

Electronic Supplementary Information

For

**Hydrogenation of CO₂ to Methanol Catalyzed by
Manganese Pincer Complex: Insights on Mechanism and
Solvent Effect**

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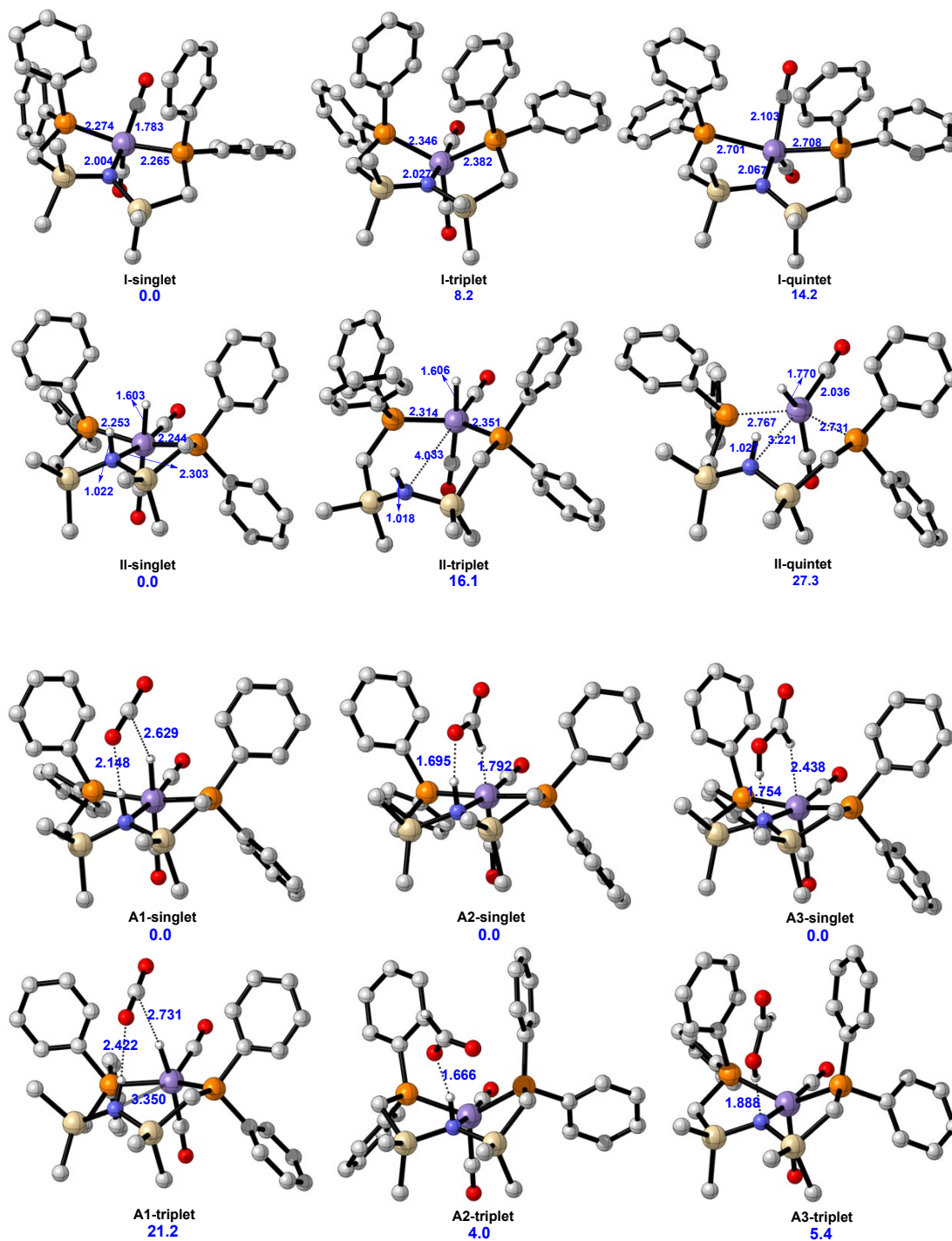
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1. Spin multiplicity of the manganese complexes



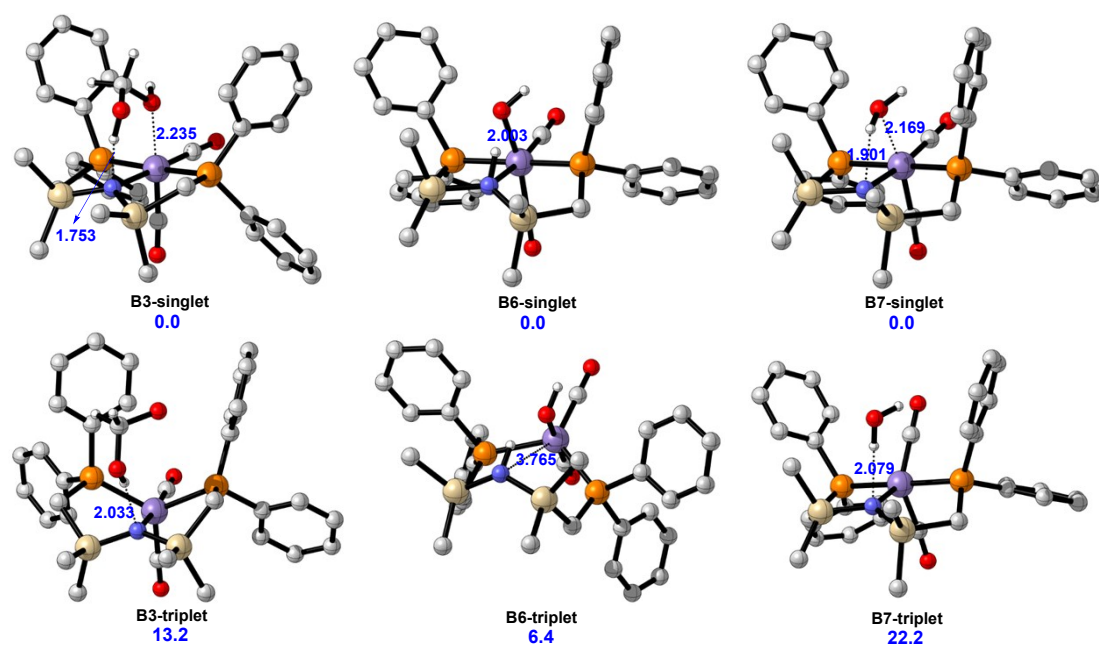


Figure S1. Free energies of manganese complexes with different spin multiplicity. All stationary points take the energy of the singlet state as the zero point reference.

2. Key scan curve

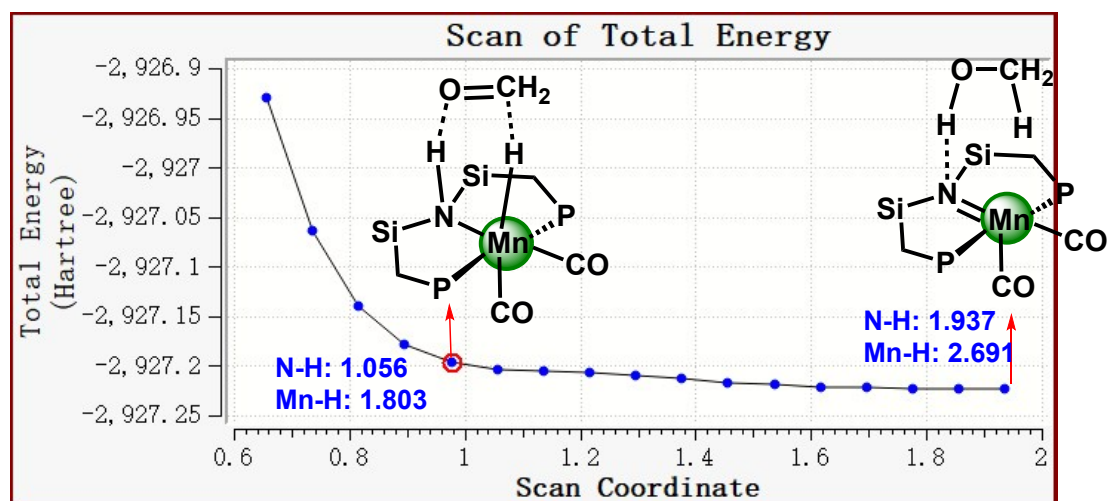


Figure S2. Scanning curve of formaldehyde hydrogenation process. The key bond lengths are given in Å.

3. DFT functional test.

Table S1. The relative Gibbs free energies (in kcal/mol) of key intermediates and transition states in the process of hydrogen activation and formic acid hydrogenation were calculated with different DFT functionals.

Complex	ω B97X-D	B3LYP-D3	B3LYP-D3(BJ)	PBE0
I	0.0	0.0	0.0	0.0
TSH	15.0	18.9	20.0	16.3
II	2.8	3.8	6.5	2.9
B1	1.7	3.2	5.5	6.8
TSB1	13.2	12.1	12.4	15.6

4. 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_{corr}	G	ΔG
Solvent-free				
I	-2811.627053	0.528803	-2811.62705269	0.0
H₂	-1.175282	-0.001321	-1.17528202745	/
I-H₂	-2812.80491	0.548467	-2812.80490951	11.6
TSH	-2812.79714	0.546176	-2812.79714031	15.0
II	-2812.822214	0.551772	-2812.82221402	2.8
CO₂	-188.526945	-0.008885	-188.52694462	6.1
A1	-3001.359467	0.558539	-3001.35946688	13.2
TSA1	-3001.351379	0.561759	-3001.35137895	8.7
A2	-3001.362053	0.565184	-3001.36205266	12.7
TSA2	-3001.352343	0.561939	-3001.35234251	14.4
A3	-3001.354197	0.566447	-3001.35419746	11.1
HCOOH	-189.704812	0.010049	-189.704811924	/
B1	-3002.549965	0.583129	-3002.54996501	1.7
TSB1	-3002.535869	0.587221	-3002.5358694	13.2
B2	-3002.547209	0.588002	-3002.54720861	6.5
B3	-3002.559074	0.589391	-3002.55907373	-0.1
TSB2	-3002.552707	0.587727	-3002.55270715	2.9
B4	-3002.552438	0.589027	-3002.55243817	3.9
TSB3	-3002.546217	0.588657	-3002.54621715	7.6
B5	-3002.549573	0.586162	-3002.54957274	3.9
HCHO	-114.469663	0.005476	-114.469663193	/
B6	-2888.055647	0.555636	-2888.05564722	3.4
TSB4	-2888.050727	0.554114	-2888.0507271	5.4

B7	-2888.05927	0.557784	-2888.05927006	2.5
H₂O	-76.409542	0.004014	-76.4095420279	/
C1	-2927.337663	0.584692	-2927.33766339	-8.7
C2	-2927.348351	0.581259	-2927.34835128	-11.0
TSC	-2927.342696	0.579326	-2927.34269584	-8.7
C3	-2927.345608	0.584100	-2927.3456083	-7.5
CH₃OH	-115.695162	0.029428	-115.69516238	/
In H₂O solvent				
I	-2811.63666	0.529121	-2811.63665975	0.0
H₂	-1.172617	-0.001323	-1.17261716177	/
I-H₂	-2812.812861	0.546944	-2812.81286089	9.8
TSH	-2812.803766	0.546477	-2812.80376647	15.2
II	-2812.837532	0.551704	-2812.83753197	-2.7
CO₂	-188.523432	-0.009116	-188.523432205	/
A1	-3001.372547	0.561168	-3001.37254748	1.7
TSA1	-3001.36528	0.561677	-3001.36527952	6.5
A2	-3001.393377	0.563964	-3001.40535711	-9.7
TSA2	-3001.385686	0.564764	-3001.38568559	-4.3
A3	-3001.385148	0.565176	-3001.38514806	-3.7
HCOOH	-189.722251	0.009993	-189.722251031	/
B1	-3002.572765	0.584796	-3002.57276471	3.6
TSB1	-3002.559408	0.586372	-3002.55940842	13.0
B2	-3002.577962	0.59263	-3002.57796198	5.3
B3	-3002.575593	0.590101	-3002.57559254	5.2
TSB2	-3002.573399	0.583685	-3002.57339904	2.5
B4	-3002.579566	0.589431	-3002.57956632	2.3
TSB3	-3002.562588	0.58535	-3002.56258757	10.4
B5	-3002.564605	0.582947	-3002.56460524	7.6
HCHO	-114.474004	0.005704	-114.474003782	/

B6	-2888.079064	0.560108	-2888.0790636	4.1
TSB4	-2888.065892	0.556553	-2888.06589233	10.1
B7	-2888.071039	0.558717	-2888.07103933	8.2
H₂O	-76.423948	0.00375	-76.4239475152	/
C1	-2927.357843	0.585289	-2927.35784266	-14.3
C2	-2927.365749	0.5845	-2927.36574897	-24.7
TSC	-2927.35093	0.579921	-2927.35092963	-18.3
C3	-2927.355098	0.579829	-2927.35509788	-21.0
CH₃OH	-115.703841	0.029418	-115.703840724	/
In toluene solvent				
I	-2811.657851	0.531819	-2811.65785113	0.0
H₂	-1.174797	-0.001323	-1.17479680828	/
I-H₂	-2812.836105	0.548379	-2812.83610522	9.1
TSH	-2812.82784	0.546936	-2812.82784	13.3
II	-2812.854522	0.552121	-2812.85452229	-0.2
CO₂	-188.527216	-0.008978	-188.527215523	/
A1	-3001.391214	0.560486	-3001.39121386	4.8
TSA1	-3001.384091	0.561364	-3001.38409061	9.8
A2	-3001.398184	0.566187	-3001.39818395	4.0
TSA2	-3001.389201	0.56048	-3001.38920057	6.0
A3	-3001.39007	0.565467	-3001.39007018	8.6
HCOOH	-189.7115	0.010063	-189.711500042	/
B1	-3002.583269	0.582658	-3002.58326855	1.9
TSB1	-3002.56945	0.587504	-3002.56945026	13.6
B3	-3002.590761	0.589784	-3002.5907605	1.6
TSB2	-3002.585249	0.588043	-3002.58524931	4.0
B4	-3002.584837	0.590088	-3002.58483658	5.5
TSB3	-3002.577257	0.588184	-3002.5772571	9.1
B5	-3002.580151	0.584346	-3002.58015106	4.9

HCHO	-114.472126	0.005572	-114.472126342	/
B6	-2888.088256	0.557469	-2888.08825582	3.9
TSB4	-2888.082686	0.555094	-2888.08268606	5.9
B7	-2888.090769	0.558075	-2888.0907689	2.7
H₂O	-76.414179	0.003906	-76.414179262	/
C1	-2927.369783	0.584659	-2927.36978333	-10.3
C2	-2927.380376	0.584441	-2927.38037556	-9.8
TSC	-2927.373115	0.580369	-2927.37311494	-7.8
C3	-2927.376174	0.581859	-2927.37617383	-8.8
CH₃OH	-115.698475	0.029242	-115.698475427	-16.7

In THF solvent

I	-2811.6618	0.528653	-2811.66179956	0.0
H₂	-1.174753	-0.001325	-1.17475282034	/
I-H₂	-2812.839334	0.545542	-2812.83933393	9.7
TSH	-2812.8307	0.546288	-2812.83069991	15.6
II	-2812.860836	0.552809	-2812.86083639	0.8
CO₂	-188.528522	-0.009031	-188.528521619	/
A1	-3001.395765	0.560523	-3001.3957646	7.2
TSA1	-3001.389471	0.563315	-3001.38947111	12.9
A2	-3001.407249	0.567448	-3001.40724918	4.4
TSA2	-3001.399213	0.561155	-3001.39921262	5.5
A3	-3001.399864	0.563886	-3001.39986448	6.8
HCOOH	-189.716718	0.010055	-189.716717917	/
B1	-3002.589046	0.584004	-3002.58904581	6.8
TSB1	-3002.574387	0.585746	-3002.57438727	17.1
B2	-3002.589978	0.591373	-3002.58997824	10.8
B3	-3002.594728	0.589744	-3002.59472847	6.8
TSB2	-3002.589309	0.582481	-3002.58930898	5.7
B4	-3002.590515	0.586653	-3002.59051466	7.5

TSB3	-3002.581541	0.588158	-3002.58154114	14.1
B5	-3002.585025	0.58332	-3002.58502504	8.9
HCHO	-114.474537	0.005613	-114.47453654	/
B6	-2888.093458	0.55857	-2888.09345806	7.6
TSB4	-2888.086347	0.554428	-2888.08634658	9.4
B7	-2888.093676	0.557655	-2888.09367582	6.9
H₂O	-76.416923	0.003779	-76.416922737	/
C1	-2927.375936	0.584503	-2927.37593628	-8.3
C2	-2927.384422	0.585606	-2927.38442236	-8.2
TSC	-2927.375686	0.580262	-2927.3756864	-6.0
C3	-2927.379101	0.583219	-2927.37910141	-6.3
CH₃OH	-115.700314	0.029155	-115.700313636	/

5. Imaginary frequencies of transition states

Table S3. Calculated imaginary frequencies of transition states at ω B97X-D/6-31G* level.

