

Supporting Information

For

The Mechanism of Direct Reductive Amination of Aldehyde and Amine with Formic Acid Catalyzed by Boron Trifluoride Complexes: Insights from a DFT Study

*Zhewei Li,^a Huili Zhang,^{*a,b} Tianwei Tan^{*b} and Ming Lei ^{*a}*

^a. State Key Laboratory of Chemical Resource Engineering, Beijing Advanced Innovation Center for Soft Matter Science and Engineering, Institute of Computational Chemistry, Beijing University of Chemical Technology, Beijing, 100029, China.

^b. Beijing Key Laboratory of Bioprocess, College of Life Science and Technology, Beijing University of Chemical Technology, Beijing, 100029, China.

*Email: zhhl@mail.buct.edu.cn (H. Zhang); twtan@mail.buct.edu.cn (T. Tan);

leim@mail.buct.edu.cn (M. Lei)

1. Details of DFT calculations	2
2. The Possible Forms of Boron Trifluoride in the Model Reaction	4
3. The Imine Formation through Path C	5
4. The Imine Formation through Path D	6
5. The Imine Formation through Path E	7
6. The Formylation Reaction through Path F	8
7. The Imine Formation through Path G	9
8. The Imine Formation through Path H	10

9. The Imine Reduction Catalyzed by BF₃-Imine	11
10. Transformation of BF₃-Imine and BF₃-H₂O	12
11. The hydrogen-transfer step with the single point correction using different methods	13
12. Discussion on Reversible Combination of Active Catalytic Species with Hydrogen	14
13. Energies of All the Structures	15
14. Imaginary Frequencies of Transition States	20
15. Cartesian coordinates of All the Structures	22
References	124

1. Details of DFT calculations

Details of DFT calculations: All structures optimized at the M06-2X/def-TZVP level using Gaussian 09 program.¹⁻³ The solvation effect of acetonitrile ($\epsilon=35.69$) was simulated by the SMD continuum solvent mode.⁴ All transition states (TSs) were further confirmed by vibrational analysis and characterized by the only one imaginary frequency. Intrinsic reaction coordinates (IRC) calculations were performed in order to confirm intermediates along the reaction pathway.⁵ MEP⁶⁻⁸ (molecular electrostatic potential) on hydrogen nuclei, and atomic Hirshfeld charge⁹ were calculated via the Multiwfn package¹⁰ under M06-2X/def-TZVP level. Additionally, single point energies were calculated with ORCA package^{11,12} with the ω B97M-V¹³ method and def2-TZVPP¹⁴ basis set, using optimized geometries under M06-2X/def-TZVP level. All energies discussed in the following parts are Gibbs free energies calculated at 298.15 K and compared to BF₃-PhNH₂ (**B1**) in the imine formation unless otherwise stated. A correction factor of 1.9 kcal/mol was applied for the standard state change from 1 atm

to 1 M. The DLPNO-CCSD(T)¹⁵/cc-pVTZ¹⁶ were calculated by ORCA package. The NormalPNO settings and the TightSCF convergence were used.

2. The Possible Forms of Boron Trifluoride in the Model Reaction

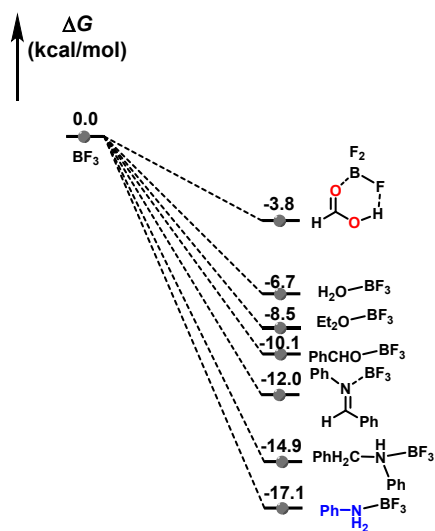


Figure S1. Binding energy (in kcal/mol) of different Lewis bases with boron trifluoride.

3. The Imine Formation through Path C

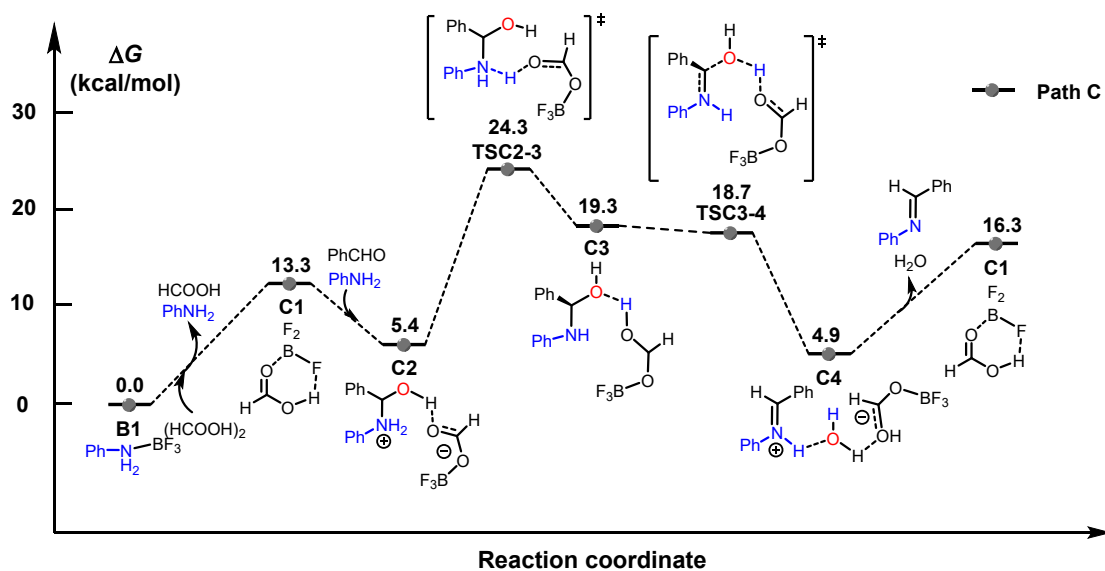


Figure S2. The Gibbs free energy profiles (in kcal/mol) of imine formation catalyzed by C1.

4. The Imine Formation through Path D

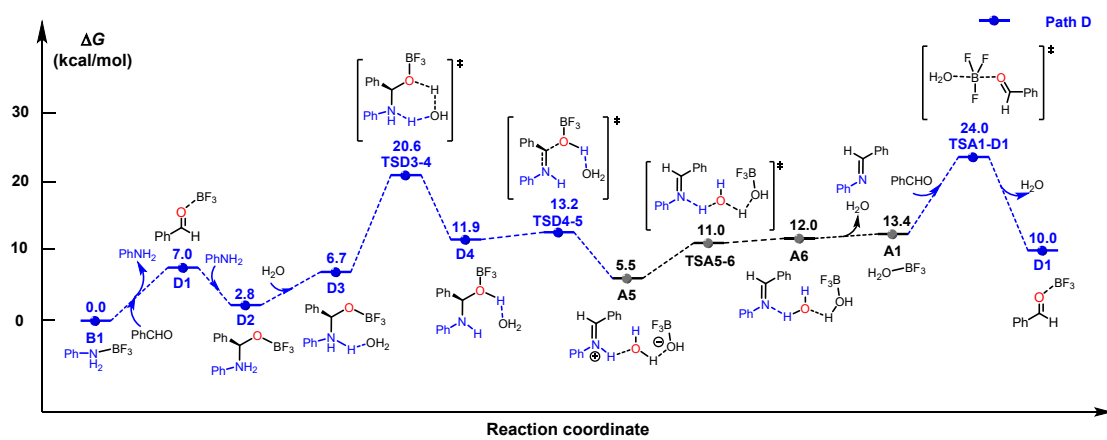


Figure S3. The Gibbs free energy profiles (in kcal/mol) of imine formation catalyzed by **D1**.

5. The Imine Formation through Path E

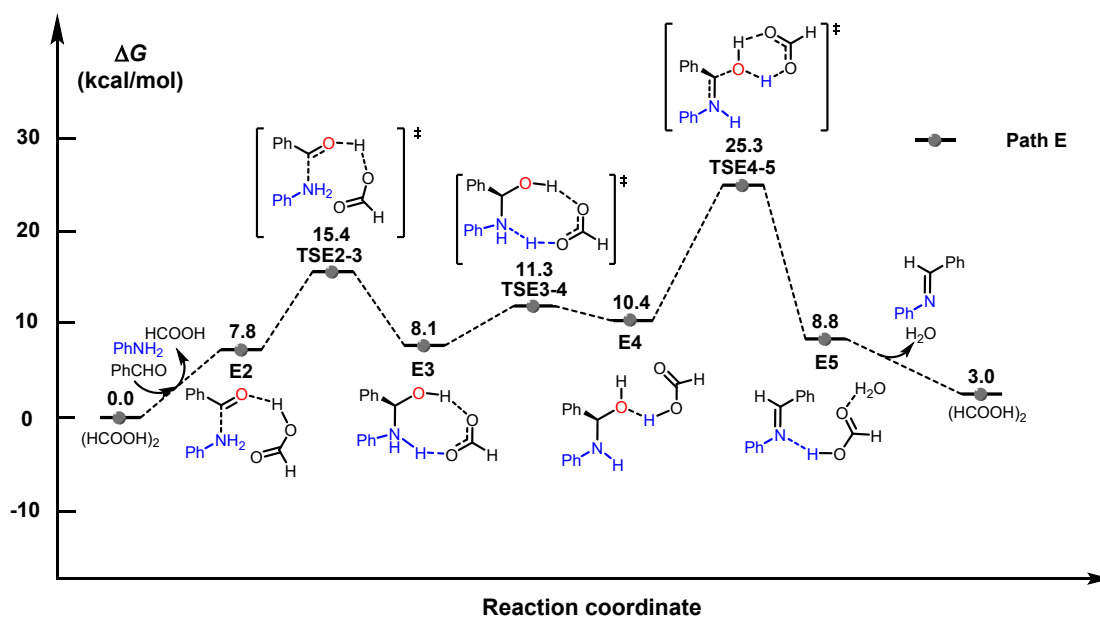


Figure S4. The Gibbs free energy profiles (in kcal/mol) of imine formation catalyzed by HCOOH.

6. The Formylation Reaction through Path F

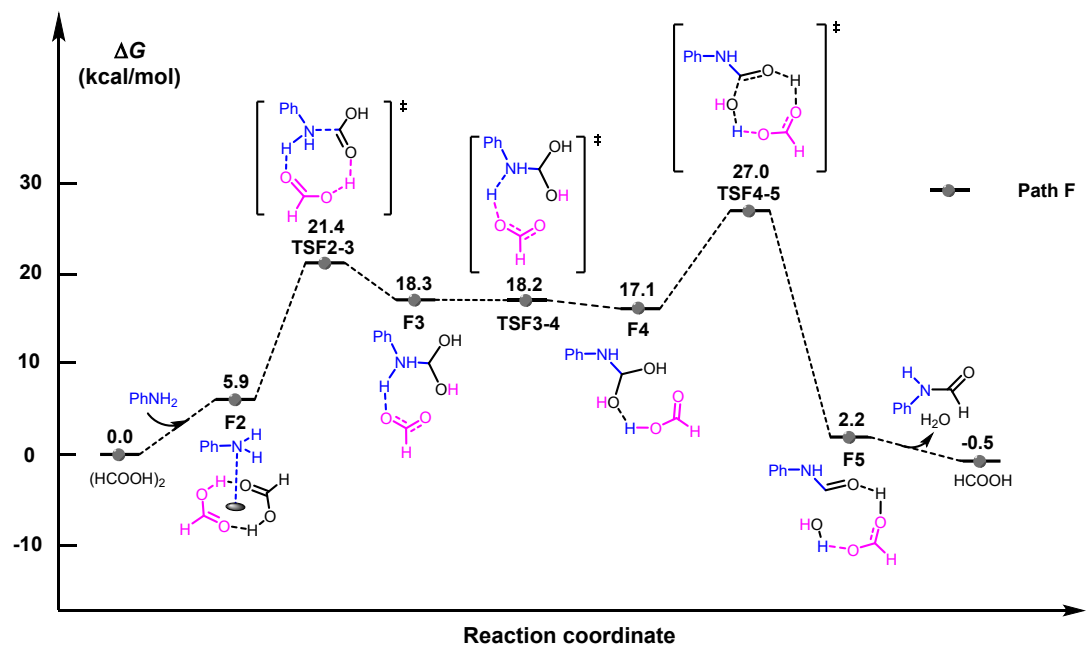


Figure S5. The Gibbs free energy profiles (in kcal/mol) of formylation reaction catalyzed by HCOOH.

7. The Imine Formation through Path G

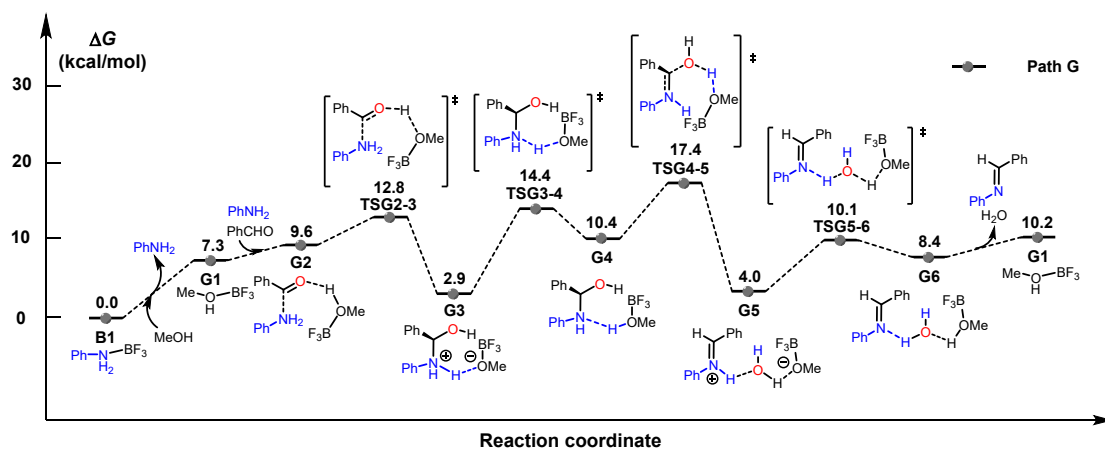


Figure S6. The Gibbs free energy profiles (in kcal/mol) of imine formation catalyzed by G1.

8. The Imine Formation through Path H

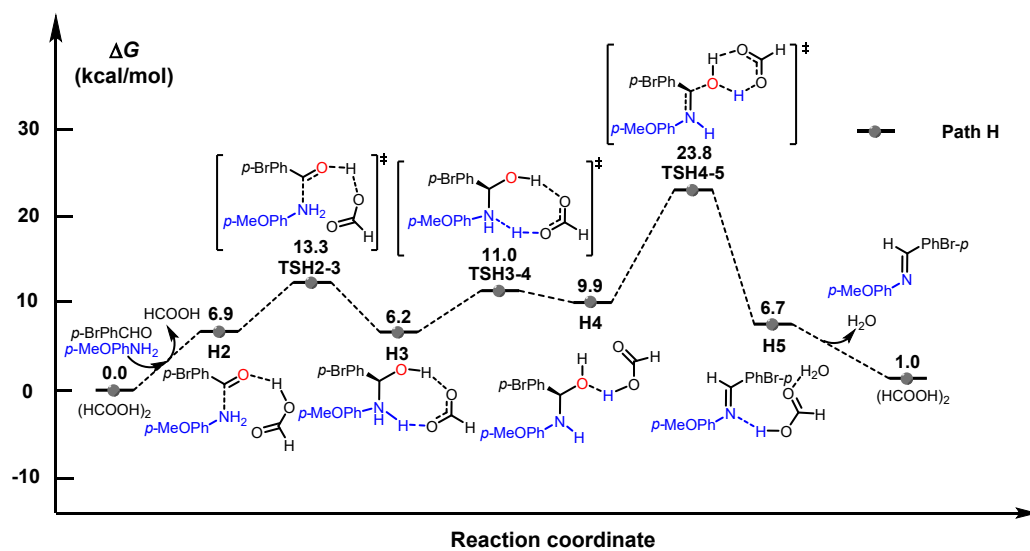


Figure S7. The Gibbs free energy profiles (in kcal/mol) of imine formation in the absence of catalyst.

9. The Imine Reduction Catalyzed by BF_3 -Imine

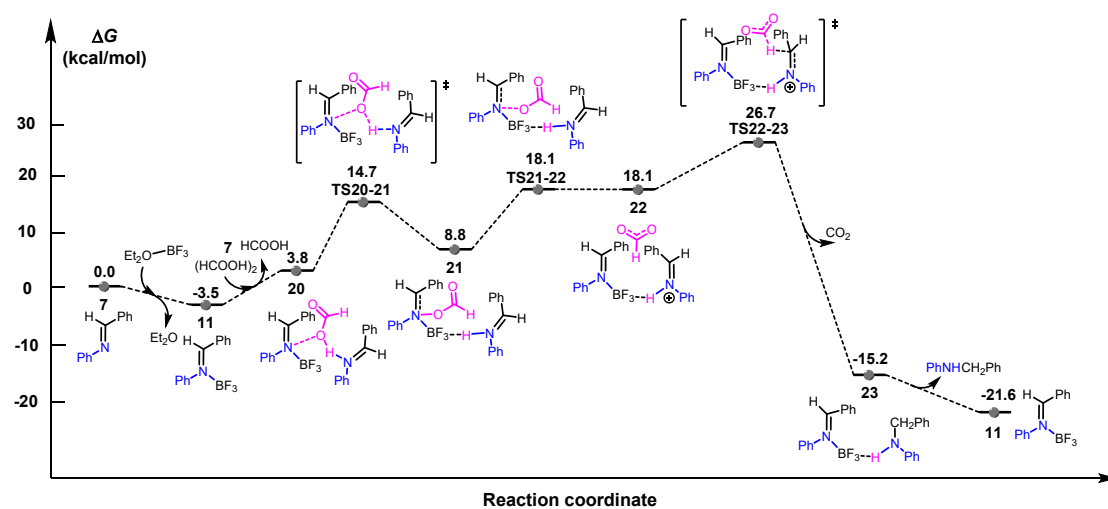


Figure S8. The Gibbs free energy profiles (in kcal/mol) of imine reduction catalyzed by BF_3 -imine.

10. Transformation of BF_3 -Imine and $\text{BF}_3\text{-H}_2\text{O}$

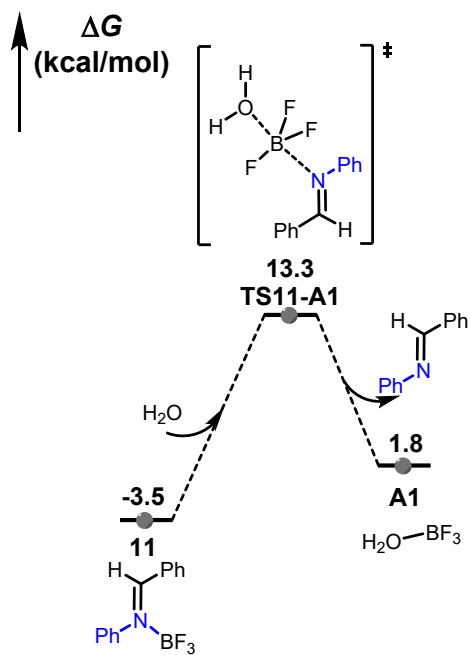


Figure S9. Transformation of BF_3 -imine and $\text{BF}_3\text{-H}_2\text{O}$.

11. The hydrogen-transfer step with the single point correction using different methods

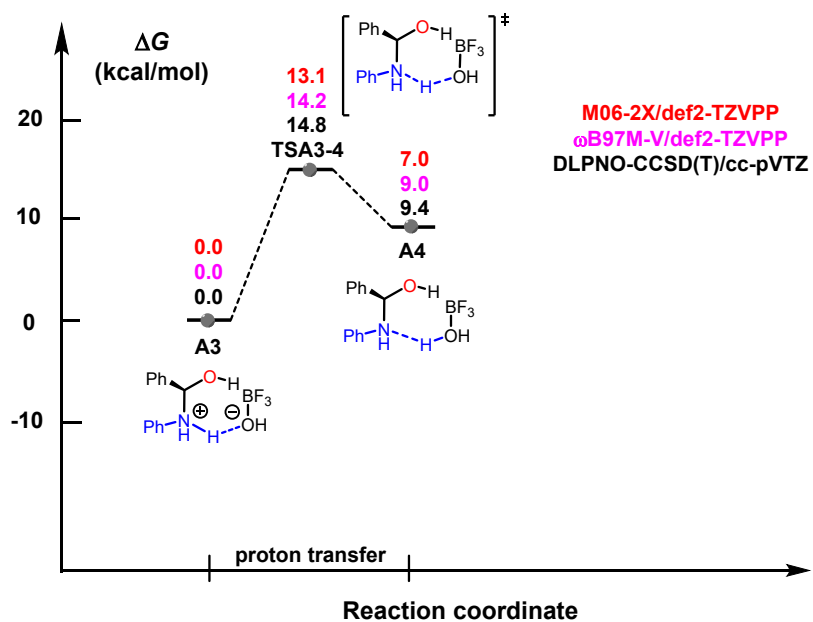


Figure S10. The calculated Gibbs free energy profiles for the hydrogen-transfer step with the single point correction using different methods (unit: kcal/mol).

12. Discussion on Reversible Combination of Active Catalytic Species with Hydrogen

Table S1. The APT charge, Hirshfield charge, MEP on hydrogen atoms of different active catalytic species and the HOMO orbital of its conjugated base.

Active Catalytic Species	APT Charge of Hydrogen (a.u.)	Hirshfeld Charge of Hydrogen (a.u.)	MEP of Hydrogen (a.u.)	HOMO Orbitals of Conjugated Bases (eV)
PhNH₂-BF₃	0.352	0.187	-0.916	-6.51
MeOH-BF₃	0.410	0.244	-0.856	-8.82
H₂O-BF₃	0.465	0.258	-0.833	-9.77

In order to explore the reversible binding ability of various Lewis acid-base pairs to hydrogen, we calculated the APT charge, Hirshfield charge, MEP on hydrogen atoms of different active catalytic species and the HOMO orbital of its conjugated base. For the PhNH₂-BF₃, MeOH-BF₃ and H₂O-BF₃, the calculated results are consistent with the trend of binding energy. PhNH₂ with the largest binding energy shows the weakest acidity, and its conjugated base has the highest HOMO orbital energy. These calculation results confirm that the greater the binding energy of different Lewis bases with BF₃, the weaker the ability of provide protons and the acidity.

13. Energies of All the Structures

Table S2. The calculated absolute electronic energies (E , in a.u.), thermal free energies (G , in a.u.), and relative Gibbs energies (ΔG , in kcal/mol) (Calculated at 298.15 K and 1 atm).

Complex	E	G	ΔG
A1	-401.1047952	-401.0952242	10.4
PhCHO	-345.5872593	-345.5077043	/
PhNH₂	-287.6092808	-287.5212638	/
H₂O	-76.44121348	-76.43743548	/
A2	-1034.3313553	-1034.1154533	12.1
TSA2-3	-1034.3306270	-1034.1156610	12.0
A3	-1034.3515308	-1034.1288128	3.7
TSA3-4	-1034.3279908	-1034.1062028	17.9
A4	-1034.3334036	-1034.1144216	12.7
TSA4-5	-1034.3259582	-1034.1067102	17.6
A5	-1034.3426619	-1034.1259809	5.5
TSA5-6	-1034.3287984	-1034.1180704	10.4
A6	-1034.3308018	-1034.1156358	12.0
B1	-612.2941488	-612.1956288	0.0
B2	-1245.5095587	-1245.2049997	8.8
TSB2-3	-1245.4965770	-1245.1886010	18.8
B3	-1245.5065929	-1245.1954059	14.5
TSB3-4	-1245.5023955	-1245.1936285	15.6
B4	-1245.5164149	-1245.2072439	7.1
TSB4-5	-1245.4824299	-1245.1753769	27.1

B5	-1245.4974858	-1245.1935548	15.7
TSB5-6	-1245.4862557	-1245.1875777	19.4
B6	-1245.5127571	-1245.2070421	7.2
C1	-514.4602984	-514.4429934	13.3
C2	-1147.7102253	-1147.4784793	5.4
TSC2-3	-1147.6777476	-1147.4483536	24.3
C3	-1147.6867080	-1147.4562730	19.3
TSC3-4	-1147.6851895	-1147.4573435	18.7
C4	-1147.7044269	-1147.4792099	4.9
D1	-670.2577974	-670.1708974	7.0
D2	-957.8995142	-957.6958242	2.8
D3	-1034.3476754	-1034.1240134	6.7
TSD3-4	-1034.3218458	-1034.1018728	20.6
D4	-1034.3362967	-1034.1157437	12.0
TSD4-5	-1034.3307747	-1034.1136007	13.4
TSA1-D1	-746.6855736	-746.5829666	24.0
(HCOOH)₂	-379.6138131	-379.5746501	0.0
E2	-823.0163499	-822.8003309	7.8
TSE2-3	-823.0067492	-822.7881132	15.4
E3	-823.0211814	-822.7998964	8.1
TSE3-4	-823.0165779	-822.7946709	11.3
E4	-823.0188517	-822.7961377	10.4
TSE4-5	-822.9901532	-822.7724832	25.3
E5	-823.0136188	-822.7986838	8.8
F2	-667.2301063	-667.0835183	5.9
TSF2-3	-667.2087010	-667.0587550	21.4
F3	-667.2166820	-667.0636630	18.3
TSF3-4	-667.2137216	-667.0638816	18.2
F4	-667.2175387	-667.0657047	17.1

TSF4-5	-667.1985881	-667.0499041	27.0
F5	-667.2323538	-667.0893388	2.2
PhNHCHO	-400.9698751	-400.8744741	-0.5
MeOH	-115.7232566	-115.6943866	/
G1	-440.3946274	-440.3571714	7.3
G2	-1073.6204312	-1073.3763892	9.6
TSG2-3	-1073.6170551	-1073.3712021	12.8
G3	-1073.6373569	-1073.3870509	2.9
TSG3-4	-1073.6193969	-1073.3686779	14.4
G4	-1073.6229798	-1073.3750648	10.4
TSG4-5	-1073.6122503	-1073.3639063	17.4
G5	-1073.6288476	-1073.3853096	4.0
TSG5-6	-1073.6162158	-1073.3755468	10.1
G6	-1073.6204352	-1073.3782492	8.4
7	-556.7523640	-556.5868180	0.0
8	-936.3755510	-936.1527480	3.6
TS8-9	-936.3710561	-936.1495891	5.6
9	-936.3731635	-936.1503585	5.1
TS9-10	-936.3397383	-936.1179233	25.4
CO₂	-188.6234075	-188.6322785	/
10	-747.7644058	-747.5458618	-10.5
PhNHCH₂Ph	-557.9601618	-557.7731248	-18.1
TS9	-1147.6511689	-1147.4303249	23.8
TS10	-746.5252873	-746.3329963	25.5
TS11	-1337.460689	-1337.210317	30.6
TS12	-1261.002008	-1260.771424	33.4
TS13	-1358.833562	-1358.520812	25.3
TS14	-1186.940698	-1186.692722	22.2
BF₃·Et₂O	-558.3072210	-558.1890960	/

Et₂O	-233.6355361	-233.5284451	/
11	-881.4289401	-881.2530561	-3.5
12	-1261.0465443	-1260.8112743	4.9
TS12-13	-1260.9727975	-1260.7392905	50.1
13	-1072.4556850	-1072.2261130	-22.8
14	-1439.4036792	-1439.0190912	-19.0
TS14-15	-1439.3702161	-1438.9886321	0.1
15	-1439.3952373	-1439.0138813	-15.7
16	-1358.8600657	-1358.5450047	2.8
TS16-17	-1358.8155097	-1358.5025097	29.5
17	-1170.2538575	-1169.9441545	-15.0
TS17-18	-1170.2486886	-1169.9394826	-12.1
18	-1170.2655557	-1169.9568627	-23.0
TS18	-1071.1581496	-1070.9559246	47.3
20	-1628.0031586	-1627.6119916	3.8
TS20-21	-1627.9915332	-1627.5946532	14.7
21	-1628.0037784	-1627.6040504	8.8
TS21-22	-1627.9860680	-1627.5891950	18.1
22	-1627.9870475	-1627.5891455	18.1
TS22-23	-1627.9701017	-1627.5754487	26.7
23	-1439.4028204	-1439.0130204	-15.2
TS11-A1	-957.8505481	-957.6606881	13.3
<i>p</i>-BrPhCHO	-2919.0080241	-2918.9417811	/
<i>p</i>-MeOPhNH₂	-402.1393743	-402.0219933	/
H2	-3510.9683149	-3510.7366119	6.9
TSH2-3	-3510.9611247	-3510.7263737	13.3
H3	-3510.9766674	-3510.7377084	6.2
TSH3-4	-3510.9685707	-3510.7300837	11.0
H4	-3510.9715337	-3510.7317377	9.9

TSH4-5	-3510.9433388	-3510.7096758	23.8
H5	-3510.9676314	-3510.7368124	6.7

14. Imaginary Frequencies of Transition States

Table S3. Calculated imaginary frequencies of transition states at M06-2X/def-TZVP

level.

