

## Supporting Information

For

### **Mechanistic Insight of Amides Formation from Aryl Epoxides and Amines Catalyzed by Ruthenium Pincer Complexes: A DFT Study**

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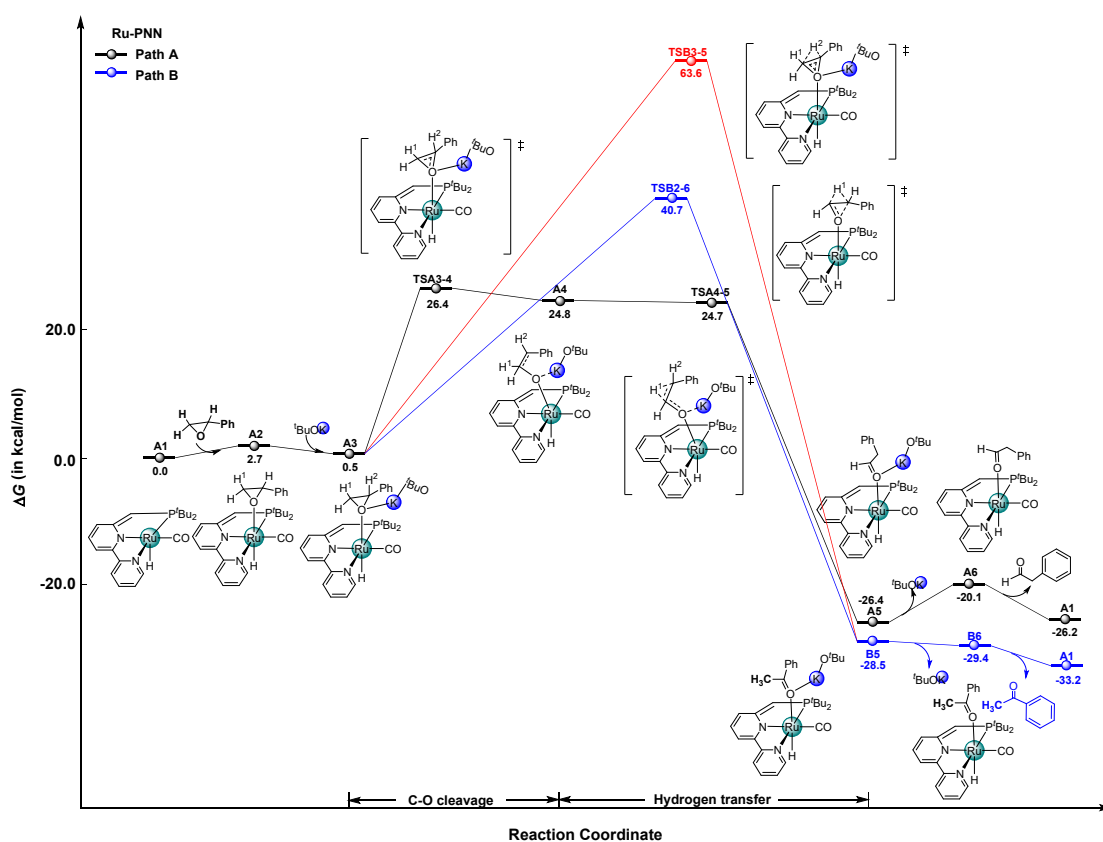
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## Content

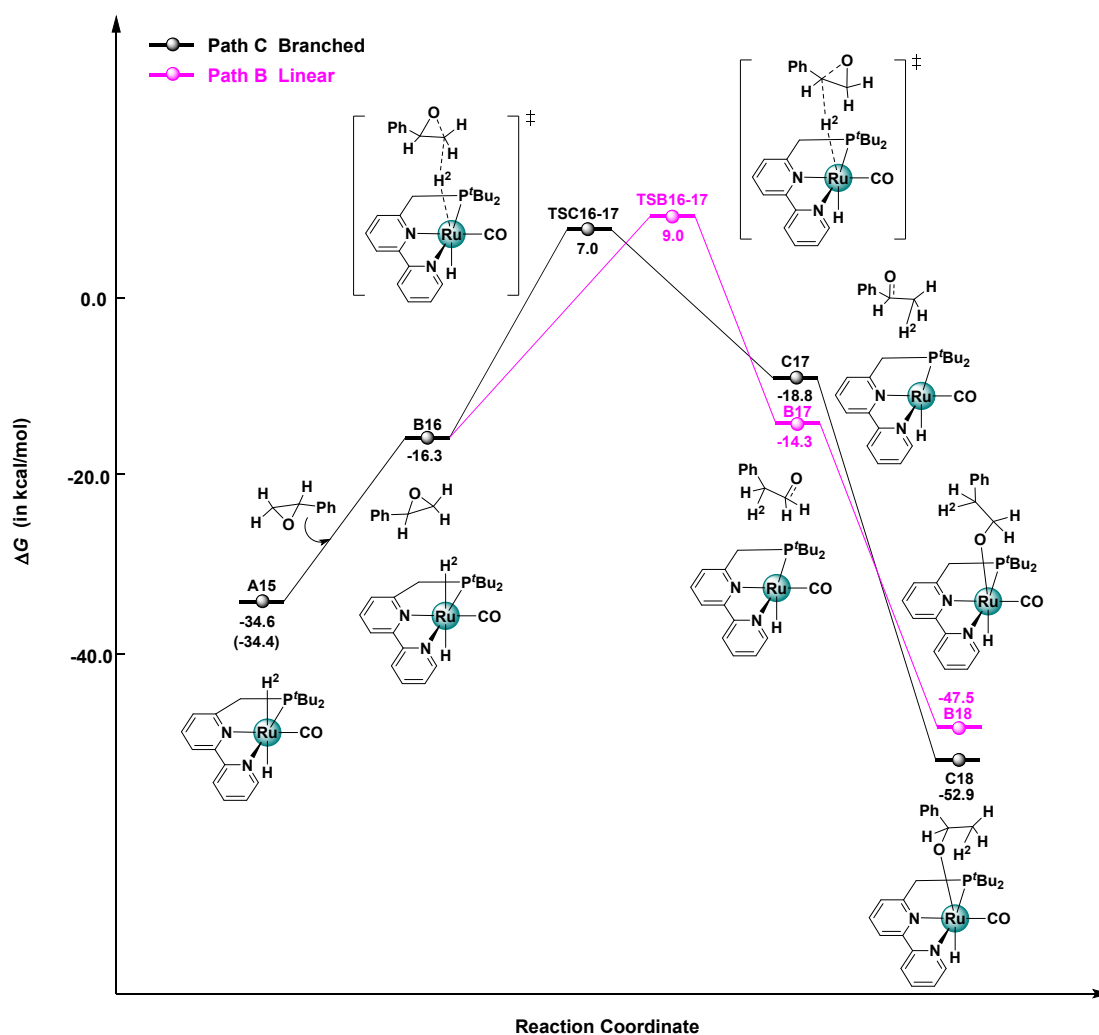
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1. The Gibbs free energy profiles of isomerization of epoxides to aldehydes catalyzed by Ru-PNN complex A1



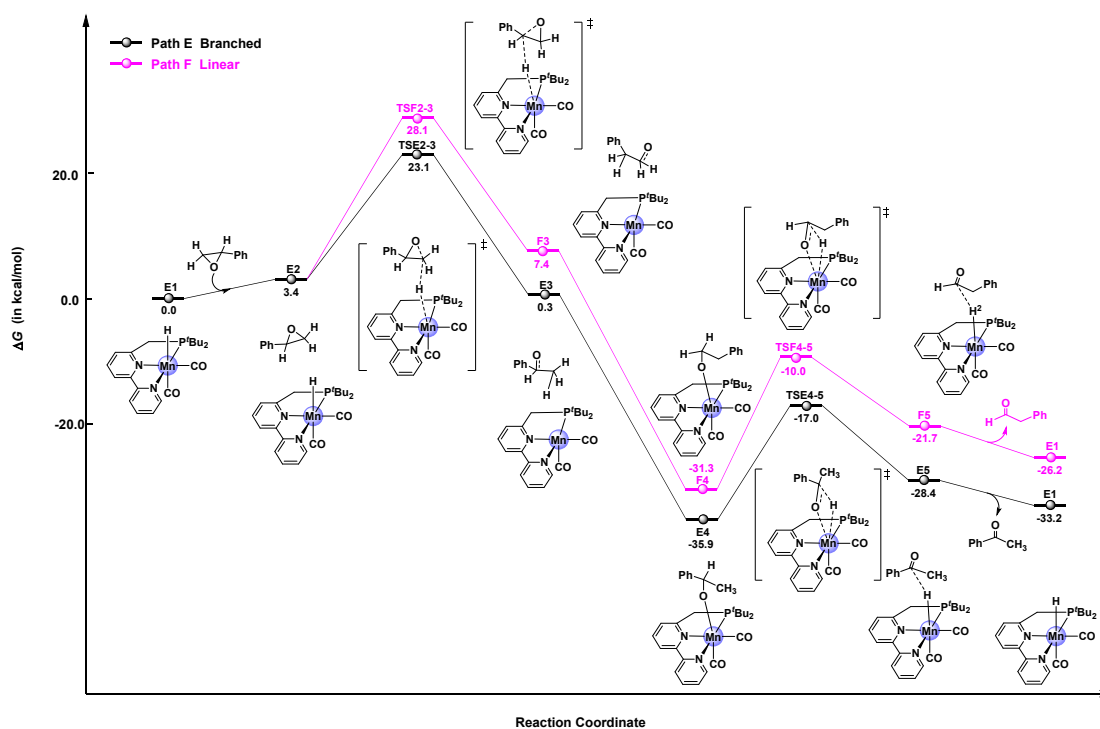
**Figure S1.** The Gibbs free energy profiles of isomerization of epoxides to aldehydes catalyzed by Ru-PNN complex A1 (in kcal/mol at 298.15 K and 1.0 atm pressure).

2. The Gibbs free energy profiles of the epoxide ring-opening through the branched (Path C) and linear (Path B) pathways



**Figure S2.** The Gibbs free energy profiles of the epoxide ring-opening through the branched (Path C) and linear (Path B) pathways catalyzed by Ru-PNN complex **A15** (in kcal/mol at 298.15 K and 1.0 atm pressure).

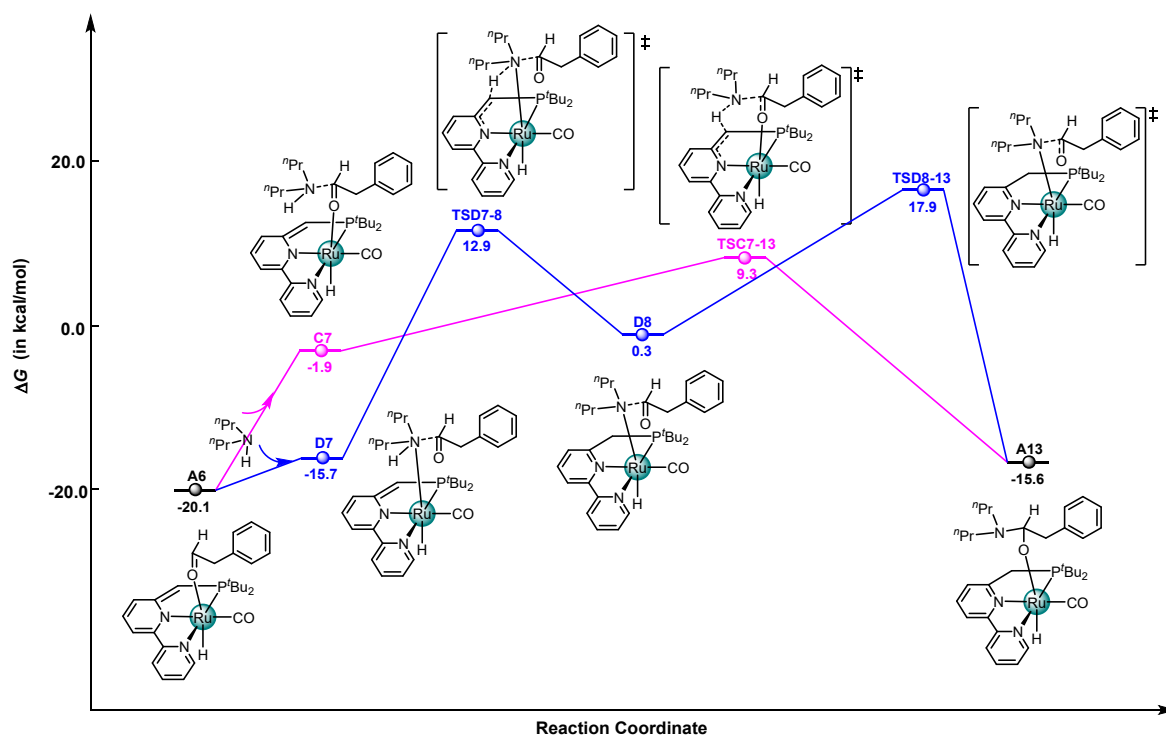
### 3. The Gibbs free energy profiles of the epoxide ring-opening through the branched (Path E) and linear (Path F) pathways



**Figure S3.** The Gibbs free energy profiles of the epoxide ring-opening through the branched (Path E) and linear (Path F) pathways catalyzed by Mn-PNN complex **E1** (in kcal/mol at 298.15 K and 1.0 atm pressure).

#### 4. The Gibbs free energy profiles of aldimine condensation catalyzed by Ru-PNN

complex



**Figure S4.** The Gibbs free energy profiles of aldimine condensation catalyzed by Ru-PNN complex (in kcal/mol at 298.15 K and 1.0 atm pressure).

## 5. Energies of all the structures

**Table S1.** The calculated absolute electronic energies ( $E$ , in a.u.), thermal free energies ( $G$ , in a.u.), and relative Gibbs energies ( $\Delta G$ , in kcal/mol) (Calculated at 298.15 K and 1.0 atm).

