106835	0.098139	-2734.038652	-2734.029956
TS4b	-2642.243385	-2432.388149	0.451576	-2641.756273	0.103071	0.094708	-2641.859344	-2641.850982
TS4c	-2681.528774	-2471.660837	0.479245	-2681.012087	0.107822	0.098492	-2681.119909	-2681.110579
TS4d	-2756.69188	-2546.793072	0.484709	-2756.16909	0.108414	0.099543	-2756.277504	-2756.268633
TS4e	-2925.782161	-2715.823905	0.44072	-2925.301536	0.112513	0.103254	-2925.414049	-2925.404790
TS4f	-2939.818297	-2729.841063	0.426607	-2939.353519	0.109559	0.100104	-2939.463077	-2939.453623
TS4g	-2820.007601	-2610.086461	0.498444	-2819.468927	0.114479	0.104028	-2819.583406	-2819.572955
TS4h	-2970.333845	-2760.350087	0.509241	-2969.782978	0.116928	0.106736	-2969.899906	-2969.889714
TS4i	-2833.611348	-2623.684757	0.442063	-2833.131109	0.109025	0.099904	-2833.240133	-2833.231013
TS4j	-2840.627995	-2630.691985	0.435127	-2840.155666	0.106864	0.097966	-2840.262529	-2840.253632
TS4k	-2780.721929	-2570.813645	0.471046	-2780.212727	0.108894	0.099835	-2780.321621	-2780.312562
TS4l	-2855.887454	-2645.948685	0.476513	-2855.372003	0.110602	0.101298	-2855.482605	-2855.473300
3	-1829.195654	-1619.673294	0.275161	-1828.898491	0.073355	0.068251	-1828.971846	-1828.966741
Int9	-2136.45787	-1926.826165	0.381963	-2136.046579	0.091597	0.083065	-2136.138176	-2136.129644
TS7	-2136.40325	-1926.777928	0.380431	-2135.994164	0.08919	0.081798	-2136.083354	-2136.075962
TS7 <sub>o</sub>	-2136.40164	-1926.774921	0.379917	-2135.993006	0.090436	0.082204	-2136.083442	-2136.075210
TMG	-362.324329	-362.195601	0.190426	-362.123021	0.042134	0.041829	-362.165155	-362.164850
Int10	-2498.809165	-2289.054109	0.573863	-2498.194758	0.115464	0.104654	-2498.310222	-2498.299412
TS8	-2498.779674	-2289.033091	0.574247	-2498.165684	0.110874	0.102336	-2498.276558	-2498.268020
TS8 <sub>o</sub>	-2498.778027	-2289.029538	0.573027	-2498.164669	0.115643	0.104638	-2498.280311	-2498.269307
TMG.HCl	-823.038455	-822.875491	0.20412	-822.821048	0.049352	0.047957	-822.8704	-822.869005
Int11	-2498.810258	-2289.058511	0.574361	-2498.195302	0.11477	0.1045	-2498.310072	-2498.299802
Int12	-1675.723065	-1466.131516	0.368907	-1675.327532	0.083619	0.076909	-1675.411152	-1675.404441
TS9	-1675.697439	-1466.110853	0.367796	-1675.303552	0.081528	0.075819	-1675.38508	-1675.379371
TS9 <sub>o</sub>	-1675.685574	-1466.09682	0.366316	-1675.292431	0.086786	0.078333	-1675.379218	-1675.370765
Ph <sub>2</sub> BiCl	-1137.68061	-928.263806	0.182451	-1137.48353	0.056739	0.053425	-1137.540269	-1137.536955
Int13	-538.089011	-537.912321	0.186411	-537.891408	0.04564	0.043909	-537.937048	-537.935317
7	-538.108304	-537.929409	0.186917	-537.910477	0.045567	0.043583	-537.956044	-537.954060
1-OH	-1300.594993	-1091.048788	0.18359	-1300.395045	0.056834	0.055694	-1300.451879	-1300.450739
1-OmCB	-2104.233326	-1894.550035	0.266886	-2103.942667	0.076214	0.071701	-2104.018881	-2104.014368
Int14a	-2338.551969	-2128.787151	0.408392	-2338.110102	0.098008	0.090558	-2338.20811	-2338.200660
Int14b	-2530.148668	-2320.325036	0.462326	-2529.649889	0.105531	0.096539	-2529.75542	-2529.746427
Int14c	-2644.598934	-2434.731192	0.495197	-2644.064675	0.111969	0.101944	-2644.176644	-2644.166620
Int14d	-2734.540264	-2524.636884	0.464829	-2734.036271	0.113953	0.102858	-2734.150224	-2734.139129
Int14e	-2721.744945	-2511.862358	0.516015	-2721.189273	0.115955	0.103994	-2721.305227	-2721.293267
Int14f	-2836.195105	-2626.268455	0.549229	-2835.603794	0.120492	0.108459	-2835.724286	-2835.712253
Int14g	-2926.136842	-2716.174493	0.51922	-2925.575593	0.120975	0.108568	-2925.696568	-2925.684161
TS10a	-2338.478948	-2128.718066	0.404336	-2338.041105	0.098336	0.090823	-2338.139441	-2338.131929
TS10b	-2530.083537	-2320.26357	0.45866	-2529.588721	0.105236	0.096188	-2529.693957	-2529.684909
TS10c	-2644.53304	-2434.669515	0.491537	-2644.002752	0.110969	0.101307	-2644.113722	-2644.104059
TS10d	-2734.479545	-2524.578937	0.462119	-2733.978973	0.11048	0.100767	-2734.089453	-2734.079741
TS10e	-2721.68365	-2511.804889	0.513173	-2721.131558	0.112046	0.101596	-2721.243604	-2721.233154
TS10f	-2836.133187	-2626.21101	0.545782	-2835.545783	0.118535	0.107071	-2835.664318	-2835.652854
TS10g	-2926.078396	-2716.119796	0.51605	-2925.520921	0.118641	0.10689	-2925.639563	-2925.627811
Int15a	-2528.006444	-2318.178297	0.433297	-2527.537914	0.103493	0.094447	-2527.641407	-2527.632361
Int15b	-2719.606977	-2509.720387	0.487208	-2719.081594	0.111511	0.100599	-2719.193104	-2719.182193
Int15c	-2413.751102	-2203.954933	0.412473	-2413.304888	0.098361	0.090988	-2413.403249	-2413.395876
Int15d	-2605.351183	-2395.497082	0.466388	-2604.847196	0.110199	0.099613	-2604.957395	-2604.946809
Int15e	-2796.946225	-2587.033479	0.520516	-2796.385137	0.118504	0.105933	-2796.503642	-2796.491070
Int15f	-2605.346089	-2395.49155	0.466467	-2604.842024	0.109116	0.099233	-2604.95114	-2604.941257
TS11a	-2527.996621	-2318.172637	0.431914	-2527.530088	0.100138	0.09263	-2527.630226	-2527.622718
TS11b	-2719.596469	-2509.714469	0.485638	-2719.073059	0.108753	0.099143	-2719.181812	-2719.172202
TS11c	-2413.739554	-2203.947562	0.41169	-2413.294097	0.097632	0.090784	-2413.391729	-2413.384881
TS11d	-2605.339759	-2395.489524	0.465249	-2604.837496	0.106654	0.0976	-2604.94415	-2604.935096
TS11e	-2796.939061	-2587.029071	0.519424	-2796.379758	0.11467	0.103662	-2796.494428	-2796.483420
TS11f	-2605.338876	-2395.486539	0.465891	-2604.836274	0.105691	0.096917	-2604.941965	-2604.933191
TS11a <sub>o</sub>	-2527.974961	-2318.152814	0.43041	-2527.509286	0.103325	0.094384	-2527.612611	-2527.603670

<b>TS11b<sub>0</sub></b>	-2719.576293	-2509.695608	0.484281	-2719.05369	0.111667	0.100813	-2719.165357	-2719.154503
<b>TS11c<sub>0</sub></b>	-2413.717141	-2203.928236	0.410247	-2413.272505	0.100346	0.092482	-2413.372851	-2413.364987
<b>TS11d<sub>0</sub></b>	-2605.318263	-2395.470943	0.463694	-2604.816945	0.109658	0.099431	-2604.926603	-2604.916376
<b>TS11e<sub>0</sub></b>	-2796.914503	-2587.008207	0.517562	-2796.356311	0.11971	0.106477	-2796.476021	-2796.462788
<b>TS11f<sub>0</sub></b>	-2605.311222	-2395.461686	0.464355	-2604.809381	0.110347	0.099733	-2604.919728	-2604.909114

## Cartesian Coordinates for the Species

### *m*CPBA

C -1.87780100 -0.04523800 -0.00000100  
C -2.04140100 1.33869700 0.00000000  
C -0.91399400 2.15724000 0.00000300  
C 0.36211100 1.60481000 0.00000500  
C 0.50593300 0.21360300 0.00000400  
C -0.61503500 -0.62132900 0.00000100  
H -3.03874900 1.76810300 -0.00000100  
H -1.03736600 3.23638800 0.00000400  
H 1.23567100 2.24835700 0.00000700  
H -0.48945000 -1.69924300 0.00000000  
C 1.82711300 -0.44311300 0.00000600  
O 2.03640600 -1.64224200 -0.00000200  
O 2.84426800 0.43943300 0.00000000  
O 4.09579000 -0.22206600 -0.00000400  
H 3.80653800 -1.16935100 0.00000600  
Cl -3.28058300 -1.07136900 -0.00000400

### Int6h

Bi -0.24487400 -0.59037400 0.66139400  
S -3.45162500 0.39080600 -0.44362800  
F 3.50086400 -5.11825000 2.98200900  
O -3.65792800 0.11730400 0.98198600  
O -4.56970000 0.84635000 -1.27452400  
C -2.15672400 1.63083700 -0.54441000  
C -0.88750400 1.46712500 0.02449200  
C -0.02985200 2.55317100 0.08463700  
H 0.95553400 2.44661700 0.52412500  
C -0.42044700 3.79525900 -0.41848700  
H 0.26891500 4.62902400 -0.34124200  
C -1.67661500 3.94550200 -1.00858900  
C -2.54984500 2.85169900 -1.06976900  
H -3.53566300 2.96983100 -1.50895600  
C -2.82097500 -1.12287300 -1.14720100  
C -1.70195300 -1.73494700 -0.58938900  
C -1.35042200 -3.00262000 -1.05473600  
H -0.47707400 -3.51301300 -0.65531900  
C -2.10835800 -3.63430400 -2.03123500  
H -1.84582300 -4.62763900 -2.38382400  
C -3.22417200 -2.99609100 -2.58750800

C -3.59084600 -1.72272100 -2.13930200  
H -4.45873400 -1.19826200 -2.52316800  
C 1.13427100 -2.16161600 1.47416500  
C 1.06286100 -2.44977400 2.83216800  
H 0.38868300 -1.89641400 3.47856600  
C 1.87326200 -3.46123700 3.34834300  
H 1.85250200 -3.71674400 4.40349800  
C 2.71694200 -4.14109300 2.48400200  
C 2.79034300 -3.86174100 1.12726000  
H 3.46891800 -4.42178400 0.49086200  
C 1.98122000 -2.85035600 0.61167500  
H 2.02753200 -2.61236500 -0.44650700  
O 1.09071700 -0.57439500 -1.25889200  
C 5.37925200 1.27291400 -2.25182300  
C 4.34019700 1.04719400 -1.35906100  
C 3.21338900 0.34705500 -1.79679000  
C 3.13597000 -0.11773900 -3.11184600  
C 4.18862800 0.11938100 -3.99038700  
C 5.31853800 0.81656300 -3.56710300  
H 4.38971600 1.40183400 -0.33483900  
H 2.25003800 -0.65607800 -3.43293300  
H 4.13463300 -0.23740600 -5.01526600  
H 6.14316900 1.00538200 -4.24778400  
C 2.09605000 0.10724200 -0.84082600  
O 2.14665300 0.55295700 0.32628600  
Cl 6.78877000 2.14623400 -1.71684400  
O -0.98396100 -0.28021300 2.69123700  
C -0.90720500 0.97807900 3.16684000  
C 0.32232500 1.50434300 3.59702800  
C -2.05605600 1.77978000 3.24222400  
C 0.39697000 2.80145100 4.09619400  
H 1.21443300 0.88461800 3.52791400  
C -1.97159200 3.07508000 3.74602000  
H -2.99474200 1.37019600 2.88373300  
C -0.74896000 3.59537400 4.17322700  
H 1.35630400 3.19474000 4.42561300  
H -2.86975500 3.68692300 3.79649500  
H -0.68882600 4.60894800 4.56170700  
C -5.02967300 -3.07553100 -4.12242100  
H -4.76672900 -2.14108300 -4.63312900  
H -5.40312200 -3.79407600 -4.85373300

H -5.80594400 -2.88497900 -3.37137000  
C -1.31465200 6.24119100 -1.46886100  
H -0.37915900 6.08811900 -2.02102700  
H -1.88384600 7.04487800 -1.93862300  
H -1.09449400 6.51164200 -0.42872200  
O -3.88779900 -3.67990600 -3.53783200  
O -2.14285700 5.09339800 -1.53534500

#### **TS4e**

Bi -0.30269200 0.01444300 -0.62114000  
S -3.33821300 -1.21091800 -0.70746800  
O -2.81702400 -0.12775100 -1.57823700  
O -4.70117400 -1.71236700 -0.85666900  
C -2.15871300 -2.53498500 -0.89785600  
C -0.80895700 -2.18939600 -0.96309200  
C 0.12990900 -3.19812900 -1.14379500  
H 1.18893400 -2.96508600 -1.21008700  
C -0.28465400 -4.52684300 -1.25552600  
H 0.43087400 -5.32989500 -1.40528000  
C -1.63773800 -4.82109400 -1.17521200  
C -2.60796500 -3.84686500 -0.99293300  
H -3.66284100 -4.10006100 -0.94457800  
C -3.06195000 -0.59750100 0.93844800  
C -1.84952600 0.06204600 1.12958700  
C -1.59446600 0.60063400 2.38849300  
H -0.65802400 1.11360800 2.59149400  
C -2.53773400 0.48259100 3.40764700  
H -2.34432400 0.91219500 4.38650100  
C -3.74353800 -0.19777100 3.18107300  
C -4.01898000 -0.75967700 1.92808000  
H -4.94914500 -1.28646200 1.73626200  
C 0.40852600 2.35912900 -0.31614500  
C -0.71082100 3.17619800 -0.14851500  
H -1.61827500 3.01715500 -0.72409300  
C -0.66443000 4.21273500 0.77645000  
H -1.52707900 4.85887900 0.91281300  
C 0.49191900 4.41528300 1.54267500  
C 1.60077100 3.57019200 1.38370800  
H 2.49399300 3.72833800 1.98159900  
C 1.55741400 2.53949700 0.45351600  
H 2.43031500 1.90769000 0.31848100  
O 1.10281800 -0.60631300 1.11006900  
C 5.72234600 -1.81836100 0.98809000  
C 4.56325700 -1.40859700 0.34244900

C 3.40097800 -1.22491500 1.09639400  
C 3.40396100 -1.45056900 2.47542400  
C 4.57617300 -1.86122500 3.10136400  
C 5.74317200 -2.04769600 2.36280300  
H 4.54829100 -1.23256200 -0.72816900  
H 2.48959900 -1.30489100 3.04131700  
H 4.58800800 -2.04093400 4.17267400  
H 6.66052400 -2.36858900 2.84706200  
C 2.15947600 -0.78882500 0.41155700  
O 2.13569200 -0.59823700 -0.83199000  
Cl 7.17659600 -2.05154500 0.06126700  
O -0.22773700 0.50552200 -2.88071100  
C 0.00647400 1.77031800 -3.02347700  
C -0.97238700 2.65550200 -3.55836400  
C 1.22455700 2.32726200 -2.52638200  
C -0.69475400 3.99725900 -3.67422100  
H -1.91916600 2.23563600 -3.88697100  
C 1.50449900 3.69966600 -2.70449600  
H 2.00669700 1.63763300 -2.22083800  
C 0.55074500 4.52802800 -3.25005100  
H -1.43669800 4.66593300 -4.10434200  
H 2.46145400 4.09727900 -2.37698000  
H 0.74813200 5.58995900 -3.36875700  
C 0.53828200 5.47719700 2.49650600  
N 0.57709900 6.33997700 3.27443700  
C -4.70079700 -0.31850800 4.23678900  
N -5.47542900 -0.41712700 5.09649900  
F -2.02901200 -6.10287500 -1.28308300

#### **TS4g**

Bi -0.42663900 0.13983800 -0.50790600  
S -3.43098700 -1.13699300 -0.47575800  
O -2.99212500 0.00886000 -1.31618900  
O -4.79831400 -1.64940900 -0.56643800  
C -2.25531800 -2.42299400 -0.85028700  
C -0.92182000 -2.04455900 -0.99068800  
C 0.00639900 -3.02401200 -1.32289100  
H 1.05524300 -2.77009500 -1.45223300  
C -0.41229700 -4.34293500 -1.50477500  
H 0.32341400 -5.09882500 -1.77347400  
C -1.75223000 -4.72065100 -1.35384200  
C -2.68406500 -3.73575900 -1.01526700  
H -3.73701300 -3.98004100 -0.89795000  
C -3.04985300 -0.62215400 1.18044200

C -1.84065400 0.04974200 1.32558900  
C -1.51291200 0.50468600 2.60077200  
H -0.57629800 1.02985900 2.77420200  
C -2.38485700 0.28534500 3.66772000  
H -2.11768900 0.65577400 4.65612800  
C -3.59527400 -0.40326500 3.50632300  
C -3.92593600 -0.87115500 2.23211500  
H -4.85649600 -1.40535800 2.05574900  
C 0.36937600 2.45595000 -0.04706300  
C -0.72301400 3.26198100 0.27283100  
H -1.66245300 3.17985200 -0.26638700  
C -0.61616000 4.18205500 1.31552900  
H -1.45250500 4.81846800 1.59015600  
C 0.57912600 4.26078000 2.01247600  
C 1.67030800 3.45754100 1.71608400  
H 2.58932000 3.55145400 2.28756500  
C 1.56058500 2.54354200 0.66896100  
H 2.41830300 1.93015000 0.40925500  
O 1.12308000 -0.62157700 1.03098000  
C 5.73510300 -1.77620500 0.59087700  
C 4.54394700 -1.32855700 0.03502900  
C 3.41862600 -1.21185100 0.85480800  
C 3.49124500 -1.54145200 2.21043600  
C 4.69475000 -1.98833100 2.74656600  
C 5.82573600 -2.10872200 1.94114200  
H 4.47451900 -1.07194900 -1.01706000  
H 2.60403300 -1.44618100 2.82802300  
H 4.75952500 -2.24789100 3.79962400  
H 6.76775100 -2.45703100 2.35401000  
C 2.14159300 -0.73021200 0.26236300  
O 2.06612700 -0.43438900 -0.95395200  
Cl 7.14479400 -1.92540400 -0.42100100  
O -0.50069400 0.86119800 -2.73231500  
C -0.22972600 2.12305300 -2.75974200  
C -1.20333900 3.09281700 -3.13968100  
C 1.03247600 2.59017200 -2.27523800  
C -0.87928500 4.42858100 -3.14640100  
H -2.18445900 2.74015300 -3.44651000  
C 1.35981600 3.96393800 -2.35234500  
H 1.80447600 1.84816700 -2.09024000  
C 0.41183600 4.87316200 -2.75804600  
H -1.61858400 5.16070200 -3.46338900  
H 2.35024300 4.29370200 -2.04945100  
H 0.64546900 5.93393900 -2.79213500

C -2.17467200 -6.14571600 -1.56611000  
H -1.59138600 -6.82867600 -0.93731000  
H -3.23377100 -6.28857400 -1.33075000  
H -2.01819700 -6.44987400 -2.60839400  
C -4.51137200 -0.62336800 4.67571300  
H -4.84874600 0.33124300 5.09754500  
H -5.39873700 -1.19528800 4.38727100  
H -4.00240400 -1.17058400 5.47839500  
F 0.68426100 5.14977400 3.02618300

### **Int7**

F 4.30447900 -0.42171600 -0.56603800  
C 0.35397000 0.11878100 0.47531100  
C 0.73331800 -0.95323800 -0.33860500  
H -0.01920600 -1.65028800 -0.69939800  
C 2.06496900 -1.14297200 -0.69700200  
H 2.37202200 -1.97100400 -1.32877600  
C 3.00769300 -0.24219800 -0.22685700  
C 2.67122000 0.83314800 0.57860100  
H 3.44131600 1.51616300 0.92408900  
C 1.33316100 1.00712900 0.92527200  
H 1.04983400 1.85076300 1.54905800  
O -1.45444400 2.23303100 -0.60146100  
C -1.79597500 1.09080400 -0.32431300  
C -2.84776400 0.39176400 -1.05774800  
C -1.11020200 0.34123800 0.82660600  
C -3.31896600 -0.80167500 -0.62807200  
H -3.25469200 0.89011200 -1.93351700  
C -1.76774100 -0.93979500 1.23546500  
H -1.13508600 1.03097800 1.68222300  
C -2.79534100 -1.46906300 0.55091600  
H -4.12641100 -1.28655600 -1.17359100  
H -1.35573500 -1.44497900 2.10685400  
H -3.24684500 -2.40753500 0.86163300

### **Int6a**

Bi 0.56468800 0.57732200 0.13231600  
S 3.68758700 -0.34872200 -1.11081900  
O 3.89333900 0.39863400 0.13648300  
O 4.82698700 -0.88565000 -1.85770100  
C 2.60553900 -1.71270100 -0.69826700  
C 1.41068600 -1.52719100 0.00142400  
C 0.70684400 -2.62412300 0.47504600  
H -0.21406200 -2.48775200 1.03040100



C 1.20013200 -3.90972100 0.23771300  
H 0.65497700 -4.76540100 0.62727200  
C 2.37281000 -4.09633400 -0.48663000  
H 2.74622400 -5.09844200 -0.67728400  
C 3.08380500 -2.99556200 -0.95757300  
H 4.01401200 -3.11452100 -1.50523800  
C 2.78379200 0.75598100 -2.17308600  
C 1.65185000 1.40033400 -1.67043200  
C 1.05267500 2.39441300 -2.43532200  
H 0.16971700 2.91586800 -2.07432100  
C 1.58909900 2.73591900 -3.68013400  
H 1.12356700 3.52536900 -4.26433200  
C 2.70663700 2.06967900 -4.17504400  
H 3.11418500 2.33281200 -5.14701400  
C 3.31658500 1.07009100 -3.41875000  
H 4.20284400 0.55153000 -3.77236200  
C -0.90724400 2.22590100 0.60536500  
C -0.72959900 2.93966400 1.78505600  
H 0.07390400 2.68613400 2.46890500  
C -1.60939600 3.97877300 2.07759500  
H -1.49468900 4.54967000 2.99425700  
C -2.64679800 4.28341200 1.18755600  
C -2.80979200 3.55265200 0.00307600  
H -3.61964800 3.79497900 -0.67864700  
C -1.93153300 2.51443200 -0.29143500  
H -2.06043900 1.94203900 -1.20510200  
O -1.00768900 -0.19504900 -1.41677100  
C -5.05999200 -2.65325100 -0.82684700  
C -3.94182800 -2.02345200 -0.29713300  
C -3.02424300 -1.43167500 -1.16886400  
C -3.22954600 -1.47342200 -2.55013100  
C -4.35666500 -2.11006300 -3.05974600  
C -5.28013200 -2.70468000 -2.20205600  
H -3.77165000 -1.98424200 0.77367300  
H -2.50185400 -1.01219400 -3.20999000  
H -4.52292000 -2.14914300 -4.13270900  
H -6.16106200 -3.20415900 -2.59370600  
C -1.82140600 -0.76480100 -0.60431200  
O -1.61048700 -0.76015800 0.63139300  
Cl -6.21044000 -3.39550400 0.24909800  
O 1.46886900 0.93799500 2.07757600  
C 1.65321800 -0.14728700 2.85691900  
C 0.58205700 -0.68045900 3.59294100  
C 2.91589400 -0.75138200 2.94910700

C 0.77476000 -1.79213900 4.40688900  
H -0.39789300 -0.21505400 3.51177200  
C 3.09891800 -1.86143000 3.76973100  
H 3.72922500 -0.34242200 2.35890900  
C 2.03340700 -2.39046400 4.49878400  
H -0.06294800 -2.19469700 4.97202500  
H 4.08250300 -2.32153200 3.83298400  
H 2.18105200 -3.26040500 5.13362800  
C -3.55033300 5.35150500 1.48851100  
N -4.28391900 6.21929600 1.72935900

## Int2

Bi 0.34337700 -0.00020200 -0.84451000  
S -1.89435700 0.00029000 1.70937700  
O -0.47411600 0.00016900 2.10868100  
C -2.07679300 1.42081300 0.64995300  
C -1.11653800 1.63609400 -0.34074700  
C -1.21430400 2.76284100 -1.14716100  
H -0.49933600 2.93058500 -1.94921800  
C -2.24979900 3.67695000 -0.92966600  
H -2.31758400 4.56534000 -1.55206100  
C -3.19746200 3.45304200 0.06654600  
H -4.00147900 4.16632600 0.22435100  
C -3.12336700 2.31132300 0.86373700  
H -3.85154800 2.11594500 1.64557600  
C -2.07701600 -1.42046500 0.65029600  
C -1.11677600 -1.63611200 -0.34031900  
C -1.21462900 -2.76296300 -1.14657300  
H -0.49961200 -2.93088700 -1.94855000  
C -2.25027800 -3.67687500 -0.92896600  
H -2.31818700 -4.56536200 -1.55120900  
C -3.19794100 -3.45264000 0.06717100  
H -4.00208200 -4.16576400 0.22506900  
C 2.33009700 0.00005600 0.17732700  
C 2.55040200 0.00015400 1.55174600  
H 1.72503800 0.00022600 2.25463800  
C 3.86327200 0.00017200 2.02132600  
H 4.08222000 0.00025500 3.08493600  
C 4.90064800 0.00008500 1.09998800  
C 4.69335500 -0.00001200 -0.27098600  
H 5.53937900 -0.00007700 -0.95174100  
C 3.38045500 -0.00004600 -0.73911600  
H 3.17692900 -0.00015300 -1.80922800  
F 6.16865500 0.00009100 1.55975200

O -2.95687500 0.00044000 2.71420200  
O 0.74999300 -0.00056500 -2.77592900  
C -3.12371700 -2.31080200 0.86417600  
H -3.85190000 -2.11518500 1.64595800

### TS5

F 4.61077300 -0.11065000 -0.39597100  
C 0.49579500 -0.21168600 -0.02291700  
C 1.10866100 0.60758800 -0.97942100  
H 0.49590700 1.22895100 -1.62405900  
C 2.49364700 0.64411400 -1.11195900  
H 2.97280400 1.27170100 -1.85754500  
C 3.26423300 -0.14428000 -0.27169400  
C 2.70195400 -0.96149500 0.69440900  
H 3.33761700 -1.56180200 1.33843300  
C 1.31369300 -0.98264500 0.81420700  
H 0.86387100 -1.61713400 1.57563200  
O -1.40244800 2.05061300 -0.12967700  
C -1.82746400 0.85787400 -0.29912100  
C -3.16954300 0.58730300 -0.70845400  
C -1.00016100 -0.28481300 0.10410100  
C -3.68479000 -0.68460900 -0.66752900  
H -3.77377800 1.43343500 -1.02464100  
C -1.59704200 -1.59184500 0.10147900  
H -1.01030700 0.29585100 1.41403300  
C -2.91093000 -1.78922400 -0.22982000  
H -4.71724900 -0.84918800 -0.96986100  
H -0.96802500 -2.44474500 0.34793500  
H -3.34594900 -2.78403500 -0.20543300  
O -0.81016800 1.27420200 2.16800600  
H -0.91671800 1.89562500 1.33716100  
H 0.13747800 1.25097700 2.38577200

### TS4<sub>o</sub>

Bi 0.78330600 0.02886900 -0.12165100  
S 3.60771100 -1.52149600 0.17254800  
F 2.27816600 5.90367500 -2.06844000  
O 4.94703100 -2.09336800 0.28295400  
O 3.42355400 -0.08451600 -0.18140600  
C 2.70692500 -1.69809900 1.69543500  
C 1.49479600 -1.01452600 1.76650200  
C 0.76439000 -1.06391300 2.94548100  
H -0.17727100 -0.52703600 3.03271000  
C 1.25688600 -1.80195500 4.02637800  
H 0.68874100 -1.83731900 4.95243200

C 2.46650900 -2.49019900 3.93116900  
H 2.83804000 -3.05710500 4.78021500  
C 3.21067300 -2.44713800 2.75286300  
H 4.16281700 -2.96225900 2.66139700  
C 2.63972400 -2.38252100 -1.04532600  
C 1.41284100 -1.80893200 -1.37920800  
C 0.63320800 -2.43337000 -2.34448700  
H -0.32693200 -2.01621500 -2.63588700  
C 1.09153900 -3.60642400 -2.95317600  
H 0.48036000 -4.08685400 -3.71313700  
C 2.31817000 -4.16538300 -2.59752000  
H 2.66330300 -5.07565400 -3.07961500  
C 3.10953100 -3.55566200 -1.62576000  
H 4.07242400 -3.96666700 -1.33521700  
C 1.06606400 2.37591300 -0.48235400  
C 0.25161900 2.96652900 -1.43084700  
H -0.68458800 2.51438100 -1.74155300  
C 0.67897400 4.17808300 -1.97776000  
H 0.08620700 4.68667400 -2.73221200  
C 1.87288200 4.72842500 -1.53825300  
C 2.66829400 4.12584800 -0.57436000  
H 3.59396500 4.59595100 -0.25586000  
C 2.25495300 2.91386500 -0.02006000  
H 2.85252800 2.42576000 0.74229900  
C -1.24756100 2.50687100 1.43251900  
C -2.51647700 1.89369700 1.48298600  
C -1.17581100 3.90652300 1.59482700  
C -3.66232400 2.65435700 1.69173800  
H -2.58033800 0.81411100 1.38640200  
C -2.33135900 4.65661200 1.78300200  
H -0.19986900 4.38354000 1.55926300  
C -3.58393700 4.04056700 1.83550900  
H -4.62842600 2.15566600 1.73936800  
H -2.25247500 5.73605500 1.89553600  
H -4.48315900 4.63105700 1.99011100  
O -0.14310000 1.80766600 1.22232100  
O -1.30972000 0.23570100 -1.68201800  
C -1.87118000 -0.50522600 -0.84731100  
O -1.22690300 -0.95359200 0.17465700  
C -3.29524200 -0.89829200 -0.99348900  
C -3.87827000 -1.75628300 -0.05713500  
C -4.04581700 -0.39079700 -2.05643700  
C -5.21692000 -2.09549300 -0.20282700  
H -3.28945000 -2.14485400 0.76693500

C -5.38506100 -0.74349000 -2.18275400  
H -3.57264700 0.27924400 -2.76697400  
C -5.98054000 -1.59849800 -1.25699300  
H -5.97707800 -0.35034600 -3.00442700  
H -7.02624100 -1.87601800 -1.34935600  
Cl -5.95605400 -3.16170900 0.95844700

#### **TS4<sub>O,H2O</sub>**

Bi 0.69919200 -0.91601900 -0.09732700  
S -1.59226400 -3.71724200 0.30985100  
F 6.13131400 1.05747800 -2.76040200  
O -2.81584700 -4.48859300 0.52933700  
O -0.32975700 -4.48046400 0.14195200  
C -1.34346500 -2.64250900 1.71516600  
C -0.33124900 -1.68235300 1.75827300  
C -0.06933000 -1.01412100 2.94309400  
H 0.72520600 -0.26993000 2.97374900  
C -0.83008200 -1.29364800 4.08172000  
H -0.61960700 -0.76800600 5.00942000  
C -1.85885700 -2.22840000 4.02467500  
H -2.46128700 -2.43537000 4.90464800  
C -2.11792500 -2.91552200 2.83950200  
H -2.90322500 -3.66331200 2.78299900  
C -1.79656600 -2.73503200 -1.16684600  
C -0.85554800 -1.77680400 -1.54887500  
C -1.02722000 -1.14005200 -2.77573900  
H -0.33046700 -0.36782200 -3.09553900  
C -2.10873900 -1.46250000 -3.59862700  
H -2.22538100 -0.95904400 -4.55500700  
C -3.04483800 -2.40799900 -3.18960300  
H -3.89677900 -2.64608900 -3.82015600  
C -2.89510600 -3.05109800 -1.96333600  
H -3.61482500 -3.78981100 -1.62373500  
C 2.82528200 0.04270700 -0.61564700  
C 2.77910200 1.19529500 -1.38604000  
H 1.89548600 1.82460400 -1.40782800  
C 3.91274800 1.53392200 -2.12645600  
H 3.92434300 2.42305900 -2.75008000  
C 5.03377100 0.72277800 -2.04598500  
C 5.07578600 -0.41676300 -1.25600600  
H 5.98195400 -1.01349000 -1.20641600  
C 3.94504300 -0.76995400 -0.51788900  
H 3.96158000 -1.64023700 0.12971400  
C 2.24143500 1.75149000 1.70349800  
C 1.11000500 2.53581000 2.00769500

C 3.51294600 2.35848300 1.76578200  
C 1.25174700 3.87102100 2.37034200  
H 0.12661200 2.07720600 1.96621200  
C 3.63968800 3.70069000 2.10685400  
H 4.38705900 1.75605900 1.53209300  
C 2.51355900 4.46737900 2.41480800  
H 0.36473600 4.45344900 2.61105400  
H 4.62912200 4.15213700 2.13940600  
H 2.61837700 5.51372800 2.68973100  
O 2.13088700 0.47870200 1.34529500  
O 1.93767600 -3.14521800 -0.19441900  
H 1.20777900 -3.79846600 -0.05712600  
O -0.21113200 1.06483900 -0.48475800  
C -1.47636100 1.18608800 -0.17771700  
O -2.14894000 0.28239600 0.30934900  
C -2.05619200 2.53562000 -0.45937500  
C -3.43912200 2.69709900 -0.34721200  
C -1.24619200 3.61896300 -0.80730500  
C -3.99359700 3.94493900 -0.59731300  
H -4.05692800 1.84996300 -0.06744100  
C -1.82103700 4.86452400 -1.04285800  
H -0.17207600 3.48252300 -0.87175000  
C -3.20011300 5.03676800 -0.94391700  
H -1.19425700 5.71305100 -1.30378800  
H -3.65545800 6.00493100 -1.12946000  
Cl -5.71983500 4.15252300 -0.47010300  
H 2.32616400 -3.35815200 -1.05688600

#### **TS4<sub>H2O</sub>**

Bi -0.60534300 -0.15832900 -0.19741200  
S -3.02726900 -2.31965600 -0.90116900  
F -1.35360000 5.11189900 3.11988400  
O -2.57988500 -1.21635900 -1.78477700  
O -4.07465300 -3.24946500 -1.32485200  
C -1.52906700 -3.20883400 -0.52859600  
C -0.37431500 -2.45946400 -0.29261200  
C 0.82088400 -3.13604800 -0.07943100  
H 1.73488600 -2.57513400 0.08533800  
C 0.84207500 -4.53502000 -0.09382700  
H 1.78443300 -5.05496600 0.06111000  
C -0.32442700 -5.26389100 -0.31325600  
H -0.29734800 -6.34993900 -0.32663600  
C -1.52996500 -4.59956600 -0.53394300  
H -2.45090200 -5.14234300 -0.72908500

C -3.46946100 -1.51297000 0.61351000  
C -2.61772500 -0.48166100 1.00617200  
C -2.93846000 0.19001500 2.18609000  
H -2.30293100 0.99235100 2.55149900  
C -4.07876200 -0.16249000 2.91463800  
H -4.32042200 0.38126200 3.82508600  
C -4.90708400 -1.20174100 2.49017600  
H -5.79118500 -1.46658000 3.06368100  
C -4.59988200 -1.90210700 1.32596000  
H -5.22411800 -2.71604200 0.96745200  
C -0.57738700 2.30069100 0.25854300  
C -1.87267400 2.79109900 0.38943300  
H -2.68061000 2.44395200 -0.24855800  
C -2.13755600 3.75420900 1.36296600  
H -3.13651700 4.16023500 1.49444200  
C -1.09709100 4.18170100 2.17337800  
C 0.19604600 3.69319800 2.05389700  
H 0.98148100 4.06130500 2.70771700  
C 0.46060800 2.73792900 1.07343400  
H 1.47118200 2.36684400 0.93141700  
O 1.76171000 -0.30545400 0.42004400  
C 6.52330600 -0.40810400 0.19430900  
C 5.30926200 0.16154200 -0.16560000  
C 4.12680200 -0.35427600 0.36996000  
C 4.17995500 -1.42738800 1.26259300  
C 5.40641900 -1.98366900 1.61598400  
C 6.59022800 -1.47955400 1.08227600  
H 5.25981100 0.99762500 -0.85539600  
H 3.25977200 -1.82325500 1.68004500  
H 5.44757500 -2.81708400 2.31246200  
H 7.55090500 -1.90900600 1.34981100  
C 2.82129600 0.28051700 -0.03797000  
O 2.83226500 1.28732300 -0.74648800  
Cl 7.99888700 0.23249400 -0.47777100  
O -0.37620200 0.41593000 -2.39805600  
C -0.65104200 1.68152200 -2.50447100  
C -1.87475500 2.12910500 -3.07818600  
C 0.23380700 2.64404400 -1.93318600  
C -2.13255800 3.47714400 -3.16755000  
H -2.56951900 1.38409200 -3.45633000  
C -0.03419200 4.02326900 -2.08626700  
H 1.20458000 2.29068500 -1.59103100  
C -1.20545800 4.43475300 -2.67840900  
H -3.05586800 3.82029700 -3.62883900

H 0.67864800 4.74867600 -1.70275100  
H -1.42708800 5.49370500 -2.78261200  
O 0.02685800 -0.36887200 2.23429300  
H 0.97951900 -0.48417900 2.02461400  
H -0.28891600 -1.19477300 2.63217000