TSA2-3	356.17 <i>i</i>
TSA3-4	327.09 <i>i</i>
TSA4-5	253.51 <i>i</i>
TSA5-6	414.27 <i>i</i>
TSB2-3	211.98 <i>i</i>
TSB3-4	943.76 <i>i</i>
TSB4-5	323.88 <i>i</i>
TSB5-6	1160.03 <i>i</i>
TSC2-3	168.89 <i>i</i>
TSC3-4	532.38 <i>i</i>
TSD3-4	431.68 <i>i</i>
TSD4-5	217.19 <i>i</i>
TSA1-D1	95.08 <i>i</i>
TSE2-3	207.77 <i>i</i>
TSE3-4	136.77 <i>i</i>
TSE4-5	305.36 <i>i</i>
TSF2-3	248.68 <i>i</i>
TSF3-4	789.72 <i>i</i>
TSF4-5	391.82 <i>i</i>
TSG2-3	206.88 <i>i</i>
TSG3-4	150.08 <i>i</i>
TSG4-5	251.42 <i>i</i>
TSG5-6	382.46 <i>i</i>
TS8-9	510.90 <i>i</i>

TS9-10	951.47 <i>i</i>
TS9	976.87 <i>i</i>
TS10	751.46 <i>i</i>
TS11	933.95 <i>i</i>
TS12	1022.91 <i>i</i>
TS13	933.57 <i>i</i>
TS14	953.79 <i>i</i>
TS12-13	921.09 <i>i</i>
TS14-15	121.00 <i>i</i>
TS16-17	860.77 <i>i</i>
TS17-18	967.91 <i>i</i>
TS18	1623.83 <i>i</i>
TS20-21	244.13 <i>i</i>
TS21-22	229.89 <i>i</i>
TS22-23	825.61 <i>i</i>
TS11-A1	124.69 <i>i</i>
TSH2-3	158.58 <i>i</i>
TSH3-4	106.54 <i>i</i>
TSH4-5	315.65 <i>i</i>

15. Cartesian coordinates of All the Structures

Table S4. Atomic cartesian coordinates of intermediates and transition states (presented in Å).

A1			

Coordinates (Angstroms)			
X	Y	Z	

H	1.86638900	0.78996000	0.20759700
O	1.41784400	-0.00226500	-0.14524100
B	-0.17766400	0.00022600	0.00054400
F	-0.56368600	-1.14481600	-0.63552900
F	-0.55841500	1.15376600	-0.62335200
F	-0.45402400	-0.00639300	1.34162800
H	1.86430600	-0.79597200	0.20688700

PhCHO			

Coordinates (Angstroms)			
X	Y	Z	

C	1.99439200	0.46669500	-0.00041900
O	2.83988700	-0.39752100	-0.00008400
H	2.27821300	1.54680600	-0.00014400
C	0.53386600	0.21143800	-0.00015300
C	-0.35590400	1.29180700	-0.00013400
C	0.04324200	-1.10175000	0.00005800
C	-1.73075400	1.06236000	0.00008500
H	0.03525300	2.31328900	-0.00030300
C	-1.32864000	-1.32920300	0.00028100
H	0.75314300	-1.93202000	0.00004200
C	-2.21460900	-0.24678500	0.00029300
H	-2.42771800	1.90322100	0.00009400
H	-1.71536700	-2.35075900	0.00044700
H	-3.29219000	-0.42773700	0.00046900

PhNH₂

Coordinates (Angstroms)

	X	Y	Z
C	-1.16658200	1.19833000	0.00421000
C	0.22095000	1.20427700	-0.00721800
C	0.93456600	0.00000000	-0.00936100
C	0.22095000	-1.20427700	-0.00721800
C	-1.16658200	-1.19833000	0.00421000
C	-1.87387300	0.00000000	0.00753200
H	-1.69961500	2.14191500	0.00963200
H	0.76623900	2.14158500	-0.00898700
H	0.76623900	-2.14158500	-0.00898700
H	-1.69961500	-2.14191500	0.00963200
H	-2.95635800	0.00000000	0.01727400
N	2.32469900	0.00000000	-0.07559700
H	2.76682400	0.83750900	0.27884300
H	2.76682400	-0.83750900	0.27884300

H₂O

Coordinates (Angstroms)

	X	Y	Z
O	0.00000000	0.00000000	0.12036200
H	0.00000000	0.75333000	-0.48145000
H	0.00000000	-0.75333000	-0.48145000

A2

Coordinates (Angstroms)

	X	Y	Z
C	0.68160100	1.42826300	-0.49779300
O	1.48955600	1.88649200	0.31841400
H	1.04365800	0.88444900	-1.37627500
C	-0.75302700	1.63922100	-0.39339500
C	-1.57668500	1.08593900	-1.37489500
C	-1.30364400	2.33108400	0.68875000
C	-2.95252000	1.23210500	-1.28191500
H	-1.13223500	0.54202000	-2.20086500
C	-2.67755900	2.47436500	0.77700900
H	-0.65115700	2.74506600	1.44777200

C	-3.49905900	1.92268400	-0.20540300
H	-3.59785400	0.80243900	-2.03756200
H	-3.11541700	3.00793100	1.61101300
H	-4.57404200	2.03295900	-0.12844100
C	-3.10630500	-1.43201900	1.28387900
C	-1.75500000	-1.12363000	1.34008200
C	-0.89373000	-1.53255900	0.31534800
C	-1.41958700	-2.25458300	-0.76192900
C	-2.77297100	-2.55847600	-0.80753900
C	-3.62899400	-2.14660300	0.20927100
H	-3.75816900	-1.10427500	2.08540700
H	-1.35274000	-0.56217900	2.17628600
H	-0.75739000	-2.57039700	-1.56077600
H	-3.16180100	-3.12015500	-1.64883100
H	-4.68445400	-2.38394000	0.16884300
N	0.43964100	-1.14204400	0.32163200
H	0.83524800	-0.95221400	1.23368900
H	1.06525500	-1.69931000	-0.24665700
H	4.22045300	1.55878800	-0.77236600
O	3.76972000	1.13566500	-0.02366000
B	3.90295100	-0.38008000	0.01167900
F	3.28208600	-0.78001300	1.18160600
F	5.25043900	-0.67951300	-0.00271200
F	3.26207200	-0.91560800	-1.09899700
H	2.74771200	1.51774400	0.11301300

TSA2-3

Coordinates (Angstroms)

	X	Y	Z
C	-0.64260200	-1.39333000	-0.50126600
O	-1.45839100	-1.89356600	0.30050500
H	-1.01311300	-0.84323600	-1.36882300
C	0.78202800	-1.61438300	-0.39387900
C	1.61167500	-1.05524200	-1.36894500
C	1.32577200	-2.31973400	0.68467500
C	2.98568700	-1.21198300	-1.27403800
H	1.17237700	-0.50316000	-2.19187800
C	2.69791600	-2.47217000	0.77355600
H	0.67036600	-2.73719200	1.43907600
C	3.52464600	-1.91648100	-0.20263000
H	3.63548100	-0.78011600	-2.02441700
H	3.13091900	-3.01638200	1.60303100

H	4.59861400	-2.03534900	-0.12488600
C	3.07561800	1.49027200	1.26189300
C	1.73969700	1.12680000	1.34842700
C	0.84093100	1.50120300	0.34358100
C	1.31113800	2.24195800	-0.74591300
C	2.64970400	2.60073900	-0.82210800
C	3.54367300	2.22451500	0.17550100
H	3.75854100	1.19035800	2.04819200
H	1.37913900	0.55011800	2.19322500
H	0.61833000	2.52918500	-1.52929500
H	2.99662800	3.17703700	-1.67171600
H	4.58741300	2.50467800	0.11144200
N	-0.47556600	1.05311300	0.37874100
H	-0.84523300	0.86249700	1.30216400
H	-1.13607600	1.57995900	-0.18056600
H	-4.12144600	-1.51950400	-0.91520200
O	-3.69164400	-1.14528900	-0.13371200
B	-3.87235800	0.33146500	0.00865100
F	-3.29063600	0.67797200	1.22358500
F	-5.22756800	0.62750400	-0.01494000
F	-3.22041500	0.99215900	-1.03832300
H	-2.56864600	-1.56885500	0.07484700

A3

Coordinates (Angstroms)

	X	Y	Z
C	-0.05973200	-1.13003200	0.03337100
O	0.52010900	-2.28442900	-0.44895300
H	0.41624300	-0.76628000	0.94623400
C	-1.54256800	-1.28716700	0.21570400
C	-2.17078800	-0.69930900	1.30787800
C	-2.29222900	-1.97740300	-0.73378600
C	-3.54956100	-0.80139300	1.45337600
H	-1.58084400	-0.16295800	2.04303100
C	-3.66886600	-2.07827300	-0.58618800
H	-1.79863000	-2.43806400	-1.58188600
C	-4.29836100	-1.48828800	0.50579100
H	-4.03658400	-0.34466400	2.30586000
H	-4.25166700	-2.61666300	-1.32326400
H	-5.37261200	-1.56818300	0.61870700
N	0.20765200	-0.02629800	-1.00696700
H	-0.20478400	-0.32872500	-1.89598700

H	1.25576200	0.01481600	-1.12887400
H	1.46603900	-2.26911800	-0.22134100
C	-0.29762100	1.28827700	-0.63063000
C	-1.49240400	1.73910200	-1.16669500
C	0.41854100	2.02525900	0.29950700
C	-1.98010500	2.97493000	-0.76182500
H	-2.02887000	1.13115500	-1.88664100
C	-0.08152400	3.25840000	0.69775700
H	1.34908200	1.64004300	0.70186900
C	-1.27782500	3.73111100	0.17005300
H	-2.91088800	3.34377300	-1.17331300
H	0.46594100	3.84846500	1.42156500
H	-1.66274200	4.69302400	0.48456600
O	2.91236500	0.00715400	-1.02715000
H	3.36827400	0.75116500	-1.43686900
B	3.59090100	-0.46428000	0.16298700
F	3.41645000	0.41036900	1.25064300
F	3.00245300	-1.71261500	0.50709300
F	4.96072600	-0.64612700	-0.05294500

TSA3-4

Coordinates (Angstroms)

	X	Y	Z
C	1.19229300	-0.26738700	0.75728100
O	0.73448500	0.98894100	1.25928000
H	1.12407600	-1.02401000	1.54209500
C	2.62709900	-0.12008000	0.32121800
C	3.58385100	-1.03581000	0.74314500
C	2.99330100	0.92338300	-0.52721000
C	4.90289200	-0.91220400	0.31942900
H	3.29679700	-1.84436000	1.40598700
C	4.30997800	1.04570100	-0.94992600
H	2.24976600	1.64337400	-0.85067500
C	5.26668400	0.12730300	-0.52709100
H	5.64517900	-1.62654900	0.65361200
H	4.59184600	1.85907200	-1.60729100
H	6.29415100	0.22518100	-0.85565500
N	0.37107500	-0.62746200	-0.38465600
H	0.89246600	-0.87078900	-1.21835000
H	-0.40558600	1.22845000	-0.38607300
H	0.08451500	0.84967200	1.96086000
C	-0.81826100	-1.35957800	-0.22918100

C	-1.41174500	-1.91272200	-1.36994300
C	-1.46180300	-1.49262500	1.00269000
C	-2.61800400	-2.58621600	-1.27693700
H	-0.91219400	-1.80646600	-2.32661000
C	-2.67485800	-2.16939400	1.08210300
H	-1.04064000	-1.07339100	1.90764400
C	-3.26185100	-2.71824200	-0.04902100
H	-3.05966100	-3.01005600	-2.17079200
H	-3.16175000	-2.26174000	2.04544800
H	-4.20690600	-3.24119700	0.02190700
O	-1.06281000	1.85117200	-0.79507700
H	-1.17067700	1.60850400	-1.73322300
B	-2.41516500	2.02146800	-0.00979200
F	-3.28177300	1.06215500	-0.47896700
F	-2.07879100	1.84390100	1.31038000
F	-2.84987500	3.29122500	-0.29144600

A4

Coordinates (Angstroms)

	X	Y	Z
C	-1.23421300	0.17844600	0.52528300
O	-0.46556800	-1.01264100	0.17304300
H	-1.08190400	0.36764900	1.58847400
C	-2.70043100	-0.05098100	0.25006700
C	-3.64785900	0.33940600	1.18985300
C	-3.10916100	-0.61615600	-0.95566600
C	-5.00209000	0.17133400	0.92484500
H	-3.32410300	0.77332700	2.12930600
C	-4.46241400	-0.78389000	-1.21869800
H	-2.36927700	-0.93107900	-1.68278400
C	-5.41006800	-0.38922600	-0.27946300
H	-5.73674400	0.47506500	1.66030800
H	-4.77856900	-1.22480600	-2.15604800
H	-6.46492900	-0.52321600	-0.48556300
N	-0.74701200	1.26952400	-0.23979300
H	-1.13224700	1.34275700	-1.17361600
H	0.90829900	-0.99227500	-0.38950300
H	-0.66842400	-1.73974300	0.78343100
C	0.55509700	1.75494800	-0.09917100
C	1.07689900	2.57821900	-1.10555400
C	1.35303000	1.45417000	1.00962000
C	2.36054000	3.08765200	-1.00095600

H	0.46217400	2.80738100	-1.96880400
C	2.63991700	1.97540100	1.10258600
H	0.98909800	0.80504600	1.79601600
C	3.15480800	2.79124100	0.10419900
H	2.74502400	3.71963300	-1.79244300
H	3.24403700	1.72553400	1.96651800
H	4.15928800	3.18681700	0.18101900
O	1.86569300	-1.07969600	-0.77210600
H	2.28640800	-0.20004000	-0.77451900
B	2.68704300	-2.16130900	-0.03142000
F	3.73984900	-2.49692200	-0.84918600
F	3.12017300	-1.62507100	1.16593600
F	1.79669000	-3.19765700	0.15710500

TSA4-5

Coordinates (Angstroms)

	X	Y	Z
C	-0.86260500	-0.41811400	-0.08704300
O	-0.52059900	0.40031400	1.44794200
H	-0.36707000	0.30602900	-0.72244600
C	-2.34515900	-0.36414000	-0.13524700
C	-2.94458800	0.56179000	-0.98516500
C	-3.13084300	-1.19532600	0.66337400
C	-4.32933600	0.64063200	-1.05604400
H	-2.32441800	1.21367600	-1.58989800
C	-4.51301900	-1.10862600	0.59267200
H	-2.67180200	-1.89886200	1.34925900
C	-5.11233900	-0.19417600	-0.26869800
H	-4.79463800	1.35547300	-1.72282600
H	-5.12434100	-1.75110000	1.21366500
H	-6.19220000	-0.13030100	-0.32064300
N	-0.28285700	-1.62526700	-0.01567400
H	-0.83269300	-2.39057100	0.35757700
H	0.30957300	1.03783300	1.39858600
H	-1.28990000	0.93756700	1.70209300
C	1.10126000	-1.87388300	-0.12696300
C	1.55376300	-3.16020800	0.16497600
C	2.00668100	-0.89213700	-0.52274200
C	2.90259900	-3.46173900	0.05944100
H	0.84246000	-3.91701300	0.47559200
C	3.35636800	-1.20734300	-0.62329600
H	1.68722700	0.11368500	-0.75918400

C	3.81305500	-2.48693500	-0.33483700
H	3.24165000	-4.46429200	0.28930400
H	4.05224300	-0.43635700	-0.93086500
H	4.86654700	-2.72269700	-0.41446100
O	1.40202400	1.96183700	1.30500000
H	2.20243200	1.83112400	1.82567600
B	1.59797400	2.74460800	0.08535200
F	2.79558800	2.38446600	-0.55135400
F	0.50561600	2.45721200	-0.75311900
F	1.62753400	4.11761800	0.35618700

A5

Coordinates (Angstroms)

	X	Y	Z
C	-2.13315800	1.04673200	-0.07877000
O	0.18722900	-1.80808300	0.09463900
H	-2.35395200	2.10743600	-0.15910000
C	-3.24722200	0.12819200	-0.02978500
C	-4.51894800	0.66575400	-0.25979300
C	-3.09937200	-1.24090200	0.23521400
C	-5.63243100	-0.15897300	-0.24715000
H	-4.62149000	1.72690800	-0.45406800
C	-4.21673000	-2.05448300	0.25042700
H	-2.12335700	-1.66571700	0.43820800
C	-5.48013600	-1.51643200	0.00752600
H	-6.61536600	0.25521700	-0.43006300
H	-4.10973900	-3.11118800	0.45870200
H	-6.34928800	-2.16248600	0.02215800
N	-0.89237700	0.70595200	-0.05098500
H	-0.60640500	-0.30194700	-0.03960900
H	1.05969500	-1.65490500	0.53522200
H	0.41172900	-2.23442800	-0.74206500
C	0.20005100	1.62346100	-0.04510700
C	1.38336300	1.22860900	-0.66023900
C	0.08574500	2.85902600	0.58084100
C	2.46121200	2.10315000	-0.66807200
H	1.45550800	0.25769100	-1.13561500
C	1.17017500	3.72394600	0.56076200
H	-0.82534400	3.13246900	1.09793100
C	2.35613900	3.34972600	-0.06158000
H	3.38348200	1.80615900	-1.15045000
H	1.09166900	4.68644000	1.04984300

H	3.20059000	4.02721400	-0.06754400
O	2.61990900	-1.30556900	1.11277900
H	2.71725500	-0.37930700	1.35858900
B	3.55656300	-1.67146100	0.06974500
F	4.51341000	-0.65777600	-0.13015600
F	4.21228900	-2.86987300	0.39966500
F	2.86536700	-1.88474400	-1.15161500

TSA5-6

Coordinates (Angstroms)

	X	Y	Z
C	2.06258100	1.02082700	0.13905300
O	-0.29164500	-1.61444000	-0.41016100
H	2.30381400	2.05966300	0.37349400
C	3.19573200	0.09671100	0.07452100
C	4.42110200	0.53334300	0.58258200
C	3.09477100	-1.18141800	-0.48351000
C	5.52648000	-0.30579300	0.56162800
H	4.49898800	1.53111300	0.99937000
C	4.20163800	-2.01375200	-0.50814300
H	2.16080500	-1.51687000	-0.91577800
C	5.41652600	-1.57952700	0.01764200
H	6.47224600	0.03566900	0.96287800
H	4.12303100	-3.00101600	-0.94567400
H	6.27879700	-2.23455500	-0.00513000
N	0.84781400	0.67462700	-0.03909000
H	0.23781500	-0.72370100	-0.23840800
H	-1.45060900	-1.44785600	-0.72315200
H	-0.24244400	-2.16760200	0.38528100
C	-0.17132400	1.66371900	-0.02061000
C	-1.36399200	1.37005800	0.63973200
C	-0.01961600	2.88147200	-0.68292600
C	-2.38781000	2.30712700	0.66263400
H	-1.47576100	0.42343700	1.15689200
C	-1.05195400	3.80948600	-0.65952600
H	0.89242300	3.08760200	-1.23040500
C	-2.23560400	3.52747900	0.01311300
H	-3.30725100	2.07996900	1.18736100
H	-0.93340700	4.75217900	-1.17938400
H	-3.03898300	4.25335600	0.02619800
O	-2.60052300	-1.35015000	-1.00390700
H	-2.83167700	-0.51109600	-1.42905000

B	-3.54836300	-1.77655200	0.07796000
F	-4.12231900	-0.65111400	0.66001800
F	-4.53307800	-2.59090600	-0.46371600
F	-2.77510400	-2.48260000	0.99866900

A6

Coordinates (Angstroms)

	X	Y	Z
C	2.75730700	2.53953000	0.23852500
C	1.99883000	2.98998900	-0.83782400
C	0.67116200	2.60380900	-0.96016200
C	0.10477200	1.73527600	-0.02404100
C	0.86587200	1.29586800	1.06317300
C	2.18713900	1.70052300	1.19266900
H	3.79045300	2.84818500	0.33965700
H	2.43957200	3.64948200	-1.57471700
H	0.07060800	2.95975300	-1.78951300
H	0.41612000	0.65493100	1.81233200
H	2.77237800	1.36560100	2.03949900
C	-1.28938300	1.31072100	-0.20355000
H	-1.94516600	1.99436200	-0.74795800
N	-1.71641000	0.18974300	0.22703400
C	-3.09091800	-0.12808800	0.09029700
C	-4.09004400	0.82243700	0.30393500
C	-3.43906800	-1.43998700	-0.22912900
C	-5.42455200	0.46404400	0.16735500
H	-3.82253300	1.82982900	0.59951500
C	-4.77457400	-1.78755700	-0.37270100
H	-2.66249500	-2.17945300	-0.38309700
C	-5.77146100	-0.83776600	-0.17540300
H	-6.19596800	1.20436200	0.34030800
H	-5.03713600	-2.80530100	-0.63367600
H	-6.81345700	-1.11369500	-0.27813200
H	-0.55498200	-1.03572200	0.47015300
O	0.19754700	-1.70626600	0.48989200
H	-0.16541100	-2.57128000	0.25510000
H	1.31560100	-1.33488900	-0.20867400
O	2.21033600	-1.04147100	-0.73717700
B	3.53534000	-1.52510600	-0.14524200
F	4.51950400	-0.72107500	-0.69109100
F	3.66926400	-2.84868700	-0.51462000
F	3.48205500	-1.39899500	1.23319500

H	2.19961700	-0.08092200	-0.89177000
---	------------	-------------	-------------

B1

Coordinates (Angstroms)

	X	Y	Z
C	2.48421000	-1.20394900	-0.13551900
C	1.17733600	-1.20966300	0.33501100
C	0.54220000	-0.00001300	0.56647300
C	1.17731400	1.20965000	0.33502400
C	2.48418900	1.20396300	-0.13550700
C	3.13749000	0.00001400	-0.37224200
H	2.99078900	-2.14359700	-0.31614700
H	0.65497500	-2.14037000	0.52278200
H	0.65493900	2.14034700	0.52280500
H	2.99075200	2.14362100	-0.31612600
H	4.15646900	0.00002500	-0.73809700
N	-0.84263200	-0.00003000	1.01584200
H	-1.01786400	-0.81807600	1.60574300
H	-1.01787000	0.81798100	1.60579100
B	-1.93828800	0.00000200	-0.17687200
F	-1.73569900	1.14481200	-0.92378300
F	-1.73565200	-1.14473200	-0.92388700
F	-3.17740000	-0.00005100	0.43958900

B2

Coordinates (Angstroms)

	X	Y	Z
C	0.26759400	1.21688200	-0.19116900
O	-0.46694500	1.21757300	-1.16337800
H	-0.10684300	0.90099600	0.79364200
C	1.66856200	1.66533000	-0.22638700
C	2.41418100	1.62849200	0.95019200
C	2.25547200	2.08953200	-1.41912500
C	3.74452700	2.02484700	0.94018800
H	1.94765700	1.28423600	1.86713400
C	3.58433800	2.48266100	-1.42787800
H	1.66424700	2.10510000	-2.32693900
C	4.32747500	2.44940500	-0.24908400
H	4.32796000	1.99521800	1.85203100

H	4.04693100	2.81270800	-2.34966900
H	5.36699500	2.75428900	-0.26026800
C	4.85886100	-1.18972200	-0.55722300
C	3.49473700	-1.24682800	-0.80167400
C	2.59788100	-1.50308500	0.24325200
C	3.10663000	-1.69851600	1.53366000
C	4.47323100	-1.63990100	1.76599900
C	5.36211700	-1.38001600	0.72700200
H	5.53535900	-0.98677500	-1.37950800
H	3.10818900	-1.09131600	-1.80306300
H	2.41841100	-1.89249900	2.34910100
H	4.84603200	-1.79492300	2.77183500
H	6.42748200	-1.33296200	0.91316800
N	1.23164800	-1.47163100	0.02111300
H	0.92336900	-1.64139000	-0.92668300
H	0.65247100	-1.94207600	0.70318600
C	-6.24744700	0.55445700	0.29015200
C	-5.25875900	0.01853000	-0.52510900
C	-3.93092300	0.31484800	-0.25897000
C	-3.57229400	1.13049800	0.80349400
C	-4.56842300	1.66130400	1.61334700
C	-5.90452200	1.37440900	1.35902000
H	-7.28688100	0.32987100	0.08680300
H	-5.51175000	-0.62229400	-1.36172300
H	-2.52809100	1.34703600	0.99734800
H	-4.29681300	2.30102500	2.44350200
H	-6.67781400	1.79088900	1.99210900
N	-2.88801200	-0.27405100	-1.08352200
H	-3.23376600	-0.40959700	-2.03680700
H	-2.07684700	0.36830100	-1.14924600
B	-2.32458700	-1.68227600	-0.54570000
F	-1.79454100	-1.46196300	0.71559000
F	-3.37483000	-2.58100600	-0.50603200
F	-1.34537200	-2.07970100	-1.44530100

TSB2-3

Coordinates (Angstroms)

	X	Y	Z
C	0.53695500	0.66124400	-0.52043600
O	-0.35338100	0.97199000	-1.37533100
H	0.23053400	0.12180800	0.38964800
C	1.67645500	1.60571000	-0.26778300

C	2.32666400	1.59815900	0.96226100
C	2.09650400	2.47711200	-1.26982300
C	3.39425700	2.45941300	1.19275500
H	1.99582500	0.91681800	1.73940200
C	3.16652600	3.33170300	-1.04261100
H	1.57569300	2.47934400	-2.22022100
C	3.81689300	3.32268400	0.18908100
H	3.89635000	2.45375700	2.15243400
H	3.49502500	4.00740100	-1.82295300
H	4.64989000	3.99227600	0.36585000
C	4.70538000	-1.53910600	0.35013600
C	3.76412900	-1.02413700	-0.53106500
C	2.42853300	-1.38405600	-0.39108500
C	2.02547800	-2.24127500	0.62735900
C	2.97452700	-2.74974900	1.50446700
C	4.31387600	-2.39962100	1.37018400
H	5.74689700	-1.26335100	0.24054500
H	4.05686900	-0.34494800	-1.32427500
H	0.97792500	-2.50420300	0.72418400
H	2.66452600	-3.42075200	2.29590800
H	5.05028900	-2.79832000	2.05648600
N	1.44024500	-0.78919900	-1.22792600
H	1.82855100	-0.43553700	-2.10212500
H	0.66904900	-1.42622500	-1.43641200
C	-5.74606700	0.89922800	0.38751900
C	-4.85919900	0.21103600	-0.43093400
C	-3.49483600	0.33069200	-0.20810300
C	-3.00539100	1.12524000	0.82008900
C	-3.89956000	1.80838200	1.63454700
C	-5.26886600	1.69750200	1.42060700
H	-6.81133800	0.81023400	0.21486500
H	-5.21976700	-0.41532400	-1.23889100
H	-1.93652800	1.20562400	0.97985100
H	-3.52277900	2.43067500	2.43662400
H	-5.96232200	2.23303000	2.05679700
N	-2.55900600	-0.40317900	-1.03609200
H	-2.97380100	-0.56733300	-1.95584700
H	-1.65950900	0.18634300	-1.20179700
B	-2.11098900	-1.81039700	-0.44542500
F	-1.56489600	-1.60747700	0.81370100
F	-3.20933200	-2.65240200	-0.38675100
F	-1.14261600	-2.31562900	-1.32196900

B3

Coordinates (Angstroms)			
X	Y	Z	

C	1.46444600	-1.26974500	0.03351100
O	1.25915400	-2.44254900	0.73370300
H	1.10787100	-1.32085900	-0.99723600
C	2.90235300	-0.83967100	0.09621500
C	3.50147000	-0.26079700	-1.01685200
C	3.61606200	-0.97235600	1.28471700
C	4.81583600	0.18629400	-0.94371700
H	2.93884500	-0.16046700	-1.93852300
C	4.92863200	-0.52589600	1.35519800
H	3.14679700	-1.42834000	2.14886600
C	5.52818200	0.05602700	0.24217200
H	5.28152500	0.63538900	-1.81208700
H	5.48470400	-0.63122000	2.27852100
H	6.55236100	0.40372800	0.29970100
C	1.53664000	3.34300300	0.05137500
C	1.45009000	2.10084600	0.66673500
C	0.66345200	1.12180400	0.08224600
C	-0.02781800	1.34098500	-1.09875900
C	0.06709800	2.58737600	-1.70473400
C	0.84803900	3.58512600	-1.13205800
H	2.14391900	4.11995600	0.49789000
H	1.98389300	1.89165900	1.58703400
H	-0.63067400	0.54818000	-1.52808800
H	-0.47176300	2.77702400	-2.62438600
H	0.91858600	4.55493700	-1.60830500
N	0.58532300	-0.19713700	0.69480100
H	0.84893900	-0.14588700	1.68454800
H	-0.41924800	-0.56899500	0.64728000
H	0.44373100	-2.86640800	0.41300300
C	-4.22669700	1.53570700	-0.43190300
C	-3.42404500	0.40704600	-0.54218000
C	-2.86709700	-0.17637900	0.60155800
C	-3.13715300	0.40248300	1.84750400
C	-3.94150500	1.52826600	1.94714700
C	-4.49099000	2.10708700	0.80753800
H	-4.65003700	1.97061200	-1.32970300
H	-3.22892300	-0.02058000	-1.51702800
H	-2.70861300	-0.04467600	2.73822300
H	-4.13778000	1.95641500	2.92305500
H	-5.11769900	2.98638900	0.88519900

N	-2.00221900	-1.28429700	0.52268600
H	-1.98509500	-1.78549100	1.40745700
B	-1.99899400	-2.23902300	-0.66851200
F	-3.25908500	-2.77627300	-0.96332900
F	-1.49841600	-1.61259200	-1.82406900
F	-1.12064300	-3.31214200	-0.33251000

TSB3-4

Coordinates (Angstroms)