Solvent-free	
TSH	1162.07 <i>i</i>
TSA1	383.90 <i>i</i>
TSA2	689.81 <i>i</i>
TSB1	318.19 <i>i</i>
TSB2	384.44 <i>i</i>
TSB3	82.09 <i>i</i>
TSB4	1146.00 <i>i</i>
TSC	1134.83 <i>i</i>

In H ₂ O solvent	
TSH	1249.42 <i>i</i>
TSA1	503.90 <i>i</i>
TSA2	325.64 <i>i</i>
TSB1	588.74 <i>i</i>
TSB2	1216.12 <i>i</i>
TSB3	143.56 <i>i</i>
TSB4	1287.49 <i>i</i>
TSC	1239.61 <i>i</i>

In toluene solvent	
TSH	1185.86 <i>i</i>
TSA1	388.74 <i>i</i>
TSA2	1130.23 <i>i</i>
TSB1	370.68 <i>i</i>

TSB2	670.02 <i>i</i>
TSB3	111.68 <i>i</i>
TSB4	1147.96 <i>i</i>
TSC	1170.64 <i>i</i>

In THF solvent

TSH	1220.88 <i>i</i>
TSA1	392.41 <i>i</i>
TSA2	1116.59 <i>i</i>
TSB1	428.18 <i>i</i>
TSB2	892.30 <i>i</i>
TSB3	117.07 <i>i</i>
TSB4	1230.64 <i>i</i>
TSC	1198.74 <i>i</i>

6. Cartesian coordinates of all the structures

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

I			

Coordinates (Angstroms)			
	X	Y	Z

25	0.100839000	0.456603000	-0.463886000
7	0.081077000	-1.289111000	-1.449333000
6	0.102111000	1.626972000	0.881118000
8	0.093494000	2.377515000	1.765113000
6	3.008886000	-1.101940000	-1.351227000
1	3.616006000	-0.522989000	-2.056259000
1	3.656094000	-1.847344000	-0.877134000
6	-2.783889000	-0.804211000	-1.563425000
6	0.120570000	1.745199000	-1.662833000
8	0.130989000	2.528129000	-2.518257000
15	-2.158858000	0.302032000	-0.260305000
15	2.307900000	0.067864000	-0.135882000
6	2.252511000	-0.857620000	1.451351000
6	2.599923000	-0.245885000	2.660539000
6	1.689925000	-2.140215000	1.480628000
6	2.403699000	-0.908438000	3.869145000
1	3.020947000	0.755042000	2.662552000
6	1.501563000	-2.803353000	2.689024000
1	1.352353000	-2.605890000	0.560593000
6	1.857750000	-2.189276000	3.887436000
1	2.676687000	-0.418749000	4.799166000
1	1.058703000	-3.794957000	2.691836000
1	1.706138000	-2.703791000	4.831965000
6	3.581377000	1.346896000	0.133263000
6	4.894591000	0.992451000	0.468320000
6	3.257888000	2.695200000	-0.027487000
6	5.864126000	1.971993000	0.642395000
1	5.152947000	-0.055120000	0.600692000
6	4.231565000	3.677451000	0.144922000
1	2.243362000	2.978238000	-0.289678000
6	5.532507000	3.317252000	0.479359000
1	6.879908000	1.689484000	0.902775000
1	3.970740000	4.723308000	0.015170000
1	6.291372000	4.082666000	0.612956000

6	-2.660862000	-0.556635000	1.280162000
6	-1.691824000	-0.941947000	2.209530000
6	-3.999002000	-0.893808000	1.517967000
6	-2.048225000	-1.661127000	3.348253000
1	-0.646189000	-0.699538000	2.044299000
6	-4.357181000	-1.604780000	2.657195000
1	-4.766199000	-0.589365000	0.810498000
6	-3.379926000	-1.992886000	3.573207000
1	-1.277482000	-1.959082000	4.052469000
1	-5.398903000	-1.857489000	2.831257000
1	-3.659931000	-2.551861000	4.461414000
6	-3.170909000	1.827141000	-0.279033000
6	-3.356072000	2.497107000	-1.493466000
6	-3.673521000	2.396860000	0.893780000
6	-4.051616000	3.700012000	-1.537212000
1	-2.944824000	2.087049000	-2.411903000
6	-4.366750000	3.603822000	0.848684000
1	-3.525720000	1.899429000	1.847467000
6	-4.561157000	4.254942000	-0.365439000
1	-4.190421000	4.206824000	-2.487463000
1	-4.754353000	4.035152000	1.766878000
1	-5.101981000	5.196064000	-0.399258000
14	-1.412562000	-2.111951000	-1.756082000
14	1.505800000	-1.851748000	-2.258365000
6	-1.692978000	-3.528137000	-0.540349000
1	-2.683408000	-3.983615000	-0.659530000
1	-0.942646000	-4.313171000	-0.697784000
1	-1.600845000	-3.181029000	0.494678000
6	-1.634605000	-2.791914000	-3.509572000
1	-0.899559000	-3.556198000	-3.782905000
1	-2.628314000	-3.248193000	-3.601668000
1	-1.569487000	-1.986645000	-4.250539000
6	1.732151000	-3.732317000	-2.209324000
1	1.814569000	-4.098611000	-1.178832000
1	0.908308000	-4.274371000	-2.685579000
1	2.654651000	-4.012390000	-2.732859000
6	1.609314000	-1.269394000	-4.049456000
1	2.579966000	-1.514703000	-4.497888000
1	0.829532000	-1.722544000	-4.671065000
1	1.478113000	-0.181499000	-4.094378000
1	-3.783136000	-1.202134000	-1.359680000
1	-2.813968000	-0.241571000	-2.504287000

I_H₂

Coordinates (Angstroms)			
	X	Y	Z

25	0.008007000	-0.123549000	-0.124302000
7	0.035464000	1.950650000	0.392711000
6	0.022164000	-1.858770000	-0.518112000
8	0.039623000	-2.982619000	-0.807005000
6	-2.539643000	1.329663000	1.448902000
1	-3.593247000	1.558779000	1.632996000
1	-2.052877000	1.161009000	2.417558000
6	2.730014000	1.781361000	-0.646352000
6	-0.241899000	0.424082000	-1.802550000
8	-0.374842000	0.860559000	-2.863591000
15	2.290227000	0.042938000	-0.331679000
15	-2.240005000	-0.158708000	0.448839000
6	-2.816872000	-1.594238000	1.446810000
6	-2.914865000	-2.852068000	0.839858000
6	-3.116067000	-1.480138000	2.806128000
6	-3.300803000	-3.966364000	1.575566000
1	-2.693322000	-2.967165000	-0.217020000
6	-3.498867000	-2.597960000	3.544812000
1	-3.061991000	-0.515602000	3.300522000
6	-3.591389000	-3.843070000	2.932597000
1	-3.373858000	-4.933385000	1.087170000
1	-3.727809000	-2.489585000	4.600986000
1	-3.890575000	-4.714168000	3.507982000
6	-3.470088000	-0.135253000	-0.909275000
6	-4.704926000	0.509813000	-0.792463000
6	-3.182214000	-0.827842000	-2.089436000
6	-5.623425000	0.474428000	-1.836281000
1	-4.958316000	1.048731000	0.114555000
6	-4.104982000	-0.873580000	-3.130124000
1	-2.227773000	-1.333852000	-2.200232000
6	-5.325804000	-0.217799000	-3.007338000
1	-6.575158000	0.986956000	-1.732828000
1	-3.863401000	-1.413536000	-4.040629000
1	-6.044101000	-0.243958000	-3.821269000
6	3.169170000	-0.456361000	1.197282000
6	2.987021000	-1.772696000	1.642408000
6	3.985139000	0.398226000	1.939261000
6	3.604693000	-2.220692000	2.802638000
1	2.358766000	-2.452361000	1.071562000
6	4.598662000	-0.049025000	3.109431000
1	4.143455000	1.422152000	1.618447000
6	4.410347000	-1.356117000	3.543244000

1	3.454996000	-3.244558000	3.132012000
1	5.224940000	0.630080000	3.680357000
1	4.888725000	-1.703474000	4.454089000
6	3.204205000	-0.916033000	-1.602953000
6	2.539195000	-1.418328000	-2.723548000
6	4.586328000	-1.109967000	-1.491697000
6	3.240785000	-2.097422000	-3.717111000
1	1.468095000	-1.283652000	-2.826811000
6	5.286125000	-1.789813000	-2.481600000
1	5.115749000	-0.734829000	-0.620024000
6	4.613664000	-2.285202000	-3.597228000
1	2.710125000	-2.484577000	-4.581674000
1	6.357285000	-1.937168000	-2.380129000
1	5.159843000	-2.819230000	-4.369318000
14	1.466606000	2.878779000	0.274614000
14	-1.483396000	2.696661000	0.642644000
6	2.170598000	3.400240000	1.952388000
1	3.169505000	3.846627000	1.862790000
1	1.516140000	4.151390000	2.410805000
1	2.232387000	2.553158000	2.644693000
6	1.306420000	4.448969000	-0.771533000
1	0.616261000	5.175947000	-0.327079000
1	2.276550000	4.947857000	-0.888777000
1	0.928420000	4.203850000	-1.771362000
6	-1.464390000	4.137011000	1.871021000
1	-1.024995000	3.831177000	2.827690000
1	-0.887145000	4.991238000	1.498593000
1	-2.483596000	4.493733000	2.064209000
6	-2.348653000	3.292955000	-0.926151000
1	-3.376969000	3.618380000	-0.724191000
1	-1.805950000	4.142599000	-1.357602000
1	-2.389842000	2.507645000	-1.688379000
1	3.788870000	1.999436000	-0.471110000
1	2.542736000	1.930041000	-1.718012000
1	0.215128000	-0.737543000	1.609835000
1	0.320146000	0.030848000	1.672390000

TSH

Coordinates (Angstroms)			
	X	Y	Z

25	0.016815000	-0.150240000	0.146481000
7	-0.077228000	1.976691000	-0.441095000
6	0.017244000	-1.920303000	0.263124000

8	0.016698000	-3.078176000	0.327910000
6	2.560602000	1.403354000	-1.369536000
1	3.623905000	1.641378000	-1.472788000
1	2.174725000	1.204613000	-2.378092000
6	-2.675072000	1.685380000	0.830109000
6	0.337288000	0.147457000	1.880122000
8	0.543274000	0.412206000	2.987269000
15	-2.250105000	-0.035645000	0.389653000
15	2.236616000	-0.134985000	-0.431652000
6	2.857897000	-1.465661000	-1.537093000
6	4.193101000	-1.881701000	-1.517611000
6	1.982808000	-2.037084000	-2.466345000
6	4.643261000	-2.848676000	-2.411399000
1	4.885498000	-1.454744000	-0.797843000
6	2.435841000	-2.999567000	-3.363677000
1	0.941732000	-1.728353000	-2.484768000
6	3.766139000	-3.408330000	-3.336924000
1	5.681695000	-3.165790000	-2.382897000
1	1.744652000	-3.435438000	-4.079077000
1	4.118086000	-4.163910000	-4.033214000
6	3.439959000	-0.177622000	0.946466000
6	4.442624000	0.775332000	1.131427000
6	3.331275000	-1.230712000	1.863742000
6	5.316509000	0.683058000	2.212995000
1	4.544490000	1.605131000	0.440413000
6	4.208855000	-1.329390000	2.936099000
1	2.552327000	-1.978296000	1.735413000
6	5.202845000	-0.368752000	3.115328000
1	6.085728000	1.437743000	2.347810000
1	4.111330000	-2.151029000	3.639181000
1	5.884400000	-0.439714000	3.957769000
6	-3.189601000	-0.404088000	-1.143523000
6	-2.907430000	-1.602604000	-1.811065000
6	-4.171880000	0.439320000	-1.665670000
6	-3.594088000	-1.947198000	-2.968831000
1	-2.143366000	-2.269837000	-1.422059000
6	-4.852693000	0.100646000	-2.834186000
1	-4.407554000	1.377267000	-1.174345000
6	-4.566625000	-1.092841000	-3.486814000
1	-3.366278000	-2.882384000	-3.471701000
1	-5.605875000	0.774900000	-3.231228000
1	-5.096176000	-1.357771000	-4.397197000
6	-3.141372000	-1.065709000	1.620409000
6	-2.438835000	-1.739345000	2.621451000