### Int3

Bi -1.16976500 0.41105300 0.08385600  
S 0.22749000 -2.60064700 -0.04320700  
F -6.66736900 3.49507500 -0.08256000  
O 1.09858600 -1.42638600 0.13652200  
O 0.76356100 -3.95805500 -0.10987600  
C -0.95686000 -2.49302500 1.28632600  
C -1.50534200 -1.24104800 1.57101300  
C -2.38015700 -1.10311300 2.64003200  
H -2.83322100 -0.14146500 2.86918800  
C -2.67660700 -2.21934300 3.42936400  
H -3.34791700 -2.11052300 4.27701800  
C -2.12286900 -3.46340600 3.13696600  
H -2.36128000 -4.32405300 3.75535000  
C -1.25776000 -3.61270700 2.05290400  
H -0.80901500 -4.57238600 1.81298200  
C -0.69980400 -2.25335200 -1.52775400  
C -1.21369200 -0.96543400 -1.69327100  
C -1.88172500 -0.63936800 -2.86598700  
H -2.30388000 0.35238700 -3.00987100  
C -2.00566400 -1.60280300 -3.87260500  
H -2.51317200 -1.34483400 -4.79833800  
C -1.48766300 -2.88371100 -3.69769500  
H -1.58955400 -3.62419700 -4.48592600  
C -0.83179400 -3.22337200 -2.51432300  
H -0.41357100 -4.21418100 -2.36159000  
C -3.12641800 1.45589800 0.01902800  
C -4.32040000 0.74948000 -0.12999000  
H -4.32716700 -0.33465000 -0.22135000  
C -5.52929700 1.44157300 -0.16477400  
H -6.47849800 0.92705700 -0.28035000  
C -5.49919000 2.82433200 -0.04844300  
C -4.32375300 3.54528500 0.10048800  
H -4.35627600 4.62713500 0.18734500  
C -3.11833800 2.84596900 0.13449900  
H -2.18034700 3.38486000 0.25029400  
O 0.16248000 1.85689800 0.31920500  
O 3.11044700 3.48044000 0.08106200

C 3.45752000 2.31103000 0.13071800  
C 4.89897600 1.90497300 0.07739000  
O 2.64687800 1.28129400 0.23359200  
C 5.87825600 2.89529600 -0.01894900  
C 5.26481600 0.55681500 0.12170900  
C 7.22270500 2.54145000 -0.06920000  
H 5.56901400 3.93541900 -0.05245100  
C 6.61301300 0.22504900 0.07020200  
H 4.50219800 -0.21105400 0.19599800  
C 7.60193400 1.20085200 -0.02513900  
H 7.98727400 3.31026400 -0.14336700  
Cl 7.07967700 -1.45573800 0.12597100  
H 8.64890100 0.91526100 -0.06374300  
H 1.65402500 1.55234600 0.26250900

### Int6j

Bi -0.49040900 -0.61686000 0.32754100  
S -3.52146900 -0.40931900 -1.35097900  
F 3.22007400 -4.16236800 4.03560700  
O -3.74870200 -0.49662900 0.09826000  
O -4.64673300 -0.29158800 -2.28068900  
C -2.44387500 0.99619000 -1.59912200  
C -1.27451900 1.16705700 -0.85380100  
C -0.56108200 2.35245800 -0.95375300  
H 0.34201300 2.50072000 -0.37237100  
C -1.02235600 3.36316200 -1.80128900  
H -0.47022700 4.29752700 -1.85942100  
C -2.17282000 3.18135400 -2.56196200  
H -2.52166100 3.96729000 -3.22576000  
C -2.89095400 1.99251900 -2.46439200  
H -3.80212200 1.83262100 -3.03324900  
C -2.58899600 -1.86606600 -1.75947200  
C -1.48376900 -2.18734500 -0.96995100  
C -0.85191100 -3.40859100 -1.17258600  
H 0.01166600 -3.69135300 -0.57571800  
C -1.32950700 -4.28817700 -2.14869000  
H -0.83823700 -5.24734200 -2.29044700  
C -2.42205600 -3.94247800 -2.93948400  
H -2.78412200 -4.62735600 -3.70104600  
C -3.06538200 -2.72073300 -2.74748100  
H -3.93395700 -2.43751800 -3.33492100  
C 0.86255600 -1.85804300 1.63152600  
C 0.55760000 -1.94897700 2.98581800  
H -0.28431000 -1.40481000 3.40138100

C 1.36221000 -2.73866400 3.80743000  
H 1.16058400 -2.83365300 4.87022200  
C 2.44016000 -3.40123500 3.24169700  
C 2.75381600 -3.31426500 1.89357100  
H 3.61265400 -3.84824400 1.49801100  
C 1.94786700 -2.52643500 1.07246900  
H 2.18347000 -2.44002100 0.01605200  
O 1.22265700 -0.64610100 -1.25904800  
C 5.36463300 1.72368500 -1.45025700  
C 4.15928500 1.44844600 -0.81850800  
C 3.28384600 0.53133900 -1.40525600  
C 3.61655800 -0.09739800 -2.60752000  
C 4.82948800 0.19315500 -3.22391800  
C 5.71275700 1.10534800 -2.64969900  
H 3.89037400 1.92892300 0.11634800  
H 2.91973200 -0.80273100 -3.04871600  
H 5.09508600 -0.29014400 -4.16006100  
H 6.66074800 1.33653100 -3.12590100  
C 1.99205400 0.23499700 -0.73132700  
O 1.66869300 0.82657400 0.32539400  
Cl 6.46412100 2.86525800 -0.72876600  
O -1.50316000 0.04102800 2.14495500  
C -1.71012300 1.36672800 2.25765900  
C -0.66872600 2.21354300 2.67371400  
C -2.96521100 1.92352700 1.96519100  
C -0.87069300 3.58461800 2.79289200  
H 0.30572500 1.78358100 2.89198700  
C -3.17669200 3.29401000 2.08534400  
H -3.75798700 1.26547600 1.62680500  
C -2.12341700 4.09825400 2.49089900  
H -0.07300500 4.24970400 3.11107400  
H -4.14173800 3.73809500 1.85838800  
F -2.32271800 5.43610100 2.59624800

### TS1<sub>H2O</sub>

Bi -1.09705200 0.21969600 -0.60564200  
S -2.63478600 -2.68695700 0.05703000  
F -1.35834400 6.19732800 1.47668000  
O -1.54913600 -2.67547300 -0.95077400  
O -3.33417100 -3.92899700 0.37897400  
C -1.92322900 -1.98618600 1.53045100  
C -1.18058200 -0.81094700 1.40076700  
C -0.58119200 -0.27878000 2.53817300  
H -0.00169300 0.63954500 2.47739100

C -0.72288700 -0.92642100 3.76871900  
H -0.24146800 -0.51034900 4.64987800  
C -1.47432400 -2.09492600 3.87545800  
H -1.57936500 -2.59097400 4.83615100  
C -2.09189500 -2.63550300 2.74883200  
H -2.67951400 -3.54723000 2.80592300  
C -3.80153300 -1.46714800 -0.51762300  
C -3.31387000 -0.22806300 -0.93287000  
C -4.20742800 0.71613000 -1.42424400  
H -3.85914900 1.69454800 -1.74757800  
C -5.56998800 0.40776200 -1.49466300  
H -6.26560100 1.14626900 -1.88504600  
C -6.04109600 -0.83200100 -1.06772500  
H -7.10098200 -1.06263300 -1.12655700  
C -5.15502300 -1.78424500 -0.56581700  
H -5.49834500 -2.75835100 -0.22906000  
C -1.23180700 2.32811300 0.11943200  
C -2.29864700 2.75297800 0.91585800  
H -3.09973500 2.06891600 1.18755700  
C -2.34728000 4.06627500 1.37932600  
H -3.16354700 4.42263000 2.00077900  
C -1.31524900 4.92520900 1.02980500  
C -0.24282600 4.53274500 0.24424600  
H 0.54242600 5.24240500 0.00166900  
C -0.20608200 3.21607400 -0.21475400  
H 0.63255000 2.89292500 -0.82760900  
O 0.99973700 0.21038500 -1.40989500  
O 2.85822200 0.40375400 -1.63598500  
C 3.50641900 -0.40571000 -0.87252600  
C 4.93583700 0.01387800 -0.63408200  
O 3.08396800 -1.44980600 -0.35782500  
C 5.41349900 1.26253700 -1.03892800  
C 5.78543500 -0.88865000 0.00937200  
C 6.73915200 1.60924100 -0.79367800  
H 4.74356500 1.95249900 -1.54119000  
C 7.10492000 -0.52387400 0.24165000  
H 5.40272400 -1.85502900 0.32009100  
C 7.59722000 0.71821400 -0.15238900  
H 7.11434300 2.58069900 -1.10450700  
Cl 8.17094100 -1.64638300 1.04539100  
H 8.63316000 0.98126400 0.03928300  
H 1.02983100 -0.73267200 -1.77411400  
H 1.84027000 -2.34808200 -1.28867800  
O 1.12474500 -2.38278400 -1.96430100

H 0.34930300 -2.78412200 -1.53865600

### **1-p-F-Ar**

Bi 0.17882300 -0.00000100 -1.32744400  
S -2.91705800 0.00000000 -0.00336000  
O -2.76483900 -0.00000100 -1.47365300  
O -4.25038600 0.00000100 0.60423800  
C -1.98620500 -1.40296000 0.58021100  
C -0.69504300 -1.57068300 0.07771600  
C 0.02728800 -2.68083300 0.51409900  
H 1.04619300 -2.84239200 0.16835700  
C -0.54132300 -3.58717500 1.41281100  
H 0.03372200 -4.45040700 1.73929900  
C -1.83246000 -3.39009400 1.90056400  
H -2.26734500 -4.09789400 2.60095100  
C -2.56869200 -2.28102000 1.48941000  
H -3.57626100 -2.10041100 1.85315500  
C -1.98620500 1.40296100 0.58021000  
C -0.69504200 1.57068300 0.07771400  
C 0.02728800 2.68083400 0.51409600  
H 1.04619300 2.84239100 0.16835500  
C -0.54132200 3.58717600 1.41280800  
H 0.03372300 4.45040900 1.73929500  
C -1.83245900 3.39009600 1.90056100  
H -2.26734500 4.09789600 2.60094800  
C -2.56869100 2.28102200 1.48940800  
H -3.57626100 2.10041300 1.85315300  
C 2.16091400 0.00000000 -0.21533900  
C 3.35151000 -0.00000200 -0.94987800  
C 2.23537700 0.00000200 1.18317300  
C 4.59549100 -0.00000200 -0.31422500  
H 3.32957700 -0.00000400 -2.03911200  
C 3.46492900 0.00000300 1.83919200  
H 1.32613000 0.00000400 1.78091400  
C 4.61963700 0.00000100 1.07018700  
H 5.52611600 -0.00000300 -0.87444900  
H 3.53519500 0.00000500 2.92329400  
F 5.81698000 0.00000100 1.69960300

### **Int8**

Bi 0.02312000 0.20720300 -0.25652300  
S 2.88184400 -0.82961200 1.04176500  
F -4.23659200 -4.05552800 1.55589900  
O 4.12423100 -1.28652000 1.66083600

O 1.56661200 -1.32087600 1.51683100  
C 2.88836200 -1.15614000 -0.70158800  
C 1.71493600 -0.84988700 -1.39422500  
C 1.67485000 -1.10076100 -2.76196200  
H 0.78669800 -0.84525600 -3.33185900  
C 2.78491200 -1.66770700 -3.39681400  
H 2.74246800 -1.87231500 -4.46378400  
C 3.94434200 -1.96558100 -2.68261300  
H 4.80049500 -2.40325800 -3.18836100  
C 4.01090300 -1.70045800 -1.31585000  
H 4.90251800 -1.92003100 -0.73524300  
C 2.74932800 0.93963800 1.16282800  
C 1.53938000 1.52640600 0.78992200  
C 1.37436800 2.89857600 0.90798300  
H 0.43052600 3.35509100 0.62886300  
C 2.42936900 3.66669700 1.41296200  
H 2.29991500 4.74070100 1.51871100  
C 3.63449400 3.07356600 1.78198600  
H 4.44426200 3.68185000 2.17487500  
C 3.80635600 1.69553900 1.65694800  
H 4.73147700 1.20804400 1.95134300  
C -1.39921800 -1.35181300 0.44135400  
C -2.27875000 -1.83660700 -0.52022500  
H -2.23139300 -1.49664900 -1.55197300  
C -3.24717900 -2.76651900 -0.14234300  
H -3.95575200 -3.16948400 -0.85951300  
C -3.29776100 -3.16110700 1.18510400  
C -2.42802500 -2.67658100 2.15205700  
H -2.50872800 -3.02117000 3.17855600  
C -1.45912800 -1.75014100 1.77222600  
H -0.76530200 -1.36345800 2.51149700  
O -1.35983700 1.82950200 0.48628800  
O -0.70840900 0.68571400 -2.16513600  
C -2.60915600 1.93493900 0.03802700  
C -3.65853500 1.19295800 0.61610800  
C -2.91866200 2.80203400 -1.03058600  
C -4.95767900 1.30595300 0.13177700  
H -3.43055400 0.53140700 1.44755500  
C -4.22270400 2.90644300 -1.50959200  
H -2.11971700 3.40446200 -1.46018900  
C -5.25040800 2.15599800 -0.93694300  
H -5.75134200 0.72196500 0.59324100  
H -4.43747800 3.58320500 -2.33395100  
H -6.26682000 2.23753700 -1.31308100

H -1.49753600 1.24778600 -2.07640200

### Int6f

Bi 0.39596200 0.55092200 0.48400300  
S 3.58405300 -0.21913700 -0.67512900  
F -3.34441000 5.05170200 2.89134900  
O 3.62748800 0.13419500 0.74801900  
O 4.79659400 -0.60444400 -1.39746000  
C 2.40112200 -1.55450900 -0.81780900  
C 1.13337000 -1.47678100 -0.23760000  
C 0.31776700 -2.60093100 -0.22619300  
H -0.66444600 -2.56166900 0.23104700  
C 0.76443700 -3.79415000 -0.79407300  
H 0.14654800 -4.68679400 -0.77865500  
C 2.01786500 -3.82890700 -1.38133100  
C 2.85936000 -2.72838200 -1.40874700  
H 3.84722700 -2.78393800 -1.85536300  
C 2.86078300 1.19496500 -1.47794800  
C 1.70488700 1.74954200 -0.92754100  
C 1.23412000 2.94988500 -1.45086600  
H 0.33790800 3.41709400 -1.05101600  
C 1.90971500 3.58085400 -2.49672900  
H 1.56167300 4.52428600 -2.90638900  
C 3.04325200 2.97961600 -3.02009400  
C 3.55043400 1.78520800 -2.52995500  
H 4.45569100 1.34476700 -2.93605900  
C -0.96554400 2.13307800 1.32488800  
C -0.82862400 2.46139800 2.66960500  
H -0.11152000 1.94269700 3.29733900  
C -1.64136200 3.46112000 3.20449800  
H -1.57001900 3.74534800 4.25007600  
C -2.55749000 4.08752300 2.37412700  
C -2.70195700 3.76460100 1.03308400  
H -3.43870600 4.27985100 0.42409200  
C -1.88856500 2.76645300 0.49793600  
H -1.99409200 2.49405500 -0.54790100  
O -1.09588100 0.40973600 -1.31597100  
C -5.40206800 -1.63841300 -1.60577400  
C -4.25781400 -1.32802600 -0.88342000  
C -3.23169400 -0.62093500 -1.51514800  
C -3.35575700 -0.23289600 -2.85148700  
C -4.51064100 -0.55506400 -3.55712700  
C -5.54241400 -1.25955700 -2.93965700  
H -4.15128100 -1.62188100 0.15548700

H -2.54513800 0.31176100 -3.32475400  
H -4.61410800 -0.25982600 -4.59758000  
H -6.44574900 -1.51393200 -3.48588200  
C -2.00539400 -0.28999600 -0.74374400  
O -1.86657100 -0.68332300 0.43985600  
Cl -6.68679100 -2.51985600 -0.82845300  
O 1.10759000 0.18733400 2.50766200  
C 1.18144300 -1.10194300 2.89381800  
C 0.01501300 -1.80996800 3.22801200  
C 2.42313300 -1.74940800 2.97882200  
C 0.09221900 -3.13799000 3.63545100  
H -0.94597400 -1.30545200 3.15362200  
C 2.48991700 -3.07751200 3.39189700  
H 3.31562600 -1.19738200 2.70422000  
C 1.32921900 -3.78085900 3.71647700  
H -0.81892500 -3.67492300 3.89007200  
H 3.45820800 -3.56931200 3.45272300  
H 1.38722100 -4.81950000 4.03190500  
F 2.44377200 -4.97538400 -1.93905800  
F 3.68613700 3.58100700 -4.03568700

#### **TS4k**

Bi -0.61306800 -0.09567700 -0.38765000  
S -3.34548000 -1.87729800 -0.13859100  
O -3.18303300 -0.66014900 -0.97625400  
O -4.60805800 -2.61643100 -0.12816300  
C -2.00627100 -2.93655000 -0.64843500  
C -0.77267600 -2.33158100 -0.89224500  
C 0.27985700 -3.12300000 -1.33433700  
H 1.25026000 -2.68221000 -1.54554100  
C 0.08421200 -4.49512200 -1.52131200  
H 0.90916600 -5.10795300 -1.87626200  
C -1.15268300 -5.08231700 -1.26097100  
H -1.29360700 -6.14903000 -1.41165100  
C -2.21723500 -4.30120800 -0.81503500  
H -3.19497100 -4.73154900 -0.61661100  
C -2.91178900 -1.33527900 1.49577400  
C -1.82209200 -0.47025000 1.56166900  
C -1.45545100 0.01636600 2.81350400  
H -0.60533100 0.68694600 2.91404800  
C -2.17906500 -0.35999000 3.94903500  
H -1.89209900 0.03283000 4.92171700  
C -3.26065400 -1.23623600 3.85103100  
H -3.81379700 -1.52243100 4.74148400

C -3.63743600 -1.74498100 2.60956300  
H -4.47794500 -2.42529500 2.50302200  
C -0.14676000 2.30655900 0.07134300  
C -1.31143500 2.93758600 0.50276100  
H -2.27490600 2.72445800 0.04795900  
C -1.23095700 3.85715000 1.54644800  
H -2.14218900 4.34878500 1.88373600  
C -0.01302900 4.15123700 2.17118700  
C 1.13309700 3.48967100 1.72005800  
H 2.09482600 3.69882500 2.18537300  
C 1.07747300 2.56947900 0.67192300  
H 1.99136800 2.09681600 0.32402500  
O 1.17067800 -0.62917700 0.99308200  
C 5.85099000 -0.98764400 0.12144400  
C 4.55730100 -0.73455700 -0.31509000  
C 3.50541100 -0.83187400 0.59919800  
C 3.75185500 -1.17964500 1.92956700  
C 5.05563400 -1.43002100 2.34542200  
C 6.11493100 -1.33558400 1.44476300  
H 4.35282200 -0.46571700 -1.34626900  
H 2.91949800 -1.25183800 2.62212100  
H 5.25576000 -1.70243000 3.37803100  
H 7.13460400 -1.52994700 1.76330800  
C 2.11820600 -0.55819800 0.13578100  
O 1.88498800 -0.26233400 -1.06080500  
Cl 7.17133400 -0.86841100 -1.00839600  
O -1.01945400 0.61893200 -2.57679100  
C -0.94548100 1.90876800 -2.60181900  
C -2.08504500 2.71900500 -2.87914500  
C 0.26920200 2.56130200 -2.22484900  
C -1.97086600 4.08901300 -2.89108100  
H -3.02408100 2.22070100 -3.10520400  
C 0.37311800 3.96896900 -2.30028200  
H 1.15884800 1.94673600 -2.11824800  
C -0.73452100 4.72444800 -2.60625100  
H -2.83854700 4.69980400 -3.13044200  
H 1.32370500 4.44595400 -2.07610500  
H -0.66900700 5.80872500 -2.63941200  
C 0.04816200 5.13944400 3.30083700  
H -0.40917900 6.09550300 3.01925300  
H -0.49372700 4.76985700 4.18082900  
H 1.08118500 5.33691500 3.60465100

#### **Int6l**



Bi -0.38373800 -0.75849900 0.41687700  
S -3.30422700 -1.24603100 -1.39987100  
F 3.69488600 -3.06388000 4.68303500  
O -3.61939300 -1.15418300 0.03239900  
O -4.36664600 -1.43732700 -2.38987800  
C -2.42289700 0.25468100 -1.81217800  
C -1.34520700 0.70657100 -1.04700700  
C -0.80406700 1.95977600 -1.29358800  
H 0.02743600 2.32325100 -0.70040300  
C -1.34535800 2.75566500 -2.30596100  
H -0.93033300 3.74516800 -2.48001900  
C -2.40236100 2.29349200 -3.08394500  
H -2.81363600 2.91341900 -3.87553300  
C -2.94765000 1.03591900 -2.83995800  
H -3.78535600 0.65904000 -3.41921000  
C -2.15282600 -2.59470100 -1.53204000  
C -1.06976100 -2.63400900 -0.65265800  
C -0.26671500 -3.76851600 -0.63362400  
H 0.58487000 -3.83213100 0.03980700  
C -0.55476000 -4.84215800 -1.48133400  
H 0.06927300 -5.73159700 -1.44937100  
C -1.62791900 -4.77695300 -2.36618600  
H -1.84216100 -5.61120400 -3.02822200  
C -2.44134200 -3.64530100 -2.39623700  
H -3.29832000 -3.57846800 -3.06016800  
C 1.10106800 -1.55945900 1.91320600  
C 0.77383100 -1.46942700 3.26257900  
H -0.15036400 -0.99502900 3.57663600  
C 1.65900400 -1.98513700 4.20960300  
H 1.44239900 -1.93122700 5.27234400  
C 2.83668000 -2.56760400 3.76840500  
C 3.17318100 -2.66156700 2.42630400  
H 4.11037900 -3.12343100 2.13023100  
C 2.28664400 -2.14703900 1.48085400  
H 2.53804900 -2.20373600 0.42596500  
O 1.36803500 -0.77660500 -1.11981400  
C 5.18237400 2.03021600 -1.71112400  
C 4.01233200 1.71303000 -1.03416800  
C 3.25784100 0.61966200 -1.46634300  
C 3.67508500 -0.13991300 -2.56203200  
C 4.84944800 0.19677200 -3.22764600  
C 5.61256400 1.28415100 -2.80679900  
H 3.67993100 2.29421900 -0.18041000  
H 3.07237500 -0.98313200 -2.88364400

H 5.17845100 -0.38717000 -4.08282400  
H 6.53034100 1.55218000 -3.32145100  
C 2.00318600 0.27428400 -0.74377100  
O 1.58848900 0.98337100 0.20037400  
Cl 6.13303300 3.38956300 -1.17902800  
O -1.56556400 0.00516100 2.08679000  
C -1.95942100 1.28851500 1.95754700  
C -1.07830600 2.33649400 2.25263400  
C -3.25530000 1.60656400 1.51457200  
C -1.46449300 3.66746600 2.10691300  
H -0.07010100 2.09861000 2.58459200  
C -3.64624600 2.92832200 1.37068200  
H -3.93267500 0.79597400 1.26819600  
C -2.75403600 3.96905800 1.65617600  
H -0.75356100 4.45295700 2.34204700  
H -4.64532200 3.17752400 1.02267200  
O -3.22511600 5.22871200 1.46492000  
C -2.35430200 6.30573800 1.73177900  
H -1.46351400 6.27247700 1.08969900  
H -2.92058500 7.21300000 1.51072800  
H -2.04529100 6.32294800 2.78541300

#### TS4i

Bi -0.51540400 -0.37356900 -0.34501400  
S -2.93296500 -2.54124100 -0.36793700  
F -0.80332300 4.06473300 3.97632200  
O -2.95124100 -1.19941800 -1.01235600  
O -4.07909600 -3.44124400 -0.48040700  
C -1.46409400 -3.30889700 -1.02238000  
C -0.33693500 -2.50022600 -1.17404600  
C 0.81707600 -3.05246600 -1.71293400  
H 1.70812500 -2.44664600 -1.85363400  
C 0.82505800 -4.39958200 -2.08946600  
H 1.72698000 -4.82748000 -2.51981100  
C -0.30682800 -5.19517200 -1.92169400  
H -0.28842300 -6.23961300 -2.21993500  
C -1.47031100 -4.65315900 -1.37822000  
H -2.36871400 -5.25006900 -1.24746300  
C -2.55681300 -2.18841400 1.33104100  
C -1.60009600 -1.19512000 1.52955500  
C -1.28800000 -0.84492800 2.83985500  
H -0.54155600 -0.08074200 3.04330100  
C -1.93490000 -1.48066300 3.90408900  
H -1.69415300 -1.19391300 4.92500400

C -2.88189000 -2.47899400 3.67330900  
H -3.37638400 -2.96547700 4.50950900  
C -3.20038300 -2.85339300 2.36912700  
H -3.93770800 -3.62364200 2.16041500  
C -0.49960700 1.99211900 0.46253300  
C -1.76317800 2.31362400 0.95610400  
H -2.66886500 2.01574400 0.43542100  
C -1.86662800 3.02307600 2.15192600  
H -2.83591700 3.28598700 2.56542800  
C -0.70392400 3.38136400 2.81678600  
C 0.55829100 3.05963200 2.33990600  
H 1.44435800 3.36207500 2.89052500  
C 0.65981300 2.35484900 1.14113000  
H 1.64285200 2.12228800 0.74312300  
O 1.36400600 -0.76595800 0.92741000  
C 6.01166100 -0.15588100 0.02030100  
C 4.68329000 -0.07242100 -0.37536400  
C 3.68736900 -0.48465700 0.51384900  
C 4.02294700 -0.97426600 1.77873300  
C 5.36024900 -1.04944400 2.15438200  
C 6.36411500 -0.64056600 1.27853600  
H 4.41086100 0.30273900 -1.35640300  
H 3.23415400 -1.29249600 2.45258300  
H 5.63026700 -1.42977600 3.13559200  
H 7.40954000 -0.69729300 1.56622600  
C 2.26450400 -0.39368800 0.09450200  
O 1.94901500 0.03974100 -1.03949600  
Cl 7.26209700 0.35452900 -1.07805100  
O -1.07161500 0.60620400 -2.43080800  
C -1.22484800 1.86707800 -2.25327700  
C -2.48516600 2.50892800 -2.45720600  
C -0.14993200 2.64445200 -1.71021700  
C -2.62184300 3.85414000 -2.24332000  
H -3.31640800 1.90451500 -2.80907400  
C -0.28601300 4.04085400 -1.56626700  
H 0.83686300 2.19079800 -1.68605100  
C -1.51227700 4.63492700 -1.79677500  
H -3.57381800 4.34740100 -2.41896200  
H 0.55828500 4.63802200 -1.23516800  
C -1.67749900 6.03877400 -1.59954400  
N -1.82113500 7.18116900 -1.43742900

**5**

C -0.42485100 -0.13052300 0.03324100

C -1.16292800 -1.14441500 -0.59324800  
C -2.55509000 -1.12651700 -0.60450500  
C -3.20315900 -0.07503200 0.02169100  
C -2.51532800 0.95032500 0.65100800  
C -1.12444700 0.91640100 0.65001500  
H -0.64062100 -1.95355600 -1.09728900  
H -3.12983800 -1.90584100 -1.09587900  
H -3.06223500 1.75491900 1.13342100  
H -0.57579100 1.71169100 1.14379100  
C 1.05363800 -0.20513900 0.06212600  
C 1.86912000 0.90655100 -0.21948100  
C 1.68949500 -1.41729200 0.35928500  
C 3.26009600 0.79177600 -0.19870000  
C 3.07565200 -1.54047800 0.37997900  
H 1.07016400 -2.27860000 0.59827500  
C 3.86312400 -0.42631100 0.09922600  
H 3.87189700 1.66411500 -0.42529200  
H 3.53477500 -2.49492500 0.62183300  
H 4.94756900 -0.49862300 0.11284400  
F -4.55618300 -0.04565300 0.01606000  
O 1.26249200 2.08384600 -0.52976800  
H 1.93785200 2.74484700 -0.74192300

### **mCBA**

C -2.22415000 -0.59198700 -0.00000400  
O -2.34317900 -1.79974200 -0.00001900  
C -0.92643900 0.12665500 0.00000100  
C -0.85272200 1.52240300 0.00000700  
C 0.23834800 -0.64552800 -0.00000100  
C 0.39237200 2.14358000 0.00001200  
H -1.76211100 2.11362500 0.00000800  
C 1.46912700 -0.00459500 0.00000400  
H 0.16753700 -1.72830000 -0.00000600  
C 1.56135100 1.38617400 0.00001000  
H 0.45879100 3.22788000 0.00001700  
H 2.53468600 1.86729100 0.00001400  
Cl 2.92605700 -0.95629000 0.00000200  
O -3.28289400 0.23477000 -0.00001000  
H -4.08062000 -0.32399900 -0.00002100

### **Int6i**

Bi -0.35841800 -0.69792400 0.35527500  
S -3.25905500 -1.15426600 -1.51206100  
F 3.48809100 -3.01480400 4.80073500

O -3.62063500 -1.10804200 -0.08991800  
O -4.28560900 -1.31988600 -2.54228500  
C -2.37847800 0.36647300 -1.84745600  
C -1.30636100 0.79559900 -1.06017000  
C -0.77182700 2.06163500 -1.24301900  
H 0.05856100 2.40042900 -0.63405600  
C -1.31771800 2.90114200 -2.21783900  
H -0.91038300 3.90084300 -2.34312200  
C -2.36826900 2.46683600 -3.01908700  
H -2.78286200 3.12034700 -3.78122600  
C -2.90366100 1.19406600 -2.83770100  
H -3.73576300 0.83920800 -3.43861100  
C -2.09212500 -2.48881300 -1.65190900  
C -1.02491700 -2.54423700 -0.75385800  
C -0.21579900 -3.67388000 -0.74094400  
H 0.62432000 -3.74665500 -0.05426800  
C -0.48329400 -4.73140200 -1.61530500  
H 0.14450600 -5.61823800 -1.58997700  
C -1.54002500 -4.65238700 -2.51822700  
H -1.73764500 -5.47359900 -3.20125300  
C -2.35867900 -3.52413500 -2.54099200  
H -3.20336000 -3.44862100 -3.21955100  
C 1.03712100 -1.48764700 1.92575100  
C 0.61621900 -1.45618000 3.25038500  
H -0.34239900 -1.02373700 3.51735500  
C 1.45479600 -1.98047700 4.23383500  
H 1.16755700 -1.97269000 5.28089700  
C 2.67667800 -2.51112100 3.85081800  
C 3.10190300 -2.54630900 2.53095700  
H 4.06994300 -2.96983100 2.28083800  
C 2.26385400 -2.02397300 1.54698200  
H 2.58338600 -2.03870800 0.50963500  
O 1.43609600 -0.68817800 -1.10768100  
C 5.27636400 2.11565000 -1.52771000  
C 4.07666000 1.80012700 -0.90402300  
C 3.34204300 0.70639800 -1.36907400  
C 3.80737800 -0.05557000 -2.44381100  
C 5.01116300 0.27923300 -3.05533800  
C 5.75491100 1.36653600 -2.60120600  
H 3.70687900 2.38302800 -0.06694900  
H 3.21977500 -0.89907900 -2.79140600  
H 5.37871200 -0.30620500 -3.89351800  
H 6.69563100 1.63285300 -3.07348700  
C 2.06026600 0.36068300 -0.69985700

O 1.60973800 1.05926000 0.23513900  
Cl 6.20305000 3.47423700 -0.95639200  
O -1.66897500 -0.04385700 2.00030600  
C -2.09000900 1.22197400 1.96809800  
C -1.20614200 2.27807200 2.26547800  
C -3.42416700 1.52113200 1.63769900  
C -1.63587800 3.59346700 2.22085800  
H -0.17407700 2.04561800 2.51792300  
C -3.85765600 2.83612500 1.59419700  
H -4.09177800 0.70244300 1.39326100  
C -2.96653000 3.88401200 1.87790000  
H -0.94763700 4.40377700 2.44452700  
H -4.88613200 3.06296400 1.32747800  
C -3.40670400 5.23832300 1.80888000  
N -3.76284800 6.34435800 1.74604500

### Int6d

Bi 0.58133900 0.58859100 0.04256800  
S 3.66779600 -0.41285300 -1.31837800  
O 4.02220800 0.53778800 -0.25925800  
O 4.71505000 -1.06423900 -2.10994500  
C 2.69804200 -1.70174000 -0.53586600  
C 1.56138200 -1.44104000 0.23525200  
C 0.98333600 -2.45477400 0.98517200  
H 0.10130200 -2.25963200 1.58415600  
C 1.54369000 -3.73405100 0.95844400  
H 1.09720800 -4.51979400 1.56205600  
C 2.65451700 -4.00339600 0.16626700  
H 3.07809000 -5.00326500 0.13612600  
C 3.23800400 -2.98608200 -0.58393600  
H 4.11761600 -3.16771200 -1.19414700  
C 2.60494600 0.48186000 -2.43383000  
C 1.48691600 1.15148500 -1.93415500  
C 0.77380300 1.99306700 -2.78089400  
H -0.10689400 2.51987600 -2.42072100  
C 1.18720200 2.16520500 -4.10444300  
H 0.63415300 2.83721900 -4.75553500  
C 2.29398400 1.47620400 -4.59287700  
H 2.60552500 1.60399400 -5.62575500  
C 3.01452100 0.62618600 -3.75566200  
H 3.89175600 0.09252200 -4.10889000  
C -0.98532600 2.13649500 0.42410100  
C -0.77400800 3.04684900 1.45719600  
H 0.11661300 2.98367200 2.07476900

C -1.72568900 4.03194600 1.68371900  
H -1.59394000 4.75459400 2.48417700  
C -2.87663500 4.10463700 0.88750600  
C -3.06859700 3.18403700 -0.14886300  
H -3.95144400 3.21875300 -0.77814700  
C -2.11434900 2.19192800 -0.37982900  
H -2.27550700 1.47780100 -1.18176100  
O -0.97805200 -0.53836300 -1.28259700  
C -4.88936200 -3.11576700 -0.36650900  
C -3.80030600 -2.37724900 0.07647700  
C -2.90971800 -1.85529600 -0.86466300  
C -3.11347500 -2.07536000 -2.22898900  
C -4.20999900 -2.82060500 -2.65156900  
C -5.10707400 -3.34601300 -1.72353000  
H -3.63190600 -2.19896900 1.13338800  
H -2.40716700 -1.66484800 -2.94343100  
H -4.37279800 -2.99920700 -3.71099100  
H -5.96478200 -3.92818900 -2.04668600  
C -1.74109900 -1.06081300 -0.38940200  
O -1.52721800 -0.90679800 0.83085700  
Cl -6.00817600 -3.76882300 0.79901200  
O 1.73165600 1.39967700 1.71080200  
C 2.01342800 0.53280300 2.70294200  
C 1.01844100 0.14530000 3.61629400  
C 3.30667500 0.00592300 2.83964000  
C 1.31430800 -0.74481400 4.64463600  
H 0.01291500 0.54662400 3.50334500  
C 3.59363400 -0.88038800 3.87469700  
H 4.05988800 0.29365600 2.11344600  
C 2.60323800 -1.26404600 4.78007600  
H 0.53271000 -1.03580600 5.34310300  
H 4.60004700 -1.28282300 3.96800600  
H 2.83234500 -1.96063800 5.58257800  
O -3.74262300 5.09291600 1.19405100  
C -4.93795700 5.19304200 0.44268100  
H -5.48514400 6.03742500 0.86547300  
H -4.72899500 5.39212500 -0.61607000  
H -5.54548200 4.28413100 0.53743700

#### TS4f

Bi -0.42545000 0.12009400 -0.48939500  
S -3.41765900 -1.22169000 -0.42868800  
O -3.01774100 -0.06418300 -1.26674300  
O -4.76985600 -1.77166500 -0.49657800

C -2.21460300 -2.48042900 -0.82012400  
C -0.88900800 -2.07538900 -0.97266100  
C 0.05881400 -3.02914400 -1.32665600  
H 1.09920400 -2.74912400 -1.46708100  
C -0.32130700 -4.35907200 -1.51955600  
H 0.40202000 -5.11699700 -1.80529000  
C -1.65107200 -4.71203700 -1.34514400  
C -2.63015300 -3.79584100 -0.99173700  
H -3.66821000 -4.09229100 -0.87537600  
C -3.02113100 -0.70988600 1.22684200  
C -1.82380300 -0.01332300 1.36275100  
C -1.48486000 0.44419300 2.63479500  
H -0.55622400 0.98568300 2.79735200  
C -2.33036800 0.20840300 3.72069900  
H -2.08539000 0.56570000 4.71682800  
C -3.50650200 -0.50151400 3.52075700  
C -3.88707600 -0.98654100 2.27944600  
H -4.81508900 -1.53318600 2.14180600  
C 0.29798200 2.45399400 -0.03512900  
C -0.81120100 3.22569600 0.30831400  
H -1.76074000 3.11167800 -0.20691900  
C -0.70455200 4.15702700 1.34105000  
H -1.55194600 4.77053900 1.63340400  
C 0.50644300 4.27768500 2.00450900  
C 1.61390600 3.50615200 1.68439500  
H 2.54443600 3.63301300 2.23025200  
C 1.50487300 2.58116900 0.64677100  
H 2.37344200 1.99174100 0.36815500  
O 1.14444800 -0.60776700 1.04619100  
C 5.77790400 -1.63697700 0.51269800  
C 4.56320500 -1.22345500 -0.01794800  
C 3.45183000 -1.14142300 0.82501500  
C 3.56087800 -1.47137600 2.17827900  
C 4.78744600 -1.88397400 2.68868200  
C 5.90481700 -1.96935400 1.86019200  
H 4.46586800 -0.96670500 -1.06778300  
H 2.68447900 -1.40360800 2.81462600  
H 4.88092100 -2.14405400 3.73938300  
H 6.86468500 -2.29072700 2.25329800  
C 2.15139300 -0.69623800 0.26037800  
O 2.03965300 -0.40856200 -0.95694500  
Cl 7.17013500 -1.74272700 -0.52714900  
O -0.55527300 0.81691100 -2.70795000  
C -0.34348700 2.09123800 -2.74690200