Complex	$E$	$G$	$\Delta G$
<b>A1</b>	-1399.607935	-1399.226145	0.0
<b><sup>t</sup>BuOK</b>	-833.057608	-832.968038	/
<b>C<sub>8</sub>H<sub>8</sub>O</b>	-384.871459	-384.762524	/
<b>(CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>)<sub>2</sub>NH</b>	-292.457353	-292.28358	/
<b>PhCH<sub>2</sub>CON(CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>)<sub>2</sub></b>	-676.200014	-675.913835	/
<b>PhCOCH<sub>3</sub></b>	-384.919532	-384.812468	/
<b>H<sub>2</sub></b>	-1.176146	-1.177473	/
<b>A2</b>	-1784.496067	-1783.981389	2.7
<b>A3</b>	-2617.581542	-2616.952873	0.5
<b>A4</b>	-2617.542536	-2616.914109	24.8
<b>A5</b>	-2617.622362	-2616.995787	-26.4
<b>A6</b>	-1784.530272	-1784.017713	-20.1
<b>A7</b>	-384.906207	-384.801336	-26.2
<b>A8</b>	-1510.464381	-1510.04859	-23.5
<b>A9</b>	-1510.482959	-1510.061844	-31.8
<b>A10</b>	-1510.476652	-1510.056047	-28.2
<b>A11</b>	-677.377075	-677.068878	-16.2
<b>A12</b>	-2077.012826	-2076.295688	-16.6
<b>A13</b>	-2077.013877	-2076.294021	-15.6
<b>A14</b>	-2077.031916	-2076.319325	-31.4
<b>A15</b>	-1400.812725	-1400.410477	-34.6
<b>A16</b>	-1693.285311	-1692.685145	-29.0
<b>A17</b>	-1693.258944	-1692.654729	-9.9

<b>A18</b>	-1693.267731	-1692.670188	-19.6
<b>B8</b>	-969.844622	-969.343923	-10.8
<b>B9</b>	-969.850825	-969.344596	-11.2
<b>B16</b>	-1785.698624	-1785.166681	-16.3
<b>B17</b>	-1785.699311	-1785.163483	-14.3
<b>B18</b>	-1785.756748	-1785.216469	-47.5
<b>C7</b>	-2076.990162	-2076.272286	-1.9
<b>C17</b>	-1785.708288	-1785.17061	-18.8
<b>C18</b>	-1785.762783	-1785.22499	-52.9
<b>D7</b>	-2077.013877	-2076.294021	-15.7
<b>D8</b>	-2076.979113	-2076.268718	0.3
<b>TSA3-4</b>	-2617.539609	-2616.911603	26.4
<b>TSA4-5</b>	-2617.540032	-2616.914386	24.7
<b>TSA8-9</b>	-1510.459717	-1510.039448	-17.8
<b>TSA9-10</b>	-1510.475671	-1510.055402	-27.8
<b>TSA12-13</b>	-2076.988555	-2076.276319	-4.4
<b>TSA12-14</b>	-2076.967474	-2076.25333	10.0
<b>TSA13-14</b>	-2076.973874	-2076.258187	6.9
<b>TSA15-1</b>	-1400.75813	-1400.36144	-3.8
<b>TSA16-17</b>	-1693.24998	-1692.649544	-6.6
<b>TSA17-18</b>	-1693.254754	-1692.657377	-11.5
<b>TSB2-6</b>	-1784.431502	-1783.920832	40.7
<b>TSB3-5</b>	-2617.477337	-2616.852384	63.3
<b>TSB8-9</b>	-969.81141	-969.304998	13.6
<b>TSB16-17</b>	-1785.658718	-1785.126319	9.0
<b>TSC7-13</b>	-2076.971745	-2076.254475	9.3
<b>TSC16-17</b>	-1785.66456	-1785.129539	7.0
<b>TSD7-8</b>	-2077.004705	-2076.294297	12.9
<b>TSD8-13</b>	-2076.960626	-2076.240643	17.9

<b>E1</b>	-2569.5923	-2569.188313	0.0
<b>E2</b>	-2954.47817	-2953.942474	3.4
<b>E3</b>	-2954.482573	-2953.947393	0.3
<b>E4</b>	-2954.543584	-2954.005065	-35.9
<b>E5</b>	-2954.528229	-2953.993131	-28.4
<b>F3</b>	-2954.472452	-2953.936086	7.4
<b>F4</b>	-2954.538144	-2953.99765	-31.3
<b>F5</b>	-2954.513055	-2953.982349	-21.7
<b>TSE2-3</b>	-2954.442798	-2953.911054	23.1
<b>TSE4-5</b>	-2954.510719	-2953.974849	-17.0
<b>TSF2-3</b>	-2954.436899	-2953.903103	28.1
<b>TSF4-5</b>	-2954.499753	-2953.963824	-10.0

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## 6. Frequencies of transition states

**Table S2.** Calculated imaginary frequencies of transition states at  $\omega$ B97X-D/BS-I level.

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<b>TSA3-4</b>	142.32 <i>i</i>
<b>TSA4-5</b>	530.20 <i>i</i>
<b>TSA8-9</b>	109.40 <i>i</i>
<b>TSA9-10</b>	406.04 <i>i</i>
<b>TSA12-13</b>	1424.16 <i>i</i>
<b>TSA12-14</b>	998.99 <i>i</i>
<b>TSA13-14</b>	584.77 <i>i</i>
<b>TSA15-1</b>	1473.38 <i>i</i>
<b>TSA16-17</b>	814.93 <i>i</i>
<b>TSA17-18</b>	1069.26 <i>i</i>
<b>TSB2-6</b>	261.46 <i>i</i>
<b>TSB3-5</b>	602.48 <i>i</i>
<b>TSB8-9</b>	1164.38 <i>i</i>
<b>TSB16-17</b>	855.52 <i>i</i>
<b>TSC7-13</b>	1489.38 <i>i</i>
<b>TSC16-17</b>	875.01 <i>i</i>
<b>TSD7-8</b>	1352.24 <i>i</i>
<b>TSD8-13</b>	111.07 <i>i</i>
<b>TSE2-3</b>	851.25 <i>i</i>
<b>TSE4-5</b>	515.04 <i>i</i>
<b>TSF2-3</b>	844.38 <i>i</i>
<b>TSF4-5</b>	413.84 <i>i</i>

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## 7. Cartesian coordinates of all the structures

**Table S3.** Atomic cartesian coordinates of intermediates and transition states

(presented in Å).

**A1**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
44	-0.365377000	-0.755300000	-0.032090000
6	-3.176845000	0.268339000	-0.013246000
6	-4.571483000	0.303335000	-0.007835000
6	-5.290013000	-0.882403000	0.021320000
6	-4.602684000	-2.090602000	0.044670000
6	-3.217856000	-2.058045000	0.037297000
7	-2.517791000	-0.914886000	0.010657000
1	-6.374890000	-0.861638000	0.024547000
1	-5.093156000	1.251725000	-0.028889000
1	-5.120974000	-3.041868000	0.066244000
1	-2.633486000	-2.970864000	0.049488000
6	-2.330942000	1.491169000	-0.048307000
6	-2.847785000	2.766089000	-0.078209000
6	-1.926788000	3.843107000	-0.126751000
6	-0.584493000	3.613223000	-0.148662000
6	-0.068692000	2.266602000	-0.121899000
7	-0.999812000	1.245617000	-0.053477000
1	-2.302259000	4.862213000	-0.149338000
1	-3.912390000	2.956455000	-0.071047000
1	0.123413000	4.434220000	-0.190085000
6	1.279918000	1.957073000	-0.154899000
1	2.010775000	2.757975000	-0.175560000
15	1.742852000	0.247911000	-0.031620000
6	0.196424000	-2.530259000	-0.112507000
8	0.537580000	-3.636907000	-0.219077000
6	2.559018000	0.018249000	1.669640000
6	1.554716000	0.600913000	2.680113000
6	2.758790000	-1.466224000	2.010062000
6	3.888576000	0.767115000	1.812063000
1	1.404015000	1.672514000	2.530519000
1	0.575338000	0.110464000	2.610045000
1	1.927548000	0.441503000	3.698986000
1	3.441673000	-1.975164000	1.327879000
1	3.180839000	-1.552779000	3.019194000
1	1.808719000	-2.008095000	1.999979000

1	4.213493000	0.744019000	2.860021000
1	4.683175000	0.307784000	1.217258000
1	3.795213000	1.818061000	1.519670000
6	2.971079000	-0.076224000	-1.428528000
6	3.720127000	-1.399499000	-1.233217000
6	2.143545000	-0.164230000	-2.722359000
6	3.975198000	1.076389000	-1.590773000
1	4.458584000	-1.342196000	-0.428222000
1	3.036397000	-2.228217000	-1.023050000
1	4.262958000	-1.646356000	-2.153750000
1	1.487055000	0.704248000	-2.837837000
1	2.823750000	-0.195930000	-3.582298000
1	1.524286000	-1.064618000	-2.744252000
1	4.658977000	0.841909000	-2.415622000
1	3.466325000	2.011808000	-1.839447000
1	4.582520000	1.243130000	-0.699106000
1	-0.350364000	-0.800329000	-1.574553000

A2

Coordinates (Angstroms)

	X	Y	Z
44	0.190816000	-0.080888000	-0.585399000
6	-1.847899000	2.108403000	-0.567783000
6	-3.038848000	2.806253000	-0.769902000
6	-4.106181000	2.180770000	-1.397507000
6	-3.965524000	0.863740000	-1.816490000
6	-2.761484000	0.221966000	-1.574983000
7	-1.730930000	0.818390000	-0.962985000
1	-5.034090000	2.718799000	-1.561738000
1	-3.127104000	3.837064000	-0.450848000
1	-4.769490000	0.332819000	-2.311666000
1	-2.605773000	-0.810221000	-1.863083000
6	-0.642220000	2.716646000	0.057773000
6	-0.603674000	4.016776000	0.516547000
6	0.623242000	4.478338000	1.052666000
6	1.719458000	3.668192000	1.088884000
6	1.652710000	2.316500000	0.590597000
7	0.422117000	1.889313000	0.126323000
1	0.690939000	5.494475000	1.431455000
1	-1.461772000	4.673631000	0.466028000
1	2.662940000	4.026802000	1.487155000
6	2.733681000	1.452437000	0.555287000
1	3.690599000	1.785487000	0.944099000

15	2.471254000	-0.208236000	-0.013381000
6	0.022824000	-1.770917000	-1.337577000
8	-0.071332000	-2.808106000	-1.859785000
6	2.895046000	-1.367781000	1.444252000
6	2.321050000	-0.723269000	2.717135000
6	2.203020000	-2.723335000	1.229686000
6	4.393801000	-1.588421000	1.690276000
1	2.841592000	0.204710000	2.967236000
1	1.258668000	-0.504172000	2.608882000
1	2.442872000	-1.422054000	3.555216000
1	2.522878000	-3.218001000	0.308748000
1	2.440244000	-3.395778000	2.064220000
1	1.116813000	-2.602857000	1.187768000
1	4.518785000	-2.164189000	2.616189000
1	4.881959000	-2.153402000	0.892836000
1	4.925159000	-0.641124000	1.824700000
6	3.711768000	-0.502644000	-1.422337000
6	3.772706000	-1.986408000	-1.808079000
6	3.225424000	0.289581000	-2.648059000
6	5.115393000	0.027801000	-1.085075000
1	4.241876000	-2.605151000	-1.038873000
1	2.775529000	-2.389277000	-2.012040000
1	4.366532000	-2.100846000	-2.723438000
1	3.017381000	1.334795000	-2.398198000
1	4.010043000	0.273105000	-3.414641000
1	2.321049000	-0.144523000	-3.078962000
1	5.768019000	-0.110856000	-1.955725000
1	5.083335000	1.099381000	-0.866051000
1	5.587289000	-0.480751000	-0.244747000
6	-1.441739000	0.261526000	2.480366000
6	-1.804843000	-1.141427000	2.255779000
8	-0.649660000	-0.565921000	1.631352000
1	-0.952732000	0.558965000	3.404892000
1	-1.529048000	-1.863116000	3.024367000
1	0.649316000	0.410070000	-1.988581000
6	-2.940680000	-1.538577000	1.373367000
6	-4.165448000	-0.875502000	1.440472000
6	-2.783594000	-2.606791000	0.486690000
6	-5.223853000	-1.272922000	0.627318000
1	-4.291858000	-0.048068000	2.132834000
6	-3.836209000	-2.995634000	-0.334943000
1	-1.829728000	-3.122468000	0.429929000
6	-5.059336000	-2.329687000	-0.263940000
1	-6.175156000	-0.753442000	0.687380000

1	-3.701796000	-3.817183000	-1.031547000
1	-5.882541000	-2.636983000	-0.901752000
1	-1.999407000	1.041553000	1.967815000

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**A3**

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Coordinates (Angstroms)

	X	Y	Z
44	1.127489000	0.052226000	0.812902000
6	-0.500137000	2.546333000	0.929343000
6	-1.377790000	3.527392000	1.385994000
6	-2.180240000	3.274566000	2.488155000
6	-2.090798000	2.041998000	3.121996000
6	-1.192653000	1.113174000	2.623368000
7	-0.418054000	1.350734000	1.557706000
1	-2.870750000	4.031655000	2.843996000
1	-1.433772000	4.483457000	0.882574000
1	-2.697095000	1.798330000	3.986391000
1	-1.071885000	0.143788000	3.093508000
6	0.397764000	2.738456000	-0.240183000
6	0.341586000	3.838233000	-1.068159000
6	1.239228000	3.874868000	-2.162157000
6	2.134446000	2.866154000	-2.370590000
6	2.184921000	1.735791000	-1.478966000
7	1.270289000	1.727334000	-0.443260000
1	1.214404000	4.721256000	-2.842849000
1	-0.377121000	4.632343000	-0.917828000
1	2.829003000	2.899367000	-3.203301000
6	3.078890000	0.682144000	-1.608572000
15	3.101106000	-0.540578000	-0.324556000
6	1.063769000	-1.406582000	1.944029000
8	1.018767000	-2.322772000	2.671950000
6	4.670282000	-0.247964000	0.715433000
6	4.765611000	1.268552000	0.956342000
6	4.572147000	-0.952000000	2.077669000
6	5.957294000	-0.686357000	0.004258000
1	4.956744000	1.810054000	0.026223000
1	3.851629000	1.673512000	1.400058000
1	5.593307000	1.468814000	1.647633000
1	4.445578000	-2.033635000	1.990411000
1	5.496533000	-0.775244000	2.641583000
1	3.739361000	-0.560680000	2.667115000
1	6.822434000	-0.322641000	0.572057000
1	6.050706000	-1.773664000	-0.059799000

1	6.030983000	-0.267472000	-1.004638000
6	3.199263000	-2.233349000	-1.169422000
6	3.448193000	-3.348909000	-0.147219000
6	1.826816000	-2.455663000	-1.818116000
6	4.243926000	-2.307017000	-2.294337000
1	4.455813000	-3.308804000	0.273857000
1	2.729645000	-3.313618000	0.678178000
1	3.341234000	-4.323454000	-0.639342000
1	1.639948000	-1.699404000	-2.584530000
1	1.798589000	-3.441248000	-2.298306000
1	1.018233000	-2.401542000	-1.084977000
1	4.129553000	-3.262021000	-2.822147000
1	4.099321000	-1.508584000	-3.028416000
1	5.270423000	-2.259182000	-1.931326000
1	3.839564000	0.726415000	-2.381091000
1	2.067677000	0.684470000	1.872460000
6	-0.686705000	-0.327807000	-2.270248000
1	-0.185506000	0.602235000	-2.529630000
6	-1.931662000	-0.309522000	-1.508625000
1	-2.570574000	-1.197906000	-1.505695000
1	-0.484695000	-1.166023000	-2.932207000
8	-0.642369000	-0.633336000	-0.873867000
6	-2.665985000	0.923994000	-1.118158000
6	-3.623835000	0.806147000	-0.103927000
6	-2.519741000	2.135817000	-1.793993000
6	-4.413479000	1.898736000	0.236543000
1	-3.763133000	-0.177722000	0.347976000
6	-3.317626000	3.225854000	-1.454609000
1	-1.792318000	2.230537000	-2.593893000
6	-4.263404000	3.108842000	-0.439665000
1	-5.160692000	1.802460000	1.018807000
1	-3.203839000	4.164316000	-1.989090000
1	-4.890132000	3.957608000	-0.181092000
19	-1.442524000	-2.678127000	0.761239000
8	-3.645533000	-2.398737000	-0.062092000
6	-4.930930000	-2.731336000	-0.399294000
6	-5.358348000	-2.027189000	-1.708924000
1	-6.388444000	-2.262316000	-2.007671000
1	-5.277038000	-0.940594000	-1.592057000
1	-4.690846000	-2.328138000	-2.525822000
6	-5.058527000	-4.258253000	-0.609950000
1	-4.798310000	-4.784159000	0.317440000
1	-6.066903000	-4.575453000	-0.908105000
1	-4.354855000	-4.578348000	-1.387818000