	X	Y	Z
C	1.47510100	-1.28860400	0.03820300
O	1.30285800	-2.47376200	0.74479800
H	1.17063300	-1.38251900	-1.00651900
C	2.90273400	-0.82040600	0.13358000
C	3.53473200	-0.28755100	-0.98426700
C	3.57161400	-0.86474000	1.35474200
C	4.83395100	0.19878700	-0.88505700
H	3.00954300	-0.25544900	-1.93247600
C	4.86961000	-0.38197800	1.45183600
H	3.07900100	-1.28391800	2.22474500
C	5.50088500	0.15334000	0.33268800
H	5.32295800	0.61180900	-1.75865700
H	5.39003200	-0.42166000	2.40084400
H	6.51326900	0.53039400	0.41088900
C	1.26246300	3.36133200	0.17662300
C	1.18112500	2.10657200	0.76799700
C	0.63207600	1.05224100	0.05165700
C	0.17382100	1.23010700	-1.24766500
C	0.26582500	2.48622200	-1.83264300
C	0.80932100	3.55205100	-1.12347200
H	1.68647100	4.18795000	0.73275400
H	1.53973800	1.94374400	1.77823800
H	-0.25777700	0.39413000	-1.78601400
H	-0.09209900	2.63155800	-2.84425800
H	0.87753000	4.53000700	-1.58311800
N	0.54419000	-0.26241700	0.64675300
H	0.76718500	-0.20693000	1.64414400
H	-0.62097500	-0.71448900	0.55329900
H	0.50444000	-2.91864700	0.41799200
C	-4.05231100	1.65072000	-0.43636500
C	-3.18857300	0.56971300	-0.55885000
C	-2.80652700	-0.14491100	0.57582300

C	-3.29282400	0.23799400	1.82440500
C	-4.15448900	1.32097500	1.93825300
C	-4.53698400	2.03480200	0.80882400
H	-4.34461800	2.19741700	-1.32471000
H	-2.81341100	0.28280900	-1.53238400
H	-2.99576000	-0.32144300	2.70478100
H	-4.52569200	1.60601000	2.91512700
H	-5.20900100	2.87907000	0.89719300
N	-1.87443900	-1.22933400	0.48427400
H	-1.92621400	-1.77522400	1.34565300
B	-1.95071800	-2.21108800	-0.71930900
F	-3.24301700	-2.68226800	-0.93092400
F	-1.47141300	-1.60141800	-1.88225800
F	-1.09913500	-3.29707100	-0.39286500

B4

Coordinates (Angstroms)

	X	Y	Z
C	1.94551700	-0.84827500	0.68037600
O	1.15311100	0.24406600	1.18294400
H	1.93082800	-1.65520800	1.41667100
C	3.37386700	-0.41917900	0.43135000
C	4.42725800	-1.23754100	0.82428300
C	3.63772400	0.78364600	-0.21979100
C	5.73972700	-0.85906600	0.56475700
H	4.21911600	-2.17057400	1.33632000
C	4.94892700	1.16053700	-0.48028700
H	2.81638200	1.42740700	-0.51379300
C	6.00153600	0.33941800	-0.08843400
H	6.55684400	-1.49819200	0.87612600
H	5.15018600	2.09694000	-0.98618600
H	7.02389000	0.63599400	-0.28854600
N	1.35763400	-1.30774800	-0.53444400
H	1.64158400	-0.81292600	-1.37089900
H	1.46898300	0.50373400	2.05947000
C	0.09231800	-1.89051500	-0.58024600
C	-0.51211500	-2.08973400	-1.82965700
C	-0.58933700	-2.30023100	0.57011400
C	-1.74854500	-2.70762100	-1.92350900
H	0.00899400	-1.76466100	-2.72365400
C	-1.82730000	-2.92499900	0.46059400
H	-0.16776500	-2.12564500	1.55138000

C	-2.41678800	-3.13610900	-0.77881000
H	-2.19496200	-2.85303500	-2.90012700
H	-2.33916700	-3.23531200	1.36408800
H	-3.38435000	-3.61580300	-0.85377500
C	-3.57857200	0.12091200	2.08668100
C	-2.38792200	0.58368000	1.54296900
C	-2.27466700	0.69330400	0.16449500
C	-3.32525100	0.36156900	-0.67525700
C	-4.51291900	-0.10170100	-0.12132600
C	-4.64012000	-0.22508200	1.25680200
H	-3.67386200	0.02649100	3.16107500
H	-1.55179800	0.84806100	2.17934800
H	-3.21004800	0.45723400	-1.74898100
H	-5.33634200	-0.37005300	-0.77121700
H	-5.56535000	-0.59008800	1.68466100
N	-1.02971400	1.18352300	-0.40637000
H	-0.23237700	0.83630200	0.15417300
H	-0.91093900	0.79792500	-1.34767200
B	-0.90598100	2.78589000	-0.49472800
F	-1.96734800	3.25679200	-1.24688200
F	-0.93867100	3.27720900	0.79939200
F	0.31042800	3.04721300	-1.10732000

TSB4-5

Coordinates (Angstroms)

	X	Y	Z
C	1.28800400	-1.49261100	0.60193100
O	0.96453600	0.16843800	1.42765000
H	1.10006500	-2.04084800	1.51738200
C	2.70337300	-1.26409800	0.24756600
C	3.68600700	-1.85219800	1.03871800
C	3.06073800	-0.47710500	-0.84734600
C	5.02633600	-1.67549400	0.72093800
H	3.39861100	-2.45056100	1.89551700
C	4.40047800	-0.29575800	-1.15415600
H	2.30107900	0.01360900	-1.44720100
C	5.38324200	-0.89851800	-0.37395600
H	5.79022100	-2.14050000	1.33115300
H	4.67952200	0.32099400	-1.99903500
H	6.42859700	-0.75539400	-0.61804600
N	0.41301600	-1.67795200	-0.37938000
H	0.69135500	-1.43127800	-1.32357200

H	0.27979200	0.10019800	2.11154400
C	-0.91756600	-2.13499000	-0.23224400
C	-1.56267700	-2.61862400	-1.36845000
C	-1.58172800	-2.08954100	0.98915800
C	-2.87061000	-3.06692500	-1.27863400
H	-1.03260100	-2.63956700	-2.31371200
C	-2.89254200	-2.54651600	1.06672100
H	-1.10021200	-1.70361800	1.87841400
C	-3.54191100	-3.03337700	-0.06036600
H	-3.36682000	-3.44281100	-2.16471300
H	-3.40942100	-2.50563400	2.01743800
H	-4.56537200	-3.37952600	0.00802200
C	-3.38097600	1.51214500	1.25054400
C	-2.03863800	1.79670300	1.03025000
C	-1.44154700	1.46463800	-0.18903900
C	-2.21050800	0.83796600	-1.17102500
C	-3.54829300	0.54809500	-0.94001600
C	-4.14302400	0.88471500	0.27148500
H	-3.83036100	1.77765900	2.20003400
H	-1.44851400	2.27530200	1.80210600
H	-1.74746700	0.57238500	-2.11567900
H	-4.12768300	0.05595900	-1.71231800
H	-5.18643400	0.65768200	0.45104700
N	-0.05589200	1.69473400	-0.38982200
H	0.59057300	0.81697600	0.67118800
H	0.22087600	1.34142800	-1.30372100
B	0.51356500	3.11698400	-0.19170700
F	-0.24893400	4.08739300	-0.86784000
F	0.54233500	3.44867800	1.17300300
F	1.82229600	3.12133200	-0.70255800

B5

Coordinates (Angstroms)

	X	Y	Z
C	-3.24011100	0.73938000	0.27624000
O	-0.16166400	-0.97469200	-0.81127700
H	-3.77633000	1.61488400	0.63143800
C	-3.99043400	-0.47981600	0.07911700
C	-5.38353600	-0.38962300	0.17725700
C	-3.38270900	-1.71385600	-0.19174700
C	-6.16584700	-1.51627000	-0.02013800
H	-5.84117400	0.56710100	0.40010800

C	-4.17100400	-2.83332200	-0.38108800
H	-2.30394300	-1.80425200	-0.23826000
C	-5.55951300	-2.73507900	-0.29904700
H	-7.24353600	-1.44596800	0.04902000
H	-3.70673600	-3.78937400	-0.58559300
H	-6.16867900	-3.61793800	-0.44903400
N	-1.98112700	0.87205300	0.04540700
H	-1.41835500	0.08769500	-0.35823100
H	0.73554400	-0.59564200	-0.61922700
H	-0.08559400	-1.33925600	-1.70189800
C	-1.22597800	2.05713600	0.29410800
C	-0.17363000	2.34328600	-0.56829400
C	-1.51394600	2.87201200	1.38247700
C	0.58971500	3.48037900	-0.34507800
H	0.03862400	1.69159900	-1.40680200
C	-0.74736400	4.01006500	1.58817600
H	-2.30630000	2.60943800	2.07212300
C	0.30272400	4.31542700	0.72900000
H	1.40970100	3.71103000	-1.01325200
H	-0.96163700	4.64913600	2.43524700
H	0.90195400	5.20039900	0.90197100
B	2.81430300	0.08750700	-1.84629100
F	2.35048700	1.28775300	-2.41811900
F	4.20988100	0.00565500	-2.02324200
F	2.23213700	-0.99875600	-2.54572100
N	2.39260300	0.07329300	-0.37822100
C	2.93417900	-0.80410600	0.56423100
H	2.25947800	1.00300000	0.00571000
C	3.38723500	-2.07781500	0.19377900
C	2.98842000	-0.44718200	1.91871300
C	3.87991200	-2.95474200	1.15129800
H	3.34918200	-2.37814100	-0.84596300
C	3.47965600	-1.33201200	2.86720700
H	2.63998100	0.53634600	2.21656700
C	3.93099400	-2.59424900	2.49354000
H	4.22663100	-3.93348000	0.84043400
H	3.51169200	-1.03027400	3.90768000
H	4.31585100	-3.28326200	3.23458000

TSB5-6

Coordinates (Angstroms)

X

Y

Z

C	-3.07518100	0.76232700	0.25911500
O	-0.17856800	-0.73574200	-0.89765900
H	-3.61975200	1.62885600	0.63371500
C	-3.85400500	-0.45107800	0.04856600
C	-5.24491600	-0.33854000	0.12846500
C	-3.27118500	-1.69651200	-0.21291100
C	-6.04819000	-1.45040300	-0.07791100
H	-5.68918300	0.62587100	0.34621600
C	-4.07791200	-2.80363300	-0.41175100
H	-2.19449100	-1.80385900	-0.24517200
C	-5.46463200	-2.68187900	-0.34883500
H	-7.12520800	-1.35750500	-0.02202200
H	-3.62738600	-3.76799800	-0.60943500
H	-6.08889800	-3.55286300	-0.50607700
N	-1.82432700	0.88025600	0.01652600
H	-1.05777500	0.01008200	-0.49271200
H	0.88798200	-0.37912200	-0.66798200
H	-0.24559800	-0.93298800	-1.84190200
C	-1.12553000	2.08628200	0.30738600
C	-0.15613300	2.51063300	-0.59795200
C	-1.35795700	2.79561900	1.48259300
C	0.56634900	3.66584800	-0.33452800
H	0.01847400	1.94879400	-1.50742600
C	-0.63065100	3.95074300	1.73499400
H	-2.08322200	2.43260600	2.20071400
C	0.33079800	4.38786100	0.83044500
H	1.31594200	3.99913000	-1.04146400
H	-0.80672900	4.50193700	2.65026300
H	0.89993000	5.28562300	1.03663700
B	2.84076900	0.10089100	-1.79476000
F	2.45919200	1.33269800	-2.34426200
F	4.23516000	0.02743500	-1.71442900
F	2.37113400	-0.93878400	-2.61578400
N	2.17099100	-0.00852900	-0.39313800
C	2.69646200	-0.94517400	0.54598900
H	2.13209200	0.91620000	0.03301100
C	2.91267500	-2.26956400	0.16505100
C	2.95596800	-0.55831800	1.85927700
C	3.39209400	-3.18768300	1.09023200
H	2.70420900	-2.57574300	-0.85260500
C	3.43058500	-1.48383900	2.78004400
H	2.78615700	0.47147600	2.15435400
C	3.65279700	-2.80240000	2.40080600
H	3.55938300	-4.21300100	0.78291700

H	3.62918400	-1.16947900	3.79756800
H	4.02494800	-3.52253000	3.11857200

B6

Coordinates (Angstroms)			
	X	Y	Z
C	-2.58271700	0.98975000	-0.35755000
O	-0.15385000	-1.69454400	-1.54171000
H	-2.84596500	2.03485100	-0.17129100
C	-3.65293000	0.01409000	-0.12256200
C	-4.93730600	0.49663600	0.13540900
C	-3.42447500	-1.36526600	-0.13149600
C	-5.98626600	-0.38472700	0.36134700
H	-5.10942900	1.56702600	0.15367600
C	-4.47211100	-2.24223100	0.09766200
H	-2.42727900	-1.74877900	-0.30759500
C	-5.75432500	-1.75438200	0.34197300
H	-6.98083600	-0.00344000	0.55597300
H	-4.29106300	-3.30986900	0.09343100
H	-6.56947200	-2.44447400	0.52200400
N	-1.41993000	0.67143700	-0.76791300
H	-0.71635500	-0.91323400	-1.32340300
H	1.50521100	-1.23110800	-1.05657200
H	-0.38055000	-1.95942200	-2.44080300
C	-0.43206500	1.67817700	-0.89261700
C	0.45940400	1.59734900	-1.96371200
C	-0.28723200	2.69677000	0.05142800
C	1.46131400	2.54705900	-2.10785700
H	0.35107800	0.79602400	-2.68516500
C	0.71932500	3.64166500	-0.09916600
H	-0.94343200	2.73111800	0.91317700
C	1.59484100	3.57277700	-1.17695100
H	2.14170600	2.48369500	-2.94834400
H	0.83102500	4.42397000	0.64190400
H	2.38267000	4.30758100	-1.28612700
B	3.31369800	-2.18744800	-0.33317400
F	3.58419900	-2.70455000	-1.59143300
F	4.46859900	-1.75444600	0.29663500
F	2.61793400	-3.09403300	0.44883900
N	2.36230900	-0.91159900	-0.56200200
C	1.97776300	-0.21401100	0.65469300
H	2.84082900	-0.26134600	-1.19103100

C	0.85924800	-0.64231100	1.35560600
C	2.74856800	0.84683000	1.10421900
C	0.50596300	0.01435100	2.52765300
H	0.27453100	-1.47663900	0.98697400
C	2.39040600	1.49259500	2.28123600
H	3.61743300	1.16148400	0.53729800
C	1.26942800	1.08008900	2.99205900
H	-0.36890400	-0.30977800	3.07748100
H	2.98643900	2.32386000	2.63669700
H	0.99042500	1.58922000	3.90607200

C1

Coordinates (Angstroms)			
	X	Y	Z

C	1.62870500	-0.67006100	0.00000200
O	0.41583300	-0.93558600	-0.00004200
O	2.14575200	0.50340200	0.00006000
H	2.34636100	-1.48840500	-0.00001100
H	1.46078100	1.20975600	0.00005000
B	-0.82052300	0.03678000	-0.00001100
F	-0.31888200	1.33857700	-0.00012200
F	-1.50545000	-0.24851900	1.14334500
F	-1.50560500	-0.24865900	-1.14323700

C2

Coordinates (Angstroms)			
	X	Y	Z

C	-0.21530800	-0.93752800	0.23556900
O	0.65257400	-1.87711900	-0.25443000
H	0.04760700	-0.57657500	1.23206600
C	-1.64256500	-1.40541900	0.17817800
C	-2.52326800	-1.07300000	1.20120600
C	-2.09170400	-2.12814100	-0.92413600
C	-3.85537200	-1.46306700	1.12419900
H	-2.16573600	-0.50842900	2.05536000
C	-3.42264400	-2.51590900	-0.99944500
H	-1.40014600	-2.38923600	-1.71685600
C	-4.30527900	-2.18146900	0.02312700
H	-4.53951700	-1.20560500	1.92305100

H	-3.77240700	-3.07912200	-1.85575000
H	-5.34316200	-2.48509200	-0.03792200
C	-3.01153700	2.60208700	-0.73903200
C	-2.12607700	1.59490400	-1.09964000
C	-0.98392500	1.41132200	-0.33898400
C	-0.70241300	2.19163400	0.77020900
C	-1.59708900	3.19433500	1.12159200
C	-2.74944300	3.39736700	0.37088200
H	-3.90750700	2.76157200	-1.32507700
H	-2.31853100	0.96007700	-1.95685000
H	0.19941700	2.01890200	1.34597000
H	-1.39063500	3.81554600	1.98367100
H	-3.44335800	4.18026300	0.64974000
N	-0.07756800	0.31554200	-0.67009700
H	-0.21950100	0.00962600	-1.63937200
H	0.90089700	0.62757700	-0.58700000
H	1.54477600	-1.76465100	0.14159300
O	3.00981700	-1.88159600	1.05759700
C	4.11415500	-1.37543200	1.10445500
H	4.91347100	-1.81105800	1.71385400
O	4.49799700	-0.30054000	0.47785400
B	3.58311100	0.47035400	-0.39497600
F	4.29355300	1.55877000	-0.87220000
F	2.47157200	0.92030300	0.35614700
F	3.11414900	-0.31356400	-1.44818900

TSC2-3

Coordinates (Angstroms)

	X	Y	Z
C	0.36369000	-0.75455400	-0.02976600
O	-0.61085100	-1.61810100	0.53990900
H	0.03899300	-0.42504400	-1.01495400
C	1.71948900	-1.41804700	-0.13929800
C	2.53931000	-1.12682100	-1.22557100
C	2.18401200	-2.26208000	0.86798200
C	3.81609300	-1.67341800	-1.30627000
H	2.17336800	-0.47708000	-2.01348800
C	3.45692700	-2.81011900	0.78512900
H	1.54252000	-2.49548500	1.71009500
C	4.27606500	-2.51507200	-0.30128500
H	4.44728100	-1.44571700	-2.15661300
H	3.81198400	-3.47004800	1.56738900

H	5.26810800	-2.94522500	-0.36473500
N	0.36814600	0.39383700	0.86630600
H	0.79823600	0.14151100	1.75306400
H	-1.65901600	-0.20319000	1.29211700
H	-0.95961900	-2.20458600	-0.14498100
O	-2.34573500	-0.05765000	2.00044800
C	-3.56028600	-0.26787700	1.68406300
H	-4.26541000	-0.20176800	2.51050500
O	-4.01529400	-0.53370900	0.55454000
B	-3.31271800	-0.49967500	-0.83787200
F	-4.28886000	-0.09842700	-1.70859300
F	-2.86931500	-1.77716600	-1.09995000
F	-2.27777400	0.41121900	-0.74777400
C	0.85804600	1.63464500	0.41350700
C	1.62679700	2.41553200	1.28183200
C	0.55371200	2.13694700	-0.85529200
C	2.06984600	3.67261400	0.89651900
H	1.87258500	2.02638000	2.26389800
C	1.01270400	3.39173600	-1.23479100
H	-0.05181000	1.56337900	-1.54424000
C	1.76999400	4.16986000	-0.36672900
H	2.66178000	4.26121600	1.58718000
H	0.76670100	3.76431100	-2.22202600
H	2.12104800	5.14782700	-0.67050100

C3

Coordinates (Angstroms)

	X	Y	Z
C	1.19882800	0.17066800	-0.25892700
O	0.54274700	-0.69946300	0.72308300
H	0.86295900	-0.14440200	-1.24597000
C	2.69588800	0.01129900	-0.15074900
C	3.46321800	-0.03227300	-1.30991900
C	3.31502600	-0.04343200	1.09506300
C	4.84713500	-0.12529900	-1.22576700
H	2.97507800	0.00560600	-2.27741400
C	4.69880200	-0.13684200	1.17736800
H	2.71492100	-0.01966100	1.99725300
C	5.46598500	-0.17673800	0.01795500
H	5.44084200	-0.16160900	-2.13080600
H	5.17862100	-0.18069300	2.14736000
H	6.54443300	-0.25232800	0.08420100

N	0.81918400	1.51453100	-0.01268300
H	1.30121800	1.94511400	0.76827200
H	-0.75946300	-0.47035800	1.17910800
H	0.64292600	-1.62953600	0.45900600
O	-1.68837500	-0.16525600	1.61906900
C	-2.78432700	-0.53725600	1.12183700
H	-3.67457500	-0.02791300	1.48766600
O	-2.96473500	-1.44135900	0.26666000
B	-1.94730900	-2.47730300	-0.24478100
F	-2.70208300	-3.51212000	-0.73334100
F	-1.16542600	-2.86548400	0.83605200
F	-1.17450100	-1.88607900	-1.22528000
C	-0.49477400	1.96224300	-0.20083500
C	-0.93645800	3.07719700	0.51946500
C	-1.37336000	1.33878700	-1.09034000
C	-2.23475200	3.53842300	0.37243100
H	-0.25604100	3.56411400	1.20945900
C	-2.67528400	1.80721700	-1.22393400
H	-1.06437400	0.47370900	-1.66102300
C	-3.11950100	2.90346900	-0.49505200
H	-2.55926100	4.39792000	0.94667500
H	-3.34665100	1.30182300	-1.90835400
H	-4.13595300	3.26000000	-0.60172700

TSC3-4

Coordinates (Angstroms)

	X	Y	Z
C	1.14912100	0.22017400	-0.20670600
O	0.57271900	-0.71174800	0.82947100
H	0.76948400	-0.13101900	-1.16318300
C	2.64628600	0.08450600	-0.14277600
C	3.35843000	-0.19451400	-1.30336900
C	3.31941800	0.26308400	1.06434000
C	4.74532800	-0.28356400	-1.26188600
H	2.82785200	-0.34061100	-2.23740700
C	4.70370100	0.17289400	1.10280200
H	2.76156300	0.46550000	1.97214600
C	5.41772700	-0.09911200	-0.06049200
H	5.29830700	-0.50092900	-2.16724600
H	5.22652200	0.31108000	2.04107600
H	6.49791100	-0.17109400	-0.02760900
N	0.71925100	1.52520900	0.06797000

H	1.22653000	2.01112400	0.79755800
H	-0.55790300	-0.54648300	1.15143400
H	0.69046200	-1.64127600	0.55833000
O	-1.65974500	-0.27339400	1.59346900
C	-2.74316200	-0.68808900	1.14814000
H	-3.65700500	-0.20877400	1.50115000
O	-2.91967300	-1.63702700	0.31889200
B	-1.84167500	-2.56226300	-0.21211100
F	-2.49832400	-3.62814300	-0.77830500
F	-1.03283400	-2.96185900	0.85195100
F	-1.07722200	-1.87463500	-1.14760200
C	-0.57916000	1.99184300	-0.17647300
C	-1.00302800	3.15309900	0.47689200
C	-1.45370500	1.34731900	-1.05359000
C	-2.28283300	3.64402500	0.27229200
H	-0.32407000	3.65623300	1.15649800
C	-2.73650600	1.84649300	-1.24490700
H	-1.15831200	0.44525300	-1.57175000
C	-3.16376700	2.99251100	-0.58598100
H	-2.59464900	4.54119800	0.79337600
H	-3.40575200	1.32627100	-1.92002900
H	-4.16540400	3.37345700	-0.73834700

C4

Coordinates (Angstroms)

	X	Y	Z
C	-2.50559800	1.00388400	-0.15063100
O	0.06068900	-1.65083800	0.17069000
H	-2.80806800	2.04375400	-0.23182900
C	-3.54599400	0.00400300	-0.07436100
C	-4.86458600	0.45488000	-0.20656800
C	-3.28606000	-1.36101400	0.11632500
C	-5.91468600	-0.44801100	-0.15951800
H	-5.05481900	1.51250800	-0.34818300
C	-4.34021200	-2.25347200	0.16419100
H	-2.27192700	-1.72369700	0.23553300
C	-5.65156500	-1.79962600	0.02515600
H	-6.93379000	-0.09922000	-0.26404200
H	-4.14548800	-3.30750800	0.31411900
H	-6.47043300	-2.50747900	0.06450200
N	-1.24219400	0.75928000	-0.14514700
H	-0.88228400	-0.22111200	-0.11123200

H	0.79890000	-1.33057600	0.73096100
H	0.50555100	-2.01427800	-0.60611000
C	-0.21796000	1.75328900	-0.18366100
C	0.95974000	1.43764400	-0.85104100
C	-0.38362600	2.97462000	0.45778100
C	1.97985100	2.37643900	-0.89773100
H	1.07497900	0.47196400	-1.32745500
C	0.64425300	3.90527300	0.40017900
H	-1.28766600	3.18796900	1.01455000
C	1.82377100	3.60982300	-0.27462600
H	2.89851300	2.13974400	-1.41980400
H	0.52735900	4.85785100	0.90092900
H	2.62369500	4.33873700	-0.30872500
O	1.96314500	-0.37610600	1.64499700
C	3.06261500	0.05320300	1.35335500
H	3.47096100	0.94499900	1.84273700
O	3.88659600	-0.45000100	0.48031100
B	3.59136000	-1.68730200	-0.29328300
F	4.74209800	-1.98331900	-1.01521800
F	2.52564100	-1.45706900	-1.17829000
F	3.27114700	-2.73985300	0.56188600

D1

Coordinates (Angstroms)

	X	Y	Z
C	0.23395500	0.54206900	-0.00503400
O	1.11264000	-0.34402500	-0.00590300
H	0.53759600	1.59078000	-0.00561700
C	-1.16243200	0.22165400	-0.00342100
C	-2.07603100	1.28300200	-0.00101200
C	-1.60565000	-1.10958700	-0.00273300
C	-3.43387600	1.01300200	0.00217900
H	-1.71217200	2.30383300	-0.00149800
C	-2.96111400	-1.36732600	0.00031100
H	-0.88458500	-1.91723200	-0.00457200
C	-3.87033200	-0.30746300	0.00284800
H	-4.15049300	1.82368600	0.00422800
H	-3.32072000	-2.38788200	0.00090400
H	-4.93279000	-0.51873300	0.00541000
B	2.64180700	-0.04678200	0.00096800
F	2.81524300	1.31858800	-0.06744900
F	3.11099200	-0.57504400	1.18011200

F 3.14108600 -0.69470500 -1.10325100

D2

Coordinates (Angstroms)

	X	Y	Z
C	-0.84934000	0.14428400	0.14060000
O	-2.10366600	0.43903600	-0.30236900
H	-0.83181900	-0.40732200	1.08463300
C	0.04943200	1.34828000	0.20373400
C	1.00136300	1.45050000	1.21237700
C	-0.04531700	2.33850700	-0.77040100
C	1.86233000	2.54138600	1.24692600
H	1.06771700	0.67511000	1.96813500
C	0.81644600	3.42655700	-0.73519000
H	-0.79604200	2.25786300	-1.54777800
C	1.77124300	3.52778200	0.27222000
H	2.60184000	2.62029800	2.03409500
H	0.74242300	4.19785300	-1.49187900
H	2.44178900	4.37807900	0.29823400
B	-3.17705200	-0.47038000	0.08918000
F	-2.82752600	-1.80215500	-0.26390500
F	-3.38614300	-0.43742500	1.47480200
F	-4.33433900	-0.09453000	-0.58256300
C	3.45598700	-1.23576400	-0.75937600
C	2.19598900	-0.78762500	-1.13382100
C	1.08435600	-1.36337700	-0.54249900
C	1.18943000	-2.36100500	0.41236900
C	2.45485000	-2.79958100	0.77947700
C	3.58502000	-2.23688700	0.19661100
H	4.33549800	-0.79919300	-1.21488500
H	2.07525400	-0.00426500	-1.87343100
H	0.29602300	-2.78696000	0.85508600
H	2.55528200	-3.58187300	1.52079100
H	4.56948700	-2.58206100	0.48626300
N	-0.24247200	-0.86315000	-0.88411800
H	-0.22746300	-0.40100900	-1.80023900
H	-0.91675900	-1.63621600	-0.95032900

D3

Coordinates (Angstroms)

	X	Y	Z
C	-0.48084000	-0.13228400	-0.31354600
O	-0.11697300	1.05086300	0.26827300
H	-0.11901700	-0.23284200	-1.34067500
C	-1.96567000	-0.42137700	-0.24100200
C	-2.47663900	-1.55463200	-0.87225300
C	-2.82313900	0.44455000	0.42658600
C	-3.83541800	-1.83047400	-0.81664400
H	-1.81084400	-2.22029900	-1.41386900
C	-4.18528600	0.16903800	0.47683500
H	-2.42634100	1.33494800	0.89644500
C	-4.69186000	-0.96817500	-0.13915600
H	-4.22752700	-2.71253000	-1.30743000
H	-4.85090200	0.84732000	0.99628400
H	-5.75312000	-1.18062000	-0.09834800
N	0.26535000	-1.23157300	0.46504500
H	-0.09295200	-2.15063400	0.18706500
H	0.02710600	-1.08777000	1.46511100
C	1.71303200	-1.18667000	0.27002600
C	2.49333800	-0.45265200	1.14604800
C	2.25038400	-1.83598600	-0.82905100
C	3.86071600	-0.37445500	0.91228600
H	2.04261800	0.05005300	1.99199200
C	3.61774800	-1.75110000	-1.05174800
H	1.60688900	-2.39782400	-1.49676100
C	4.42104500	-1.01954900	-0.18357200
H	4.48590200	0.19477200	1.58819100
H	4.05399300	-2.25626100	-1.90392500
H	5.48702300	-0.95414300	-0.36170800
O	-0.53691400	0.05654000	2.82457300
H	-0.18339200	0.24905400	3.70102700
B	0.42491400	2.11311900	-0.58325000
F	1.54302300	1.66189700	-1.30337900
F	0.78621700	3.16735300	0.25500900
F	-0.54646800	2.54152600	-1.50552100
H	-0.41976100	0.85858500	2.29092700