C -1.37043700 3.01181700 -3.10665600  
C 0.90802900 2.61761200 -2.29882300  
C -1.10995900 4.36139200 -3.12362800  
H -2.34073500 2.61229800 -3.38929000  
C 1.16720400 4.00432500 -2.38172200  
H 1.71757200 1.91341100 -2.12729700  
C 0.16732800 4.86673300 -2.76611700  
H -1.89010400 5.05697200 -3.42423200  
H 2.14775400 4.38183600 -2.10375400  
H 0.34998900 5.93720500 -2.80637800  
F -4.31422500 -0.72605500 4.57556800  
F -2.01085100 -5.99555100 -1.53258600  
F 0.61125500 5.17667000 3.00792800

#### TS4h

Bi 0.25766500 -0.25537400 -0.64820600  
S 3.38317800 0.75340900 -0.77522400  
O 2.78669000 -0.25188300 -1.68984000  
O 4.77837000 1.16709600 -0.91899600  
C 2.29594700 2.16106500 -0.90968600  
C 0.92338900 1.90573800 -0.97733300  
C 0.07249400 2.98931500 -1.13392600  
H -1.00166800 2.84032700 -1.20277300  
C 0.58006100 4.28999200 -1.21794300  
H -0.11131400 5.11566900 -1.34895300  
C 1.95727500 4.51711200 -1.13643600  
C 2.83297800 3.43436900 -0.97673900  
H 3.90532600 3.59949900 -0.92721300  
C 3.07962300 0.09126200 0.84587700  
C 1.82625500 -0.49400600 1.02742200  
C 1.57087500 -1.05955100 2.27087800  
H 0.60918500 -1.52357400 2.47804400  
C 2.53745700 -1.04493800 3.28204400  
H 2.30658400 -1.50585000 4.23684800  
C 3.78064600 -0.44067900 3.06283100  
C 4.05901800 0.14730100 1.82179500  
H 5.02338500 0.61157200 1.63702700  
C -0.79118700 -2.49207600 -0.30306600  
C 0.21326000 -3.43698800 -0.09507500  
H 1.13308100 -3.42063900 -0.67270100  
C 0.04325900 -4.41871400 0.88119100  
H 0.81080500 -5.16480800 1.06595100  
C -1.12355700 -4.41727000 1.62865900  
C -2.12626900 -3.47653900 1.44490700

H -3.02638800 -3.51115300 2.05203500  
C -1.95477900 -2.50261300 0.46243800  
H -2.74814900 -1.78170700 0.28823900  
O -1.07440900 0.50062300 1.08133000  
C -5.55052900 2.15435300 1.20118900  
C -4.46627100 1.65655500 0.49066100  
C -3.29400700 1.34068400 1.18195400  
C -3.21492600 1.52415100 2.56467600  
C -4.31296700 2.02496800 3.25677500  
C -5.48920400 2.34331400 2.58049000  
H -4.51561800 1.51112000 -0.58355000  
H -2.29408300 1.27362100 3.08127700  
H -4.25924200 2.17200200 4.33195000  
H -6.34975500 2.73416400 3.11504600  
C -2.13187000 0.80099400 0.42453400  
O -2.19000100 0.63999500 -0.81722700  
Cl -7.01767500 2.55118600 0.35054800  
O 0.13313100 -0.81507900 -2.91771800  
C -0.28092800 -2.03403400 -3.01497600  
C 0.55538300 -3.07424500 -3.51558700  
C -1.56326000 -2.39223600 -2.49426400  
C 0.07910900 -4.36121200 -3.59767100  
H 1.55478700 -2.81067700 -3.85147000  
C -2.05018300 -3.71106700 -2.64697800  
H -2.23373700 -1.58440200 -2.21447500  
C -1.23430400 -4.68688300 -3.16882300  
H 0.71277700 -5.14507700 -4.00641600  
H -3.05590700 -3.95046100 -2.31152000  
H -1.59055500 -5.70915100 -3.26387900  
O 4.77291800 -0.37577600 3.97604200  
O 2.53730600 5.73303700 -1.20611700  
C 1.70057400 6.86172800 -1.37901800  
H 1.00425900 6.97403200 -0.53824400  
H 2.36855900 7.72417400 -1.41131000  
H 1.14015800 6.80210100 -2.32052500  
C 4.55683400 -0.97052200 5.24166600  
H 5.47626800 -0.80798100 5.80685200  
H 3.71981400 -0.49530600 5.76874200  
H 4.37458200 -2.04886400 5.15011600  
F -1.28922100 -5.36525900 2.57907900

#### TS4<sub>H2O</sub>

Bi -0.43900700 -0.12378600 -0.34932700  
S -2.25789800 -2.84108500 0.36200000

F -4.45200600 3.47038100 2.85684500  
O -3.11205700 -3.99132900 0.65387000  
O -2.86558000 -1.55238100 -0.08169000  
C -1.10477300 -3.22805100 -0.93151900  
C -0.35406300 -2.16236300 -1.42646700  
C 0.52199700 -2.41007800 -2.47896500  
H 1.13361600 -1.60654900 -2.88136800  
C 0.62327400 -3.69935500 -3.01120000  
H 1.30578800 -3.88491600 -3.83698100  
C -0.13287600 -4.74982100 -2.49077400  
H -0.04256900 -5.74785900 -2.91042800  
C -1.00896500 -4.52318700 -1.43120600  
H -1.61475700 -5.32114300 -1.01089100  
C -1.28943400 -2.39382900 1.78012400  
C -0.54073400 -1.21914700 1.69251200  
C 0.18262000 -0.83216300 2.81707100  
H 0.77746200 0.07715400 2.79757200  
C 0.14564700 -1.60759900 3.97979600  
H 0.70963500 -1.28815700 4.85283500  
C -0.60127900 -2.78338400 4.03199100  
H -0.62163700 -3.37984700 4.93981000  
C -1.32996200 -3.19373100 2.91813200  
H -1.92913600 -4.09996400 2.93144900  
C -1.99006600 1.80967400 0.04662300  
C -1.45173100 2.69008600 0.98075800  
H -0.39707800 2.94057000 0.97481700  
C -2.29315100 3.25533900 1.93929500  
H -1.90829000 3.94580100 2.68442200  
C -3.63768300 2.92023600 1.92820000  
C -4.18113100 2.04296300 1.00201100  
H -5.24111300 1.80741400 1.02676200  
C -3.34159800 1.47911600 0.04300500  
H -3.75652300 0.80916800 -0.70120900  
C -0.16092100 2.30328900 -2.08222300  
C 0.66621800 3.42201700 -1.77180600  
C -1.57482200 2.50633600 -2.15274400  
C 0.11508000 4.67608000 -1.66229800  
H 1.73277300 3.25426000 -1.65118100  
C -2.10595800 3.81588900 -2.09452400  
H -2.18470000 1.67476600 -2.49417000  
C -1.27958300 4.88245300 -1.83282500  
H 0.75511500 5.52963700 -1.45008600  
H -3.17583200 3.96098100 -2.21999900  
H -1.68414800 5.88862200 -1.76127000

O 0.32506300 1.10973000 -2.19532100  
O -2.78884800 -0.46367000 -2.63438600  
H -2.99134700 -1.10300400 -1.92756500  
O 1.29169700 1.40363200 0.76013300  
C 2.17006900 0.59411900 0.37051100  
O 1.84611700 -0.48397500 -0.23021400  
C 3.61133300 0.87453400 0.60428800  
C 4.57242000 -0.04965800 0.18769100  
C 3.99519100 2.06103400 1.23354800  
C 5.91371800 0.23157200 0.41171300  
H 4.26470400 -0.96720900 -0.30226100  
C 5.34451200 2.32424400 1.44560600  
H 3.23060100 2.76437300 1.54781800  
C 6.31437100 1.41081100 1.03650300  
H 5.65094900 3.24572200 1.93298300  
H 7.36951400 1.60927400 1.19891000  
Cl 7.12148500 -0.91455900 -0.10016200  
H -2.17377700 -0.92403000 -3.22282100

#### **Int6e**

Bi 0.21925800 -0.56101900 -0.62090900  
S 3.48684300 0.19874000 -0.03789600  
F -3.20425100 -5.50123700 -2.60828100  
O 3.09059100 -0.20293800 -1.39797000  
O 4.86206800 0.57100400 0.28498700  
C 2.40109600 1.55077100 0.38755200  
C 1.04227300 1.47421100 0.07597800  
C 0.22643200 2.57356300 0.30441900  
H -0.82763700 2.54043200 0.05263800  
C 0.77251500 3.74192400 0.83109000  
H 0.14209800 4.61192000 0.98868700  
C 2.13386300 3.80241600 1.15018400  
C 2.96330600 2.69637300 0.93290300  
H 4.02403300 2.73344100 1.16253600  
C 2.97429800 -1.16139200 0.98029800  
C 1.72292900 -1.70889100 0.69978900  
C 1.33454000 -2.85326600 1.38824100  
H 0.37067200 -3.31738300 1.19756700  
C 2.18516400 -3.42661000 2.33187000  
H 1.88735400 -4.32664600 2.86170500  
C 3.42870500 -2.84291500 2.60704200  
C 3.83974800 -1.69109700 1.92442500  
H 4.80838500 -1.23774800 2.11174300  
C -1.04750500 -2.29256300 -1.31346500

C -0.91303300 -2.70291100 -2.63667500  
H -0.26460400 -2.17252600 -3.32618700  
C -1.64888900 -3.80256000 -3.07776100  
H -1.57803700 -4.15329600 -4.10291400  
C -2.49070400 -4.44166500 -2.18041200  
C -2.63366800 -4.03675600 -0.86188900  
H -3.31144100 -4.56598900 -0.19877900  
C -1.89445100 -2.93964400 -0.41967600  
H -1.99783700 -2.60557000 0.60851900  
O -1.04785200 -0.50175300 1.33655700  
C -5.35386500 1.46007500 2.00956300  
C -4.27609400 1.16225300 1.18659400  
C -3.17314500 0.50080100 1.73348900  
C -3.15344200 0.14726700 3.08521800  
C -4.24230100 0.45957200 3.89239000  
C -5.35006600 1.11677100 3.36054500  
H -4.28183100 1.43053700 0.13534600  
H -2.28572600 -0.36256400 3.49108600  
H -4.23469500 0.19279100 4.94542100  
H -6.20293600 1.36157100 3.98637600  
C -2.02021900 0.18185000 0.85853400  
O -1.98719700 0.57395000 -0.33667700  
Cl -6.73514700 2.27894400 1.34002500  
O 0.39542400 0.02889900 -2.71528600  
C 0.45815200 1.35157400 -2.94906200  
C -0.72550500 2.10621600 -3.03231400  
C 1.69423700 1.99658400 -3.11902100  
C -0.66879300 3.47464600 -3.27083500  
H -1.67756600 1.60000100 -2.89670100  
C 1.73991200 3.36785000 -3.35470700  
H 2.60098500 1.40586400 -3.04751700  
C 0.56359400 4.11492300 -3.42558400  
H -1.59133900 4.04732100 -3.33457600  
H 2.70311200 3.85721300 -3.48019300  
H 0.60495700 5.18599700 -3.60635900  
C 4.28869900 -3.43375300 3.58583400  
N 4.98113900 -3.91516700 4.38394200  
C 2.68577600 5.00517500 1.69367900  
N 3.12947300 5.98237000 2.13680300

### Int6c

Bi 0.56630200 0.56380100 0.19034400  
S 3.57446500 -0.45267900 -1.30465700  
O 3.93482600 0.14500300 -0.01378200

O 4.61023900 -1.00139600 -2.18415700  
C 2.40850300 -1.76510300 -0.94923400  
C 1.25534000 -1.56420700 -0.18545200  
C 0.49433000 -2.65193600 0.21696400  
H -0.39826800 -2.50497700 0.81450800  
C 0.88760300 -3.94095400 -0.15071100  
H 0.29689800 -4.78990400 0.18330900  
C 2.01857400 -4.13907600 -0.93540900  
H 2.31441800 -5.14227200 -1.22903700  
C 2.78592900 -3.04938600 -1.33789300  
H 3.68361500 -3.17985700 -1.93486000  
C 2.70174000 0.81951100 -2.19238700  
C 1.64153200 1.47940900 -1.56866700  
C 1.08550100 2.58991400 -2.19407400  
H 0.25680100 3.12469500 -1.73639400  
C 1.59295200 3.02993400 -3.41960000  
H 1.16139400 3.90775800 -3.89350900  
C 2.63841400 2.34849500 -4.03654200  
H 3.02336600 2.68834200 -4.99392000  
C 3.20445500 1.23279600 -3.42188500  
H 4.03436600 0.69631700 -3.87213100  
C -0.75411100 2.22674300 0.92252600  
C -0.45972000 2.79772400 2.15435800  
H 0.36259900 2.42264400 2.75566200  
C -1.25014600 3.85784600 2.59754100  
H -1.02977700 4.31189700 3.56178900  
C -2.31683600 4.34282400 1.83275300  
C -2.57559600 3.74212700 0.59660500  
H -3.39845700 4.10416100 -0.01654000  
C -1.80065300 2.68001100 0.12955900  
H -2.02484900 2.22547700 -0.83074100  
O -1.12081100 0.06042300 -1.35458600  
C -5.41011700 -1.98111400 -0.87173000  
C -4.20348500 -1.56406500 -0.32613600  
C -3.25317100 -0.97216500 -1.16164300  
C -3.51467800 -0.80404200 -2.52344100  
C -4.73028800 -1.22964400 -3.04997300  
C -5.68762400 -1.82104400 -2.22791800  
H -3.98934300 -1.68750900 0.73036700  
H -2.76133700 -0.34512100 -3.15553800  
H -4.94011600 -1.10416500 -4.10868700  
H -6.63834800 -2.15524800 -2.63223800  
C -1.95958300 -0.52201300 -0.57696800  
O -1.71051100 -0.70125100 0.63638600

Cl -6.60343000 -2.71973200 0.16068900  
O 1.67162200 0.68161700 2.06386800  
C 1.79890200 -0.46826000 2.75425300  
C 0.71014800 -0.99452300 3.46983300  
C 3.02351000 -1.15279100 2.77444100  
C 0.84769700 -2.17640500 4.19154100  
H -0.24175700 -0.46758800 3.44400400  
C 3.15198200 -2.33226500 3.50328700  
H 3.84936800 -0.74927800 2.19786000  
C 2.06882100 -2.85319300 4.21255400  
H -0.00466300 -2.57210500 4.73960900  
H 4.10641300 -2.85425100 3.50874900  
H 2.17383600 -3.77751400 4.77502200  
C -3.17424000 5.46541900 2.34161700  
H -3.88715300 5.10088800 3.09256900  
H -2.57037900 6.24487600 2.81920800  
H -3.75181000 5.92695400 1.53438300

#### **TS1**

Bi -0.84460000 0.05959600 0.00375600  
S -2.44614100 -2.86360600 -0.03510600  
F -2.55852000 6.17091800 0.08732800  
O -0.96882700 -2.84845500 -0.03494300  
O -3.18517200 -4.12583800 -0.05219300  
C -2.92918400 -1.90200400 1.38736000  
C -2.28138000 -0.68461000 1.60023900  
C -2.61721100 0.06275900 2.72442200  
H -2.14204800 1.02296500 2.91264300  
C -3.58039800 -0.41950000 3.61595100  
H -3.83345700 0.16473400 4.49709500  
C -4.21967500 -1.63570900 3.38297500  
H -4.96662000 -2.00221500 4.08150300  
C -3.90175600 -2.38929000 2.25401200  
H -4.38528700 -3.34070900 2.05133300  
C -2.92909600 -1.86363600 -1.43083900  
C -2.28126400 -0.64083400 -1.61051300  
C -2.61737300 0.13672900 -2.71398100  
H -2.14232100 1.10188400 -2.87518000  
C -3.58023100 -0.32133200 -3.61847500  
H -3.83325600 0.28651300 -4.48351300  
C -4.21929000 -1.54357700 -3.41866000  
H -4.96611600 -1.89115600 -4.12691300  
C -3.90150700 -2.32737400 -2.31041400  
H -4.38511800 -3.28394500 -2.13382600

C -1.47972700 2.20676900 0.03186600  
C -2.83101100 2.56596400 0.03687800  
H -3.60911300 1.80546900 0.02666900  
C -3.20418600 3.90859600 0.05548800  
H -4.24707300 4.21186700 0.05969300  
C -2.20248700 4.86853900 0.06897800  
C -0.85441600 4.54781200 0.06463800  
H -0.10782000 5.33651300 0.07571800  
C -0.49596800 3.19950800 0.04569600  
H 0.55850100 2.93298900 0.04183100  
O 1.42694500 0.49908100 -0.03642700  
O 3.14001700 1.10950000 -0.07763600  
C 3.85808800 0.03443900 -0.01613700  
C 5.33736900 0.26013000 -0.03874800  
O 3.38101000 -1.10613700 0.05608000  
C 5.88182100 1.54251700 -0.13942400  
C 6.16968500 -0.85843000 0.04231900  
C 7.26365800 1.70415800 -0.15960000  
H 5.22347200 2.40282100 -0.20213400  
C 7.54572600 -0.67321700 0.02199100  
H 5.73448800 -1.84923500 0.11926800  
C 8.10687000 0.59791800 -0.07889400  
H 7.69381200 2.69876500 -0.23892100  
Cl 8.59346400 -2.06133300 0.12454100  
H 9.18590800 0.71810500 -0.09383100  
H 1.82572300 -0.42288500 0.01361300

#### **TS4**

Bi -0.60848200 -0.09200300 -0.38597700  
S -3.34498300 -1.86041000 -0.17627500  
F 0.01247700 4.94916600 3.23618100  
O -3.16717300 -0.63264700 -0.99615300  
O -4.61236400 -2.59041700 -0.18595300  
C -2.00848200 -2.92072100 -0.69097700  
C -0.77031500 -2.31937700 -0.92031600  
C 0.28218900 -3.10953300 -1.36381200  
H 1.25596300 -2.67077900 -1.56343200  
C 0.08150900 -4.47867300 -1.56722400  
H 0.90608700 -5.09131000 -1.92326500  
C -1.15975000 -5.06298900 -1.32182000  
H -1.30424400 -6.12730200 -1.48533600  
C -2.22411700 -4.28242000 -0.87425700  
H -3.20491700 -4.71085200 -0.68717300  
C -2.91983200 -1.34184400 1.46780600



C -1.82700400 -0.48216300 1.55249700  
C -1.46627300 -0.01294500 2.81238900  
H -0.61388000 0.65234100 2.92804800  
C -2.19903100 -0.40058800 3.93832700  
H -1.91724500 -0.02052900 4.91747900  
C -3.28321900 -1.27115700 3.82191300  
H -3.84338600 -1.56613900 4.70502100  
C -3.65391800 -1.76282700 2.57169300  
H -4.49634000 -2.43843600 2.45133400  
C -0.14984100 2.30425400 0.11028300  
C -1.32140800 2.92180100 0.54659000  
H -2.28015000 2.70981600 0.08199600  
C -1.26699300 3.82576600 1.60732900  
H -2.16385200 4.31920500 1.97070400  
C -0.04210100 4.07608400 2.20537800  
C 1.13002300 3.46062800 1.79170400  
H 2.06997300 3.68543200 2.28767400  
C 1.07153800 2.56243000 0.72698200  
H 1.98830200 2.09813600 0.37607200  
O 1.17025400 -0.63250800 0.99648800  
C 5.85129600 -0.97892800 0.12094000  
C 4.55714200 -0.72382300 -0.31293300  
C 3.50592200 -0.82892200 0.60139800  
C 3.75317700 -1.18622500 1.92918000  
C 5.05749900 -1.43788700 2.34241600  
C 6.11607200 -1.33590400 1.44174100  
H 4.35205600 -0.44771300 -1.34206100  
H 2.92144500 -1.26456000 2.62183300  
H 5.25858400 -1.71717800 3.37295700  
H 7.13611700 -1.53126500 1.75846700  
C 2.11900700 -0.55243100 0.14100600  
O 1.88472700 -0.24373600 -1.05259000  
Cl 7.17055700 -0.85065600 -1.00869200  
O -0.99586300 0.66831700 -2.56070000  
C -0.92329600 1.95774800 -2.56166900  
C -2.06224300 2.77281900 -2.82744800  
C 0.29001300 2.60270300 -2.16593400  
C -1.94741500 4.14259100 -2.81287400  
H -3.00035100 2.27904100 -3.06677100  
C 0.39542700 4.01156100 -2.21655600  
H 1.17852200 1.98504500 -2.06744400  
C -0.71123700 4.77212500 -2.51255700  
H -2.81366400 4.75841900 -3.04399700  
H 1.34569300 4.48440900 -1.98260300

H -0.64541900 5.85675700 -2.52680400

### Int6b

Bi -0.58017700 -0.42515800 0.51868200  
S -3.36291100 -0.08094000 -1.59399900  
O -3.86594100 0.09931400 -0.22742400  
O -4.27128700 0.01862900 -2.73932200  
C -2.06620800 1.13454900 -1.81883500  
C -0.99480100 1.26710300 -0.93115400  
C -0.13557300 2.35048400 -1.03788000  
H 0.69404900 2.46234600 -0.34911000  
C -0.34783100 3.29995400 -2.04030700  
H 0.31766700 4.15658800 -2.10712300  
C -1.39493200 3.15274700 -2.94382000  
H -1.54903800 3.88650600 -3.72994700  
C -2.26133000 2.06817800 -2.83545600  
H -3.09850200 1.94343100 -3.51586100  
C -2.60984700 -1.69399000 -1.61513500  
C -1.67399000 -2.02359200 -0.63311200  
C -1.23282600 -3.33933800 -0.54413000  
H -0.50164700 -3.62812900 0.20730900  
C -1.73176600 -4.30459600 -1.42320200  
H -1.39275600 -5.33363800 -1.33662500  
C -2.65039300 -3.95466000 -2.40894600  
H -3.02780000 -4.70615500 -3.09673400  
C -3.09970600 -2.63912100 -2.51057200  
H -3.83189900 -2.34585800 -3.25700800  
C 0.50316300 -1.58589900 2.11113700  
C 0.06048200 -1.44856500 3.42037600  
H -0.75124700 -0.76930300 3.66173100  
C 0.69290800 -2.20258100 4.41207400  
H 0.36410100 -2.10653500 5.44379700  
C 1.73658100 -3.06514800 4.08374600  
C 2.15818700 -3.18484400 2.76022800  
H 2.97379900 -3.85566900 2.50188300  
C 1.53979000 -2.44034600 1.75418900  
H 1.87090900 -2.53115000 0.72416200  
O 1.20884000 -0.91160000 -0.91341500  
C 5.67425200 0.75873200 -1.17081900  
C 4.41558400 0.76348400 -0.58490900  
C 3.42921900 -0.08313600 -1.09654400  
C 3.70655900 -0.91928700 -2.18060500  
C 4.97404200 -0.90654700 -2.75457500  
C 5.96797900 -0.06802300 -2.25348400

H 4.18888100 1.40727700 0.25851200  
H 2.92493300 -1.56686500 -2.56455700  
H 5.19662800 -1.55167800 -3.60007500  
H 6.95925000 -0.05432700 -2.69647500  
C 2.07983600 -0.08092400 -0.46656400  
O 1.81465300 0.70209900 0.47282000  
Cl 6.91274300 1.80811900 -0.53827300  
O -1.79242200 0.49662800 2.07907400  
C -1.80132900 1.84413600 2.09766000  
C -0.70279700 2.55762800 2.60619700  
C -2.91038800 2.55343100 1.61251200  
C -0.71797000 3.94900200 2.62996500  
H 0.16006300 2.00624000 2.97474800  
C -2.91763200 3.94545700 1.64536900  
H -3.74191700 1.99083600 1.20113200  
C -1.82441500 4.65181100 2.14873700  
H 0.14037600 4.48766500 3.02559900  
H -3.78293500 4.48323900 1.26394600  
H -1.83333400 5.73873500 2.16597200  
H 2.22522500 -3.64559500 4.86200900

#### TS4I

Bi -0.58688200 -0.36973300 -0.35699500  
S -3.24182800 -2.27995000 -0.32269400  
F 0.06301500 4.27060100 3.84267300  
O -3.12966800 -0.96029800 -0.99916100  
O -4.47852800 -3.05770000 -0.40210400  
C -1.87127500 -3.21689100 -0.96896900  
C -0.66368000 -2.53953700 -1.13839400  
C 0.41457100 -3.23073400 -1.67679700  
H 1.36715300 -2.73139100 -1.83282300  
C 0.26914000 -4.57578600 -2.03125100  
H 1.11395000 -5.10908700 -2.46028400  
C -0.94348200 -5.23704100 -1.84282800  
H -1.04515000 -6.28183200 -2.12305100  
C -2.03317900 -4.55796900 -1.30085400  
H -2.99216600 -5.04680400 -1.15236700  
C -2.81305400 -1.93420900 1.36570000  
C -1.75234300 -1.04740500 1.53745400  
C -1.39451700 -0.71335800 2.84121900  
H -0.56820800 -0.03112400 3.02707400  
C -2.09542200 -1.25814200 3.92135800  
H -1.81451600 -0.98383300 4.93555500  
C -3.14752600 -2.15123800 3.71498300

H -3.68381200 -2.56848900 4.56291100  
C -3.51604100 -2.50879200 2.41945300  
H -4.33380100 -3.19817400 2.22824300  
C -0.20836100 1.96597100 0.45730600  
C -1.36959700 2.46670400 1.04608900  
H -2.35109900 2.25357500 0.63172200  
C -1.28102600 3.25407800 2.19468700  
H -2.17057800 3.65493000 2.67236800  
C -0.02802500 3.50670900 2.72970900  
C 1.13726600 3.00031900 2.17309900  
H 2.09948900 3.21776700 2.62829700  
C 1.04002100 2.22010900 1.02152900  
H 1.95057100 1.84648100 0.56199800  
O 1.24353400 -0.99753100 0.90666700  
C 5.92748700 -0.95768000 -0.01337400  
C 4.61663600 -0.73398000 -0.41315700  
C 3.58091600 -1.01375500 0.48177500  
C 3.86047300 -1.51223700 1.75652600  
C 5.18102100 -1.73130800 2.13567300  
C 6.22446900 -1.45479600 1.25414800  
H 4.38626100 -0.34870400 -1.40106100  
H 3.04037400 -1.72365400 2.43496400  
H 5.40690100 -2.12063400 3.12457200  
H 7.25704100 -1.62276200 1.54492800  
C 2.17550800 -0.76553500 0.05914200  
O 1.91320500 -0.33421700 -1.08812900  
Cl 7.22784500 -0.60924100 -1.11896600  
O -1.04774100 0.69982100 -2.40351500  
C -1.07963500 1.96995400 -2.19327800  
C -2.30432000 2.70775700 -2.24227200  
C 0.09688000 2.67131600 -1.78955100  
C -2.31088300 4.05426200 -2.00646200  
H -3.21643000 2.17231400 -2.49129300  
C 0.09281700 4.06813300 -1.61292500  
H 1.03824300 2.13094000 -1.82838800  
C -1.10663700 4.74972900 -1.68857000  
H -3.23076600 4.63105800 -2.05811500  
H 1.01944700 4.57320300 -1.36393600  
O -1.26175600 6.07244100 -1.48856600  
C -0.11959600 6.82185400 -1.11641600  
H 0.64407500 6.79692200 -1.90372500  
H -0.46578000 7.84783100 -0.98074800  
H 0.30476300 6.45105100 -0.17484700

**TS6**

Bi 0.07582900 -0.43537400 0.19332100  
S 3.40708900 0.64637300 0.78104400  
F -4.44969900 3.79111000 -0.57270500  
O 2.73284100 0.38200300 2.06714600  
O 4.80279400 1.09255000 0.78488900  
C 3.28913700 -0.85519200 -0.17663600  
C 2.05061900 -1.47936900 -0.34647800  
C 2.00685400 -2.69180200 -1.02947900  
H 1.05480900 -3.19547200 -1.17467300  
C 3.18531600 -3.26762400 -1.51419800  
H 3.14087700 -4.22133400 -2.03429800  
C 4.40958500 -2.62840200 -1.33778900  
H 5.32239500 -3.07699000 -1.71992000  
C 4.46945600 -1.40935200 -0.66474100  
H 5.41334800 -0.89577600 -0.50620100  
C 2.41841700 1.85152600 -0.08632000  
C 1.04824800 1.62505200 -0.25181000  
C 0.30313600 2.62651400 -0.87590200  
H -0.76520500 2.49898200 -1.03336600  
C 0.91076300 3.81250200 -1.29833900  
H 0.30831600 4.58491600 -1.77029800  
C 2.27784200 4.00790400 -1.12119800  
H 2.74913400 4.92860500 -1.45398400  
C 3.04726500 3.01852000 -0.51206400  
H 4.11481700 3.14636500 -0.35780300  
C -2.28108200 0.38606700 0.13507600  
C -2.86592300 0.57734800 -1.11636200  
H -2.75970900 -0.15878000 -1.90696800  
C -3.60700500 1.73416600 -1.35553100  
H -4.07552800 1.91207900 -2.31947300  
C -3.73259100 2.66913700 -0.33818200  
C -3.14275200 2.50033200 0.90481800  
H -3.25854000 3.25999400 1.67265800  
O 0.04854800 -0.45158300 2.27761500  
C -2.24698500 -2.39996500 0.00713500  
C -2.82803600 -1.63571000 1.07111300  
C -4.23539300 -1.50081500 1.16165800  
H -2.20617500 -1.41804000 1.93614900  
C -4.46137600 -2.64694100 -0.95729700  
C -5.03792400 -1.97063600 0.15126000  
H -4.66443400 -0.98534500 2.01680400  
H -5.11062100 -3.01848000 -1.74697200  
H -6.11592300 -1.84232800 0.19841300

O -0.96953900 -2.56538600 -0.04273500  
C -2.40269700 1.34194500 1.14290600  
H -1.92880500 1.19143000 2.10965600  
C -3.10512600 -2.85176600 -1.03839900  
H -2.65899600 -3.38335600 -1.87511600  
H 0.94465900 -0.19369400 2.56258200

**Int4**

Bi -0.75997700 0.52230000 -0.55848200  
S -3.75586500 -1.19078600 -0.07290200  
F 2.47299000 5.92780100 -0.34992700  
O -3.97851700 -0.19602700 -1.13716200  
O -4.84785700 -2.07567600 0.33349600  
C -2.38971300 -2.19979200 -0.63117800  
C -1.17828400 -1.64401100 -1.05757800  
C -0.23146000 -2.45197300 -1.66961100  
H 0.71119700 -2.03136200 -2.00274800  
C -0.49195600 -3.81484900 -1.83862000  
H 0.25195400 -4.43942600 -2.32614100  
C -1.68220100 -4.37115200 -1.38239500  
H -1.87473900 -5.43325900 -1.50418300  
C -2.64173100 -3.56201600 -0.77936500  
H -3.58995300 -3.96761800 -0.43921200  
C -3.19923700 -0.28207900 1.35252200  
C -2.12295800 0.59764400 1.22542800  
C -1.78097100 1.39670600 2.31080500  
H -0.94037100 2.08393700 2.24496100  
C -2.51775400 1.31833300 3.49528000  
H -2.25205100 1.95525300 4.33493500  
C -3.58096700 0.42583100 3.60841300  
H -4.14495600 0.36234400 4.53467100  
C -3.93087300 -0.38658600 2.53159400  
H -4.76322300 -1.08146300 2.59221100  
C 0.44513600 2.39640800 -0.48350600  
C 0.16207200 3.36632600 -1.43951400  
H -0.58905800 3.18732400 -2.20203800  
C 0.86032500 4.57307300 -1.39514400  
H 0.67767000 5.35604200 -2.12489200  
C 1.80118800 4.75993500 -0.39459600  
C 2.08051300 3.79935500 0.56615800  
H 2.82593700 3.99343300 1.33136600  
C 1.39016100 2.58931700 0.51801300  
H 1.59837500 1.82305400 1.25784600  
O 0.81348200 -0.40078100 0.99770300

C 5.33550900 -1.83454200 0.44525400  
C 4.15811600 -1.32052300 -0.08155900  
C 3.05468500 -1.15908700 0.75977800  
C 3.13767200 -1.51007800 2.10927600  
C 4.32659700 -2.02518000 2.61678600  
C 5.43527100 -2.19076500 1.78873300  
H 4.08285900 -1.04132900 -1.12734200  
H 2.26761200 -1.37991000 2.74479800  
H 4.39740200 -2.30321100 3.66483700  
H 6.36627500 -2.59122400 2.17859200  
C 1.78944300 -0.60566400 0.19627400  
O 1.70548300 -0.34416500 -1.02731200  
Cl 6.71777200 -2.03794300 -0.59576700  
H -2.67589400 0.86351000 -2.23535000  
O -1.81854200 1.32322500 -2.21072200

### TS3

Bi -0.35988500 -0.66392800 0.03261300  
S 1.35780300 -3.79747100 -0.21241300  
F -4.79910300 2.39332000 3.26375000  
O 2.42139500 -4.79895600 -0.29624000  
O -0.04060600 -4.24537800 -0.35757100  
C 1.63513300 -2.59440000 -1.51229400  
C 0.86808500 -1.43698600 -1.67507100  
C 0.98259000 -0.67478700 -2.82658300  
H 0.37794500 0.21639200 -2.94951700  
C 1.88764000 -1.06305800 -3.81707600  
H 1.97126200 -0.46885200 -4.72301200  
C 2.67935300 -2.19363300 -3.64445600  
H 3.39245100 -2.48593900 -4.40985800  
C 2.55029500 -2.96928500 -2.49531300  
H 3.13753500 -3.87186900 -2.35589500  
C 1.49873000 -2.95966500 1.35360800  
C 0.73349300 -1.82440600 1.63226700  
C 0.81861300 -1.27260800 2.90803000  
H 0.26052000 -0.37037400 3.15041800  
C 1.62925800 -1.85838700 3.88214400  
H 1.67632400 -1.42068600 4.87592000  
C 2.38630200 -2.98794000 3.58139800  
H 3.02677600 -3.43593300 4.33586700  
C 2.32990000 -3.54531500 2.30673700  
H 2.91562900 -4.42217200 2.04800100  
C -1.87100900 0.50372900 1.17262600  
C -2.12971600 1.83767000 0.88958600

H -1.58959600 2.36321700 0.11109800  
C -3.13221300 2.48385200 1.60979500  
H -3.38542600 3.52067200 1.41156300  
C -3.82600700 1.76747400 2.57283900  
C -3.57146600 0.43332300 2.85305200  
H -4.14876500 -0.08586300 3.61195000  
C -2.57566700 -0.21936000 2.12770800  
H -2.38403200 -1.27381100 2.30466700  
C -3.14626300 0.21756300 -1.81454300  
C -2.99062700 1.44175000 -2.48352200  
C -4.35243100 -0.03785800 -1.14186200  
C -4.01128500 2.38662500 -2.46870700  
H -2.05072400 1.63984100 -2.99123200  
C -5.36730800 0.91512400 -1.13262700  
H -4.47962800 -0.98170300 -0.61705200  
C -5.20601500 2.13449400 -1.79096000  
H -3.87167200 3.33128700 -2.99039400  
H -6.29196800 0.70238700 -0.60032700  
H -6.00046600 2.87619400 -1.77899300  
O -2.13823100 -0.66666400 -1.81398900  
O -1.96241700 -2.28639400 -0.13381600  
H -1.54195600 -3.14121100 -0.34769400  
O 0.12779700 1.61650000 -1.13802300  
C 1.10700900 1.74619800 -0.36211300  
O 1.36498300 0.85859100 0.51968200  
C 1.98892100 2.94029000 -0.44765700  
C 3.06655400 3.06506600 0.43268200  
C 1.73504200 3.92847500 -1.40177200  
C 3.87913300 4.18750300 0.34289000  
H 3.25657800 2.29199400 1.16964700  
C 2.56268900 5.04413100 -1.47549200  
H 0.89152200 3.81081600 -2.07470900  
C 3.64097800 5.18223100 -0.60327700  
H 2.37220100 5.81702100 -2.21497100  
H 4.29010100 6.05118400 -0.65482700  
Cl 5.22403800 4.35511600 1.43672000  
H -2.27736800 -1.66227900 -1.08943600

### Int6

Bi -0.56807500 0.54874700 -0.23317400  
S -3.58382500 -0.40242300 1.24522000  
F 2.91877200 5.29513600 -2.54895000  
O -3.87357700 0.10551800 -0.10152900  
O -4.66251700 -0.89565600 2.10484700

C -2.39398400 -1.72419700 1.04091400  
C -1.21843600 -1.56317800 0.30264900  
C -0.42096800 -2.66321100 0.02384200  
H 0.48855200 -2.54996300 -0.55517200  
C -0.80333800 -3.92439200 0.48782800  
H -0.18477000 -4.78559700 0.24919500  
C -1.95962100 -4.08046300 1.24481900  
H -2.24739400 -5.06160400 1.61172700  
C -2.76196000 -2.97783300 1.52576000  
H -3.67855700 -3.07654700 2.09969200  
C -2.75875100 0.93256300 2.08185900  
C -1.69063600 1.56697700 1.44518400  
C -1.16365700 2.71982900 2.01596500  
H -0.33202500 3.24032900 1.54752300  
C -1.70724400 3.22490600 3.20060000  
H -1.29830000 4.13524600 3.63121400  
C -2.76026800 2.56844000 3.83161100  
H -3.17343300 2.96061900 4.75662500  
C -3.29804000 1.41089400 3.27126000  
H -4.13387300 0.89191300 3.73115100  
C 0.70659500 2.21368400 -1.05004900  
C 0.40670400 2.70175100 -2.31735600  
H -0.39434100 2.26343500 -2.90388900  
C 1.16225400 3.75698700 -2.82919700  
H 0.96393400 4.16542700 -3.81561100  
C 2.18650200 4.27714700 -2.05377900  
C 2.49345500 3.79561600 -0.78985200  
H 3.30921900 4.23377800 -0.22270700  
C 1.73720600 2.74194300 -0.27815000  
H 1.96728300 2.34593700 0.70637900  
O 1.11781000 0.20308600 1.35276800  
C 5.43196900 -1.81173200 0.98863400  
C 4.22284400 -1.43668900 0.41851700  
C 3.26104600 -0.81852900 1.22144600  
C 3.51307900 -0.58321400 2.57523400  
C 4.73083900 -0.96878600 3.12668500  
C 5.69976000 -1.58523400 2.33735200  
H 4.01675400 -1.61338900 -0.63199500  
H 2.75076600 -0.10543100 3.18207800  
H 4.93333200 -0.79184200 4.17940700  
H 6.65250500 -1.88787200 2.76122300  
C 1.96441000 -0.41591100 0.61329400  
O 1.71342700 -0.66990700 -0.58773400  
Cl 6.63993300 -2.58114900 -0.00231600