6	-4.538287000	-1.157032000	1.593246000
6	-3.118718000	-2.484139000	3.583015000
1	-1.356009000	-1.687636000	2.653537000
6	-5.216377000	-1.900891000	2.551157000
1	-5.098308000	-0.652632000	0.810188000
6	-4.506537000	-2.566275000	3.549515000
1	-2.559006000	-3.004053000	4.354709000
1	-6.299864000	-1.967519000	2.515831000
1	-5.036464000	-3.150680000	4.295993000
14	-1.541354000	2.852869000	-0.157489000
14	1.454420000	2.756716000	-0.627485000
6	-2.359318000	3.383687000	-1.772162000
1	-3.348260000	3.831013000	-1.611749000
1	-1.734368000	4.132922000	-2.273269000
1	-2.474633000	2.538037000	-2.458867000
6	-1.304838000	4.390051000	0.913722000
1	-0.656799000	5.136236000	0.439820000
1	-2.271951000	4.871142000	1.105091000
1	-0.862509000	4.127762000	1.881483000
6	1.409092000	4.199094000	-1.846243000
1	1.019468000	3.873216000	-2.817657000
1	0.770699000	5.016162000	-1.490006000
1	2.411623000	4.614526000	-2.004743000
6	2.180560000	3.367590000	1.001024000
1	3.206182000	3.735202000	0.871363000
1	1.583702000	4.194369000	1.402027000
1	2.198787000	2.573690000	1.755305000
1	-3.746892000	1.905036000	0.779400000
1	-2.375080000	1.784101000	1.881781000
1	-0.235005000	0.818295000	-1.294131000
1	-0.270145000	-0.113051000	-1.558899000

II

Coordinates (Angstroms)

	X	Y	Z
25	0.027514000	-0.119357000	0.404511000
7	-0.165248000	1.867078000	-0.745452000
6	0.043258000	-1.777210000	1.025714000
8	0.043008000	-2.876052000	1.394326000
6	2.323444000	0.889881000	-1.734862000
1	3.364266000	1.043609000	-2.034594000
1	1.773368000	0.512426000	-2.604787000
6	-2.656019000	1.765717000	0.812111000

6	0.227391000	0.657719000	1.988556000
8	0.336965000	1.167286000	3.035068000
15	-2.220762000	0.020779000	0.406436000
15	2.121995000	-0.339780000	-0.370105000
6	2.536342000	-1.958990000	-1.146711000
6	3.484997000	-2.825940000	-0.599476000
6	1.833437000	-2.366064000	-2.286139000
6	3.733656000	-4.065876000	-1.185796000
1	4.034563000	-2.540881000	0.292137000
6	2.091243000	-3.595588000	-2.879272000
1	1.058934000	-1.724511000	-2.696477000
6	3.043562000	-4.451548000	-2.329304000
1	4.470015000	-4.730191000	-0.742880000
1	1.540398000	-3.891531000	-3.767595000
1	3.239297000	-5.416755000	-2.787170000
6	3.634358000	-0.019235000	0.636666000
6	4.897503000	0.137404000	0.051055000
6	3.524990000	0.073659000	2.024401000
6	6.014667000	0.411364000	0.831597000
1	5.016512000	0.024539000	-1.023336000
6	4.643357000	0.345717000	2.810731000
1	2.556749000	-0.057434000	2.493504000
6	5.887347000	0.523051000	2.215795000
1	6.986123000	0.534462000	0.361582000
1	4.535699000	0.424312000	3.888391000
1	6.758723000	0.742463000	2.826053000
6	-3.073913000	-0.292676000	-1.195231000
6	-2.702066000	-1.430042000	-1.923740000
6	-4.085218000	0.525526000	-1.706305000
6	-3.326793000	-1.737921000	-3.126895000
1	-1.906234000	-2.064305000	-1.545398000
6	-4.697593000	0.230316000	-2.923611000
1	-4.409546000	1.406030000	-1.161795000
6	-4.320998000	-0.903223000	-3.635289000
1	-3.029861000	-2.627844000	-3.674185000
1	-5.472192000	0.886864000	-3.309235000
1	-4.799126000	-1.136737000	-4.582087000
6	-3.232904000	-0.950527000	1.592232000
6	-2.718422000	-1.149021000	2.878327000
6	-4.491694000	-1.470547000	1.278176000
6	-3.452817000	-1.842607000	3.834145000
1	-1.736391000	-0.762067000	3.132480000
6	-5.222076000	-2.172340000	2.233662000
1	-4.905285000	-1.334917000	0.283392000

6	-4.705602000	-2.358262000	3.512794000
1	-3.038306000	-1.990144000	4.826910000
1	-6.196073000	-2.577796000	1.975413000
1	-5.275512000	-2.909162000	4.255358000
14	-1.480658000	2.904260000	-0.135988000
14	1.474515000	2.453446000	-1.121745000
6	-2.350062000	3.711523000	-1.596457000
1	-3.222568000	4.288511000	-1.267336000
1	-1.676673000	4.395967000	-2.124971000
1	-2.698842000	2.961878000	-2.315967000
6	-0.796996000	4.204453000	1.027653000
1	-0.178990000	4.947474000	0.512237000
1	-1.631816000	4.737823000	1.497996000
1	-0.201657000	3.748408000	1.825336000
6	1.414969000	3.758798000	-2.478551000
1	0.892441000	3.389443000	-3.368518000
1	0.897976000	4.663671000	-2.136718000
1	2.426443000	4.053565000	-2.782229000
6	2.333422000	3.140541000	0.396656000
1	3.418539000	3.044598000	0.272265000
1	2.104813000	4.198745000	0.556352000
1	2.061722000	2.587614000	1.300088000
1	-3.717274000	2.007283000	0.692530000
1	-2.422706000	1.863348000	1.879676000
1	-0.505068000	1.361969000	-1.566475000
1	-0.124463000	-0.747407000	-1.062209000

A1

Coordinates (Angstroms)			
	X	Y	Z

25	-0.066777000	-0.263766000	0.437408000
7	0.114253000	-0.923771000	-1.754600000
6	-0.081301000	0.494953000	2.031879000
8	-0.076493000	1.032158000	3.061292000
6	-2.410271000	0.408918000	-1.801054000
1	-3.450034000	0.512458000	-2.126736000
1	-1.875056000	1.301592000	-2.146787000
6	2.585891000	-1.992258000	-0.560572000
6	-0.398315000	-1.914674000	1.017348000
8	-0.611449000	-2.997175000	1.393672000
15	2.174126000	-0.502071000	0.437372000
15	-2.184297000	0.382700000	0.027723000
6	-2.754102000	2.059317000	0.542766000

6	-4.114355000	2.358807000	0.683588000
6	-1.816499000	3.074840000	0.749451000
6	-4.525385000	3.646294000	1.013098000
1	-4.861196000	1.582603000	0.546554000
6	-2.228932000	4.364301000	1.074726000
1	-0.760843000	2.850417000	0.648954000
6	-3.583044000	4.653436000	1.207493000
1	-5.584539000	3.860621000	1.123427000
1	-1.485312000	5.140672000	1.228780000
1	-3.904655000	5.658394000	1.465908000
6	-3.556872000	-0.674190000	0.651842000
6	-4.698679000	-1.011406000	-0.080757000
6	-3.436160000	-1.160478000	1.958477000
6	-5.686759000	-1.823264000	0.471217000
1	-4.830092000	-0.645614000	-1.094477000
6	-4.425089000	-1.963389000	2.515728000
1	-2.553333000	-0.912651000	2.540910000
6	-5.551761000	-2.302059000	1.770669000
1	-6.563191000	-2.080904000	-0.116672000
1	-4.308738000	-2.334321000	3.529589000
1	-6.319887000	-2.938627000	2.199835000
6	3.152867000	0.853288000	-0.325494000
6	2.941165000	2.147675000	0.166661000
6	4.086422000	0.670324000	-1.347242000
6	3.646343000	3.227876000	-0.349705000
1	2.201106000	2.306239000	0.946156000
6	4.779261000	1.756555000	-1.882430000
1	4.281581000	-0.320204000	-1.744614000
6	4.562990000	3.035930000	-1.383654000
1	3.467578000	4.223858000	0.043679000
1	5.492447000	1.596653000	-2.685873000
1	5.103335000	3.882299000	-1.797190000
6	3.099669000	-0.793961000	1.999455000
6	2.442337000	-1.422104000	3.061591000
6	4.448867000	-0.453690000	2.144366000
6	3.120218000	-1.707522000	4.243057000
1	1.393803000	-1.684480000	2.966722000
6	5.124469000	-0.734881000	3.327593000
1	4.974841000	0.040985000	1.332847000
6	4.461481000	-1.362419000	4.379431000
1	2.594940000	-2.191459000	5.061062000
1	6.170653000	-0.461139000	3.429508000
1	4.987765000	-1.576482000	5.305116000
14	1.449821000	-2.060875000	-2.069840000

14	-1.505226000	-1.099183000	-2.474846000
6	2.343723000	-1.509016000	-3.630526000
1	3.278653000	-2.063279000	-3.775326000
1	1.718342000	-1.670815000	-4.515798000
1	2.586876000	-0.441461000	-3.586535000
6	0.815003000	-3.815859000	-2.249175000
1	0.235617000	-3.966789000	-3.166160000
1	1.670222000	-4.501622000	-2.283407000
1	0.194917000	-4.101483000	-1.392656000
6	-1.392983000	-1.016726000	-4.352642000
1	-0.836666000	-0.128250000	-4.672859000
1	-0.882685000	-1.897903000	-4.760112000
1	-2.388791000	-0.973595000	-4.809035000
6	-2.342006000	-2.690946000	-1.944982000
1	-3.418769000	-2.612598000	-2.134062000
1	-1.970591000	-3.555570000	-2.502359000
1	-2.213935000	-2.887308000	-0.876357000
1	3.652900000	-2.100305000	-0.783823000
1	2.309449000	-2.831641000	0.090425000
1	0.445025000	0.009191000	-2.013992000
1	0.192138000	1.200485000	-0.180257000
6	0.770955000	2.856093000	-2.139354000
8	0.615107000	3.812378000	-1.497477000
8	0.920226000	1.933310000	-2.841897000

TSA1

Coordinates (Angstroms)

	X	Y	Z
25	-0.037787000	0.007418000	0.355106000
7	0.084259000	-1.535045000	-1.303566000
6	-0.034191000	1.369275000	1.484768000
8	-0.016625000	2.274791000	2.209518000
6	-2.540369000	-0.517714000	-1.781182000
1	-3.599825000	-0.633721000	-2.030288000
1	-2.100817000	0.143819000	-2.538157000
6	2.617540000	-1.994459000	0.134208000
6	-0.339739000	-1.228848000	1.598789000
8	-0.528686000	-2.051559000	2.398453000
15	2.222166000	-0.238281000	0.498993000
15	-2.234856000	0.315576000	-0.172303000
6	-2.923220000	2.000482000	-0.427612000
6	-4.301011000	2.185087000	-0.599188000
6	-2.077257000	3.108430000	-0.490676000

6	-4.819454000	3.451986000	-0.835827000
1	-4.976149000	1.335814000	-0.535693000
6	-2.598410000	4.379126000	-0.727362000
1	-1.008816000	2.980836000	-0.371424000
6	-3.966533000	4.553426000	-0.900151000
1	-5.889654000	3.582531000	-0.966905000
1	-1.925919000	5.230037000	-0.777181000
1	-4.372512000	5.544314000	-1.082194000
6	-3.474432000	-0.390435000	0.987853000
6	-4.562519000	-1.175789000	0.600180000
6	-3.314503000	-0.094064000	2.346813000
6	-5.464158000	-1.661450000	1.544818000
1	-4.718888000	-1.421804000	-0.445325000
6	-4.217364000	-0.570117000	3.289860000
1	-2.473647000	0.513603000	2.670238000
6	-5.293749000	-1.359671000	2.891618000
1	-6.300247000	-2.276295000	1.224349000
1	-4.074433000	-0.331452000	4.339391000
1	-5.995822000	-1.737706000	3.628789000
6	3.250134000	0.741785000	-0.658204000
6	3.097860000	2.132719000	-0.617768000
6	4.175331000	0.191271000	-1.547751000
6	3.855160000	2.952066000	-1.444905000
1	2.365188000	2.573081000	0.052693000
6	4.926359000	1.012279000	-2.387461000
1	4.320724000	-0.882784000	-1.599391000
6	4.769405000	2.393134000	-2.335755000
1	3.715895000	4.027784000	-1.406539000
1	5.634729000	0.568602000	-3.080962000
1	5.354433000	3.032862000	-2.989664000
6	3.099832000	0.051270000	2.090480000
6	2.395066000	-0.010803000	3.295409000
6	4.480288000	0.282240000	2.126282000
6	3.054915000	0.151093000	4.510832000
1	1.324575000	-0.181965000	3.291769000
6	5.138523000	0.445676000	3.340090000
1	5.043271000	0.345408000	1.199393000
6	4.426623000	0.380720000	4.535867000
1	2.491790000	0.104484000	5.438096000
1	6.209100000	0.628508000	3.352068000
1	4.939608000	0.513941000	5.483825000
14	1.498282000	-2.621640000	-1.252787000
14	-1.532695000	-2.109584000	-1.789441000
6	2.336445000	-2.540776000	-2.932176000

1	3.303525000	-3.057244000	-2.929075000
1	1.707488000	-3.012886000	-3.695870000
1	2.503993000	-1.502122000	-3.237682000
6	1.017589000	-4.387566000	-0.835509000
1	0.398454000	-4.856836000	-1.607530000
1	1.931515000	-4.986095000	-0.737904000
1	0.483468000	-4.441636000	0.119208000
6	-1.467432000	-2.822147000	-3.529712000
1	-1.022555000	-2.101844000	-4.225887000
1	-0.870425000	-3.741412000	-3.567599000
1	-2.471520000	-3.067189000	-3.895369000
6	-2.225586000	-3.378920000	-0.595584000
1	-3.299423000	-3.499999000	-0.779634000
1	-1.759548000	-4.359004000	-0.731793000
1	-2.104446000	-3.083339000	0.450536000
1	3.685826000	-2.180371000	-0.021414000
1	2.330767000	-2.532096000	1.047300000
1	0.319551000	-0.806581000	-1.991657000
1	0.201670000	1.088014000	-0.886207000
6	0.513233000	1.683966000	-2.452589000
8	0.553919000	2.850170000	-2.279644000
8	0.556370000	0.691435000	-3.115689000

A2

Coordinates (Angstroms)

	X	Y	Z
25	0.033926000	-0.171124000	0.226407000
7	-0.115429000	1.928587000	-0.471192000
6	0.076067000	-1.923514000	0.553486000
8	0.100473000	-3.059361000	0.766588000
6	2.540308000	1.339459000	-1.378710000
1	3.593334000	1.589809000	-1.543152000
1	2.103186000	1.094231000	-2.355888000
6	-2.608327000	1.662412000	1.075289000
6	0.358342000	0.297329000	1.906357000
8	0.550451000	0.660393000	2.990234000
15	-2.242787000	-0.059306000	0.570399000
15	2.280682000	-0.154133000	-0.352411000
6	3.024239000	-1.537426000	-1.300326000
6	4.410228000	-1.741276000	-1.301134000
6	2.209827000	-2.380146000	-2.060888000
6	4.969814000	-2.768652000	-2.050959000
1	5.056129000	-1.103681000	-0.704289000
6	2.775887000	-3.405537000	-2.815350000