TSD3-4

Coordinates (Angstroms)		
X	Y	Z

C	-0.31668700	-0.06857600	-0.17624400
O	-0.39409900	1.21557400	0.42558400
H	0.05115400	0.04810600	-1.19941100
C	-1.65394200	-0.77805300	-0.17709900
C	-1.83973900	-1.84683400	-1.05099000
C	-2.67327300	-0.40904700	0.69257900
C	-3.03938500	-2.54522400	-1.05339500
H	-1.04387400	-2.12635000	-1.73351100
C	-3.87381300	-1.11123400	0.69019400
H	-2.53980700	0.43307600	1.36036400
C	-4.05853500	-2.17808800	-0.18043100
H	-3.18134300	-3.37079200	-1.73976100
H	-4.66737800	-0.81924700	1.36689000
H	-4.99660700	-2.71938400	-0.18399300
N	0.65522400	-0.86915000	0.60552000
H	0.33238000	-1.83080800	0.68367500
H	0.59940500	-0.20580400	2.01768400
C	2.02664200	-0.83572600	0.19033400
C	2.80457600	-1.97973800	0.35173700
C	2.59392200	0.33166800	-0.31144400
C	4.14690000	-1.95620600	0.00275300
H	2.35315500	-2.88360000	0.74531200
C	3.93936300	0.34094200	-0.66376400
H	1.99731100	1.22712600	-0.43288000
C	4.72069500	-0.79628100	-0.50767800
H	4.74433900	-2.85103300	0.12668600
H	4.37500500	1.25009400	-1.05957100
H	5.76778100	-0.78104100	-0.78224700
O	0.31790500	0.62280600	2.62156600
H	1.09365800	1.04991200	3.02723900
B	-0.71859400	2.40546100	-0.40232900
F	0.30121200	2.62381300	-1.33379100
F	-0.81198600	3.47505800	0.48135000
F	-1.92049900	2.20773000	-1.08069100
H	-0.04811700	1.16442000	1.75820400

D4

Coordinates (Angstroms)

	X	Y	Z
C	-0.44582700	-0.26015900	-0.33217100
O	-0.29376200	0.99705100	0.47540100
H	-0.25628200	0.04059900	-1.36217500

C	-1.85903200	-0.74854700	-0.16610000
C	-2.60662800	-1.07004100	-1.29231100
C	-2.40489600	-0.90700100	1.10491800
C	-3.89993100	-1.55916800	-1.14944400
H	-2.17745400	-0.93354900	-2.27851600
C	-3.69680500	-1.39564900	1.24500800
H	-1.82444100	-0.64083300	1.98139300
C	-4.44490000	-1.72263700	0.11820500
H	-4.48226400	-1.80641800	-2.02834200
H	-4.12247400	-1.51661600	2.23341100
H	-5.45431000	-2.09914900	0.22957100
N	0.48759500	-1.21644100	0.09707800
H	0.19886400	-1.82029100	0.85614800
H	2.59651600	0.91577000	1.52040800
C	1.86351800	-1.10935100	-0.11862000
C	2.70817500	-2.04424800	0.49082300
C	2.41930200	-0.10047600	-0.90956400
C	4.07857700	-1.97174900	0.30666500
H	2.27485500	-2.82201200	1.10954800
C	3.79846900	-0.04311000	-1.08790000
H	1.79339100	0.64949600	-1.37649800
C	4.63653500	-0.97128600	-0.48574300
H	4.71674700	-2.70361300	0.78700300
H	4.21393400	0.74603600	-1.70290200
H	5.70824400	-0.91649400	-0.62675500
O	1.75663500	1.10156700	1.96838000
H	1.87100200	1.93599100	2.44474900
B	-0.60871400	2.35403300	-0.15688900
F	0.25116500	2.55407600	-1.22659400
F	-0.39162900	3.27983600	0.84496300
F	-1.92107300	2.31533300	-0.57842000
H	0.54558900	1.00439200	1.06547600

TSD4-5

Coordinates (Angstroms)

	X	Y	Z
C	-0.41310600	-0.52879900	-0.41833600
O	-0.36257100	1.07078300	0.65124200
H	-0.20153600	0.02702600	-1.32283800
C	-1.81412300	-0.92839800	-0.20942400
C	-2.72101500	-0.68102000	-1.23698800
C	-2.24107600	-1.53390600	0.97289700

C	-4.04861900	-1.06371500	-1.09583500
H	-2.38362000	-0.19050300	-2.14278600
C	-3.56797900	-1.90811700	1.11128300
H	-1.54937600	-1.69358700	1.79250900
C	-4.47106100	-1.67722000	0.07635900
H	-4.75162900	-0.87698500	-1.89757900
H	-3.90294400	-2.37281900	2.02994400
H	-5.50742900	-1.97055000	0.18998700
N	0.56285300	-1.29456300	0.04277200
H	0.33725300	-2.01285200	0.72384300
H	2.02020700	1.05866200	3.02571200
C	1.93997100	-1.09537100	-0.20709000
C	2.83037600	-2.05829100	0.26259900
C	2.40886000	0.04027600	-0.86349800
C	4.19201400	-1.89138500	0.06167100
H	2.44913100	-2.92972300	0.78260100
C	3.77595800	0.18970400	-1.06433100
H	1.73184600	0.81557000	-1.19949800
C	4.67114100	-0.76821600	-0.60448700
H	4.87995600	-2.64255900	0.42889000
H	4.13926000	1.07371500	-1.57324400
H	5.73452700	-0.63890500	-0.76014800
O	1.98739300	1.11239100	2.06268300
H	2.74480800	0.60978100	1.73591900
B	-0.72557700	2.33749800	0.00486300
F	-0.17979100	2.39479300	-1.29514300
F	-0.23431100	3.41156500	0.75523100
F	-2.11778800	2.41305000	-0.09340400
H	0.48784200	1.10485100	1.14248700

TSA1-D1

Coordinates (Angstroms)

	X	Y	Z
B	-2.62412400	0.12308700	-0.00376900
F	-2.94533600	1.40721200	0.02364600
F	-2.49364200	-0.50352900	-1.16472700
F	-2.48280200	-0.55054200	1.12958900
H	-5.48279300	-0.19117900	-0.72058800
H	-5.42831900	-0.31420700	0.80737100
O	-4.93400100	-0.51552300	0.00362500
O	-0.37629100	0.65322800	-0.00102700
C	0.39836800	-0.28367100	-0.00454200

H	0.01865900	-1.31817400	-0.00983300
C	1.86105200	-0.14180600	-0.00180900
C	2.64291000	-1.29585100	-0.00341700
C	2.46104200	1.11963400	0.00265400
C	4.02737100	-1.19206400	-0.00030800
H	2.16150100	-2.26768600	-0.00694300
C	3.84171600	1.21907000	0.00556500
H	1.83872900	2.00637400	0.00375900
C	4.62294900	0.06385800	0.00413400
H	4.63972600	-2.08477800	-0.00137400
H	4.31600500	2.19237100	0.00893100
H	5.70301600	0.14692600	0.00649500

HCOOH

Coordinates (Angstroms)

	X	Y	Z
C	0.13073500	0.40169700	-0.00017800
O	1.12715100	-0.26653000	0.00008500
O	-1.10679900	-0.08895800	0.00002400
H	0.11504600	1.49605200	0.00008400
H	-1.06227000	-1.06233200	0.00011300

E2

Coordinates (Angstroms)

	X	Y	Z
C	1.28468100	1.20517800	-0.48122600
O	2.15135100	1.64391000	0.25765800
H	1.54865400	0.49777800	-1.28328100
C	-0.13249700	1.56293500	-0.38338400
C	-1.00756300	1.08824600	-1.36055400
C	-0.60735200	2.32856500	0.68361100
C	-2.35943200	1.39108000	-1.28075500
H	-0.62234200	0.48765500	-2.17733900
C	-1.95915100	2.61789400	0.76601200
H	0.08540600	2.68133500	1.43813800
C	-2.83188300	2.15033200	-0.21566300
H	-3.04404200	1.02811300	-2.03680200
H	-2.33964000	3.20525700	1.59216400
H	-3.88852100	2.37912400	-0.14603900

C	-2.84621300	-1.44322000	0.79034700
C	-1.62600100	-1.14320000	1.37684500
C	-0.42932100	-1.55412900	0.77476200
C	-0.49372600	-2.27933600	-0.42165000
C	-1.72133100	-2.57399200	-0.99882400
C	-2.90806800	-2.16023600	-0.40192100
H	-3.75928300	-1.10698000	1.26815300
H	-1.58489900	-0.57832000	2.30200700
H	0.42711200	-2.60127100	-0.89583200
H	-1.74829200	-3.13218200	-1.92754200
H	-3.86280200	-2.38996400	-0.85754800
N	0.79161800	-1.27962900	1.37038300
H	0.79725100	-0.50151400	2.01600900
H	1.60706300	-1.30413000	0.76797500
H	3.64648600	1.01311000	0.03047900
O	4.54952000	0.60896400	-0.12841800
C	4.44775400	-0.69400100	-0.26587900
H	5.42259900	-1.16486800	-0.43151100
O	3.41344600	-1.31942900	-0.22199500

TSE2-3

Coordinates (Angstroms)

	X	Y	Z
C	0.95042500	-1.06482900	0.28412900
O	1.85647400	-1.78311100	-0.21570600
H	1.20104700	-0.37014100	1.09785700
C	-0.46251100	-1.53185400	0.29072000
C	-1.36447700	-0.98069800	1.19628000
C	-0.88726900	-2.50141200	-0.61562200
C	-2.69008100	-1.40022000	1.20045400
H	-1.02568100	-0.22457300	1.89664000
C	-2.21166000	-2.91424300	-0.61490600
H	-0.17358300	-2.92495100	-1.31226200
C	-3.11372600	-2.36368700	0.29310400
H	-3.39041100	-0.97345600	1.90780300
H	-2.54458900	-3.66660600	-1.31933900
H	-4.14671700	-2.68967300	0.29297600
C	-2.44744000	2.28387200	-0.73185000
C	-1.48163600	1.38401600	-1.16145300
C	-0.19606400	1.44216300	-0.62724100
C	0.11553500	2.39232500	0.34391000
C	-0.85820000	3.28628800	0.76856600

C	-2.14223900	3.23544200	0.23568900
H	-3.44445000	2.23693500	-1.15255000
H	-1.71630600	0.63294200	-1.90785400
H	1.11700000	2.42552700	0.75802300
H	-0.61141100	4.02531200	1.52098600
H	-2.89854200	3.93422400	0.57010700
N	0.76381700	0.47036100	-0.97877600
H	0.57902200	0.01560100	-1.86943100
H	1.73205400	0.79515700	-0.92340400
H	3.15650600	-1.35401700	0.11604800
O	4.13905100	-1.05646400	0.40415300
C	4.33830700	0.21617900	0.24266300
H	5.34709400	0.52953200	0.54015800
O	3.52678300	1.01652500	-0.18731900

E3

Coordinates (Angstroms)

	X	Y	Z
C	0.53548300	-1.11558100	0.26519200
O	1.19217700	-2.25024800	-0.13577200
H	0.88498200	-0.73579800	1.23002500
C	-0.95736300	-1.30032700	0.26967200
C	-1.73301000	-0.69580900	1.25283500
C	-1.56762400	-2.03622000	-0.74295200
C	-3.11708200	-0.82624600	1.22661200
H	-1.25194000	-0.12418100	2.03906100
C	-2.94999500	-2.16572900	-0.76824800
H	-0.95856400	-2.51125200	-1.50320700
C	-3.72581600	-1.55889600	0.21489200
H	-3.71777500	-0.35649700	1.99562600
H	-3.42369800	-2.74023200	-1.55478600
H	-4.80388900	-1.66177100	0.19375700
C	-1.38087800	2.92759500	-0.91704800
C	-0.78362800	1.71021400	-1.21737200
C	0.29699000	1.28615600	-0.45995900
C	0.78945000	2.04449800	0.59203600
C	0.18223800	3.25860400	0.88670200
C	-0.90186600	3.69909600	0.13576900
H	-2.22355800	3.26936600	-1.50450000
H	-1.15007200	1.09246400	-2.02962400
H	1.63684600	1.68973400	1.16676100
H	0.55901600	3.86032100	1.70404700

H	-1.37215000	4.64607500	0.36907700
N	0.90742100	-0.00254900	-0.73128300
H	0.64871100	-0.33143700	-1.66607200
H	2.00134600	0.07515100	-0.67500200
H	2.16352900	-2.14501000	0.10738200
O	3.65960600	-1.80135600	0.51911100
C	4.11439100	-0.70142100	0.14512400
H	5.18409300	-0.50826600	0.33793300
O	3.48114800	0.21955100	-0.43221900

TSE3-4

Coordinates (Angstroms)

	X	Y	Z
C	-0.75052900	0.31216900	-0.51213200
O	-0.59144200	1.72133700	-0.42806800
H	-0.47904800	-0.01714100	-1.51981400
C	-2.20613100	-0.03216300	-0.26355800
C	-2.58153300	-1.37452700	-0.20903200
C	-3.17392300	0.95469400	-0.11554900
C	-3.90844400	-1.72474300	-0.00386400
H	-1.83046300	-2.14779800	-0.32978700
C	-4.50382600	0.60173500	0.09599600
H	-2.88642100	1.99597900	-0.16486700
C	-4.87450100	-0.73497800	0.15192300
H	-4.18962300	-2.77006400	0.03398300
H	-5.25071100	1.37727600	0.21542100
H	-5.91026100	-1.00694500	0.31458100
N	0.08918500	-0.36472400	0.44537700
H	-0.38677000	-0.81077400	1.21811400
H	0.80487600	1.72765300	1.09086600
H	0.18975500	2.00062200	-0.93178900
O	1.62708600	2.11187700	1.46677900
C	2.32533400	2.71964000	0.52400500
H	3.25596000	3.13461200	0.92248500
O	1.99456300	2.81996800	-0.63288100
C	1.34272800	-0.88236100	0.13827700
C	1.91363700	-1.83423300	0.99537100
C	2.07470400	-0.45617600	-0.97543500
C	3.17516600	-2.34466400	0.74048100
H	1.35165500	-2.16562500	1.86172500
C	3.33761100	-0.98351600	-1.22314900
H	1.67857200	0.29388600	-1.64824100

C	3.89971800	-1.92669800	-0.37340100
H	3.59474700	-3.07978200	1.41698100
H	3.88659100	-0.64097100	-2.09226800
H	4.88512900	-2.32838300	-0.57126400

E4

Coordinates (Angstroms)			
	X	Y	Z

C	-0.78842500	-0.34507000	-0.71561600
O	-0.37573500	0.93255600	-1.21681400
H	-0.66971500	-1.08210800	-1.51026300
C	-2.24579400	-0.26426500	-0.32517700
C	-2.98569500	-1.44220700	-0.25189800
C	-2.84398100	0.94601100	0.00698100
C	-4.31379100	-1.41099800	0.14979000
H	-2.51574000	-2.38468900	-0.51130000
C	-4.17550600	0.97623100	0.41112000
H	-2.27867400	1.86726100	-0.05704800
C	-4.91174500	-0.19917300	0.48258200
H	-4.88376500	-2.33063700	0.20013800
H	-4.63715500	1.92222700	0.66667000
H	-5.94878900	-0.17280500	0.79396000
N	-0.01693400	-0.76201400	0.42968000
H	-0.29487600	-0.28427900	1.28063600
H	0.26650500	1.98788200	0.05773800
H	0.49051700	0.83971500	-1.64679400
O	0.90822800	2.40095900	0.68713500
C	2.10426100	2.39786200	0.11940100
H	2.87726100	2.76425100	0.80298500
O	2.32359100	2.05399000	-1.01569800
C	1.37221900	-0.91814800	0.31758300
C	2.18127500	-0.64553600	1.42610600
C	1.97415000	-1.36185600	-0.86368100
C	3.55548200	-0.81424700	1.35390800
H	1.71992500	-0.29121200	2.34147700
C	3.35267200	-1.52592000	-0.92462200
H	1.37651400	-1.58762300	-1.73839600
C	4.15432500	-1.25398700	0.17689300
H	4.16295800	-0.59480500	2.22397600
H	3.80035100	-1.87023400	-1.84930000
H	5.22786700	-1.38105900	0.12055100

TSE4-5

Coordinates (Angstroms)

	X	Y	Z
C	-0.72572000	-0.76269800	-0.35402300
O	-0.47150400	0.71367000	-1.65048700
H	-0.50550000	-1.48991700	-1.12195600
C	-2.14493000	-0.51844700	-0.05466000
C	-3.09485500	-1.35833000	-0.63110000
C	-2.54470400	0.53113900	0.77400500
C	-4.44227800	-1.17120900	-0.35370600
H	-2.77464800	-2.15915700	-1.28735900
C	-3.89222000	0.71883200	1.03922400
H	-1.81282400	1.21935100	1.18393000
C	-4.84029900	-0.13467100	0.48151500
H	-5.17980200	-1.83058600	-0.79343100
H	-4.20593600	1.53626600	1.67600200
H	-5.89172200	0.01553100	0.69349800
N	0.17753500	-0.58303000	0.58941700
H	-0.08692800	-0.02084700	1.39278600
H	-0.24774000	1.47539700	-0.96053800
H	0.38403200	0.60268700	-2.09683900
O	0.26364900	2.34906700	0.08337500
C	1.49828600	2.50635400	-0.18333300
H	2.08784000	3.00713800	0.60983500
O	2.07442600	2.16686000	-1.22074800
C	1.57018100	-0.79509500	0.45250700
C	2.39356900	-0.27500200	1.44741100
C	2.11604600	-1.46647600	-0.63680400
C	3.76834000	-0.42630100	1.35160200
H	1.95209100	0.25493300	2.28421800
C	3.49493900	-1.61071000	-0.72037500
H	1.49123100	-1.87818900	-1.41876000
C	4.32546100	-1.09294800	0.26611900
H	4.40466800	-0.01641400	2.12591700
H	3.91988600	-2.13115700	-1.56953700
H	5.39914900	-1.20723500	0.18890300

E5

Coordinates (Angstroms)

	X	Y	Z
--	---	---	---

C	4.42948300	-0.75607900	-0.36679700
C	3.84464500	-1.69421200	0.47539500
C	2.46162500	-1.79338800	0.54312300
C	1.65567300	-0.94453600	-0.21948500
C	2.25029400	-0.01363600	-1.07584500
C	3.63120800	0.07734900	-1.14672600
H	5.50825800	-0.67915700	-0.42502800
H	4.46390200	-2.34887900	1.07556300
H	1.99630200	-2.52461800	1.19525700
H	1.63543400	0.61853600	-1.70359700
H	4.08953400	0.79566700	-1.81498600
C	0.20242500	-1.06025000	-0.06795500
H	-0.15678700	-1.96138700	0.43506500
N	-0.61832700	-0.16497200	-0.45299300
C	-2.00849900	-0.38463500	-0.28258700
C	-2.60304500	-1.60857000	-0.58860200
C	-2.79112200	0.67666800	0.17132500
C	-3.97132200	-1.77166700	-0.41637900
H	-1.99779100	-2.41765400	-0.97983800
C	-4.15611300	0.50163700	0.34900300
H	-2.32219800	1.62639400	0.40132400
C	-4.75057100	-0.72116000	0.05497500
H	-4.43081100	-2.72136400	-0.66143800
H	-4.75780700	1.32458700	0.71455300
H	-5.81743500	-0.85214100	0.18577400
H	-0.27072100	1.36238900	-0.89217300
O	-0.13331900	2.34098700	-1.17794500
C	0.47239500	3.02511500	-0.24237000
H	0.64331700	4.06779300	-0.53365200
O	0.81995900	2.59118500	0.83545200
O	0.74975900	0.40779400	2.66959800
H	1.51915400	-0.13374000	2.46341200
H	0.73228500	1.08282300	1.97142900

F2

Coordinates (Angstroms)

X

Y

Z

C	-2.93415000	0.88734700	0.37404000
C	-1.71799500	0.67819200	1.01165900
C	-1.00558500	-0.50860400	0.80440600
C	-1.54281000	-1.47552200	-0.05463700

C	-2.75747600	-1.25564900	-0.68548800
C	-3.46300000	-0.07194300	-0.48249000
H	-3.47082500	1.81251800	0.54952300
H	-1.30931900	1.43162900	1.67600000
H	-0.99382800	-2.39570400	-0.22256400
H	-3.15653000	-2.01652300	-1.34615900
H	-4.41040600	0.09525700	-0.97877100
N	0.25226400	-0.68442500	1.36389500
H	0.43451600	-0.14520000	2.19964700
H	0.55574800	-1.64497500	1.45382600
H	1.76965300	-0.57574800	-1.10064000
O	0.78979600	0.69114300	-1.55894800
C	0.57888700	1.66919700	-0.86723000
H	-0.19341800	2.40241200	-1.11308200
O	1.24690500	1.98125600	0.21224900
H	1.93473600	1.28401700	0.40353000
C	3.19713000	-0.92674200	0.10297400
O	3.18680600	0.17109200	0.62474800
O	2.40675300	-1.30937400	-0.86455200
H	3.90173100	-1.70730800	0.40404000

TSF2-3

Coordinates (Angstroms)

	X	Y	Z
C	3.52267100	0.45715900	0.13834500
C	2.35789500	1.11238900	-0.23930500
C	1.21755900	0.36752300	-0.51504700
C	1.22566400	-1.01729500	-0.40451800
C	2.39503700	-1.66311500	-0.02575200
C	3.54414900	-0.92908800	0.24717100
H	4.41547700	1.03312000	0.34780000
H	2.33074600	2.19245800	-0.32830200
H	0.32394300	-1.57927700	-0.62183300
H	2.40678800	-2.74284100	0.05608400
H	4.45472300	-1.43619700	0.54049100
N	-0.00455200	1.03694600	-0.82255300
H	0.14471000	1.90945700	-1.32859100
H	-0.63428300	0.44748300	-1.37008800
H	-1.78698000	-0.67871400	1.05919500
O	-1.02321300	0.40929100	1.38151200
C	-0.97465900	1.45428500	0.66075800
H	-0.34452600	2.27957800	1.00063100

O	-2.10467600	1.94135400	0.07732000
H	-2.61732900	1.17503100	-0.25460200
C	-2.93941100	-1.45919500	-0.32179800
O	-2.94030400	-0.44985800	-1.01719100
O	-2.34189800	-1.57979300	0.81546100
H	-3.47410900	-2.36265500	-0.63886100

F3

Coordinates (Angstroms)

	X	Y	Z
C	2.55741900	1.41388200	0.66334700
C	1.26838700	1.02249800	0.32578400
C	1.08978800	-0.16625300	-0.36513900
C	2.16198700	-0.96961700	-0.72108300
C	3.44687400	-0.56849000	-0.37876600
C	3.64447800	0.62084600	0.31294100
H	2.71074200	2.34159400	1.19986900
H	0.41342200	1.63281900	0.58991000
H	1.99061400	-1.89288900	-1.26272300
H	4.29206100	-1.18609000	-0.65483500
H	4.64745000	0.93137100	0.57764400
N	-0.25967800	-0.59207700	-0.70053900
H	-0.24455700	-1.14919400	-1.55925500
H	-2.75946500	-1.11055100	-0.05218800
O	-2.14134500	-1.86705500	-0.13286100
C	-0.93558300	-1.45827000	0.37775500
H	-0.28716700	-2.31870000	0.52550400
O	-1.01714700	-0.73606400	1.53556900
H	-1.74783200	-0.09012700	1.42118400
C	-2.84508200	1.49491900	-0.36279600
O	-1.83162400	1.47983600	-1.09915800
O	-3.14607600	0.62706700	0.49307300
H	-3.53260200	2.34901600	-0.48213200
H	-0.90500100	0.26991700	-0.88445100

TSF3-4

Coordinates (Angstroms)

	X	Y	Z
C	-2.55278400	-1.33318200	0.76232700

C	-1.25378600	-0.95976700	0.44255600
C	-1.04489900	0.16957300	-0.33805300
C	-2.11357300	0.92591100	-0.80053300
C	-3.40988100	0.54358600	-0.47925400
C	-3.63046800	-0.58395600	0.30312500
H	-2.72192900	-2.21406000	1.36884500
H	-0.40944000	-1.54126400	0.79217600
H	-1.92769500	1.80340300	-1.40974600
H	-4.24617700	1.12850900	-0.84109100
H	-4.64156000	-0.88030400	0.55298200
N	0.31061000	0.56324800	-0.66265600
H	0.30264700	1.09449300	-1.53575200
H	2.77919700	1.13204400	-0.08467900
O	2.16297100	1.88540000	-0.13811500
C	0.95146000	1.46359900	0.37036800
H	0.30929900	2.33217400	0.50420000
O	1.04293000	0.79952700	1.57052900
H	1.73002900	0.11332500	1.47177200
C	2.75049100	-1.55076700	-0.40062600
O	1.69990100	-1.47571600	-1.11513100
O	3.10334200	-0.71809000	0.44642600
H	3.37385900	-2.43877600	-0.57507100
H	1.02498600	-0.45123100	-0.87417600

F4

Coordinates (Angstroms)

	X	Y	Z
C	-2.94889700	-0.60887400	-1.07933900
C	-1.61326400	-0.79368000	-0.73523100
C	-1.06988300	-0.07263400	0.32633600
C	-1.87078100	0.83177200	1.02677200
C	-3.19867000	1.00978800	0.67215200
C	-3.74707100	0.28935800	-0.38480500
H	-3.36249400	-1.17628600	-1.90431800
H	-1.00201400	-1.48582300	-1.29703300
H	-1.44261400	1.39022300	1.85194900
H	-3.80767500	1.71352700	1.22633800
H	-4.78465000	0.42780800	-0.66112600
N	0.29991700	-0.18659100	0.70737500
H	1.08642600	1.16386300	0.05301200
H	0.39242800	0.00646400	1.70307400
H	2.72771900	-0.82413700	0.94632500

O	2.11490000	-1.51834600	1.24123900
C	0.99440500	-1.45594000	0.42614600
H	0.35731700	-2.30701800	0.67120200
O	1.30059000	-1.55960400	-0.92554800
H	1.96147000	-0.88041900	-1.13406300
C	2.81381700	1.66237200	-0.57853600
O	1.57772300	1.98097700	-0.30676300
O	3.28361600	0.54651000	-0.44667500
H	3.40209500	2.50867100	-0.94598500

TSF4-5

Coordinates (Angstroms)

	X	Y	Z
C	-3.18261000	-0.86444100	0.59489300
C	-1.84859200	-1.01089300	0.23194600
C	-1.18332900	0.05121700	-0.37920600
C	-1.85307100	1.25640500	-0.59742400
C	-3.17903900	1.39183800	-0.21879100
C	-3.85513300	0.33014900	0.37483300
H	-3.69229700	-1.69558600	1.06674500
H	-1.33686500	-1.94003200	0.44291200
H	-1.32529600	2.07784000	-1.06860200
H	-3.68756600	2.33218600	-0.39295400
H	-4.89199900	0.43629700	0.66715600
N	0.15370600	-0.04304700	-0.79883800
H	1.76674300	-0.52524000	1.24245600
H	0.64220700	0.82802800	-0.97587400
H	1.78802000	-2.18523500	1.08782600
O	1.21502200	-1.41008400	0.97217500
C	0.90141700	-1.17759500	-0.75593100
H	0.36046100	-2.10565500	-0.89978100
O	2.09285000	-1.14290100	-1.30753800
H	2.55309500	-0.24736400	-1.06225400
C	3.00270900	1.32864800	0.64992900
O	2.41669600	0.66296100	1.54028600
O	3.08043200	1.04473900	-0.56699200
H	3.49345000	2.25641100	0.97930300

F5

Coordinates (Angstroms)

	X	Y	Z
C	-3.74774100	-0.60646500	0.34226100
C	-2.46282900	-1.13386500	0.36062700
C	-1.38717300	-0.32546600	0.00167600
C	-1.59544000	1.01019600	-0.33496000
C	-2.88139600	1.53039700	-0.32977300
C	-3.96429800	0.72289400	-0.00002000
H	-4.58240800	-1.23915400	0.61772300
H	-2.30511200	-2.15921400	0.66894900
H	-0.74702600	1.63122500	-0.59887900
H	-3.03601100	2.57005300	-0.59050500
H	-4.96794600	1.12859800	-0.00177900
N	-0.05973000	-0.81249400	-0.00818500
H	1.67827800	3.79042300	0.84141300
H	0.69788600	-0.13112800	0.07420200
H	2.25175700	2.59281300	0.07442600
O	2.12844900	3.55391000	0.02429800
C	0.30680100	-2.07543400	-0.23144900
H	-0.50538000	-2.78172600	-0.42170900
O	1.48124600	-2.45468000	-0.23761500
H	2.79034300	-1.60689600	-0.05054400
C	3.52489200	0.15575800	0.13243900
O	2.44652700	0.72383800	0.11608100
O	3.68330900	-1.13233200	0.04401200
H	4.47058700	0.69848600	0.22499400

PhNHCHO

Coordinates (Angstroms)			
	X	Y	Z
C	-1.81966700	1.31818300	-0.02776600
C	-0.45366300	1.09717100	-0.15028100
C	0.03857800	-0.20701000	-0.11302300
C	-0.84533700	-1.27863500	0.00784000
C	-2.20917000	-1.04625700	0.10620000
C	-2.70372800	0.25353000	0.09850100
H	-2.19400000	2.33422700	-0.05272800
H	0.21680300	1.93460600	-0.29317400
H	-0.45374200	-2.28911500	0.02802900
H	-2.88668500	-1.88644000	0.19635500
H	-3.76787800	0.43408300	0.18156400

N	1.41635700	-0.48238600	-0.22068700
H	1.68084900	-1.41136600	-0.53144000
C	2.42475300	0.32245600	0.19046800
H	2.09150000	1.26771200	0.63646000
O	3.60100700	0.02954700	0.08851400

CH₃OH

Coordinates (Angstroms)			
	X	Y	Z
O	-0.04760500	-0.75701400	0.00000000
H	0.86848900	-1.05435500	0.00000000
C	-0.04760500	0.66409000	0.00000000
H	-1.08767500	0.98748800	0.00000000
H	0.44283000	1.06922100	0.88966600
H	0.44283000	1.06922100	-0.88966600