O -1.57281300 0.46547000 -2.16175800  
C -1.67895800 -0.75384800 -2.72622100  
C -0.57102100 -1.34304200 -3.35800900  
C -2.89840000 -1.44676000 -2.69812500  
C -0.68526400 -2.59659000 -3.95109700  
H 0.37600300 -0.80740900 -3.36815800  
C -3.00336600 -2.69878800 -3.29844400  
H -3.73968000 -0.99079300 -2.18710600  
C -1.90113400 -3.28289000 -3.92384600  
H 0.18090800 -3.04118000 -4.43633300  
H -3.95400800 -3.22667400 -3.26833400  
H -1.98760400 -4.26312200 -4.38581000

#### TS4<sub>CBA</sub>

Bi -0.68630600 0.24753000 -0.28759200  
S -3.45573500 -0.31459100 1.29763500  
F -1.77799100 6.32610500 0.60984500  
O -4.68192300 -0.45200300 2.07997000  
O -2.73677800 0.98770000 1.23421500  
C -3.72404100 -0.75139000 -0.40343200  
C -2.65344800 -0.50671300 -1.26249400  
C -2.79810100 -0.85089800 -2.60242100  
H -1.97404700 -0.70754300 -3.29736400  
C -4.00045200 -1.40601400 -3.05242200  
H -4.11016200 -1.66581800 -4.10255700  
C -5.05529800 -1.63982800 -2.16994800  
H -5.98305000 -2.07406100 -2.53198300  
C -4.92182500 -1.32322500 -0.81898800  
H -5.72527600 -1.50212000 -0.10959600  
C -2.21245400 -1.45608900 1.86680700  
C -0.92309600 -1.28979800 1.35923300  
C 0.09223300 -2.12435600 1.80967400  
H 1.10326300 -2.01521900 1.43114100  
C -0.20328200 -3.11305800 2.75319100  
H 0.59157400 -3.76685600 3.10280800  
C -1.49837600 -3.27206800 3.24269900  
H -1.71267300 -4.04308500 3.97748000  
C -2.52454300 -2.43810800 2.80003300  
H -3.53790700 -2.53141500 3.18042100  
C -0.26098700 2.64465300 -0.17216400  
C -0.77539900 3.36958800 -1.23452900  
H -0.77433500 2.98369900 -2.24860300  
C -1.29822500 4.63230500 -0.95550600  
H -1.72702400 5.24028500 -1.74654500

C -1.26648400 5.10289600 0.34851800  
C -0.73144700 4.36615200 1.39416600  
H -0.72684500 4.76903300 2.40253000  
C -0.20264500 3.10215400 1.13411600  
H 0.22601500 2.50578000 1.93312500  
C 0.92842000 -2.02376100 -1.56155500  
C 0.08758800 -3.13635700 -1.40278900  
C 2.31781100 -2.20264700 -1.48731700  
C 0.62942000 -4.39619200 -1.16137000  
H -0.98941500 -2.99729900 -1.46223000  
C 2.85057300 -3.46559400 -1.24755900  
H 2.96238500 -1.33787400 -1.61556100  
C 2.01126200 -4.56911700 -1.07710500  
H -0.03503000 -5.24815100 -1.03538300  
H 3.93011800 -3.58758800 -1.18954900  
H 2.43106900 -5.55340700 -0.88633400  
O 0.42912400 -0.79537100 -1.80842900  
O 1.64235500 2.11304700 -0.73238500  
C 2.22417800 1.23184700 -0.02363100  
O 1.61769900 0.39599500 0.70024400  
C 3.71837000 1.18742100 -0.07648700  
C 4.37819600 0.11195900 0.52255300  
C 4.44369500 2.18652300 -0.72855400  
C 5.76290300 0.04925200 0.45248600  
H 3.80342700 -0.66021200 1.02261700  
C 5.83238500 2.11006100 -0.77852000  
H 3.91219400 3.01252200 -1.19036900  
C 6.50335100 1.03921000 -0.19043000  
H 6.40358300 2.88639400 -1.28031000  
H 7.58626000 0.97067500 -0.23147100  
Cl 6.59161400 -1.30188400 1.17945100

#### **TS4k**

Bi -0.58372300 -0.24044400 -0.36855500  
S -3.22433700 -2.17133500 -0.25862400  
F -0.00974200 4.49574300 3.68474500  
O -3.13219800 -0.87778500 -0.98478200  
O -4.44919700 -2.96997800 -0.30301800  
C -1.84283500 -3.11384500 -0.87324500  
C -0.64379900 -2.42963200 -1.07521000  
C 0.44106500 -3.12574300 -1.59275900  
H 1.38590400 -2.62010600 -1.77281200  
C 0.31097100 -4.48506400 -1.89515800  
H 1.16052200 -5.02327900 -2.30826900

C -0.89199100 -5.15374300 -1.67515200  
H -0.98159600 -6.20964900 -1.91484000  
C -1.98794900 -4.46838900 -1.15401900  
H -2.93998800 -4.96330700 -0.98277700  
C -2.79557900 -1.75577300 1.41347100  
C -1.74849900 -0.84676600 1.54776400  
C -1.39097400 -0.45584600 2.83534800  
H -0.57448800 0.24559400 2.99034800  
C -2.08100600 -0.96758000 3.93841600  
H -1.80187400 -0.64864700 4.93993700  
C -3.11976300 -1.88408000 3.77084600  
H -3.64741600 -2.27527900 4.63641600  
C -3.48636900 -2.29856400 2.49180900  
H -4.29387200 -3.00751900 2.33085800  
C -0.22314000 2.11665800 0.35199500  
C -1.39655800 2.61960000 0.91334200  
H -2.37047400 2.38666700 0.49216100  
C -1.32602900 3.43314000 2.04439200  
H -2.22426700 3.83541500 2.50411400  
C -0.08120500 3.70911100 2.58699100  
C 1.09476300 3.20377000 2.05242300  
H 2.05032700 3.44342100 2.51013000  
C 1.01821500 2.39729800 0.91781200  
H 1.93614400 2.02420200 0.47335100  
O 1.24470700 -0.80786000 0.93225200  
C 5.92599100 -0.77412500 -0.00237900  
C 4.61257100 -0.57576100 -0.40716100  
C 3.58133800 -0.82719400 0.50124800  
C 3.86746100 -1.27289300 1.79401100  
C 5.19044600 -1.46693700 2.17798700  
C 6.22956100 -1.21811900 1.28319900  
H 4.37721900 -0.23135600 -1.40886400  
H 3.05066700 -1.46326200 2.48259200  
H 5.42157600 -1.81447300 3.18112500  
H 7.26410200 -1.36647300 1.57765300  
C 2.17342200 -0.60543600 0.07475700  
O 1.90375100 -0.22233300 -1.08903700  
Cl 7.22082200 -0.46087400 -1.12439600  
O -1.08269200 0.71581300 -2.44597100  
C -1.10504900 1.99879300 -2.30268800  
C -2.31583700 2.74606300 -2.40322100  
C 0.07533600 2.69957800 -1.91158400  
C -2.30063100 4.10761400 -2.23521200  
H -3.23154300 2.21029800 -2.63930400

C 0.07021700 4.10709800 -1.80554500  
H 1.01275300 2.15053900 -1.92208800  
C -1.10100100 4.82162100 -1.94020800  
H -3.22718100 4.67051600 -2.33751700  
H 0.99848400 4.62391600 -1.57265500  
C -1.14743900 6.31199700 -1.78989000  
H -1.52618800 6.79166100 -2.70153000  
H -1.81908300 6.60372900 -0.97207200  
H -0.15681800 6.72481400 -1.57569700

#### **TS4a**

Bi -0.57223500 -0.23938300 -0.39811900  
S -3.23802400 -2.06783600 -0.01609400  
O -3.09459600 -0.92560800 -0.95821500  
O -4.47675800 -2.84199500 0.04073500  
C -1.85813000 -3.12405800 -0.41078600  
C -0.64058800 -2.50562500 -0.69876000  
C 0.44530600 -3.29404700 -1.05370100  
H 1.40245200 -2.84049300 -1.29585200  
C 0.29743100 -4.68373600 -1.11310300  
H 1.14707700 -5.29807400 -1.40036700  
C -0.92276800 -5.28577300 -0.81226900  
H -1.02596200 -6.36597700 -0.86409200  
C -2.01953300 -4.50459900 -0.45214000  
H -2.98449100 -4.94926700 -0.22484400  
C -2.84916400 -1.36387200 1.56612400  
C -1.78795900 -0.46105500 1.56594100  
C -1.45576900 0.15233400 2.77013800  
H -0.62674900 0.85386100 2.82223000  
C -2.18755000 -0.13789500 3.92583600  
H -1.92951100 0.35497700 4.86015100  
C -3.24004600 -1.05323200 3.89608600  
H -3.79932500 -1.27095100 4.80180700  
C -3.57989100 -1.68975900 2.70376300  
H -4.39762200 -2.40328000 2.65097700  
C -0.28802300 2.20965000 -0.20821700  
C -1.51139400 2.80002600 0.11951000  
H -2.43936100 2.46095100 -0.33166400  
C -1.54417600 3.83618300 1.04451800  
H -2.48999000 4.30414500 1.30293700  
C -0.35812700 4.26825400 1.65482600  
C 0.86207200 3.65203600 1.33704800  
H 1.77916800 3.98535000 1.81478700  
C 0.89504300 2.62173200 0.40658000

H 1.84736000 2.16802800 0.14938400  
O 1.21490900 -0.52279000 1.03959600  
C 5.90888600 -0.77970700 0.20429200  
C 4.60788400 -0.62363900 -0.25540800  
C 3.55784600 -0.66844700 0.66544100  
C 3.81257300 -0.86840000 2.02456700  
C 5.12362300 -1.02298600 2.46303000  
C 6.18105900 -0.97952000 1.55644600  
H 4.39756200 -0.47012300 -1.30884300  
H 2.98167400 -0.90231700 2.72173100  
H 5.33086800 -1.18003200 3.51789000  
H 7.20645400 -1.09945000 1.89268700  
C 2.16369800 -0.50095700 0.17953500  
O 1.91645100 -0.33836700 -1.04023100  
Cl 7.22718400 -0.72584600 -0.93164600  
O -0.94392900 0.21783600 -2.64758100  
C -0.95750100 1.49908700 -2.81773200  
C -2.13926800 2.18995600 -3.21196000  
C 0.19853800 2.27183700 -2.48553900  
C -2.11895900 3.55654100 -3.36331700  
H -3.03354300 1.60492500 -3.40920600  
C 0.20750100 3.66829000 -2.70285900  
H 1.12483700 1.73550100 -2.29842000  
C -0.94032000 4.30593800 -3.11257300  
H -3.01770300 4.07588500 -3.68806000  
H 1.11551900 4.23306500 -2.50825900  
H -0.94980600 5.38288500 -3.25716700  
C -0.39310200 5.32790200 2.61110100  
N -0.42013000 6.18951400 3.39122800

#### **Int6k**

Bi -0.47354800 -0.61884600 0.34957600  
S -3.48754800 -0.56893800 -1.37323100  
F 3.34444200 -3.91923000 4.17523000  
O -3.73315500 -0.62000900 0.07424200  
O -4.60242600 -0.51953300 -2.32191400  
C -2.45457800 0.86365400 -1.65383700  
C -1.30259000 1.09891000 -0.89948500  
C -0.62773500 2.30356600 -1.03047500  
H 0.26034200 2.50165900 -0.44098600  
C -1.10887700 3.26789400 -1.91983100  
H -0.58648400 4.21734100 -2.00376300  
C -2.24106900 3.02136400 -2.68979200  
H -2.60513000 3.77117200 -3.38648700

C -2.92153600 1.81372500 -2.55976600  
H -3.81867800 1.60390000 -3.13481800  
C -2.50074300 -2.00503600 -1.72277000  
C -1.39844800 -2.26471700 -0.90700200  
C -0.72706700 -3.47220000 -1.06030400  
H 0.13460400 -3.70928000 -0.44131200  
C -1.16257400 -4.39787200 -2.01324900  
H -0.64054400 -5.34575300 -2.11556300  
C -2.25226600 -4.11224500 -2.83151000  
H -2.58131400 -4.83239900 -3.57531800  
C -2.93529100 -2.90550200 -2.68919500  
H -3.80289100 -2.66851300 -3.29812000  
C 0.91850900 -1.77354000 1.69224200  
C 0.62997800 -1.80654500 3.05273800  
H -0.21873800 -1.25942600 3.45042800  
C 1.45776700 -2.54166400 3.90157200  
H 1.26915100 -2.59016500 4.96987000  
C 2.54187400 -3.21036200 3.35527400  
C 2.84007100 -3.18081400 2.00118200  
H 3.70486100 -3.71683800 1.62160900  
C 2.01095100 -2.44715300 1.15328800  
H 2.23542500 -2.40432000 0.09168100  
O 1.24890800 -0.65071100 -1.23136600  
C 5.33970700 1.80073000 -1.47438700  
C 4.13590100 1.52084700 -0.84171500  
C 3.28209500 0.56998200 -1.40599100  
C 3.63462600 -0.08685700 -2.58735200  
C 4.84532200 0.20940600 -3.20551300  
C 5.70739500 1.15484200 -2.65326000  
H 3.85174800 2.02296200 0.07715700  
H 2.95439800 -0.81853800 -3.01122600  
H 5.12588500 -0.29575400 -4.12564800  
H 6.65378600 1.39046500 -3.13053000  
C 1.99218300 0.26684000 -0.73005000  
O 1.64831800 0.88749600 0.30294400  
Cl 6.41284500 2.98380800 -0.77984300  
O -1.52348400 0.05117200 2.13611400  
C -1.78957700 1.37119400 2.20592000  
C -0.78716800 2.28135600 2.57855300  
C -3.06868200 1.86320800 1.91059700  
C -1.06358800 3.64154500 2.65450400  
H 0.21153500 1.90732500 2.79394600  
C -3.33047600 3.22750800 1.99491300  
H -3.83508900 1.16170200 1.59874800

C -2.33925700 4.14346900 2.36416700  
H -0.27057000 4.33036100 2.94186000  
H -4.32924700 3.59013900 1.75688300  
C -2.63763500 5.61187100 2.47513300  
H -2.90671800 5.88632000 3.50436500  
H -1.77118900 6.22158200 2.19429100  
H -3.47681600 5.89990400 1.83236600

### TS<sub>2H2O</sub>

Bi -0.91117400 0.33213800 -0.76535900  
S -3.16069800 -1.89320600 0.41059500  
F 2.16504400 5.62773400 0.70813000  
O -2.67599400 -2.08657600 -0.97129100  
O -4.12540400 -2.81856200 1.00287100  
C -1.69074500 -1.84438000 1.41242200  
C -0.61097300 -1.07865800 0.97065600  
C 0.55125300 -1.04305400 1.73055800  
H 1.39680800 -0.43859900 1.41658200  
C 0.63236900 -1.80362700 2.90080500  
H 1.55015900 -1.78676100 3.48272600  
C -0.44675300 -2.57647100 3.32264800  
H -0.37362500 -3.16670000 4.23161800  
C -1.62719000 -2.59507600 2.58149600  
H -2.48293600 -3.18882100 2.88992200  
C -3.80180100 -0.23142400 0.47394800  
C -3.02105600 0.79737900 -0.06112100  
C -3.53887400 2.08868700 -0.05246100  
H -2.95911200 2.91734500 -0.45305300  
C -4.81321700 2.32977000 0.47076200  
H -5.21291800 3.34058800 0.46275500  
C -5.57110600 1.28844200 1.00126300  
H -6.55984300 1.48352800 1.40685000  
C -5.06508400 -0.01068900 1.01166700  
H -5.63838700 -0.83968900 1.41642100  
C 0.15616500 2.20096500 -0.24778000  
C 1.07919700 2.72430500 -1.15120100  
H 1.27818600 2.22547200 -2.09588700  
C 1.76402100 3.89404300 -0.82902900  
H 2.49169000 4.33107700 -1.50621800  
C 1.50097200 4.49812800 0.39214300  
C 0.58645000 3.99255600 1.30392000  
H 0.41836900 4.50398200 2.24690300  
C -0.09813000 2.82354100 0.97298300  
H -0.81960100 2.41404200 1.67665400



O 1.70028100 -2.58351000 -1.72967700  
C 5.34878300 -0.54994900 0.54123200  
C 4.07651500 -0.47208800 -0.00823500  
C 3.53152500 -1.60272100 -0.62207800  
C 4.26164500 -2.79149000 -0.68354800  
C 5.53661200 -2.84809100 -0.12809500  
C 6.09050300 -1.72835000 0.48952100  
H 3.50506100 0.45007400 0.02464400  
H 3.82493200 -3.66000500 -1.16521800  
H 6.10992900 -3.76991500 -0.17414600  
H 7.08503100 -1.76684300 0.92356800  
C 2.15197000 -1.50956900 -1.18828000  
O 1.53532700 -0.43201400 -1.09460700  
Cl 6.03117700 0.85738000 1.31069600  
H -0.70295400 -1.36059800 -2.86950500  
O -0.99857800 0.00078000 -2.72711300  
O -0.45249800 -2.40794800 -2.82250900  
H -1.15954300 -2.79484900 -2.27919500  
H 0.66856400 -2.48503200 -2.22168200

#### **Int5**

Bi -0.59965800 -0.80157000 -0.05306000  
S 1.40347300 -3.53606600 -0.80142000  
F -5.59042600 1.53238100 2.99163400  
O 2.48845000 -4.49659800 -1.00072800  
O 0.03460700 -3.88335300 -1.22664600  
C 1.81505100 -2.03151700 -1.67126700  
C 0.97846400 -0.91443100 -1.64320300  
C 1.26105000 0.18613700 -2.43652000  
H 0.62165900 1.06168900 -2.41011200  
C 2.38642200 0.16248000 -3.26344400  
H 2.60427700 1.02347300 -3.88980500  
C 3.23137700 -0.94344100 -3.27691800  
H 4.11377100 -0.95031200 -3.91032100  
C 2.94869300 -2.04986700 -2.47995000  
H 3.58774400 -2.92790900 -2.48304000  
C 1.29449400 -3.15205200 0.93579000  
C 0.36203400 -2.21522700 1.38541700  
C 0.19183000 -2.02502300 2.75017700  
H -0.51748700 -1.28755800 3.12095200  
C 0.94999400 -2.77487900 3.65316100  
H 0.81020300 -2.62864800 4.72098800  
C 1.88999600 -3.69274600 3.19302900  
H 2.48678600 -4.26338900 3.89884600

C 2.06947600 -3.88896200 1.82415200  
H 2.78888800 -4.60860500 1.44522100  
C -2.33042800 0.10035000 1.01402000  
C -2.31051800 1.41239200 1.47316900  
H -1.44723200 2.04564200 1.30747200  
C -3.42776000 1.90089300 2.14855800  
H -3.46301700 2.92296400 2.51303800  
C -4.50994300 1.05599700 2.34114400  
C -4.53266100 -0.25602100 1.89315000  
H -5.40648500 -0.87683900 2.06618700  
C -3.42137300 -0.74286300 1.20701600  
H -3.42336700 -1.75367100 0.81047300  
C -2.91589000 1.27903400 -2.04400000  
C -2.55317500 2.62653700 -2.02841200  
C -4.24900600 0.90610300 -1.86695800  
C -3.52851500 3.59919600 -1.83084900  
H -1.50928900 2.89602600 -2.16596000  
C -5.21567000 1.88960200 -1.66904600  
H -4.52216700 -0.14651100 -1.87400200  
C -4.86383700 3.23842000 -1.64726400  
H -3.24099800 4.64787100 -1.81926900  
H -6.25218700 1.59398000 -1.52597000  
H -5.62226400 4.00058900 -1.49053100  
O -1.92641000 0.36039700 -2.22172700  
O -2.05283300 -1.98642200 -1.14351800  
H -1.60123600 -2.78643200 -1.46392200  
O 0.38991300 1.23162200 0.36903800  
C 1.66185000 1.16334500 0.62962900  
O 2.25501300 0.11568900 0.88588600  
C 2.38821800 2.47386200 0.57914100  
C 3.76117500 2.48520300 0.83439600  
C 1.72288900 3.66143700 0.26621200  
C 4.44871900 3.68989900 0.77284400  
H 4.26757900 1.55519100 1.07165000  
C 2.42950500 4.85942300 0.21027400  
H 0.65642400 3.63498400 0.06721300  
C 3.79959200 4.88338700 0.46296100  
H 1.91559200 5.78584900 -0.03227600  
H 4.35815600 5.81353900 0.42037200  
Cl 6.16383700 3.71096100 1.08664500  
H -2.26290100 -0.57302800 -2.14502100

#### **Int6<sub>H2O</sub>**

Bi -0.95101300 0.33246600 -0.80630100

S -3.21494900 -1.83453900 0.44275000  
F 2.35000800 5.48487200 0.71267400  
O -2.76567900 -2.04918800 -0.94781400  
O -4.18732900 -2.73257700 1.06429600  
C -1.72360900 -1.80764900 1.41375400  
C -0.64011400 -1.06303500 0.94519500  
C 0.53146700 -1.03346200 1.69164000  
H 1.37963800 -0.44001500 1.36377700  
C 0.61951100 -1.78189800 2.86909800  
H 1.54490700 -1.76903900 3.43903700  
C -0.46319100 -2.53643300 3.31441200  
H -0.38523700 -3.11733900 4.22898000  
C -1.65440300 -2.54550500 2.59077100  
H -2.51488400 -3.12123500 2.91943800  
C -3.81793500 -0.15798800 0.50654900  
C -3.02989100 0.84936200 -0.05745000  
C -3.51754800 2.15223100 -0.04574200  
H -2.92953400 2.96437100 -0.46767700  
C -4.77167800 2.42591600 0.50924900  
H -5.14850000 3.44548900 0.50417300  
C -5.53813000 1.40585300 1.06802000  
H -6.51086000 1.62641600 1.49852200  
C -5.06103400 0.09577800 1.07579900  
H -5.64139900 -0.71685900 1.50295700  
C 0.18708600 2.15989100 -0.27505100  
C 1.11913500 2.66256500 -1.18135700  
H 1.28455800 2.17359700 -2.13778500  
C 1.85646900 3.79716200 -0.84881400  
H 2.59285400 4.21589600 -1.52822700  
C 1.63462300 4.38979100 0.38598400  
C 0.71073200 3.90693800 1.30059900  
H 0.57507700 4.40886500 2.25386700  
C -0.02513800 2.77259700 0.95884100  
H -0.75425600 2.38192000 1.66510000  
O 1.74832500 -2.68635900 -1.66752300  
C 5.35431500 -0.52292800 0.54533400  
C 4.08923800 -0.47784100 -0.02311100  
C 3.55873700 -1.63923100 -0.59091200  
C 4.29423800 -2.82657800 -0.58919700  
C 5.56228800 -2.84931400 -0.01587200  
C 6.10190100 -1.69906700 0.55642700  
H 3.51154900 0.44095500 -0.03830500  
H 3.87019100 -3.72030100 -1.03458400  
H 6.14100900 -3.76879300 -0.01247700

H 7.09097300 -1.71249700 1.00424000  
C 2.18801000 -1.56864600 -1.16974900  
O 1.55481200 -0.50872900 -1.14106500  
Cl 6.01843300 0.92083900 1.25877300  
H -0.72441400 -1.53465200 -2.86831000  
O -1.01485800 -0.01785000 -2.75809300  
O -0.51210300 -2.53247300 -2.74900300  
H -1.23635000 -2.85267800 -2.18715800  
H 0.78871800 -2.59794500 -2.09263900

### Int6c

Bi 0.39485400 0.54823300 0.49297300  
S 3.57204600 -0.22816700 -0.69875300  
F -3.39485500 4.99458000 2.92523200  
O 3.66588900 0.10884500 0.72741100  
O 4.76526500 -0.61635300 -1.45501400  
C 2.38083700 -1.55751400 -0.81791900  
C 1.12115400 -1.47876700 -0.21720600  
C 0.31253800 -2.60320100 -0.18746700  
H -0.66447100 -2.56509300 0.28126000  
C 0.76560500 -3.79494800 -0.75855400  
H 0.12641300 -4.67381800 -0.71166300  
C 2.01009600 -3.88176400 -1.38244800  
C 2.81797000 -2.73951000 -1.40533400  
H 3.80373100 -2.76576200 -1.86323300  
C 2.84756300 1.20232700 -1.46813700  
C 1.69900000 1.75596900 -0.89829800  
C 1.23834600 2.96585100 -1.40044200  
H 0.34632900 3.43353500 -0.99066700  
C 1.92290700 3.60124500 -2.44020000  
H 1.55531000 4.55616300 -2.80948400  
C 3.06172900 3.03725300 -3.01815000  
C 3.52445800 1.81509000 -2.51309900  
H 4.42075400 1.34930200 -2.91523900  
C -0.98755700 2.10383900 1.34475400  
C -0.86409700 2.41884800 2.69384900  
H -0.14642000 1.89774900 3.31923300  
C -1.68637600 3.40793700 3.23409300  
H -1.62486300 3.68055100 4.28341300  
C -2.59820700 4.03971400 2.40334000  
C -2.72860200 3.73254200 1.05725500  
H -3.46157500 4.25234900 0.44753500  
C -1.90558100 2.74466100 0.51783500  
H -1.99916800 2.48472600 -0.53221900

O -1.10504200 0.40768800 -1.30388000  
C -5.40984500 -1.62931500 -1.66723500  
C -4.27294700 -1.33147900 -0.92814000  
C -3.24089500 -0.61261300 -1.53609400  
C -3.35272200 -0.20083500 -2.86621800  
C -4.50071200 -0.50997600 -3.58903400  
C -5.53820900 -1.22622900 -2.99508900  
H -4.17551200 -1.64389900 0.10623100  
H -2.53756700 0.35280900 -3.32090300  
H -4.59434200 -0.19510300 -4.62473000  
H -6.43628200 -1.47054300 -3.55445000  
C -2.02193300 -0.29331300 -0.74410600  
O -1.90371000 -0.69576500 0.43651100  
Cl -6.70186100 -2.52638600 -0.91855300  
O 1.14390000 0.22253100 2.51326000  
C 1.20774900 -1.05705800 2.93035800  
C 0.03886200 -1.74585200 3.29520500  
C 2.44356500 -1.71550900 3.01791700  
C 0.10777200 -3.06356800 3.73682100  
H -0.91892400 -1.23558200 3.21734200  
C 2.50219100 -3.03279100 3.46538400  
H 3.33734100 -1.18063100 2.71468000  
C 1.33907800 -3.71624300 3.82249100  
H -0.80613900 -3.58466900 4.01378800  
H 3.46651600 -3.53254100 3.52678200  
H 1.39069600 -4.74678100 4.16472500  
C 3.79072300 3.71446100 -4.14136500  
H 4.82779900 3.93420000 -3.86093800  
H 3.82486200 3.07374600 -5.03070600  
H 3.30864800 4.65637400 -4.42029100  
C 2.49338900 -5.16011700 -2.00157600  
H 2.74702700 -5.01550900 -3.05840700  
H 3.39776000 -5.52164600 -1.49737600  
H 1.73427900 -5.94560600 -1.93847500

#### **TS4j**

Bi -0.57337700 -0.23732000 -0.36422000  
S -3.22299000 -2.14098900 -0.26341400  
F -0.06889000 4.43882900 3.73203500  
O -3.11007500 -0.84736600 -0.98857200  
O -4.45719800 -2.92373400 -0.31696500  
C -1.84802100 -3.09774200 -0.87025300  
C -0.64209000 -2.42414500 -1.06735800  
C 0.44053500 -3.12986600 -1.57602300

H 1.39057100 -2.63248900 -1.75197100  
C 0.30110400 -4.48910300 -1.87480000  
H 1.14870800 -5.03561500 -2.28086000  
C -0.90858300 -5.14729100 -1.66002900  
H -1.00510500 -6.20319300 -1.89691000  
C -2.00238000 -4.45185400 -1.14759000  
H -2.95916200 -4.93896000 -0.98048900  
C -2.79910800 -1.72982200 1.41101300  
C -1.74264200 -0.83247900 1.55029100  
C -1.38687400 -0.44383300 2.83877300  
H -0.56399500 0.24936100 2.99698900  
C -2.08805600 -0.94712100 3.93873400  
H -1.81072600 -0.63013000 4.94133200  
C -3.13584600 -1.85241400 3.76670500  
H -3.67205600 -2.23681900 4.63002200  
C -3.50097100 -2.26417600 2.48631200  
H -4.31550400 -2.96429100 2.32226500  
C -0.23037300 2.13383000 0.34659100  
C -1.41259600 2.62750300 0.89828600  
H -2.37991200 2.40439600 0.45687800  
C -1.35946600 3.41604000 2.04743100  
H -2.26444900 3.81098400 2.50002300  
C -0.12319000 3.67823900 2.61645100  
C 1.06087000 3.18458600 2.08900600  
H 2.00920000 3.41433200 2.56634400  
C 1.00249500 2.40257300 0.93622700  
H 1.92728300 2.03761000 0.49915500  
O 1.25337000 -0.79483900 0.93615600  
C 5.93431200 -0.75298200 -0.00117200  
C 4.62026400 -0.55772300 -0.40539000  
C 3.59017100 -0.80882800 0.50448400  
C 3.87778000 -1.25114900 1.79813800  
C 5.20137500 -1.44190000 2.18154700  
C 6.23933100 -1.19341100 1.28534300  
H 4.38373800 -0.21621000 -1.40779700  
H 3.06198200 -1.44152100 2.48788800  
H 5.43387900 -1.78656000 3.18533500  
H 7.27432200 -1.33924000 1.57946500  
C 2.18225100 -0.59007200 0.07858000  
O 1.91019100 -0.20692200 -1.08471400  
Cl 7.22755700 -0.44047200 -1.12476800  
O -1.04698000 0.71959300 -2.45740900  
C -1.08333900 1.99964000 -2.31586400  
C -2.30091400 2.73343900 -2.45519400

C 0.08426100 2.70741200 -1.88797200  
C -2.31130900 4.09677400 -2.29829700  
H -3.20304800 2.18763600 -2.71650000  
C 0.07838200 4.11697000 -1.79472800  
H 1.02632300 2.16721800 -1.88903000  
C -1.11108000 4.76587100 -1.97317000  
H -3.21950900 4.67916700 -2.42629900  
H 0.97739500 4.67034900 -1.54231800  
F -1.16472100 6.10892400 -1.85336800

## TS2

Bi -0.94503600 -0.47070900 -0.18525600  
S -4.10110600 -1.15355900 0.68243700  
F 2.52434900 4.68912100 -1.29193200  
O -3.18000800 -2.28998400 0.53491500  
O -5.50281900 -1.33430900 1.05069300  
C -3.31715200 -0.07018300 1.85878400  
C -1.94994400 0.17382000 1.72040200  
C -1.30047700 0.97722800 2.64730800  
H -0.24284500 1.20444300 2.53988400  
C -2.02052700 1.49288700 3.72832900  
H -1.51071400 2.10586600 4.46613000  
C -3.38150000 1.23358000 3.86301800  
H -3.93154300 1.64146300 4.70564000  
C -4.04632400 0.45171800 2.92004200  
H -5.10671800 0.23514200 3.00636900  
C -4.01167900 -0.28594200 -0.87285300  
C -2.75667100 -0.07260400 -1.44713300  
C -2.66682800 0.53350800 -2.69292400  
H -1.69883000 0.72513300 -3.14821400  
C -3.83868400 0.89298100 -3.36461900  
H -3.77112200 1.35088200 -4.34729400  
C -5.08460500 0.67127800 -2.78577600  
H -5.98859900 0.95490800 -3.31620500  
C -5.18098400 0.08083500 -1.52686300  
H -6.14230800 -0.10983500 -1.05976500  
C 0.31521200 1.32223800 -0.60704900  
C -0.33305000 2.53929300 -0.82143900  
H -1.41812200 2.60733000 -0.80984400  
C 0.41745700 3.68717700 -1.05774600  
H -0.05349400 4.64956200 -1.23098800  
C 1.80220900 3.58533900 -1.06696900  
C 2.46250600 2.38506700 -0.84785200  
H 3.54746900 2.35249000 -0.85709700

C 1.70659700 1.23914700 -0.61576900  
H 2.20936600 0.29575300 -0.42839700  
O 0.00847400 -2.20102300 -0.33875100  
O 3.06878700 -2.90836200 -1.59247300  
C 3.30307900 -2.19399000 -0.63698600  
C 4.66286900 -1.61757400 -0.38834300  
O 2.41585500 -1.81792000 0.26735200  
C 5.69553700 -1.93371500 -1.27174900  
C 4.89695400 -0.74984000 0.68055000  
C 6.95890600 -1.38433600 -1.09040300  
H 5.48480700 -2.60868700 -2.09480700  
C 6.16449300 -0.20499100 0.84026400  
H 4.09792500 -0.50928500 1.37239700  
C 7.20393400 -0.51131300 -0.03290100  
H 7.76471300 -1.62991900 -1.77609100  
Cl 6.45773100 0.89238200 2.16481200  
H 8.18609800 -0.07361000 0.11388400  
H 1.43875600 -2.07533200 -0.01458200

## TS4b

Bi -0.59950100 0.05837000 -0.31485800  
S -3.33123100 -1.74592800 -0.34592800  
O -3.17211600 -0.41834600 -0.99446500  
O -4.58952600 -2.48501500 -0.44958600  
C -1.98654800 -2.71241000 -1.00307000  
C -0.75542100 -2.07318100 -1.15413800  
C 0.30084400 -2.78453000 -1.70875300  
H 1.26929900 -2.31272800 -1.85059200  
C 0.11086100 -4.11396000 -2.09905800  
H 0.93811100 -4.66314600 -2.54185000  
C -1.12331900 -4.73884700 -1.92909900  
H -1.25945400 -5.77187700 -2.23683700  
C -2.19095400 -4.03801400 -1.37105900  
H -3.16629200 -4.49789100 -1.23781700  
C -2.90692400 -1.44729100 1.35211400  
C -1.82169600 -0.59661800 1.55008000  
C -1.46918700 -0.28958400 2.86151300  
H -0.62653700 0.36695600 3.06558600  
C -2.20051300 -0.82632400 3.92536800  
H -1.92474300 -0.57318000 4.94644500  
C -3.27663200 -1.68409200 3.69428300  
H -3.83616600 -2.09537100 4.53001700  
C -3.64051700 -2.01276300 2.38982100  
H -4.47780300 -2.67250700 2.17964200

C -0.15647800 2.35925600 0.52876900  
C -1.32900600 2.88291300 1.06843300  
H -2.29259500 2.72911300 0.59047000  
C -1.25410500 3.61431000 2.25496200  
H -2.16645600 4.02496600 2.68152200  
C -0.02937300 3.80583800 2.89241200  
C 1.13082900 3.26090500 2.34213600  
H 2.09173500 3.40496400 2.83107900  
C 1.07470200 2.53355300 1.15256700  
H 1.98852600 2.14017900 0.71668100  
O 1.18166500 -0.68002800 0.96717200  
C 5.86668300 -0.84208200 0.06106000  
C 4.56962400 -0.54375900 -0.33484800  
C 3.51938000 -0.79208300 0.55238000  
C 3.77062400 -1.33232900 1.81599400  
C 5.07784000 -1.62454800 2.19189000  
C 6.13563400 -1.38128200 1.31762700  
H 4.36161100 -0.12480900 -1.31394100  
H 2.93932000 -1.51787800 2.48835300  
H 5.28190700 -2.04638000 3.17215900  
H 7.15805000 -1.60689000 1.60554900  
C 2.12921800 -0.46855700 0.13305200  
O 1.89215000 0.00384400 -1.00482000  
Cl 7.18429900 -0.53650600 -1.03619800  
O -1.00724100 1.11300800 -2.35941600  
C -0.96718400 2.39092400 -2.17035400  
C -2.12964900 3.20424000 -2.30518300  
C 0.23340400 3.00471100 -1.69706200  
C -2.05185300 4.55975200 -2.08851600  
H -3.05698000 2.72502100 -2.60765700  
C 0.29948000 4.40698400 -1.53533900  
H 1.14002700 2.40598900 -1.69910100  
C -0.83057300 5.17229100 -1.70599900  
H -2.93728200 5.17786700 -2.21912500  
H 1.23917600 4.86588300 -1.23916000  
H -0.79416600 6.24818200 -1.55722200  
H 0.02130800 4.37607300 3.81622800

## 6

F -4.53668200 -0.85132900 -0.04564600  
C -0.73608800 0.69165500 -0.08930400  
C -1.69062900 1.23735100 0.76419000  
H -1.41593600 2.06585900 1.41027800  
C -2.98444700 0.72008100 0.77922700

H -3.74803300 1.12766700 1.43461600  
C -3.28412400 -0.33967200 -0.06083800  
C -2.34734500 -0.89540800 -0.91963300  
H -2.62732200 -1.71996000 -1.56820900  
C -1.05961200 -0.36818400 -0.93699800  
H -0.30818400 -0.77908200 -1.60505200  
O 0.50298100 1.28463800 -0.12387800  
C 1.62614600 0.50363300 -0.01349200  
C 1.64949500 -0.68793500 0.71167600  
C 2.78425900 0.99346800 -0.61554800  
C 2.84676600 -1.39340900 0.81908000  
H 0.74681000 -1.05841300 1.18845500  
C 3.97403200 0.28104900 -0.49390100  
C 4.01160700 -0.91718400 0.21942900  
H 2.86503000 -2.32159100 1.38492300  
H 4.87544000 0.66453800 -0.96526800  
H 4.94076200 -1.47329100 0.30889500  
H 2.73736400 1.92647600 -1.17013600