1	1.135767000	-2.235927000	-2.100693000
6	4.151965000	-3.603852000	-2.810179000
1	6.045329000	-2.919826000	-2.039916000
1	2.130539000	-4.045683000	-3.408651000
1	4.589682000	-4.407967000	-3.394659000
6	3.441645000	-0.027149000	1.060728000
6	4.458003000	0.924696000	1.159469000
6	3.310646000	-0.979470000	2.078905000
6	5.314435000	0.936670000	2.258879000
1	4.592382000	1.668334000	0.380767000
6	4.169520000	-0.974867000	3.170558000
1	2.530466000	-1.733468000	2.015725000
6	5.171978000	-0.011857000	3.265759000
1	6.094855000	1.689019000	2.323461000
1	4.053425000	-1.721463000	3.950215000
1	5.840648000	-0.002798000	4.121285000
6	-3.295655000	-0.398384000	-0.883615000
6	-3.104720000	-1.619560000	-1.538640000
6	-4.278207000	0.477421000	-1.352752000
6	-3.880044000	-1.957608000	-2.640399000
1	-2.326336000	-2.299420000	-1.204987000
6	-5.050488000	0.140796000	-2.461433000
1	-4.444857000	1.432782000	-0.866377000
6	-4.853105000	-1.076958000	-3.104898000
1	-3.703993000	-2.899066000	-3.149844000
1	-5.802719000	0.835351000	-2.823322000
1	-5.449509000	-1.335405000	-3.974778000
6	-3.044815000	-1.076519000	1.872537000
6	-2.289978000	-1.595067000	2.927683000
6	-4.426512000	-1.300936000	1.854185000
6	-2.903340000	-2.316134000	3.948926000
1	-1.217196000	-1.442222000	2.959096000
6	-5.038073000	-2.022544000	2.873128000
1	-5.026722000	-0.919097000	1.033243000
6	-4.277320000	-2.531019000	3.923769000
1	-2.302078000	-2.714631000	4.760477000
1	-6.110294000	-2.192370000	2.843516000
1	-4.755142000	-3.097100000	4.717912000
14	-1.553416000	2.852296000	0.049430000
14	1.468470000	2.723834000	-0.669563000
6	-2.435088000	3.438485000	-1.498163000
1	-3.430452000	3.840864000	-1.276668000
1	-1.854747000	4.231203000	-1.984507000
1	-2.538069000	2.620152000	-2.219066000

6	-1.127444000	4.303412000	1.164200000
1	-0.527318000	5.067728000	0.658980000
1	-2.060023000	4.781085000	1.488779000
1	-0.591591000	3.980419000	2.063204000
6	1.329570000	4.108383000	-1.932158000
1	0.883305000	3.724631000	-2.856713000
1	0.702160000	4.931076000	-1.569112000
1	2.312732000	4.527084000	-2.176182000
6	2.144682000	3.367451000	0.958417000
1	3.205345000	3.617439000	0.840274000
1	1.630326000	4.278201000	1.278018000
1	2.069032000	2.629223000	1.762688000
1	-3.678300000	1.896570000	1.087039000
1	-2.256851000	1.730122000	2.113114000
1	-0.345165000	1.633327000	-1.455214000
1	-0.269046000	-0.505296000	-1.507531000
6	-0.489283000	-0.312996000	-2.694601000
8	-0.570770000	-1.361076000	-3.303407000
8	-0.558414000	0.895079000	-2.966471000

TSA2

Coordinates (Angstroms)			
	X	Y	Z

25	0.023327000	-0.159244000	0.264854000
7	-0.110050000	1.895713000	-0.327239000
6	0.050399000	-1.927098000	0.500808000
8	0.065524000	-3.071936000	0.670977000
6	2.565175000	1.408828000	-1.247306000
1	3.621734000	1.676954000	-1.346307000
1	2.178768000	1.230619000	-2.259192000
6	-2.652965000	1.632691000	1.116281000
6	0.357281000	0.187703000	1.966741000
8	0.554262000	0.485875000	3.067442000
15	-2.255565000	-0.066594000	0.590994000
15	2.274985000	-0.145012000	-0.331607000
6	2.974847000	-1.473548000	-1.386514000
6	4.360738000	-1.660681000	-1.466412000
6	2.135676000	-2.275444000	-2.163384000
6	4.893325000	-2.627265000	-2.310687000
1	5.026186000	-1.054002000	-0.858397000
6	2.671765000	-3.240593000	-3.012683000
1	1.059935000	-2.148250000	-2.132902000
6	4.048608000	-3.419279000	-3.086797000

1	5.969391000	-2.764623000	-2.362832000
1	2.005931000	-3.848880000	-3.616609000
1	4.465175000	-4.173627000	-3.747827000
6	3.434442000	-0.153167000	1.086706000
6	4.441705000	0.795715000	1.267706000
6	3.305939000	-1.187865000	2.021740000
6	5.296146000	0.721780000	2.365768000
1	4.565804000	1.606167000	0.557798000
6	4.162301000	-1.266549000	3.112862000
1	2.530119000	-1.938559000	1.894971000
6	5.158038000	-0.307786000	3.290056000
1	6.069549000	1.472925000	2.495778000
1	4.047983000	-2.073387000	3.830324000
1	5.823374000	-0.364167000	4.146350000
6	-3.221942000	-0.380601000	-0.929132000
6	-3.027728000	-1.606539000	-1.576876000
6	-4.128451000	0.534250000	-1.468391000
6	-3.721427000	-1.907683000	-2.741415000
1	-2.315671000	-2.324195000	-1.177011000
6	-4.818419000	0.234737000	-2.640916000
1	-4.297105000	1.491417000	-0.987015000
6	-4.615729000	-0.984480000	-3.278340000
1	-3.547338000	-2.854953000	-3.241084000
1	-5.511836000	0.960118000	-3.055786000
1	-5.146082000	-1.212776000	-4.197760000
6	-3.093583000	-1.151008000	1.809446000
6	-2.371181000	-1.735910000	2.852199000
6	-4.475292000	-1.364643000	1.737219000
6	-3.017281000	-2.515371000	3.808716000
1	-1.299045000	-1.588942000	2.923662000
6	-5.119087000	-2.143990000	2.691108000
1	-5.048655000	-0.928117000	0.924163000
6	-4.390654000	-2.721354000	3.729297000
1	-2.442712000	-2.966270000	4.612085000
1	-6.190583000	-2.305686000	2.620257000
1	-4.893718000	-3.334056000	4.471518000
14	-1.503848000	2.831061000	0.187354000
14	1.434818000	2.717016000	-0.463315000
6	-2.373059000	3.585000000	-1.303760000
1	-3.335659000	4.031323000	-1.025468000
1	-1.752593000	4.379808000	-1.734498000
1	-2.544536000	2.845011000	-2.091911000
6	-1.130310000	4.219607000	1.407578000
1	-0.504572000	5.008296000	0.974986000

1	-2.073948000	4.685626000	1.717810000
1	-0.632081000	3.843116000	2.307831000
6	1.328378000	4.185288000	-1.639896000
1	0.901159000	3.875231000	-2.600308000
1	0.698139000	4.986209000	-1.235122000
1	2.319588000	4.613633000	-1.829897000
6	2.168909000	3.293309000	1.173211000
1	3.213726000	3.594571000	1.029398000
1	1.632767000	4.161694000	1.567478000
1	2.151309000	2.510295000	1.937797000
1	-3.721022000	1.869278000	1.063090000
1	-2.367468000	1.673790000	2.175660000
1	-0.380148000	1.592269000	-1.667888000
1	-0.315368000	-0.471134000	-1.640969000
6	-0.464681000	-0.056005000	-2.698349000
8	-0.521087000	-0.855452000	-3.599515000
8	-0.534890000	1.229399000	-2.728867000

A3

Coordinates (Angstroms)

	X	Y	Z
25	-0.011062000	-0.375544000	-0.164306000
7	-0.104622000	-0.210424000	1.896786000
6	-0.033875000	-0.160144000	-1.932813000
8	-0.051110000	-0.049355000	-3.086990000
6	2.582361000	0.776486000	1.629994000
1	3.646060000	0.770880000	1.887544000
1	2.230845000	1.812296000	1.718573000
6	-2.800221000	-1.306336000	1.460769000
6	0.332448000	-2.099031000	-0.309859000
8	0.543933000	-3.236913000	-0.321400000
15	-2.287926000	-0.597568000	-0.135057000
15	2.228156000	0.272610000	-0.087715000
6	2.841924000	1.651304000	-1.132428000
6	4.218935000	1.860674000	-1.280169000
6	1.952680000	2.542597000	-1.736042000
6	4.692258000	2.943141000	-2.011020000
1	4.923689000	1.166567000	-0.829878000
6	2.427473000	3.631988000	-2.462630000
1	0.881864000	2.400284000	-1.645924000
6	3.795861000	3.833414000	-2.600989000
1	5.761980000	3.093412000	-2.122229000
1	1.721551000	4.321555000	-2.914357000

1	4.166830000	4.681821000	-3.168351000
6	3.402898000	-1.064763000	-0.514960000
6	4.410393000	-1.517837000	0.337570000
6	3.271120000	-1.651876000	-1.779830000
6	5.266051000	-2.543062000	-0.061754000
1	4.531891000	-1.084539000	1.324440000
6	4.128358000	-2.668605000	-2.180395000
1	2.493604000	-1.309325000	-2.457622000
6	5.127166000	-3.119603000	-1.319201000
1	6.040165000	-2.889875000	0.616197000
1	4.012298000	-3.114637000	-3.163420000
1	5.794235000	-3.918380000	-1.629042000
6	-3.026120000	1.072039000	-0.232354000
6	-2.886231000	1.777784000	-1.436068000
6	-3.630657000	1.702933000	0.855392000
6	-3.330037000	3.088907000	-1.539537000
1	-2.424425000	1.299912000	-2.296163000
6	-4.067215000	3.022766000	0.751877000
1	-3.754341000	1.179595000	1.797087000
6	-3.913329000	3.718194000	-0.441138000
1	-3.206272000	3.626098000	-2.474538000
1	-4.518814000	3.506427000	1.612415000
1	-4.238970000	4.750811000	-0.516040000
6	-3.209735000	-1.517406000	-1.420815000
6	-2.561920000	-2.476384000	-2.202128000
6	-4.580313000	-1.298744000	-1.604774000
6	-3.272920000	-3.210251000	-3.148910000
1	-1.499075000	-2.652841000	-2.077654000
6	-5.288381000	-2.029595000	-2.551283000
1	-5.091054000	-0.543921000	-1.012617000
6	-4.634572000	-2.987796000	-3.324593000
1	-2.757428000	-3.951098000	-3.752450000
1	-6.350296000	-1.849830000	-2.689615000
1	-5.187658000	-3.556695000	-4.066115000
14	-1.494212000	-0.818775000	2.763255000
14	1.439646000	-0.285737000	2.712702000
6	-2.209315000	0.460304000	3.955833000
1	-3.215801000	0.170717000	4.283144000
1	-1.584445000	0.535722000	4.853079000
1	-2.262970000	1.461432000	3.516153000
6	-1.181627000	-2.391089000	3.761829000
1	-0.492882000	-2.228978000	4.598629000
1	-2.127650000	-2.753531000	4.183468000
1	-0.767685000	-3.187072000	3.132039000

6	1.383726000	0.487383000	4.433330000
1	0.936589000	1.487431000	4.397731000
1	0.798095000	-0.118402000	5.135014000
1	2.393520000	0.583778000	4.849959000
6	2.167867000	-2.018896000	2.860199000
1	3.189656000	-1.970618000	3.257411000
1	1.580985000	-2.639701000	3.544075000
1	2.207152000	-2.533457000	1.894769000
1	-3.839581000	-1.079941000	1.722343000
1	-2.727701000	-2.393282000	1.326979000
1	-0.358990000	2.029641000	0.030035000
6	-0.435037000	2.896118000	0.729024000
8	-0.500400000	4.026014000	0.325185000
8	-0.432736000	2.528749000	1.996918000
1	-0.353192000	1.521209000	2.020807000

B1

Coordinates (Angstroms)			
	X	Y	Z

25	0.011633000	-0.211460000	0.519286000
7	0.106034000	-1.349794000	-1.452440000
6	0.079686000	0.903833000	1.881589000
8	0.176448000	1.674077000	2.747981000
6	-2.470737000	-0.198061000	-1.693731000
1	-3.533477000	-0.251913000	-1.949230000
1	-1.991951000	0.546605000	-2.340535000
6	2.789600000	-1.879545000	-0.369364000
6	-0.109306000	-1.698876000	1.487473000
8	-0.152519000	-2.670661000	2.132711000
15	2.258288000	-0.302406000	0.417355000
15	-2.156990000	0.271955000	0.054719000
6	-2.691882000	2.030454000	0.176259000
6	-3.127560000	2.769724000	-0.926606000
6	-2.663778000	2.650758000	1.430395000
6	-3.494860000	4.107986000	-0.785486000
1	-3.183763000	2.308553000	-1.906848000
6	-3.033724000	3.983261000	1.572524000
1	-2.349195000	2.091606000	2.305716000
6	-3.443116000	4.719694000	0.462735000
1	-3.829666000	4.666787000	-1.655052000
1	-2.998286000	4.448242000	2.553168000
1	-3.727200000	5.762054000	0.573767000
6	-3.578969000	-0.517367000	0.930099000
6	-4.892278000	-0.348848000	0.473696000

6	-3.361704000	-1.271037000	2.083038000
6	-5.957005000	-0.947538000	1.135860000
1	-5.089047000	0.269391000	-0.398771000
6	-4.428371000	-1.868521000	2.753385000
1	-2.353217000	-1.398769000	2.458555000
6	-5.725333000	-1.714103000	2.277546000
1	-6.969268000	-0.811152000	0.766196000
1	-4.239809000	-2.455323000	3.647536000
1	-6.557088000	-2.182957000	2.795397000
6	3.058936000	1.024851000	-0.564375000
6	3.670925000	0.822036000	-1.800038000
6	2.973167000	2.330228000	-0.058038000
6	4.182780000	1.900695000	-2.524614000
1	3.745337000	-0.174901000	-2.222032000
6	3.496459000	3.401455000	-0.769787000
1	2.482677000	2.503508000	0.896429000
6	4.099787000	3.189345000	-2.011725000
1	4.643807000	1.726677000	-3.492150000
1	3.428188000	4.404934000	-0.359808000
1	4.501180000	4.027780000	-2.573093000
6	3.294533000	-0.271985000	1.937744000
6	2.728008000	-0.581507000	3.176028000
6	4.667313000	-0.004508000	1.868534000
6	3.516682000	-0.620331000	4.323940000
1	1.666499000	-0.790050000	3.249933000
6	5.454229000	-0.043513000	3.013784000
1	5.123110000	0.242841000	0.913498000
6	4.878762000	-0.350490000	4.245524000
1	3.060081000	-0.855803000	5.280532000
1	6.517491000	0.167455000	2.945155000
1	5.492083000	-0.376126000	5.141672000
14	1.493764000	-2.450772000	-1.624828000
14	-1.539615000	-1.809629000	-1.960015000
6	2.151167000	-2.329312000	-3.381828000
1	3.136578000	-2.800056000	-3.478729000
1	1.472984000	-2.823909000	-4.086142000
1	2.231281000	-1.281459000	-3.691973000
6	0.989292000	-4.208557000	-1.208399000
1	0.294514000	-4.626654000	-1.945004000
1	1.878146000	-4.850686000	-1.191998000
1	0.518541000	-4.262378000	-0.220784000
6	-1.553296000	-2.275028000	-3.782076000
1	-1.061769000	-1.496236000	-4.376018000
1	-1.027113000	-3.221080000	-3.958028000