G1

Coordinates (Angstroms)			
	X	Y	Z
O	0.81165400	-0.67357700	-0.26861800
B	-0.55854500	0.04607200	0.00691500
F	-1.48885200	-0.95581100	-0.10338500
F	-0.66264700	1.00865300	-0.96231300
F	-0.49036900	0.58083000	1.27124800
H	0.84609000	-1.57554400	0.10017700
C	2.04379900	0.05728200	0.00222000
H	2.85585900	-0.48914800	-0.46739200
H	1.92457800	1.03350100	-0.45787000
H	2.18698600	0.14271300	1.07618000

G2

Coordinates (Angstroms)			
	X	Y	Z
C	-0.55987700	1.34629300	0.31793000
O	-1.36212700	1.70463000	-0.54617200
H	-0.91531300	0.82191000	1.21292500

C	0.86647400	1.63765200	0.25354200
C	1.68117800	1.19183300	1.29470800
C	1.41870900	2.29876500	-0.84632600
C	3.04910600	1.41484000	1.24344500
H	1.23628400	0.67061100	2.13511500
C	2.78473400	2.51948600	-0.89313500
H	0.77382800	2.62896900	-1.65163900
C	3.59741400	2.07588000	0.14951700
H	3.68745500	1.06820500	2.04634100
H	3.22352200	3.03062800	-1.74065300
H	4.66628500	2.24705300	0.10590200
C	3.48296300	-1.39413900	-1.12842400
C	2.11969000	-1.17888200	-1.26665400
C	1.23532900	-1.57371700	-0.25581100
C	1.75206600	-2.18438800	0.89284200
C	3.11778200	-2.39542700	1.02022400
C	3.99586200	-1.99850000	0.01626500
H	4.15177000	-1.07917100	-1.92108700
H	1.72494000	-0.70262300	-2.15754300
H	1.07256500	-2.48751700	1.68196600
H	3.49905200	-2.87136500	1.91611600
H	5.06070100	-2.16348100	0.12039400
N	-0.11687500	-1.27434000	-0.34993000
H	-0.47715500	-1.15369200	-1.28769200
H	-0.73692000	-1.83200000	0.22355700
O	-3.61078800	0.79084900	-0.14244100
B	-3.63986800	-0.72727200	-0.20027400
F	-2.94552700	-1.06828800	-1.34714500
F	-4.96272500	-1.11839300	-0.24625600
F	-3.01224900	-1.22822500	0.93431800
H	-2.65425400	1.20216800	-0.34549200
C	-4.22405600	1.43423200	0.99679900
H	-4.11957100	2.50782100	0.86265800
H	-5.27620900	1.16302200	1.00541100
H	-3.73592800	1.11294700	1.91571900

TSG2-3

Coordinates (Angstroms)

	X	Y	Z
C	-0.44881700	1.19474900	0.28009000
O	-1.27964600	1.70565900	-0.51757700
H	-0.81519300	0.65751500	1.15659100

C	0.95889700	1.54696300	0.23854000
C	1.78071400	1.11885500	1.28253900
C	1.49486400	2.24609300	-0.84581900
C	3.13872300	1.39990600	1.24927900
H	1.34923000	0.57312300	2.11363400
C	2.85175400	2.52056100	-0.87510600
H	0.84770900	2.56138500	-1.65512400
C	3.67150800	2.09535500	0.16922100
H	3.78070400	1.07187900	2.05692000
H	3.27736100	3.06002000	-1.71163000
H	4.73283100	2.31013100	0.13889900
C	3.44988500	-1.56814200	-0.96810000
C	2.15706700	-1.15626400	-1.25798400
C	1.11235500	-1.46877200	-0.38569000
C	1.37954700	-2.19735200	0.77516600
C	2.67587200	-2.60713300	1.05469900
C	3.71946700	-2.29031100	0.19081300
H	4.25334500	-1.31810200	-1.65074900
H	1.94614600	-0.58951300	-2.15804000
H	0.56629400	-2.43218500	1.45328400
H	2.87165500	-3.17386000	1.95710100
H	4.72992800	-2.60805800	0.41454700
N	-0.16828800	-0.95364300	-0.61214000
H	-0.37630000	-0.76124200	-1.58683400
H	-0.92176900	-1.48035100	-0.18030100
O	-3.45912600	0.85820300	0.02379700
B	-3.60748600	-0.58970000	-0.22627200
F	-3.04351300	-0.83716800	-1.47734900
F	-4.95100200	-0.94528300	-0.19426500
F	-2.90646300	-1.31854500	0.75201000
H	-2.33258800	1.33437700	-0.29122500
C	-3.99121500	1.37615200	1.24759800
H	-3.71066000	2.42567100	1.31783900
H	-5.07728700	1.29577200	1.23247600
H	-3.59072300	0.83154500	2.10414400

G3

Coordinates (Angstroms)

	X	Y	Z
C	-0.36278800	-1.21276500	0.13607700
O	0.15913400	-2.39760300	-0.34196200
H	0.06773100	-0.91523800	1.09469300

C	-1.86269500	-1.25928000	0.19935200
C	-2.52980600	-0.66697600	1.26538200
C	-2.58352100	-1.84587100	-0.83800900
C	-3.91969700	-0.66322700	1.29867000
H	-1.96117400	-0.20984200	2.06768100
C	-3.97128500	-1.84194300	-0.80199500
H	-2.05986000	-2.30886900	-1.66664400
C	-4.63981200	-1.24866100	0.26483200
H	-4.43736000	-0.20310700	2.13102700
H	-4.53255600	-2.30108900	-1.60628600
H	-5.72266700	-1.24641000	0.29010400
N	0.06528400	-0.10739000	-0.84158300
H	-0.29864700	-0.35085000	-1.76842200
H	1.13118200	-0.13603500	-0.88272400
H	1.09958600	-2.43818200	-0.09640300
C	-0.36228500	1.23328400	-0.46335900
C	-1.45782500	1.80481200	-1.08903000
C	0.32957500	1.88285300	0.54748000
C	-1.86812900	3.07091600	-0.69163500
H	-1.97898600	1.26634900	-1.87255800
C	-0.09228900	3.14735500	0.93770500
H	1.18280100	1.40624300	1.01811500
C	-1.18862300	3.73934800	0.32056000
H	-2.72089400	3.53236600	-1.17290500
H	0.43847200	3.66890500	1.72385400
H	-1.51304700	4.72550100	0.62811900
O	2.72047300	-0.10012400	-0.76074100
B	3.41247100	-0.77447600	0.31543600
F	3.44383000	0.00566000	1.48313400
F	2.68583300	-1.96468500	0.59026900
F	4.72442800	-1.11048600	-0.03729700
C	3.29852300	1.10539200	-1.24259800
H	4.24955200	0.90379700	-1.74020800
H	2.61400800	1.54813000	-1.96705000
H	3.46278700	1.81841000	-0.43041400

TSG3-4

Coordinates (Angstroms)

	X	Y	Z
C	1.25861900	0.43853200	-0.89858500
O	0.79147800	-0.71886100	-1.58318800
H	1.22174900	1.30323500	-1.56598800

C	2.67589300	0.20620300	-0.43616400
C	3.56818000	1.27215800	-0.38442500
C	3.07478000	-1.05389700	0.00153800
C	4.85818300	1.07909000	0.09558500
H	3.25289000	2.25193700	-0.72634000
C	4.36414100	-1.24506500	0.48317900
H	2.38123300	-1.88513700	-0.04696000
C	5.25669700	-0.17947000	0.53145800
H	5.55212400	1.91010900	0.12680600
H	4.67325000	-2.22721500	0.81947000
H	6.26253100	-0.33104200	0.90369100
N	0.41470900	0.65471100	0.26765100
H	0.92895500	0.79588600	1.12931800
H	-0.38186900	-1.13598000	0.05914500
H	0.22728900	-0.46285600	-2.32353700
C	-0.75146100	1.43617600	0.18234600
C	-1.30441600	1.94737200	1.36171400
C	-1.40955300	1.65868400	-1.02856300
C	-2.49115300	2.66097000	1.32752500
H	-0.79063300	1.77760300	2.30167500
C	-2.59948600	2.37836600	-1.05020500
H	-1.01695000	1.26968600	-1.95918400
C	-3.15006000	2.88061700	0.12068400
H	-2.90321000	3.05008800	2.25077700
H	-3.09855800	2.53969300	-1.99807000
H	-4.07869200	3.43619800	0.09580800
O	-0.98009400	-1.82527300	0.44654900
B	-2.37507900	-1.90221100	-0.22377500
F	-3.19020500	-0.96496000	0.37800400
F	-2.15124400	-1.63125200	-1.55439700
F	-2.83207300	-3.18219800	-0.00456100
C	-0.92568700	-1.76513000	1.89484300
H	0.10619400	-1.93276200	2.19069200
H	-1.28181200	-0.79536200	2.23652800
H	-1.55949300	-2.56489000	2.26760200

G4

Coordinates (Angstroms)

	X	Y	Z
C	-1.36708600	0.16282500	0.57010600
O	-0.58056700	-1.02911500	0.28450600
H	-1.24053100	0.39591200	1.62915800

C	-2.82479900	-0.09218500	0.26975000
C	-3.80088800	0.34827300	1.15684000
C	-3.19651300	-0.73293200	-0.90988100
C	-5.14608000	0.15346600	0.86552500
H	-3.50610600	0.84215900	2.07611400
C	-4.54099200	-0.92690400	-1.19960800
H	-2.43426700	-1.08668400	-1.59465200
C	-5.51694000	-0.48367000	-0.31272200
H	-5.90304500	0.49548100	1.56046700
H	-4.82764400	-1.42769800	-2.11619500
H	-6.56476900	-0.63915800	-0.53857400
N	-0.87703400	1.23132500	-0.21942900
H	-1.27431900	1.32209600	-1.14542400
H	0.80344600	-1.11591100	-0.32679100
H	-0.76413400	-1.71795900	0.94298100
C	0.38293300	1.79456900	-0.03082100
C	0.83218600	2.75246100	-0.94975300
C	1.20818200	1.44596400	1.04237400
C	2.07361600	3.34428500	-0.79611600
H	0.19400300	3.02000800	-1.78463100
C	2.44884200	2.05838700	1.19059100
H	0.90246700	0.68986300	1.75461600
C	2.89474500	3.00371200	0.27742600
H	2.40388500	4.07926600	-1.52046500
H	3.07596000	1.77394100	2.02712700
H	3.86506800	3.46846300	0.39607800
O	1.70219900	-1.36585500	-0.74366000
B	2.64853200	-2.12599000	0.18476900
F	3.35152500	-3.02224100	-0.59434800
F	3.50099900	-1.22344400	0.79260600
F	1.81703700	-2.75137900	1.09568000
C	2.23498600	-0.39796800	-1.67468800
H	1.41433800	-0.06039600	-2.30262900
H	2.68079600	0.43398700	-1.13252200
H	2.97917400	-0.91106200	-2.27885800

TSG4-5

Coordinates (Angstroms)

	X	Y	Z
C	1.42418900	0.29954100	-0.45835700
O	0.69571400	-1.28713300	0.15787400
H	1.09515100	0.17166000	-1.48196900

C	2.85464700	0.02868100	-0.20973000
C	3.66021100	-0.28323500	-1.30120700
C	3.39939500	0.08033900	1.07367400
C	5.01650800	-0.52091200	-1.11537200
H	3.22483900	-0.33113200	-2.29260400
C	4.75150400	-0.16299600	1.25412000
H	2.77178800	0.28741100	1.93339700
C	5.56119300	-0.46010200	0.16032400
H	5.64364300	-0.75608700	-1.96593200
H	5.17579300	-0.12876100	2.24950200
H	6.61719600	-0.65008400	0.30742000
N	0.82137200	1.26437600	0.22820500
H	1.25991600	1.59056100	1.08302000
H	-0.31894100	-1.24180600	0.38817000
H	0.81869300	-2.01213600	-0.47582300
C	-0.45267700	1.80664500	-0.05805300
C	-0.89087900	2.87195700	0.72615400
C	-1.25998900	1.30337100	-1.07372500
C	-2.13079900	3.44228100	0.48405800
H	-0.25480000	3.24704100	1.52029700
C	-2.49580400	1.89179100	-1.31304100
H	-0.95501600	0.44998200	-1.66576800
C	-2.93832400	2.95772600	-0.53981900
H	-2.46505000	4.26887400	1.09849800
H	-3.12237700	1.49579800	-2.10246700
H	-3.90607000	3.40427500	-0.72923500
O	-1.72290900	-1.27797000	0.75249300
B	-2.61345900	-2.10648200	-0.04156600
F	-3.26834000	-3.05889300	0.75980400
F	-3.59211500	-1.33617600	-0.69203100
F	-1.81313500	-2.76133000	-0.99242100
C	-2.28570400	-0.38030900	1.69426300
H	-1.47632100	0.04429600	2.28891400
H	-2.82104900	0.42946800	1.19164800
H	-2.97065900	-0.90783100	2.36249300

G5

Coordinates (Angstroms)

	X	Y	Z
C	-2.24932000	1.05565900	-0.01139600
O	-0.01494500	-1.76143000	-0.72002300
H	-2.43714100	2.10421000	0.20313700

C	-3.37541700	0.15070600	0.02177600
C	-4.64021900	0.72330700	0.19840200
C	-3.24467300	-1.23964900	-0.10714200
C	-5.76785500	-0.08166500	0.22745500
H	-4.72819700	1.79809200	0.30531000
C	-4.37507400	-2.03443100	-0.07283100
H	-2.26961000	-1.69826500	-0.22266300
C	-5.63407800	-1.45803800	0.09228700
H	-6.74626700	0.36162000	0.35922200
H	-4.28004800	-3.10835900	-0.16842300
H	-6.51340800	-2.08981800	0.11831700
N	-1.03920100	0.71904700	-0.29191100
H	-0.79492400	-0.26585500	-0.55412300
H	0.84748800	-1.65183500	-0.23464900
H	0.19990400	-2.13409600	-1.58302600
C	0.07671400	1.60878300	-0.27486000
C	1.09752800	1.38581800	-1.19142700
C	0.15161200	2.63629500	0.65777000
C	2.19742500	2.23190500	-1.19208400
H	1.02482900	0.56910200	-1.89889100
C	1.25653600	3.47507800	0.64457900
H	-0.62740800	2.76435400	1.39880500
C	2.27809700	3.27627600	-0.27809900
H	2.99454200	2.06902800	-1.90603200
H	1.32594500	4.27541200	1.37020200
H	3.14090200	3.93029500	-0.27883000
O	2.18524600	-1.29203500	0.62799700
B	3.47902900	-1.63533700	0.09179000
F	4.19948700	-0.49183500	-0.31716900
F	4.27018700	-2.31957100	1.04025500
F	3.26717600	-2.46996500	-1.02008900
C	2.13327400	-0.32919900	1.66203900
H	1.09836200	-0.23623300	1.99577300
H	2.74345800	-0.63844300	2.51610100
H	2.47947800	0.64914000	1.31462500

TSG5-6

Coordinates (Angstroms)

	X	Y	Z
C	-2.21095000	0.99908300	-0.09648900
O	0.09870200	-1.64992700	-0.17079500
H	-2.41983400	2.06979600	-0.07568200

C	-3.37585000	0.12020000	-0.03383600
C	-4.63477400	0.72220800	-0.10085000
C	-3.28013300	-1.26985500	0.09262400
C	-5.78513400	-0.05279200	-0.06165600
H	-4.70458100	1.80033800	-0.18896700
C	-4.43046800	-2.03893500	0.13486600
H	-2.31414200	-1.75118900	0.17034300
C	-5.68291500	-1.43310900	0.05545900
H	-6.75754800	0.41948400	-0.11873900
H	-4.35475600	-3.11424500	0.23565200
H	-6.57862900	-2.04106400	0.08906400
N	-1.00084900	0.60211000	-0.19363800
H	-0.47356800	-0.69697400	-0.23562200
H	1.12742000	-1.47540100	0.24337200
H	0.16849400	-2.07817600	-1.03858900
C	0.06063300	1.55067400	-0.19706100
C	1.10123300	1.36861200	-1.10512600
C	0.09683100	2.60207700	0.71625000
C	2.15859700	2.26774600	-1.12456300
H	1.06922500	0.54049900	-1.80413000
C	1.16520400	3.48847000	0.69668600
H	-0.69624500	2.70884500	1.44683700
C	2.19462500	3.32691800	-0.22423300
H	2.96082900	2.13279800	-1.83909100
H	1.19677700	4.30214100	1.41067100
H	3.02644600	4.02003200	-0.23509500
O	2.29969000	-1.27409800	0.73454300
B	3.45961900	-1.64367200	-0.09101800
F	4.10900300	-0.50287200	-0.57381400
F	4.36738400	-2.39872100	0.65809000
F	2.95274000	-2.40349700	-1.15135800
C	2.45036700	-0.26226800	1.72746300
H	1.53211700	-0.22122700	2.31230700
H	3.27916300	-0.51802800	2.38911400
H	2.63380700	0.70981500	1.26565500

G6

Coordinates (Angstroms)

	X	Y	Z
C	2.49742200	3.04404400	0.29474100
C	1.69221300	3.44145500	-0.76697500
C	0.40765900	2.92959500	-0.89083100

C	-0.06698100	1.99704700	0.03279800
C	0.73998800	1.61166200	1.10673300
C	2.01641300	2.13708300	1.23575800
H	3.49697500	3.44853000	0.39684800
H	2.06246800	4.15417500	-1.49317200
H	-0.22899500	3.23916300	-1.71201300
H	0.35989900	0.92106200	1.84919600
H	2.63799300	1.84302800	2.07222700
C	-1.40752300	1.43548300	-0.16498300
H	-2.10862600	2.03619100	-0.74997900
N	-1.74455900	0.29168200	0.28534000
C	-3.07723000	-0.15776400	0.10760300
C	-4.16928100	0.68355000	0.32120400
C	-3.28521000	-1.48996900	-0.24828300
C	-5.45874800	0.19635900	0.15157200
H	-4.00717400	1.70584500	0.64146300
C	-4.57652000	-1.96556700	-0.42556400
H	-2.43416900	-2.14159200	-0.40753300
C	-5.66699600	-1.12522900	-0.22556000
H	-6.30362100	0.85125000	0.32586200
H	-4.73119700	-2.99747700	-0.71561400
H	-6.67406200	-1.50149000	-0.35445400
H	-0.60786300	-0.84257600	0.81917200
O	0.12033400	-1.50315200	1.04771100
H	-0.28715500	-2.37120900	1.16849100
H	1.20147300	-1.48024900	0.17247100
O	1.99852300	-1.44775900	-0.53145800
B	3.38981800	-1.75686100	-0.02088700
F	4.12690500	-2.24518800	-1.08663800
F	3.21640500	-2.70319900	0.97341600
F	3.96374600	-0.59549600	0.47568400
C	1.82753800	-0.41817000	-1.52564000
H	2.35337600	-0.73011400	-2.42491900
H	0.76208500	-0.33573200	-1.73166900
H	2.22060100	0.52849100	-1.15695400

7

Coordinates (Angstroms)

X

Y

Z

C	-4.60356900	-0.16111800	0.05508400
C	-4.06902400	1.03671900	-0.40247500
C	-2.69066000	1.19838700	-0.46870900

C	-1.84033700	0.16335700	-0.07953400
C	-2.38410600	-1.03882300	0.38164100
C	-3.75854700	-1.19813900	0.44686600
H	-5.67773800	-0.28987600	0.10850300
H	-4.72355800	1.84398900	-0.70675200
H	-2.26623000	2.13078800	-0.82442600
H	-1.72063700	-1.83884700	0.68596300
H	-4.17732800	-2.13047500	0.80515400
C	-0.38741900	0.37402100	-0.16117000
H	-0.06887400	1.36564300	-0.50003900
N	0.45212700	-0.53491900	0.12710300
C	1.83002000	-0.23430600	0.07291300
C	2.35491900	0.97129600	0.54514800
C	2.69315000	-1.21109300	-0.42653100
C	3.72320400	1.20292300	0.48489800
H	1.69405900	1.71239100	0.97883000
C	4.05683400	-0.96636700	-0.49776400
H	2.27747000	-2.15174200	-0.76754000
C	4.57778700	0.24067400	-0.04108800
H	4.12332600	2.13687900	0.86072000
H	4.71719400	-1.72462600	-0.90073500
H	5.64391500	0.42512400	-0.08507800

8

Coordinates (Angstroms)

	X	Y	Z
C	0.03256200	-1.20466400	-0.34540600
H	-0.26381700	-2.11486100	0.18128300
C	1.46402400	-1.06170000	-0.62028100
C	2.34000800	-1.94010300	0.02068500
C	1.97389600	-0.07129200	-1.46415400
C	3.71079800	-1.82285600	-0.16514500
H	1.93970200	-2.71025000	0.67086900
C	3.34205100	0.03697900	-1.65444500
H	1.30269700	0.59609200	-1.98954900
C	4.21199200	-0.83434100	-1.00287700
H	4.38540800	-2.50333800	0.33920100
H	3.73454700	0.80018500	-2.31479300
H	5.28061400	-0.74299800	-1.15406500
C	-3.91326900	-1.17776800	1.24790100
C	-2.56737100	-1.03394300	0.93742900
C	-2.19682800	-0.52985700	-0.30942200

C	-3.17528700	-0.14143300	-1.22359400
C	-4.51755000	-0.29711000	-0.90807900
C	-4.89053000	-0.81554000	0.32762800
H	-4.19846800	-1.56302100	2.21915100
H	-1.80733200	-1.28897700	1.66610700
H	-2.87307000	0.26438500	-2.18180000
H	-5.27387200	-0.00658100	-1.62672000
H	-5.93850000	-0.92688900	0.57635600
N	-0.83905500	-0.33551000	-0.67369700
H	2.37291000	-0.45623100	2.84578700
C	2.05743700	0.41488500	2.25993500
O	0.74133100	0.44258600	2.11901800
O	2.82033400	1.23896900	1.82763400
C	-0.35390100	2.96234600	-0.42694800
O	-0.10626100	2.59585800	0.70571800
O	-0.62475600	2.18212400	-1.43495400
H	-0.37286500	4.02321500	-0.69759500
H	-0.63285100	1.18895400	-1.15638900
H	0.46489600	1.21096700	1.55934600

TS8-9

Coordinates (Angstroms)

	X	Y	Z
C	0.18368200	-1.29828900	-0.22584300
H	-0.11960500	-2.18926900	0.32113700
C	1.60819100	-1.12191300	-0.46460100
C	2.48476700	-1.87848900	0.31846800
C	2.11433900	-0.21950200	-1.40655300
C	3.85541900	-1.71234500	0.18594100
H	2.08289900	-2.58339400	1.03745600
C	3.48381400	-0.07264000	-1.54653000
H	1.44348400	0.35349200	-2.03362700
C	4.35373600	-0.81102700	-0.74733700
H	4.53266100	-2.29009800	0.80189100
H	3.87796600	0.61854800	-2.28064400
H	5.42379500	-0.68594000	-0.85886700
C	-3.87138200	-1.33184000	1.16036700
C	-2.51226400	-1.21718400	0.90421300
C	-2.09264500	-0.62970500	-0.28620200
C	-3.01725300	-0.12686500	-1.19723600
C	-4.37359500	-0.24713100	-0.92959000
C	-4.80307000	-0.85095600	0.24673000

H	-4.20230800	-1.78443800	2.08666900
H	-1.78800500	-1.55983700	1.63289700
H	-2.66891900	0.33866500	-2.11109900
H	-5.09494400	0.13476900	-1.64096700
H	-5.86171400	-0.93821800	0.45661100
N	-0.71332400	-0.46541800	-0.59757300
H	2.27249000	0.17355300	2.73137300
C	1.80490400	0.91622700	2.07272700
O	0.49817000	0.75279900	2.01630300
O	2.43031000	1.77284500	1.49850700
C	-0.61686200	2.72014200	-0.66600200
O	-0.69947800	2.54632500	0.55731100
O	-0.39857500	1.82499200	-1.54031200
H	-0.74751400	3.73924500	-1.06074300
H	-0.47450000	0.60875400	-1.07555800
H	0.06337800	1.43550700	1.41069400

9

Coordinates (Angstroms)

	X	Y	Z
C	0.25116200	-1.46922100	-0.09724900
H	-0.08765100	-2.40333300	0.34208000
C	1.67693300	-1.29654300	-0.27482300
C	2.50135400	-2.32399300	0.19709100
C	2.24366500	-0.15830200	-0.86523600
C	3.87881600	-2.21680400	0.08510000
H	2.05339400	-3.19862100	0.65412000
C	3.61867800	-0.06301200	-0.97895500
H	1.61634400	0.64395000	-1.23655600
C	4.43570900	-1.08724200	-0.50226600
H	4.51545400	-3.01048900	0.45416200
H	4.06013800	0.81494500	-1.43303300
H	5.51167200	-1.00128800	-0.59191800
C	-3.86226300	-1.59060300	1.14413700
C	-2.49483400	-1.46035900	0.94784000
C	-2.03748200	-0.76778600	-0.16808100
C	-2.92332700	-0.17636900	-1.06313400
C	-4.28788000	-0.31151200	-0.85176700
C	-4.75915400	-1.02038200	0.24746000
H	-4.22638300	-2.12548400	2.01209000
H	-1.79696000	-1.87104000	1.66708000
H	-2.54163500	0.36908700	-1.91743200

H	-4.98306300	0.13945300	-1.54840900
H	-5.82470300	-1.12044900	0.41127100
N	-0.64300200	-0.60420600	-0.41492900
H	2.48253100	1.03254400	2.12864500
C	1.79096000	1.70360200	1.60062800
O	0.55905400	1.25414900	1.63546900
O	2.15787400	2.72835600	1.07454300
C	-0.88514000	2.67718800	-0.89719100
O	-1.05169700	2.71359700	0.34292600
O	-0.34273600	1.75106100	-1.54689400
H	-1.25325800	3.54182700	-1.47471800
H	-0.39190800	0.34120700	-0.86402300
H	-0.09611500	1.86785600	1.11145400

TS9-10

Coordinates (Angstroms)

	X	Y	Z
C	0.73551800	-0.99770300	-0.40679100
H	0.57462300	-2.05907400	-0.58214000
C	2.12902600	-0.52074100	-0.51960200
C	3.12401300	-1.44312500	-0.83896300
C	2.46191100	0.81488900	-0.28685400
C	4.44382400	-1.02802400	-0.95116000
H	2.85853200	-2.48043300	-1.00660500
C	3.78256400	1.22277400	-0.39774100
H	1.69959600	1.53496400	-0.00940400
C	4.77346800	0.30396400	-0.73136400
H	5.21383200	-1.74451900	-1.20792700
H	4.04142500	2.25836200	-0.21662900
H	5.80355400	0.62749600	-0.81598400
C	-3.88468300	-0.01225800	-1.38290300
C	-2.53532600	0.29878900	-1.39452200
C	-1.62360600	-0.54377900	-0.75440700
C	-2.06835000	-1.69660400	-0.10831300
C	-3.42529900	-1.99970700	-0.11380100
C	-4.33680900	-1.16322100	-0.74311000
H	-4.58617000	0.64455400	-1.88209200
H	-2.17717400	1.18260100	-1.90911700
H	-1.37808400	-2.35812900	0.39951500
H	-3.76679700	-2.89613800	0.38862800
H	-5.39199800	-1.40488800	-0.73811700
N	-0.26333300	-0.18369100	-0.77157700

H	-0.07279500	0.81242100	-0.87507700
H	0.62269700	-1.16077600	0.99296600
C	0.37517800	-0.75890500	2.17787400
O	-0.14356900	0.34374800	2.13680900
O	0.73993500	-1.57330900	2.98503600
C	-1.43287000	2.97824900	0.28284700
O	-1.78816900	2.28643500	1.34116400
O	-0.48933900	2.72232400	-0.43122400
H	-2.09520000	3.83295500	0.11328300
H	-1.16492900	1.53526900	1.50832500

CO₂

Coordinates (Angstroms)

	X	Y	Z
C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.15472700
O	0.00000000	0.00000000	-1.15472700

10

Coordinates (Angstroms)

	X	Y	Z
C	0.61333200	-1.02814300	0.71595200
H	0.50449400	-2.09921800	0.90790200
C	2.04274900	-0.71174200	0.36161500
C	2.70132200	-1.45004100	-0.62210100
C	2.71166700	0.34102300	0.97940100
C	4.00685600	-1.14053100	-0.97896100
H	2.18469000	-2.27163200	-1.10651900
C	4.02111400	0.65228900	0.62547800
H	2.20553600	0.91805400	1.74671900
C	4.66988600	-0.08746700	-0.35468900
H	4.51045400	-1.72182100	-1.74190900
H	4.53171000	1.47244600	1.11538500
H	5.68904400	0.15301700	-0.63180600
C	-3.82546700	-0.05959000	-1.07280700
C	-2.44640800	-0.03725300	-1.19117200
C	-1.63542800	-0.67415100	-0.23570900
C	-2.25511300	-1.32796400	0.83785700
C	-3.64223800	-1.34518600	0.93942900

C	-4.43929300	-0.71256600	-0.00516400
H	-4.42842600	0.43986300	-1.82220200
H	-1.97744300	0.46651400	-2.02930800
H	-1.65935600	-1.82437600	1.59251500
H	-4.10009300	-1.85813400	1.77723400
H	-5.51792900	-0.72747400	0.08428700
N	-0.25966700	-0.65434200	-0.39005400
H	0.08715000	0.11434900	-0.95146500
H	0.33836000	-0.50477400	1.64147100
C	-0.98066100	2.58548900	-0.10151300
O	-0.84015300	2.22072600	1.16915200
O	-0.14540000	2.42187700	-0.95054200
H	-1.95012700	3.06492500	-0.26785600
H	0.03012000	1.79282800	1.28135000

PhNHCH₂Ph

Coordinates (Angstroms)