## Int1

Bi 1.43696900 0.35147900 1.16314200  
S 3.41949300 -1.95708500 -0.25116500  
F -2.39582100 4.76137200 -1.46435700  
O 3.36180900 -1.83766500 1.22146000  
O 4.27984600 -2.96303200 -0.87940600  
C 1.73412300 -2.17775900 -0.78675300  
C 0.77909400 -1.30055100 -0.27008500  
C -0.53435200 -1.45592300 -0.70914700  
H -1.30363100 -0.76472700 -0.37822500  
C -0.87310400 -2.47245100 -1.60534800  
H -1.90643600 -2.57982600 -1.92719300  
C 0.10267900 -3.33878400 -2.09523900  
H -0.16462800 -4.12849200 -2.79191400  
C 1.42925400 -3.18572200 -1.69643300  
H 2.21391300 -3.83644200 -2.07218700  
C 3.83774100 -0.33292100 -0.85578700  
C 3.12555800 0.74703000 -0.33107800  
C 3.45895800 2.01972600 -0.79367500  
H 2.91817000 2.89204300 -0.43214500  
C 4.47625300 2.18859600 -1.73690500  
H 4.72565000 3.18881800 -2.08319700  
C 5.16673300 1.08835400 -2.24350400  
H 5.95553400 1.22693900 -2.97788100  
C 4.84280600 -0.19507000 -1.80831500

H 5.36013500 -1.07169900 -2.18797800  
C 0.08834900 1.89526000 0.17153300  
C -0.17036900 1.91743400 -1.20416700  
H 0.27904100 1.17444900 -1.85960500  
C -1.00596900 2.88168600 -1.76701500  
H -1.21650600 2.90435600 -2.83266400  
C -1.57418300 3.82823100 -0.92773600  
C -1.34073700 3.85317800 0.43750200  
H -1.80574200 4.61588800 1.05581500  
C -0.50300400 2.87424300 0.97800500  
H -0.32622600 2.88550400 2.05283300  
O -1.16271700 -0.59031600 3.21982600  
O -2.02389700 -0.04994300 2.23380700  
C -2.91212100 -0.97223800 1.80401800  
C -3.78045600 -0.45528900 0.73028000  
O -2.93047300 -2.09153500 2.27828400  
C -3.63136800 0.83409400 0.20869600  
C -4.74391700 -1.33001500 0.21947100  
C -4.45962000 1.24660900 -0.82912400  
H -2.87177800 1.50369000 0.59823300  
C -5.55702900 -0.89373600 -0.81713300  
H -4.84277300 -2.32982900 0.62949500  
C -5.42633200 0.38865200 -1.34844400  
H -4.35080300 2.24493200 -1.24272400  
Cl -6.75720000 -1.96968900 -1.46773800  
H -6.07189000 0.70873000 -2.16065700  
H -1.50805800 -1.51726700 3.28513200

#### TS4d

Bi -0.52160700 -0.35263900 -0.45193000  
S -3.05240600 -2.37261500 0.00377100  
O -2.98891300 -1.28164500 -1.00435800  
O -4.22904500 -3.23720900 0.09722000  
C -1.59010500 -3.34133600 -0.31113500  
C -0.41890100 -2.64719800 -0.61649300  
C 0.72820300 -3.37429000 -0.90843400  
H 1.65536600 -2.86611400 -1.16021700  
C 0.68572100 -4.77209100 -0.88986600  
H 1.58400100 -5.33636500 -1.12835500  
C -0.49192100 -5.44681000 -0.57252300  
H -0.51334600 -6.53303700 -0.56295800  
C -1.64943000 -4.73051100 -0.27357700  
H -2.58281300 -5.23228500 -0.03351100  
C -2.74402700 -1.54889500 1.54663400

C -1.75730600 -0.56673400 1.50423200  
C -1.49989700 0.14347900 2.67409300  
H -0.73573700 0.91732200 2.69073400  
C -2.22504400 -0.13706500 3.83598900  
H -2.02282200 0.42821100 4.74290300  
C -3.20015200 -1.13542300 3.84847600  
H -3.75516300 -1.34525200 4.75883100  
C -3.46783900 -1.86503400 2.69173600  
H -4.22570800 -2.64338200 2.67034600  
C -0.39260100 2.11823100 -0.30410200  
C -1.64331500 2.63513000 0.01132300  
H -2.55042300 2.23745600 -0.43549800  
C -1.75040600 3.68167500 0.93079800  
H -2.73602500 4.06696400 1.17069200  
C -0.60083800 4.19980100 1.53299100  
C 0.65342900 3.66378600 1.21085300  
H 1.54056400 4.07603200 1.68449300  
C 0.75976200 2.62769300 0.29283100  
H 1.74377700 2.24610000 0.03632500  
O 1.25725000 -0.47341200 1.02238100  
C 5.97609200 -0.36189800 0.30471300  
C 4.67873000 -0.33586800 -0.18957500  
C 3.61273700 -0.43102000 0.70854000  
C 3.84920800 -0.55129700 2.08015200  
C 5.15713400 -0.57638100 2.55361700  
C 6.23032800 -0.48151800 1.66964200  
H 4.48253600 -0.24412500 -1.25286300  
H 3.00618700 -0.62450200 2.75954700  
H 5.34978700 -0.67067200 3.61874900  
H 7.25336600 -0.50020200 2.03294200  
C 2.22115900 -0.39879400 0.18322000  
O 1.99752700 -0.29607600 -1.04664500  
Cl 7.31393400 -0.24222500 -0.80434100  
O -0.90163900 0.01395100 -2.73353200  
C -1.00235300 1.28774800 -2.92349400  
C -2.22786700 1.89021300 -3.33233200  
C 0.09494900 2.14575400 -2.60105800  
C -2.29935100 3.25047800 -3.51883700  
H -3.08020500 1.24153300 -3.51655000  
C 0.01195100 3.53334700 -2.85739700  
H 1.05412800 1.67914700 -2.39382900  
C -1.17313300 4.08243900 -3.28810900  
H -3.22998200 3.69972800 -3.85843100  
H 0.87924000 4.16227300 -2.67381800

H -1.25244300 5.15217300 -3.46291100  
O -0.59949300 5.20824400 2.43639900  
C -1.84119000 5.79142900 2.77766800  
H -2.51405500 5.05882100 3.24202700  
H -1.61398500 6.57834700 3.49937000  
H -2.32909600 6.23549300 1.90041100

### TS7

Bi 0.42592800 -0.16057300 -0.08233400  
C 3.55977900 -0.77125100 -0.08245700  
C 2.32116400 -1.40215600 -0.17078400  
C 2.22890300 -2.78345800 -0.32434100  
H 1.26150700 -3.27510600 -0.39582800  
C 3.39690400 -3.54444300 -0.38961900  
C 4.64210700 -2.92342400 -0.30092700  
H 5.55063500 -3.51842900 -0.35202400  
C 4.72357700 -1.54045200 -0.14787900  
H 5.69354600 -1.05320200 -0.08024300  
C 1.78087800 2.36234400 1.31893900  
C 1.28892600 1.91202800 0.09167300  
C 1.30650200 2.74993500 -1.02441000  
H 0.92724900 2.40428300 -1.98310300  
C 1.82236600 4.04169600 -0.91047100  
H 1.83705100 4.69263800 -1.78165100  
C 2.31775100 4.49432300 0.31147800  
H 2.71950800 5.50116400 0.39662100  
C 2.29830100 3.65446600 1.42412300  
H 2.68603200 4.00179200 2.37905900  
C -2.08051900 0.63982000 0.12515500  
C -2.62166800 0.73694600 -1.14435400  
H -2.65194800 -0.10984200 -1.82205600  
C -3.11010000 1.98401300 -1.53932100  
H -3.52285500 2.09125000 -2.53953100  
C -3.05822200 3.07621100 -0.67400300  
C -2.50877700 2.93196900 0.59934400  
H -2.45399200 3.77939000 1.27844200  
C -2.01336000 1.69710500 1.02172100  
H -1.57566300 1.57733400 2.00927600  
C -2.25959600 -2.14990600 0.53324800  
C -2.98151700 -2.77233600 -0.49315800  
C -2.82054700 -1.06210400 1.25139100  
C -4.30229900 -2.41679400 -0.68854900  
H -2.50127000 -3.54050900 -1.09158700  
C -4.21523400 -0.80874400 1.10413800

H -2.30356400 -0.72077000 2.14491700  
C -4.93656800 -1.45374600 0.13274000  
H -4.87174700 -2.90543400 -1.47489100  
H -4.67173000 -0.04270300 1.72416800  
H -5.98851800 -1.22914500 -0.01592300  
O -0.99923800 -2.52980000 0.74235000  
H -0.63526300 -2.11539100 1.57211400  
H 3.63311200 0.30778300 0.03259600  
H 1.76460500 1.71742000 2.19426900  
Cl 0.33477100 -0.61711000 2.67402100  
H 3.33103300 -4.62319600 -0.51092800  
Cl 0.20523400 -0.16686400 -2.67023100  
H -3.43846700 4.04194600 -0.99527000

### TS8

Bi 0.70637800 -0.37854100 -0.27353300  
C -1.60845800 -2.61898400 -0.13068300  
C -1.13036200 -1.57751100 -0.92531000  
C -1.78277500 -1.24715800 -2.11200400  
H -1.39626900 -0.45431300 -2.74796500  
C -2.93073700 -1.94683100 -2.49249000  
C -3.41987100 -2.97949700 -1.69297200  
H -4.30967700 -3.52797900 -1.99406000  
C -2.75323500 -3.31995900 -0.51599000  
H -3.11798900 -4.13765100 0.10259800  
C 2.11461300 -2.89486200 1.21450200  
C 2.20902200 -2.07117100 0.09108200  
C 3.26153200 -2.24698000 -0.80911600  
H 3.34916500 -1.61125900 -1.68657900  
C 4.20959200 -3.24798800 -0.59004100  
H 5.02724100 -3.37706200 -1.29605000  
C 4.10950400 -4.07757800 0.52547800  
H 4.84826500 -4.85780500 0.69415400  
C 3.06098500 -3.89985200 1.42664200  
H 2.97862000 -4.53970900 2.30289300  
C 2.32938900 1.38505400 0.55101300  
C 3.17087200 1.81918800 -0.46964700  
H 2.77571600 2.12413500 -1.43248100  
C 4.54811500 1.83042400 -0.24399000  
H 5.20987600 2.15550900 -1.04400800  
C 5.07253200 1.42336900 0.98187300  
C 4.21097800 0.99419200 1.99119700  
H 4.60675500 0.66697900 2.95024700  
C 2.83213600 0.97171600 1.78354100

H 2.16490600 0.62917500 2.56995200  
C 0.01818800 2.66908500 -0.32195100  
C 0.35427100 3.61438800 -1.33144200  
C 0.65102400 2.79882700 0.95635500  
C 1.14514900 4.69931000 -1.02817200  
H -0.04664100 3.46203000 -2.33005500  
C 1.38614400 3.97342800 1.26392900  
H 0.29575900 2.15640200 1.75837600  
C 1.65525600 4.89479200 0.28163300  
H 1.37740600 5.42789500 -1.80207300  
H 1.78472300 4.09991700 2.26736600  
H 2.25601300 5.77407400 0.49863900  
O -0.73583000 1.64917200 -0.56464200  
H -2.19641300 1.30687200 0.38267800  
H -1.10411900 -2.88703900 0.79414000  
H 1.31634600 -2.75116300 1.93838400  
Cl -0.25469500 -0.60510700 2.30778600  
H -3.43615500 -1.68829000 -3.42089000  
Cl 1.42331400 -0.04801500 -2.76848500  
H 6.14672400 1.43264800 1.14753400  
H -2.31725600 0.07162000 1.54812400  
N -2.82437800 0.74503500 0.97430000  
C -4.12595800 0.63557100 0.77288200  
N -4.87799300 -0.09007000 1.63330100  
N -4.71578900 1.25385000 -0.26828700  
C -4.31286200 -0.50925900 2.90365800  
C -5.97728600 -0.91676200 1.15879000  
C -6.06985600 1.77466000 -0.18782100  
C -3.92072700 1.78041300 -1.36372200  
H -3.69332700 -1.41108900 2.79852600  
H -3.70949200 0.29046200 3.33908900  
H -5.13739000 -0.73070500 3.58711600  
H -6.90257500 -0.68656900 1.69894700  
H -6.13712900 -0.77394000 0.08993200  
H -5.72672200 -1.97241400 1.32230700  
H -6.71553000 1.31568800 -0.94543600  
H -6.49392500 1.59961100 0.80153000  
H -6.04462900 2.85727100 -0.36325900  
H -3.58621000 2.80711500 -1.16189600  
H -3.04965000 1.15182100 -1.54970200  
H -4.54164000 1.78453300 -2.26434800

**3**

Bi -0.08226000 -1.06447200 0.45229000

C 0.47792600 -1.01746700 -2.64536600  
C 1.05532000 -0.66913000 -1.42955800  
C 2.31196100 -0.08079500 -1.34175900  
H 2.73792100 0.20413100 -0.38456500  
C 3.01654800 0.15641600 -2.52296000  
C 2.45574300 -0.17531300 -3.75497100  
H 3.00724900 0.01991800 -4.67103500  
C 1.19010900 -0.75578400 -3.81669400  
H 0.75001100 -1.01399500 -4.77641100  
C 1.37444900 -3.50602400 1.80936600  
C 0.84822600 -2.25191500 2.09875900  
C 0.87569700 -1.70983800 3.37901200  
H 0.47877600 -0.71986400 3.58332100  
C 1.44705000 -2.46224700 4.40617400  
H 1.46965900 -2.05689900 5.41442500  
C 1.98957800 -3.71808200 4.13941800  
H 2.43924700 -4.29546400 4.94303700  
C 1.95765700 -4.23619700 2.84596300  
H 2.38088100 -5.21499600 2.63546100  
C -2.16058800 -0.27787900 0.71737100  
C -2.36980200 1.09651300 0.68309800  
H -1.54581600 1.79020400 0.54680100  
C -3.67077400 1.57420700 0.84810300  
H -3.85221800 2.64545300 0.81709600  
C -4.72486500 0.68684200 1.05725800  
C -4.48848700 -0.68604800 1.09520800  
H -5.30821800 -1.38082900 1.25884000  
C -3.19687500 -1.18360700 0.91640400  
H -3.01813900 -2.25445300 0.92015500  
H -0.49631100 -1.49454700 -2.69326400  
H 1.32534100 -3.92302500 0.80797500  
Cl -1.02101500 -3.27210000 -0.60037600  
H 4.00401700 0.60782200 -2.47222400  
Cl 0.90493600 1.12712300 1.49374200  
H -5.73447200 1.06670000 1.19078500

**Int11**

Bi -1.07679000 -0.32075900 0.15217600  
C 0.79415700 -2.85302300 0.21701000  
C 0.52598400 -1.69451400 0.93523000  
C 1.17064400 -1.40110400 2.12897400  
H 0.92538200 -0.49962600 2.68235600  
C 2.13947800 -2.28819400 2.60215100  
C 2.44209900 -3.44655000 1.88603900



H 3.19505900 -4.13553800 2.26133700  
C 1.76656900 -3.73230700 0.70035400  
H 1.98514400 -4.64448900 0.14968900  
C -3.55140800 -1.69705100 -1.32462200  
C -2.70223400 -1.84678400 -0.23007600  
C -2.85112900 -2.92569600 0.63896800  
H -2.19717700 -3.03846400 1.50172900  
C -3.85676900 -3.86573800 0.40793900  
H -3.97562400 -4.70766300 1.08621300  
C -4.70931300 -3.72075000 -0.68610700  
H -5.49409100 -4.45220200 -0.86398000  
C -4.55821200 -2.63727300 -1.55113800  
H -5.22242400 -2.52212200 -2.40467900  
C -2.08926700 1.54880100 -0.58299400  
C -3.29949600 1.88685200 0.00535700  
H -3.72685500 1.28691000 0.80434800  
C -3.95482900 3.03622300 -0.44212500  
H -4.90449300 3.31818700 0.00601000  
C -3.38895900 3.81875600 -1.44689400  
C -2.17200600 3.45343000 -2.02069500  
H -1.72623700 4.06658600 -2.79998300  
C -1.50982100 2.30235000 -1.59275200  
H -0.56570000 2.00738400 -2.03813100  
C 0.78188300 2.50249000 0.58076200  
C 0.01254300 3.14589200 1.57070800  
C 1.52731600 3.31192500 -0.30376100  
C -0.01282400 4.53372500 1.66151700  
H -0.57422300 2.53158500 2.24886000  
C 1.50529200 4.69932000 -0.19533700  
H 2.10674200 2.83182000 -1.09056500  
C 0.73275500 5.32500700 0.78484400  
H -0.62666800 5.00410300 2.42735700  
H 2.08828200 5.29910600 -0.89235800  
H 0.70829400 6.40912200 0.86124000  
O 0.81398600 1.18006600 0.48274200  
H 2.09579100 0.53930200 -0.32144100  
H 0.26862700 -3.07421200 -0.70867100  
H -3.43372000 -0.85737200 -2.00723400  
Cl -0.12429400 -0.75612400 -2.32547500  
H 2.65428500 -2.07069000 3.53526700  
Cl -1.91710500 0.05071100 2.59180300  
H -3.89719400 4.71915700 -1.78293200  
H 2.15742100 -0.69915900 -1.50935900  
N 2.70088700 -0.09170800 -0.90375200

C 3.99812000 -0.27326000 -0.76164000  
N 4.67515300 -1.03482300 -1.65948700  
N 4.67277700 0.30782900 0.25052400  
C 4.03483000 -1.40335900 -2.90892200  
C 5.73211000 -1.93908200 -1.23349800  
C 6.05156100 0.74195400 0.10534000  
C 3.96451500 0.89994100 1.37249500  
H 3.35471300 -2.25973700 -2.78978900  
H 3.47722300 -0.55861800 -3.32006000  
H 4.81482400 -1.67982100 -3.62387400  
H 6.64518800 -1.77719900 -1.81754900  
H 5.95514300 -1.80468500 -0.17480000  
H 5.40166100 -2.97586300 -1.37927200  
H 6.70321800 0.24206100 0.83164600  
H 6.41584000 0.54303600 -0.90308700  
H 6.10226200 1.82337500 0.28197900  
H 3.73456700 1.95746800 1.18944600  
H 3.03503800 0.36575200 1.56737600  
H 4.60190000 0.82595900 2.25902700

#### **BiPh<sub>2</sub>Cl**

Bi 0.20098000 -1.46163600 0.89157400  
C 0.40157600 -1.10835200 -2.24142400  
C 0.97224900 -0.62567600 -1.05859800  
C 2.01100500 0.30455900 -1.12546800  
H 2.45928600 0.69583500 -0.21479300  
C 2.46902000 0.75408300 -2.36556200  
C 1.89696700 0.27251000 -3.54206500  
H 2.25531600 0.62451500 -4.50630800  
C 0.86171200 -0.65970000 -3.47980600  
H 0.40804000 -1.03509500 -4.39417900  
C -1.80217200 -0.44575700 0.69994500  
C -1.99795400 0.67642400 -0.11116700  
H -1.16788600 1.10113700 -0.67126400  
C -3.26084700 1.26005700 -0.20523500  
H -3.40620200 2.13506500 -0.83451600  
C -4.33540600 0.72389500 0.50518900  
C -4.14722700 -0.39525600 1.31433000  
H -4.98241300 -0.81381200 1.87111900  
C -2.88262100 -0.97794800 1.41213200  
H -2.74960500 -1.84817400 2.05398700  
H -0.41832100 -1.82578200 -2.21373300  
H 3.27416700 1.48397900 -2.40986600  
Cl 1.27278900 0.31847900 2.31212500

H -5.31943500 1.17999600 0.42873600

### TS9

Bi -0.34110400 0.32780400 -0.70265100  
C -3.50650900 -0.33028700 -0.88134400  
C -2.35178000 -0.61462600 -0.15371900  
C -2.40878600 -1.47398200 0.94753100  
H -1.51743100 -1.71508400 1.52192800  
C -3.62895500 -2.03841900 1.32410100  
H -3.66981800 -2.70354200 2.18392300  
C -4.78519500 -1.75359700 0.59954200  
H -5.73405700 -2.19650600 0.89232600  
C -4.72298500 -0.90105200 -0.50159500  
H -5.62262300 -0.67470600 -1.06927500  
C 0.69457700 2.90482300 0.78542100  
C -0.15384100 1.81289700 0.97107500  
C -0.85816400 1.65765700 2.16536800  
H -1.53774700 0.82038500 2.30758900  
C -0.69870600 2.59624600 3.18603900  
H -1.24700100 2.47807400 4.11777800  
C 0.15229800 3.68643700 3.00730200  
H 0.27023000 4.41874200 3.80228900  
C 0.84406200 3.84377800 1.80688600  
H 1.49815100 4.70030800 1.66138500  
C 1.00633600 -1.56780500 0.06922500  
C 1.37847100 -1.32680000 1.39691700  
H 1.78681800 -0.36567200 1.69674700  
C 1.22651800 -2.33834700 2.34776700  
H 1.50822900 -2.14340200 3.38005700  
C 0.72468400 -3.58476500 1.97887900  
C 0.35220800 -3.81810400 0.65237700  
H -0.05177700 -4.78422600 0.35902100  
C 0.48022300 -2.81269100 -0.30052900  
H 0.17505500 -3.00231900 -1.32712000  
O 1.74332100 0.99930200 -1.74296600  
C 2.64876200 0.28323500 -1.17929100  
C 3.57453700 0.82060400 -0.23253600  
C 2.66670100 -1.13608400 -1.39477200  
C 4.53729600 0.01584200 0.32719600  
H 3.52372600 1.88237700 -0.00829600  
C 3.71661000 -1.92574600 -0.86362800  
H 2.05749500 -1.52127200 -2.20696800  
C 4.61976000 -1.36571300 0.00636300  
H 5.26101800 0.44302300 1.01772100

H 3.76756300 -2.98229800 -1.11328500

H 5.40761400 -1.97076400 0.44697000

H 0.61896700 -4.37204900 2.72071200

H -3.46873300 0.33942300 -1.73684800

H 1.22877500 3.03004500 -0.15368200

Cl -1.34930000 1.84213700 -2.50686200

### TS8<sub>o</sub>

Bi 1.28529400 0.06069400 -0.11648600  
C 0.48175800 -2.98231200 -0.68814400  
C 0.28638700 -1.68420500 -1.15709800  
C -0.54124600 -1.44094900 -2.25067500  
H -0.67313400 -0.43008300 -2.62837600  
C -1.19507200 -2.50738900 -2.87094200  
C -1.01460200 -3.80795400 -2.40120600  
H -1.52023300 -4.63805400 -2.88923900  
C -0.17238100 -4.04502300 -1.31495400  
H -0.01559400 -5.05970600 -0.95522800  
C 4.07717400 -1.11859000 -1.12092100  
C 3.43841800 -0.62835900 0.01751700  
C 4.11852800 -0.54646000 1.23199800  
H 3.62027800 -0.17818600 2.12551300  
C 5.44920000 -0.96166000 1.30643100  
H 5.98137200 -0.89638700 2.25270400  
C 6.09047300 -1.46164400 0.17403600  
H 7.12609600 -1.78755500 0.23504300  
C 5.40448200 -1.54243500 -1.03724400  
H 5.90175300 -1.93119500 -1.92298300  
C 0.45944900 2.14482400 0.88322800  
C 0.84207400 3.27761400 0.18259200  
H 0.98329700 3.25705600 -0.89369600  
C 1.04097300 4.45151500 0.91228500  
H 1.35135400 5.34878900 0.38179300  
C 0.84177300 4.47886000 2.29179300  
C 0.44283300 3.31746300 2.95286500  
H 0.27980300 3.32448600 4.02847500  
C 0.24262000 2.12572400 2.25216400  
H -0.05683300 1.21828600 2.76561600  
C -1.94842500 2.27957400 -0.53027600  
C -1.86478100 2.71129500 -1.86860100  
C -2.87441800 2.91542400 0.32194100  
C -2.70398900 3.71568600 -2.34153900  
H -1.12652500 2.24377400 -2.51590000  
C -3.70320500 3.92460700 -0.15812000

H -2.91953100 2.60458400 1.36351900  
C -3.63079600 4.32681400 -1.49393400  
H -2.62790300 4.03154300 -3.38007000  
H -4.40963100 4.40549400 0.51566900  
H -4.28011100 5.11498800 -1.86663400  
O -1.16242000 1.31022700 -0.07620400  
H -2.04412400 0.01024200 0.72637100  
H 1.13027200 -3.17262000 0.16313600  
H 3.55456400 -1.16759600 -2.07335100  
Cl 0.82489800 -1.25135000 2.25868000  
H -1.83989800 -2.31858800 -3.72651100  
Cl 1.73251700 1.18595300 -2.43594400  
H 0.99146300 5.40048500 2.84757700  
H -1.34662800 -1.24587800 1.66703400  
N -2.18830100 -0.89492100 1.20589500  
C -3.21675700 -1.70020400 0.99612100  
N -3.36319900 -2.80595500 1.76321800  
N -4.13283000 -1.43066000 0.04752800  
C -2.60525800 -2.94251000 2.99438400  
H -1.59739700 -3.34073400 2.81514300  
H -2.52139900 -1.97836500 3.50046900  
H -3.14258500 -3.63263500 3.65159700  
C -3.83992000 -4.05882300 1.19933700  
H -4.71722900 -4.42869100 1.74247400  
H -4.09136100 -3.93665500 0.14540600  
H -3.04156800 -4.80814500 1.27025300  
C -5.53161500 -1.79111600 0.19937800  
H -5.84872800 -2.49346400 -0.58040400  
H -5.71356200 -2.23372500 1.17951400  
H -6.13986400 -0.88255800 0.11421400  
C -3.86081800 -0.47724200 -1.01356300  
H -4.21399600 0.52754700 -0.75096800  
H -2.79345100 -0.43872700 -1.22950500  
H -4.38194000 -0.80979600 -1.91682300

### Int10

Bi 1.22905100 -0.31281800 -0.12469700  
C -0.50888400 -2.89761200 -0.30184500  
C -0.30452400 -1.70173400 -0.97755600  
C -0.94894800 -1.39154200 -2.16620800  
H -0.75649800 -0.45557100 -2.67919300  
C -1.85809500 -2.31591600 -2.68274400  
C -2.09435200 -3.51948000 -2.01953200  
H -2.80399600 -4.23373900 -2.42962200

C -1.41690300 -3.81350100 -0.83783100  
H -1.58901700 -4.75630100 -0.32426700  
C 3.79629900 -1.35103200 1.38278400  
C 3.05065800 -1.55307700 0.22392100  
C 3.42826700 -2.50403900 -0.72115200  
H 2.85029900 -2.64681200 -1.63140900  
C 4.57305400 -3.26962000 -0.49597100  
H 4.87478300 -4.01446800 -1.22829000  
C 5.32867600 -3.07459200 0.65959600  
H 6.22197200 -3.67041400 0.82987400  
C 4.94297900 -2.11670900 1.59664300  
H 5.53182000 -1.96371000 2.49771100  
C 1.72961200 1.74547600 0.59654600  
C 2.82666400 2.35970700 0.00878800  
H 3.38285600 1.88365600 -0.79356800  
C 3.19233900 3.62832100 0.46326600  
H 4.04884100 4.12685400 0.01653000  
C 2.46014200 4.25011100 1.47222100  
C 1.36381000 3.60622300 2.04306100  
H 0.78483100 4.09321800 2.82339300  
C 0.98791000 2.33482300 1.60915700  
H 0.13862800 1.82821200 2.05454900  
C -1.23966500 2.55256300 -0.62353000  
C -0.43979800 3.29314600 -1.49994200  
C -2.13640200 3.21274200 0.22552900  
C -0.53419400 4.68069600 -1.51924400  
H 0.25821200 2.76575300 -2.14472800  
C -2.22708400 4.60274000 0.18883600  
H -2.74457900 2.63292600 0.91500700  
C -1.42755700 5.34685000 -0.67826400  
H 0.09962300 5.24669900 -2.19818200  
H -2.92623000 5.10689900 0.85274700  
H -1.49779700 6.43130000 -0.69780000  
O -1.10282800 1.20777300 -0.61479500  
H -1.84825000 0.74015100 -0.06937100  
H 0.00731000 -3.11916600 0.62797900  
H 3.49153600 -0.61329700 2.12184700  
Cl 0.31311900 -0.88877500 2.29660700  
H -2.38097400 -2.08762800 -3.60829900  
Cl 1.98574700 0.28517200 -2.54981600  
H 2.74269800 5.24272900 1.81344200  
H -2.14879600 -0.66338500 1.46276700  
N -2.76614100 -0.17507600 0.81773800  
C -3.95544800 -0.69304800 0.76489400

N -4.43670700 -1.61315000 1.67654200  
N -4.83139600 -0.32786700 -0.22719500  
C -3.65569900 -1.86278000 2.86851100  
C -5.17818300 -2.77465500 1.21608300  
C -6.23541000 -0.10457400 0.06190600  
C -4.32703600 0.45064600 -1.33705800  
H -2.77887500 -2.50160100 2.67551200  
H -3.31396600 -0.92228900 3.30907300  
H -4.29238400 -2.37026600 3.60028400  
H -6.00455000 -2.99764600 1.90162000  
H -5.58240100 -2.60330000 0.21796700  
H -4.51947200 -3.65547900 1.16799200  
H -6.86659100 -0.55745600 -0.71268200  
H -6.50262000 -0.53028700 1.02983200  
H -6.45059700 0.97437500 0.09224600  
H -4.21869400 1.51647600 -1.08651100  
H -3.35804900 0.06668900 -1.65780600  
H -5.03209100 0.36167100 -2.17068100

#### **TS9<sub>o</sub>**

Bi -0.49979500 0.01770300 -0.36138700  
C -2.44026300 2.15671500 0.95530300  
C -1.09691300 1.91619900 0.66466000  
C -0.10576800 2.83254400 1.01190400  
H 0.93735900 2.62182000 0.78305900  
C -0.46938700 4.01090100 1.66439300  
H 0.29590400 4.73283000 1.93875700  
C -1.80883100 4.26188000 1.96192200  
H -2.08784500 5.18207200 2.46932800  
C -2.79234800 3.33802300 1.61005300  
H -3.83636000 3.53515800 1.84138600  
C -2.83260400 -1.93432300 0.54957300  
C -2.52336100 -1.02323800 -0.46453900  
C -3.44218200 -0.76298800 -1.48153600  
H -3.20223500 -0.06551300 -2.28113900  
C -4.68112900 -1.40622700 -1.47404400  
H -5.39865200 -1.20234100 -2.26540300  
C -4.99673200 -2.30827200 -0.45820500  
H -5.96171700 -2.80898500 -0.45701800  
C -4.07385600 -2.57330400 0.55233900  
H -4.31498300 -3.28056500 1.34243300  
C 1.08590500 -1.21459900 0.89570200  
C 1.69718900 -2.32010300 0.31696500  
H 1.83591400 -2.39451600 -0.75791400

C 2.14757000 -3.33330900 1.16265900  
H 2.62775900 -4.20725200 0.72900800  
C 1.98361600 -3.23426600 2.54560700  
C 1.37331700 -2.10740700 3.09347100  
H 1.25813400 -2.01277300 4.17078700  
C 0.92432300 -1.07160600 2.26995300  
H 0.48502100 -0.17407200 2.69820700  
C 3.13572800 0.50588700 -0.28405400  
C 3.40938500 0.38588400 -1.66392500  
C 4.22165300 0.49603900 0.61815100  
C 4.72022700 0.27796100 -2.11690400  
H 2.57848500 0.40877600 -2.36477100  
C 5.52491300 0.36592300 0.15422800  
H 4.01006900 0.57994300 1.68120400  
C 5.78600000 0.26130900 -1.21502900  
H 4.91184500 0.20266400 -3.18527400  
H 6.34836400 0.35149800 0.86529400  
H 6.80803700 0.17081300 -1.57384100  
O 1.89519900 0.58784000 0.16437300  
H -2.11987200 -2.15642100 1.34231500  
H -3.21128200 1.44042700 0.67965700  
H 2.34092300 -4.02946200 3.19398500  
Cl -0.38013100 0.69506200 -2.78716500

#### **Int9**

Bi -0.84670500 0.01414100 -0.18552100  
C -0.81394000 2.92348900 1.04638700  
C -0.69805200 2.25228200 -0.16494500  
C -0.50705200 2.91688800 -1.37006900  
H -0.43791800 2.37828500 -2.30955700  
C -0.41728900 4.30969300 -1.35120400  
C -0.53161900 5.00715200 -0.15083700  
H -0.46295600 6.09183100 -0.14472100  
C -0.73354400 4.31652000 1.04205900  
H -0.82354800 4.85570000 1.98151400  
C -3.48098300 -0.60132500 1.44203200  
C -2.80852700 -0.94109600 0.27257100  
C -3.31795700 -1.86723700 -0.63202400  
H -2.79032500 -2.10961400 -1.54983100  
C -4.53963500 -2.47756800 -0.34477400  
H -4.94656200 -3.20834900 -1.03887700  
C -5.23359500 -2.14721600 0.81769000  
H -6.18723300 -2.62225500 1.03290400  
C -4.70829500 -1.21029800 1.70602900

H -5.24806200 -0.95120700 2.61323100  
C 0.84452500 -1.39374400 -0.51276600  
C 1.79145200 -1.10931300 -1.48828700  
H 1.74015700 -0.20213700 -2.08284600  
C 2.82662600 -2.02204100 -1.68814900  
H 3.59075300 -1.80706000 -2.42993600  
C 2.88612300 -3.19266600 -0.93481700  
C 1.91809500 -3.45844000 0.03161900  
H 1.96482000 -4.37077000 0.62073800  
C 0.88458500 -2.54869000 0.25907000  
H 0.14393700 -2.74521300 1.02945500  
C 3.41110700 0.63773600 0.84874100  
C 4.29804700 1.13332000 -0.11088500  
C 3.73156100 -0.51689900 1.56669700  
C 5.49763100 0.47028200 -0.35021100  
H 4.03167000 2.03402800 -0.65790400  
C 4.93477500 -1.17189000 1.31571500  
H 3.03612100 -0.90467300 2.30765800  
C 5.82472900 -0.68700400 0.35835900  
H 6.18309100 0.86318400 -1.09771200  
H 5.17323200 -2.07363200 1.87491800  
H 6.76269500 -1.20193300 0.16828300  
O 2.25104500 1.31335400 1.03379000  
H 1.69377800 0.86326800 1.69833300  
H -0.94310800 2.38892400 1.98181000  
H -3.06304800 0.10690300 2.15088700  
Cl -0.25975600 -0.07529800 2.42445900  
H -0.26035300 4.84347900 -2.28498400  
Cl -1.32484900 -0.02721900 -2.73540500  
H 3.69670500 -3.89808100 -1.09733600

### TS7<sub>o</sub>

Bi 0.74275200 -0.15475900 -0.30767100  
C 3.68936100 -1.20756600 -0.88306400  
C 2.50425800 -1.58438800 -0.25258100  
C 2.39351800 -2.81206300 0.39602400  
H 1.47244800 -3.09940400 0.89641200  
C 3.49348900 -3.67228300 0.42036000  
C 4.68578800 -3.30303500 -0.19943800  
H 5.54019400 -3.97507500 -0.17789500  
C 4.78398400 -2.07252200 -0.84816700  
H 5.71302400 -1.78057900 -1.33214000  
C 2.29735700 1.44290400 1.94883100  
C 1.63915400 1.61783300 0.73087600

C 1.51512900 2.88957900 0.17056200  
H 1.01396300 3.02928600 -0.78464800  
C 2.05539200 3.99184500 0.83448000  
H 1.96107000 4.98326400 0.39752500  
C 2.71705500 3.82131500 2.04981600  
H 3.13962000 4.68120500 2.56393000  
C 2.83915200 2.54820000 2.60567300  
H 3.35709400 2.41164300 3.55203700  
C -1.74264700 0.65149700 -0.55076400  
C -2.06913600 0.86353100 -1.87279900  
H -1.84267100 0.14496000 -2.65243100  
C -2.65219300 2.09953000 -2.16338200  
H -2.89155600 2.32971600 -3.19849400  
C -2.91715100 3.02203800 -1.15128600  
C -2.59819800 2.72114500 0.17147500  
H -2.79759900 3.43448100 0.96708000  
C -2.01703400 1.49395600 0.50649300  
H -1.76086000 1.24593600 1.53215300  
C -3.55113200 -1.29658700 0.24454900  
C -4.43703600 -1.42905300 -0.82117900  
C -3.99809100 -1.22762700 1.56235200  
C -5.80128200 -1.49862800 -0.55612600  
H -4.05429200 -1.48228000 -1.83569700  
C -5.36577700 -1.31003500 1.81147100  
H -3.28639200 -1.12155200 2.37672000  
C -6.26894700 -1.44075000 0.75728400  
H -6.50154800 -1.60375100 -1.38041600  
H -5.72390000 -1.26738200 2.83650400  
H -7.33510000 -1.49934200 0.95828200  
O -2.20807500 -1.20426200 -0.05528200  
H -1.64932700 -1.31306500 0.77996000  
H 3.77133300 -0.25452100 -1.39945500  
H 2.39028600 0.45472600 2.39380400  
Cl -0.22375900 -1.20233100 2.11708500  
H 3.41360100 -4.63063600 0.92808400  
Cl 1.29995200 0.72960600 -2.67690700  
H -3.37856600 3.97476500 -1.39417400

### 7

C -1.18610100 -0.52239200 0.04147900  
C -2.25403500 -1.05589500 -0.67641600  
H -2.09608100 -1.94927800 -1.27402900  
C -3.49994800 -0.43578000 -0.61306700  
H -4.33259900 -0.85245800 -1.17422600

C -3.67900700 0.71290000 0.15682000  
C -2.60164700 1.23416500 0.87338200  
H -2.73250300 2.12413700 1.48398000  
C -1.35245600 0.61989600 0.82518100  
H -0.51531100 1.02036800 1.38979900  
O -0.00009300 -1.21296000 -0.00049900  
C 1.18603600 -0.52253400 -0.04192300  
C 1.35305000 0.61920600 -0.82628400  
C 2.25338600 -1.05560100 0.67712900  
C 2.60230300 1.23338700 -0.87394900  
H 0.51636800 1.01935100 -1.39182400  
C 3.49940700 -0.43559900 0.61430500  
C 3.67909700 0.71254900 -0.15620800  
H 2.73366400 2.12293800 -1.48504800  
H 4.33159500 -0.85196200 1.17637900  
H 4.65101800 1.19646100 -0.19991900  
H 2.09496200 -1.94856600 1.27524000  
H -4.65087500 1.19688000 0.20095200