1	-2.577441000	-2.394625000	-4.154393000
6	-2.259531000	-3.194408000	-0.918601000
1	-3.354003000	-3.132079000	-0.954045000
1	-1.967781000	-4.182081000	-1.289004000
1	-1.965859000	-3.121058000	0.131809000
1	3.815677000	-1.845343000	-0.752046000
1	2.780637000	-2.604867000	0.454196000
1	0.335082000	-0.529149000	-2.023241000
1	0.114806000	1.108080000	-0.399377000
6	0.520729000	1.865311000	-2.752503000
1	1.314360000	2.295521000	-2.129680000
8	0.665966000	0.881688000	-3.438405000
8	-0.638165000	2.532455000	-2.740732000
1	-0.665204000	3.138984000	-1.984279000

TSB1

Coordinates (Angstroms)			
	X	Y	Z

25	-0.036668000	-0.064182000	0.323078000
7	-0.095119000	1.817644000	-0.845486000
6	-0.101428000	-1.691485000	1.013818000
8	-0.180772000	-2.765837000	1.448224000
6	2.517553000	0.942651000	-1.548465000
1	3.572850000	1.116856000	-1.778046000
1	2.030944000	0.514085000	-2.435146000
6	-2.807070000	1.862893000	0.326550000
6	0.162617000	0.798107000	1.863399000
8	0.265101000	1.400062000	2.852108000
15	-2.302664000	0.099226000	0.427335000
15	2.205801000	-0.240879000	-0.195779000
6	2.899393000	-1.850797000	-0.756774000
6	3.468293000	-2.022134000	-2.021225000
6	2.877305000	-2.936789000	0.125828000
6	3.993229000	-3.256218000	-2.398960000
1	3.488403000	-1.199540000	-2.727247000
6	3.403760000	-4.167443000	-0.250620000
1	2.450004000	-2.825143000	1.117385000
6	3.962084000	-4.331241000	-1.516165000
1	4.428155000	-3.373877000	-3.387128000
1	3.376711000	-4.998609000	0.447615000
1	4.372585000	-5.292249000	-1.811680000
6	3.428183000	0.168935000	1.117154000
6	4.655871000	0.778968000	0.843358000

6	3.141914000	-0.197292000	2.435413000
6	5.563477000	1.038958000	1.864894000
1	4.915698000	1.056045000	-0.173441000
6	4.053172000	0.051170000	3.457627000
1	2.195976000	-0.677955000	2.665974000
6	5.263287000	0.677222000	3.175767000
1	6.508976000	1.521931000	1.636122000
1	3.811236000	-0.236106000	4.476470000
1	5.972019000	0.881149000	3.972869000
6	-3.195622000	-0.755944000	-0.920180000
6	-3.682414000	-0.093029000	-2.045797000
6	-3.294842000	-2.152325000	-0.856354000
6	-4.264733000	-0.809592000	-3.089589000
1	-3.593754000	0.984279000	-2.132056000
6	-3.882107000	-2.865621000	-1.894114000
1	-2.910034000	-2.682670000	0.011121000
6	-4.367737000	-2.194043000	-3.015701000
1	-4.629082000	-0.280989000	-3.965002000
1	-3.958321000	-3.946930000	-1.828818000
1	-4.820597000	-2.750478000	-3.830859000
6	-3.231714000	-0.501077000	1.895744000
6	-2.573446000	-0.808024000	3.087631000
6	-4.627802000	-0.607964000	1.845732000
6	-3.294802000	-1.211056000	4.209996000
1	-1.493551000	-0.736480000	3.147060000
6	-5.347101000	-1.011114000	2.963837000
1	-5.152266000	-0.386219000	0.920037000
6	-4.680027000	-1.313794000	4.150065000
1	-2.768718000	-1.448461000	5.129737000
1	-6.428553000	-1.094557000	2.908991000
1	-5.241011000	-1.632123000	5.023904000
14	-1.496798000	2.882211000	-0.587568000
14	1.530210000	2.488971000	-1.119419000
6	-2.136266000	3.453878000	-2.258927000
1	-3.142256000	3.883013000	-2.183415000
1	-1.478630000	4.217405000	-2.689093000
1	-2.159838000	2.611578000	-2.959667000
6	-1.049435000	4.342703000	0.505466000
1	-0.375810000	5.046640000	0.004858000
1	-1.959863000	4.892316000	0.773394000
1	-0.571906000	4.010909000	1.434163000
6	1.523025000	3.658897000	-2.590335000
1	1.032098000	3.183769000	-3.446992000
1	0.992824000	4.592118000	-2.366258000

1	2.544913000	3.924245000	-2.885828000
6	2.229662000	3.348948000	0.395866000
1	3.314970000	3.455472000	0.280726000
1	1.809870000	4.351266000	0.525113000
1	2.054806000	2.785289000	1.316803000
1	-3.823751000	1.985127000	-0.063170000
1	-2.819055000	2.210060000	1.367500000
1	-0.316729000	1.337959000	-1.759941000
1	-0.227369000	-0.744763000	-1.229369000
6	-0.451598000	-0.751331000	-2.643328000
1	-1.282127000	-1.474353000	-2.575113000
8	-0.667878000	0.414706000	-3.054469000
8	0.719645000	-1.341871000	-3.100102000
1	0.831036000	-2.197311000	-2.661399000

B2

Coordinates (Angstroms)

	X	Y	Z
25	-0.045353000	-0.051692000	0.356243000
7	-0.097502000	1.858736000	-0.423091000
6	-0.116933000	-1.787578000	0.734835000
8	-0.197942000	-2.912553000	1.013434000
6	2.561414000	1.248288000	-1.290669000
1	3.617265000	1.502948000	-1.420099000
1	2.143339000	0.969460000	-2.267172000
6	-2.838072000	1.804694000	0.626988000
6	0.184055000	0.434761000	2.034414000
8	0.305393000	0.849993000	3.108687000
15	-2.329144000	0.061219000	0.487121000
15	2.235100000	-0.166024000	-0.201311000
6	2.921064000	-1.649161000	-1.052823000
6	3.575354000	-1.550861000	-2.284648000
6	2.802525000	-2.907624000	-0.452253000
6	4.085109000	-2.687512000	-2.908502000
1	3.677791000	-0.587346000	-2.771858000
6	3.315737000	-4.041473000	-1.073262000
1	2.309947000	-3.011901000	0.508563000
6	3.954765000	-3.935124000	-2.306114000
1	4.584465000	-2.592806000	-3.868139000
1	3.211351000	-5.009721000	-0.593102000
1	4.351746000	-4.820737000	-2.793237000
6	3.391052000	-0.039625000	1.219097000
6	4.565976000	0.715124000	1.174295000

6	3.105083000	-0.771387000	2.376326000
6	5.428282000	0.747336000	2.265999000
1	4.815370000	1.290528000	0.288853000
6	3.971593000	-0.748971000	3.463854000
1	2.192744000	-1.358305000	2.433622000
6	5.133881000	0.014915000	3.412533000
1	6.333532000	1.345401000	2.218762000
1	3.731283000	-1.319626000	4.355814000
1	5.807978000	0.041038000	4.263486000
6	-3.107065000	-0.599749000	-1.032012000
6	-3.641854000	0.220223000	-2.024637000
6	-3.089696000	-1.987041000	-1.230950000
6	-4.154813000	-0.332797000	-3.196415000
1	-3.649049000	1.297245000	-1.901384000
6	-3.605644000	-2.538150000	-2.397123000
1	-2.676018000	-2.640544000	-0.467087000
6	-4.138828000	-1.709963000	-3.384965000
1	-4.558319000	0.320281000	-3.963968000
1	-3.589649000	-3.614909000	-2.537195000
1	-4.538180000	-2.139920000	-4.298647000
6	-3.270628000	-0.818296000	1.792007000
6	-2.632170000	-1.310354000	2.931579000
6	-4.658620000	-0.965222000	1.673641000
6	-3.365883000	-1.935676000	3.937755000
1	-1.558186000	-1.211375000	3.040767000
6	-5.389911000	-1.590009000	2.676111000
1	-5.166096000	-0.598177000	0.785411000
6	-4.743308000	-2.077054000	3.811217000
1	-2.856168000	-2.316255000	4.817649000
1	-6.464781000	-1.702343000	2.570169000
1	-5.314078000	-2.568577000	4.593622000
14	-1.479492000	2.886924000	-0.160809000
14	1.448777000	2.632558000	-0.628177000
6	-2.138933000	3.657069000	-1.754575000
1	-3.126802000	4.106019000	-1.591376000
1	-1.471870000	4.452447000	-2.105413000
1	-2.216917000	2.921756000	-2.562185000
6	-1.173803000	4.293629000	1.062531000
1	-0.471838000	5.039397000	0.671474000
1	-2.114529000	4.813597000	1.282734000
1	-0.767168000	3.912273000	2.006564000
6	1.421204000	4.007766000	-1.919761000
1	0.961693000	3.658014000	-2.851229000
1	0.863577000	4.886672000	-1.575003000

1	2.441544000	4.338732000	-2.148278000
6	2.209756000	3.316341000	0.957535000
1	3.264755000	3.570832000	0.795731000
1	1.696670000	4.224147000	1.291546000
1	2.167675000	2.589159000	1.774915000
1	-3.853795000	1.985620000	0.259125000
1	-2.839366000	2.017298000	1.703616000
6	-0.382651000	-0.382721000	-2.868147000
1	-0.362617000	-0.700177000	-1.792202000
8	-0.687567000	0.943326000	-2.988973000
8	0.883185000	-0.625691000	-3.443380000
1	1.170525000	-1.516117000	-3.200014000
1	-1.160816000	-0.979464000	-3.362675000
1	-0.422806000	1.382544000	-2.139210000

B3

Coordinates (Angstroms)

	X	Y	Z
25	0.016264000	0.273298000	-0.027846000
7	-0.054456000	-1.279739000	-1.545632000
6	0.128438000	1.488027000	1.266626000
8	0.220001000	2.289630000	2.101587000
6	2.724006000	-1.601406000	-0.879476000
1	3.768182000	-1.598192000	-1.203367000
1	2.545897000	-2.511400000	-0.298779000
6	-2.769246000	-0.210097000	-1.849202000
6	0.177557000	1.455018000	-1.336598000
8	0.224956000	2.188658000	-2.232657000
15	-2.269546000	0.445394000	-0.223950000
15	2.296129000	-0.164830000	0.169318000
6	2.874797000	-0.554741000	1.869732000
6	2.691854000	-1.833115000	2.407617000
6	3.409852000	0.449952000	2.681413000
6	3.053695000	-2.101981000	3.723509000
1	2.245093000	-2.618125000	1.805177000
6	3.764982000	0.180261000	4.000271000
1	3.556867000	1.450032000	2.284081000
6	3.590858000	-1.096833000	4.524523000
1	2.911643000	-3.101104000	4.125933000
1	4.181146000	0.971839000	4.616647000
1	3.869966000	-1.307830000	5.552806000
6	3.486071000	1.143135000	-0.329540000
6	4.833063000	0.837852000	-0.561915000
6	3.079049000	2.476271000	-0.420092000

6	5.739429000	1.833173000	-0.906181000
1	5.185436000	-0.184068000	-0.456867000
6	3.986497000	3.476768000	-0.761779000
1	2.048761000	2.741807000	-0.214990000
6	5.315767000	3.156684000	-1.013071000
1	6.779369000	1.577936000	-1.086960000
1	3.648369000	4.506121000	-0.833810000
1	6.022999000	3.934365000	-1.285741000
6	-3.199427000	-0.515013000	1.030043000
6	-3.951712000	-1.651922000	0.733046000
6	-3.076320000	-0.116848000	2.369948000
6	-4.556537000	-2.386911000	1.753083000
1	-4.059665000	-1.982323000	-0.294724000
6	-3.674785000	-0.852402000	3.386929000
1	-2.517877000	0.785917000	2.613916000
6	-4.413008000	-1.995570000	3.079485000
1	-5.134430000	-3.272388000	1.505392000
1	-3.568312000	-0.532103000	4.419108000
1	-4.878555000	-2.572400000	3.872736000
6	-3.118216000	2.069537000	-0.092153000
6	-2.392412000	3.261713000	-0.073063000
6	-4.517107000	2.127333000	-0.041972000
6	-3.049799000	4.488568000	-0.006129000
1	-1.309315000	3.241375000	-0.106765000
6	-5.172960000	3.349998000	0.025356000
1	-5.095790000	1.206920000	-0.044890000
6	-4.438358000	4.535056000	0.043547000
1	-2.471625000	5.407520000	0.010282000
1	-6.257787000	3.380395000	0.067753000
1	-4.949826000	5.491394000	0.099921000
14	-1.526655000	-1.557394000	-2.394962000
14	1.466681000	-1.611036000	-2.303545000
6	-2.239048000	-3.273567000	-2.041763000
1	-3.236925000	-3.401024000	-2.480387000
1	-1.585074000	-4.037527000	-2.479338000
1	-2.303484000	-3.487001000	-0.969035000
6	-1.444237000	-1.366867000	-4.276222000
1	-0.755560000	-2.076010000	-4.748166000
1	-2.435601000	-1.528664000	-4.717936000
1	-1.119561000	-0.355487000	-4.548215000
6	1.529173000	-3.344332000	-3.060909000
1	1.241727000	-4.094776000	-2.314922000
1	0.857958000	-3.453968000	-3.920406000
1	2.542607000	-3.583547000	-3.405404000

6	2.050130000	-0.368319000	-3.597936000
1	3.001522000	-0.700427000	-4.032306000
1	1.327620000	-0.265321000	-4.414857000
1	2.209445000	0.626290000	-3.168515000
1	-3.828944000	-0.482706000	-1.906594000
1	-2.619402000	0.628405000	-2.542358000
6	-0.530459000	-2.656454000	1.404663000
1	-1.603630000	-2.737097000	1.176723000
8	0.264045000	-3.161461000	0.419182000
8	-0.219634000	-1.260755000	1.580554000
1	-0.847593000	-0.894738000	2.219999000
1	-0.309476000	-3.180573000	2.341633000
1	0.094822000	-2.582610000	-0.382706000

TSB2

----- Coordinates (Angstroms) -----			
	X	Y	Z
25	0.024106000	-0.248117000	-0.110588000
7	0.068200000	1.988773000	-0.045280000
6	-0.001016000	-2.027080000	-0.070393000
8	-0.019271000	-3.185427000	-0.045902000
6	-2.659015000	1.628363000	0.764222000
1	-3.725154000	1.869315000	0.701878000
1	-2.363125000	1.741148000	1.814171000
6	2.784869000	1.478894000	-1.096592000
6	-0.229311000	-0.171077000	-1.868096000
8	-0.365268000	-0.079182000	-3.014852000
15	2.309425000	-0.149717000	-0.411491000
15	-2.270378000	-0.103693000	0.317241000
6	-3.075076000	-1.118485000	1.619370000
6	-2.302290000	-1.854936000	2.519716000
6	-4.470505000	-1.148863000	1.730267000
6	-2.917824000	-2.607792000	3.518263000
1	-1.220539000	-1.815278000	2.450486000
6	-5.081411000	-1.897256000	2.728890000
1	-5.083585000	-0.593550000	1.024984000
6	-4.304075000	-2.630728000	3.624492000
1	-2.307870000	-3.178641000	4.212240000
1	-6.164623000	-1.914222000	2.806657000
1	-4.781983000	-3.219065000	4.402540000
6	-3.325962000	-0.505447000	-1.129560000
6	-4.303461000	0.348870000	-1.641514000
6	-3.139106000	-1.753927000	-1.736333000