6	-5.915071000	-2.312214000	0.717405000
1	-6.957242000	-2.581558000	0.500151000
1	-5.627290000	-2.790593000	1.661423000
1	-5.872211000	-1.226525000	0.865321000

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#### A4

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Coordinates (Angstroms)			
	X	Y	Z
44	1.067848000	-1.190517000	0.210054000
6	-1.455548000	-0.875475000	1.820610000
6	-2.640364000	-1.167777000	2.494508000
6	-3.123277000	-2.463712000	2.510717000
6	-2.402492000	-3.456922000	1.855890000
6	-1.242323000	-3.095860000	1.192475000
7	-0.784004000	-1.835002000	1.146629000
1	-4.047366000	-2.697071000	3.028574000
1	-3.188436000	-0.378593000	2.992742000
1	-2.725597000	-4.491636000	1.857150000
1	-0.633226000	-3.837504000	0.684236000
6	-0.844553000	0.477772000	1.827501000
6	-1.294826000	1.521266000	2.596001000
6	-0.601853000	2.760796000	2.512254000
6	0.484772000	2.895626000	1.706943000
6	0.966640000	1.771746000	0.946393000
7	0.219570000	0.609650000	0.986270000
1	-0.947657000	3.602268000	3.104623000
1	-2.133067000	1.412065000	3.271391000
1	1.025751000	3.833747000	1.647049000
6	2.125102000	1.793200000	0.181198000
15	2.909457000	0.208896000	-0.143182000
6	1.841675000	-2.754156000	-0.402190000
8	2.331123000	-3.742530000	-0.779544000
6	4.227263000	0.045062000	1.238183000
6	3.572496000	0.482754000	2.560563000
6	4.669755000	-1.419662000	1.384664000
6	5.458475000	0.938151000	1.032626000
1	3.383825000	1.559521000	2.582607000
1	2.628410000	-0.035655000	2.744210000
1	4.255060000	0.243992000	3.385361000
1	5.110923000	-1.827265000	0.472433000
1	5.428245000	-1.487881000	2.174653000
1	3.826968000	-2.055913000	1.664836000
1	6.064633000	0.922241000	1.946981000

1	6.102109000	0.594779000	0.219414000
1	5.183272000	1.980936000	0.844813000
6	3.788343000	0.336389000	-1.821569000
6	4.735939000	-0.858963000	-2.001063000
6	2.721746000	0.262245000	-2.927581000
6	4.553966000	1.653823000	-2.025247000
1	5.588939000	-0.828197000	-1.319749000
1	4.214964000	-1.811706000	-1.861802000
1	5.138432000	-0.848133000	-3.021010000
1	2.184686000	1.211345000	-3.012624000
1	3.223175000	0.091579000	-3.888422000
1	1.981826000	-0.524152000	-2.755777000
1	4.877440000	1.712597000	-3.072094000
1	3.912989000	2.520769000	-1.836345000
1	5.446858000	1.742615000	-1.406567000
1	2.696989000	2.717004000	0.152154000
1	1.685631000	-1.510737000	1.641604000
6	-0.251764000	0.639207000	-1.844823000
1	0.633300000	1.283298000	-1.594341000
6	-1.342692000	1.120858000	-1.000002000
1	-2.083009000	0.378285000	-0.637448000
1	-0.507824000	0.977487000	-2.878474000
8	0.020881000	-0.688871000	-1.761827000
6	-1.658321000	2.495415000	-0.776278000
6	-2.797314000	2.779772000	0.002521000
6	-0.863354000	3.563214000	-1.250334000
6	-3.135192000	4.092416000	0.304145000
1	-3.397792000	1.947036000	0.354047000
6	-1.203861000	4.867124000	-0.943334000
1	0.028787000	3.357455000	-1.832317000
6	-2.335363000	5.131657000	-0.162637000
1	-4.014977000	4.305960000	0.902324000
1	-0.589701000	5.687755000	-1.299794000
1	-2.592228000	6.159594000	0.075366000
19	-1.837854000	-2.383101000	-1.819430000
8	-3.421552000	-0.874386000	-0.676684000
6	-4.755582000	-0.705232000	-0.915667000
6	-4.995721000	0.396889000	-1.975725000
1	-6.056675000	0.546587000	-2.216475000
1	-4.590728000	1.352718000	-1.625202000
1	-4.467481000	0.136387000	-2.901680000
6	-5.382729000	-2.021145000	-1.444813000
1	-5.186764000	-2.828624000	-0.728292000
1	-6.467153000	-1.959352000	-1.605227000



1	-4.926092000	-2.295500000	-2.406466000
6	-5.515901000	-0.315776000	0.375474000
1	-6.589340000	-0.153322000	0.210660000
1	-5.401107000	-1.104931000	1.127225000
1	-5.096384000	0.605961000	0.795933000

A5

Coordinates (Angstroms)

	X	Y	Z
44	1.319787000	-0.549025000	0.747190000
6	-0.935863000	1.019808000	1.936499000
6	-2.073054000	1.357800000	2.672087000
6	-2.736650000	0.386613000	3.402778000
6	-2.232249000	-0.909902000	3.417348000
6	-1.089208000	-1.174720000	2.683545000
7	-0.466490000	-0.248450000	1.937908000
1	-3.630678000	0.639049000	3.962738000
1	-2.436386000	2.376973000	2.666448000
1	-2.705931000	-1.700235000	3.987432000
1	-0.632703000	-2.159415000	2.694740000
6	-0.171394000	2.006577000	1.131461000
6	-0.602976000	3.294620000	0.911401000
6	0.220533000	4.129334000	0.118198000
6	1.388414000	3.662940000	-0.409448000
6	1.797545000	2.297622000	-0.193804000
7	0.981904000	1.526958000	0.610092000
1	-0.089795000	5.152147000	-0.075038000
1	-1.550454000	3.655624000	1.286348000
1	2.017604000	4.299490000	-1.022684000
6	2.922257000	1.727291000	-0.771203000
15	3.286427000	0.032364000	-0.397837000
6	1.618428000	-2.374414000	0.845142000
8	1.777539000	-3.529156000	0.921056000
6	4.844102000	0.008346000	0.694155000
6	4.637912000	1.081697000	1.777272000
6	5.010131000	-1.354273000	1.383187000
6	6.124384000	0.364409000	-0.073821000
1	4.608421000	2.085582000	1.345331000
1	3.708843000	0.928025000	2.332866000
1	5.470601000	1.036827000	2.489892000
1	5.127571000	-2.177191000	0.674499000
1	5.907587000	-1.334965000	2.014269000
1	4.153296000	-1.578906000	2.023799000

1	6.947313000	0.489579000	0.640565000
1	6.425080000	-0.416275000	-0.776884000
1	6.020841000	1.308176000	-0.619332000
6	3.642849000	-0.816688000	-2.057152000
6	4.278916000	-2.198638000	-1.861994000
6	2.282302000	-1.005408000	-2.743812000
6	4.514678000	0.040716000	-2.987702000
1	5.304823000	-2.137829000	-1.490040000
1	3.697981000	-2.820677000	-1.173363000
1	4.315543000	-2.720128000	-2.826372000
1	1.765625000	-0.048109000	-2.860358000
1	2.434146000	-1.432787000	-3.742642000
1	1.635819000	-1.679845000	-2.176857000
1	4.624130000	-0.472955000	-3.950832000
1	4.048728000	1.010682000	-3.183134000
1	5.517524000	0.213954000	-2.596069000
1	3.597798000	2.352352000	-1.345431000
1	2.156884000	-0.428750000	2.056489000
6	-0.741907000	0.405149000	-1.667003000
1	-0.107596000	1.301784000	-1.768233000
6	-2.105987000	0.462783000	-2.275559000
1	-2.640644000	-0.479868000	-2.085871000
1	-1.997149000	0.662249000	-3.348538000
8	-0.326615000	-0.551851000	-1.027269000
6	-2.834794000	1.606766000	-1.591329000
6	-3.592810000	1.318349000	-0.453251000
6	-2.721415000	2.925753000	-2.034429000
6	-4.252709000	2.346188000	0.215881000
1	-3.672924000	0.270069000	-0.152156000
6	-3.374411000	3.950814000	-1.355774000
1	-2.127051000	3.152665000	-2.916244000
6	-4.143004000	3.662202000	-0.229260000
1	-4.858218000	2.115598000	1.088295000
1	-3.286891000	4.973937000	-1.709084000
1	-4.660694000	4.461716000	0.292998000
19	-1.475872000	-2.793425000	-0.221284000
8	-3.622934000	-1.836314000	-0.665349000
6	-4.948412000	-2.158558000	-0.780002000
6	-5.591392000	-1.428609000	-1.981825000
1	-6.656276000	-1.662750000	-2.112739000
1	-5.493461000	-0.345083000	-1.851775000
1	-5.065531000	-1.702891000	-2.904262000
6	-5.122428000	-3.683514000	-0.989389000
1	-4.696929000	-4.223896000	-0.132878000

1	-6.169539000	-3.996446000	-1.097559000
1	-4.580447000	-3.995097000	-1.891183000
6	-5.723372000	-1.762465000	0.499831000
1	-6.787382000	-2.032315000	0.463552000
1	-5.272416000	-2.255960000	1.369744000
1	-5.654873000	-0.679949000	0.659474000

**A6**

Coordinates (Angstroms)

	X	Y	Z
44	-0.760316000	1.118806000	0.361604000
6	1.649726000	2.465907000	-0.805823000
6	2.700836000	3.364996000	-0.990868000
6	2.871938000	4.416302000	-0.102481000
6	1.986486000	4.554442000	0.960170000
6	0.963246000	3.628808000	1.087922000
7	0.795285000	2.609871000	0.234818000
1	3.684535000	5.121779000	-0.240923000
1	3.381659000	3.243873000	-1.823888000
1	2.077862000	5.360872000	1.678287000
1	0.240332000	3.693630000	1.892859000
6	1.395897000	1.308821000	-1.707307000
6	2.167468000	1.030611000	-2.815854000
6	1.797189000	-0.088990000	-3.600457000
6	0.697879000	-0.830886000	-3.283681000
6	-0.108701000	-0.498124000	-2.134051000
7	0.344881000	0.542793000	-1.341452000
1	2.392342000	-0.349218000	-4.471342000
1	3.015987000	1.640009000	-3.096358000
1	0.400809000	-1.676350000	-3.895626000
6	-1.271439000	-1.162733000	-1.790543000
15	-2.087674000	-0.703944000	-0.282141000
6	-1.853147000	1.722121000	1.741807000
8	-2.563464000	2.124517000	2.570386000
6	-1.963875000	-2.209576000	0.876523000
6	-0.521912000	-2.727669000	0.740620000
6	-2.197873000	-1.767809000	2.329691000
6	-2.900394000	-3.374034000	0.529704000
1	-0.358195000	-3.205323000	-0.228570000
1	0.211501000	-1.927306000	0.839949000
1	-0.322455000	-3.467162000	1.526403000
1	-3.185400000	-1.324261000	2.480690000
1	-2.123873000	-2.638497000	2.994096000
1	-1.447232000	-1.038088000	2.643585000

1	-2.642807000	-4.237264000	1.156823000
1	-3.952652000	-3.145178000	0.716523000
1	-2.790183000	-3.686701000	-0.513615000
6	-3.904408000	-0.378205000	-0.719769000
6	-4.778985000	-0.299021000	0.538301000
6	-3.972463000	0.978111000	-1.441977000
6	-4.462986000	-1.434434000	-1.687716000
1	-4.894503000	-1.267197000	1.032459000
1	-4.380495000	0.414815000	1.266109000
1	-5.783220000	0.043842000	0.260010000
1	-3.253455000	1.031203000	-2.265436000
1	-4.978721000	1.111989000	-1.858230000
1	-3.770888000	1.809008000	-0.762306000
1	-5.500928000	-1.179442000	-1.935195000
1	-3.895676000	-1.450463000	-2.622947000
1	-4.468826000	-2.442363000	-1.271786000
6	1.848782000	-0.248497000	2.244662000
8	0.692621000	0.052552000	2.024427000
1	-1.621025000	1.964284000	-0.619301000
1	-1.596148000	-2.007875000	-2.388888000
1	2.107129000	-0.694523000	3.223489000
6	2.984140000	-0.129536000	1.267374000
1	2.680978000	0.485155000	0.421216000
1	3.829965000	0.344551000	1.777711000
6	3.356755000	-1.526929000	0.810759000
6	2.798343000	-2.042496000	-0.360790000
6	4.202378000	-2.331877000	1.576888000
6	3.088215000	-3.342090000	-0.763769000
1	2.133493000	-1.424604000	-0.956406000
6	4.489263000	-3.633447000	1.175206000
1	4.645034000	-1.936101000	2.487707000
6	3.931972000	-4.141262000	0.004109000
1	2.648747000	-3.728286000	-1.678301000
1	5.149484000	-4.250566000	1.776926000
1	4.155455000	-5.156774000	-0.308157000

A7

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Coordinates (Angstroms)

	X	Y	Z
6	-1.830822000	1.313906000	-0.055953000
6	-0.504167000	1.137588000	0.323517000
6	0.041283000	-0.144554000	0.427762000
6	-0.763857000	-1.245876000	0.129735000

6	-2.090269000	-1.071508000	-0.255113000
6	-2.627283000	0.209058000	-0.347438000
1	-2.243850000	2.315351000	-0.126272000
1	0.115907000	2.001978000	0.545987000
1	-0.350550000	-2.248131000	0.208220000
1	-2.704816000	-1.937944000	-0.479238000
1	-3.663106000	0.346690000	-0.641216000
6	1.497810000	-0.323634000	0.793137000
1	1.839896000	0.433035000	1.503448000
1	1.651714000	-1.312838000	1.243334000
6	2.371199000	-0.256798000	-0.441502000
8	3.342580000	0.452081000	-0.553597000
1	2.050804000	-0.923874000	-1.270369000

**A8**

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Coordinates (Angstroms)			
	X	Y	Z
-----			
19	1.287287000	-0.691944000	-2.181290000
8	3.110972000	-0.036050000	-0.789640000
6	4.342660000	0.135251000	-0.208819000
6	4.583030000	-0.929279000	0.885255000
1	4.513941000	-1.932395000	0.448251000
1	5.563007000	-0.833709000	1.370710000
1	3.811650000	-0.846594000	1.660470000
6	5.453764000	0.001144000	-1.271911000
1	5.391173000	-0.985840000	-1.745426000
1	5.312679000	0.758522000	-2.052000000
1	6.463666000	0.119839000	-0.858059000
6	4.453004000	1.531233000	0.443895000
1	3.677377000	1.645054000	1.211465000
1	5.427177000	1.706988000	0.918357000
1	4.295579000	2.310070000	-0.311392000
6	-1.655296000	-0.276434000	-0.778298000
8	-1.306880000	-1.079853000	-1.625596000
6	-2.434368000	-0.640424000	0.457313000
1	-2.020086000	-0.085967000	1.303527000
1	-2.330400000	-1.712462000	0.643150000
7	0.771311000	0.189082000	0.665140000
6	0.772754000	-0.818402000	1.715455000
1	1.552783000	-0.617314000	2.474199000
1	-0.184849000	-0.801012000	2.255984000
6	1.003305000	-2.202588000	1.115508000
1	0.182277000	-2.428667000	0.422317000