### Int13

C 0.76311600 0.02741300 0.38297100  
C 1.03440000 -1.01624700 -0.50730700  
H 0.22301100 -1.65140300 -0.85625800  
C 2.33472700 -1.24609500 -0.95025700  
H 2.53168200 -2.05997300 -1.64378100  
C 3.37953900 -0.43566000 -0.50715400  
C 3.11465600 0.60717700 0.37864700  
H 3.92252200 1.24517500 0.72846200  
C 1.81287600 0.83772800 0.82036600  
H 1.60877100 1.65771100 1.50460300  
O -1.00231400 2.27782500 -0.47959100  
C -1.37727000 1.13790800 -0.23803700  
C -2.49692900 0.52040300 -0.94407400  
C -0.66480300 0.30417600 0.83555600  
C -2.99929200 -0.67021100 -0.54321200  
H -2.92670200 1.07752700 -1.77224800  
C -1.36003800 -0.96293000 1.22424400  
H -0.60254100 0.95330800 1.72045700  
C -2.44575100 -1.41428900 0.57437500  
H -3.85591400 -1.09311500 -1.06483600  
H -0.92572600 -1.52626800 2.04780200  
H -2.92285000 -2.34591100 0.86704100  
H 4.39487700 -0.61589200 -0.85123500

### 1-OH

Bi 1.45354500 0.14137600 -0.43070700  
S -1.74729000 -0.16979800 -1.06606900  
O -0.68218300 -0.06602600 -2.09996200  
O -3.15021300 -0.30629100 -1.45741600  
C -1.23714400 -1.52207100 -0.02771300  
C 0.11249500 -1.54470400 0.32301000  
C 0.54457100 -2.56023200 1.17138100  
H 1.58128800 -2.59397300 1.49835000  
C -0.35917100 -3.52536100 1.62637400  
H -0.01122700 -4.31630700 2.28640900  
C -1.70167900 -3.48036900 1.25159400  
H -2.39476300 -4.23640500 1.61022900  
C -2.16087600 -2.45878300 0.42150100  
H -3.20360200 -2.39216000 0.12368700  
C -1.50734500 1.25519800 -0.02739500  
C -0.18734200 1.53746600 0.32325200  
C 0.04104200 2.61730200 1.17153500  
H 1.05185700 2.85040500 1.49829100  
C -1.03171100 3.39031300 1.62639600  
H -0.84270500 4.23375200 2.28609700  
C -2.34042600 3.08733200 1.25182200  
H -3.16619400 3.69570300 1.61036000  
C -2.59426200 1.99627900 0.42195900  
H -3.60459500 1.72995200 0.12407900  
O 2.45971200 0.23785900 1.46120100  
H 3.41488600 0.33302300 1.33537600

### 1-OmCB

Bi 0.71938300 -0.38789500 -1.27235700  
S 3.54756400 0.05516800 0.20464400  
O 3.30506200 -0.43501600 -1.18735200  
O 4.91169500 0.17898800 0.71292800  
C 2.67197600 1.59918400 0.27708300  
C 1.41396500 1.59129700 -0.32401900  
C 0.67099300 2.76883300 -0.26491600  
H -0.32566600 2.80976900 -0.69728800  
C 1.19621500 3.90086500 0.36571300  
H 0.60838600 4.81496700 0.40104600  
C 2.45965100 3.87153100 0.95651700  
H 2.85632700 4.75829800 1.44305700  
C 3.21556200 2.70103900 0.92763500  
H 4.19979000 2.64634300 1.38460600  
C 2.57001500 -1.03434000 1.21401100

C 1.30946600 -1.35829500 0.71080800  
C 0.50624100 -2.20270800 1.47327500  
H -0.48073100 -2.48609800 1.11827800  
C 0.97310600 -2.69446600 2.69647000  
H 0.33954800 -3.35639000 3.28174300  
C 2.23618300 -2.34823800 3.17426900  
H 2.58789500 -2.74027400 4.12451800  
C 3.05406700 -1.49861400 2.43103600  
H 4.04391300 -1.21379300 2.77677400  
O -1.30277900 0.25762500 -0.49221400  
C -2.04478300 -0.79593700 -0.60883000  
C -3.47823200 -0.65188800 -0.22717500  
O -1.58677900 -1.87784400 -1.01363000  
C -4.34338900 -1.73859300 -0.37411100  
C -3.94980400 0.56306800 0.27625700  
C -5.68233200 -1.60861100 -0.02014300  
H -3.95491200 -2.67288500 -0.76701500  
C -5.28965600 0.67095400 0.62547900  
H -3.27210800 1.40194500 0.39182600  
C -6.16640000 -0.40217300 0.48291400  
H -6.36087200 -2.44952700 -0.13424900  
Cl -5.88562600 2.18277400 1.25500300  
H -7.21038500 -0.29437000 0.76151700

### Int15f

Bi 0.55829600 0.40163900 0.18838100  
S 3.86440800 -0.33975200 -0.40634800  
O 3.67215300 0.72269600 0.59204800  
O 5.20575600 -0.80444700 -0.76547900  
C 2.91931100 -1.73535400 0.18850200  
C 1.62003100 -1.56688100 0.67157800  
C 0.95389600 -2.64428400 1.23672600  
H -0.05599500 -2.52660100 1.61532200  
C 1.59460700 -3.88327700 1.32091700  
H 1.07295100 -4.71982400 1.77879200  
C 2.88497400 -4.05057600 0.82626200  
H 3.37564600 -5.01767900 0.88953100  
C 3.55529600 -2.97322600 0.25289500  
H 4.56708600 -3.07354100 -0.12926100  
C 3.03757800 0.24536700 -1.86511200  
C 1.75930600 0.78064800 -1.70582400  
C 1.14128400 1.36575200 -2.80505000  
H 0.14172000 1.78651600 -2.71704300  
C 1.80656800 1.41504500 -4.03371200

H 1.32296100 1.88548600 -4.88604200  
C 3.07799900 0.86292100 -4.17478700  
H 3.58607800 0.90046200 -5.13432900  
C 3.70842700 0.26777800 -3.08293400  
H 4.70598600 -0.15458100 -3.16235700  
C -0.99411600 3.08597900 0.51849300  
H -0.10747000 3.32808500 1.10307600  
O -0.79763600 -0.92595900 -1.20728800  
C -4.85927900 -3.25982000 -0.26962100  
C -3.78330500 -2.48928500 0.15063100  
C -2.80836600 -2.12472900 -0.78110600  
C -2.91503000 -2.53168000 -2.11316300  
C -4.00021700 -3.30549400 -2.51266500  
C -4.98139000 -3.67458100 -1.59434300  
H -3.69045600 -2.16624400 1.18224800  
H -2.14527400 -2.23985300 -2.82026800  
H -4.08886700 -3.62791000 -3.54648700  
H -5.83134600 -4.27708300 -1.90051600  
C -1.65326900 -1.29875700 -0.33260300  
O -1.53267900 -0.97453000 0.87474500  
Cl -6.08201600 -3.71738800 0.88390500  
O 1.09615000 1.41029800 2.03529600  
C 1.57366400 -0.23573500 3.67565900  
H 0.56276100 -0.63470500 3.58224500  
C 1.92154300 0.80904200 2.90179900  
H 2.93238800 1.22105800 2.94527400  
C 2.49959000 -0.89481800 4.64190100  
H 2.09826500 -0.87999000 5.66475800  
H 2.65940000 -1.95111400 4.38130600  
H 3.47927400 -0.40338200 4.65527800  
C -1.09274300 1.87732300 -0.03802400  
H -1.91804900 1.49921000 -0.63679000  
C -1.98850000 4.16467300 0.42369700  
C -1.63989800 5.43212600 0.91084900  
C -3.26490800 3.98437000 -0.13092400  
C -2.53370000 6.49695000 0.83334800  
H -0.65624000 5.57900800 1.35178600  
C -4.15775200 5.04624500 -0.20542400  
H -3.56755800 3.00521200 -0.49275400  
C -3.79504100 6.30754900 0.27295000  
H -2.24516900 7.47325200 1.21433200  
H -5.14509800 4.89041500 -0.63285200  
H -4.49717100 7.13529800 0.21423900

**TS10e**

Bi 0.39433500 -0.67327200 -0.38763400  
S 1.33036700 -3.80910300 0.18047300  
O 1.67843700 -5.20664300 0.43901300  
O -0.06466100 -3.42261900 -0.14443500  
C 2.29696700 -3.16453100 -1.16444900  
C 1.95111500 -1.88593000 -1.59682000  
C 2.64373500 -1.34969100 -2.67647400  
H 2.40834100 -0.35033700 -3.03990700  
C 3.65247300 -2.09314400 -3.29826800  
H 4.18712800 -1.67045800 -4.14547400  
C 3.98312600 -3.36783200 -2.83905600  
H 4.76918800 -3.93637500 -3.32835300  
C 3.30465000 -3.92049200 -1.75312200  
H 3.53739000 -4.91495600 -1.38241000  
C 1.75177300 -2.79739700 1.58476200  
C 1.34041400 -1.46393900 1.57445400  
C 1.61061300 -0.67753800 2.68710000  
H 1.29375500 0.36014100 2.71697800  
C 2.28190700 -1.23097900 3.78227400  
H 2.48237900 -0.61123100 4.65281700  
C 2.69537100 -2.56134800 3.76883900  
H 3.21681700 -2.98102300 4.62456900  
C 2.43385700 -3.36132300 2.65834200  
H 2.73430000 -4.40493900 2.62535300  
C -1.96800900 -1.00307700 -0.54849800  
C -2.80301500 -0.38245500 0.30538700  
H -2.53015200 0.60707100 0.67565300  
O 0.02350100 1.43906600 0.92727400  
C 1.09836800 1.90444400 0.46398700  
O 1.87013100 1.19364400 -0.26017900  
C 1.47736200 3.31593200 0.75183800  
C 2.69506000 3.81590100 0.28461700  
C 0.60702400 4.13362900 1.47697200  
C 3.02477300 5.13776700 0.55483000  
H 3.36415300 3.17378100 -0.27843500  
C 0.95588600 5.45551500 1.73404400  
H -0.33447500 3.72292300 1.82798800  
C 2.16822300 5.96772400 1.27521500  
H 0.28324500 6.09801000 2.29567300  
H 2.44711900 6.99847700 1.47252300  
Cl 4.54175400 5.77179600 -0.02093000  
H -2.20685500 -1.96038500 -1.01167500  
C -0.96144400 0.37019400 -1.96720400

C -1.39549100 1.65320000 -1.87304300  
H -0.64962500 2.42756800 -1.67884200  
H -1.08675600 -0.43769500 -2.68115000  
C -2.77178700 2.08748200 -1.75625100  
C -3.04705400 3.39365000 -1.30394700  
C -3.85718500 1.23357800 -2.03250700  
C -4.35466200 3.82721300 -1.13184200  
H -2.21600500 4.05931300 -1.07796400  
C -5.16559700 1.67148700 -1.85916300  
H -3.66627600 0.22825100 -2.39370200  
C -5.42091000 2.96472200 -1.40374200  
H -4.54782200 4.83719100 -0.77823900  
H -5.99069200 0.99620000 -2.07103900  
H -6.44492100 3.30166800 -1.26315700  
C -4.09077500 -0.88748000 0.78718100  
C -4.97229300 0.00506500 1.41789400  
C -4.48964300 -2.22575000 0.63687000  
C -6.22051900 -0.41816000 1.86467500  
H -4.67354500 1.04414000 1.54024500  
C -5.73638500 -2.64776700 1.08345800  
H -3.80937600 -2.94260600 0.18402100  
C -6.60993100 -1.74642500 1.69632600  
H -6.89105300 0.29099200 2.34427600  
H -6.02614400 -3.68893400 0.96313700  
H -7.58286500 -2.08111800 2.04744900

**Int14b**

Bi -0.87425300 0.49958000 0.50247600  
S -4.13953200 -0.16751400 -0.39149600  
O -5.47833500 -0.54668000 -0.84964400  
O -3.97314200 0.80541800 0.70355000  
C -3.20410100 0.46750500 -1.75645200  
C -1.90866700 0.91119900 -1.49098000  
C -1.16230800 1.42298600 -2.54766500  
H -0.13316000 1.73827300 -2.38718200  
C -1.72408600 1.51734300 -3.82419900  
H -1.13454700 1.92886500 -4.63966300  
C -3.02414600 1.07585100 -4.06179500  
H -3.45231500 1.14674000 -5.05783900  
C -3.77705500 0.53262900 -3.02240100  
H -4.79019800 0.17420100 -3.18031400  
C -3.26305700 -1.63022700 0.13163400  
C -1.97039000 -1.52430300 0.65466500  
C -1.38250400 -2.66492700 1.18758300



H -0.39272400 -2.61529300 1.62719900  
C -2.06677700 -3.88326800 1.17346200  
H -1.59129400 -4.76396300 1.59798200  
C -3.34003200 -3.97769400 0.61919600  
H -3.86421800 -4.92910300 0.60245300  
C -3.95048600 -2.84142000 0.09592400  
H -4.95304000 -2.87621100 -0.32075300  
C -1.59615400 1.53215700 2.33571200  
C -0.74910000 2.28425200 3.03658000  
H 0.27840100 2.41554100 2.68725900  
O 0.94198100 -0.73829100 1.49826100  
C 1.37868100 -1.26409600 0.41881600  
O 0.80402500 -1.09447400 -0.68209200  
C 2.61981800 -2.09243400 0.49576100  
C 3.11025600 -2.69071000 -0.66742800  
C 3.28717900 -2.25877800 1.71162500  
C 4.26982700 -3.45103900 -0.59392100  
H 2.58284900 -2.55358200 -1.60570400  
C 4.44807500 -3.02449500 1.76318000  
H 2.88924700 -1.78341000 2.60249400  
C 4.94867400 -3.62660700 0.61033500  
H 4.97252800 -3.15749400 2.70555900  
H 5.85384500 -4.22546700 0.64321100  
Cl 4.89082500 -4.20160100 -2.03898800  
C -1.09994100 2.98800200 4.30924700  
H -0.93266600 4.06849200 4.20980600  
H -2.14376400 2.82090700 4.59267100  
H -0.45494600 2.64108400 5.12725000  
H -2.63024300 1.33845500 2.61038000  
C 0.74430700 2.00386600 0.04544200  
C 2.06745700 1.85160000 -0.00973800  
H 2.50191400 0.86590600 0.14428500  
H 0.25157500 2.96799800 -0.09948900  
C 3.06462100 2.90140300 -0.27037400  
C 4.41354900 2.52839100 -0.35627000  
C 2.73368200 4.25540000 -0.43492600  
C 5.40446800 3.47528500 -0.60308200  
H 4.68303600 1.48163300 -0.22912000  
C 3.72196500 5.20092700 -0.67985700  
H 1.69679500 4.57453400 -0.36715100  
C 5.06189200 4.81578300 -0.76590500  
H 6.44423600 3.16459900 -0.66747100  
H 3.44794100 6.24579600 -0.80328000  
H 5.83214600 5.55857700 -0.95700600

### TS11e

Bi 0.97667800 -0.45867500 -0.33384700  
S 4.13013000 -1.46111600 -0.24211300  
O 3.08492000 -2.17621400 -1.00899600  
O 5.52201900 -1.91114900 -0.25394800  
C 4.03388000 0.22088800 -0.82470700  
C 2.77261700 0.77367600 -1.04720900  
C 2.67297200 2.05110300 -1.57728500  
H 1.70130300 2.49381100 -1.77468700  
C 3.84015300 2.76350800 -1.87186300  
H 3.76092100 3.76126400 -2.29609400  
C 5.09500300 2.20888400 -1.63058600  
H 5.99474200 2.77133500 -1.86378900  
C 5.20199100 0.92444600 -1.10103300  
H 6.16833900 0.46186100 -0.92049900  
C 3.50135700 -1.42170000 1.41654700  
C 2.13830900 -1.15504600 1.53377300  
C 1.57303600 -1.17344400 2.80477800  
H 0.51472000 -0.96286300 2.94079800  
C 2.37011300 -1.46271000 3.91690400  
H 1.91978300 -1.48702700 4.90623600  
C 3.73367100 -1.71666300 3.77199600  
H 4.34263200 -1.93949800 4.64381200  
C 4.31981100 -1.69301200 2.50736400  
H 5.37736300 -1.89728700 2.36522400  
C -1.04298200 -1.43099300 0.22586900  
C -1.97533500 -0.77316100 0.91545400  
H -1.96305600 0.31518100 0.94958800  
O 0.43781100 1.35273500 1.00159400  
C -2.24182900 5.20219900 0.10349200  
C -1.66384500 4.00972900 -0.31115900  
C -0.86437100 3.29947000 0.58797100  
C -0.64889000 3.78193100 1.88136000  
C -1.23638100 4.97978300 2.27526800  
C -2.03763200 5.69830800 1.38980700  
H -1.82428500 3.62524000 -1.31304400  
H -0.02298900 3.21453500 2.56254400  
H -1.07274800 5.36336500 3.27851100  
H -2.49910000 6.63358600 1.69212500  
C -0.25263200 2.01729700 0.15188900  
O -0.41393300 1.58684700 -1.01563600  
Cl -3.24285200 6.09463600 -1.00687500  
O 0.68662100 -1.26475700 -2.42705400

C -1.66241100 -1.27381600 -2.41018800  
H -1.64802300 -0.19479500 -2.26796900  
C -0.45066800 -1.89181800 -2.56295600  
H -0.38411000 -2.97571500 -2.71699700  
H -0.96115700 -2.51493300 0.16581500  
C -2.96472600 -1.91528600 -2.37573600  
C -4.08516700 -1.13136400 -2.04507500  
C -3.16735800 -3.29228100 -2.59380400  
C -5.35203100 -1.69339000 -1.93091300  
H -3.94598000 -0.06740400 -1.86463900  
C -4.43513600 -3.85109000 -2.48652700  
H -2.32922000 -3.93237800 -2.85559000  
C -5.53460000 -3.05794100 -2.15015500  
H -6.19821600 -1.06530400 -1.66327200  
H -4.56795500 -4.91565700 -2.66495400  
H -6.52304800 -3.50113600 -2.05989500  
C -3.08012000 -1.38831000 1.66595000  
C -3.77543000 -0.60660300 2.60008300  
C -3.48247200 -2.71750400 1.46946200  
C -4.83018300 -1.14245600 3.33401900  
H -3.48114900 0.43065900 2.74944700  
C -4.53689000 -3.25100100 2.20065100  
H -2.98956100 -3.32643900 0.71670500  
C -5.21288400 -2.46853500 3.13901500  
H -5.35626300 -0.52194100 4.05532900  
H -4.84350600 -4.27956500 2.02742400  
H -6.04043600 -2.88810400 3.70538600

#### **TS10d**

Bi -0.89683800 -0.57405200 0.22966400  
S -3.74275500 -2.16145500 -0.29666400  
O -4.96089400 -2.92961800 -0.54988600  
O -2.42899100 -2.84044300 -0.16542000  
C -3.89899300 -1.21034400 1.19497800  
C -2.74177900 -0.55875800 1.61728100  
C -2.79082800 0.16798500 2.80107000  
H -1.91058500 0.69789100 3.16093400  
C -3.98107500 0.22429100 3.53414300  
H -4.01306100 0.78912200 4.46259000  
C -5.12701700 -0.43107300 3.08469100  
H -6.04586700 -0.37990800 3.66214800  
C -5.09889600 -1.15849400 1.89526100  
H -5.97594200 -1.68448400 1.52839200  
C -3.48676700 -0.96184600 -1.58768100

C -2.28159300 -0.25777200 -1.59371900  
C -2.04042400 0.64423200 -2.62135900  
H -1.10812200 1.19846100 -2.66067600  
C -3.00189600 0.82684300 -3.62107900  
H -2.80396800 1.52857500 -4.42748800  
C -4.20376600 0.12307100 -3.59399800  
H -4.94294200 0.27287100 -4.37590900  
C -4.45919000 -0.78263700 -2.56616900  
H -5.38282600 -1.35349600 -2.52757700  
C 0.63600700 -2.40449400 -0.13135700  
C 1.51773800 -2.32908200 -1.13597200  
H 1.93322100 -1.35617400 -1.40690800  
O 0.67916700 0.92586900 -1.04521200  
C 0.25652200 1.90058900 -0.37167600  
O -0.70722800 1.75878500 0.45541900  
C 0.88466800 3.24074900 -0.51894700  
C 0.37715800 4.32632200 0.19915300  
C 1.98479000 3.40165300 -1.36522200  
C 0.98390000 5.56733400 0.05559000  
H -0.47637700 4.19109100 0.85489800  
C 2.57904400 4.65295000 -1.49187500  
H 2.36327000 2.54367000 -1.91191600  
C 2.08251700 5.74542900 -0.78295800  
H 3.43600500 4.78603100 -2.14636800  
H 2.54123000 6.72489500 -0.87885100  
Cl 0.35801100 6.92848500 0.94318200  
C 1.98160900 -3.49360000 -1.95310100  
H 1.67340100 -3.36969000 -3.00039800  
H 3.07766800 -3.55863900 -1.95216400  
H 1.57137300 -4.43985900 -1.58611400  
H 0.21077900 -3.35204000 0.20283600  
C 0.95652000 -0.98737700 1.54670700  
C 2.11972700 -0.28736800 1.44822300  
H 2.06120000 0.80276500 1.46028600  
H 0.59466600 -1.80761400 2.15731900  
C 3.41187000 -0.82587700 1.10663500  
C 4.46035300 0.05608800 0.76206800  
C 3.66727600 -2.21429800 1.06806600  
C 5.70310000 -0.41664800 0.38594000  
H 4.27634000 1.12773100 0.78312100  
C 4.90908200 -2.69982000 0.69379200  
H 2.88627600 -2.90968100 1.35383800  
C 5.91423200 -1.79740000 0.34794800  
H 6.50555400 0.25991300 0.11422800

H 5.10965800 -3.76522700 0.66798300  
N 7.21044100 -2.30273600 -0.05576500  
O 8.08134100 -1.48952700 -0.34844100  
O 7.37386300 -3.51826000 -0.08796400

### **TS11d**

Bi -0.72503700 0.45202200 -0.13929900  
S -3.99119500 0.44665600 -0.55718500  
O -3.10724100 1.57240700 -0.94580500  
O -5.43154100 0.49671200 -0.80808900  
C -3.27861700 -0.97362400 -1.36532300  
C -1.88847600 -1.08780200 -1.38323600  
C -1.30598600 -2.14933200 -2.06035200  
H -0.22561800 -2.25150700 -2.10337900  
C -2.12281600 -3.08415800 -2.70504500  
H -1.66392600 -3.90989400 -3.24308800  
C -3.51056000 -2.96637900 -2.66746200  
H -4.13467000 -3.69822700 -3.17258000  
C -4.10406600 -1.90274600 -1.99040700  
H -5.18297000 -1.77892600 -1.95835000  
C -3.65984900 0.21328500 1.17033000  
C -2.31881500 0.31483900 1.53597400  
C -2.00235800 0.18731900 2.88550600  
H -0.96764100 0.24748300 3.21467400  
C -3.01634500 -0.02499700 3.82480000  
H -2.76122800 -0.11270500 4.87826100  
C -4.34896300 -0.13071400 3.42673300  
H -5.12794100 -0.29731300 4.16563500  
C -4.68666400 -0.01851500 2.07905600  
H -5.71679000 -0.09073300 1.74139800  
C 0.72769400 1.91568400 0.97400400  
C 1.68327300 1.46565200 1.77862600  
H 2.13169500 0.48590100 1.61412200  
O 0.20214200 -1.32394300 1.00775600  
C 4.04423800 -4.01611000 0.11925300  
C 3.19767300 -2.97065900 -0.22512100  
C 2.09913200 -2.69537100 0.59316500  
C 1.85646800 -3.46047400 1.73662300  
C 2.71707400 -4.50366900 2.06247000  
C 3.81767500 -4.78887300 1.25670900  
H 3.37440900 -2.37140600 -1.11234100  
H 0.99511000 -3.23194200 2.35579200  
H 2.53438500 -5.10449000 2.94906700  
H 4.49331300 -5.60172800 1.50529200

C 1.18797800 -1.57811000 0.22943500  
O 1.37526200 -0.90086200 -0.80874400  
Cl 5.41704100 -4.36966900 -0.89204900  
O -0.35643300 1.71721400 -2.02146600  
C 1.78309800 2.41918200 -1.37288400  
H 2.11649100 1.38380800 -1.40131400  
C 0.49504700 2.66580900 -1.78631200  
H 0.11222100 3.69314800 -1.84508100  
H 0.24676000 2.88920100 1.06956100  
C 2.25323000 2.26395400 2.91272900  
H 2.18167800 1.70798600 3.85685000  
H 3.31802700 2.46278200 2.73233600  
H 1.74165600 3.22397100 3.03118100  
C 2.75952100 3.40960500 -0.96123100  
C 4.08799000 2.99956000 -0.74510200  
C 2.43637200 4.75615100 -0.70405300  
C 5.05846700 3.89699800 -0.31267000  
H 4.35214800 1.95961600 -0.92662300  
C 3.40816600 5.65283400 -0.27611900  
H 1.41507400 5.10471600 -0.83167100  
C 4.72429800 5.23073300 -0.07758400  
H 6.07904000 3.55481700 -0.15828400  
H 3.13568800 6.68840100 -0.08659200  
H 5.47976900 5.93442600 0.26250900

### **Int15e**

Bi 0.03160800 -0.68730100 -0.17193600  
S -2.96407700 -1.17064700 -1.82476500  
O -2.87815100 -1.97800200 -0.59864600  
O -4.16311800 -1.20895200 -2.66440400  
C -2.68291100 0.52053900 -1.31924200  
C -1.62855900 0.86006800 -0.46842000  
C -1.51343000 2.16132900 -0.00320800  
H -0.69940000 2.43625900 0.65882200  
C -2.46367900 3.11358100 -0.37923900  
H -2.38137200 4.12555600 0.00861200  
C -3.50926900 2.77486300 -1.23279800  
H -4.24470200 3.51995200 -1.52212100  
C -3.62119200 1.47292200 -1.71204700  
H -4.43246400 1.17921800 -2.37172500  
C -1.55848600 -1.65522100 -2.79841500  
C -0.31684400 -1.71412400 -2.16528700  
C 0.76887100 -2.21965300 -2.87111400  
H 1.75173000 -2.26936400 -2.40707200

C 0.59950600 -2.66501000 -4.18531900  
H 1.44973500 -3.07092200 -4.72747700  
C -0.64603500 -2.58650800 -4.80446300  
H -0.76914800 -2.92878400 -5.82817500  
C -1.74253100 -2.07598000 -4.11107300  
H -2.72676500 -2.01855300 -4.56674800  
C 2.02011500 -2.55838500 1.34015000  
H 1.08454400 -2.95610200 1.73053500  
O 1.36137000 0.77264000 -1.42515300  
C 4.00337100 4.53752600 -0.13641100  
C 3.12942600 3.50784000 0.18602500  
C 2.67382500 2.66516700 -0.83080600  
C 3.09123400 2.85742600 -2.14996400  
C 3.96647500 3.89615600 -2.45146400  
C 4.42973100 4.74376100 -1.44694200  
H 2.79925200 3.34831000 1.20719700  
H 2.72238500 2.19357700 -2.92519600  
H 4.29395400 4.05340400 -3.47546600  
H 5.11304300 5.55588300 -1.67601600  
C 1.73093600 1.56515600 -0.48852800  
O 1.31456800 1.42174200 0.68577700  
Cl 4.57810900 5.59425800 1.12367200  
O -0.86264900 -1.56843000 1.62984100  
C -2.28399800 0.10254900 2.50433500  
H -1.41920800 0.74762800 2.65907400  
C -2.06190500 -1.13612300 2.00517900  
H -2.87715300 -1.84887300 1.87293100  
C 1.98097000 -1.53701000 0.48253100  
H 2.82862800 -1.03162900 0.02526700  
C -3.58850200 0.65613300 2.84162100  
C -3.66836800 1.78003700 3.68222800  
C -4.78869700 0.13908900 2.31864500  
C -4.89516800 2.34782100 4.01227300  
H -2.75020500 2.20357800 4.08514800  
C -6.01418600 0.70266500 2.65485800  
H -4.75683300 -0.69488500 1.62247600  
C -6.07719300 1.80882500 3.50461000  
H -4.92854600 3.21435900 4.66876700  
H -6.92741100 0.28586800 2.23625000  
H -7.03688300 2.25184100 3.75878700  
C 3.23313200 -3.22567000 1.83371600  
C 3.08205800 -4.38095300 2.61324300  
C 4.52902700 -2.76039500 1.56276500  
C 4.19392300 -5.06278200 3.10070700

H 2.08090600 -4.74420300 2.83521000  
C 5.63816100 -3.43951800 2.05124800  
H 4.67127700 -1.85535800 0.97808500  
C 5.47560800 -4.59457800 2.81988400  
H 4.05781000 -5.95760600 3.70258000  
H 6.63601600 -3.06465400 1.83793100  
H 6.34607500 -5.12180700 3.20180200

### TS11a<sub>o</sub>

Bi 0.72437600 0.35582800 -0.08554500  
S 3.51767200 -1.30802900 -0.07730800  
O 4.84093100 -1.92899100 -0.08897500  
O 3.36933800 0.15996200 -0.28674100  
C 2.68626800 -1.60480200 1.46603900  
C 1.49608200 -0.90606700 1.65687400  
C 0.81944300 -1.06640100 2.85942100  
H -0.10867200 -0.52929900 3.04159500  
C 1.34037100 -1.91993200 3.83686900  
H 0.81110800 -2.04170100 4.77872900  
C 2.52934100 -2.61671000 3.61851800  
H 2.92425400 -3.27470200 4.38765300  
C 3.21975300 -2.46801300 2.41671400  
H 4.15290900 -2.99101300 2.22641000  
C 2.46405800 -2.02456000 -1.31770000  
C 1.24249200 -1.38694200 -1.53291700  
C 0.39891200 -1.89964100 -2.51172700  
H -0.56025200 -1.43053400 -2.71446300  
C 0.78855200 -3.02376600 -3.24702600  
H 0.12582100 -3.41545800 -4.01487100  
C 2.01167400 -3.64831200 -3.00592700  
H 2.30280000 -4.52081500 -3.58417600  
C 2.86770200 -3.15259500 -2.02441100  
H 3.82942400 -3.61540900 -1.82052800  
C 1.11698600 2.75808000 -0.18588900  
C 0.34028600 3.46827200 -1.07805900  
H -0.61048900 3.08712500 -1.44004600  
C 0.82979700 4.70975000 -1.49348000  
H 0.25102500 5.29329500 -2.20576800  
C 2.04013000 5.19561700 -0.99942800  
C 2.77711600 4.44183500 -0.08727000  
H 3.71790700 4.81901200 0.30685700  
C 2.31803400 3.19202200 0.34114100  
H 2.88721800 2.60092200 1.05141500  
C -2.43289200 2.82692500 1.08623700

H -2.50713000 2.39325600 0.09055000  
O -0.23643000 1.97572600 1.36755200  
O -1.44337800 0.67987300 -1.50710300  
C -1.97918900 -0.09443000 -0.68099600  
O -1.29207100 -0.64678600 0.25082000  
C -3.43323100 -0.40163700 -0.74755600  
C -4.00674600 -1.24439900 0.20772800  
C -4.21721500 0.16450800 -1.75538800  
C -5.36810300 -1.50832000 0.13736600  
H -3.39081900 -1.67626000 0.98919800  
C -5.57912100 -0.11415900 -1.80774900  
H -3.75081600 0.81843500 -2.48548000  
C -6.16516000 -0.95286900 -0.86140200  
H -6.19548600 0.32281400 -2.58852900  
H -7.22768400 -1.17400200 -0.89588100  
Cl -6.09516800 -2.55471700 1.32501000  
H 2.40788800 6.16558900 -1.32301700  
C -1.28886600 2.63845500 1.79092900  
H -1.20250000 3.08304900 2.79274400  
C -3.60933000 3.57952900 1.60554900  
H -3.86255200 4.42974900 0.95589800  
H -4.50581600 2.94383800 1.64700500  
H -3.42620200 3.97014500 2.61348200

#### **TS11c<sub>0</sub>**

Bi 0.75666500 0.67496900 -0.11591800  
S 3.77499700 -0.50878500 -0.08056900  
O 5.18425600 -0.89646700 -0.08895200  
O 3.37746100 0.90256900 -0.35455300  
C 3.01994500 -0.86892200 1.48921500  
C 1.72967200 -0.37431100 1.66748000  
C 1.09939500 -0.59212400 2.88606800  
H 0.09520400 -0.21174600 3.05965200  
C 1.76549900 -1.29902900 3.89194100  
H 1.27178800 -1.46552900 4.84621700  
C 3.05424200 -1.79243900 3.68646700  
H 3.56168900 -2.33686400 4.47802600  
C 3.70048700 -1.58338500 2.46897600  
H 4.70834300 -1.94692600 2.28853600  
C 2.84150300 -1.45328900 -1.26495400  
C 1.52541000 -1.04512500 -1.47873200  
C 0.76487400 -1.74993200 -2.40497500  
H -0.26513500 -1.46499700 -2.60307100  
C 1.32853700 -2.82966700 -3.09247700

H 0.72916600 -3.37117900 -3.82036200  
C 2.64582200 -3.22054100 -2.85469900  
H 3.07268700 -4.06021500 -3.39607600  
C 3.42120600 -2.53278600 -1.92300200  
H 4.45131000 -2.81328500 -1.72086100  
C 0.78496900 3.07575500 -0.38870600  
C 0.01290100 3.61819900 -1.30937500  
H -0.87469200 3.08955600 -1.65946500  
C -2.63880100 2.82235700 1.01374900  
H -2.69189400 2.27755500 0.07287600  
O -0.35105300 2.25359200 1.30507500  
O -1.45113600 0.64914000 -1.54519600  
C -1.86952500 -0.14891300 -0.67734200  
O -1.10981100 -0.55491300 0.27615800  
C -3.26680500 -0.65826400 -0.71407000  
C -3.71562300 -1.53281700 0.27860100  
C -4.12455100 -0.24542200 -1.73631500  
C -5.02840100 -1.98310900 0.23031300  
H -3.04345500 -1.84534500 1.07045800  
C -5.43574700 -0.70845900 -1.76525200  
H -3.75364900 0.43601900 -2.49533900  
C -5.89779600 -1.58080600 -0.78161200  
H -6.10925700 -0.39082300 -2.55642700  
H -6.92060300 -1.94475400 -0.79734600  
Cl -5.60175500 -3.07195300 1.46318000  
C -1.46344400 2.83685700 1.69029000  
H -1.40455700 3.40119300 2.63298700  
C -3.87857500 3.49488700 1.49826200  
H -4.24748700 4.23656600 0.77519800  
H -4.69598700 2.77415800 1.64634800  
H -3.71032400 4.01119700 2.45107000  
C 0.28505600 4.97316900 -1.89970500  
H 0.39907800 4.90373500 -2.98865200  
H -0.56157500 5.64257800 -1.69796100  
H 1.19027600 5.42676000 -1.48480200  
H 1.66655200 3.43106200 0.13406000

#### **Int14f**

Bi -0.04530800 0.75793800 0.21357300  
S -0.17984100 4.19776400 0.56521500  
O -0.08459500 5.65344600 0.70227700  
O -1.49586400 3.54609700 0.44285600  
C 0.62942400 3.42365100 1.93940900  
C 0.62725300 2.02962800 1.98571700

C 1.24860200 1.40942300 3.06518000  
H 1.30283000 0.32356800 3.11395500  
C 1.82102000 2.17709900 4.08336800  
H 2.29445100 1.68053300 4.92668600  
C 1.80163700 3.56879900 4.01883400  
H 2.25347100 4.15952000 4.81089700  
C 1.20982400 4.20795900 2.93105000  
H 1.18694800 5.29084100 2.84981800  
C 0.74571500 3.68605700 -0.87136300  
C 0.78276200 2.33883000 -1.24454500  
C 1.38111700 2.00837000 -2.45425400  
H 1.40266400 0.97765500 -2.78998700  
C 1.94851800 3.00267400 -3.25542500  
H 2.40907900 2.72453900 -4.20010500  
C 1.93419700 4.33471500 -2.85222200  
H 2.38603200 5.10303800 -3.47335800  
C 1.32323000 4.68532100 -1.65172100  
H 1.27242700 5.71864700 -1.32090300  
C -2.19837400 0.74005700 -0.32171900  
C -2.83580200 -0.43653100 -0.35315700  
H -2.28597800 -1.34220700 -0.08315800  
O 0.73996800 -0.79586200 -1.47147000  
C 1.95618600 -0.81424000 -1.08563800  
O 2.36633300 -0.08749400 -0.14809500  
C 2.89943100 -1.74430000 -1.77615200  
C 4.23542600 -1.78318500 -1.36959100  
C 2.44968100 -2.57235700 -2.80736400  
C 5.10561600 -2.65820200 -2.00617300  
H 4.57246200 -1.13535300 -0.56709000  
C 3.33885200 -3.44091900 -3.43310000  
H 1.40690300 -2.52686600 -3.10488800  
C 4.67408700 -3.49070500 -3.03701700  
H 2.99588100 -4.08747400 -4.23628000  
H 5.37316500 -4.16635300 -3.52048100  
Cl 6.77368100 -2.71847000 -1.50476000  
H -2.62341900 1.70526200 -0.58038800  
C -0.15526700 -1.09572400 1.49462600  
C 0.49672300 -2.25342900 1.38866600  
H 1.22515500 -2.39005700 0.59206400  
H -0.90349800 -0.90374000 2.26690500  
C 0.34830100 -3.43048200 2.25820300  
C 1.09448300 -4.57760800 1.95254400  
C -0.49976800 -3.46182000 3.37612600  
C 0.99669800 -5.72531700 2.73503700