6	-5.072414000	-0.028474000	-2.740883000
1	-4.468454000	1.323277000	-1.195185000
6	-3.910255000	-2.134437000	-2.827444000
1	-2.384332000	-2.434700000	-1.352155000
6	-4.877903000	-1.269715000	-3.335674000
1	-5.822487000	0.653498000	-3.130471000
1	-3.751755000	-3.105777000	-3.286110000
1	-5.475546000	-1.563693000	-4.193429000
6	3.242590000	-0.314098000	1.157422000
6	3.622885000	0.798884000	1.912677000
6	3.449062000	-1.596515000	1.687312000
6	4.212671000	0.634006000	3.163289000
1	3.446869000	1.800542000	1.538667000
6	4.039123000	-1.758369000	2.936566000
1	3.147814000	-2.471978000	1.117200000
6	4.422742000	-0.641791000	3.677162000
1	4.496444000	1.509424000	3.739048000
1	4.195489000	-2.756978000	3.333033000
1	4.878882000	-0.767475000	4.654404000
6	3.191883000	-1.344378000	-1.488033000
6	4.592736000	-1.365395000	-1.512694000
6	2.487246000	-2.208133000	-2.327919000
6	5.271803000	-2.232207000	-2.359407000
1	5.154551000	-0.705284000	-0.856869000
6	3.168466000	-3.077160000	-3.178557000
1	1.403354000	-2.209990000	-2.322346000
6	4.558328000	-3.090674000	-3.195491000
1	6.357751000	-2.240677000	-2.367439000
1	2.606448000	-3.744129000	-3.825088000
1	5.088975000	-3.769279000	-3.856758000
14	1.497943000	2.812598000	-0.659695000
14	-1.504389000	2.761124000	-0.220532000
6	2.168845000	3.998287000	0.638751000
1	3.227029000	4.234086000	0.472778000
1	1.610821000	4.941628000	0.617396000
1	2.038889000	3.566691000	1.637422000
6	1.201527000	3.752603000	-2.265815000
1	0.535705000	4.612562000	-2.133124000
1	2.158592000	4.136670000	-2.640703000
1	0.774292000	3.104024000	-3.038945000
6	-1.495315000	4.458647000	0.590724000
1	-1.050890000	4.372848000	1.588835000
1	-0.901632000	5.179245000	0.015266000
1	-2.506549000	4.869696000	0.692250000

6	-2.107339000	2.904830000	-1.997769000
1	-3.157210000	3.223515000	-2.003344000
1	-1.539456000	3.653519000	-2.557428000
1	-2.044056000	1.957326000	-2.541192000
1	3.817714000	1.745751000	-0.845713000
1	2.742997000	1.348509000	-2.185659000
8	0.359613000	-0.306956000	2.038844000
1	0.222210000	2.001303000	1.112319000
1	1.301569000	-0.487908000	2.160779000
6	0.044379000	0.847208000	2.945764000
1	-1.049023000	0.715988000	3.067099000
8	0.446091000	2.002930000	2.450746000
1	0.525793000	0.575724000	3.904103000

B4

Coordinates (Angstroms)			
	X	Y	Z

25	-0.025788000	-0.220615000	0.175052000
7	-0.066338000	1.942302000	-0.435532000
6	-0.000055000	-1.956400000	0.569341000
8	0.023074000	-3.085769000	0.825666000
6	2.633685000	1.349597000	-1.194298000
1	3.701417000	1.586727000	-1.244475000
1	2.289798000	1.183372000	-2.222427000
6	-2.781630000	1.708382000	0.714586000
6	0.231105000	0.286970000	1.859054000
8	0.367124000	0.661934000	2.946946000
15	-2.310582000	-0.041070000	0.445820000
15	2.266115000	-0.200553000	-0.292076000
6	3.063133000	-1.530291000	-1.277169000
6	2.280478000	-2.409550000	-2.030006000
6	4.456812000	-1.662311000	-1.301787000
6	2.885436000	-3.401593000	-2.799314000
1	1.200918000	-2.299792000	-2.024376000
6	5.056665000	-2.653296000	-2.069749000
1	5.077153000	-0.997771000	-0.706325000
6	4.270414000	-3.525618000	-2.820791000
1	2.267999000	-4.078565000	-3.382431000
1	6.138531000	-2.749327000	-2.078892000
1	4.739652000	-4.301994000	-3.418275000
6	3.337105000	-0.183550000	1.198763000
6	4.341105000	0.760318000	1.420983000
6	3.140726000	-1.191415000	2.151293000
6	5.123431000	0.710080000	2.572835000

1	4.519351000	1.551189000	0.700747000
6	3.925445000	-1.247748000	3.296597000
1	2.366643000	-1.938366000	1.996833000
6	4.917124000	-0.292891000	3.513070000
1	5.893592000	1.459023000	2.732273000
1	3.757586000	-2.034617000	4.025779000
1	5.524098000	-0.331394000	4.412726000
6	-3.246289000	-0.576623000	-1.036110000
6	-3.595579000	0.319302000	-2.050565000
6	-3.477278000	-1.946356000	-1.229917000
6	-4.179079000	-0.141870000	-3.227565000
1	-3.398941000	1.378815000	-1.937938000
6	-4.061259000	-2.404264000	-2.406739000
1	-3.199364000	-2.657000000	-0.455557000
6	-4.413501000	-1.501427000	-3.408089000
1	-4.437813000	0.566718000	-4.007923000
1	-4.236962000	-3.467028000	-2.542480000
1	-4.863195000	-1.859437000	-4.329224000
6	-3.196034000	-0.931270000	1.782651000
6	-4.596878000	-0.925095000	1.820936000
6	-2.494505000	-1.583084000	2.797982000
6	-5.277986000	-1.557259000	2.853221000
1	-5.155877000	-0.430546000	1.030670000
6	-3.177906000	-2.217090000	3.834342000
1	-1.410666000	-1.602741000	2.784830000
6	-4.567763000	-2.205012000	3.863719000
1	-6.363842000	-1.546960000	2.870577000
1	-2.619001000	-2.721917000	4.616407000
1	-5.099586000	-2.700352000	4.670746000
14	-1.491916000	2.898862000	-0.019401000
14	1.520857000	2.716729000	-0.505394000
6	-2.152306000	3.747819000	-1.561462000
1	-3.211602000	4.014069000	-1.463475000
1	-1.594345000	4.670049000	-1.760223000
1	-2.015869000	3.090169000	-2.427781000
6	-1.157948000	4.173122000	1.325240000
1	-0.503026000	4.981374000	0.982112000
1	-2.106814000	4.629983000	1.632445000
1	-0.703541000	3.714809000	2.210826000
6	1.496903000	4.144084000	-1.727932000
1	1.017726000	3.806142000	-2.653776000
1	0.933502000	5.002853000	-1.343582000
1	2.509287000	4.492075000	-1.964223000
6	2.147592000	3.302795000	1.168478000

1	3.206327000	3.576888000	1.085277000
1	1.610036000	4.190974000	1.513175000
1	2.064201000	2.534116000	1.942646000
1	-3.809401000	1.910304000	0.392567000
1	-2.753999000	1.845586000	1.803207000
8	-0.366557000	-0.790810000	-1.884042000
1	-0.235584000	1.680411000	-1.500942000
1	-1.297670000	-1.042671000	-1.942070000
6	-0.110611000	0.099206000	-3.098530000
1	0.976141000	-0.080694000	-3.237646000
8	-0.483738000	1.338548000	-2.908231000
1	-0.648501000	-0.436336000	-3.907541000

TSB3

Coordinates (Angstroms)

	X	Y	Z
25	-0.002728000	-0.283767000	-0.236013000
7	0.115417000	1.956891000	0.092352000
6	-0.053640000	-2.056146000	-0.363268000
8	-0.092042000	-3.211438000	-0.435543000
6	-2.453383000	1.392948000	1.238014000
1	-3.492780000	1.650221000	1.466323000
1	-1.927520000	1.266930000	2.192526000
6	2.709124000	1.479649000	-1.232630000
6	-0.295473000	-0.027640000	-1.967277000
8	-0.462360000	0.188163000	-3.097167000
15	2.273952000	-0.162300000	-0.538203000
15	-2.250509000	-0.206464000	0.368247000
6	-2.955604000	-1.467970000	1.509382000
6	-2.192315000	-1.871456000	2.612045000
6	-4.226011000	-2.022866000	1.323001000
6	-2.697355000	-2.803660000	3.512256000
1	-1.198653000	-1.447941000	2.730198000
6	-4.724626000	-2.959737000	2.224850000
1	-4.833574000	-1.731907000	0.472190000
6	-3.963684000	-3.351009000	3.322142000
1	-2.094833000	-3.108669000	4.363410000
1	-5.711032000	-3.385715000	2.065309000
1	-4.354094000	-4.082402000	4.024140000
6	-3.482696000	-0.208802000	-0.987947000
6	-4.601432000	0.627753000	-1.023236000
6	-3.313803000	-1.146428000	-2.012818000
6	-5.518554000	0.544462000	-2.067399000

1	-4.765899000	1.355172000	-0.234630000
6	-4.234545000	-1.239675000	-3.050881000
1	-2.455759000	-1.812683000	-1.996123000
6	-5.336919000	-0.389600000	-3.083239000
1	-6.377320000	1.209199000	-2.084032000
1	-4.086760000	-1.973376000	-3.837472000
1	-6.053542000	-0.455182000	-3.896531000
6	3.222592000	-0.307498000	1.018839000
6	3.749047000	0.795065000	1.690797000
6	3.327787000	-1.574984000	1.608993000
6	4.368872000	0.638142000	2.929047000
1	3.669437000	1.788144000	1.263160000
6	3.946800000	-1.731715000	2.843755000
1	2.926383000	-2.445793000	1.094387000
6	4.468391000	-0.622086000	3.508567000
1	4.766308000	1.508561000	3.441888000
1	4.023349000	-2.719712000	3.287826000
1	4.948850000	-0.742300000	4.474826000
6	3.170860000	-1.327742000	-1.635843000
6	4.562012000	-1.467226000	-1.555038000
6	2.472860000	-2.051618000	-2.605324000
6	5.238129000	-2.316320000	-2.423041000
1	5.117402000	-0.915826000	-0.801128000
6	3.151334000	-2.899688000	-3.477925000
1	1.395159000	-1.957138000	-2.682760000
6	4.532504000	-3.035093000	-3.386673000
1	6.316268000	-2.421091000	-2.345342000
1	2.595271000	-3.459048000	-4.224162000
1	5.060899000	-3.701011000	-4.062545000
14	1.460888000	2.808609000	-0.698259000
14	-1.491435000	2.701816000	0.272019000
6	2.233901000	4.014802000	0.518811000
1	3.259400000	4.279334000	0.234377000
1	1.652500000	4.942428000	0.569026000
1	2.239184000	3.579734000	1.524503000
6	0.908304000	3.697237000	-2.257183000
1	0.313307000	4.589928000	-2.037498000
1	1.794527000	4.023600000	-2.815070000
1	0.322601000	3.042024000	-2.910864000
6	-1.374728000	4.281050000	1.279087000
1	-0.802050000	4.080497000	2.191207000
1	-0.866904000	5.077497000	0.721813000
1	-2.366472000	4.653919000	1.560493000
6	-2.286004000	3.043005000	-1.396064000

1	-3.359019000	3.220805000	-1.260815000
1	-1.863996000	3.937113000	-1.864294000
1	-2.179226000	2.208468000	-2.095690000
1	3.757117000	1.744492000	-1.051944000
1	2.593489000	1.355662000	-2.317179000
8	0.295371000	-0.341988000	1.817149000
1	0.429190000	1.842378000	1.072826000
1	0.963367000	-1.016589000	1.983961000
6	0.684922000	0.912552000	3.271028000
1	-0.245648000	0.607585000	3.779991000
8	0.813584000	2.063397000	2.827993000
1	1.570938000	0.322837000	3.565837000

B5

Coordinates (Angstroms)

	X	Y	Z
25	-0.030445000	-0.374171000	-0.234618000
7	0.118562000	1.894035000	-0.397971000
6	-0.060069000	-2.113666000	0.119098000
8	-0.072623000	-3.244219000	0.371007000
6	-2.387634000	1.590109000	0.959745000
1	-3.407428000	1.912197000	1.191763000
1	-1.801005000	1.625050000	1.885093000
6	2.675842000	1.100525000	-1.619618000
6	-0.327851000	-0.556925000	-1.974761000
8	-0.500926000	-0.609560000	-3.124211000
15	2.242575000	-0.326321000	-0.549041000
15	-2.248698000	-0.150868000	0.403726000
6	-2.862723000	-1.158099000	1.815178000
6	-2.096719000	-1.187113000	2.988002000
6	-4.047984000	-1.896757000	1.758724000
6	-2.519096000	-1.931910000	4.083228000
1	-1.162004000	-0.631923000	3.000996000
6	-4.463426000	-2.645853000	2.857754000
1	-4.654553000	-1.895399000	0.858852000
6	-3.703493000	-2.663072000	4.022633000
1	-1.917224000	-1.946405000	4.987853000
1	-5.386447000	-3.215601000	2.799323000
1	-4.030467000	-3.246744000	4.878546000
6	-3.576432000	-0.384787000	-0.838426000
6	-4.740660000	0.389234000	-0.869820000
6	-3.434293000	-1.419197000	-1.768771000
6	-5.725890000	0.153466000	-1.823534000