1	1.926220000	-2.157239000	0.522963000
6	1.115414000	-3.298296000	2.169688000
1	0.205779000	-3.359581000	2.778073000
1	1.273726000	-4.278614000	1.710053000
1	1.955843000	-3.108416000	2.845830000
6	0.606405000	1.545822000	1.161054000
1	-0.399455000	1.668537000	1.594488000
1	1.318790000	1.772104000	1.977115000
6	0.818321000	2.553330000	0.033504000
1	0.026931000	2.426926000	-0.718120000
1	1.765168000	2.304953000	-0.461190000
6	0.838146000	3.997329000	0.522430000
1	0.970966000	4.698228000	-0.307253000
1	-0.095779000	4.259853000	1.032646000
1	1.659317000	4.160480000	1.228699000
6	-3.883527000	-0.250865000	0.239302000
6	-4.398994000	0.930149000	0.775422000
6	-4.710010000	-1.054565000	-0.550496000
6	-5.721711000	1.295365000	0.538506000
1	-3.763689000	1.562521000	1.390143000
6	-6.031379000	-0.691979000	-0.786105000
1	-4.312139000	-1.970143000	-0.979512000
6	-6.540765000	0.484734000	-0.241571000
1	-6.113252000	2.212390000	0.967773000
1	-6.664759000	-1.328494000	-1.396072000
1	-7.573264000	0.765993000	-0.423238000
1	-1.511155000	0.808282000	-0.932637000
1	1.719921000	0.147146000	0.218317000

**A9**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
19	-2.221246000	1.487765000	-0.661045000
8	0.211771000	2.559896000	-0.775486000
6	1.040397000	3.007523000	0.284120000
6	2.426593000	2.368250000	0.158702000
1	2.876473000	2.638674000	-0.802247000
1	3.096153000	2.705994000	0.957837000
1	2.345249000	1.275522000	0.203034000
6	1.134135000	4.527088000	0.158098000
1	1.571065000	4.799245000	-0.807269000
1	0.139226000	4.981780000	0.221849000
1	1.756416000	4.953023000	0.952165000
6	0.408441000	2.632443000	1.632964000

1	0.290450000	1.546566000	1.710609000
1	1.023265000	2.962552000	2.477270000
1	-0.578048000	3.102439000	1.738889000
6	0.167861000	-0.768627000	-0.056905000
8	-0.160431000	0.065627000	-1.062040000
6	-0.733563000	-2.057579000	-0.081609000
1	-0.485725000	-2.708431000	0.765219000
1	-0.528320000	-2.607824000	-1.005584000
7	1.613493000	-1.093289000	-0.061138000
6	2.089719000	-1.570314000	-1.351521000
1	2.100317000	-2.676910000	-1.402129000
1	1.376962000	-1.210829000	-2.098915000
6	3.477301000	-1.033333000	-1.703449000
1	3.415843000	0.059718000	-1.744984000
1	4.192366000	-1.275925000	-0.907048000
6	3.992896000	-1.582238000	-3.030814000
1	3.302773000	-1.346303000	-3.848695000
1	4.968709000	-1.157891000	-3.286743000
1	4.103589000	-2.672183000	-2.995488000
6	2.103931000	-1.891038000	1.049370000
1	1.664131000	-2.909202000	1.067885000
1	3.179757000	-2.040155000	0.895558000
6	1.918662000	-1.246542000	2.423950000
1	0.855661000	-1.204853000	2.687990000
1	2.271058000	-0.209460000	2.372903000
6	2.670729000	-2.005783000	3.513860000
1	2.520156000	-1.545951000	4.495473000
1	2.332023000	-3.045950000	3.579413000
1	3.748128000	-2.020831000	3.315406000
6	-2.175323000	-1.655595000	-0.018634000
6	-2.731806000	-1.192882000	1.182602000
6	-2.967249000	-1.595386000	-1.172783000
6	-4.022960000	-0.667558000	1.226469000
1	-2.140684000	-1.238569000	2.093776000
6	-4.262032000	-1.080305000	-1.134410000
1	-2.552018000	-1.944048000	-2.113481000
6	-4.793631000	-0.602118000	0.064683000
1	-4.430960000	-0.315001000	2.169312000
1	-4.856533000	-1.050061000	-2.043004000
1	-5.801894000	-0.201132000	0.097641000
1	-0.009169000	-0.324426000	0.951005000
1	0.287472000	1.545692000	-0.877769000

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**A10**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
19	-2.117866000	-1.550333000	0.842279000
8	0.209368000	-2.212314000	0.676406000
6	1.394592000	-2.907606000	0.504726000
6	2.584798000	-2.082585000	1.029922000
1	2.456029000	-1.887730000	2.100951000
1	3.543416000	-2.596990000	0.888971000
1	2.628297000	-1.113130000	0.521535000
6	1.328096000	-4.238359000	1.276041000
1	1.164586000	-4.042286000	2.341551000
1	0.488779000	-4.842418000	0.910964000
1	2.245571000	-4.830877000	1.172119000
6	1.608622000	-3.207203000	-0.990956000
1	1.633815000	-2.267644000	-1.551278000
1	2.540914000	-3.751101000	-1.188859000
1	0.774318000	-3.806582000	-1.374673000
6	0.269855000	0.851510000	-0.146772000
8	-0.007168000	0.180120000	1.030106000
6	-0.793116000	1.964096000	-0.341597000
1	-0.554671000	2.545348000	-1.239864000
1	-0.758900000	2.646283000	0.512965000
7	1.652971000	1.341175000	-0.211669000
6	1.982801000	2.447470000	0.685219000
1	3.036184000	2.693486000	0.503007000
1	1.415673000	3.367480000	0.440902000
6	1.830742000	2.147383000	2.175303000
1	0.783891000	1.951366000	2.415412000
1	2.368617000	1.219906000	2.397698000
6	2.368187000	3.294429000	3.027552000
1	1.841240000	4.232564000	2.816374000
1	2.247931000	3.083508000	4.094616000
1	3.434582000	3.467708000	2.842283000
6	2.107158000	1.608072000	-1.574302000
1	1.433342000	2.296880000	-2.121514000
1	3.065073000	2.134660000	-1.498054000
6	2.340180000	0.356337000	-2.420123000
1	1.399669000	-0.180035000	-2.588510000
1	2.989596000	-0.322542000	-1.857390000
6	2.967972000	0.690548000	-3.770865000
1	3.137175000	-0.215659000	-4.359848000
1	2.323811000	1.353441000	-4.359881000
1	3.934362000	1.191788000	-3.647269000
6	-2.170999000	1.374437000	-0.466432000



6	-2.516959000	0.613457000	-1.591609000
6	-3.112134000	1.494733000	0.562339000
6	-3.754440000	-0.021174000	-1.679523000
1	-1.801711000	0.511845000	-2.403680000
6	-4.355227000	0.867406000	0.477805000
1	-2.860013000	2.077078000	1.444056000
6	-4.679274000	0.099281000	-0.641035000
1	-3.999849000	-0.604589000	-2.561812000
1	-5.073003000	0.979905000	1.285015000
1	-5.647101000	-0.386970000	-0.711023000
1	0.175541000	0.156728000	-0.997537000
1	0.278783000	-0.849160000	0.904916000

## A11

### Coordinates (Angstroms)

	X	Y	Z
6	0.416167000	0.242130000	1.273706000
8	-0.031703000	-0.963303000	1.843422000
7	1.182286000	-0.043379000	0.066606000
6	2.234142000	-1.045259000	0.277461000
1	2.364459000	-1.242512000	1.348135000
1	3.195158000	-0.655320000	-0.084009000
6	1.627413000	1.109230000	-0.710112000
1	2.180902000	0.717478000	-1.571561000
1	0.755323000	1.622052000	-1.134360000
6	-0.772761000	1.192843000	1.032416000
1	-0.437462000	2.105582000	0.530488000
1	-1.122136000	1.500918000	2.022138000
6	-1.936163000	0.573941000	0.285513000
6	-3.211379000	0.589687000	0.858808000
6	-1.783897000	-0.029635000	-0.969690000
6	-4.305301000	0.034964000	0.201461000
1	-3.347914000	1.044581000	1.836404000
6	-2.875882000	-0.590742000	-1.626609000
1	-0.797338000	-0.086997000	-1.415785000
6	-4.140679000	-0.557812000	-1.046799000
1	-5.285086000	0.062058000	0.668537000
1	-2.734753000	-1.058167000	-2.596595000
1	-4.990899000	-0.995789000	-1.560522000
6	2.503269000	2.131335000	0.026742000
1	3.355884000	1.617812000	0.487845000
1	1.933819000	2.582774000	0.848388000
6	3.003696000	3.228874000	-0.907500000

1	3.613759000	3.961906000	-0.371658000
1	3.615810000	2.812520000	-1.715168000
1	2.167905000	3.765823000	-1.369741000
6	1.928034000	-2.357532000	-0.441775000
1	1.761156000	-2.146729000	-1.505327000
1	0.985130000	-2.754357000	-0.049666000
6	3.039674000	-3.389090000	-0.277340000
1	2.795490000	-4.325661000	-0.787501000
1	3.985630000	-3.022551000	-0.692446000
1	3.210501000	-3.620668000	0.779835000
1	-0.636840000	-1.358704000	1.202489000
1	1.051124000	0.686425000	2.058768000

**A12**

Coordinates (Angstroms)

	X	Y	Z
44	-1.140391000	0.207676000	-0.940119000
6	0.534424000	-2.156787000	-1.658674000
6	1.438986000	-2.983054000	-2.326183000
6	2.251066000	-2.455213000	-3.318071000
6	2.137302000	-1.105855000	-3.637334000
6	1.200546000	-0.346204000	-2.955340000
7	0.419587000	-0.850896000	-1.989750000
1	2.960419000	-3.090368000	-3.838146000
1	1.503997000	-4.033246000	-2.070643000
1	2.749736000	-0.647745000	-4.404926000
1	1.056479000	0.705438000	-3.175890000
6	-0.332844000	-2.634087000	-0.549725000
6	-0.168296000	-3.862492000	0.057130000
6	-1.049895000	-4.181222000	1.116744000
6	-2.009397000	-3.297629000	1.519730000
6	-2.138027000	-2.011907000	0.882020000
7	-1.273843000	-1.752117000	-0.161244000
1	-0.955098000	-5.140982000	1.617009000
1	0.606669000	-4.554479000	-0.244674000
1	-2.682151000	-3.541007000	2.335501000
6	-3.052265000	-1.039477000	1.264764000
15	-3.086812000	0.478903000	0.346681000
6	-1.012027000	1.939639000	-1.592945000
8	-0.930586000	3.023559000	-2.011830000
6	-3.161640000	1.868573000	1.637880000
6	-1.761429000	1.955886000	2.263962000
6	-3.472071000	3.223529000	0.989155000
6	-4.153355000	1.591893000	2.778739000

1	-1.479704000	0.997626000	2.718761000
1	-1.016820000	2.251715000	1.520476000
1	-1.759904000	2.710085000	3.059544000
1	-4.504005000	3.289371000	0.635597000
1	-3.334029000	4.021286000	1.729628000
1	-2.804362000	3.435274000	0.147967000
1	-4.071101000	2.390119000	3.527276000
1	-5.192070000	1.565567000	2.448459000
1	-3.929357000	0.646919000	3.281849000
6	-4.680815000	0.496282000	-0.696635000
6	-4.592620000	1.555350000	-1.806025000
6	-4.786372000	-0.891710000	-1.351868000
6	-5.956664000	0.714300000	0.127677000
1	-4.473687000	2.569249000	-1.417026000
1	-3.755878000	1.352134000	-2.478583000
1	-5.516294000	1.538013000	-2.398453000
1	-4.967885000	-1.671637000	-0.607356000
1	-5.622863000	-0.890091000	-2.061608000
1	-3.877794000	-1.154138000	-1.900126000
1	-6.831459000	0.537635000	-0.510513000
1	-6.021732000	0.015261000	0.968080000
1	-6.042632000	1.734179000	0.511767000
6	1.849904000	0.684885000	0.635097000
8	0.473743000	0.290978000	0.770699000
1	-2.094706000	-0.102699000	-2.142320000
7	2.771910000	-0.246915000	1.214927000
6	2.513330000	-0.607572000	2.610271000
1	2.199871000	0.305496000	3.126808000
1	3.464286000	-0.889627000	3.078982000
6	1.468655000	-1.722210000	2.876145000
1	0.731092000	-1.734904000	2.068778000
1	0.921050000	-1.462188000	3.790454000
6	2.052653000	-3.123070000	3.055085000
1	2.802744000	-3.140383000	3.854217000
1	1.265695000	-3.835735000	3.321120000
1	2.530772000	-3.491667000	2.142648000
6	3.129155000	-1.365901000	0.351209000
1	3.134315000	-1.000242000	-0.681801000
1	2.377190000	-2.169814000	0.388969000
6	4.509282000	-1.942415000	0.654067000
1	5.253294000	-1.144001000	0.553880000
1	4.557249000	-2.291025000	1.692101000
6	4.838785000	-3.104595000	-0.278796000
1	4.825621000	-2.786685000	-1.327533000

1	5.828999000	-3.519190000	-0.068369000
1	4.108920000	-3.915449000	-0.169949000
1	-3.787913000	-1.278432000	2.025692000
1	0.148418000	0.502485000	1.651041000
6	2.023578000	2.129401000	1.126301000
1	1.180642000	2.704670000	0.730295000
1	1.960126000	2.174406000	2.219881000
6	3.317395000	2.729624000	0.636893000
6	4.531665000	2.454631000	1.271792000
6	3.324771000	3.536959000	-0.503090000
6	5.723330000	2.979016000	0.780725000
1	4.539890000	1.817946000	2.151302000
6	4.516000000	4.061319000	-0.998976000
1	2.385831000	3.757904000	-1.005547000
6	5.719294000	3.784502000	-0.356525000
1	6.658520000	2.760394000	1.287812000
1	4.501913000	4.689876000	-1.884548000
1	6.648899000	4.195169000	-0.738866000
1	2.014956000	0.683110000	-0.443693000

### A13

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Coordinates (Angstroms)			
	X	Y	Z
-----			
44	-1.028872000	-1.284196000	-0.447156000
6	1.148774000	-2.306037000	1.337185000
6	2.132318000	-3.138987000	1.866279000
6	2.651407000	-4.163934000	1.087964000
6	2.176103000	-4.330712000	-0.206986000
6	1.197938000	-3.464103000	-0.671972000
7	0.690405000	-2.475386000	0.074576000
1	3.413974000	-4.823029000	1.488515000
1	2.483972000	-2.996398000	2.880652000
1	2.552388000	-5.112942000	-0.855542000
1	0.794064000	-3.556221000	-1.673136000
6	0.543439000	-1.182629000	2.096627000
6	0.986957000	-0.736393000	3.337994000
6	0.357624000	0.362345000	3.912333000
6	-0.657725000	1.015358000	3.225821000
6	-1.043289000	0.537802000	1.974797000
7	-0.473059000	-0.565751000	1.471100000
1	0.682185000	0.726434000	4.881475000
1	1.815412000	-1.216467000	3.843280000
1	-1.130769000	1.899511000	3.637761000