H 1.75696000 -4.56400600 1.08923200  
C -0.59737000 -4.60652200 4.15767900  
H -1.08509400 -2.58447800 3.63957300  
C 0.14939800 -5.74383900 3.84074200  
H 1.58372100 -6.60426500 2.48068400  
H -1.25826200 -4.61368000 5.02096000  
H 0.07077000 -6.63697200 4.45534400  
C -4.23418300 -0.67377500 -0.71819600  
C -4.71495600 -1.98705000 -0.73799900  
C -5.13035000 0.35799900 -1.05323800  
C -6.03240100 -2.28374100 -1.08148100  
H -4.04143300 -2.80254300 -0.48160900  
C -6.44020600 0.08143900 -1.39525600  
H -4.79580600 1.39183600 -1.04373500  
C -6.90385200 -1.24366200 -1.41363700  
H -6.36223600 -3.31704200 -1.08597300  
H -7.13161700 0.87883200 -1.65309200  
O -8.19913500 -1.41105700 -1.76134300  
C -8.71181900 -2.72811100 -1.80058200  
H -9.75716200 -2.63336700 -2.10027200  
H -8.17873400 -3.34236500 -2.53758800  
H -8.66089200 -3.20664800 -0.81418600

#### TS10c

Bi -0.86635400 -0.55494100 0.18353300  
S -3.92569200 -1.71764200 -0.36889700  
O -5.24033400 -2.30404100 -0.63479100  
O -2.71114100 -2.57032800 -0.33273400  
C -3.92465300 -0.86788200 1.19254400  
C -2.68607400 -0.39239600 1.61834100  
C -2.62303600 0.24560300 2.85271900  
H -1.67556700 0.63686100 3.22097600  
C -3.77953900 0.39148300 3.62602800  
H -3.72162100 0.88765600 4.59192700  
C -5.00700200 -0.08812000 3.16899800  
H -5.89948300 0.03055000 3.77731200  
C -5.09378500 -0.72549600 1.93161600  
H -6.03617200 -1.11532000 1.55666300  
C -3.55239400 -0.46385800 -1.57742600  
C -2.26836800 0.08092800 -1.56887500  
C -1.94888700 1.02711000 -2.53558100  
H -0.95649700 1.46586300 -2.56868600  
C -2.90586100 1.40900200 -3.48134000  
H -2.64378200 2.14509000 -4.23752100

C -4.18661400 0.85991900 -3.46380200  
H -4.92298400 1.16408400 -4.20246800  
C -4.52419900 -0.08747700 -2.49971200  
H -5.51162400 -0.53972900 -2.46725500  
C 0.44893900 -2.55946900 -0.16162200  
C 1.35901700 -2.59686900 -1.14096800  
H 1.87993300 -1.67863900 -1.41827700  
O 0.89322200 0.77959200 -1.08927900  
C 0.61139300 1.77604500 -0.37584800  
O -0.35541400 1.74947100 0.45622400  
C 1.42414400 3.02145900 -0.48581100  
C 1.08227000 4.14185700 0.27499300  
C 2.52888800 3.05637100 -1.34018600  
C 1.85789500 5.28886200 0.16599500  
H 0.22286900 4.10450600 0.93608900  
C 3.29384600 4.21475000 -1.43235000  
H 2.77548600 2.17236400 -1.91994200  
C 2.96388700 5.34061700 -0.67977200  
H 4.15516200 4.24875400 -2.09407200  
H 3.55577800 6.24843300 -0.74709800  
Cl 1.43920200 6.69376800 1.10758400  
C 1.72794400 -3.82418800 -1.91469400  
H 2.80846000 -4.01188100 -1.84924200  
H 1.19543600 -4.70985000 -1.55250500  
H 1.49122300 -3.69398600 -2.97966400  
H -0.08635200 -3.44778000 0.17730100  
C 0.94292700 -1.16569200 1.53272500  
C 2.18740000 -0.63549100 1.42921800  
H 2.27138200 0.45448300 1.44260200  
H 0.48030300 -1.93429900 2.14321000  
C 3.40271200 -1.33104000 1.06690700  
C 4.52658900 -0.59600800 0.65344600  
C 3.51071600 -2.73806700 1.07749200  
C 5.70889100 -1.21655300 0.26879500  
H 4.46569000 0.49034700 0.62697900  
C 4.68366300 -3.36829100 0.70199700  
H 2.66578900 -3.33479300 1.40567400  
C 5.79140700 -2.61473000 0.28934000  
H 6.55168100 -0.61010800 -0.04541600  
H 4.76872000 -4.45139500 0.72280400  
O 6.89061700 -3.31979200 -0.06148700  
C 8.04008500 -2.60453800 -0.46843600  
H 8.79800100 -3.35816000 -0.69056500  
H 7.84445400 -2.01263700 -1.37183900

H 8.40691900 -1.94834500 0.33129400

#### Int14c

Bi -1.03299500 -0.62324400 -0.52805700  
S -4.29380200 -1.11458100 0.52377400  
O -5.65380400 -1.20295500 1.06198900  
O -3.88522000 -1.96393500 -0.60929700  
C -3.12652200 -1.42699900 1.82048000  
C -1.77299400 -1.40403100 1.48481800  
C -0.84539500 -1.65919200 2.49020600  
H 0.22019900 -1.60584700 2.27545100  
C -1.27664700 -1.96634600 3.78375000  
H -0.54228200 -2.17420500 4.55795900  
C -2.63550100 -1.99306000 4.09121700  
H -2.96351200 -2.22641200 5.10042300  
C -3.57883700 -1.71015800 3.10532700  
H -4.64403000 -1.71532800 3.31760600  
C -3.98072700 0.56411100 0.00521000  
C -2.75583200 0.90762400 -0.57597600  
C -2.61555200 2.18437700 -1.10637400  
H -1.68935700 2.47533500 -1.58917000  
C -3.66951100 3.09884900 -1.03283600  
H -3.54155400 4.09200300 -1.45624800  
C -4.87006100 2.75182000 -0.42013200  
H -5.68335700 3.46935800 -0.35614200  
C -5.03368700 1.47153800 0.10098300  
H -5.96691200 1.16187800 0.56264600  
C -1.47561400 -1.80556800 -2.36081100  
C -0.46860600 -2.23395400 -3.12054900  
H 0.56279900 -2.03223100 -2.81933200  
O 0.21176600 1.19761700 -1.52495900  
C 0.48541800 1.80291300 -0.43405700  
O 0.04736200 1.40979700 0.67267100  
C 1.36685600 3.00795600 -0.50332800  
C 1.67577200 3.69118200 0.67523500  
C 1.88367400 3.44046800 -1.72688000  
C 2.50389400 4.80379900 0.60940000  
H 1.26782800 3.34501000 1.61917800  
C 2.71101600 4.55873000 -1.77083200  
H 1.63255800 2.89328800 -2.63001600  
C 3.02774000 5.24949000 -0.60256300  
H 3.11624300 4.90063200 -2.71937700  
H 3.67232700 6.12297100 -0.62956600  
Cl 2.89827600 5.66105500 2.07476000

C -0.63770200 -2.99540000 -4.39718900  
H -0.13089300 -3.96736800 -4.33489500  
H -1.69268300 -3.16677400 -4.63278300  
H -0.17642100 -2.45014500 -5.23111400  
H -2.52954700 -1.95241100 -2.58513300  
C 1.01275300 -1.50337500 -0.19636700  
C 2.21032300 -0.91531500 -0.19828600  
H 2.27766800 0.15967400 -0.35373500  
H 0.87487900 -2.57721000 -0.05207600  
C 3.51162600 -1.56376000 -0.00495200  
C 4.66258100 -0.76923900 0.01298600  
C 3.67199400 -2.95085700 0.16694200  
C 5.93210100 -1.31396300 0.19740000  
H 4.56564200 0.30683500 -0.11826700  
C 4.92328300 -3.50792600 0.35063000  
H 2.80441600 -3.60556700 0.15373000  
C 6.06664100 -2.69365300 0.36911500  
H 6.79674800 -0.65877600 0.20513800  
H 5.04548600 -4.57946800 0.48228800  
O 7.24260000 -3.33303200 0.55607200  
C 8.42438900 -2.55717100 0.58355000  
H 9.24161200 -3.26293700 0.74355200  
H 8.58080700 -2.03328700 -0.36805300  
H 8.40716500 -1.83168600 1.40687300

### **TS11b<sub>o</sub>**

Bi 1.14108900 0.37062000 -0.20404400  
S 4.31038900 -0.00901900 0.36943900  
O 5.75477000 -0.03003300 0.59091800  
O 3.64166500 1.22386900 -0.13818400  
C 3.42533700 -0.38576600 1.86503100  
C 2.04513800 -0.20430500 1.81144600  
C 1.29919600 -0.44535600 2.95803200  
H 0.22081500 -0.30438600 2.94894000  
C 1.94417100 -0.86560000 4.12529800  
H 1.35960500 -1.05121400 5.02298000  
C 3.32694300 -1.05023900 4.15187000  
H 3.81564600 -1.37446200 5.06647300  
C 4.08975500 -0.81328200 3.00931500  
H 5.16899000 -0.93891200 3.00808600  
C 3.81908000 -1.26627300 -0.78840300  
C 2.49438900 -1.21837800 -1.22138600  
C 2.07083900 -2.16846600 -2.14338000  
H 1.04744900 -2.16460900 -2.50948100

C 2.96921800 -3.13400100 -2.60928400  
H 2.63265000 -3.87052100 -3.33482200  
C 4.28692300 -3.16475900 -2.15419300  
H 4.97529200 -3.91893600 -2.52525400  
C 4.72768200 -2.22484000 -1.22439500  
H 5.75056200 -2.22221700 -0.85788700  
C 0.54909700 2.69620700 -0.72157400  
C -0.37400500 2.87405200 -1.72893100  
H -1.07064200 2.09042100 -2.01376200  
C -0.37959000 4.12058200 -2.36172700  
H -1.08666500 4.29893400 -3.16851300  
C 0.50437800 5.12203200 -1.96031600  
C 1.40760800 4.88742800 -0.92474200  
H 2.09350600 5.66772100 -0.60331600  
C 1.44382700 3.64776500 -0.27624400  
H 2.14338000 3.45817700 0.53139900  
C -2.82808200 1.50972800 0.41114900  
H -2.58881600 0.80673400 -0.38235300  
O -0.53678700 1.71364600 0.93602300  
O -0.77770500 -0.39239700 -1.85348400  
C -1.10604100 -1.16511000 -0.92625000  
O -0.40379900 -1.25566300 0.14613300  
C -2.34009900 -1.99104600 -1.01791200  
C -2.75946600 -2.73722000 0.08603300  
C -3.09292400 -1.98018300 -2.19482100  
C -3.93848500 -3.46500800 -0.00641300  
H -2.17375700 -2.73231800 0.99887400  
C -4.26729800 -2.72213600 -2.26817900  
H -2.75169700 -1.38613700 -3.03681500  
C -4.70000800 -3.46838000 -1.17341800  
H -4.85750200 -2.72042000 -3.18045500  
H -5.61872500 -4.04508000 -1.22230000  
Cl -4.47773500 -4.38999200 1.36643800  
H 0.48602200 6.09010000 -2.45346500  
C -1.78790300 2.00651400 1.14500600  
H -1.98211400 2.70249400 1.97083000  
C -4.23991500 1.77087000 0.62347600  
C -5.18223600 0.95858000 -0.03722600  
C -4.73036600 2.79729900 1.45583000  
C -6.54871300 1.14971100 0.13477900  
H -4.82521900 0.16023300 -0.68488100  
C -6.09594200 2.98607300 1.62648500  
H -4.03586500 3.46192500 1.96259900  
C -7.01571400 2.16397000 0.97044700



H -7.25211400 0.50265300 -0.38421300  
H -6.44869700 3.78707200 2.27205700  
H -8.08319500 2.31731900 1.10675200

### **Int15b**

Bi -0.06035400 -0.85181200 0.54328300  
S -2.86436900 -1.49565600 -1.38352900  
O -3.17220100 -1.52857400 0.05351500  
O -3.91386200 -1.72397100 -2.37898900  
C -2.13055500 0.10219700 -1.69363900  
C -1.12865700 0.61308400 -0.86619400  
C -0.67020300 1.90654300 -1.06824100  
H 0.10545100 2.31889800 -0.43232900  
C -1.22447800 2.68490200 -2.08681300  
H -0.87676700 3.70587300 -2.22112700  
C -2.21552500 2.16860100 -2.91634900  
H -2.64177200 2.77806700 -3.70796000  
C -2.67184300 0.86814300 -2.72476100  
H -3.45123200 0.44203000 -3.34974300  
C -1.57953300 -2.70248700 -1.61171900  
C -0.49334200 -2.68171600 -0.73533500  
C 0.44104500 -3.70864600 -0.81247300  
H 1.30004900 -3.72507500 -0.14558200  
C 0.27879300 -4.73279900 -1.75024100  
H 1.00750900 -5.53826400 -1.79447100  
C -0.80335100 -4.72589600 -2.62690800  
H -0.92018400 -5.52168300 -3.35725600  
C -1.74801000 -3.70286700 -2.56284300  
H -2.61159100 -3.68456500 -3.22140200  
C 1.41359300 -1.65352800 2.05618000  
C 0.99671700 -1.78664500 3.37642200  
H 0.00527800 -1.47197800 3.68242000  
C 1.89384200 -2.32280100 4.30326600  
H 1.58597000 -2.42761400 5.34065700  
C 3.17144400 -2.71220200 3.90667300  
C 3.56475200 -2.57022200 2.57722400  
H 4.56174200 -2.87031200 2.26383000  
C 2.68283500 -2.03640600 1.63564100  
H 2.99518500 -1.92208500 0.60201800  
O 1.75061300 -0.53896200 -0.89220900  
C 5.20955100 2.75168900 -0.97806400  
C 4.05695900 2.22616400 -0.40969500  
C 3.47338900 1.09632000 -0.98818000  
C 4.04162200 0.50613900 -2.11979000

C 5.19607100 1.04991500 -2.67421700  
C 5.78903100 2.17637700 -2.10728700  
H 3.60815800 2.67467300 0.47048900  
H 3.57031300 -0.36865700 -2.55614000  
H 5.64259600 0.59845000 -3.55588400  
H 6.69002000 2.60523800 -2.53541700  
C 2.23578900 0.53489700 -0.38264100  
O 1.68849500 1.09412500 0.59492300  
Cl 5.94661100 4.15973000 -0.26526300  
O -1.39003000 -0.41425300 2.23828500  
C -2.26759800 1.73799600 1.81998400  
H -1.26119100 2.15239200 1.87847300  
H 3.86400900 -3.12485600 4.63575800  
C -2.41205800 0.40875700 2.03431200  
H -3.39540700 -0.06341400 2.03338100  
C -3.34319800 2.66504600 1.49616300  
C -3.12864000 4.04780100 1.63263400  
C -4.58955100 2.23887200 0.99932300  
C -4.12370900 4.96709400 1.31473900  
H -2.16638500 4.39801500 2.00156300  
C -5.58527500 3.15775600 0.68920100  
H -4.76874500 1.18038000 0.83037400  
C -5.36132600 4.52720700 0.84585200  
H -3.93223600 6.03109300 1.43390400  
H -6.53929800 2.80338400 0.30556500  
H -6.14018400 5.24287100 0.59480500

### **TS10f**

Bi 0.98091500 -0.44213400 -0.38226100  
S 3.27500800 -2.78980300 0.13642300  
O 4.23451800 -3.86926500 0.37415100  
O 1.84725700 -3.09173700 -0.13013200  
C 3.78792300 -1.79444600 -1.24396000  
C 2.88141100 -0.82037700 -1.65758600  
C 3.21541500 -0.04407200 -2.76184600  
H 2.53709300 0.73222300 -3.11347300  
C 4.42908800 -0.25559500 -3.42461500  
H 4.68175900 0.35143300 -4.29071900  
C 5.32046500 -1.23310600 -2.98294600  
H 6.26093400 -1.38892100 -3.50435100  
C 5.00733200 -2.01777900 -1.87338000  
H 5.68037300 -2.79173300 -1.51487100  
C 3.24410100 -1.67630100 1.52626700  
C 2.27221000 -0.67522600 1.53840700

C 2.20512000 0.16619800 2.64213500  
H 1.45440800 0.94855300 2.69314600  
C 3.10098400 -0.00338000 3.70275700  
H 3.03633100 0.65559400 4.56522700  
C 4.07197500 -1.00201900 3.66515700  
H 4.76376700 -1.12444700 4.49389800  
C 4.15363900 -1.85231900 2.56461000  
H 4.89309100 -2.64677300 2.51286000  
C -0.97501600 -1.81044600 -0.47042000  
C -1.97479000 -1.61811300 0.40923500  
H -2.15690200 -0.60606800 0.77399300  
O -0.29489900 1.26220400 0.98373000  
C 0.42300400 2.17131800 0.49080500  
O 1.41270500 1.90107800 -0.26592600  
C 0.11076000 3.59967100 0.78161400  
C 0.93127000 4.60696200 0.26877000  
C -1.00644600 3.92213400 1.55594600  
C 0.61736100 5.93199200 0.54253500  
H 1.79613600 4.34637400 -0.33204500  
C -1.30415900 5.25596900 1.81607300  
H -1.62891300 3.12162300 1.94331100  
C -0.49388700 6.27158100 1.31144600  
H -2.17213100 5.51450800 2.41659000  
H -0.71973500 7.31477700 1.51100700  
Cl 1.63476900 7.19672900 -0.09042900  
H -0.77189500 -2.77653200 -0.93222900  
C -0.75158500 -0.13077800 -1.91564600  
C -1.73129200 0.80283600 -1.79209600  
H -1.42456100 1.83531800 -1.60710100  
H -0.52531100 -0.91181300 -2.63515900  
C -3.14328900 0.54751800 -1.62185400  
C -3.97759200 1.55753700 -1.11198000  
C -3.72855100 -0.70824100 -1.89298600  
C -5.32928000 1.34085200 -0.87549400  
H -3.54923800 2.53216600 -0.88549800  
C -5.07356400 -0.93532000 -1.66782700  
H -3.11402300 -1.50702600 -2.29553500  
C -5.88446100 0.08328000 -1.14908200  
H -5.93644900 2.14604200 -0.47563300  
H -5.51921700 -1.90445800 -1.87314300  
C -2.89493800 -2.63476600 0.92274500  
C -4.06942400 -2.21580900 1.56824200  
C -2.66419000 -4.01356700 0.78687600  
C -4.99491300 -3.14054400 2.04248900

H -4.25809300 -1.15012600 1.68096600  
C -3.58825000 -4.93675700 1.26217700  
H -1.74542600 -4.36267500 0.32230500  
C -4.76009400 -4.50625300 1.88875500  
H -5.90251400 -2.79393900 2.53102600  
H -3.38984300 -6.00036600 1.15288000  
H -5.47934000 -5.23153600 2.26095200  
O -7.18285200 -0.23562100 -0.95020900  
C -8.04280500 0.75893400 -0.43148400  
H -9.02625000 0.29177600 -0.35154800  
H -7.71861100 1.08928300 0.56385700  
H -8.10762400 1.62358800 -1.10452500

### TS11f<sub>0</sub>

Bi 0.80896900 0.12619900 0.37013400  
S 4.04133000 -0.69995600 0.03479600  
O 3.62485600 0.45772300 0.85446800  
O 5.45295000 -1.05589300 -0.11452600  
C 3.13942900 -2.06991100 0.72595300  
C 1.80967700 -1.85523300 1.07672800  
C 1.08978400 -2.87275400 1.68589800  
H 0.04994100 -2.72426400 1.96336800  
C 1.71957900 -4.09790200 1.93372000  
H 1.16020200 -4.89520200 2.41693000  
C 3.04772900 -4.30609200 1.56728300  
H 3.52472800 -5.26195800 1.76515700  
C 3.77347600 -3.28753200 0.95154100  
H 4.81346000 -3.42037400 0.66608200  
C 3.31114200 -0.40921300 -1.56181000  
C 1.99225400 0.04563400 -1.57465900  
C 1.41122200 0.32246200 -2.81009500  
H 0.37735600 0.65528100 -2.86904500  
C 2.14896600 0.15768200 -3.98600800  
H 1.68770200 0.38434100 -4.94407900  
C 3.46371800 -0.30346400 -3.94273000  
H 4.02791400 -0.43284900 -4.86218700  
C 4.05926900 -0.60121300 -2.71817400  
H 5.08301500 -0.95915900 -2.65538000  
C -0.53768500 2.05866300 0.07897900  
C -1.73276700 2.12036300 0.66107800  
H -1.97817600 1.44118000 1.47574500  
O -0.73985700 -1.09327300 -0.84020500  
C -5.19021000 -2.58985000 0.01429200  
C -3.98325500 -2.07314100 0.46588500

C -2.94596600 -1.87774900 -0.44906300  
C -3.12273300 -2.20230400 -1.79588700  
C -4.33907900 -2.72267200 -2.22719600  
C -5.38328100 -2.91965400 -1.32558200  
H -3.83502600 -1.81758800 1.51002700  
H -2.30514000 -2.04206700 -2.49118900  
H -4.48278300 -2.97778800 -3.27360900  
H -6.33567800 -3.32305400 -1.65607100  
C -1.65819800 -1.30016700 0.03391900  
O -1.49989500 -1.01847500 1.24094600  
Cl -6.49199600 -2.83043700 1.14827600  
O 1.29778100 2.23925700 1.24751100  
C 2.23552500 4.32518200 1.79648100  
H 1.53055100 4.42189600 2.62226000  
C 2.18583200 3.19393600 1.05265600  
H 2.88603400 3.05697700 0.21975800  
H -0.13219600 2.66748800 -0.72505700  
C 3.18871800 5.44057200 1.54360100  
H 3.85692800 5.21821700 0.70373500  
H 2.66298200 6.38013600 1.31998200  
H 3.81053400 5.63844400 2.42836000  
C -2.81429700 3.00346800 0.20012800  
C -4.14366200 2.61947700 0.43325100  
C -2.56718000 4.20965700 -0.47324700  
C -5.19847800 3.41122000 -0.01005400  
H -4.34447600 1.68852400 0.95932100  
C -3.62342600 4.99800700 -0.91709100  
H -1.54307900 4.54200500 -0.62391100  
C -4.94235300 4.60123700 -0.69095700  
H -6.22271600 3.09849600 0.17707500  
H -3.41728600 5.93409200 -1.43029800  
H -5.76572800 5.22242300 -1.03411500

#### **Int14a**

Bi -0.70492100 -0.70936100 -0.28701300  
S -3.62200500 1.19774700 -0.19023600  
O -4.75575200 2.11377300 -0.03976200  
O -3.67618000 0.11124900 -1.18314400  
C -3.27800400 0.43056000 1.36915800  
C -2.22425500 -0.48365400 1.42430000  
C -2.00006000 -1.13472900 2.63420000  
H -1.18028400 -1.84288200 2.72477400  
C -2.82056200 -0.88545100 3.73843500  
H -2.63709700 -1.41232300 4.67169600

C -3.86099600 0.03649000 3.65550400  
H -4.49107100 0.23253900 4.51864900  
C -4.09575300 0.71106300 2.45909000  
H -4.90221400 1.43200800 2.36110300  
C -2.16444200 2.14540500 -0.58678300  
C -0.93587800 1.51413200 -0.80789400  
C 0.11814300 2.27640700 -1.29423200  
H 1.07199300 1.81554900 -1.51748300  
C -0.04735100 3.64432200 -1.52394700  
H 0.78947700 4.22165600 -1.90865400  
C -1.26314300 4.26702800 -1.25950200  
H -1.38465900 5.33332800 -1.42831900  
C -2.33604900 3.51280400 -0.79447800  
H -3.30770200 3.96166200 -0.61014400  
C -1.49818900 -1.77371400 -2.06534100  
C -0.70723600 -2.61676800 -2.72878700  
H 0.31706900 -2.78785500 -2.39039300  
O 1.51428100 -0.46082600 -1.30732600  
C 2.11097400 0.03121400 -0.29487700  
O 1.50205100 0.36652900 0.75049200  
C 3.59380600 0.21515300 -0.37546500  
C 4.26775800 0.79121000 0.70398900  
C 4.29904000 -0.18479500 -1.51276300  
C 5.64443500 0.95662900 0.62780900  
H 3.70920000 1.10176900 1.58089200  
C 5.67873300 -0.01073700 -1.56912900  
H 3.75589600 -0.62956600 -2.34043300  
C 6.36315900 0.56165600 -0.49843300  
H 6.23243000 -0.32086900 -2.45132200  
H 7.43930700 0.70140100 -0.53555000  
Cl 6.49330100 1.67498900 1.97123000  
C -1.11998300 -3.36353000 -3.95783800  
H -1.01991000 -4.44607300 -3.80436800  
H -2.15513500 -3.14455900 -4.23805800  
H -0.46720900 -3.10079900 -4.80072500  
H -2.51674500 -1.52769800 -2.35445100  
C 1.82134200 -3.73719400 2.19382400  
H 1.64304100 -3.78283900 3.27630800  
H 1.40224900 -4.63740800 1.73288300  
H 2.91019000 -3.74769400 2.05253500  
C 0.32868700 -2.46995700 0.64803100  
C 1.23814000 -2.48414600 1.61801300  
H 1.60681700 -1.54362700 2.02527800  
H -0.09030500 -3.37969300 0.21138800

**Int14e**

Bi 0.74683800 -0.19506400 0.12035500  
S 3.23600000 -2.52470100 0.69636500  
O 4.18141600 -3.61403500 0.95240400  
O 3.72533400 -1.19049600 0.30530900  
C 2.22190400 -2.27469800 2.12853700  
C 1.27078200 -1.25606000 2.07138700  
C 0.48219100 -1.03218600 3.19552900  
H -0.29696900 -0.27264000 3.17368400  
C 0.67596200 -1.79210600 4.35262200  
H 0.06145600 -1.59973300 5.22853400  
C 1.63841100 -2.79897700 4.38741000  
H 1.78010500 -3.38946000 5.28834000  
C 2.41864700 -3.05703400 3.26181800  
H 3.17191800 -3.83955400 3.25824400  
C 2.11122300 -3.02058000 -0.59658500  
C 1.13013000 -2.13628000 -1.05645800  
C 0.38251400 -2.50245700 -2.16852400  
H -0.36581400 -1.82901700 -2.57078800  
C 0.59888500 -3.73619500 -2.78787100  
H 0.00678000 -4.00356100 -3.65954000  
C 1.55525800 -4.61995800 -2.29679600  
H 1.71283500 -5.58231200 -2.77567800  
C 2.32514600 -4.26087600 -1.19407000  
H 3.09727200 -4.91723600 -0.80310600  
C 2.25829300 1.16656000 -0.77570900  
C 1.90998200 2.43459800 -1.01645900  
H 0.90595000 2.77011000 -0.74430500  
O -1.00478600 0.12881900 -1.52535800  
C -1.87237800 -0.60172500 -0.94137300  
O -1.60411900 -1.24209700 0.10498200  
C -3.24380400 -0.67530000 -1.52846200  
C -4.20564800 -1.47690800 -0.90874700  
C -3.56387800 0.05486200 -2.67552800  
C -5.48251800 -1.53441500 -1.45144900  
H -3.94428500 -2.03865900 -0.01796600  
C -4.84958500 -0.01743000 -3.20319800  
H -2.80176600 0.67296300 -3.13936700  
C -5.81900600 -0.81285500 -2.59514700  
H -5.10585000 0.54814200 -4.09496300  
H -6.82399000 -0.87372200 -3.00175800  
Cl -6.69121500 -2.52896800 -0.68530300  
H 3.21245100 0.71001900 -1.02132300

C -0.33855100 1.44593300 1.22228700  
C -1.61075400 1.83593600 1.14762900  
H -2.29594800 1.31115100 0.48512500  
H 0.39620800 1.93149700 1.86833500  
C -2.23816900 2.93743300 1.89408300  
C -3.61029800 3.16316200 1.71388600  
C -1.53347100 3.76897900 2.77842300  
C -4.26375400 4.18545500 2.39741200  
H -4.16696500 2.52485300 1.03049100  
C -2.18474900 4.78976400 3.45992400  
H -0.46805700 3.61966100 2.93401100  
C -3.55281400 5.00232100 3.27379200  
H -5.32851400 4.34285200 2.24480500  
H -1.62373900 5.42530800 4.14063300  
H -4.05848600 5.80176900 3.80931500  
C 2.74531800 3.47418300 -1.63331900  
C 2.16504600 4.71955000 -1.91308800  
C 4.09796200 3.27684500 -1.95140300  
C 2.90798700 5.73820000 -2.50431400  
H 1.11796500 4.88410800 -1.66648800  
C 4.84003300 4.29381600 -2.53931800  
H 4.57323700 2.32460100 -1.73122900  
C 4.24851200 5.52787900 -2.82020100  
H 2.43941100 6.69587000 -2.71678600  
H 5.88728700 4.12621400 -2.77821400  
H 4.83302200 6.32062500 -3.28020700

**TS11c**

Bi -0.69444600 0.63685900 -0.28740300  
S -3.61485400 -0.89797300 -0.42536200  
O -3.34613900 0.41039700 -1.06719600  
O -4.91954600 -1.54824200 -0.55028300  
C -2.33625600 -1.97003700 -1.05309100  
C -1.04562800 -1.45263500 -1.16861900  
C -0.04822200 -2.24396800 -1.71991700  
H 0.96018700 -1.85814800 -1.83642400  
C -0.35390600 -3.54181500 -2.14222400  
H 0.42754300 -4.15597900 -2.58275100  
C -1.64375600 -4.05106400 -2.00812000  
H -1.86988700 -5.06042200 -2.34031000  
C -2.65246000 -3.26334100 -1.45685300  
H -3.67001700 -3.63034100 -1.35573000  
C -3.20649900 -0.63595900 1.28129600  
C -2.05854600 0.12028300 1.51107100

C -1.71418300 0.39445000 2.83156900  
H -0.81709900 0.96598700 3.05696500  
C -2.51839700 -0.07289700 3.87573600  
H -2.24803500 0.15508800 4.90407000  
C -3.65851600 -0.83274700 3.61453000  
H -4.27455600 -1.19231700 4.43416100  
C -4.01297800 -1.13138900 2.30011500  
H -4.89796000 -1.71693100 2.06692400  
C -0.02480700 2.74781700 0.46461100  
C 1.02611400 2.89653800 1.26529300  
H 1.86446200 2.20196600 1.21481100  
O 0.92303000 -0.33804200 1.05963500  
C 5.54475800 -1.23695900 0.25832300  
C 4.32347200 -0.72533600 -0.15977400  
C 3.22415300 -0.81761400 0.69742100  
C 3.35174400 -1.41714600 1.95280700  
C 4.58443600 -1.92426500 2.35120300  
C 5.69016000 -1.83769000 1.50740000  
H 4.21126400 -0.25969100 -1.13340000  
H 2.48373600 -1.48244900 2.60087700  
H 4.69203400 -2.39369700 3.32513400  
H 6.65446000 -2.23229500 1.81318000  
C 1.91383800 -0.27346600 0.25171000  
O 1.77975300 0.23433100 -0.88732900  
Cl 6.92234500 -1.12646400 -0.80141600  
O -0.95058700 1.57196200 -2.33431800  
C 0.67028700 3.25425400 -2.03439100  
H 1.44905100 2.50184300 -1.92226900  
C -0.59569300 2.82770100 -2.32093800  
H -1.39736800 3.56922800 -2.45161400  
H -0.89145600 3.40935800 0.46769500  
C 1.05579500 4.68725900 -1.94732200  
H 0.20403400 5.35079000 -2.13696700  
H 1.45533500 4.92361500 -0.94991100  
H 1.84787800 4.93279900 -2.66787000  
C 1.16490400 4.01359700 2.25710500  
H 1.28858800 3.61615900 3.27343800  
H 2.05945100 4.61196700 2.03831700  
H 0.29415100 4.67690800 2.24823700

**TS10g**

Bi -0.74931000 -0.72831300 0.42201200  
S -0.88358800 -3.98888600 -0.15889500  
O -0.87931500 -5.42851400 -0.41669600

O 0.35135500 -3.29114900 0.27692900  
C -2.08630900 -3.58069000 1.08449500  
C -2.08330100 -2.25646900 1.51828200  
C -2.97273200 -1.88985600 2.52140300  
H -3.00592500 -0.86199800 2.87950500  
C -3.83465200 -2.84492900 3.07100200  
H -4.52442600 -2.55531100 3.85988400  
C -3.82195900 -4.16226300 2.61373000  
H -4.49655100 -4.89566300 3.04671300  
C -2.94218400 -4.54629700 1.60189600  
H -2.90783500 -5.56822300 1.23478800  
C -1.39943400 -3.10175100 -1.61437000  
C -1.30596400 -1.70945500 -1.59791800  
C -1.65334400 -1.00458700 -2.74274400  
H -1.58324300 0.07829300 -2.76645700  
C -2.08408200 -1.69765300 -3.87892400  
H -2.34636900 -1.14021200 -4.77472700  
C -2.18148400 -3.08729000 -3.87382600  
H -2.51784400 -3.61535300 -4.76164200  
C -1.84017200 -3.80640500 -2.73011500  
H -1.89626400 -4.89109900 -2.70246200  
C 1.59901600 -0.51729400 0.80029900  
C 2.35509000 0.28595100 0.02502900  
H 1.90245200 1.18532200 -0.39434500  
O -0.74278600 1.41800900 -0.89398700  
C -1.93387800 1.61934800 -0.53818300  
O -2.57867800 0.74604400 0.13291200  
C -2.61007700 2.89780800 -0.88951000  
C -3.94525700 3.09526800 -0.52957700  
C -1.90312300 3.89468100 -1.56653500  
C -4.55718600 4.29815300 -0.85750000  
H -4.48505400 2.31539900 -0.00308500  
C -2.53481900 5.09286200 -1.88348300  
H -0.86601500 3.71887600 -1.83433500  
C -3.86694800 5.30345200 -1.53172400  
H -1.99185800 5.87386600 -2.40866300  
H -4.36581800 6.23614100 -1.77697000  
Cl -6.22190900 4.55501000 -0.41522500  
H 2.00950100 -1.39250800 1.30390600  
C 0.20010100 0.58440600 2.08743800  
C 0.35556800 1.93262000 2.01094600  
H -0.51406300 2.52903000 1.72588700  
H 0.43505000 -0.16994100 2.83234100  
C 1.61139100 2.65112300 2.02153200

C 1.64719000 3.98381200 1.56324800  
C 2.82059100 2.05053400 2.42398600  
C 2.84369900 4.68491300 1.50418200  
H 0.72048600 4.45663600 1.24325800  
C 4.01664600 2.75755300 2.36727300  
H 2.81209500 1.03120600 2.79668600  
C 4.03607400 4.07172100 1.90083400  
H 2.85285600 5.71046700 1.14333200  
H 4.94033700 2.27788600 2.68111900  
H 4.97415800 4.61860500 1.84998000  
C 3.76744000 0.10592800 -0.29154800  
C 4.45926300 1.17004900 -0.89933800  
C 4.47565400 -1.07619200 -0.00337500  
C 5.80995300 1.07643400 -1.19219500  
H 3.92340300 2.08836600 -1.12569600  
C 5.82518500 -1.18479500 -0.28980200  
H 3.95884000 -1.92401600 0.43689600  
C 6.48185000 -0.10340000 -0.87930000  
H 6.34518100 1.89970700 -1.65195600  
H 6.37317200 -2.09464900 -0.07163400  
N 7.89787000 -0.21188000 -1.17663700  
O 8.46945500 -1.25769500 -0.88900300  
O 8.45301700 0.74900000 -1.69833100

#### **Int14d**

Bi -1.10250500 -0.63326500 -0.56376200  
S -4.25128400 -1.52118500 0.51932400  
O -5.57998600 -1.79806600 1.06936000  
O -3.77433300 -2.23567300 -0.67881400  
C -3.02511500 -1.79592100 1.76996600  
C -1.68902500 -1.61178500 1.41284200  
C -0.71459700 -1.84672800 2.37734900  
H 0.33540700 -1.67790800 2.14741200  
C -1.07979200 -2.28655500 3.65308300  
H -0.30828300 -2.47662000 4.39498200  
C -2.42067400 -2.46916700 3.98377200  
H -2.69788200 -2.80518300 4.97906400  
C -3.41265400 -2.21340200 3.03887200  
H -4.46614900 -2.34200600 3.26999900  
C -4.13159500 0.21174100 0.11853700  
C -2.96860300 0.71514900 -0.47214200  
C -2.97214200 2.03220500 -0.91370000  
H -2.09958200 2.44791600 -1.40475000  
C -4.10719800 2.82931900 -0.74307900

H -4.09252700 3.85649500 -1.09861400  
C -5.24482300 2.32298600 -0.12136600  
H -6.12127700 2.94960400 0.01767900  
C -5.26413500 0.99985300 0.31047500  
H -6.14542900 0.56662400 0.77465300  
C -1.42093700 -1.75597100 -2.45766600  
C -0.39437000 -1.95359700 -3.28288800  
H 0.60192400 -1.59481700 -3.01147800  
O -0.07418800 1.32894600 -1.55501600  
C 0.17265500 1.91431400 -0.45012400  
O -0.18414200 1.42408100 0.65117100  
C 0.91650300 3.20812300 -0.48220800  
C 1.16286100 3.87983800 0.71778100  
C 1.36807500 3.73604200 -1.69419400  
C 1.86305200 5.07867600 0.68486500  
H 0.80515600 3.46028900 1.65230300  
C 2.06814900 4.93873000 -1.70472900  
H 1.16677600 3.19711900 -2.61451100  
C 2.32111800 5.61931900 -0.51514400  
H 2.42285000 5.35526100 -2.64351500  
H 2.86664600 6.55817600 -0.51669800  
Cl 2.17705500 5.92350800 2.17569300  
C -0.49688000 -2.64955900 -4.60317500  
H 0.17074700 -3.52063200 -4.63162900  
H -1.51804700 -2.98548800 -4.80813400  
H -0.17931700 -1.97954400 -5.41283600  
H -2.44527600 -2.06533500 -2.65079100  
C 1.05101300 -1.29749400 -0.32524500  
C 2.15364800 -0.58008600 -0.10763100  
H 2.08669600 0.50122700 -0.01266200  
H 1.06936100 -2.38491300 -0.43050200  
C 3.52021900 -1.10385000 0.02655400  
C 4.57765200 -0.18393100 0.10341500  
C 3.81473100 -2.47618800 0.08738200  
C 5.89298000 -0.60913000 0.22530100  
H 4.36053400 0.88056700 0.06269900  
C 5.12135400 -2.91792100 0.21120400  
H 3.01339600 -3.20782000 0.04653500  
C 6.14695000 -1.97569400 0.27647200  
H 6.71156300 0.09968600 0.28135800  
H 5.35482000 -3.97555700 0.26179000  
N 7.52271500 -2.43723800 0.40780500  
O 8.40767600 -1.59373000 0.46456500  
O 7.71958700 -3.64456000 0.45396400