	X	Y	Z
C	-0.43704800	-0.82751500	0.19540700
H	-0.24889200	-1.25551800	1.18327400
C	-1.88099000	-0.40782000	0.09927200
C	-2.65789800	-0.77105600	-0.99660300
C	-2.44793200	0.38004800	1.10171700
C	-3.98471500	-0.36042900	-1.08977900
H	-2.22198000	-1.38107700	-1.77999600
C	-3.77002700	0.79313000	1.01047700
H	-1.84612500	0.66518300	1.95798200
C	-4.54213100	0.42269400	-0.08743300
H	-4.58016800	-0.65137300	-1.94674600
H	-4.20165500	1.40076500	1.79667800
H	-5.57460600	0.74266800	-0.15795000
C	3.83417600	-1.05837700	0.42865800
C	2.44492400	-0.97621000	0.43802500
C	1.80493700	0.18260800	-0.02018400
C	2.59725400	1.24018900	-0.49854900
C	3.97695800	1.14136200	-0.50665000
C	4.61224600	-0.00901100	-0.03971200
H	4.30748800	-1.96371600	0.79055900
H	1.86634000	-1.81459300	0.80252800
H	2.10931900	2.13913200	-0.85935900
H	4.56503300	1.97100700	-0.88142500
H	5.69218700	-0.08254400	-0.04622000

N	0.42718900	0.33266200	0.01805700
H	-0.22638400	-1.60547100	-0.54850300
H	0.07058800	1.00922400	-0.64508900

TS9

Coordinates (Angstroms)

	X	Y	Z
C	-1.84058600	0.41058300	0.61830400
H	-1.62594000	0.54222700	1.67705900
C	-3.06591300	-0.37080400	0.31646700
C	-3.87218600	-0.79137000	1.37189500
C	-3.40431200	-0.70405000	-0.99569200
C	-5.02778800	-1.51729300	1.11500300
H	-3.59684900	-0.54004300	2.38952700
C	-4.55768600	-1.43233700	-1.24678900
H	-2.76418300	-0.41076900	-1.82059800
C	-5.37164300	-1.83665300	-0.19298900
H	-5.65773100	-1.83462800	1.93648100
H	-4.81848000	-1.69149400	-2.26518700
H	-6.27156600	-2.40503300	-0.39302700
C	0.80576400	4.22522000	-0.73427800
C	-0.29322500	3.39426400	-0.86016500
C	-0.44835600	2.30818400	0.00556600
C	0.50963700	2.05675500	0.98816600
C	1.60683900	2.90430800	1.10393300
C	1.76236500	3.98662100	0.25033500
H	0.91800200	5.06428600	-1.40964800
H	-1.03916600	3.57305300	-1.62596700
H	0.41757000	1.21638000	1.66441300
H	2.34732400	2.70376700	1.86829800
H	2.62127600	4.63840500	0.34561900
N	-1.56462000	1.48024900	-0.16597400
H	-2.04783800	1.56326500	-1.05339900
H	-0.86937500	-0.46927200	0.41646900
C	0.13976700	-0.96550500	-0.32099800
O	0.16418900	-0.43258300	-1.38130600
O	0.68491600	-1.82089800	0.36099300
H	3.07338100	-3.59414100	-0.24362700
O	2.91232900	-2.65523200	-0.44116100
B	4.03407900	-1.68245900	0.00130100
F	3.51476600	-0.42961300	-0.23873400
F	5.13238900	-1.97281900	-0.77349300

F	4.28334600	-1.89469400	1.34229500
H	1.97346900	-2.36915200	-0.12247200

TS10

Coordinates (Angstroms)			
	X	Y	Z
C	0.45562100	-0.20558300	0.61735700
H	0.17827500	-0.02696400	1.65146900
C	1.88693300	-0.39568300	0.33600400
C	2.77391600	-0.39199200	1.41295700
C	2.36990500	-0.55359900	-0.96503700
C	4.13238100	-0.57048400	1.19452100
H	2.39346600	-0.25604100	2.41850900
C	3.72875000	-0.72805000	-1.17677800
H	1.69883100	-0.52073800	-1.81563300
C	4.61015300	-0.73970900	-0.09951400
H	4.81698400	-0.57498900	2.03322100
H	4.10322500	-0.84746600	-2.18551000
H	5.67073100	-0.87534700	-0.27156500
C	-4.05324000	-1.36804100	-0.62724400
C	-2.67837600	-1.44994000	-0.77075300
C	-1.85226400	-0.65575400	0.02381700
C	-2.40052900	0.23125800	0.94774400
C	-3.78219100	0.29671000	1.08514400
C	-4.61158800	-0.49766000	0.30475400
H	-4.69118100	-1.98782300	-1.24479600
H	-2.23433800	-2.12632400	-1.49184400
H	-1.77325300	0.87501700	1.55068500
H	-4.20835800	0.98571500	1.80360700
H	-5.68659800	-0.43660600	0.41652500
N	-0.46073200	-0.76558800	-0.16007100
H	-0.16546400	-1.16830300	-1.04357000
H	0.33406600	1.28454000	0.32486800
C	0.04116300	2.18678600	-0.46649200
O	-0.32669800	1.72892300	-1.53298500
O	0.20981400	3.28168600	0.04244100

TS11

Coordinates (Angstroms)			
	X	Y	Z

C	1.52619100	-0.28618300	-1.08981300
H	1.15421300	-0.60569600	-2.06226800
C	2.84869900	-0.84898500	-0.71476900
C	3.45438800	-1.76629000	-1.57124100
C	3.46592400	-0.50638000	0.48879700
C	4.68325600	-2.32034800	-1.23877500
H	2.96381400	-2.03618500	-2.49926400
C	4.69342900	-1.06366800	0.81677000
H	2.99363600	0.18849400	1.17479100
C	5.30330200	-1.96970900	-0.04539700
H	5.15482800	-3.02646300	-1.91063100
H	5.17231100	-0.79607400	1.75028400
H	6.26089400	-2.40311200	0.21539500
C	-1.18865500	3.71625000	-1.10440100
C	-0.01323500	3.04017100	-0.82935000
C	0.08479700	1.67011200	-1.09679700
C	-1.00457000	0.99136400	-1.64673500
C	-2.17676600	1.68811700	-1.92378300
C	-2.27861200	3.04469200	-1.65412900
H	-1.25266500	4.77676700	-0.89426400
H	0.84074900	3.56636300	-0.41913700
H	-0.95988800	-0.06763200	-1.86920000
H	-3.01730700	1.15278700	-2.34819400
H	-3.19584600	3.57761800	-1.86964900
N	1.28456500	1.01757500	-0.78482400
H	1.86111500	1.46659500	-0.07687400
H	0.69944000	-1.00984600	-0.40089200
C	-0.14312100	-1.25415400	0.65066300
O	-0.03284800	-0.36473700	1.43697700
O	-0.68750700	-2.30812600	0.42469100
C	1.16144800	2.82776900	2.38082900
O	0.00958500	2.19948400	2.50943600
O	2.08328000	2.44706300	1.69931200
H	1.18793900	3.74742900	2.97267800
H	0.01881300	1.36270500	1.99852700
H	-2.16650700	-2.69705900	0.89269600
O	-3.15270300	-2.76986900	1.06091000
H	-3.45489900	-3.68430700	0.91451400
B	-3.95388700	-1.66595800	0.28923800
F	-3.32826700	-0.49549300	0.64393700
F	-5.24621400	-1.76310600	0.73534600
F	-3.84112600	-1.93169800	-1.05736700

TS12

Coordinates (Angstroms)

	X	Y	Z
C	-1.22278500	1.71999600	-0.05390000
H	-1.28942300	2.79238600	0.11521900
C	-2.51669200	1.01106600	-0.19259300
C	-3.69728300	1.75092400	-0.17313900
C	-2.56389600	-0.37792000	-0.32086600
C	-4.92027600	1.10719900	-0.30871700
H	-3.65370800	2.82807000	-0.06125000
C	-3.78841300	-1.01572200	-0.45168600
H	-1.65090800	-0.96249700	-0.29482500
C	-4.96646200	-0.27470600	-0.44909300
H	-5.83610000	1.68477200	-0.30271500
H	-3.82434100	-2.09372200	-0.54802500
H	-5.92060500	-0.77674100	-0.55190000
C	3.35408600	1.88321600	-1.58883000
C	2.06897900	1.37187100	-1.63093000
C	1.09185000	1.87217800	-0.76555800
C	1.41474400	2.87924200	0.14442300
C	2.70994600	3.38711300	0.16936500
C	3.68219500	2.89540800	-0.68921600
H	4.10485100	1.49096200	-2.26360600
H	1.80760700	0.58668200	-2.33026800
H	0.67660100	3.27682000	0.82931800
H	2.95421600	4.17078100	0.87575200
H	4.68839000	3.29359700	-0.66007200
N	-0.19321600	1.31364600	-0.82691200
H	-0.23869100	0.38034800	-1.22512600
H	-0.87640000	1.44543200	1.23262300
C	-0.20188300	0.67274100	2.07592200
O	0.26223600	-0.23585600	1.41022600
O	-0.28058300	1.09274100	3.18931800
H	1.36061800	-1.21965000	1.51390500
O	2.23986300	-1.72733500	1.70684800
C	2.65134900	-2.67438300	0.97434600
H	3.61510300	-3.09233400	1.25921600
O	2.08458000	-3.17570800	-0.02099700
B	0.68281700	-2.81928000	-0.58033400
F	0.44107700	-3.75491300	-1.55195100
F	0.76447300	-1.53909600	-1.09779700
F	-0.20558400	-2.90422500	0.46991000

TS13

Coordinates (Angstroms)

	X	Y	Z
C	-1.35355300	-1.90853100	-0.17451900
H	-2.02319600	-2.70317700	0.14457700
C	0.04350300	-2.29721300	-0.46536200
C	0.63661700	-3.26327600	0.35239700
C	0.77083700	-1.74056100	-1.51614400
C	1.94329200	-3.66053400	0.12718300
H	0.06662300	-3.68958800	1.17079400
C	2.07920300	-2.15034900	-1.74427100
H	0.32900100	-1.00881600	-2.18324000
C	2.66801900	-3.10275700	-0.92343100
H	2.39840300	-4.40484400	0.76826100
H	2.63726900	-1.72036100	-2.56634200
H	3.69040200	-3.41277500	-1.10152400
C	-5.35835100	-0.48281300	0.45805100
C	-4.06013800	-0.96529700	0.33607200
C	-3.23425000	-0.44631800	-0.65849500
C	-3.69427600	0.56393800	-1.50346100
C	-4.98737100	1.03872900	-1.36494300
C	-5.82760800	0.51375200	-0.38669800
H	-6.00043900	-0.88787300	1.23014000
H	-3.70855400	-1.72821800	1.01878500
H	-3.03261400	0.96452400	-2.26310500
H	-5.34112600	1.82123200	-2.02448000
H	-6.83902700	0.88494100	-0.28167300
N	-1.90926900	-0.89044900	-0.82903600
H	-1.22746900	-1.46751300	1.20018800
C	-1.06557100	-0.58722100	2.08393200
O	-0.93521800	0.50727200	1.55658700
O	-1.07870800	-1.07504900	3.18818700
C	3.70579800	-0.36351200	1.21296900
C	2.46332400	0.23098600	1.03065700
C	2.22968500	0.96101300	-0.12518600
C	3.20927000	1.11275900	-1.09416600
C	4.44873700	0.51602400	-0.90100600
C	4.69817100	-0.22353600	0.24930800
H	3.89411800	-0.94031100	2.10987800
H	1.68619500	0.12968700	1.77962400
H	2.99983800	1.68534400	-1.99000100

H	5.21795800	0.62673600	-1.65505000
H	5.66389500	-0.69126700	0.39452300
N	0.93343700	1.59452000	-0.31761400
H	0.66024900	1.53048000	-1.30195200
H	0.21277400	1.09376700	0.22911300
B	0.86626500	3.14637100	0.11956400
F	1.23570800	3.22061800	1.44951900
F	1.73681700	3.85415600	-0.69165000
F	-0.44678100	3.54437200	-0.07453200
H	-1.29711800	-0.24412500	-1.31533700

TS14

Coordinates (Angstroms)

	X	Y	Z
C	-2.02769400	0.37843800	0.62420000
H	-1.79073800	0.49171800	1.68016700
C	-3.20918900	-0.46615800	0.32426100
C	-3.96673300	-0.96300900	1.38271000
C	-3.55602700	-0.78166400	-0.99036700
C	-5.08321700	-1.74839500	1.12781300
H	-3.68535300	-0.72377400	2.40151100
C	-4.66958900	-1.57005600	-1.23940500
H	-2.95176700	-0.42831300	-1.81880800
C	-5.43576500	-2.05099100	-0.18183500
H	-5.67594300	-2.12486800	1.95202100
H	-4.93645800	-1.81599400	-2.25949100
H	-6.30502700	-2.66563500	-0.38058200
C	0.35256800	4.37612200	-0.69380400
C	-0.69444700	3.47987500	-0.81281000
C	-0.75548900	2.36424300	0.02643400
C	0.24491100	2.14719600	0.97429400
C	1.28882500	3.06057400	1.08384500
C	1.35010900	4.17318700	0.25755600
H	0.39157800	5.23856700	-1.34757800
H	-1.47241800	3.63111000	-1.55238000
H	0.22789800	1.28417300	1.62808900
H	2.06344500	2.88707200	1.82048400
H	2.16798300	4.87639300	0.34841700
N	-1.82531900	1.47519500	-0.13969900
H	-2.33548900	1.55367100	-1.01230600
H	-1.00458900	-0.45374800	0.38031800
C	0.01331900	-0.86425300	-0.37223500

O	-0.02956500	-0.33799200	-1.43808400
O	0.64982300	-1.66965400	0.29228200
O	3.03495400	-2.17034700	-0.38721900
B	3.94397700	-0.99191800	-0.01168100
F	3.20186800	0.13327700	-0.30650800
F	5.08316300	-1.10198300	-0.77953000
F	4.23544300	-1.07959100	1.33793000
H	2.05805200	-1.99160800	-0.14871300
C	3.44160100	-3.50345500	0.00403200
H	3.38881400	-3.60339500	1.08619900
H	2.77283300	-4.20689500	-0.48425200
H	4.45945300	-3.64655800	-0.34779300

BF₃·Et₂O

Coordinates (Angstroms)

	X	Y	Z
C	0.87713900	1.20629500	-0.82130700
H	1.82027800	0.96869700	-1.30957600
H	0.24122200	1.74086400	-1.52254100
C	1.07611200	1.97785100	0.46068400
H	1.60417400	2.90113200	0.21495200
H	0.12331700	2.24411700	0.91684600
H	1.67477500	1.42121400	1.18044600
C	1.07691800	-1.27138500	-0.58962800
H	1.54495600	-1.30670400	-1.57212500
H	0.38862600	-2.10714600	-0.49526900
C	2.09140900	-1.24675000	0.52604300
H	2.81645400	-0.44296300	0.39846700
H	1.60762800	-1.15007300	1.49788400
H	2.63322900	-2.19381200	0.50217100
O	0.21858600	-0.08527700	-0.60460800
B	-1.16625600	-0.15204200	0.09110700
F	-1.80687900	-1.25494000	-0.42953600
F	-0.95635400	-0.28398100	1.44923400
F	-1.80360500	1.02459100	-0.22910700

Et₂O

Coordinates (Angstroms)

	X	Y	Z
--	---	---	---

C	-1.17447100	-0.51222200	-0.00010600
H	-1.18246500	-1.16130600	-0.88528800
H	-1.18252600	-1.16135400	0.88504100
C	-2.37867800	0.40013000	-0.00011900
H	-3.29592100	-0.19088500	-0.00024600
H	-2.37925800	1.03647500	0.88617400
H	-2.37911600	1.03663000	-0.88630100
C	1.17447100	-0.51222200	0.00017900
H	1.18255300	-1.16150500	-0.88485700
H	1.18243800	-1.16115500	0.88547200
C	2.37867800	0.40013000	0.00008000
H	2.37930500	1.03630900	-0.88633300
H	2.37906900	1.03679700	0.88614200
H	3.29592100	-0.19088500	0.00036300
O	0.00000000	0.27824800	-0.00004600

11

Coordinates (Angstroms)

	X	Y	Z
C	4.67698300	-0.61421400	-0.22629200
C	3.95039900	0.50635500	-0.62034300
C	2.56633500	0.48770300	-0.59219600
C	1.89823000	-0.66755700	-0.17212800
C	2.63350200	-1.80719200	0.17495200
C	4.01883700	-1.77179400	0.17178200
H	5.75965400	-0.58785000	-0.24488800
H	4.46693300	1.39654400	-0.95593500
H	2.01070600	1.35462200	-0.91970600
H	2.11005500	-2.71262300	0.45964800
H	4.58286300	-2.64912700	0.46121100
C	0.44904400	-0.81560000	-0.14812000
H	0.08996300	-1.83192500	-0.29830400
N	-0.45197200	0.08762700	0.01940000
C	-1.83129800	-0.33680000	-0.07690000
C	-2.29760600	-1.37151300	0.72109500
C	-2.66714200	0.31585500	-0.97348900
C	-3.62357900	-1.77089400	0.60442500
H	-1.63374300	-1.84844500	1.43223000
C	-3.98861600	-0.09278700	-1.08317700
H	-2.28238400	1.12550800	-1.58138500
C	-4.46848100	-1.13493200	-0.29615700
H	-3.99466000	-2.57555200	1.22659400

H	-4.64451300	0.40506500	-1.78619800
H	-5.50156200	-1.44715200	-0.38306200
B	-0.21846200	1.63524700	0.44812200
F	-1.37578500	2.04810900	1.08293300
F	0.85476200	1.68467000	1.31792300
F	0.00915300	2.38072400	-0.69944900

12

Coordinates (Angstroms)

	X	Y	Z
C	-0.96965400	-1.30420300	-0.27190000
H	-0.84145700	-2.06453000	-1.03927100
C	-2.33562100	-0.82312400	-0.11075600
C	-3.33680700	-1.69360600	-0.55941200
C	-2.68752800	0.44415500	0.36959500
C	-4.67146600	-1.33091200	-0.47244900
H	-3.05947100	-2.65973600	-0.96501000
C	-4.02134700	0.81055400	0.42767100
H	-1.92969200	1.15285300	0.67125300
C	-5.01335100	-0.07751500	0.02018100
H	-5.44053200	-2.01667200	-0.80372000
H	-4.28976600	1.79575300	0.78702800
H	-6.05449400	0.21583300	0.07537700
C	2.67889600	-3.52925000	-0.39330200
C	1.48524000	-2.95277300	0.02550100
C	1.33286600	-1.57790600	-0.06792900
C	2.34719000	-0.76802600	-0.55921400
C	3.53496200	-1.35363000	-0.97316300
C	3.70265200	-2.73249600	-0.88987000
H	2.80745000	-4.60199900	-0.32318900
H	0.68217300	-3.55879400	0.42787000
H	2.18983400	0.30029700	-0.63646800
H	4.32933700	-0.73115300	-1.36553500
H	4.63196400	-3.18442900	-1.21318100
N	0.09578700	-0.96166900	0.36300700
H	-1.94220000	1.61837700	-2.35368300
C	-0.90702100	1.66686800	-1.99859900
O	-0.64958400	2.82964900	-1.42794400
O	-0.11333400	0.76900300	-2.12941600
B	0.20302200	0.01090000	1.63273000
F	1.39203800	-0.26943000	2.27450600
F	-0.87498000	-0.20635500	2.46221000

F	0.22496500	1.34317400	1.17174700
C	2.82077100	3.20443200	0.07013800
O	1.97731800	3.29831700	-0.79191500
O	2.65142100	2.60464100	1.22855000
H	3.82566700	3.62356800	-0.02972100
H	1.75455400	2.20966000	1.27652400
H	0.28755000	2.86336600	-1.12227500

TS12-13

Coordinates (Angstroms)			
	X	Y	Z
C	0.50874300	-0.99184000	0.74943400
H	0.20616300	-1.75259400	1.47051600
C	1.93440200	-1.16021700	0.31482100
C	2.24523500	-1.49980700	-0.99895900
C	2.95358200	-1.06767400	1.26270300
C	3.56703400	-1.72939000	-1.36319200
H	1.45536800	-1.59557400	-1.73270000
C	4.27177800	-1.29523500	0.89549600
H	2.71204600	-0.81340200	2.28854700
C	4.58214900	-1.62252900	-0.42078100
H	3.80158900	-1.99458500	-2.38681700
H	5.05765800	-1.21730300	1.63664900
H	5.61139100	-1.79934900	-0.70795300
C	-3.00098500	-3.39026800	0.09659400
C	-1.79761700	-2.72080400	-0.08003200
C	-1.74056300	-1.33247500	0.04423500
C	-2.89856300	-0.61903300	0.34898400
C	-4.10231300	-1.29447400	0.51197200
C	-4.15893200	-2.67785500	0.38745300
H	-3.03438700	-4.46821200	-0.00409200
H	-0.89279100	-3.26595000	-0.32515400
H	-2.84789500	0.45393600	0.46754300
H	-4.99873000	-0.73446300	0.74938200
H	-5.09971600	-3.19811600	0.51823000
N	-0.48241700	-0.67777500	-0.13698900
H	0.61364900	-0.04691100	1.61883000
C	0.53800100	1.29517300	1.92404200
O	-0.58189400	1.62487600	1.57959600
O	1.55708000	1.66403400	2.39696600
B	-0.34804500	0.42225500	-1.19367300
F	-1.43577100	1.30491900	-1.19568900

F	-0.18458600	-0.07964700	-2.48029900
F	0.80697900	1.22827700	-0.86248400
C	-0.76332100	4.20967900	-0.52372200
O	-1.30629700	3.73815400	0.50337000
O	0.16361000	3.67481900	-1.20286200
H	-1.10739800	5.18152200	-0.86859600
H	0.42965700	2.73726300	-0.96009000
H	-0.96082700	2.83038300	0.89838200

13

Coordinates (Angstroms)

	X	Y	Z
C	0.48698900	0.60872300	-1.57404000
H	0.00409200	1.47093400	-2.03162000
C	1.76680300	0.99700100	-0.88860000
C	1.82780800	2.17429500	-0.14476600
C	2.88298800	0.16613600	-0.94723900
C	2.98855700	2.51281800	0.53883000
H	0.96108600	2.82612900	-0.10218200
C	4.04653400	0.50541900	-0.26616700
H	2.83714700	-0.74907800	-1.52721500
C	4.09906700	1.67703400	0.47979400
H	3.02856000	3.42991100	1.11363600
H	4.91057800	-0.14569100	-0.31707900
H	5.00471000	1.94095300	1.01213700
C	0.74060700	-2.15348200	2.15303900
C	0.23874200	-1.04662900	1.47868600
C	0.00509000	-1.13264800	0.11506700
C	0.26984900	-2.29812800	-0.58991900
C	0.77269300	-3.39760100	0.09342700
C	1.00836300	-3.32829300	1.46213600
H	0.92635200	-2.09138200	3.21782100
H	0.03484700	-0.12199700	2.00661500
H	0.09158800	-2.34782200	-1.65627100
H	0.98180400	-4.31094400	-0.44917100
H	1.40241000	-4.18889800	1.98792000
N	-0.50658200	0.04389900	-0.58728200
H	0.65462500	-0.15212400	-2.33324900
B	-1.95642100	-0.16834300	-1.25436900
F	-1.84237800	-0.98963200	-2.35288200
F	-2.43004500	1.08775300	-1.58790200
F	-2.77424000	-0.74488800	-0.27185300

C	-2.93792200	1.94407200	1.72386500
O	-1.77895400	1.76615100	1.43487100
O	-3.93510100	1.16405000	1.35379700
H	-3.28600900	2.78256400	2.33401300
H	-3.59197800	0.43024300	0.80278600
H	-0.67623300	0.76862500	0.12437800

14

Coordinates (Angstroms)

	X	Y	Z
C	-2.07753600	-2.07845100	-0.01493800
H	-1.90830100	-2.04626600	-1.08808000
C	-0.83090000	-2.49379100	0.71464000
C	0.38991600	-2.55625700	0.05003300
C	-0.89105400	-2.81406100	2.06992700
C	1.54059200	-2.93354500	0.73265600
H	0.44108700	-2.30484300	-1.00377000
C	0.25913200	-3.18096300	2.75557500
H	-1.84372900	-2.77554100	2.58881800
C	1.47787500	-3.24083100	2.08648400
H	2.48671900	-2.97919100	0.20683200
H	0.20481200	-3.42609500	3.80922300
H	2.37570600	-3.52992900	2.61932500
C	-5.32044400	-0.07592900	-2.01633400
C	-4.05717000	-0.36315000	-1.51610800
C	-3.87467400	-0.41344900	-0.14120000
C	-4.92434300	-0.18186000	0.73326400
C	-6.18392000	0.10659600	0.22191500
C	-6.38367700	0.15914400	-1.15153500
H	-5.47086500	-0.03307600	-3.08761500
H	-3.22758300	-0.53753700	-2.18940800
H	-4.75777800	-0.22223200	1.80382100
H	-7.00664500	0.28984700	0.90134800
H	-7.36560500	0.38380900	-1.54851600
N	-2.54668200	-0.70432700	0.40317500
H	-2.89932700	-2.76161400	0.19882100
B	-1.47395800	0.48784900	0.09834900
F	-0.47703500	0.39901100	1.05244600
F	-2.16079300	1.68471300	0.21021600
F	-0.98334300	0.29449800	-1.18101900
H	-2.64103600	-0.72484100	1.42325200
C	3.18568100	0.89717300	-0.09096000

H	3.59133400	1.15445300	0.89325400
C	3.63879800	-0.38537900	-0.64953500
C	4.64207700	-1.08883100	0.01773300
C	3.09577300	-0.90980200	-1.82580600
C	5.11232000	-2.29370700	-0.49025900
H	5.05705300	-0.68388000	0.93415200
H	2.30853000	-0.36692300	-2.33463800
C	4.57107000	-2.80850000	-1.66209600
H	5.89620500	-2.83073700	0.02921800
H	4.93241900	-3.74956900	-2.05846400
C	0.32807700	4.57833600	0.21278300
C	0.73130400	3.36787900	-0.33198100
C	2.03167200	2.90331400	-0.13012400
C	2.94143300	3.69450100	0.57685700
C	2.53591500	4.91323700	1.10504400
C	1.22883500	5.35627800	0.93368400
H	-0.68925700	4.92001200	0.06456600
H	0.04515300	2.76092600	-0.90952200
H	3.96763700	3.36676000	0.69195100
H	3.24920800	5.52407800	1.64520400
H	0.91775200	6.30727000	1.34781800
N	2.37640900	1.66062700	-0.70465600
C	3.55917200	-2.11620800	-2.32613200
H	3.13320000	-2.52269300	-3.23527900

TS14-15

Coordinates (Angstroms)

	X	Y	Z
C	-3.17436000	0.30962800	-0.80014800
H	-2.56768100	0.70313400	-1.62167700
C	-3.36978600	-1.17418900	-1.00530200
C	-4.26953000	-1.58310700	-1.99185300
C	-2.69347700	-2.14778100	-0.27355500
C	-4.48449100	-2.92942600	-2.24776200
H	-4.80721800	-0.83249000	-2.56144600
C	-2.91484700	-3.49987000	-0.52376800
H	-1.98291400	-1.86835800	0.49517900
C	-3.80669000	-3.89596200	-1.51069300
H	-5.18634900	-3.22575700	-3.01794600
H	-2.38407900	-4.24414500	0.05755300
H	-3.97626300	-4.94813300	-1.70359100
C	-2.77267600	4.32760700	0.57091600

C	-2.78920500	3.02957500	0.06974700
C	-2.57601900	1.94719400	0.92692800
C	-2.35233700	2.19360500	2.28765800
C	-2.34117800	3.48985600	2.77466300
C	-2.54916300	4.57003300	1.91925100
H	-2.93800700	5.15557900	-0.10827400
H	-2.95857900	2.86746800	-0.98664400
H	-2.18647300	1.35387900	2.95401800
H	-2.16881400	3.65903500	3.83092200
H	-2.53940600	5.58270100	2.30170800
N	-2.51274500	0.62623000	0.46041300
H	-4.15219800	0.80145200	-0.86481700
B	0.04972700	0.33313500	0.09811300
F	0.10150900	-0.22295000	1.29969300
F	0.16443800	1.64459700	-0.02935000
F	-0.20225800	-0.39654700	-0.98023000
H	-2.75912200	-0.02750300	1.19633700
C	3.31904400	-0.85934000	0.11150600
H	4.39694300	-0.71010000	-0.00577900
C	2.92502200	-2.15905200	0.67528100
C	3.86172100	-2.84712400	1.44949600
C	1.67491400	-2.73286300	0.43681000
C	3.53774000	-4.07109100	2.01823700
H	4.84163100	-2.41205500	1.61144500
H	0.96574400	-2.22928900	-0.20546200
C	2.28448900	-4.62859400	1.79265200
H	4.26426600	-4.59303300	2.62832400
H	2.03209700	-5.58776100	2.22793300
C	3.51576900	3.59159600	-0.75121700
C	2.95742400	2.46134100	-0.17129500
C	3.08157100	1.22535900	-0.80383300
C	3.74694700	1.13292300	-2.02487000
C	4.29087000	2.27283800	-2.60596800
C	4.17871100	3.50370500	-1.97210800
H	3.42888800	4.54710800	-0.24841200
H	2.43744900	2.52359400	0.77601900
H	3.82475800	0.17054400	-2.51699200
H	4.80308500	2.19448300	-3.55723200
H	4.60459300	4.39037100	-2.42489500
N	2.50723300	0.06793300	-0.20784400
C	1.35842300	-3.96233400	0.99483700
H	0.39108200	-4.40860900	0.80051300