6	-2.016007000	1.258886000	1.084015000
15	-2.845649000	0.111390000	-0.128666000
6	-1.475331000	-1.937472000	-2.120315000
8	-1.749815000	-2.372786000	-3.162713000
6	-3.454767000	1.247093000	-1.517358000
6	-2.307544000	1.362270000	-2.540855000
6	-4.657823000	0.636383000	-2.251911000
6	-3.814904000	2.648660000	-0.999240000
1	-1.321159000	1.459065000	-2.078330000
1	-2.265589000	0.468181000	-3.169906000
1	-2.502582000	2.220910000	-3.195069000
1	-5.581251000	0.650673000	-1.668018000
1	-4.838960000	1.222340000	-3.160593000
1	-4.457957000	-0.392311000	-2.567360000
1	-4.217736000	3.241514000	-1.828732000
1	-4.572106000	2.630954000	-0.211143000
1	-2.935241000	3.179118000	-0.622481000
6	-4.300626000	-0.594437000	0.854201000
6	-4.925217000	-1.766975000	0.081538000
6	-3.746312000	-1.145184000	2.181158000
6	-5.372274000	0.451444000	1.193141000
1	-5.442439000	-1.445988000	-0.824225000
1	-4.163214000	-2.500650000	-0.197044000
1	-5.663169000	-2.266783000	0.720134000
1	-3.375885000	-0.351803000	2.837650000
1	-4.558561000	-1.652067000	2.715233000
1	-2.944642000	-1.869842000	2.018015000
1	-6.131313000	-0.009964000	1.836226000
1	-4.957257000	1.302367000	1.743486000
1	-5.887174000	0.834145000	0.309942000
6	1.460470000	0.638492000	-0.732748000
8	0.124098000	0.569536000	-0.976842000
1	-1.865446000	-2.517678000	0.163080000
7	1.949012000	1.986192000	-0.392904000
6	1.666919000	3.036228000	-1.362590000
1	1.770634000	2.586741000	-2.353080000
1	2.457667000	3.799273000	-1.298602000
6	0.295632000	3.750039000	-1.302924000
1	-0.444968000	3.028899000	-0.951218000
1	0.002562000	4.006979000	-2.328358000
6	0.249437000	5.026558000	-0.462650000
1	1.011245000	5.743097000	-0.791895000
1	-0.724101000	5.521408000	-0.555896000
1	0.418940000	4.834898000	0.601273000

6	1.731764000	2.351541000	0.989760000
1	1.828062000	1.438851000	1.588442000
1	0.708850000	2.727974000	1.184576000
6	2.746809000	3.362233000	1.522858000
1	3.750819000	2.953607000	1.361923000
1	2.693168000	4.297126000	0.953151000
6	2.519898000	3.659712000	3.002904000
1	2.605266000	2.747196000	3.604520000
1	3.248724000	4.380801000	3.386124000
1	1.520061000	4.076388000	3.175192000
1	-2.697397000	1.894060000	1.655489000
1	-1.389178000	1.886240000	0.438715000
6	2.297056000	0.043150000	-1.901775000
1	1.865881000	-0.942575000	-2.104909000
1	2.149719000	0.641032000	-2.807490000
6	3.757012000	-0.082986000	-1.563383000
6	4.645876000	0.981108000	-1.751787000
6	4.249595000	-1.249028000	-0.971471000
6	5.980294000	0.878336000	-1.372473000
1	4.280305000	1.901128000	-2.198491000
6	5.583231000	-1.358168000	-0.584545000
1	3.573551000	-2.084711000	-0.813830000
6	6.456545000	-0.293439000	-0.785831000
1	6.653135000	1.716017000	-1.533651000
1	5.940367000	-2.278090000	-0.129210000
1	7.498871000	-0.374911000	-0.491598000
1	1.764936000	0.037000000	0.150243000

#### A14

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Coordinates (Angstroms)

	X	Y	Z
44	-1.355962000	1.139316000	-0.710849000
6	0.958015000	0.457689000	-2.465244000
6	2.184954000	0.552037000	-3.120172000
6	2.799109000	1.789196000	-3.242376000
6	2.169221000	2.906895000	-2.709079000
6	0.961526000	2.739104000	-2.050996000
7	0.369861000	1.545415000	-1.913489000
1	3.757360000	1.877048000	-3.742881000
1	2.668731000	-0.337340000	-3.499914000
1	2.608865000	3.894669000	-2.780929000
1	0.445325000	3.577216000	-1.599264000
6	0.215545000	-0.814745000	-2.328212000
6	0.625185000	-2.026613000	-2.878748000

6	-0.181654000	-3.142858000	-2.709070000
6	-1.382363000	-3.026448000	-2.017621000
6	-1.745272000	-1.789746000	-1.493962000
7	-0.934263000	-0.727375000	-1.632920000
1	0.122941000	-4.098979000	-3.121444000
1	1.566380000	-2.107395000	-3.403712000
1	-2.039618000	-3.879357000	-1.889691000
6	-3.065882000	-1.548944000	-0.812462000
15	-3.003351000	-0.079139000	0.337160000
6	-1.688938000	2.777113000	0.085748000
8	-1.882192000	3.807407000	0.594048000
6	-2.530238000	-0.860774000	2.004415000
6	-1.331024000	-1.786963000	1.735641000
6	-2.064972000	0.245693000	2.964700000
6	-3.630199000	-1.699150000	2.668113000
1	-1.606440000	-2.673830000	1.155425000
1	-0.529948000	-1.253691000	1.217721000
1	-0.939853000	-2.141422000	2.696808000
1	-2.867701000	0.938542000	3.230316000
1	-1.703293000	-0.212209000	3.893826000
1	-1.246452000	0.819506000	2.522314000
1	-3.205483000	-2.212587000	3.539214000
1	-4.463236000	-1.092551000	3.031269000
1	-4.025603000	-2.470710000	1.998666000
6	-4.803255000	0.511606000	0.377740000
6	-4.980345000	1.485497000	1.553185000
6	-5.072196000	1.289891000	-0.921268000
6	-5.840151000	-0.619584000	0.472331000
1	-4.944200000	0.981878000	2.522507000
1	-4.219213000	2.271790000	1.542736000
1	-5.959381000	1.972308000	1.473409000
1	-4.912904000	0.682245000	-1.816956000
1	-6.118148000	1.620472000	-0.920212000
1	-4.424801000	2.163728000	-1.009056000
1	-6.843497000	-0.181902000	0.409945000
1	-5.751481000	-1.333348000	-0.352950000
1	-5.788118000	-1.173520000	1.408988000
6	3.549733000	-1.326939000	-0.244768000
8	3.334194000	-1.777323000	-1.370988000
1	-3.787629000	-1.279767000	-1.592699000
7	2.909788000	-1.823447000	0.847530000
6	1.914382000	-2.867890000	0.632301000
1	1.331612000	-2.610412000	-0.255704000
1	1.230989000	-2.856648000	1.485473000

6	2.514882000	-4.262671000	0.466217000
1	3.113169000	-4.512300000	1.351527000
1	3.193423000	-4.248561000	-0.392021000
6	1.425663000	-5.311388000	0.260035000
1	0.833989000	-5.086623000	-0.634556000
1	1.851977000	-6.311472000	0.137380000
1	0.735954000	-5.342919000	1.111411000
6	3.185010000	-1.439817000	2.227430000
1	4.043883000	-0.769313000	2.239976000
1	3.482336000	-2.336806000	2.787275000
6	2.002618000	-0.752845000	2.926354000
1	1.466840000	-0.135320000	2.199249000
1	1.290773000	-1.504214000	3.285589000
6	4.566664000	-0.201266000	-0.064212000
1	5.430469000	-0.584287000	0.492120000
1	4.918737000	0.013632000	-1.076692000
6	4.060829000	1.070525000	0.587761000
6	4.948028000	1.916688000	1.260217000
6	2.715472000	1.431002000	0.524926000
6	4.498076000	3.094288000	1.851298000
1	6.000142000	1.649524000	1.326592000
6	2.258311000	2.599646000	1.126240000
1	1.992697000	0.783469000	0.038382000
6	3.148699000	3.438815000	1.788981000
1	5.201059000	3.738153000	2.371770000
1	1.197202000	2.827516000	1.078842000
1	2.793873000	4.349853000	2.261163000
6	2.465265000	0.116187000	4.091140000
1	3.109311000	0.927531000	3.733858000
1	1.611257000	0.569211000	4.603133000
1	3.029878000	-0.464561000	4.830121000
1	-3.435333000	-2.457428000	-0.328020000
1	-0.267995000	0.739289000	0.517148000
1	-2.374126000	1.466859000	-2.029308000

## A15

Coordinates (Angstroms)

	X	Y	Z
44	-0.392026000	-0.804343000	-0.035622000
6	-3.174125000	0.287766000	-0.038552000
6	-4.565030000	0.361613000	0.032225000
6	-5.307320000	-0.804331000	0.142338000
6	-4.639369000	-2.022741000	0.174467000



6	-3.255861000	-2.025439000	0.097458000
7	-2.531968000	-0.902931000	-0.003656000
1	-6.389622000	-0.760500000	0.200222000
1	-5.067272000	1.320438000	-0.004594000
1	-5.173179000	-2.962238000	0.257208000
1	-2.691865000	-2.949901000	0.116232000
6	-2.309394000	1.481169000	-0.178647000
6	-2.775143000	2.794023000	-0.199100000
6	-1.861547000	3.825080000	-0.370619000
6	-0.516362000	3.527399000	-0.551012000
6	-0.107337000	2.197874000	-0.527877000
7	-0.996013000	1.214599000	-0.304719000
1	-2.199887000	4.855868000	-0.376773000
1	-3.827700000	3.014500000	-0.074226000
1	0.213875000	4.312201000	-0.713214000
6	1.309551000	1.779450000	-0.812261000
15	1.720500000	0.116486000	-0.070275000
6	0.109605000	-2.572545000	0.198429000
8	0.424278000	-3.683189000	0.346722000
6	2.466783000	0.568831000	1.618902000
6	1.512168000	1.583780000	2.274703000
6	2.505306000	-0.692417000	2.495748000
6	3.861392000	1.205732000	1.569190000
1	1.550922000	2.562007000	1.784299000
1	0.480443000	1.222312000	2.273748000
1	1.816062000	1.732778000	3.317404000
1	3.187308000	-1.452700000	2.106269000
1	2.853556000	-0.422635000	3.500210000
1	1.509917000	-1.134616000	2.583699000
1	4.132266000	1.539136000	2.578351000
1	4.633855000	0.504046000	1.246261000
1	3.894798000	2.086891000	0.919690000
6	3.071934000	-0.538056000	-1.230025000
6	3.779934000	-1.723809000	-0.556405000
6	2.391559000	-1.063998000	-2.505055000
6	4.102341000	0.521566000	-1.654701000
1	4.407922000	-1.417984000	0.284070000
1	3.063455000	-2.471356000	-0.201491000
1	4.432656000	-2.214679000	-1.287762000
1	1.824088000	-0.288854000	-3.028900000
1	3.167550000	-1.430383000	-3.188507000
1	1.697545000	-1.876911000	-2.287685000
1	4.809894000	0.064260000	-2.356615000
1	3.634770000	1.362431000	-2.176755000

1	4.684063000	0.918389000	-0.823398000
1	1.389560000	1.644814000	-1.897657000
1	2.019325000	2.562518000	-0.531366000
1	-0.500296000	-0.585759000	1.638857000
1	-0.405191000	-0.952108000	-1.726461000

**A16**

Coordinates (Angstroms)

	X	Y	Z
44	0.319754000	-0.912774000	-0.887880000
6	-2.378463000	-2.001216000	-0.202550000
6	-3.624873000	-2.615826000	-0.317739000
6	-4.062398000	-3.048386000	-1.560354000
6	-3.241454000	-2.850586000	-2.664436000
6	-2.016569000	-2.229018000	-2.481195000
7	-1.586727000	-1.810920000	-1.283417000
1	-5.029335000	-3.528482000	-1.664694000
1	-4.252685000	-2.751063000	0.554276000
1	-3.538552000	-3.167870000	-3.657258000
1	-1.342469000	-2.051936000	-3.310225000
6	-1.850797000	-1.485298000	1.080723000
6	-2.495682000	-1.614754000	2.308711000
6	-1.920360000	-1.033273000	3.430451000
6	-0.739090000	-0.312894000	3.301436000
6	-0.134230000	-0.218633000	2.051748000
7	-0.677283000	-0.831846000	0.985339000
1	-2.401077000	-1.128525000	4.398153000
1	-3.428429000	-2.157275000	2.397078000
1	-0.285935000	0.175260000	4.156912000
6	1.100600000	0.602791000	1.799817000
15	2.068505000	-0.025135000	0.333254000
6	1.166195000	-0.975424000	-2.535633000
8	1.692673000	-1.005607000	-3.572731000
6	3.267044000	-1.282862000	1.107133000
6	2.436367000	-2.206142000	2.017238000
6	3.884385000	-2.139027000	-0.009860000
6	4.379806000	-0.666207000	1.964859000
1	2.076919000	-1.688469000	2.912628000
1	1.583607000	-2.635600000	1.485039000
1	3.073097000	-3.031610000	2.356770000
1	4.530835000	-1.559699000	-0.673513000
1	4.498007000	-2.929158000	0.439775000
1	3.103242000	-2.609695000	-0.612455000
1	4.931206000	-1.473673000	2.461597000

1	5.103800000	-0.099050000	1.375552000
1	3.984245000	-0.014753000	2.751225000
6	3.019352000	1.508783000	-0.243499000
6	4.167586000	1.078822000	-1.169152000
6	2.050922000	2.375350000	-1.063624000
6	3.561820000	2.377995000	0.903526000
1	4.980035000	0.582244000	-0.633065000
1	3.818221000	0.412511000	-1.964231000
1	4.591061000	1.969249000	-1.648411000
1	1.183710000	2.698467000	-0.481285000
1	2.584199000	3.274653000	-1.396365000
1	1.677916000	1.845078000	-1.941418000
1	4.066840000	3.250338000	0.471826000
1	2.758289000	2.759775000	1.540715000
1	4.286899000	1.864598000	1.535228000
1	0.766621000	1.609425000	1.514471000
1	1.702219000	0.703074000	2.707776000
1	0.846318000	-2.472706000	-0.523660000
1	-0.329580000	0.622973000	-1.222763000
7	-1.230926000	2.926193000	0.331051000
6	-1.957688000	2.845259000	1.588980000
1	-1.274816000	2.448771000	2.352938000
1	-2.207142000	3.868531000	1.903692000
6	-3.229055000	1.988797000	1.588716000
1	-3.945272000	2.380505000	0.857213000
1	-2.964905000	0.978278000	1.255184000
6	-3.886551000	1.927742000	2.964192000
1	-4.747431000	1.251429000	2.968992000
1	-3.180171000	1.571262000	3.722447000
1	-4.238370000	2.916435000	3.280218000
6	-1.954353000	3.605999000	-0.737979000
1	-2.863830000	3.064233000	-1.053225000
1	-2.293659000	4.578405000	-0.352945000
6	-1.070403000	3.824568000	-1.962045000
1	-0.682493000	2.854005000	-2.294015000
1	-0.202682000	4.426648000	-1.668751000
6	-1.818975000	4.503942000	-3.105352000
1	-1.164518000	4.663413000	-3.967745000
1	-2.666948000	3.896425000	-3.441350000
1	-2.211515000	5.481242000	-2.800559000
1	-0.987879000	1.989274000	0.002481000