**TS11d<sub>o</sub>**

Bi -1.16705800 -0.58859200 -0.31037000  
S -4.35809700 -0.48460000 0.21202000  
O -5.80509400 -0.59077000 0.38635800  
O -3.59011400 -1.59721300 -0.42096400  
C -3.53737400 -0.23056000 1.76910600  
C -2.14633900 -0.30061900 1.73632800  
C -1.44732900 -0.13445300 2.92527100  
H -0.36119200 -0.18940200 2.93437100  
C -2.14853300 0.10073900 4.11193700  
H -1.59977600 0.22770400 5.04187300  
C -3.54182600 0.17592700 4.11730500  
H -4.07388100 0.35695900 5.04715900  
C -4.25850900 0.01359500 2.93271300  
H -5.34393400 0.05879000 2.91206900  
C -3.92958600 0.93980400 -0.76441200  
C -2.59446400 1.03825400 -1.15457200  
C -2.21841800 2.13108500 -1.92763900  
H -1.18883900 2.24521700 -2.25676100  
C -3.17157000 3.08811100 -2.29111900  
H -2.87097100 3.93694200 -2.90057700  
C -4.49884900 2.96878600 -1.88057600  
H -5.22963200 3.71849800 -2.17066600  
C -4.89375200 1.88457900 -1.09885100  
H -5.92193600 1.76486700 -0.76825900  
C -0.46540300 -2.77497600 -1.14603600  
C 0.34163900 -2.81684800 -2.18559600  
H 0.99385300 -1.97076700 -2.40794600  
C 2.81655400 -1.68543500 0.15812600  
H 2.53753900 -0.90385300 -0.54376500  
O 0.54128000 -2.04317600 0.67022300  
O 0.70327400 0.47673100 -1.81956300  
C 1.01480600 1.11445500 -0.78912900  
O 0.31424800 1.02602800 0.28476500  
C 2.22705900 1.97573500 -0.76204100  
C 2.63840500 2.56188900 0.43722300  
C 2.97327300 2.15024300 -1.93017400  
C 3.80429500 3.31649800 0.44794000  
H 2.05816200 2.41299000 1.34140100  
C 4.13402200 2.91591300 -1.89846800  
H 2.63783000 1.67803100 -2.84807000  
C 4.55989600 3.50230100 -0.70796800  
H 4.71902800 3.05741600 -2.80309200

H 5.46867500 4.09558200 -0.67477000  
Cl 4.33438300 4.04247900 1.93884300  
C 1.80588000 -2.31241400 0.82925300  
H 2.03647400 -3.10935000 1.54850700  
C 0.43341400 -4.01039800 -3.09496700  
H 0.19832400 -3.72518300 -4.12778200  
H 1.45856800 -4.40302900 -3.08501800  
H -0.24755300 -4.81124000 -2.79179200  
H -1.14759500 -3.49039900 -0.69974500  
C 4.24209600 -1.90796300 0.32372500  
C 5.13865700 -1.01728400 -0.29830600  
C 4.79120000 -2.96493000 1.07739800  
C 6.51519500 -1.16646000 -0.16901500  
H 4.73763900 -0.19119100 -0.88240400  
C 6.16656900 -3.11218200 1.20571500  
H 4.13493100 -3.68286100 1.56175100  
C 7.04007900 -2.21527800 0.58549200  
H 7.18106100 -0.45889300 -0.65780400  
H 6.56339800 -3.93773000 1.79218400  
H 8.11543300 -2.33597200 0.68864900

**Int14g**

Bi 0.10501900 0.72276500 0.26691600  
S -0.15415800 4.15243300 0.63722600  
O -0.10620500 5.60968200 0.77463200  
O -1.44938100 3.45081100 0.58489700  
C 0.75496600 3.40626900 1.96379000  
C 0.80469000 2.01308300 2.00880300  
C 1.49646000 1.41310300 3.05606600  
H 1.58946900 0.32971000 3.10192900  
C 2.08939000 2.20057600 4.04724100  
H 2.61816700 1.72075800 4.86693300  
C 2.01895800 3.59061400 3.98556700  
H 2.48677000 4.19653400 4.75650900  
C 1.35393600 4.20949500 2.92860000  
H 1.28855500 5.29095100 2.85191200  
C 0.70714900 3.67854100 -0.85152700  
C 0.77586200 2.33477400 -1.23286400  
C 1.31776100 2.02753600 -2.47439300  
H 1.36227700 0.99867400 -2.81348400  
C 1.79852200 3.04470400 -3.30336000  
H 2.21537700 2.78613500 -4.27346200  
C 1.75363700 4.37453300 -2.89569400  
H 2.13822400 5.16075600 -3.53920100

C 1.19905400 4.70002100 -1.66109600  
H 1.12667300 5.73045600 -1.32526400  
C -2.07841500 0.66318100 -0.19265300  
C -2.70981700 -0.51486800 -0.18648000  
H -2.15519600 -1.41937800 0.07480300  
O 0.84366600 -0.80976100 -1.47203200  
C 2.07224000 -0.77578100 -1.13382600  
O 2.48038700 -0.03401500 -0.20366700  
C 3.03548900 -1.65162800 -1.86268000  
C 4.38608900 -1.62161100 -1.50652500  
C 2.59074900 -2.49644500 -2.88251500  
C 5.27666100 -2.44524600 -2.18228400  
H 4.71917500 -0.96119700 -0.71276100  
C 3.50012800 -3.31348500 -3.54715000  
H 1.53678400 -2.50413300 -3.14149500  
C 4.85017300 -3.29406900 -3.20196000  
H 3.16176800 -3.97305200 -4.34157500  
H 5.56492900 -3.92905400 -3.71659600  
Cl 6.96318300 -2.41776200 -1.74622100  
H -2.52584100 1.61672400 -0.45822800  
C 0.06578900 -1.13743500 1.53545200  
C 0.71532000 -2.28998000 1.37260000  
H 1.39217000 -2.41037900 0.52923800  
H -0.63486500 -0.95440900 2.35306200  
C 0.62467800 -3.48025700 2.23146500  
C 1.36221700 -4.61625000 1.86883200  
C -0.16193700 -3.53424700 3.39252000  
C 1.31501600 -5.77581500 2.63848400  
H 1.97763100 -4.58460200 0.97182100  
C -0.20913300 -4.69082000 4.16094900  
H -0.73850900 -2.66567900 3.70023500  
C 0.52815200 -5.81702400 3.78729900  
H 1.89407000 -6.64620000 2.34047000  
H -0.82275000 -4.71622100 5.05803200  
H 0.48887700 -6.71968000 4.39160800  
C -4.12226400 -0.74408400 -0.51771700  
C -4.58328800 -2.06731800 -0.59935000  
C -5.02875400 0.30308200 -0.75341600  
C -5.90351900 -2.34940000 -0.92028200  
H -3.89139100 -2.88492100 -0.41329200  
C -6.35004700 0.03900500 -1.07339600  
H -4.70037800 1.33532700 -0.68006000  
C -6.77063400 -1.28770200 -1.15543900  
H -6.26224400 -3.37016700 -0.98879400

H -7.05462700 0.84258700 -1.25575800  
N -8.15925500 -1.57038600 -1.49498300  
O -8.90401800 -0.62080500 -1.69946500  
O -8.50646800 -2.74261200 -1.55860400

### TS10a

Bi 0.65657500 0.58076900 0.41708500  
S 3.54901800 -0.79959500 -0.41658500  
O 4.86643800 -1.31825000 -0.78824800  
O 3.38772900 0.61253200 0.01528100  
C 2.84804200 -1.75334900 0.90868000  
C 1.65961400 -1.25502300 1.43792900  
C 1.08149300 -1.94633000 2.49801200  
H 0.14721900 -1.59894200 2.93632400  
C 1.69459800 -3.09776700 3.00250500  
H 1.23816500 -3.62957900 3.83402300  
C 2.88172100 -3.57490900 2.44657900  
H 3.34990100 -4.47042600 2.84597800  
C 3.47392400 -2.90345700 1.37759300  
H 4.40113000 -3.25089900 0.93007800  
C 2.40461600 -0.98183400 -1.76950200  
C 1.15138700 -0.38193500 -1.63762600  
C 0.26248800 -0.48431100 -2.70235300  
H -0.71920700 -0.02429900 -2.64311000  
C 0.63458300 -1.17350700 -3.86102400  
H -0.06677800 -1.24173200 -4.68921800  
C 1.88814500 -1.77333700 -3.96440200  
H 2.16715600 -2.30744600 -4.86850600  
C 2.79066100 -1.68452100 -2.90662200  
H 3.77813500 -2.13437400 -2.96183200  
C 1.36056600 2.93899100 0.45614300  
C 0.87070500 3.71887400 -0.51245500  
H -0.12489500 3.51726300 -0.91315300  
O -1.53328400 1.26941400 -0.73855400  
C -2.06291500 0.23882000 -0.25303100  
O -1.38124500 -0.61161400 0.41341100  
C -3.51921900 -0.01613900 -0.44503600  
C -4.09301100 -1.17921200 0.07415000  
C -4.30222400 0.90898600 -1.13940500  
C -5.45193400 -1.39788300 -0.11124800  
H -3.47718800 -1.89318800 0.61063000  
C -5.66189100 0.67106500 -1.31297700  
H -3.83472900 1.80537400 -1.53433500  
C -6.24765000 -0.48489100 -0.79995500



H -6.27689900 1.38744000 -1.85079800  
H -7.30814400 -0.67732400 -0.93190100  
Cl -6.17733000 -2.84576400 0.53183100  
C 1.60523300 4.87419300 -1.12426400  
H 1.03935900 5.80830100 -1.00281300  
H 2.59442100 5.00824200 -0.67443500  
H 1.73682500 4.72070000 -2.20393000  
H 2.35287500 3.09477400 0.88179400  
C -1.39191500 4.27050700 1.86553800  
H -2.26700700 4.63204800 2.41955000  
H -0.50815300 4.82938600 2.18390700  
H -1.56478700 4.49679600 0.80180100  
C -0.04850200 2.15567800 2.06597100  
C -1.22428500 2.79786100 2.06525800  
H -2.14050300 2.20197500 2.03977600  
H 0.87521800 2.15749000 2.63048500

#### **TS10b**

Bi -0.73252000 -0.43601800 0.19440400  
S -4.00415100 -0.34475200 -0.32271900  
O -5.44481300 -0.38807200 -0.57607200  
O -3.20624300 -1.59568300 -0.27426800  
C -3.66268600 0.46134800 1.22370900  
C -2.33242200 0.42788700 1.63691800  
C -2.01460000 1.00883800 2.85987400  
H -0.98567800 1.01010000 3.21668000  
C -3.01755500 1.59976800 3.63556400  
H -2.76266200 2.04836000 4.59276300  
C -4.33970400 1.62468100 3.19185200  
H -5.11092600 2.08664700 3.80209500  
C -4.67861200 1.05367900 1.96555100  
H -5.70237000 1.05242300 1.60170300  
C -3.18813900 0.65074100 -1.55361100  
C -1.79277600 0.65794900 -1.56025100  
C -1.14151700 1.39172800 -2.54438900  
H -0.05706900 1.41233300 -2.58798900  
C -1.88682500 2.09818300 -3.49407500  
H -1.36856000 2.66327800 -4.26500800  
C -3.27979800 2.08669200 -3.46221300  
H -3.84889700 2.63940400 -4.20452700  
C -3.94774400 1.35869600 -2.47978800  
H -5.03287200 1.32342400 -2.43619400  
C -0.31422600 -2.78728000 -0.20185200  
C 0.49589300 -3.15751800 -1.19997700

H 1.33748700 -2.51616300 -1.46831400  
O 1.38346900 0.13104300 -1.07540200  
C 1.50827200 1.16100700 -0.36366100  
O 0.61067400 1.49896600 0.47808000  
C 2.72829800 2.00710500 -0.48852000  
C 2.83572500 3.18238100 0.25856400  
C 3.76094100 1.61412900 -1.34341600  
C 3.98471200 3.95287600 0.13503000  
H 2.02876000 3.47826600 0.92049500  
C 4.90415500 2.39963000 -1.45041700  
H 3.65563800 0.69483800 -1.91095700  
C 5.02446200 3.57589500 -0.71241000  
H 5.71229300 2.09967300 -2.11197300  
H 5.91350200 4.19411000 -0.79246600  
Cl 4.12937600 5.42156400 1.06093400  
C 0.33607200 -4.40636600 -2.00950700  
H 1.25831100 -5.00259300 -1.98690300  
H -0.49190300 -5.02446900 -1.64693900  
H 0.14316000 -4.15915000 -3.06254300  
H -1.15281400 -3.40094800 0.13092700  
C 0.70165000 -1.73848800 1.50252400  
C 2.05160700 -1.71981000 1.38540100  
H 2.54762800 -0.74691900 1.42597800  
H -0.02688600 -2.27385800 2.10109600  
C 2.90409800 -2.82036900 0.98018200  
C 4.22028500 -2.55230400 0.55625000  
C 2.45621500 -4.15519100 0.96270900  
C 5.05560900 -3.57628500 0.12930300  
H 4.57511600 -1.52328900 0.55761800  
C 3.29710800 -5.17898400 0.53839100  
H 1.45113000 -4.38389200 1.30248500  
C 4.59570200 -4.89574000 0.11440100  
H 6.06741100 -3.34856300 -0.19736300  
H 2.93775900 -6.20534800 0.53970000  
H 5.24875100 -5.69805800 -0.21977300

#### **Int15d**

Bi -0.02925900 -0.80755900 0.80023300  
S -2.69095000 -1.55793200 -1.30375000  
O -3.16522800 -1.36516800 0.07396800  
O -3.63428500 -1.86343100 -2.38142100  
C -1.80876200 -0.06384900 -1.73641400  
C -0.84896500 0.49339000 -0.88806100  
C -0.27999800 1.71803800 -1.20424000

H 0.47088300 2.15669000 -0.55575200  
C -0.68794000 2.39006300 -2.35874300  
H -0.25526300 3.36048700 -2.58752100  
C -1.63945800 1.83077300 -3.20597900  
H -1.95179400 2.35657300 -4.10364600  
C -2.20200300 0.59505200 -2.89983000  
H -2.95257200 0.14041400 -3.53974100  
C -1.48527400 -2.86186000 -1.20643300  
C -0.49494700 -2.77171200 -0.22759400  
C 0.36645900 -3.84882500 -0.04970500  
H 1.15700700 -3.80438400 0.69681000  
C 0.22247800 -4.99543900 -0.83596800  
H 0.89223200 -5.83785300 -0.68324200  
C -0.76480000 -5.06139500 -1.81636800  
H -0.86667100 -5.95237700 -2.42958900  
C -1.63156300 -3.98697600 -2.01101500  
H -2.41826700 -4.02041300 -2.75908900  
C 0.80891400 -1.55873000 3.71666800  
H -0.24730000 -1.37799900 3.91060100  
O 1.93416800 -0.89210400 -0.46606000  
C 5.73965800 1.98313000 -0.70393400  
C 4.48102700 1.68538900 -0.19878600  
C 3.83810100 0.52215500 -0.62908000  
C 4.45308600 -0.32571000 -1.55335100  
C 5.71429500 -0.00809500 -2.04766400  
C 6.36772600 1.14838000 -1.62618300  
H 3.99360100 2.33563200 0.52024900  
H 3.93484900 -1.22267200 -1.87678800  
H 6.19811500 -0.66167500 -2.76831500  
H 7.35218600 1.40154300 -2.00785400  
C 2.48609800 0.20283300 -0.09140200  
O 1.91416300 0.98301200 0.70491100  
Cl 6.55077500 3.43148300 -0.17459500  
O -1.47750000 -0.10208300 2.29307800  
C -2.23747000 1.99296100 1.50692900  
H -1.22263400 2.38391800 1.57987500  
C -2.44883900 0.71471400 1.89848500  
H -3.44965100 0.28040200 1.89786500  
C 1.64866500 -1.96648800 4.88570500  
H 1.60471400 -1.19429200 5.66455600  
H 1.25857200 -2.89103800 5.33009700  
H 2.69539400 -2.12346400 4.60756000  
C 1.29457000 -1.39498700 2.49064100  
H 2.33264300 -1.51906400 2.18623700

C -3.25482400 2.89175000 0.97762700  
C -3.01635000 4.27702100 0.95988500  
C -4.46579100 2.42614900 0.43158100  
C -3.95757600 5.16448700 0.44695900  
H -2.07962700 4.65606700 1.36442600  
C -5.40890300 3.31434400 -0.07290200  
H -4.65579700 1.35737300 0.37859400  
C -5.16348600 4.68885000 -0.06768800  
H -3.74909400 6.23198300 0.44995000  
H -6.33643400 2.92925000 -0.49050900  
H -5.89986500 5.37972900 -0.47061500

### TS11f

Bi 0.84566900 0.23726900 0.57608000  
S 4.11181400 -0.00909100 -0.03675800  
O 3.59862200 0.73530400 1.13288500  
O 5.54790000 -0.14701200 -0.28204800  
C 3.37112400 -1.62506900 0.10363800  
C 2.03516500 -1.71574900 0.49664200  
C 1.47058200 -2.96497600 0.70618700  
H 0.43819200 -3.05687200 1.02942600  
C 2.24812400 -4.11104000 0.51037900  
H 1.80627300 -5.08897500 0.68415200  
C 3.57491600 -4.01083900 0.09886600  
H 4.16928700 -4.90752500 -0.05245600  
C 4.14992000 -2.75856700 -0.10790900  
H 5.18826000 -2.65211800 -0.40922900  
C 3.31915600 0.75587300 -1.42729800  
C 1.97197700 1.06945300 -1.25690000  
C 1.31439400 1.72732300 -2.29155200  
H 0.25928000 1.97606100 -2.20369800  
C 2.01187900 2.06621300 -3.45534500  
H 1.49495600 2.59091000 -4.25517300  
C 3.35802100 1.73366600 -3.60342400  
H 3.88887300 1.99955700 -4.51340900  
C 4.02955000 1.06280600 -2.58259900  
H 5.07991500 0.79875500 -2.66799100  
C -0.64296800 1.98020400 0.72823200  
C -1.84206700 1.96559700 0.14459300  
H -2.32323700 1.01408200 -0.07812100  
O -0.51971200 -0.71798100 -1.06225100  
C -4.41112500 -3.43914000 -0.53888600  
C -3.34824800 -2.73245600 0.00780200  
C -2.44987600 -2.09471300 -0.85165000

C -2.61695100 -2.16901400 -2.23672800  
C -3.68800600 -2.88410900 -2.76281700  
C -4.59315000 -3.52379400 -1.91794600  
H -3.20863400 -2.66818700 1.08194300  
H -1.90632000 -1.66655300 -2.88503100  
H -3.82532500 -2.94803000 -3.83864000  
H -5.43155100 -4.08280900 -2.32250000  
C -1.31713500 -1.32688200 -0.27225300  
O -1.15024500 -1.26761700 0.97316900  
Cl -5.54044100 -4.23485100 0.52088900  
O 1.18756300 0.40609900 2.76614800  
C -0.94906000 1.20600200 3.38636800  
H -1.41482200 0.30648400 2.98602400  
C 0.40487200 1.29963300 3.33791600  
H 0.90376200 2.19801700 3.72629600  
H -0.09596900 2.88194100 0.99976900  
C -1.83162900 2.25830900 3.95774200  
H -1.25423800 3.09067600 4.37677500  
H -2.50154700 2.66566800 3.18604800  
H -2.47640300 1.85601800 4.75087600  
C -2.64386500 3.14174600 -0.22518600  
C -3.95239000 2.93711700 -0.68673000  
C -2.16197200 4.45763800 -0.14259300  
C -4.76192300 4.01233000 -1.04392600  
H -4.33566400 1.92121000 -0.75981800  
C -2.96902700 5.53021000 -0.50192100  
H -1.14636300 4.64491900 0.19650400  
C -4.27347500 5.31396600 -0.95205000  
H -5.77479800 3.83188900 -1.39520700  
H -2.57866000 6.54263200 -0.43352500  
H -4.90124300 6.15607100 -1.23176700

### **Int15a**

Bi 0.62995100 0.52835800 0.43817900  
S 3.52386100 -0.96838000 -0.67215200  
O 3.67273300 -0.27513700 0.61631300  
O 4.64968600 -1.68064500 -1.28020400  
C 2.17648100 -2.11848600 -0.45032100  
C 1.00279000 -1.72503100 0.19487200  
C 0.02361300 -2.67061200 0.46302000  
H -0.89109300 -2.38287100 0.97020400  
C 0.22477500 -4.00033500 0.08384900  
H -0.54157600 -4.73732200 0.31018500  
C 1.38930200 -4.38343600 -0.57612800

H 1.53612300 -5.41748300 -0.87497700  
C 2.37528900 -3.43926300 -0.84759700  
H 3.30021500 -3.71138900 -1.34789100  
C 2.94163500 0.27523500 -1.79840500  
C 1.90062500 1.09877800 -1.36712600  
C 1.52345900 2.16545300 -2.17550300  
H 0.71793600 2.83116500 -1.87444700  
C 2.18499600 2.39396700 -3.38588200  
H 1.89162100 3.23853100 -4.00427800  
C 3.21042900 1.54965300 -3.80478100  
H 3.71640200 1.73072400 -4.74901900  
C 3.59957200 0.47464300 -3.00719200  
H 4.40920600 -0.18743400 -3.30036200  
C -0.39632800 2.49279200 0.88069400  
C 0.00252500 3.19613200 2.01308100  
H 0.74111700 2.78416100 2.69176100  
C -0.58500100 4.43808500 2.26528800  
H -0.28879000 4.99579200 3.15035500  
C -1.54497600 4.95484500 1.39773200  
C -1.92643500 4.23331300 0.26803600  
H -2.67643300 4.63157500 -0.41107600  
C -1.35107500 2.98975700 -0.00053800  
H -1.65469300 2.43091900 -0.88050700  
O -1.06614000 0.14093400 -1.13094800  
C -5.62965800 -1.14706900 -0.56215300  
C -4.38111200 -0.85730600 -0.02827500  
C -3.33516300 -0.53255300 -0.89562700  
C -3.54368800 -0.50041300 -2.27652700  
C -4.80219700 -0.79666000 -2.79053000  
C -5.85490000 -1.12140500 -1.93713700  
H -4.20771000 -0.87540600 1.04270300  
H -2.71683000 -0.24798100 -2.93249700  
H -4.97207700 -0.77669400 -3.86349200  
H -6.83977700 -1.35244700 -2.33174400  
C -1.99578700 -0.22201800 -0.32606800  
O -1.78853400 -0.31066700 0.90661600  
Cl -6.94279600 -1.55072300 0.50878900  
O 1.44621300 0.62784000 2.45143600  
C 1.31181000 -1.52069800 3.45027600  
H 0.22453700 -1.50579900 3.36474700  
H -1.99915300 5.92076300 1.60341600  
C 2.00521300 -0.46239100 2.99044800  
H 3.09669900 -0.45330900 3.03281600  
C 1.94959800 -2.72624200 4.05446200

H 1.58559600 -2.91069100 5.07474500  
H 1.72211700 -3.63009300 3.47087800  
H 3.04000800 -2.62306600 4.09717700

### **Int15c**

Bi -0.60715300 -0.37355900 0.75650500  
S -3.34134200 0.44367100 -1.23162400  
O -3.71943900 0.50704500 0.18586700  
O -4.31138600 0.76837000 -2.28012400  
C -1.93480900 1.53429900 -1.41681900  
C -0.84340000 1.48326100 -0.54626500  
C 0.15540700 2.44147300 -0.64052500  
H 1.01044500 2.40552700 0.02583600  
C 0.05629900 3.44890500 -1.60359700  
H 0.83588700 4.20414600 -1.66267100  
C -1.02251600 3.48669300 -2.48187800  
H -1.09004600 4.26623200 -3.23552100  
C -2.02534600 2.52533600 -2.39233400  
H -2.88430700 2.53990600 -3.05685400  
C -2.74989300 -1.21264800 -1.49384500  
C -1.80826500 -1.72794900 -0.60257600  
C -1.44567600 -3.06568400 -0.71693800  
H -0.70581500 -3.49535400 -0.04490200  
C -2.03088700 -3.86677500 -1.70134100  
H -1.75177600 -4.91472100 -1.77568200  
C -2.95995300 -3.33034500 -2.58978100  
H -3.40569500 -3.95607900 -3.35794600  
C -3.32809500 -1.98948000 -2.49245700  
H -4.06116700 -1.55124800 -3.16336900  
C 0.02496000 -1.96332700 3.37783400  
H -0.81517600 -1.38542000 3.75979200  
O 1.16140700 -0.89781000 -0.70476400  
C 5.79449800 0.25826600 -0.68410800  
C 4.52195800 0.36063100 -0.13803300  
C 3.46924900 -0.33010100 -0.74288000  
C 3.69621800 -1.11006800 -1.87920300  
C 4.97898200 -1.19819100 -2.41112700  
C 6.03871700 -0.51518900 -1.81714200  
H 4.33427400 0.96254400 0.74504800  
H 2.86363400 -1.63625500 -2.33491100  
H 5.16244400 -1.80147500 -3.29604500  
H 7.04219300 -0.58026700 -2.22696800  
C 2.10141700 -0.21924000 -0.16044400  
O 1.89061900 0.51413100 0.83396900

Cl 7.11408300 1.11626300 0.06383600  
O -1.67429300 0.41229900 2.47616300  
C -1.48022200 2.78079700 2.46573900  
H -0.39227400 2.70545400 2.50884500  
C -2.19996600 1.64480400 2.43327300  
H -3.28970700 1.67938300 2.36444300  
C -2.08430200 4.14489400 2.42296200  
H -1.79821400 4.74496700 3.29799000  
H -1.74930700 4.70150400 1.53577800  
H -3.17889000 4.09543000 2.39050000  
C 0.68245800 -2.91180600 4.32979300  
H 1.05952700 -2.36401100 5.20308800  
H -0.04655600 -3.64290100 4.70206500  
H 1.51616200 -3.44972300 3.86788000  
C 0.42878800 -1.79195100 2.12347100  
H 1.27113500 -2.28932100 1.64491400

### **TS11a**

Bi -0.65589500 0.27921200 -0.45816900  
S -3.58126200 -1.22110900 -0.29237600  
O -3.28303800 -0.07756400 -1.18889900  
O -4.89667800 -1.86157200 -0.29931500  
C -2.31392200 -2.41807000 -0.66633500  
C -1.01554800 -1.94998200 -0.87234600  
C -0.02197900 -2.85420100 -1.22077500  
H 0.99412800 -2.51537500 -1.40140100  
C -0.33910000 -4.20996400 -1.35404900  
H 0.43980600 -4.91385500 -1.63637100  
C -1.63759300 -4.66413300 -1.13296500  
H -1.87297700 -5.71932800 -1.24019800  
C -2.64277400 -3.76479300 -0.78231400  
H -3.66597000 -4.09147700 -0.61853100  
C -3.18362100 -0.61649500 1.32796700  
C -2.03008000 0.16102400 1.40534500  
C -1.69004800 0.70080600 2.64227000  
H -0.79335100 1.30636900 2.75092700  
C -2.50251200 0.46161500 3.75486700  
H -2.23568700 0.89547600 4.71564300  
C -3.64711600 -0.32890500 3.64859200  
H -4.26880800 -0.50902100 4.52133400  
C -3.99922900 -0.88777700 2.42143800  
H -4.88795300 -1.50246200 2.30827300  
C 0.02121000 2.52918400 -0.06705200  
C -1.06605200 3.36013100 0.18734100

H -2.05604500 3.12863000 -0.20178700  
C -0.87664000 4.50979700 0.95517700  
H -1.72151300 5.16558200 1.15233900  
C 0.38439700 4.81015900 1.47092000  
C 1.45992400 3.96215400 1.21298600  
H 2.44614200 4.18931600 1.61150100  
C 1.28365100 2.81340300 0.43698500  
H 2.13358500 2.17150000 0.22619800  
O 0.96122500 -0.37751600 1.08125100  
C 5.61288200 -1.25288000 0.43429900  
C 4.36829800 -0.89717200 -0.06817400  
C 3.28045100 -0.83483600 0.80638000  
C 3.44239700 -1.12629000 2.16302100  
C 4.69833600 -1.48067000 2.64502300  
C 5.79279500 -1.54631100 1.78470600  
H 4.22962600 -0.66909600 -1.11994100  
H 2.58345500 -1.07311600 2.82414400  
H 4.83325100 -1.70970800 3.69848800  
H 6.77537900 -1.82230900 2.15549300  
C 1.94828700 -0.44793000 0.27288900  
O 1.79428800 -0.18817800 -0.94756800  
Cl 6.97679100 -1.33357400 -0.64544300  
O -0.87771300 0.79625700 -2.65538000  
C 0.60753000 2.62159300 -2.66067400  
H 1.43259600 1.96174600 -2.39604600  
C 0.88587000 4.06977600 -2.84527300  
H 1.25159700 4.52073900 -1.91172700  
H 1.66773600 4.23175700 -3.60013400  
H -0.01050700 4.61790700 -3.15649600  
C -0.61745900 2.05388000 -2.87494300  
H -1.46701800 2.69617700 -3.14753900  
H 0.52778500 5.70436300 2.07185900

### TS11e<sub>0</sub>

Bi 1.16722700 0.32545400 0.08854400  
S 4.36090700 0.70431000 0.38308000  
O 5.77643900 1.03476000 0.52922000  
O 3.33229900 1.78535800 0.34138300  
C 3.80790100 -0.35654100 1.69900800  
C 2.43376900 -0.57761700 1.76231300  
C 1.93506900 -1.37377200 2.78505500  
H 0.86672400 -1.56006200 2.86597300  
C 2.81670400 -1.93142700 3.71628600  
H 2.42503000 -2.55105100 4.51914800

C 4.19019200 -1.70297900 3.62810800  
H 4.86305200 -2.14012200 4.36059200  
C 4.70624700 -0.90811400 2.60575900  
H 5.77051300 -0.70602800 2.52219800  
C 4.06579800 -0.21967400 -1.10873600  
C 2.72967200 -0.42618000 -1.45033700  
C 2.45090600 -1.13076500 -2.61551700  
H 1.42307400 -1.31104400 -2.91988800  
C 3.50103400 -1.60527900 -3.40836500  
H 3.27643500 -2.14970000 -4.32233400  
C 4.82889200 -1.39061900 -3.04093100  
H 5.63524900 -1.76328000 -3.66638800  
C 5.12763400 -0.69390400 -1.87125600  
H 6.15360500 -0.50887400 -1.56487700  
C 0.06632600 2.45470800 0.29871800  
C -0.94831200 2.73233700 -0.50328500  
H -1.53875800 1.90445000 -0.90291900  
C -2.84994700 0.41954800 1.13234100  
H -2.51797400 -0.08913800 0.23112900  
O -0.61064300 0.89658400 1.70315100  
O -0.71092200 -0.34586600 -1.61787700  
C -0.73496700 -1.43127800 -0.99684600  
O 0.08692500 -1.66431800 -0.03552000  
C -1.72969300 -2.48426200 -1.33046000  
C -1.78069000 -3.65676900 -0.57274300  
C -2.62835400 -2.27711500 -2.38019200  
C -2.74044100 -4.61180000 -0.88105200  
H -1.08418400 -3.80627300 0.24517300  
C -3.58024700 -3.24818500 -2.67306400  
H -2.57287900 -1.35583700 -2.95153600  
C -3.64421700 -4.42221900 -1.92453000  
H -4.28287300 -3.09493000 -3.48753900  
H -4.38696500 -5.18266600 -2.14607200  
Cl -2.81688800 -6.07542600 0.05843800  
C -1.88543600 0.92390800 1.95936100  
H -2.17221400 1.41546900 2.89794500  
H 0.72857300 3.06099700 0.90674100  
C -4.28435600 0.43674700 1.35836300  
C -5.10929600 -0.33955200 0.52116300  
C -4.90943800 1.20036700 2.36474900  
C -6.49010900 -0.36214000 0.68449500  
H -4.64807400 -0.93761600 -0.26256300  
C -6.28869400 1.17400700 2.52826100  
H -4.31084600 1.83087500 3.01645400

C -7.09020500 0.39322000 1.69165900  
H -7.10025000 -0.97428900 0.02425900  
H -6.74585700 1.77465600 3.31123200  
H -8.16922500 0.37887800 1.82233900  
C -1.41185700 4.07947800 -0.86313600  
C -2.70389500 4.22249800 -1.38906300  
C -0.61919300 5.22559500 -0.69907600  
C -3.19920300 5.48005100 -1.72274700  
H -3.32543900 3.33954800 -1.52167300  
C -1.11591200 6.47982900 -1.03440600  
H 0.39656600 5.13044400 -0.32319400  
C -2.40849400 6.61410500 -1.54532200  
H -4.20584300 5.57260700 -2.12291200  
H -0.48823400 7.35802800 -0.90426300  
H -2.79238800 7.59618100 -1.80924700

### **TS11b**

Bi 0.79573700 -0.32677000 -0.28667900  
S 4.06515000 -0.49907000 -0.62434400  
O 3.12133400 -1.51955300 -1.14322600  
O 5.50653100 -0.62636600 -0.84062700  
C 3.47425800 1.03570100 -1.31215300  
C 2.09501000 1.24108700 -1.35293600  
C 1.60439100 2.40047300 -1.93729100  
H 0.53464000 2.57943200 -1.99465100  
C 2.49834300 3.33668000 -2.46722100  
H 2.11031700 4.23931600 -2.93267300  
C 3.87401000 3.12355000 -2.40730300  
H 4.55908400 3.85721800 -2.82294600  
C 4.37717300 1.96303000 -1.82239100  
H 5.44469900 1.76625800 -1.77592700  
C 3.69460600 -0.41094100 1.10926000  
C 2.34031200 -0.46210800 1.43269000  
C 1.99153500 -0.45012500 2.78008000  
H 0.94610600 -0.48178400 3.07804600  
C 2.98881400 -0.39417300 3.75857800  
H 2.70859900 -0.39566900 4.80926800  
C 4.33665600 -0.33299900 3.40381800  
H 5.10219700 -0.28821600 4.17363400  
C 4.70661800 -0.33413900 2.06010900  
H 5.74851900 -0.29464300 1.75472300  
C -0.86332500 -1.73275000 0.73180000  
C -0.29964300 -2.92480700 1.17569600  
H 0.59213100 -3.33931900 0.70812200

C -0.89475300 -3.59664500 2.24482000  
H -0.46212300 -4.53132100 2.59433000  
C -2.02969200 -3.07034800 2.86077500  
C -2.57233200 -1.87006000 2.40699500  
H -3.46216600 -1.45712300 2.87654800  
C -1.99006000 -1.19173300 1.33378600  
H -2.44210900 -0.27337300 0.97172300  
O -0.04177600 1.40011300 1.00905800  
C -3.78403100 4.29210600 0.35672200  
C -2.95389600 3.27245300 -0.08969200  
C -1.87824900 2.87937400 0.71062500  
C -1.64092600 3.50410700 1.93738800  
C -2.48357300 4.52545100 2.36398900  
C -3.56207000 4.92619600 1.57757500  
H -3.12782400 2.78144400 -1.04164900  
H -0.79950500 3.18250500 2.54245800  
H -2.30541100 5.01757900 3.31611800  
H -4.22445400 5.72136700 1.90599300  
C -0.99631700 1.77660700 0.24503400  
O -1.18887200 1.22009300 -0.86378200  
Cl -5.13117400 4.78818200 -0.62927600  
O 0.36030800 -1.47523100 -2.24971900  
C -1.86094400 -1.96179400 -1.69506600  
H -2.07007800 -0.89343800 -1.67773200  
C -0.59064100 -2.33241400 -2.08240400  
H -0.32629000 -3.39349300 -2.18083300  
C -2.96956400 -2.85058900 -1.41163000  
C -2.81145200 -4.22802800 -1.16782400  
C -4.26480100 -2.30736200 -1.32782900  
C -3.90979400 -5.02757600 -0.87809400  
H -1.81955400 -4.67036100 -1.18361700  
C -5.36266900 -3.10874900 -1.03701400  
H -4.40021800 -1.24183600 -1.50201400  
C -5.19056400 -4.47466400 -0.81244800  
H -3.76623300 -6.08874500 -0.68928700  
H -6.35491100 -2.66751700 -0.98279000  
H -6.04611900 -5.10377000 -0.58012500  
H -2.49270700 -3.59786600 3.69053400

### **Ph<sub>2</sub>BiCl**

Bi 0.20098000 -1.46163600 0.89157400  
C 0.40157600 -1.10835200 -2.24142400  
C 0.97224900 -0.62567600 -1.05859800  
C 2.01100500 0.30455900 -1.12546800

H 2.45928600 0.69583500 -0.21479300  
C 2.46902000 0.75408300 -2.36556200  
C 1.89696700 0.27251000 -3.54206500  
H 2.25531600 0.62451500 -4.50630800  
C 0.86171200 -0.65970000 -3.47980600  
H 0.40804000 -1.03509500 -4.39417900  
C -1.80217200 -0.44575700 0.69994500  
C -1.99795400 0.67642400 -0.11116700  
H -1.16788600 1.10113700 -0.67126400  
C -3.26084700 1.26005700 -0.20523500  
H -3.40620200 2.13506500 -0.83451600  
C -4.33540600 0.72389500 0.50518900  
C -4.14722700 -0.39525600 1.31433000  
H -4.98241300 -0.81381200 1.87111900  
C -2.88262100 -0.97794800 1.41213200  
H -2.74960500 -1.84817400 2.05398700  
H -0.41832100 -1.82578200 -2.21373300  
H 3.27416700 1.48397900 -2.40986600  
Cl 1.27278900 0.31847900 2.31212500  
H -5.31943500 1.17999600 0.42873600