Coordinates (Angstroms)			
	X	Y	Z

C	2.71779800	1.78361100	0.86864500
H	1.97391900	1.30899400	1.51439200
C	3.77187400	0.77101500	0.49851400
C	5.10498200	0.96731300	0.84637100
C	3.41731700	-0.38007800	-0.20734500
C	6.07253800	0.02869700	0.49896800
H	5.38779800	1.86105500	1.39150600
C	4.38208300	-1.31391000	-0.56104700
H	2.37858800	-0.53868500	-0.47966600
C	5.71364300	-1.11180900	-0.20757700
H	7.10677200	0.19347800	0.77626000
H	4.09550800	-2.20362500	-1.10936100
H	6.46592000	-1.84080000	-0.48319600
C	-0.62686800	4.46723500	0.97556200
C	0.42206300	3.55299700	0.95959600
C	1.05081100	3.22394600	-0.24861200
C	0.61262100	3.85533900	-1.42551800
C	-0.42718700	4.76669100	-1.39218700
C	-1.06419600	5.07883100	-0.19111000
H	-1.10290300	4.70173200	1.92065100
H	0.74226800	3.09414600	1.88579400
H	1.09785400	3.60914500	-2.36382300
H	-0.74795000	5.23782300	-2.31403900
H	-1.87976900	5.79028700	-0.16924000
N	2.04627100	2.26584400	-0.32828000
H	3.17404600	2.60234400	1.43854000
B	-0.97554400	-0.03958000	-0.24438000
F	-0.05476600	-0.50995700	-1.16322000
F	-1.59487200	1.10382000	-0.70915100
F	-0.40319700	0.18517500	1.00066700
H	2.64921500	2.35741300	-1.13583000
C	-1.95988000	-2.44349200	-0.03558400
H	-2.86728300	-3.04379700	-0.00400600
C	-0.71707500	-3.20698100	-0.05870700
C	-0.80126700	-4.49089800	-0.61055000
C	0.49068500	-2.76860400	0.49498700
C	0.32165200	-5.30091800	-0.66973800
H	-1.74871400	-4.84244700	-1.00260600
H	0.55685600	-1.80270600	0.97472700
C	1.52280400	-4.85358800	-0.13221200

H	0.25565400	-6.28450400	-1.11661500
H	2.39807700	-5.49099400	-0.16031400
C	-5.45543500	0.32823200	-0.76743500
C	-4.14797600	-0.09876900	-0.94858300
C	-3.48317200	-0.69608600	0.11435300
C	-4.09576000	-0.86569600	1.34732300
C	-5.40435800	-0.42811300	1.51907800
C	-6.08296900	0.16807800	0.46462300
H	-5.98535200	0.78821900	-1.59196000
H	-3.64722700	0.02003700	-1.90043700
H	-3.54875500	-1.32904900	2.15970700
H	-5.88902900	-0.55476600	2.47890700
H	-7.10223600	0.50777700	0.59966200
N	-2.12498700	-1.16758700	-0.05791400
C	1.60045400	-3.59654800	0.46117100
H	2.52990000	-3.26129600	0.90362200

16

Coordinates (Angstroms)

	X	Y	Z
C	-1.44622500	-1.13697100	-0.66083600
H	-1.23085600	-1.43871600	-1.68335500
C	-2.82482000	-0.71002400	-0.45467200
C	-3.71261100	-1.11136700	-1.46292000
C	-3.29109400	0.11182500	0.57975000
C	-5.04923500	-0.74973500	-1.41260100
H	-3.34582700	-1.71748100	-2.28324900
C	-4.62391100	0.48536000	0.61337200
H	-2.62073700	0.48595100	1.33722800
C	-5.50550300	0.05044300	-0.37256800
H	-5.72763000	-1.07830400	-2.18933700
H	-4.97587700	1.13094100	1.40793500
H	-6.54624100	0.34802600	-0.33497200
C	2.67687600	-3.10109600	-0.56029900
C	1.47138300	-2.74793300	0.03066600
C	0.81118000	-1.60913800	-0.41306500
C	1.33772900	-0.82569800	-1.43326800
C	2.54372600	-1.19002300	-2.01835700
C	3.21609000	-2.32400900	-1.58040000
H	3.19352800	-3.99116700	-0.22384300
H	1.04054700	-3.35334200	0.81638100
H	0.80681300	0.06119100	-1.75785400

H	2.95882300	-0.57946000	-2.81046300
H	4.15898100	-2.60423000	-2.03332300
N	-0.46167300	-1.23564400	0.16584100
H	-2.72072400	2.13542800	-1.68400200
C	-1.93887000	2.44049100	-0.97708500
O	-0.81912800	1.77096700	-1.16593200
O	-2.10215900	3.29860500	-0.14393300
B	-0.51714100	-0.93067900	1.75074000
F	0.61480900	-1.45766400	2.34039200
F	-1.65645900	-1.52636600	2.26491800
F	-0.54201300	0.45219800	1.91060300
H	-0.10436600	2.08190400	-0.49948700
C	3.89467700	0.30588000	1.07713600
C	2.68471900	0.96408800	1.25519100
C	2.32538100	2.00658100	0.40265300
C	3.18622800	2.38086000	-0.62819700
C	4.39975200	1.72526800	-0.79195800
C	4.76050300	0.68333300	0.05615900
H	4.16118500	-0.50496800	1.74497100
H	2.01384500	0.67479400	2.05491400
H	2.90241500	3.18955000	-1.29266900
H	5.06427800	2.02937200	-1.59185900
H	5.70424500	0.16990000	-0.07890300
N	1.06392900	2.63862700	0.53452400
H	0.65647300	2.50019700	1.45455600
H	1.10845900	3.63403200	0.33457500

TS16-17

Coordinates (Angstroms)

	X	Y	Z
C	0.92072300	1.05855400	0.75918000
H	1.55181600	1.35876900	1.59410200
C	-0.25053400	1.96783400	0.53800200
C	-0.00304000	3.33944100	0.56698700
C	-1.54396300	1.50229000	0.32312900
C	-1.03803900	4.23927100	0.35188000
H	1.00429200	3.69836700	0.74646900
C	-2.57924300	2.40617700	0.11456900
H	-1.74576900	0.43556000	0.31507300
C	-2.32820000	3.77312600	0.12472700
H	-0.83755800	5.30346300	0.36838500
H	-3.58430600	2.03852700	-0.05196500

H	-3.13748300	4.47429800	-0.03788100
C	5.13919200	0.39963300	0.77893800
C	3.85851100	0.86797900	0.51355700
C	2.89305600	0.00669300	-0.00420100
C	3.22008800	-1.32304900	-0.26179300
C	4.50457500	-1.78216500	-0.00463400
C	5.46765200	-0.92518400	0.51820900
H	5.88354000	1.07745600	1.17846700
H	3.60689100	1.90676400	0.69519000
H	2.46153500	-1.98886600	-0.65115600
H	4.75129700	-2.81742200	-0.20659700
H	6.46788100	-1.28808700	0.71976000
N	1.57468100	0.49098600	-0.27039300
H	0.29753500	0.07091500	1.46741500
C	-0.00690100	-1.08526500	1.95412300
O	0.35979800	-1.93927100	1.16952900
O	-0.53364600	-0.96556700	3.02890400
B	0.91132000	0.27970500	-1.66994100
F	1.84312500	-0.28412000	-2.54028100
F	0.48620900	1.50798700	-2.18881800
F	-0.20235800	-0.57254300	-1.55865700
C	-3.95219100	-1.48468300	1.27417000
C	-2.85301100	-2.23279300	0.87157000
C	-2.47257300	-2.18909400	-0.45877200
C	-3.15483900	-1.43635400	-1.39741600
C	-4.25548700	-0.69668900	-0.98360500
C	-4.64986600	-0.71595800	0.34938200
H	-4.25840900	-1.50286600	2.31228000
H	-2.29666800	-2.83414900	1.58084200
H	-2.82433600	-1.41870500	-2.42875600
H	-4.79785200	-0.09875300	-1.70490200
H	-5.50320400	-0.13042200	0.66788600
N	-1.27796500	-2.93559400	-0.86157100
H	-1.38076300	-3.93893000	-0.68104100
H	-1.07435000	-2.80746200	-1.85618300
H	-0.46516700	-2.58654600	-0.31960500

17

Coordinates (Angstroms)

	X	Y	Z
C	-1.12190900	-0.29392100	-1.09833200
H	-0.38881400	-1.09794200	-1.20804600

C	-2.38016100	-0.86653300	-0.46949900
C	-3.03062200	-0.24405400	0.59098500
C	-2.90833100	-2.05283800	-0.98094200
C	-4.19147800	-0.79415900	1.12830500
H	-2.62857400	0.67394300	1.00291100
C	-4.06705500	-2.60176400	-0.44874700
H	-2.40434400	-2.54900900	-1.80432000
C	-4.71364900	-1.97260100	0.61137200
H	-4.68594400	-0.29905900	1.95561700
H	-4.46502500	-3.52283000	-0.85778500
H	-5.61605500	-2.40046100	1.03076100
C	1.11787800	-0.99440900	2.41005900
C	0.33358600	-0.74917300	1.28933200
C	0.19833400	0.55237300	0.77641400
C	0.87399100	1.58949100	1.44690300
C	1.64460700	1.33109400	2.57012000
C	1.78199000	0.03693200	3.06187100
H	1.20279600	-2.01124700	2.77576600
H	-0.17446500	-1.58104200	0.82136300
H	0.79914100	2.60415100	1.07844900
H	2.15089900	2.15467500	3.06021500
H	2.38883700	-0.16144300	3.93621400
N	-0.51111200	0.82950700	-0.39963700
H	-1.36269700	0.03561900	-2.10904900
B	-1.07059900	2.24372600	-0.66058400
F	-1.62548000	2.82778300	0.49238400
F	-2.05213900	2.18569400	-1.65794200
F	-0.03074700	3.10210700	-1.11403300
C	4.18464700	-1.19338300	0.28168500
C	3.61510600	-0.00829300	-0.16839100
C	2.73311700	-0.05932500	-1.23196500
C	2.40733300	-1.24704100	-1.86511600
C	2.98239900	-2.42452000	-1.40619300
C	3.86508000	-2.39894100	-0.33139300
H	4.87384900	-1.17062100	1.11631800
H	3.84407800	0.93852600	0.30625700
H	1.71276600	-1.24879700	-2.69716200
H	2.73816400	-3.36201600	-1.88919700
H	4.30722100	-3.32034600	0.02591600
N	2.06206400	1.16767100	-1.66291600
H	2.09336300	1.28462700	-2.68019700
H	1.05190700	1.14146200	-1.36544700
H	2.48535800	1.99907400	-1.24027000

TS17-18

Coordinates (Angstroms)

	X	Y	Z
C	-0.68536200	-1.67501700	-1.18739400
H	-0.88411800	-2.74618100	-1.18229700
C	-1.97355600	-0.94335400	-0.88061600
C	-2.68406100	-1.22780300	0.28697000
C	-2.49149800	-0.00292300	-1.76792100
C	-3.87211600	-0.56758300	0.57278100
H	-2.29992700	-1.97463700	0.97387500
C	-3.68386400	0.65756700	-1.48744200
H	-1.95992800	0.21347900	-2.68836400
C	-4.37426300	0.38060100	-0.31419600
H	-4.41130500	-0.79778400	1.48387100
H	-4.07237300	1.38723200	-2.18763400
H	-5.30134300	0.89541800	-0.09337100
C	3.74016100	0.22039500	-0.78888300
C	2.78739700	-0.70303900	-0.36904100
C	1.44524100	-0.53446200	-0.71261600
C	1.08757700	0.57235500	-1.49012800
C	2.04378500	1.48384000	-1.91036000
C	3.37888700	1.31801400	-1.55673800
H	4.77642600	0.06835600	-0.51178700
H	3.10267300	-1.54929400	0.22285400
H	0.05041900	0.74110800	-1.74750500
H	1.73812600	2.33597400	-2.50557900
H	4.12546400	2.03266600	-1.87968500
N	0.41701400	-1.41197800	-0.21143200
H	-0.34673100	-1.41578900	-2.18921100
B	0.86217500	-2.70859300	0.54234200
F	1.57614600	-2.34643200	1.69693500
F	1.64866100	-3.53562900	-0.26590400
F	-0.29067300	-3.40019100	0.93672500
C	1.34769300	3.37628900	1.19129100
C	1.17756900	2.07962200	1.65855800
C	-0.04468800	1.44938200	1.47393200
C	-1.09847900	2.09240000	0.84049700
C	-0.91717300	3.38854800	0.37461400
C	0.30483200	4.03049200	0.54324300
H	2.29982200	3.87332600	1.32982500
H	1.98702800	1.55327500	2.15219300
H	-2.04353300	1.57721100	0.70631300

H	-1.73482400	3.89484900	-0.12361900
H	0.44248700	5.03990900	0.17652700
N	-0.19679900	0.06540200	1.85644100
H	-1.13207000	-0.12301600	2.21960800
H	-0.00503100	-0.66459500	0.87690300
H	0.48066200	-0.20418400	2.57122100

18

Coordinates (Angstroms)

	X	Y	Z
C	-0.95852700	1.33151900	-1.05621500
H	-1.56110600	2.21672400	-0.86375800
C	0.50998300	1.65301300	-1.02446600
C	0.97514600	2.81349500	-0.41183500
C	1.41911500	0.78963700	-1.63324900
C	2.33384800	3.10419500	-0.40053000
H	0.26915500	3.48701600	0.06141200
C	2.77783600	1.07874200	-1.62437000
H	1.05777600	-0.11078200	-2.12020000
C	3.23692800	2.23619800	-1.00520400
H	2.68784700	4.00887300	0.07850400
H	3.47663100	0.40217300	-2.10111500
H	4.29610400	2.46357400	-0.99790100
C	-5.03253100	0.00778700	-0.58307900
C	-3.79005000	0.55111200	-0.28408600
C	-2.66631700	-0.26305400	-0.33838300
C	-2.76702900	-1.59871700	-0.69548300
C	-4.01590900	-2.13380400	-0.98926400
C	-5.14909200	-1.33302200	-0.93313200
H	-5.91250900	0.63713100	-0.54003300
H	-3.69847800	1.59355900	-0.00768000
H	-1.87812000	-2.21566800	-0.74533500
H	-4.09760500	-3.17764200	-1.26503200
H	-6.12111200	-1.75100400	-1.16296300
N	-1.34988700	0.29587300	-0.02898100
H	-1.23198100	0.92056700	-2.02752800
B	-1.24598500	0.80724000	1.50599600
F	-1.85820200	-0.15722800	2.29364600
F	-1.88815600	2.03045700	1.60527300
F	0.09631000	0.91524300	1.82578800
C	3.87695600	-2.34350500	-0.78308000
C	2.51379700	-2.49214400	-0.56795100

C	1.90066900	-1.86780900	0.52150900
C	2.67549100	-1.08775700	1.38256900
C	4.03797100	-0.94236200	1.15680400
C	4.64975500	-1.56688500	0.07486400
H	4.33762300	-2.83804100	-1.63016900
H	1.91381100	-3.09714000	-1.23909600
H	2.20268300	-0.60040900	2.22697900
H	4.62524800	-0.33460100	1.83512100
H	5.71249800	-1.45171500	-0.09684200
N	0.51139000	-1.97316500	0.70768300
H	0.23154400	-1.83717500	1.67363900
H	-0.66134300	-0.47894700	-0.07395800
H	0.13293100	-2.84773300	0.36019900

TS18

Coordinates (Angstroms)

	X	Y	Z
C	0.38676700	0.17613400	0.78198400
H	-0.01436800	0.00904000	1.77967600
C	1.82455700	-0.11702900	0.64541600
C	2.37133800	-0.97516800	1.60205500
C	2.63589000	0.42865200	-0.35129400
C	3.71038900	-1.33019300	1.52764800
H	1.74062700	-1.37417600	2.38783100
C	3.97706400	0.08832400	-0.40472100
H	2.23204600	1.12552200	-1.07482600
C	4.51230000	-0.79833300	0.52591700
H	4.12788600	-2.01032600	2.25894300
H	4.60899200	0.51927900	-1.17059400
H	5.56112700	-1.06334400	0.47540000
C	-4.21700200	0.48892100	0.15783300
C	-2.91022900	0.68124600	-0.27281500
C	-1.90613600	-0.13833300	0.22267900
C	-2.19280400	-1.15913700	1.12033900
C	-3.50209400	-1.34475800	1.54262000
C	-4.51413200	-0.51932200	1.06621500
H	-5.00262900	1.12887500	-0.22329100
H	-2.68396200	1.45567100	-0.99541200
H	-1.40278600	-1.81242600	1.47275800
H	-3.73002700	-2.14179900	2.23893200
H	-5.53450600	-0.66705300	1.39678900
N	-0.53404200	0.04011300	-0.25119400

H	0.38441500	1.57683600	0.96954000
C	0.31475200	2.66481800	0.30922600
O	-0.24254600	2.42023400	-0.78207300
O	0.79049400	3.59210300	0.87225900
B	-0.17313800	-0.90855900	-1.55452700
F	-1.36651500	-1.13147000	-2.20645100
F	0.38078900	-2.08205100	-1.08474900
F	0.70329000	-0.19903200	-2.35255500
H	-0.46845800	1.25525800	-0.75106200

20

Coordinates (Angstroms)

	X	Y	Z
C	-1.70803900	2.61437300	-0.51911400
H	-1.68962800	3.51935800	-1.13112900
C	-2.99918600	1.92616100	-0.44451200
C	-4.09699400	2.55004100	-1.04128300
C	-3.17086400	0.69409500	0.19655100
C	-5.35430400	1.96386100	-0.98902200
H	-3.95840200	3.50129400	-1.54280400
C	-4.42742100	0.11344200	0.24729500
H	-2.32757800	0.18283500	0.64666100
C	-5.52009000	0.74598700	-0.34274300
H	-6.20048400	2.45570600	-1.45196800
H	-4.55786400	-0.83849900	0.74599800
H	-6.49884500	0.28418400	-0.29888500
C	2.94384300	2.96961300	-0.21397700
C	1.74415000	2.27718100	-0.13425900
C	0.54189900	2.97608100	-0.02853700
C	0.54949400	4.36898600	0.04383600
C	1.75580700	5.05354600	-0.02651800
C	2.95362000	4.35953800	-0.15808900
H	3.87270200	2.42088900	-0.31324400
H	1.72570500	1.19455400	-0.18226900
H	-0.37997100	4.90986000	0.17569700
H	1.75915700	6.13493000	0.03479700
H	3.89089200	4.89923300	-0.21003200
N	-0.65202700	2.21574100	0.07135800
H	-0.36568600	0.95758700	1.06357200
H	0.30799900	1.92461500	2.84924800
C	0.43199000	0.83155800	2.81823600
O	0.94978200	0.21251300	3.71300300

O	-0.03395200	0.25419900	1.72726300
C	0.55797800	-2.24368800	0.53585800
H	1.07011300	-2.39899800	1.48284300
C	-0.85255400	-2.61659500	0.53406900
N	1.27424000	-1.80137200	-0.43799800
C	-1.51147900	-2.55483600	1.76769700
C	-1.51948500	-3.12721100	-0.58325500
C	2.68965600	-1.63145100	-0.19632400
B	0.72995900	-1.28327300	-1.87436300
C	-2.83680300	-2.94467700	1.87036900
H	-0.97881900	-2.18365500	2.63529200
C	-2.83843400	-3.53736300	-0.46831200
H	-1.00606100	-3.23276100	-1.52832800
C	3.13461400	-0.97073100	0.94090000
C	3.58722700	-2.13940500	-1.12745400
F	0.67665700	-2.36310200	-2.74581400
F	1.63143900	-0.33589900	-2.32809800
F	-0.51458600	-0.71208900	-1.68431400
C	-3.49984900	-3.43866000	0.75158900
H	-3.34802500	-2.87751700	2.82227400
H	-3.34963400	-3.94372900	-1.33173900
C	4.50065100	-0.82909200	1.15320700
H	2.42115400	-0.56572500	1.64845700
C	4.94891600	-1.99414200	-0.90433000
H	3.22163100	-2.64929300	-2.01018100
H	-4.53254900	-3.75590000	0.83217900
C	5.40827800	-1.33795400	0.23308300
H	4.85065700	-0.31042100	2.03693300
H	5.65236700	-2.39496700	-1.62319300
H	6.47193300	-1.22364400	0.40027200

TS20-21

Coordinates (Angstroms)

	X	Y	Z
C	-1.23729600	2.80600800	-0.40086000
H	-1.09665600	3.77395200	-0.87326600
C	-2.56355800	2.23595800	-0.42124400
C	-3.53798000	2.92755200	-1.15021500
C	-2.90047200	1.05906300	0.26309500
C	-4.83374300	2.43981800	-1.21305700
H	-3.26813000	3.84137100	-1.66688100
C	-4.19625000	0.58325700	0.19902300

H	-2.15745200	0.51473600	0.83449000
C	-5.16100600	1.27029400	-0.53817100
H	-5.58625600	2.97189000	-1.78036900
H	-4.46079300	-0.32359800	0.72790200
H	-6.17391500	0.88914700	-0.58159200
C	3.45871400	2.57486200	0.33869500
C	2.19036200	2.02250500	0.24043900
C	1.08346600	2.86403700	0.23021600
C	1.22236800	4.24209400	0.34989300
C	2.49766400	4.78125400	0.44121400
C	3.61486000	3.95305300	0.43563000
H	4.32457100	1.92464100	0.33807200
H	2.05263200	0.95306200	0.14729100
H	0.35192700	4.88460500	0.39572400
H	2.61575900	5.85308700	0.53641900
H	4.60581100	4.38186200	0.51424000
N	-0.20340000	2.25706300	0.13400100
H	-0.25198900	1.29720600	0.54883700
H	0.50776400	1.10169600	3.01094900
C	0.48054700	0.04580300	2.68226600
O	0.83743700	-0.84159100	3.44221700
O	0.05303000	-0.11306900	1.47696800
C	0.19791800	-1.87859900	0.61944300
H	0.75149300	-2.28863500	1.45761400
C	-1.24204300	-2.24504600	0.62619900
N	0.89539400	-1.66388200	-0.48187200
C	-1.95143200	-2.17550600	1.82773400
C	-1.84784000	-2.81201700	-0.49236700
C	2.31702500	-1.84135700	-0.41694900
B	0.34084100	-0.89066000	-1.74461200
C	-3.25693900	-2.63547400	1.89807100
H	-1.47236700	-1.76039500	2.70618500
C	-3.15866500	-3.27054100	-0.41960100
H	-1.29642500	-2.91473200	-1.41713600
C	3.04659000	-1.52131300	0.72568800
C	2.97500500	-2.34077700	-1.53974300
F	0.10785600	-1.76912900	-2.80822500
F	1.29887400	0.04963700	-2.13183000
F	-0.83544800	-0.23137000	-1.39616900
C	-3.86641200	-3.18118700	0.77124600
H	-3.79966900	-2.57161800	2.83316700
H	-3.62063900	-3.70775500	-1.29609700
C	4.42322700	-1.71698100	0.74513100
H	2.55199900	-1.11964400	1.60148100

C	4.34959200	-2.52547700	-1.51372200
H	2.40598200	-2.59033300	-2.42646500
H	-4.88684200	-3.54047100	0.82587200
C	5.08061300	-2.21554100	-0.37160900
H	4.98098300	-1.46617600	1.63917100
H	4.84977100	-2.91910700	-2.39006900
H	6.15311600	-2.36316200	-0.35350500

21

Coordinates (Angstroms)

	X	Y	Z
C	-1.39668900	2.84858600	-0.15144800
H	-1.16572300	3.80287400	0.31281300
C	-2.78586800	2.47157000	-0.26954600
C	-3.72942000	3.37747900	0.22988600
C	-3.20672300	1.25439900	-0.82382300
C	-5.07987100	3.07267700	0.17574700
H	-3.39319800	4.31430200	0.65847900
C	-4.55615100	0.95838800	-0.87235900
H	-2.49455600	0.54163800	-1.22139400
C	-5.49123600	1.86371400	-0.37209400
H	-5.80858800	3.77298900	0.56259000
H	-4.88446500	0.01846100	-1.29736600
H	-6.54616100	1.62176000	-0.41262500
C	3.22491100	2.38618900	-1.14902500
C	1.88181700	2.07984200	-1.31702500
C	0.97529600	2.46904900	-0.34001300
C	1.38401900	3.12755300	0.81376700
C	2.72898000	3.43458300	0.96434700
C	3.64798700	3.06828800	-0.01381200
H	3.93940500	2.08726200	-1.90561900
H	1.53447400	1.54570600	-2.19205900
H	0.67116900	3.37701100	1.59018000
H	3.06109900	3.94457600	1.85966700
H	4.69734100	3.30107100	0.11746900
N	-0.39846300	2.13713600	-0.54178400
H	-0.55506100	1.22797300	-0.99690800
H	-1.20460500	1.18243700	2.32471500
C	-0.81529300	0.15685600	2.28870000
O	-0.77906500	-0.57930300	3.23885200
O	-0.39570300	-0.13654000	1.06506300
C	0.20458300	-1.45964500	0.83419200

H	0.73419200	-1.71843800	1.75142500
C	-0.89162700	-2.48855900	0.62622800
N	1.13047700	-1.36862100	-0.23967700
C	-0.51722100	-3.83099600	0.60672100
C	-2.23082300	-2.15141700	0.48428900
C	2.45284700	-1.03140600	0.09399900
B	0.59377600	-1.32945700	-1.67639000
C	-1.46964200	-4.82314900	0.42952000
H	0.52938000	-4.09357300	0.71855800
C	-3.18792700	-3.14676300	0.30374200
H	-2.53636100	-1.11311300	0.50631300
C	2.76701000	-0.31530100	1.25867300
C	3.51450700	-1.43672700	-0.73010100
F	0.22397900	-2.59524900	-2.16279100
F	1.51641200	-0.77121000	-2.56730000
F	-0.58357900	-0.51051100	-1.71175000
C	-2.81090300	-4.48206900	0.27408700
H	-1.16817000	-5.86343000	0.41298200
H	-4.22976000	-2.87268100	0.18828500
C	4.08703900	-0.02147700	1.58129800
H	1.98194300	0.04084100	1.91384900
C	4.82560100	-1.11868400	-0.41159800
H	3.30199400	-2.01637200	-1.61829500
H	-3.55606600	-5.25574900	0.13470300
C	5.12730800	-0.40949300	0.74812700
H	4.29474900	0.53729300	2.48665200
H	5.62236900	-1.44672100	-1.06908000
H	6.15338800	-0.16987500	0.99722600

TS21-22

Coordinates (Angstroms)

	X	Y	Z
C	-1.23902100	2.23665700	0.32621700
H	-0.96872200	2.59725700	1.30976300
C	-2.60356100	1.80116700	0.13274600
C	-3.48169000	2.01274600	1.20156400
C	-3.06681600	1.20178600	-1.04717200
C	-4.81757900	1.66246800	1.08402100
H	-3.10869700	2.46225800	2.11457700
C	-4.40017400	0.85212700	-1.15395200
H	-2.39775800	0.99763100	-1.87413300
C	-5.27578400	1.08696100	-0.09425100

H	-5.49707800	1.83452600	1.90863500
H	-4.76170200	0.38536200	-2.06119300
H	-6.31836100	0.80863900	-0.18874300
C	3.14305400	2.98300800	-1.51561500
C	1.79548000	2.66328100	-1.59927700
C	1.01833400	2.66551100	-0.44756300
C	1.56752900	2.99612200	0.78777900
C	2.91392500	3.31975700	0.85633100
C	3.70576000	3.30935800	-0.28859500
H	3.74992900	2.97363400	-2.41186600
H	1.34603100	2.39649700	-2.54834800
H	0.97351200	2.99996100	1.69054200
H	3.34781900	3.57433700	1.81494600
H	4.75776100	3.55630000	-0.22152600
N	-0.34461900	2.29027100	-0.59833900
H	-0.58215800	1.95383400	-1.53086700
H	0.58661200	1.20122100	3.06616500
C	0.36890200	0.19348300	2.65655300
O	0.48826000	-0.78081700	3.39859700
O	0.00448300	0.19135200	1.43466800
C	0.06375900	-1.61375600	0.54119100
H	0.40025000	-2.00794200	1.49327900
C	-1.38491600	-1.81432100	0.27828100
N	0.98941400	-1.49782400	-0.38585200
C	-1.83535100	-2.44053600	-0.88212700
C	-2.30026900	-1.52376600	1.29448200
C	2.34212400	-1.65023600	0.09122100
B	0.82632100	-1.02639200	-1.87487900
C	-3.18504800	-2.73835100	-1.03912000
H	-1.13624900	-2.71835600	-1.65805200
C	-3.64417400	-1.82109200	1.13485300
H	-1.94994500	-1.05824100	2.20661400
C	3.08637100	-0.52041400	0.41484300
C	2.87853300	-2.92086100	0.24570700
F	0.69731700	-2.14084800	-2.71655700
F	1.96906900	-0.32474500	-2.25177700
F	-0.29701200	-0.20151900	-2.00325200
C	-4.09190900	-2.42648000	-0.03622300
H	-3.52184600	-3.22434600	-1.94655600
H	-4.34455000	-1.58282600	1.92602700
C	4.37982400	-0.67022000	0.89609300
H	2.64677400	0.46179700	0.28281600
C	4.17567900	-3.06392800	0.72838900
H	2.27980200	-3.78651200	-0.01265300

H	-5.14322200	-2.65620400	-0.16174800
C	4.92618000	-1.94104600	1.05332800
H	4.96223700	0.20747900	1.14964200
H	4.59703300	-4.05438800	0.84835600
H	5.93606500	-2.05389800	1.42799800

22

Coordinates (Angstroms)