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A17

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Coordinates (Angstroms)			
	X	Y	Z
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44	0.052926000	-1.057457000	-0.737176000
6	-2.752882000	-1.389342000	0.267407000
6	-4.100310000	-1.747630000	0.331230000
6	-4.710012000	-2.333016000	-0.767619000
6	-3.957526000	-2.550977000	-1.916034000
6	-2.623505000	-2.174999000	-1.913618000
7	-2.029445000	-1.606800000	-0.855972000
1	-5.757239000	-2.613815000	-0.726414000
1	-4.668647000	-1.569544000	1.235564000
1	-4.387974000	-3.005351000	-2.800814000
1	-1.991654000	-2.329461000	-2.780346000
6	-2.042153000	-0.717129000	1.386261000
6	-2.641459000	-0.402757000	2.595052000
6	-1.862879000	0.290186000	3.544194000
6	-0.570464000	0.646708000	3.264132000
6	0.024986000	0.296650000	2.006353000
7	-0.765962000	-0.390821000	1.110113000
1	-2.297150000	0.543141000	4.507285000
1	-3.663883000	-0.676971000	2.817464000
1	0.031295000	1.178406000	3.993934000
6	1.332191000	0.627175000	1.628926000
15	2.027461000	-0.358636000	0.302996000
6	0.780815000	-1.702921000	-2.314567000
8	1.234724000	-2.122754000	-3.302188000
6	2.980470000	-1.779302000	1.168182000
6	2.052906000	-2.328259000	2.266789000
6	3.275006000	-2.913081000	0.174507000
6	4.281651000	-1.340809000	1.853153000
1	1.925695000	-1.609407000	3.081202000
1	1.066054000	-2.581788000	1.871504000
1	2.496976000	-3.239396000	2.687005000
1	3.943051000	-2.606062000	-0.633656000
1	3.762421000	-3.742591000	0.703120000
1	2.350914000	-3.289636000	-0.270583000
1	4.667226000	-2.173256000	2.455220000
1	5.066756000	-1.072790000	1.141633000
1	4.120031000	-0.497383000	2.532856000
6	3.286272000	0.744650000	-0.594716000
6	4.179671000	-0.092118000	-1.520322000
6	2.490559000	1.725005000	-1.463621000
6	4.147143000	1.593406000	0.354757000
1	4.880360000	-0.722558000	-0.967976000

1	3.586391000	-0.731812000	-2.181314000
1	4.776483000	0.576349000	-2.153355000
1	1.891618000	2.381040000	-0.828258000
1	3.183062000	2.358346000	-2.032312000
1	1.822656000	1.212608000	-2.158766000
1	4.776834000	2.267851000	-0.239615000
1	3.521721000	2.214417000	1.004119000
1	4.811613000	1.002643000	0.984733000
1	-0.023173000	2.346399000	0.555729000
1	1.977084000	1.060785000	2.390287000
1	0.267989000	-2.540396000	-0.051108000
1	-0.321570000	0.479925000	-1.505633000
7	-0.766262000	2.464112000	-0.152682000
6	-2.103353000	2.554901000	0.490414000
1	-2.074853000	1.946676000	1.394539000
1	-2.269689000	3.594276000	0.791670000
6	-3.200146000	2.060481000	-0.446284000
1	-3.290915000	2.728172000	-1.310740000
1	-2.910888000	1.078689000	-0.835892000
6	-4.541319000	1.958073000	0.272342000
1	-5.315112000	1.590036000	-0.406685000
1	-4.474272000	1.264254000	1.116534000
1	-4.867993000	2.929627000	0.659081000
6	-0.442517000	3.586269000	-1.070905000
1	0.198672000	3.186233000	-1.859281000
1	-1.373659000	3.910031000	-1.541969000
6	0.234277000	4.739081000	-0.342861000
1	1.137606000	4.364778000	0.155168000
1	-0.429405000	5.117715000	0.443652000
6	0.604212000	5.865917000	-1.302382000
1	1.084753000	6.690356000	-0.768993000
1	1.300517000	5.514130000	-2.070577000
1	-0.281374000	6.265698000	-1.807480000
1	-0.664918000	1.526922000	-0.697048000

## A18

Coordinates (Angstroms)

	X	Y	Z
44	0.188112000	-1.267958000	-0.574910000
6	-2.607405000	-1.653208000	0.444255000
6	-3.927750000	-2.090351000	0.551336000
6	-4.450204000	-2.944288000	-0.408145000
6	-3.642281000	-3.348249000	-1.464649000

6	-2.340496000	-2.876167000	-1.515018000
7	-1.832456000	-2.049891000	-0.591771000
1	-5.475986000	-3.288894000	-0.330560000
1	-4.544575000	-1.762086000	1.378168000
1	-4.005259000	-4.016273000	-2.236738000
1	-1.667445000	-3.160642000	-2.315407000
6	-1.981607000	-0.718206000	1.415827000
6	-2.634852000	-0.228969000	2.529150000
6	-1.933101000	0.690193000	3.342872000
6	-0.663326000	1.077893000	3.024534000
6	-0.001027000	0.535661000	1.867901000
7	-0.720271000	-0.357936000	1.102608000
1	-2.415062000	1.095302000	4.227924000
1	-3.644249000	-0.526224000	2.779504000
1	-0.122025000	1.782262000	3.647125000
6	1.296682000	0.864291000	1.490761000
15	2.081230000	-0.177381000	0.283108000
6	1.059630000	-2.181570000	-1.952470000
8	1.613757000	-2.777771000	-2.779266000
6	3.257296000	-1.315456000	1.262260000
6	2.464463000	-1.855322000	2.465394000
6	3.705619000	-2.511278000	0.409879000
6	4.480368000	-0.573824000	1.820440000
1	2.201634000	-1.058359000	3.165731000
1	1.541855000	-2.354532000	2.158545000
1	3.083795000	-2.586893000	2.998705000
1	4.265034000	-2.217621000	-0.480757000
1	4.358595000	-3.158640000	1.008550000
1	2.846415000	-3.107407000	0.091356000
1	5.033057000	-1.243685000	2.490580000
1	5.177583000	-0.253454000	1.042818000
1	4.187441000	0.302920000	2.407706000
6	3.090819000	0.944517000	-0.863520000
6	4.151667000	0.162003000	-1.649454000
6	2.109729000	1.547118000	-1.880588000
6	3.741728000	2.108332000	-0.099714000
1	4.974076000	-0.189608000	-1.022321000
1	3.717486000	-0.700455000	-2.165168000
1	4.584673000	0.817651000	-2.414704000
1	1.239868000	1.990736000	-1.392173000
1	2.619186000	2.332743000	-2.452205000
1	1.751640000	0.795123000	-2.588620000
1	4.297053000	2.737141000	-0.806317000
1	2.982747000	2.735663000	0.377057000

1	4.445461000	1.780815000	0.667358000
1	-0.330557000	2.465936000	0.143929000
1	1.877120000	1.516051000	2.136505000
1	0.578158000	-2.479260000	0.346069000
1	-0.468413000	-0.057326000	-1.962100000
7	-1.041007000	2.640132000	-0.562080000
6	-2.377272000	2.481403000	0.006660000
1	-2.295667000	1.975690000	0.972220000
1	-2.851593000	3.455981000	0.212206000
6	-3.292365000	1.659636000	-0.900938000
1	-3.376922000	2.151743000	-1.878310000
1	-2.813461000	0.690987000	-1.082455000
6	-4.676272000	1.451543000	-0.293910000
1	-5.305326000	0.822912000	-0.932016000
1	-4.596826000	0.965052000	0.685187000
1	-5.196176000	2.405229000	-0.147068000
6	-0.795596000	3.917770000	-1.216547000
1	0.033557000	3.804675000	-1.928616000
1	-1.679243000	4.167821000	-1.818363000
6	-0.472364000	5.072241000	-0.262676000
1	0.437666000	4.813257000	0.295173000
1	-1.274223000	5.168092000	0.480257000
6	-0.275992000	6.401355000	-0.986384000
1	-0.008133000	7.201026000	-0.289179000
1	0.521630000	6.331888000	-1.734681000
1	-1.190678000	6.706638000	-1.506986000
1	-0.459740000	0.492492000	-1.409218000

**B8**

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Coordinates (Angstroms)

	X	Y	Z
7	2.711517000	0.135260000	-0.506286000
6	3.554505000	1.269126000	-0.122072000
1	3.377069000	2.099572000	-0.815164000
1	4.620171000	1.008119000	-0.222462000
6	3.412007000	-1.140722000	-0.587608000
1	4.303231000	-1.078152000	-1.239956000
1	3.781400000	-1.407396000	0.410871000
6	-1.871793000	-0.042658000	-2.355618000
1	-2.149919000	-0.710656000	-3.184328000
1	-1.955497000	0.979280000	-2.733998000
6	-0.410445000	-0.338031000	-2.090734000
8	0.488215000	0.230271000	-2.676730000

1	-0.204385000	-1.174893000	-1.401156000
7	-0.194100000	0.665654000	0.543241000
1	0.800829000	0.499267000	0.366083000
6	-0.443569000	2.088084000	0.688460000
1	-1.520321000	2.230645000	0.854028000
1	0.056376000	2.510982000	1.583103000
6	-0.609320000	-0.083367000	1.717834000
1	-1.702428000	-0.014388000	1.802387000
1	-0.194114000	0.349188000	2.650216000
1	2.256750000	0.310941000	-1.398529000
6	-0.203590000	-1.549196000	1.638229000
1	0.889332000	-1.617556000	1.561846000
1	-0.613818000	-1.978849000	0.717632000
6	-0.690511000	-2.350498000	2.840536000
1	-0.392720000	-3.400962000	2.767982000
1	-0.281054000	-1.951804000	3.775351000
1	-1.783137000	-2.316276000	2.915059000
6	-0.014735000	2.877971000	-0.542060000
1	1.048027000	2.690297000	-0.739589000
1	-0.554796000	2.501366000	-1.416778000
6	-0.251505000	4.376026000	-0.379738000
1	0.310837000	4.777183000	0.470738000
1	0.056845000	4.927398000	-1.273044000
1	-1.311782000	4.591828000	-0.204748000
6	3.287941000	1.757896000	1.304364000
1	3.983240000	2.577903000	1.524243000
1	2.278590000	2.183716000	1.351490000
6	3.420147000	0.669381000	2.363968000
1	4.423539000	0.228284000	2.363338000
1	3.233290000	1.069660000	3.365282000
1	2.697058000	-0.133222000	2.185917000
6	2.495697000	-2.245223000	-1.101757000
1	2.080729000	-1.936508000	-2.069217000
1	1.648845000	-2.348949000	-0.414745000
6	3.213642000	-3.583053000	-1.249719000
1	2.527931000	-4.362529000	-1.595037000
1	4.032323000	-3.517780000	-1.974558000
1	3.638870000	-3.914086000	-0.295822000
6	-2.785170000	-0.286411000	-1.182330000
6	-2.985781000	-1.577617000	-0.689450000
6	-3.443651000	0.775601000	-0.560961000
6	-3.811769000	-1.800808000	0.408761000
1	-2.492535000	-2.419375000	-1.169610000
6	-4.278333000	0.556386000	0.530791000



1	-3.298275000	1.784737000	-0.937315000
6	-4.462451000	-0.733491000	1.022393000
1	-3.952067000	-2.810969000	0.781285000
1	-4.782426000	1.395925000	0.999694000
1	-5.111547000	-0.906876000	1.874918000

**B9**

Coordinates (Angstroms)

	X	Y	Z
7	2.852997000	-0.065377000	-0.503268000
6	3.775863000	0.912885000	0.087091000
1	3.847211000	1.790469000	-0.568195000
1	4.781345000	0.475716000	0.132847000
6	3.378611000	-1.421444000	-0.621142000
1	4.314810000	-1.374066000	-1.191530000
1	3.633751000	-1.862181000	0.359487000
6	-1.758139000	0.480375000	-1.777075000
1	-1.791963000	0.025618000	-2.772461000
1	-1.814063000	1.563273000	-1.923670000
6	-0.384136000	0.111820000	-1.184448000
8	0.563610000	0.481051000	-2.149800000
1	-0.369025000	-0.977094000	-1.043320000
7	-0.050990000	0.679155000	0.127415000
1	1.991667000	-0.062347000	0.045039000
6	-0.255602000	2.121441000	0.273079000
1	-1.325196000	2.388288000	0.204428000
1	0.043796000	2.373527000	1.298582000
6	-0.580989000	-0.024084000	1.303291000
1	-1.669863000	0.104945000	1.410470000
1	-0.127760000	0.465467000	2.175185000
1	1.453413000	0.362680000	-1.755117000
6	-0.250230000	-1.511200000	1.400105000
1	0.827450000	-1.657714000	1.257402000
1	-0.756587000	-2.076797000	0.611725000
6	-0.677730000	-2.074855000	2.752966000
1	-0.463217000	-3.145207000	2.821702000
1	-0.156064000	-1.575912000	3.577269000
1	-1.753676000	-1.939856000	2.907568000
6	0.546881000	3.009532000	-0.675730000
1	1.603001000	2.723076000	-0.623964000
1	0.241140000	2.840438000	-1.710129000
6	0.385201000	4.482329000	-0.309228000
1	0.731209000	4.680448000	0.711769000

1	0.960451000	5.122537000	-0.984435000
1	-0.663567000	4.794935000	-0.369094000
6	3.363313000	1.373063000	1.487902000
1	4.068097000	2.143480000	1.821906000
1	2.381272000	1.857730000	1.422231000
6	3.302936000	0.246119000	2.515966000
1	4.278481000	-0.238498000	2.633388000
1	2.996442000	0.623602000	3.496288000
1	2.581833000	-0.524404000	2.223267000
6	2.402858000	-2.338723000	-1.352081000
1	2.181689000	-1.905894000	-2.333661000
1	1.452240000	-2.366665000	-0.805827000
6	2.941188000	-3.758018000	-1.503524000
1	2.237450000	-4.391563000	-2.051283000
1	3.889841000	-3.766739000	-2.051369000
1	3.116955000	-4.223483000	-0.527455000
6	-2.917856000	-0.003367000	-0.942552000
6	-3.141110000	-1.373610000	-0.770384000
6	-3.764036000	0.891811000	-0.284869000
6	-4.151728000	-1.834882000	0.066456000
1	-2.509238000	-2.086679000	-1.294428000
6	-4.782316000	0.436172000	0.548337000
1	-3.614746000	1.959939000	-0.419181000
6	-4.972240000	-0.929676000	0.735983000
1	-4.301916000	-2.902550000	0.194947000
1	-5.424792000	1.149728000	1.055468000
1	-5.759226000	-1.287221000	1.392657000

C7

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Coordinates (Angstroms)

	X	Y	Z
44	0.480734000	0.970533000	-0.951296000
6	-0.494187000	3.139504000	0.854398000
6	-1.214471000	4.230901000	1.339096000
6	-2.127268000	4.874265000	0.515705000
6	-2.304931000	4.413572000	-0.782642000
6	-1.554254000	3.325784000	-1.202222000
7	-0.674617000	2.704411000	-0.411651000
1	-2.691707000	5.723740000	0.885935000
1	-1.065444000	4.576366000	2.354260000
1	-3.007831000	4.879898000	-1.462992000
1	-1.654783000	2.924818000	-2.204026000
6	0.486786000	2.385660000	1.683356000