1	-4.887956000	1.184208000	-0.145492000
6	-4.421615000	-1.662247000	-2.719086000
1	-2.543552000	-2.039909000	-1.749215000
6	-5.566412000	-0.871282000	-2.752895000
1	-6.620587000	0.769147000	-1.838749000
1	-4.290977000	-2.465092000	-3.438320000
1	-6.333382000	-1.053761000	-3.499811000
6	3.185532000	-0.076175000	1.000144000
6	3.788329000	1.133082000	1.345887000
6	3.215729000	-1.134239000	1.920086000
6	4.409196000	1.287194000	2.584811000
1	3.773649000	1.972200000	0.658916000
6	3.835299000	-0.981603000	3.154864000
1	2.748685000	-2.083540000	1.666009000
6	4.433307000	0.233079000	3.491423000
1	4.866738000	2.238414000	2.838886000
1	3.850539000	-1.810078000	3.856722000
1	4.914857000	0.354724000	4.457031000
6	3.146637000	-1.723089000	-1.321036000
6	4.535827000	-1.846256000	-1.196021000
6	2.449660000	-2.658049000	-2.089954000
6	5.211364000	-2.884639000	-1.826775000
1	5.090192000	-1.131829000	-0.593178000
6	3.127620000	-3.695737000	-2.725475000
1	1.372822000	-2.579756000	-2.194322000
6	4.507335000	-3.811908000	-2.593248000
1	6.288127000	-2.973884000	-1.716901000
1	2.572168000	-4.416076000	-3.318356000
1	5.034622000	-4.625382000	-3.082997000
14	1.444640000	2.530649000	-1.388518000
14	-1.480956000	2.664518000	-0.301170000
6	2.258075000	4.000205000	-0.546997000
1	3.245369000	4.211649000	-0.975248000
1	1.643934000	4.899836000	-0.667783000
1	2.363048000	3.826831000	0.529301000
6	0.824125000	3.010375000	-3.093574000
1	0.215226000	3.920438000	-3.076231000
1	1.682595000	3.203955000	-3.748267000
1	0.232850000	2.205837000	-3.544169000
6	-1.333836000	4.425539000	0.334775000
1	-0.692053000	4.441115000	1.223175000
1	-0.885997000	5.085122000	-0.418460000
1	-2.312219000	4.843290000	0.599414000
6	-2.344245000	2.620800000	-1.968555000

1	-3.419563000	2.784268000	-1.833240000
1	-1.973593000	3.399379000	-2.641890000
1	-2.221713000	1.652839000	-2.464858000
1	3.729820000	1.387939000	-1.533256000
1	2.530613000	0.724517000	-2.640774000
8	0.245442000	0.246790000	1.693349000
1	0.445742000	1.771773000	0.575782000
1	0.936406000	-0.294095000	2.089532000
6	0.915227000	2.158133000	3.147973000
1	-0.075088000	1.960780000	3.591898000
8	1.134821000	3.145775000	2.479921000
1	1.715179000	1.450381000	3.423848000

B6

Coordinates (Angstroms)

	X	Y	Z
25	0.030615000	0.375817000	-0.064321000
7	0.097806000	-1.648947000	-1.255621000
6	0.051960000	1.691203000	1.114252000
8	0.078928000	2.512047000	1.934284000
6	2.820032000	-0.596230000	-1.679496000
1	2.831581000	0.217319000	-2.416360000
1	3.838816000	-0.998295000	-1.639754000
6	-2.707493000	-0.853510000	-1.502793000
6	0.018252000	1.399111000	-1.520324000
8	0.017874000	2.016963000	-2.505900000
15	-2.270682000	0.219257000	-0.078720000
15	2.316326000	0.222946000	-0.117450000
6	3.035610000	-0.788280000	1.227481000
6	3.622955000	-2.038645000	1.033548000
6	2.925887000	-0.286665000	2.531940000
6	4.094017000	-2.775520000	2.119720000
1	3.721834000	-2.451478000	0.034606000
6	3.399290000	-1.018933000	3.613611000
1	2.463639000	0.683695000	2.698023000
6	3.983679000	-2.268338000	3.409427000
1	4.548407000	-3.747759000	1.953237000
1	3.307332000	-0.615761000	4.617595000
1	4.349534000	-2.843157000	4.254822000
6	3.384804000	1.714156000	-0.063193000
6	4.763562000	1.596607000	0.151659000
6	2.837308000	2.980757000	-0.276072000
6	5.576630000	2.723576000	0.151439000

1	5.201449000	0.617932000	0.330420000
6	3.652728000	4.110788000	-0.276071000
1	1.770740000	3.090874000	-0.439129000
6	5.020933000	3.984171000	-0.062290000
1	6.644092000	2.619151000	0.321821000
1	3.212680000	5.090034000	-0.438276000
1	5.655592000	4.865625000	-0.058324000
6	-3.070492000	-0.551364000	1.376854000
6	-4.134041000	-1.451348000	1.285737000
6	-2.603648000	-0.186045000	2.643375000
6	-4.722644000	-1.975927000	2.434239000
1	-4.509932000	-1.765675000	0.316668000
6	-3.197766000	-0.698307000	3.790149000
1	-1.761348000	0.490942000	2.727932000
6	-4.256626000	-1.598204000	3.688802000
1	-5.542929000	-2.682406000	2.345474000
1	-2.822698000	-0.405344000	4.766361000
1	-4.712944000	-2.007431000	4.585512000
6	-3.312662000	1.712573000	-0.334646000
6	-4.703416000	1.599797000	-0.451027000
6	-2.730036000	2.977479000	-0.428742000
6	-5.490372000	2.724009000	-0.667395000
1	-5.177139000	0.626127000	-0.358003000
6	-3.518075000	4.106812000	-0.643776000
1	-1.655893000	3.087227000	-0.331708000
6	-4.897149000	3.981960000	-0.766538000
1	-6.567769000	2.620215000	-0.756868000
1	-3.048798000	5.083386000	-0.715618000
1	-5.511295000	4.861719000	-0.935376000
14	-1.514655000	-2.321006000	-1.552208000
14	1.509556000	-1.835710000	-2.284505000
6	-1.861262000	-3.562651000	-0.192976000
1	-2.904072000	-3.899523000	-0.190399000
1	-1.218982000	-4.443328000	-0.315210000
1	-1.635664000	-3.107787000	0.777662000
6	-1.694672000	-3.134303000	-3.241679000
1	-0.926838000	-3.894423000	-3.425499000
1	-2.668728000	-3.636360000	-3.289052000
1	-1.660120000	-2.406108000	-4.058232000
6	2.175190000	-3.596254000	-2.201714000
1	2.320224000	-3.915484000	-1.163330000
1	1.468138000	-4.297274000	-2.661007000
1	3.131933000	-3.697696000	-2.727681000
6	1.121627000	-1.364111000	-4.061173000

1	2.059449000	-1.212354000	-4.609351000
1	0.548047000	-2.127105000	-4.594616000
1	0.563829000	-0.420989000	-4.095623000
1	-3.766272000	-1.131024000	-1.550484000
1	-2.493371000	-0.244766000	-2.391593000
8	-0.042921000	-1.117306000	1.269328000
1	0.285901000	-1.835616000	-0.233814000
1	0.662565000	-1.102738000	1.923419000

TSB4

Coordinates (Angstroms)			
	X	Y	Z

25	0.025374000	0.369199000	-0.116280000
7	0.065497000	-1.599561000	-1.217157000
6	0.047743000	1.686524000	1.068100000
8	0.078005000	2.522850000	1.872534000
6	2.820689000	-0.656092000	-1.662103000
1	2.811998000	0.114874000	-2.443474000
1	3.842594000	-1.049343000	-1.618321000
6	-2.736392000	-0.864937000	-1.510803000
6	0.013843000	1.398760000	-1.566027000
8	0.014606000	2.008142000	-2.553960000
15	-2.276369000	0.221000000	-0.111283000
15	2.319611000	0.230304000	-0.146989000
6	3.015765000	-0.732572000	1.248005000
6	3.639900000	-1.972265000	1.099150000
6	2.848757000	-0.209508000	2.538471000
6	4.091736000	-2.676150000	2.215105000
1	3.777707000	-2.402453000	0.112730000
6	3.304533000	-0.908538000	3.649620000
1	2.354462000	0.749770000	2.670612000
6	3.926204000	-2.146491000	3.489843000
1	4.572730000	-3.640731000	2.082796000
1	3.169514000	-0.488669000	4.641749000
1	4.276932000	-2.695501000	4.358471000
6	3.380434000	1.726271000	-0.117858000
6	4.761033000	1.612971000	0.087512000
6	2.828387000	2.989999000	-0.334840000
6	5.571539000	2.741475000	0.073998000
1	5.202552000	0.636352000	0.269001000
6	3.641286000	4.121846000	-0.347909000
1	1.760464000	3.097120000	-0.490592000
6	5.011227000	3.999491000	-0.143505000

1	6.640436000	2.640536000	0.237130000
1	3.198026000	5.099087000	-0.513263000
1	5.643896000	4.882331000	-0.149809000
6	-3.038719000	-0.530986000	1.375072000
6	-4.064060000	-1.476911000	1.321416000
6	-2.582138000	-0.102977000	2.625615000
6	-4.624618000	-1.983915000	2.491835000
1	-4.427501000	-1.843525000	0.366445000
6	-3.147635000	-0.598724000	3.793734000
1	-1.771159000	0.614882000	2.684296000
6	-4.169718000	-1.543487000	3.729841000
1	-5.415039000	-2.726431000	2.432638000
1	-2.780984000	-0.254898000	4.756484000
1	-4.605855000	-1.938930000	4.642576000
6	-3.315323000	1.718413000	-0.345528000
6	-4.708749000	1.606962000	-0.425335000
6	-2.732384000	2.981112000	-0.462278000
6	-5.498773000	2.731545000	-0.627930000
1	-5.180632000	0.634007000	-0.315378000
6	-3.523682000	4.110716000	-0.663491000
1	-1.655843000	3.089480000	-0.393548000
6	-4.905700000	3.987661000	-0.749690000
1	-6.578315000	2.629639000	-0.689288000
1	-3.054777000	5.085972000	-0.753443000
1	-5.522311000	4.867656000	-0.907818000
14	-1.501750000	-2.304581000	-1.571832000
14	1.488276000	-1.926939000	-2.165983000
6	-1.899501000	-3.606020000	-0.274972000
1	-2.920637000	-3.993380000	-0.372483000
1	-1.207178000	-4.450855000	-0.379480000
1	-1.774638000	-3.193328000	0.730991000
6	-1.674265000	-3.098538000	-3.274316000
1	-0.937258000	-3.892632000	-3.441042000
1	-2.668457000	-3.555855000	-3.351408000
1	-1.579365000	-2.368824000	-4.084855000
6	2.108350000	-3.686427000	-1.879696000
1	2.218200000	-3.900437000	-0.810470000
1	1.389718000	-4.411128000	-2.282268000
1	3.071934000	-3.870470000	-2.370063000
6	1.259171000	-1.643915000	-4.015950000
1	2.241693000	-1.556836000	-4.496643000
1	0.717959000	-2.451330000	-4.516760000
1	0.720409000	-0.705701000	-4.195255000
1	-3.791837000	-1.157221000	-1.527674000

1	-2.551406000	-0.261807000	-2.409676000
8	-0.034377000	-1.241871000	1.176199000
1	0.161414000	-1.716812000	0.024244000
1	0.738222000	-1.340651000	1.744732000

B7

Coordinates (Angstroms)			
	X	Y	Z
25	0.021347000	0.334030000	-0.126090000
7	0.105829000	-1.525014000	-1.245575000
6	0.008501000	1.690921000	1.017734000
8	0.014740000	2.560162000	1.788601000
6	2.857371000	-0.634536000	-1.658988000
1	2.859311000	0.131534000	-2.445138000
1	3.879688000	-1.023074000	-1.592305000
6	-2.727063000	-0.979484000	-1.485651000
6	0.004383000	1.316888000	-1.602491000
8	0.001041000	1.894640000	-2.607354000
15	-2.279504000	0.168469000	-0.140264000
15	2.320178000	0.244870000	-0.158036000
6	3.009726000	-0.696110000	1.257199000
6	3.608410000	-1.950956000	1.129926000
6	2.846092000	-0.151809000	2.540773000
6	4.035803000	-2.649732000	2.258883000
1	3.744095000	-2.394175000	0.149270000
6	3.274852000	-0.848260000	3.665433000
1	2.379370000	0.823929000	2.656092000
6	3.869654000	-2.102039000	3.526135000
1	4.498934000	-3.624970000	2.142174000
1	3.143102000	-0.412077000	4.650973000
1	4.200513000	-2.647909000	4.404386000
6	3.343632000	1.766571000	-0.108033000
6	4.722199000	1.687502000	0.125650000
6	2.767776000	3.015204000	-0.349647000
6	5.506355000	2.834608000	0.118843000
1	5.182929000	0.722445000	0.320924000
6	3.554129000	4.165650000	-0.356655000
1	1.701419000	3.096124000	-0.530293000
6	4.921865000	4.077321000	-0.121795000
1	6.574022000	2.759958000	0.303060000
1	3.092282000	5.130750000	-0.541296000
1	5.533723000	4.974715000	-0.123793000
6	-3.045853000	-0.504633000	1.383583000

6	-3.908942000	-1.600929000	1.392276000
6	-2.760667000	0.137782000	2.593974000
6	-4.473326000	-2.051253000	2.584486000
1	-4.138639000	-2.126249000	0.471414000
6	-3.329134000	-0.304701000	3.781711000
1	-2.087036000	0.989690000	2.608368000
6	-4.186159000	-1.404209000	3.780698000
1	-5.138244000	-2.910065000	2.573637000
1	-3.099361000	0.206223000	4.712152000
1	-4.626273000	-1.754533000	4.709728000
6	-3.323383000	1.653537000	-0.424521000
6	-4.714843000	1.520409000	-0.507780000
6	-2.756233000	2.919493000	-0.574388000
6	-5.518942000	2.627457000	-0.747066000
1	-5.172162000	0.543357000	-0.373105000
6	-3.562044000	4.031793000	-0.812225000
1	-1.681872000	3.045729000	-0.502720000
6	-4.941658000	3.887445000	-0.901937000
1	-6.596610000	2.509330000	-0.811637000
1	-3.105912000	5.010419000	-0.927940000
1	-5.569154000	4.753924000	-1.089361000
14	-1.389064000	-2.333546000	-1.539700000
14	1.513171000	-1.904581000	-2.154053000
6	-1.738537000	-3.659836000	-0.237739000
1	-2.718730000	-4.131194000	-0.382844000
1	-0.978864000	-4.448659000	-0.313660000
1	-1.703709000	-3.259709000	0.781054000
6	-1.580059000	-3.186442000	-3.217861000
1	-0.824898000	-3.964706000	-3.380267000
1	-2.563042000	-3.670830000	-3.270954000
1	-1.512931000	-2.472854000	-4.046032000
6	2.133197000	-3.665043000	-1.828632000
1	2.233560000	-3.872052000	-0.756805000
1	1.418004000	-4.394250000	-2.230133000
1	3.100002000	-3.858068000	-2.310071000
6	1.380669000	-1.697572000	-4.030059000
1	2.380919000	-1.688659000	-4.481856000
1	0.809724000	-2.498134000	-4.510199000
1	0.896124000	-0.744024000	-4.272832000
1	-3.765781000	-1.325096000	-1.459181000
1	-2.597083000	-0.400147000	-2.409291000
8	-0.016422000	-1.215043000	1.392037000
1	0.207511000	-1.807848000	0.631235000
1	0.761514000	-1.199078000	1.968271000

C1

Coordinates (Angstroms)