	X	Y	Z
C	1.43338000	-1.89806300	-0.72839500
H	1.25044300	-2.77369700	-0.11038900
C	2.78056900	-1.38235200	-0.74765800
C	3.69189900	-2.01520600	0.10824000
C	3.20306500	-0.32465600	-1.56607600
C	5.01324800	-1.59983000	0.14311000
H	3.34695400	-2.82376200	0.74277100
C	4.52459200	0.07713200	-1.52932100
H	2.51627200	0.17171200	-2.24152600
C	5.42839900	-0.55850500	-0.67784300
H	5.71706700	-2.08714800	0.80525000
H	4.85676800	0.89028600	-2.16185000
H	6.46182800	-0.23487300	-0.65685400
C	-3.13597900	-1.64124900	-2.22321800
C	-1.80896400	-1.23617200	-2.20704400
C	-0.90963700	-1.87950200	-1.36505700
C	-1.31463100	-2.92710400	-0.54099000
C	-2.64255300	-3.32434300	-0.57534800
C	-3.55617800	-2.68287600	-1.40660900
H	-3.83838200	-1.13646000	-2.87420700
H	-1.47207300	-0.42805100	-2.84382500
H	-0.62563600	-3.42193100	0.13201700
H	-2.96623800	-4.13568200	0.06419400
H	-4.59230600	-2.99668800	-1.41648900
N	0.43130600	-1.39502000	-1.36899800
H	0.56663100	-0.54048000	-1.91468400
H	0.09644300	-1.33703400	1.29624400
C	0.31107700	-1.92437600	2.22805200
O	0.80361900	-3.05713900	2.04646000
O	0.03021200	-1.34616400	3.29335100
C	-0.24376200	1.30494400	1.05021700
H	-0.49297200	0.79997000	1.98518700
C	1.16499800	1.65817900	0.91676300

N	-1.22674400	1.52578000	0.24240600
C	2.03523000	0.98054700	1.78370400
C	1.67151500	2.67719400	0.09704700
C	-2.55132300	1.16357400	0.70062500
B	-1.13685000	2.09925000	-1.26540700
C	3.39011500	1.27315100	1.79155200
H	1.63579700	0.22968500	2.45609900
C	3.02126400	2.98060300	0.12990800
H	1.01791300	3.25816700	-0.53406100
C	-2.80973800	-0.12137700	1.15317000
C	-3.55061500	2.12869300	0.66873500
F	-0.99443100	3.47704100	-1.22245400
F	-2.30387700	1.75637600	-1.91794800
F	-0.04299400	1.48994200	-1.88147000
C	3.88367600	2.27416400	0.96453900
H	4.05463900	0.73348000	2.45431400
H	3.40375600	3.77801700	-0.49454200
C	-4.08944100	-0.44286100	1.59051500
H	-2.02334600	-0.86606600	1.15354300
C	-4.82348300	1.79826100	1.11013600
H	-3.32944200	3.12598600	0.30870000
H	4.94004100	2.51412700	0.97608900
C	-5.09636800	0.51303100	1.56895500
H	-4.29513800	-1.44767000	1.93844700
H	-5.60455400	2.54800900	1.09419800
H	-6.09320800	0.25871100	1.90666500

TS22-23

Coordinates (Angstroms)

	X	Y	Z
C	-1.52589000	2.06899100	-0.54128700
H	-1.51911300	3.15501100	-0.58082400
C	-2.84581000	1.40804300	-0.65327200
C	-3.91612000	1.93862900	0.07135900
C	-3.05104500	0.31402900	-1.49248200
C	-5.17631900	1.37425100	-0.03644000
H	-3.74980600	2.78865500	0.72391200
C	-4.31994000	-0.24126200	-1.60310800
H	-2.24332300	-0.08990500	-2.09085200
C	-5.38060200	0.28265600	-0.87617200
H	-6.00108400	1.78682600	0.53084300
H	-4.47613700	-1.08659200	-2.26158100

H	-6.36684300	-0.15608200	-0.96430100
C	3.07381100	1.98266000	-1.97202100
C	1.79941300	1.44518700	-1.87658800
C	0.84281800	2.07471600	-1.08470300
C	1.15210100	3.24543300	-0.39700900
C	2.42985800	3.77845100	-0.50930800
C	3.39536800	3.14978200	-1.28730800
H	3.81636500	1.48519100	-2.58369900
H	1.54047400	0.54036100	-2.41100100
H	0.42066400	3.73271300	0.23497000
H	2.67257400	4.68570100	0.02983100
H	4.39137700	3.56778400	-1.36018900
N	-0.42811000	1.46538400	-0.97708700
H	-0.44938900	0.45916500	-1.13914400
H	-1.42700900	2.14123400	0.93099600
C	-0.91954600	2.01642500	2.05302000
O	-1.56107000	2.61145400	2.89473800
O	0.07919800	1.31967900	1.98753700
C	0.38356800	-1.47358300	1.05987000
H	0.64249900	-1.03919200	2.02157100
C	-1.02632100	-1.82360300	0.91211100
N	1.35640100	-1.61487100	0.22389400
C	-1.89848700	-1.19408400	1.81225200
C	-1.53489400	-2.78867800	0.03187900
C	2.67445800	-1.22319100	0.67933700
B	1.25554400	-2.09264200	-1.31367600
C	-3.25746000	-1.46580400	1.78666100
H	-1.49918200	-0.49400600	2.53447200
C	-2.88791700	-3.08095800	0.03608800
H	-0.88033300	-3.33675100	-0.62742900
C	2.88930500	0.06751200	1.14150600
C	3.70435200	-2.15323800	0.62359400
F	1.13708300	-3.47259300	-1.35782900
F	2.40795500	-1.68655100	-1.95822300
F	0.14323000	-1.46427900	-1.87367700
C	-3.75262000	-2.41204500	0.89822500
H	-3.92234700	-0.95813300	2.47400400
H	-3.27159900	-3.83797100	-0.63609200
C	4.16299800	0.42563700	1.56964700
H	2.06883900	0.77607700	1.16326200
C	4.97034900	-1.78369300	1.05512000
H	3.51273200	-3.15305400	0.25324900
H	-4.81176300	-2.63876500	0.88333900
C	5.20245600	-0.49467300	1.52543400

H	4.33919300	1.43232600	1.92832600
H	5.77723300	-2.50502100	1.02196700
H	6.19347700	-0.20976000	1.85604300

23

Coordinates (Angstroms)

	X	Y	Z
C	1.74377400	2.00421600	-0.32647000
H	1.84744100	3.08975900	-0.40916700
C	3.09450400	1.43139600	0.03278200
C	4.14513100	1.62687600	-0.86832700
C	3.34277700	0.72574100	1.20533700
C	5.41220200	1.13262100	-0.60375200
H	3.95828100	2.17163400	-1.78833300
C	4.61628000	0.22297800	1.47089800
H	2.55528700	0.56505700	1.93149200
C	5.65248100	0.42255800	0.57107900
H	6.21398200	1.29563500	-1.31403200
H	4.79110300	-0.32731400	2.38779700
H	6.64092500	0.03181000	0.77988600
C	-2.81795900	2.40182800	1.35786900
C	-1.54337400	1.87249800	1.43642500
C	-0.54872600	2.25323100	0.51928400
C	-0.87891500	3.18271500	-0.47490800
C	-2.16482000	3.71600800	-0.53467200
C	-3.14307800	3.33278000	0.37121600
H	-3.56744000	2.08492900	2.07404100
H	-1.29324800	1.16209600	2.21489900
H	-0.14327500	3.49333500	-1.20474500
H	-2.39748800	4.43549900	-1.31120300
H	-4.14164400	3.74694000	0.31286600
N	0.72584500	1.71746800	0.65876200
H	0.72330300	0.76635900	1.01043900
H	1.46397600	1.64253300	-1.32704200
C	-0.49019600	-1.21717300	-0.99509900
H	-0.82334500	-0.86447100	-1.96921300
C	0.92853300	-1.54093800	-0.93968500
N	-1.40830100	-1.31510600	-0.09421300
C	1.68853600	-1.03606500	-2.00495200
C	1.54110300	-2.38449400	-0.00118700
C	-2.76378400	-1.03399600	-0.51778200
B	-1.20754000	-1.67890100	1.46761100

C	3.04208900	-1.31610500	-2.10197900
H	1.20706000	-0.41945700	-2.75528200
C	2.88928900	-2.67405400	-0.11544200
H	0.97097600	-2.84013700	0.79284700
C	-3.06264100	0.15649600	-1.16380400
C	-3.74503000	-1.98802500	-0.27715000
F	-1.08276000	-3.05493100	1.59039500
F	-2.32134300	-1.22585600	2.14691900
F	-0.06664100	-1.02258300	1.91548900
C	3.64431500	-2.13337400	-1.15407200
H	3.62156200	-0.90655100	-2.91926900
H	3.35588700	-3.33232300	0.60642000
C	-4.36471600	0.38761300	-1.59073500
H	-2.28927400	0.90176100	-1.31348000
C	-5.04194600	-1.74636000	-0.70641100
H	-3.49194100	-2.90976100	0.23227200
H	4.69986100	-2.36484000	-1.23040200
C	-5.35401600	-0.56041300	-1.36399300
H	-4.60299900	1.31842800	-2.09047100
H	-5.80976200	-2.48860400	-0.52824200
H	-6.36853300	-0.37536600	-1.69403100

TS11-A1

Coordinates (Angstroms)

	X	Y	Z
C	-4.65657700	-0.91312600	0.20089000
C	-3.83032200	-0.00976300	0.86525600
C	-2.45332500	-0.15829400	0.81476700
C	-1.89096700	-1.21566600	0.09590900
C	-2.72452500	-2.13531200	-0.54297300
C	-4.10322600	-1.97649500	-0.50236200
H	-5.73218700	-0.79203200	0.24141400
H	-4.26408200	0.80684000	1.42904300
H	-1.80894500	0.53031000	1.34569000
H	-2.28575900	-2.96905000	-1.07961200
H	-4.74459000	-2.68575800	-1.01043700
C	-0.43881900	-1.42076200	0.02085300
H	-0.11740500	-2.44141400	-0.20620500
N	0.41678500	-0.49850100	0.21762600
C	1.79290300	-0.84561500	0.14981500
C	2.31141800	-1.63290200	-0.87721300
C	2.64293600	-0.33164900	1.12793700

C	3.66914900	-1.92800600	-0.90264600
H	1.65639100	-1.99434900	-1.66110200
C	3.99510700	-0.64094300	1.10292400
H	2.23007400	0.29979300	1.90584400
C	4.51322100	-1.43954200	0.08751300
H	4.06819600	-2.53529700	-1.70597100
H	4.64850400	-0.25022200	1.87341600
H	5.57073600	-1.67118400	0.06376300
B	0.17451900	1.87673200	-0.16830200
F	1.39523500	1.91376800	-0.68101100
F	-0.86709900	1.68644500	-0.96506100
F	-0.00809900	2.17556300	1.11105700
O	-0.02641500	4.27340000	-0.74173600
H	0.48504500	4.90830000	-0.22638400
H	-0.92693900	4.61917900	-0.74632100

(HCOOH)₂

Coordinates (Angstroms)

	X	Y	Z
H	-0.52447600	-1.12341700	0.00062200
O	1.14559400	-1.14359500	-0.00019300
C	1.89774100	-0.18783200	-0.00054400
H	2.98456600	-0.30264400	-0.00132900
O	1.52035300	1.06325600	0.00081900
H	0.52440900	1.12374200	0.00091300
C	-1.89784700	0.18789800	-0.00014500
O	-1.14535600	1.14343400	-0.00060700
O	-1.52049800	-1.06322800	0.00050400
H	-2.98460500	0.30298900	-0.00024600

***p*-BrPhCHO**

Coordinates (Angstroms)

	X	Y	Z
C	-3.58003400	0.31430600	0.00003000
O	-4.33289600	-0.63114700	0.00005900
H	-3.96959900	1.34650100	0.00007600
C	-2.10524100	0.20004200	-0.00004400
C	-1.33933500	1.36195200	-0.00003400
C	-1.48405500	-1.04876500	-0.00005600

C	0.04678900	1.28861200	-0.00002200
H	-1.82846700	2.32972200	-0.00001900
C	-0.10297300	-1.13767800	-0.00003300
H	-2.08760300	-1.94826200	-0.00004700
C	0.64247000	0.03653400	-0.00002000
H	0.64704000	2.18851400	-0.00000300
H	0.38680300	-2.10227400	-0.00003800
Br	2.54426500	-0.08157300	0.00001800

p-MeOPhNH₂

Coordinates (Angstroms)

	X	Y	Z
C	-0.42199200	-1.00017600	-0.00246800
C	0.95835500	-1.19159300	-0.00958400
C	1.83853000	-0.11300700	-0.00813000
C	1.29902800	1.17897900	-0.00745200
C	-0.06981800	1.37585100	0.00042300
C	-0.94466500	0.28887700	-0.00040100
H	-1.06930100	-1.86663800	-0.00023500
H	1.35397500	-2.20119900	-0.01059100
H	1.96643400	2.03364900	-0.00650700
H	-0.48134700	2.37806500	0.00541900
N	3.22521400	-0.30869200	-0.07799700
H	3.53136400	-1.19156000	0.31056300
H	3.76292500	0.45503700	0.31134400
O	-2.27724500	0.58494700	0.00614400
C	-3.18154000	-0.50595200	0.00582700
H	-3.05084700	-1.12874100	0.89490600
H	-4.17974700	-0.07442700	0.01264000
H	-3.05938700	-1.12078700	-0.89000100

H2

Coordinates (Angstroms)

	X	Y	Z
C	-2.39454700	-1.30967300	-0.54909300
O	-3.18510400	-1.94195900	0.13077500
H	-2.75797100	-0.60097400	-1.30971600
C	-0.93869600	-1.42752600	-0.42438700
C	-0.13159300	-0.73147300	-1.32198900

C	-0.36783200	-2.18400300	0.59934600
C	1.24932900	-0.79249700	-1.21128400
H	-0.58556200	-0.13961200	-2.10869200
C	1.00871200	-2.24584600	0.72628100
H	-1.00483600	-2.71421400	1.29671500
C	1.79572500	-1.54663700	-0.18289900
H	1.88276200	-0.25291100	-1.90285400
H	1.46324900	-2.82389100	1.51969200
C	1.20815700	1.86178600	1.01422400
C	0.03480300	1.33749100	1.55052200
C	-1.20407300	1.58389900	0.96237600
C	-1.24275300	2.39089600	-0.18111000
C	-0.07964100	2.91277500	-0.71995800
C	1.15708600	2.65058500	-0.13133900
H	2.14905000	1.63696800	1.49858900
H	0.08727800	0.71522400	2.43759100
H	-2.19632100	2.59957700	-0.65401700
H	-0.11449300	3.52939700	-1.61033400
N	-2.38154300	1.07772000	1.51951900
H	-2.25445600	0.23631500	2.06726700
H	-3.16220800	0.99342500	0.87689600
H	-4.77257800	-1.56065400	-0.12223000
O	-5.71943400	-1.30219100	-0.31346900
C	-5.82835200	0.00644000	-0.38583100
H	-6.85645700	0.31893300	-0.59766900
O	-4.91769500	0.78847300	-0.24097500
Br	3.68995600	-1.61853000	-0.00009200
O	2.24781300	3.19751000	-0.74535700
C	3.51457200	2.93039300	-0.17155000
H	3.72817800	1.85736500	-0.16381200
H	4.24657100	3.43612000	-0.79697700
H	3.58011200	3.31911300	0.84850200

TSH2-3

Coordinates (Angstroms)

	X	Y	Z
C	-1.41322700	-1.86006600	-0.41450000
O	-1.87484600	-2.96157300	-0.04478900
H	-1.96213200	-1.25379100	-1.14800600
C	0.04420100	-1.58011000	-0.34144900
C	0.58529800	-0.54236800	-1.09304800
C	0.86459700	-2.33486300	0.49370100

C	1.94324100	-0.25565600	-1.02265900
H	-0.05485800	0.04668200	-1.74073100
C	2.21910700	-2.05560000	0.58118600
H	0.43713100	-3.14243000	1.07547900
C	2.73905000	-1.01630600	-0.18129400
H	2.36548600	0.54901800	-1.60988500
H	2.85943200	-2.63695100	1.23125200
C	-0.05178900	2.62591800	1.09395100
C	-0.45867900	1.33782600	1.38535400
C	-1.63670100	0.82835000	0.83471000
C	-2.38186700	1.62466100	-0.02585600
C	-1.97592300	2.92176200	-0.32685000
C	-0.80418100	3.42652200	0.23131200
H	0.85806300	3.02879900	1.52170600
H	0.13445100	0.71548200	2.04698800
H	-3.29338900	1.23371900	-0.46395800
H	-2.57962500	3.51962800	-0.99530800
N	-2.00136600	-0.51584300	1.05220300
H	-1.60774000	-0.91369800	1.90061800
H	-3.00385600	-0.70032600	0.99299700
H	-3.27211700	-3.15908900	-0.41420400
O	-4.25994800	-3.31855700	-0.72212000
C	-5.05639500	-2.36630600	-0.32817600
H	-6.09479300	-2.53246100	-0.64008700
O	-4.73040100	-1.38714200	0.31399900
Br	4.60449100	-0.63092000	-0.06781500
O	-0.32205500	4.67595800	0.00108300
C	-1.06713600	5.51714400	-0.86588200
H	-2.06938200	5.70235700	-0.47091700
H	-0.52067600	6.45561900	-0.91906400
H	-1.14321200	5.08560300	-1.86716800

H3

Coordinates (Angstroms)

	X	Y	Z
C	-1.35958200	-1.70657600	-0.25129900
O	-1.66847700	-2.98396800	0.13605000
H	-1.78457400	-1.43459000	-1.22226900
C	0.12404000	-1.45810100	-0.23245700
C	0.70367600	-0.62425300	-1.18097200
C	0.91130800	-2.01936300	0.76814000
C	2.06404000	-0.34558000	-1.13842000

H	0.09238300	-0.18557800	-1.96158800
C	2.27205000	-1.75138300	0.82377000
H	0.46353800	-2.67535700	1.50497600
C	2.82878100	-0.91314900	-0.13173600
H	2.51304800	0.30298000	-1.87871400
H	2.88473600	-2.18977600	1.60035800
C	-0.61718000	2.68988300	0.91465800
C	-0.86574900	1.35138600	1.19742300
C	-1.82627200	0.65979600	0.48388000
C	-2.54806300	1.28293900	-0.52793300
C	-2.30333600	2.61135700	-0.81670700
C	-1.33477000	3.32144200	-0.10039100
H	0.13474000	3.21807000	1.48334600
H	-0.30374500	0.85010400	1.97759200
H	-3.29850200	0.72989900	-1.08054800
H	-2.85393300	3.12000200	-1.59773700
N	-2.04902800	-0.75206200	0.73843000
H	-1.72685900	-1.00230600	1.67799500
H	-3.11306600	-0.98975500	0.66400200
H	-2.62606400	-3.16245400	-0.12569500
O	-4.14251100	-3.26953100	-0.56012700
C	-4.90688600	-2.35306000	-0.19343400
H	-5.98304800	-2.48555800	-0.40150100
O	-4.58177200	-1.28864300	0.39097800
O	-1.16631000	4.61463800	-0.45662500
C	-0.18276900	5.37051600	0.23811700
H	0.81245200	4.94219000	0.09721000
H	-0.21248000	6.36863200	-0.19107100
H	-0.41180300	5.42677500	1.30478500
Br	4.69923400	-0.53839800	-0.06337700

TSH3-4

Coordinates (Angstroms)

	X	Y	Z
C	0.03860600	0.81833900	-0.52790400
O	0.15633700	2.23261800	-0.41694500
H	0.36540400	0.51509100	-1.52703400
C	-1.41772200	0.43463700	-0.35714200
C	-1.76570600	-0.91490300	-0.38167700
C	-2.41232100	1.39101000	-0.19917500
C	-3.08764300	-1.30997700	-0.24478000
H	-0.99796300	-1.66979600	-0.51098500

C	-3.74270100	1.00998000	-0.05412900
H	-2.15241600	2.44043200	-0.18790000
C	-4.06259200	-0.33634500	-0.07868100
H	-3.35003100	-2.35919500	-0.26829900
H	-4.51209600	1.75998100	0.07415300
N	0.84773600	0.15362500	0.45946800
H	0.34483300	-0.34070600	1.18379000
H	1.45344400	2.33469000	1.08414600
H	0.90494600	2.55004400	-0.94639000
O	2.25510200	2.72461300	1.49987700
C	2.98137600	3.35104200	0.59184500
H	3.88789000	3.77880000	1.03100100
O	2.69666400	3.45435500	-0.57736100
C	2.12335900	-0.34682600	0.17977600
C	2.67107300	-1.33431500	0.99831000
C	2.90099400	0.14081000	-0.87716700
C	3.95116300	-1.83006100	0.77943300
H	2.08381500	-1.72340800	1.82290400
C	4.17315600	-0.35928200	-1.10468700
H	2.52997100	0.92156700	-1.52931500
C	4.71197900	-1.34487800	-0.28134900
H	4.33456300	-2.59566600	1.43990300
H	4.76932400	0.02134400	-1.92528700
Br	-5.88537400	-0.87008500	0.11875300
O	5.97249900	-1.76686500	-0.58396500
C	6.54189600	-2.76224700	0.24965000
H	5.95579600	-3.68491600	0.22383500
H	7.53579700	-2.95709300	-0.14626700
H	6.62633700	-2.41325200	1.28232800

H4

Coordinates (Angstroms)

	X	Y	Z
C	0.00784000	0.04476200	0.87460600
O	-0.36895600	1.42323400	0.97305600
H	-0.17547500	-0.42383700	1.84322100
C	1.48813200	-0.02365700	0.56505400
C	2.06326100	-1.25691100	0.26299400
C	2.29036900	1.11080800	0.59921700
C	3.41905100	-1.35936200	-0.01057000
H	1.44717400	-2.14728000	0.23834200
C	3.65086100	1.02409100	0.32231500

H	1.85830900	2.07192000	0.84108600
C	4.19724300	-0.21114900	0.02028600
H	3.85819800	-2.32033800	-0.24377600
H	4.26827000	1.91248400	0.34566700
N	-0.73409600	-0.66759600	-0.13302500
H	-0.43460100	-0.41640200	-1.07014900
H	-1.03662900	2.13369300	-0.50473500
H	-1.22756000	1.48756700	1.42351700
O	-1.71139900	2.42184200	-1.16826000
C	-2.87070300	2.56774400	-0.54780400
H	-3.67875700	2.80330600	-1.24792500
O	-3.02883400	2.47337300	0.64511000
C	-2.14040300	-0.73525200	-0.02439600
C	-2.92781000	-0.65688900	-1.16880800
C	-2.77835100	-0.91787100	1.20739400
C	-4.31462800	-0.75731900	-1.10499700
H	-2.45078600	-0.50750400	-2.13121200
C	-4.15710500	-1.01009700	1.27890800
H	-2.20228900	-0.99456100	2.12147300
C	-4.93878700	-0.92984500	0.12691900
H	-4.88702000	-0.69209400	-2.02027000
H	-4.64753500	-1.14822700	2.23492100
O	-6.28559500	-1.02824900	0.30173500
C	-7.09733600	-0.98325500	-0.86013900
H	-8.12404400	-1.08633700	-0.51706400
H	-6.98678800	-0.03070000	-1.38507800
H	-6.85894600	-1.80465500	-1.54107400
Br	6.06358900	-0.34057800	-0.36327900

TSH4-5

Coordinates (Angstroms)

	X	Y	Z
C	-0.03474100	-0.63654400	0.67093300
O	-0.26413300	0.96106000	1.78440500
H	-0.31095300	-1.27935400	1.49536400
C	1.40586000	-0.48590000	0.39939100
C	2.29602400	-1.36611400	1.00644700
C	1.88105500	0.52222800	-0.43872500
C	3.65713900	-1.26989600	0.75311100
H	1.92652000	-2.13669300	1.67221100
C	3.23885200	0.63346400	-0.69001000
H	1.19904800	1.24589000	-0.87315200

C	4.10842600	-0.27172900	-0.09579200
H	4.34890500	-1.96104500	1.21556200
H	3.61107900	1.41926600	-1.33340000
N	-0.88668800	-0.52536200	-0.32865000
H	-0.55958600	-0.07642900	-1.17898600
H	-0.44936100	1.66953000	1.01767800
H	-1.13015000	0.91678200	2.22203300
O	-0.87771600	2.45755300	-0.09844900
C	-2.11974000	2.67465800	0.08701100
H	-2.65025600	3.11664800	-0.77890400
O	-2.75601800	2.44768300	1.11865300
C	-2.29434500	-0.65365600	-0.23448300
C	-3.05338700	-0.25853200	-1.32576000
C	-2.92660500	-1.12212700	0.91588500
C	-4.44010600	-0.33119400	-1.28966100
H	-2.55867900	0.11730400	-2.21467500
C	-4.30540200	-1.19776400	0.95558600
H	-2.36151600	-1.42552800	1.78766400
C	-5.07362300	-0.80199600	-0.14179700
H	-5.00624200	-0.01429000	-2.15409000
H	-4.80896200	-1.55749500	1.84398000
Br	5.97603500	-0.12765700	-0.44798700
O	-6.41638300	-0.90890700	0.00021900
C	-7.22831600	-0.49549200	-1.09008000
H	-8.25692200	-0.65403100	-0.77634100
H	-7.07562300	0.56305800	-1.31433300
H	-7.02427800	-1.09363300	-1.98149900

H5

Coordinates (Angstroms)

	X	Y	Z
C	3.78819000	-0.59387700	-0.13649100
C	3.17812200	-1.50223800	0.71480500
C	1.79268300	-1.56953200	0.73265800
C	1.02622600	-0.73007200	-0.07754200
C	1.66738500	0.16327600	-0.93848000
C	3.05006900	0.23551500	-0.97154600
H	3.76638900	-2.14876800	1.35199800
H	1.29972700	-2.27555800	1.39156900
H	1.09162400	0.78843500	-1.60836900
H	3.54393600	0.92466200	-1.64352500
C	-0.43359200	-0.81501400	0.02976900

H	-0.82591600	-1.70163400	0.53300400
N	-1.21983700	0.09317500	-0.39314900
C	-2.62067000	-0.08880100	-0.27388200
C	-3.24061800	-1.30308900	-0.54516800
C	-3.40215600	1.01004000	0.09398800
C	-4.62014900	-1.43864400	-0.42993000
H	-2.64879400	-2.14919600	-0.87378300
C	-4.77005100	0.88060400	0.22286000
H	-2.92609900	1.96120200	0.30180000
C	-5.38997700	-0.34476200	-0.03986600
H	-5.07661500	-2.39155500	-0.65838700
H	-5.38195200	1.72259300	0.52140000
H	-0.82525100	1.59277200	-0.87856600
O	-0.65787400	2.55504100	-1.20436900
C	-0.05836500	3.26588100	-0.28488200
H	0.14161000	4.29140300	-0.61559300
O	0.25534100	2.87056800	0.81796800
O	0.09571200	0.76547300	2.73533400
H	0.87553500	0.21924200	2.58976400
H	0.10966100	1.41073900	2.00952400
Br	5.69049800	-0.49171500	-0.17602900
O	-6.73675600	-0.37072000	0.10052800
C	-7.40655200	-1.59495900	-0.16580700
H	-8.46238000	-1.40343800	0.00807800
H	-7.25978000	-1.90756900	-1.20246300
H	-7.06492800	-2.38440100	0.50800900

References

- (1) Zhao, Y.; Truhlar, D. G. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc.* **2007**, *120*, 215-241.
- (2) Schäfer, A.; Huber, C.; Ahlrichs, R. Fully optimized contracted Gaussian basis sets of triple zeta valence quality for atoms Li to Kr. *J. Chem. Phys.* **1994**, *100*, 5829.
- (3) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Gaussian 09, Revision D. 01 ed.; Gaussian, Inc, Wallingford.: CT 2010.
- (4) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B* **2009**, *113*, 6378-6396.
- (5) Hratchian, H. P.; Schlegel, H. B. Accurate Reaction Paths Using a Hessian Based Predictor-corrector Integrator. *J. Chem. Phys.* **2004**, *120*, 9918-9924.
- (6) Liu, S.; Schauer, C. K.; Pedersen, L. G. Molecular acidity: A quantitative conceptual density functional theory description. *J. Chem. Phys.* **2009**, *131*, 164107.
- (7) Liu, S. B.; Pedersen, L. G. Estimation of Molecular Acidity via Electrostatic Potential at the Nucleus and Valence Natural Atomic Orbitals. *J. Phys. Chem. A* **2009**, *113*, 3648-3655.
- (8) Burger, S. K.; Liu, S.; Ayers, P. W. Practical calculation of molecular acidity with the aid of a reference molecule. *J. Phys. Chem. A* **2011**, *115*, 1293-1304.
- (9) Hirshfeld, F. L. Bonded-atom fragments for describing molecular charge densities. *Theor. Chem. Acc.* **1977**, *44*, 129-138.
- (10) Lu, T.; Chen, F. Multiwfn: A Multifunctional Wavefunction Analyzer. *J. Comput. Chem.* **2012**, *33*, 580-592.
- (11) Neese, F. Software update: the ORCA program system, version 4.0. *WIREs Comput. Mol. Sci.* **2018**, *8*, e1327.
- (12) Neese, F.; Wennmohs, F.; Becker, U.; Riplinger, C. The ORCA quantum chemistry program package. *J. Chem. Phys.* **2020**, *152*, 224108.
- (13) Mardirossian, N.; Head-Gordon, M. ω B97M-V: A combinatorially optimized, range-separated hybrid, meta-GGA density functional with VV10 nonlocal correlation. *J. Chem. Phys.* **2016**, *144*, 214110.
- (14) Weigend, F.; Ahlrichs, R. Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297-3305.

- (15) Riplinger, C.; Neese, F. An efficient and near linear scaling pair natural orbital based local coupled cluster method. *J. Chem. Phys.* **2013**, *138*, 034106.
- (16) Dunning, T. H. Gaussian basis sets for use in correlated molecular calculations. I. The atoms boron through neon and hydrogen. . *J. Chem. Phys.* **1989**, *90*, 1007-1023.