6	0.750195000	2.687148000	3.007416000
6	1.683154000	1.874084000	3.685056000
6	2.277760000	0.814717000	3.056340000
6	1.962487000	0.512844000	1.686979000
7	1.076617000	1.354774000	1.050629000
1	1.928176000	2.093963000	4.720596000
1	0.276046000	3.517174000	3.513679000
1	2.995606000	0.188269000	3.575858000
6	2.486047000	-0.574511000	0.982555000
15	2.313896000	-0.512026000	-0.791144000
6	0.027238000	0.721747000	-2.729588000
8	-0.226001000	0.632805000	-3.863464000
6	2.189907000	-2.296467000	-1.457083000
6	1.306259000	-3.079719000	-0.483050000
6	1.486682000	-2.261528000	-2.823468000
6	3.505512000	-3.071174000	-1.598266000
1	1.798191000	-3.236633000	0.480658000
1	0.369671000	-2.553395000	-0.314465000
1	1.060073000	-4.059179000	-0.912099000
1	2.012066000	-1.633055000	-3.547506000
1	1.437180000	-3.275961000	-3.238586000
1	0.465477000	-1.882906000	-2.735770000
1	3.272392000	-4.117699000	-1.832234000
1	4.125133000	-2.694266000	-2.414713000
1	4.093124000	-3.066421000	-0.675930000
6	3.962218000	0.252580000	-1.412837000
6	3.942231000	0.381864000	-2.940154000
6	4.102018000	1.654503000	-0.788860000
6	5.214648000	-0.518656000	-0.955298000
1	3.960824000	-0.592828000	-3.438008000
1	3.055509000	0.926644000	-3.281080000
1	4.827097000	0.934735000	-3.279971000
1	4.127031000	1.602060000	0.304091000
1	5.049018000	2.093460000	-1.125544000
1	3.297253000	2.330196000	-1.077962000
1	6.097120000	0.112106000	-1.116593000
1	5.175123000	-0.747670000	0.114936000
1	5.386412000	-1.442962000	-1.502762000
6	-1.940451000	-0.956999000	0.557195000
8	-1.461319000	0.167579000	0.135096000
1	1.562440000	1.945779000	-1.522839000
1	3.256189000	-1.172654000	1.462711000
1	-2.861903000	-0.877432000	1.170928000
7	-0.880205000	-1.506196000	1.732976000

1	0.028857000	-1.307979000	1.290522000
6	-0.890819000	-2.930834000	2.137227000
1	-0.781848000	-3.527012000	1.230558000
1	-1.870922000	-3.158650000	2.565804000
6	0.243552000	-3.281932000	3.097924000
1	0.065857000	-2.833275000	4.080894000
1	1.173360000	-2.844242000	2.714112000
6	0.396190000	-4.793455000	3.239301000
1	0.631446000	-5.257614000	2.275460000
1	1.201543000	-5.041779000	3.935889000
1	-0.523427000	-5.253649000	3.616678000
6	-0.972050000	-0.548019000	2.873893000
1	-1.079256000	0.427919000	2.399237000
1	-0.017037000	-0.554866000	3.403755000
6	-2.115545000	-0.800231000	3.847449000
1	-3.068850000	-0.872119000	3.313087000
1	-1.973531000	-1.749078000	4.377012000
6	-2.177238000	-2.046493000	-0.505544000
1	-1.308140000	-2.072220000	-1.168285000
1	-2.318385000	-3.037606000	-0.064762000
6	-3.410151000	-1.685034000	-1.299279000
6	-3.370265000	-0.642639000	-2.229948000
6	-4.620998000	-2.347281000	-1.087056000
6	-4.509906000	-0.282023000	-2.940031000
1	-2.434351000	-0.118669000	-2.386686000
6	-5.766065000	-1.986699000	-1.794949000
1	-4.668055000	-3.156245000	-0.361630000
6	-5.713084000	-0.952084000	-2.724006000
1	-4.458794000	0.522962000	-3.667465000
1	-6.698989000	-2.514757000	-1.620243000
1	-6.602847000	-0.671700000	-3.279981000
6	-2.184199000	0.340296000	4.861701000
1	-2.373444000	1.296640000	4.363540000
1	-2.983299000	0.173160000	5.589193000
1	-1.242123000	0.435442000	5.412317000

**D7**

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Coordinates (Angstroms)			
	X	Y	Z
-----			
44	-1.584816000	-0.162951000	-0.812792000
6	-2.320838000	-2.850173000	0.304491000
6	-2.518949000	-4.227325000	0.418372000
6	-2.352403000	-5.041789000	-0.690943000

6	-2.010962000	-4.461325000	-1.907211000
6	-1.814925000	-3.090677000	-1.947960000
7	-1.931981000	-2.302929000	-0.871039000
1	-2.505556000	-6.112716000	-0.608712000
1	-2.813004000	-4.658060000	1.366908000
1	-1.897496000	-5.049609000	-2.810162000
1	-1.555303000	-2.589045000	-2.872510000
6	-2.561494000	-1.901801000	1.423062000
6	-2.994673000	-2.300677000	2.670534000
6	-3.253216000	-1.285042000	3.621751000
6	-3.122918000	0.031275000	3.289619000
6	-2.690750000	0.417459000	1.969465000
7	-2.353850000	-0.607456000	1.104835000
1	-3.574547000	-1.560547000	4.622371000
1	-3.149986000	-3.341270000	2.921635000
1	-3.341799000	0.811831000	4.010621000
6	-2.580076000	1.730297000	1.546192000
15	-1.859058000	2.048230000	-0.041963000
6	-1.095246000	0.263627000	-2.551722000
8	-0.838471000	0.535790000	-3.655613000
6	-0.275810000	3.063658000	0.304706000
6	0.375863000	2.445596000	1.551388000
6	0.683825000	2.941620000	-0.887969000
6	-0.487966000	4.549861000	0.624760000
1	-0.177062000	2.704960000	2.457577000
1	0.402933000	1.354944000	1.525656000
1	1.401662000	2.812808000	1.665838000
1	0.259913000	3.350353000	-1.809215000
1	1.611873000	3.489075000	-0.679944000
1	0.941041000	1.898929000	-1.088970000
1	0.468418000	4.981936000	0.945789000
1	-0.829040000	5.128969000	-0.236332000
1	-1.196399000	4.690728000	1.446398000
6	-3.084644000	3.147216000	-0.999190000
6	-2.437375000	3.738594000	-2.258369000
6	-4.274130000	2.276035000	-1.437645000
6	-3.665803000	4.265488000	-0.116955000
1	-1.672530000	4.485136000	-2.029796000
1	-1.985252000	2.961163000	-2.882144000
1	-3.205732000	4.237779000	-2.861688000
1	-4.693791000	1.714781000	-0.597128000
1	-5.059576000	2.928443000	-1.839282000
1	-3.992596000	1.564713000	-2.216036000
1	-4.424568000	4.813528000	-0.689035000

1	-4.158090000	3.849303000	0.767112000
1	-2.925064000	4.993131000	0.211633000
6	3.624604000	0.932152000	1.595092000
8	3.418371000	1.531536000	2.624462000
1	-2.815153000	2.531125000	2.239842000
1	3.221395000	1.307259000	0.628528000
6	4.450522000	-0.328631000	1.494143000
1	4.711091000	-0.661305000	2.502358000
1	3.832010000	-1.092989000	1.011234000
6	5.678155000	-0.063259000	0.646754000
6	6.649784000	0.834211000	1.100291000
6	5.846240000	-0.668935000	-0.599302000
6	7.770051000	1.114600000	0.325672000
1	6.524136000	1.315515000	2.066743000
6	6.968078000	-0.389482000	-1.376496000
1	5.098332000	-1.370663000	-0.960510000
6	7.931743000	0.502797000	-0.915932000
1	8.516697000	1.813328000	0.690226000
1	7.088306000	-0.870914000	-2.342186000
1	8.806248000	0.721842000	-1.520691000
1	-3.079690000	-0.008687000	-1.249499000
7	0.772931000	-0.728424000	-0.123048000
1	1.013190000	0.141451000	0.341158000
6	1.708150000	-0.860655000	-1.253097000
1	1.634672000	0.047495000	-1.859443000
6	0.931611000	-1.808749000	0.868489000
1	0.240147000	-2.620512000	0.622758000
1	2.745342000	-0.916679000	-0.881940000
1	1.945906000	-2.238340000	0.807809000
6	1.449051000	-2.068055000	-2.143290000
1	1.415887000	-2.984058000	-1.541240000
1	0.467200000	-1.956160000	-2.606927000
6	2.515120000	-2.203935000	-3.226882000
1	3.509853000	-2.359361000	-2.793604000
1	2.303138000	-3.053744000	-3.882233000
1	2.559827000	-1.305053000	-3.851414000
6	0.687702000	-1.334528000	2.296168000
1	1.454529000	-0.599152000	2.571691000
1	-0.275511000	-0.820888000	2.348370000
6	0.705806000	-2.491776000	3.289422000
1	-0.075846000	-3.220281000	3.050018000
1	1.669896000	-3.013371000	3.283750000
1	0.524080000	-2.133686000	4.306422000

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**D8**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
44	-1.546750000	0.219673000	0.694714000
6	-1.853984000	3.069901000	-0.201977000
6	-1.992536000	4.457534000	-0.185735000
6	-1.989110000	5.129966000	1.026855000
6	-1.860654000	4.396755000	2.199540000
6	-1.725402000	3.019747000	2.108821000
7	-1.706331000	2.365269000	0.942628000
1	-2.094870000	6.209209000	1.054232000
1	-2.101338000	5.010761000	-1.110058000
1	-1.865747000	4.873843000	3.172342000
1	-1.629817000	2.408155000	2.997162000
6	-1.881701000	2.277626000	-1.456597000
6	-2.056278000	2.834599000	-2.720960000
6	-2.107836000	1.992557000	-3.823131000
6	-1.979435000	0.622100000	-3.643799000
6	-1.785983000	0.120635000	-2.360090000
7	-1.746611000	0.947505000	-1.300504000
1	-2.247547000	2.405904000	-4.816262000
1	-2.159748000	3.903752000	-2.852245000
1	-2.009363000	-0.059253000	-4.486579000
6	-1.526114000	-1.338841000	-2.108037000
15	-1.834552000	-1.834913000	-0.338649000
6	-1.551023000	-0.417614000	2.431733000
8	-1.611961000	-0.818872000	3.521334000
6	-0.622151000	-3.269587000	-0.114229000
6	0.781962000	-2.647725000	-0.226773000
6	-0.812940000	-3.843404000	1.296604000
6	-0.704847000	-4.404022000	-1.149515000
1	1.095658000	-2.577860000	-1.275533000
1	0.832458000	-1.632353000	0.186193000
1	1.505556000	-3.293493000	0.282492000
1	-1.779624000	-4.344255000	1.409500000
1	-0.033187000	-4.588048000	1.493326000
1	-0.731785000	-3.069815000	2.065767000
1	0.210133000	-5.002704000	-1.068531000
1	-1.545857000	-5.078314000	-0.991894000
1	-0.749822000	-4.026825000	-2.176929000
6	-3.630072000	-2.456707000	-0.347457000
6	-4.152119000	-2.510439000	1.097823000
6	-4.478729000	-1.445109000	-1.138431000

6	-3.819117000	-3.834857000	-0.993635000
1	-3.561289000	-3.178130000	1.731271000
1	-4.151376000	-1.519688000	1.557009000
1	-5.182039000	-2.887483000	1.092087000
1	-4.269394000	-1.480995000	-2.212627000
1	-5.538007000	-1.694999000	-1.006863000
1	-4.330082000	-0.423042000	-0.781412000
1	-4.892340000	-4.022108000	-1.117991000
1	-3.358524000	-3.905230000	-1.983989000
1	-3.422652000	-4.637388000	-0.367489000
6	4.016991000	-2.033809000	1.321491000
8	3.727342000	-3.145878000	1.699297000
1	-2.065627000	-1.962098000	-2.827269000
1	4.387135000	-1.269739000	2.037537000
6	3.901693000	-1.564124000	-0.111941000
1	3.802307000	-2.443834000	-0.753519000
1	2.959187000	-1.000685000	-0.171494000
6	5.061814000	-0.691451000	-0.525075000
6	6.226717000	-1.261543000	-1.046051000
6	5.009502000	0.694944000	-0.360314000
6	7.310329000	-0.464678000	-1.403875000
1	6.281462000	-2.339409000	-1.176445000
6	6.092939000	1.494655000	-0.714827000
1	4.107817000	1.149045000	0.040813000
6	7.245996000	0.917308000	-1.239280000
1	8.205629000	-0.923082000	-1.813206000
1	6.031759000	2.570904000	-0.583558000
1	8.089883000	1.540264000	-1.520073000
1	-3.164331000	0.264287000	0.798647000
7	0.735161000	0.447318000	0.536798000
6	1.458022000	0.324501000	1.781093000
1	1.239388000	-0.660478000	2.225837000
6	1.223715000	1.548286000	-0.258214000
1	0.534536000	2.416427000	-0.302908000
1	2.552106000	0.321069000	1.586585000
1	2.143838000	1.977956000	0.181922000
6	1.251067000	1.386231000	2.877636000
1	1.362185000	2.386797000	2.438078000
1	0.226008000	1.319615000	3.256182000
6	2.230675000	1.214510000	4.035834000
1	3.268314000	1.311420000	3.694111000
1	2.071109000	1.959813000	4.822499000
1	2.125888000	0.223313000	4.492711000
6	1.554024000	1.176425000	-1.711001000



1	2.362561000	0.435586000	-1.719615000
1	0.685980000	0.686713000	-2.162591000
6	1.956564000	2.386942000	-2.548668000
1	1.159839000	3.140762000	-2.558306000
1	2.856749000	2.864716000	-2.143806000
1	2.167979000	2.113841000	-3.587787000
1	-0.456316000	-1.505295000	-2.279422000

#### TSA3-4

Coordinates (Angstroms)

	X	Y	Z
44	1.058691000	-0.179886000	-0.693827000
6	-1.019568000	1.895108000	-1.286591000
6	-2.142434000	2.519967000	-1.825200000
6	-3.123566000	1.756359000	-2.441457000
6	-2.970314000	0.377133000	-2.497309000
6	-1.820196000	-0.179980000	-1.960842000
7	-0.857504000	0.553785000	-1.387556000
1	-4.003395000	2.233571000	-2.860276000
1	-2.253559000	3.594505000	-1.756902000
1	-3.720907000	-0.266349000	-2.939917000
1	-1.665031000	-1.249759000	-1.979775000
6	0.044808000	2.632723000	-0.557389000
6	-0.038395000	3.979681000	-0.262234000
6	1.043305000	4.554654000	0.447578000
6	2.132049000	3.806756000	0.788685000
6	2.204117000	2.410073000	0.434772000
7	1.087428000	1.869944000	-0.176191000
1	1.007256000	5.608218000	0.711609000
1	-0.888707000	4.580630000	-0.555128000
1	2.971345000	4.250833000	1.313845000
6	3.307355000	1.608556000	0.667690000
1	4.172902000	2.030460000	1.168405000
15	3.234084000	-0.098584000	0.185433000
6	1.155499000	-1.888055000	-1.372753000
8	1.222098000	-2.959970000	-1.844974000
6	3.516299000	-1.140298000	1.758471000
6	2.677183000	-0.496131000	2.873204000
6	2.971415000	-2.558664000	1.525287000
6	4.968337000	-1.210924000	2.247187000
1	3.027210000	0.511424000	3.113287000
1	1.628531000	-0.450143000	2.570745000
1	2.753246000	-1.111585000	3.779662000