	X	Y	Z
25	0.012021000	-0.056203000	-0.387971000
7	0.060456000	1.879020000	0.227075000
6	0.079322000	-1.831417000	-0.528699000
8	0.139334000	-2.984384000	-0.648209000
6	-2.549808000	1.349483000	1.243264000
1	-3.603525000	1.586723000	1.410654000
1	-2.053102000	1.232313000	2.214528000
6	2.792543000	1.782904000	-0.813909000
6	-0.254476000	0.179223000	-2.110866000
8	-0.405154000	0.435183000	-3.231306000
15	2.288215000	0.058903000	-0.519624000
15	-2.234450000	-0.165203000	0.293385000
6	-2.745892000	-1.576467000	1.357949000
6	-2.832867000	-2.858870000	0.804095000
6	-3.013179000	-1.411327000	2.718885000
6	-3.176211000	-3.949735000	1.594116000
1	-2.636499000	-3.012397000	-0.252676000
6	-3.353728000	-2.505312000	3.511249000
1	-2.959265000	-0.427297000	3.172739000
6	-3.434903000	-3.776113000	2.951887000
1	-3.241321000	-4.936976000	1.146844000
1	-3.557388000	-2.358796000	4.567908000
1	-3.701263000	-4.628541000	3.569870000
6	-3.493114000	-0.230156000	-1.039067000
6	-4.722811000	0.427740000	-0.945138000
6	-3.228664000	-1.002874000	-2.174354000
6	-5.660534000	0.324647000	-1.967652000
1	-4.959036000	1.028328000	-0.073035000
6	-4.170040000	-1.115366000	-3.192811000
1	-2.276926000	-1.516700000	-2.268925000
6	-5.386516000	-0.447382000	-3.093575000
1	-6.608851000	0.846745000	-1.882047000
1	-3.945401000	-1.716362000	-4.068753000
1	-6.119396000	-0.525942000	-3.890981000
6	3.026853000	-0.424278000	1.084880000
6	2.990550000	-1.779236000	1.441496000
6	3.578546000	0.495043000	1.977868000
6	3.501475000	-2.202419000	2.661664000
1	2.566647000	-2.509269000	0.757206000

6	4.083088000	0.070739000	3.206327000
1	3.616068000	1.549922000	1.729949000
6	4.047759000	-1.276188000	3.549865000
1	3.469050000	-3.256180000	2.921567000
1	4.499956000	0.799639000	3.894632000
1	4.442656000	-1.605829000	4.506180000
6	3.266167000	-0.954655000	-1.691744000
6	2.651323000	-1.581498000	-2.776930000
6	4.650725000	-1.082966000	-1.525069000
6	3.407064000	-2.323641000	-3.682579000
1	1.579555000	-1.496280000	-2.918759000
6	5.403538000	-1.824458000	-2.426876000
1	5.137771000	-0.611056000	-0.675629000
6	4.781056000	-2.447272000	-3.508120000
1	2.917062000	-2.808592000	-4.521448000
1	6.475566000	-1.922762000	-2.284435000
1	5.368946000	-3.031574000	-4.209860000
14	1.433298000	2.902347000	-0.080255000
14	-1.489715000	2.661312000	0.379772000
6	2.060538000	3.754200000	1.486439000
1	3.098080000	4.092751000	1.372381000
1	1.451773000	4.637825000	1.708987000
1	1.999864000	3.094197000	2.358838000
6	1.126935000	4.238585000	-1.381040000
1	0.401852000	4.990872000	-1.049916000
1	2.062296000	4.764302000	-1.610562000
1	0.750361000	3.796409000	-2.311032000
6	-1.458427000	4.181186000	1.497534000
1	-0.993307000	3.941934000	2.460367000
1	-0.909042000	5.018394000	1.051739000
1	-2.480257000	4.529710000	1.690834000
6	-2.288901000	3.132177000	-1.262224000
1	-3.334608000	3.427713000	-1.109993000
1	-1.769305000	3.974310000	-1.731961000
1	-2.280594000	2.297933000	-1.971455000
1	3.816444000	1.997601000	-0.489657000
1	2.760830000	1.912164000	-1.903258000
1	0.282392000	1.495952000	2.112375000
1	0.002403000	-0.653480000	2.235385000
6	0.284691000	-0.135627000	3.170776000
1	1.301309000	-0.454133000	3.431581000
1	-0.403513000	-0.485225000	3.948197000
8	0.180667000	1.262305000	3.060248000

C2

Coordinates (Angstroms)			
	X	Y	Z

25	-0.030724000	0.007839000	0.312167000
7	-0.039485000	1.735400000	-1.179529000
6	-0.115923000	-1.484496000	1.264369000
8	-0.205195000	-2.466640000	1.874186000
6	2.553507000	0.710302000	-1.681916000
1	3.613840000	0.834734000	-1.918558000
1	2.052658000	0.181681000	-2.500078000
6	-2.803857000	1.906184000	-0.162271000
6	0.082319000	1.081624000	1.719571000
8	0.128583000	1.834442000	2.606666000
15	-2.311715000	0.185194000	0.281361000
15	2.228941000	-0.282312000	-0.176665000
6	2.772402000	-1.988243000	-0.572298000
6	2.773187000	-2.938329000	0.454396000
6	3.175451000	-2.376794000	-1.850171000
6	3.154363000	-4.251305000	0.203884000
1	2.474492000	-2.653862000	1.459287000
6	3.558268000	-3.692002000	-2.102228000
1	3.184856000	-1.657602000	-2.662441000
6	3.544509000	-4.632828000	-1.077945000
1	3.142977000	-4.978385000	1.010285000
1	3.863494000	-3.979949000	-3.104174000
1	3.836711000	-5.659960000	-1.275723000
6	3.580473000	0.226460000	0.967570000
6	4.902406000	0.367237000	0.528042000
6	3.298777000	0.437549000	2.318442000
6	5.908743000	0.741327000	1.410412000
1	5.153500000	0.168050000	-0.510399000
6	4.306619000	0.807340000	3.207240000
1	2.284484000	0.316582000	2.682224000
6	5.610984000	0.967740000	2.753446000
1	6.928189000	0.851784000	1.051973000
1	4.067979000	0.973519000	4.253488000
1	6.396327000	1.262330000	3.443383000
6	-3.142492000	-0.883049000	-0.944917000
6	-3.344977000	-2.229760000	-0.623734000
6	-3.497758000	-0.430137000	-2.215141000
6	-3.898840000	-3.101331000	-1.553121000
1	-3.062732000	-2.601212000	0.357963000
6	-4.042902000	-1.305696000	-3.151263000

1	-3.350996000	0.610378000	-2.486776000
6	-4.245925000	-2.642066000	-2.822280000
1	-4.051389000	-4.143805000	-1.290430000
1	-4.310213000	-0.939473000	-4.138282000
1	-4.670883000	-3.325082000	-3.551831000
6	-3.330327000	-0.129344000	1.777867000
6	-2.735076000	-0.299134000	3.028694000
6	-4.728101000	-0.158437000	1.682797000
6	-3.519737000	-0.492454000	4.164655000
1	-1.655468000	-0.284176000	3.124702000
6	-5.510459000	-0.350776000	2.814404000
1	-5.204594000	-0.041657000	0.712870000
6	-4.905712000	-0.518294000	4.059737000
1	-3.041979000	-0.626178000	5.130462000
1	-6.592659000	-0.374408000	2.725362000
1	-5.516031000	-0.671677000	4.944939000
14	-1.455609000	2.787448000	-1.159839000
14	1.609393000	2.323695000	-1.460970000
6	-2.029566000	3.131723000	-2.920400000
1	-3.006465000	3.628836000	-2.937844000
1	-1.315019000	3.781021000	-3.438930000
1	-2.109449000	2.206812000	-3.503082000
6	-1.041429000	4.394909000	-0.283137000
1	-0.332680000	5.009927000	-0.848830000
1	-1.952330000	4.988475000	-0.141443000
1	-0.611553000	4.198258000	0.705542000
6	1.715734000	3.352399000	-3.036151000
1	1.289483000	2.814749000	-3.890681000
1	1.176710000	4.301990000	-2.933092000
1	2.758757000	3.592698000	-3.274306000
6	2.269219000	3.322153000	-0.016787000
1	3.358964000	3.410828000	-0.103293000
1	1.852002000	4.334082000	0.004725000
1	2.054843000	2.846003000	0.944055000
1	-3.798302000	1.945611000	-0.621077000
1	-2.876523000	2.429720000	0.799572000
1	-0.193309000	0.913968000	-1.807265000
6	-0.269129000	-2.089320000	-1.989018000
1	-1.247903000	-2.203604000	-2.484434000
1	0.499004000	-2.399826000	-2.720127000
8	-0.047124000	-0.792086000	-1.553326000
1	-0.234276000	-2.828819000	-1.171027000

TSC

Coordinates (Angstroms)			
	X	Y	Z

25	0.034094000	-0.162546000	0.074303000
7	-0.049617000	2.040492000	-0.259274000
6	0.059998000	-1.934938000	-0.007200000
8	0.077438000	-3.093411000	-0.069098000
6	2.675636000	1.610628000	-1.036322000
1	3.738275000	1.873131000	-1.018187000
1	2.366226000	1.546600000	-2.086339000
6	-2.656325000	1.591054000	0.993651000
6	0.297969000	-0.069262000	1.830563000
8	0.473515000	0.068017000	2.967410000
15	-2.238886000	-0.098135000	0.425821000
15	2.319103000	-0.051857000	-0.362365000
6	3.055996000	-1.215714000	-1.576725000
6	4.421015000	-1.521360000	-1.565554000
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6	4.956868000	-2.383325000	-2.517346000
1	5.068102000	-1.094188000	-0.804377000
6	2.775880000	-2.649063000	-3.506251000
1	1.183249000	-1.539079000	-2.568889000
6	4.134757000	-2.949794000	-3.488765000
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1	2.128688000	-3.089341000	-4.259238000
1	4.552541000	-3.627503000	-4.227785000
6	3.412732000	-0.287734000	1.086266000
6	4.350486000	0.644731000	1.531620000
6	3.274331000	-1.492631000	1.787902000
6	5.129690000	0.382433000	2.657863000
1	4.476815000	1.588814000	1.011881000
6	4.057251000	-1.759308000	2.903064000
1	2.544676000	-2.227320000	1.456355000
6	4.986571000	-0.818408000	3.343605000
1	5.849926000	1.121454000	2.996293000
1	3.937420000	-2.699335000	3.433097000
1	5.593634000	-1.021331000	4.220873000
6	-3.337390000	-0.443571000	-0.997740000
6	-3.235083000	-1.708530000	-1.589259000
6	-4.238694000	0.479661000	-1.529277000
6	-4.009570000	-2.037109000	-2.694283000
1	-2.535209000	-2.437367000	-1.188160000
6	-5.010521000	0.153098000	-2.643573000

1	-4.338747000	1.466368000	-1.089198000
6	-4.895295000	-1.102659000	-3.229431000
1	-3.915841000	-3.020516000	-3.145191000
1	-5.702658000	0.884386000	-3.050787000
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6	-2.262834000	-2.065766000	2.465821000
6	-4.396373000	-1.092101000	1.920199000
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1	-1.195558000	-2.159790000	2.303350000
6	-5.005865000	-1.865802000	2.899208000
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1	-4.717477000	-3.349728000	4.434231000
14	-1.538821000	2.858906000	0.125433000
14	1.498201000	2.847210000	-0.210837000
6	-2.345135000	3.510264000	-1.448994000
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1	-2.466605000	2.717764000	-2.195808000
6	-1.347712000	4.290078000	1.339353000
1	-0.696237000	5.085762000	0.961583000
1	-2.328363000	4.737932000	1.541692000
1	-0.937538000	3.942577000	2.294246000
6	1.512565000	4.423437000	-1.250350000
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1	2.514024000	4.868842000	-1.284678000
6	2.067814000	3.246480000	1.537596000
1	3.097072000	3.625999000	1.536623000
1	1.436081000	4.017865000	1.990609000
1	2.034765000	2.362695000	2.183415000
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1	-2.357564000	1.602397000	2.050619000
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1	-1.837640000	0.582478000	-2.965016000
1	-0.386413000	0.506733000	-3.994286000
8	-0.010460000	0.361609000	-1.980952000
1	-1.012516000	-0.959034000	-3.205827000

G3

Coordinates (Angstroms)			
	X	Y	Z

25	-0.009015000	-0.103365000	0.210120000
7	-0.047434000	1.925438000	-0.554356000
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8	-0.184769000	-2.905620000	1.056702000
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1	3.734641000	1.631679000	-1.223834000
1	2.417035000	1.113619000	-2.276379000
6	-2.745596000	1.828375000	0.547777000
6	0.259027000	0.470513000	1.867581000
8	0.421924000	0.906032000	2.927868000
15	-2.305624000	0.064983000	0.398486000
15	2.280694000	-0.143872000	-0.261906000
6	3.029629000	-1.528696000	-1.223955000
6	2.562400000	-2.836083000	-1.059616000
6	4.073977000	-1.299789000	-2.126395000
6	3.122501000	-3.886699000	-1.781228000
1	1.754204000	-3.045502000	-0.369320000
6	4.630322000	-2.348406000	-2.852852000
1	4.460176000	-0.295152000	-2.268985000
6	4.153926000	-3.645645000	-2.683672000
1	2.743693000	-4.894751000	-1.640202000
1	5.437056000	-2.150055000	-3.552533000
1	4.586013000	-4.464450000	-3.251327000
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1	4.506828000	1.654710000	0.715852000
6	3.966106000	-1.149595000	3.321554000
1	2.410434000	-1.864439000	2.030773000
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1	3.808718000	-1.933281000	4.056545000
1	5.548430000	-0.199993000	4.432679000
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6	-2.979335000	-1.917108000	-1.413870000
6	-4.014025000	0.204003000	-1.882609000
6	-3.588622000	-2.467297000	-2.533089000
1	-2.331623000	-2.534260000	-0.796800000
6	-4.620793000	-0.345649000	-3.012732000

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6	-4.409194000	-1.679252000	-3.340656000
1	-3.421179000	-3.511845000	-2.779141000
1	-5.259899000	0.275137000	-3.633951000
1	-4.881543000	-2.106998000	-4.220095000
6	-3.232377000	-0.763362000	1.751354000
6	-2.573964000	-1.180283000	2.910309000
6	-4.617277000	-0.948140000	1.656253000
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6	-4.659541000	-1.945370000	3.851279000
1	-2.757724000	-2.087242000	4.849402000
1	-6.398780000	-1.676676000	2.607694000
1	-5.211801000	-2.407362000	4.664448000
14	-1.498334000	2.849515000	-0.470771000
14	1.470544000	2.717176000	-0.687980000
6	-2.197760000	3.209172000	-2.190942000
1	-3.184914000	3.686408000	-2.148715000
1	-1.525677000	3.887258000	-2.731033000
1	-2.287195000	2.291467000	-2.783437000
6	-1.359874000	4.503213000	0.439750000
1	-0.678377000	5.205123000	-0.054475000
1	-2.341771000	4.988788000	0.501724000
1	-0.996806000	4.350810000	1.463046000
6	1.523010000	4.036967000	-2.044595000
1	1.203546000	3.619570000	-3.007211000
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6	2.117152000	3.497140000	0.904751000
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1	2.136319000	2.776192000	1.728874000
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1	-0.453183000	-0.816323000	-3.886120000
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8	-0.394219000	-0.270599000	-1.898579000

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