1	3.451828000	-3.073722000	0.689517000
1	3.124455000	-3.165548000	2.426999000
1	1.898430000	-2.498413000	1.327681000
1	4.990977000	-1.726301000	3.215903000
1	5.621745000	-1.770058000	1.573431000
1	5.394899000	-0.214674000	2.400730000
6	4.687083000	-0.377157000	-1.010831000
6	4.919338000	-1.870193000	-1.276783000
6	4.327358000	0.297445000	-2.345158000
6	5.981622000	0.288624000	-0.514302000
1	5.305837000	-2.400689000	-0.402473000
1	4.000815000	-2.367225000	-1.604952000
1	5.659349000	-1.986738000	-2.078329000
1	4.005030000	1.333066000	-2.197673000
1	5.213616000	0.303805000	-2.992257000
1	3.527623000	-0.232647000	-2.865495000
1	6.763609000	0.161079000	-1.273207000
1	5.835252000	1.363326000	-0.371084000
1	6.362892000	-0.133175000	0.415591000
6	-0.715507000	0.201424000	2.003822000
6	-2.100042000	0.198549000	1.483580000
8	-0.030701000	-0.737038000	1.275468000
1	-2.528184000	-0.789510000	1.205626000
1	1.670162000	0.299121000	-2.065116000
6	-2.942315000	1.298300000	1.226899000
6	-2.638864000	2.632382000	1.599176000
6	-4.185190000	1.002883000	0.616341000
6	-3.581485000	3.622076000	1.403997000
1	-1.675145000	2.870875000	2.035289000
6	-5.121638000	2.004681000	0.423984000
1	-4.341823000	-0.026385000	0.299346000
6	-4.817122000	3.305950000	0.822532000
1	-3.366156000	4.645577000	1.691037000
1	-6.076362000	1.784039000	-0.041016000
1	-5.548590000	4.094832000	0.672772000
1	-0.267536000	1.209635000	1.955578000
19	-0.855352000	-3.050578000	0.539045000
8	-3.168846000	-2.161388000	0.212432000
6	-4.326757000	-2.892825000	0.142707000
6	-5.210320000	-2.655160000	1.389260000
6	-5.138140000	-2.510736000	-1.117773000
6	-4.018721000	-4.409611000	0.061510000
1	-4.645801000	-2.911590000	2.293895000
1	-5.488589000	-1.597281000	1.464971000

1	-6.136238000	-3.245165000	1.383675000
1	-4.528080000	-2.681177000	-2.012560000
1	-6.068761000	-3.083361000	-1.222874000
1	-5.400401000	-1.445880000	-1.089925000
1	-4.916734000	-5.032358000	-0.038748000
1	-3.374779000	-4.610784000	-0.804827000
1	-3.493270000	-4.736999000	0.969568000
1	-0.781976000	-0.033242000	3.092878000
44	-0.790718000	-1.184811000	0.243447000

**TSA4-5**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
44	1.130286000	-1.170349000	0.205484000
6	-1.382511000	-0.918285000	1.834524000
6	-2.569526000	-1.238506000	2.494292000
6	-3.018131000	-2.546805000	2.513803000
6	-2.259462000	-3.528084000	1.882277000
6	-1.101339000	-3.140876000	1.230291000
7	-0.682553000	-1.866052000	1.172802000
1	-3.942474000	-2.800264000	3.021636000
1	-3.143275000	-0.463309000	2.985018000
1	-2.551344000	-4.572022000	1.894189000
1	-0.464321000	-3.867756000	0.734993000
6	-0.798200000	0.448156000	1.844041000
6	-1.322169000	1.494733000	2.568503000
6	-0.649721000	2.740084000	2.495644000
6	0.476255000	2.884319000	1.741763000
6	1.019158000	1.766917000	1.011905000
7	0.317448000	0.579055000	1.084253000
1	-1.041747000	3.588651000	3.048513000
1	-2.210745000	1.386111000	3.175407000
1	0.993829000	3.836271000	1.690361000
6	2.189000000	1.820190000	0.263491000
15	2.953735000	0.260415000	-0.147191000
6	1.877733000	-2.701428000	-0.521132000
8	2.346633000	-3.671414000	-0.967545000
6	4.331295000	0.009417000	1.159694000
6	3.737577000	0.394251000	2.526231000
6	4.768157000	-1.462644000	1.221755000
6	5.560988000	0.899208000	0.934609000
1	3.550582000	1.469125000	2.595408000
1	2.799271000	-0.128528000	2.728881000

1	4.453373000	0.122243000	3.311915000
1	5.157708000	-1.833294000	0.270801000
1	5.565801000	-1.570721000	1.967967000
1	3.937054000	-2.106756000	1.518537000
1	6.211377000	0.842135000	1.816485000
1	6.159230000	0.581510000	0.077005000
1	5.287617000	1.950615000	0.799608000
6	3.758053000	0.438845000	-1.857284000
6	4.663890000	-0.765973000	-2.148151000
6	2.627861000	0.446693000	-2.898849000
6	4.542869000	1.747951000	-2.042776000
1	5.557570000	-0.783111000	-1.519223000
1	4.131793000	-1.713743000	-2.019043000
1	5.005612000	-0.717434000	-3.189391000
1	2.103957000	1.406960000	-2.884809000
1	3.065411000	0.335540000	-3.898983000
1	1.893481000	-0.347803000	-2.738130000
1	4.790398000	1.864118000	-3.105525000
1	3.942262000	2.616511000	-1.754165000
1	5.480557000	1.777820000	-1.487889000
1	2.757816000	2.746001000	0.267586000
1	1.817413000	-1.547509000	1.576887000
6	-0.462970000	0.633299000	-1.776969000
1	0.345736000	1.352784000	-1.978298000
6	-1.526474000	1.152885000	-0.956855000
1	-2.306736000	0.410037000	-0.643863000
1	-1.227194000	0.855507000	-2.636088000
8	-0.105132000	-0.645372000	-1.716818000
6	-1.797586000	2.547902000	-0.735559000
6	-2.971886000	2.866435000	-0.031711000
6	-0.918229000	3.584570000	-1.109107000
6	-3.272837000	4.185196000	0.281691000
1	-3.630911000	2.058487000	0.268851000
6	-1.230479000	4.899046000	-0.809586000
1	0.021127000	3.354221000	-1.599738000
6	-2.404829000	5.199187000	-0.113693000
1	-4.179571000	4.421934000	0.828391000
1	-0.552001000	5.695408000	-1.097093000
1	-2.636476000	6.232674000	0.125853000
19	-1.855567000	-2.477375000	-1.708465000
8	-3.474154000	-0.911429000	-0.716752000
6	-4.818349000	-0.771274000	-0.926413000
6	-5.100068000	0.323983000	-1.982456000
1	-6.167510000	0.451554000	-2.205234000

1	-4.710454000	1.289727000	-1.641420000
1	-4.582647000	0.072395000	-2.916753000
6	-5.425870000	-2.099524000	-1.443432000
1	-5.205792000	-2.902230000	-0.728458000
1	-6.513337000	-2.058543000	-1.588169000
1	-4.976388000	-2.365721000	-2.410451000
6	-5.552282000	-0.398514000	0.383190000
1	-6.631871000	-0.252236000	0.246846000
1	-5.404429000	-1.188506000	1.128346000
1	-5.135136000	0.526951000	0.797794000

### TSA8-9

Coordinates (Angstroms)

	X	Y	Z
19	1.249873000	-1.858515000	-1.995473000
8	2.539550000	-0.134115000	-0.903079000
6	3.787537000	0.408516000	-0.703807000
6	4.261395000	0.185381000	0.749162000
1	4.301876000	-0.887011000	0.973598000
1	5.253330000	0.612612000	0.944073000
1	3.553081000	0.647849000	1.446671000
6	4.806613000	-0.254913000	-1.655342000
1	4.823751000	-1.337439000	-1.477064000
1	4.508828000	-0.085001000	-2.697261000
1	5.828051000	0.126254000	-1.529306000
6	3.776951000	1.927653000	-0.979670000
1	3.104590000	2.430260000	-0.274867000
1	4.768479000	2.389099000	-0.885523000
1	3.402759000	2.116884000	-1.992245000
6	-1.143060000	-0.369366000	-0.173214000
8	-0.894955000	-1.503723000	-0.621976000
6	-2.173873000	-0.184914000	0.930715000
1	-1.960360000	0.720451000	1.503887000
1	-2.112419000	-1.046641000	1.602419000
7	0.562615000	0.324237000	0.905385000
6	0.856469000	-0.504647000	2.073388000
1	1.687238000	-0.060939000	2.648695000
1	-0.014629000	-0.507950000	2.744789000
6	1.234741000	-1.932654000	1.689027000
1	0.377362000	-2.412232000	1.206542000
1	2.038283000	-1.867437000	0.944749000
6	1.692122000	-2.744428000	2.896006000
1	0.913616000	-2.785997000	3.666237000

1	1.933540000	-3.774761000	2.616490000
1	2.586590000	-2.305777000	3.352401000
6	0.539518000	1.744363000	1.251240000
1	-0.194256000	1.913839000	2.052533000
1	1.518506000	2.037621000	1.668715000
6	0.223641000	2.639090000	0.054938000
1	-0.832839000	2.537683000	-0.217950000
1	0.812034000	2.291336000	-0.802027000
6	0.531559000	4.104809000	0.343435000
1	0.264581000	4.741037000	-0.505540000
1	-0.025216000	4.464032000	1.216379000
1	1.597768000	4.252105000	0.547393000
6	-3.551830000	-0.080413000	0.314227000
6	-4.223080000	1.142859000	0.268040000
6	-4.158771000	-1.200357000	-0.262889000
6	-5.475408000	1.247840000	-0.332834000
1	-3.763873000	2.022194000	0.712667000
6	-5.409541000	-1.098934000	-0.861923000
1	-3.637464000	-2.152764000	-0.244022000
6	-6.072497000	0.126273000	-0.899304000
1	-5.983531000	2.207132000	-0.356644000
1	-5.869034000	-1.978818000	-1.302270000
1	-7.048666000	0.205320000	-1.367664000
1	-1.031868000	0.510208000	-0.826651000
1	1.342333000	0.184749000	0.200372000

### TSA9-10

Coordinates (Angstroms)

	X	Y	Z
19	-2.068179000	1.671196000	-0.734009000
8	0.307707000	2.247600000	-0.528239000
6	1.549509000	2.842024000	-0.320304000
6	2.671422000	1.950657000	-0.880288000
1	2.527318000	1.804700000	-1.956883000
1	3.661840000	2.395088000	-0.724796000
1	2.645914000	0.963255000	-0.406863000
6	1.578612000	4.203285000	-1.032765000
1	1.408274000	4.063794000	-2.105807000
1	0.784006000	4.851515000	-0.644812000
1	2.536154000	4.721701000	-0.900724000
6	1.768172000	3.053035000	1.187711000
1	1.709890000	2.090504000	1.705306000
1	2.739596000	3.509569000	1.414039000

1	0.983238000	3.702776000	1.592643000
6	0.220246000	-0.836442000	0.116795000
8	-0.029623000	-0.066404000	-0.992311000
6	-0.858450000	-1.953290000	0.213505000
1	-0.649422000	-2.600557000	1.073024000
1	-0.812559000	-2.571221000	-0.688122000
7	1.600133000	-1.352100000	0.159915000
6	1.938568000	-2.354393000	-0.848704000
1	2.989117000	-2.622959000	-0.679903000
1	1.366999000	-3.294315000	-0.713069000
6	1.808457000	-1.897586000	-2.300532000
1	0.763917000	-1.683544000	-2.533752000
1	2.340923000	-0.947767000	-2.415044000
6	2.370780000	-2.944543000	-3.259184000
1	1.854398000	-3.905724000	-3.149669000
1	2.259350000	-2.627815000	-4.300847000
1	3.437404000	-3.122663000	-3.079208000
6	2.017020000	-1.785682000	1.490362000
1	1.325108000	-2.532071000	1.929390000
1	2.974174000	-2.307423000	1.377378000
6	2.231029000	-0.654963000	2.497167000
1	1.296533000	-0.112955000	2.678231000
1	2.933254000	0.067759000	2.067367000
6	2.763783000	-1.183043000	3.827018000
1	2.906995000	-0.372277000	4.547609000
1	2.070853000	-1.905501000	4.273352000
1	3.728098000	-1.686722000	3.697110000
6	-2.228457000	-1.350168000	0.347593000
6	-2.592123000	-0.667041000	1.516623000
6	-3.139304000	-1.365883000	-0.715149000
6	-3.815670000	-0.006857000	1.615127000
1	-1.901047000	-0.646370000	2.355382000
6	-4.368723000	-0.713890000	-0.620473000
1	-2.874138000	-1.886428000	-1.630857000
6	-4.709061000	-0.022459000	0.542796000
1	-4.073922000	0.515904000	2.531183000
1	-5.062617000	-0.745529000	-1.455384000
1	-5.666700000	0.482607000	0.620497000
1	0.124674000	-0.228266000	1.034862000
1	0.307314000	1.016782000	-0.784280000

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**TSA12-13**  
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Coordinates (Angstroms)  
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	X	Y	Z
44	-1.087517000	-1.365327000	-0.453342000
6	1.114087000	-2.505435000	1.255537000
6	2.078159000	-3.387553000	1.738930000
6	2.538554000	-4.411890000	0.923852000
6	2.025142000	-4.529719000	-0.362260000
6	1.066384000	-3.618745000	-0.780055000
7	0.616193000	-2.627738000	0.001135000
1	3.285871000	-5.108168000	1.288860000
1	2.459724000	-3.277695000	2.746897000
1	2.356375000	-5.309190000	-1.038111000
1	0.633154000	-3.672831000	-1.771730000
6	0.597002000	-1.358301000	2.043570000
6	1.140150000	-0.903098000	3.236774000
6	0.614550000	0.268730000	3.789072000
6	-0.370153000	0.976707000	3.125665000
6	-0.862942000	0.489040000	1.902063000
7	-0.411055000	-0.701196000	1.448915000
1	1.011735000	0.644700000	4.726782000
1	1.963583000	-1.416731000	3.716328000
1	-0.745281000	1.915323000	3.517514000
6	-1.693172000	1.235080000	0.961602000
15	-2.793525000	0.171068000	-0.038743000
6	-1.638473000	-1.964140000	-2.117690000
8	-1.983552000	-2.371631000	-3.150365000
6	-3.453995000	1.301998000	-1.410213000
6	-2.389475000	1.402365000	-2.517737000
6	-4.717111000	0.712869000	-2.055976000
6	-3.743912000	2.718176000	-0.887244000
1	-1.400973000	1.657520000	-2.136729000
1	-2.290709000	0.455455000	-3.055009000
1	-2.708754000	2.165060000	-3.238703000
1	-5.592220000	0.747677000	-1.403289000
1	-4.957835000	1.299493000	-2.950495000
1	-4.561130000	-0.321434000	-2.378429000
1	-4.172300000	3.316480000	-1.700333000
1	-4.456409000	2.732232000	-0.059577000
1	-2.827675000	3.218784000	-0.562839000
6	-4.218075000	-0.444820000	1.051615000
6	-4.976883000	-1.578114000	0.341661000
6	-3.601807000	-1.033676000	2.333074000
6	-5.179178000	0.675304000	1.470986000
1	-5.535054000	-1.236863000	-0.531256000
1	-4.289699000	-2.367946000	0.023521000



1	-5.699842000	-2.017698000	1.039616000
1	-3.119924000	-0.268100000	2.947321000
1	-4.404031000	-1.479310000	2.933130000
1	-2.871397000	-1.815544000	2.110153000
1	-5.904088000	0.278721000	2.192412000
1	-4.647187000	1.497797000	1.961369000
1	-5.748428000	1.084404000	0.633609000
6	1.399504000	0.765698000	-0.665350000
8	0.027467000	0.664144000	-0.886610000
1	-1.932541000	-2.572379000	0.136627000
7	1.869851000	2.122921000	-0.444359000
6	1.444754000	3.116732000	-1.423891000
1	1.345276000	2.598651000	-2.380246000
1	2.252484000	3.850750000	-1.561614000
6	0.130508000	3.885421000	-1.146547000
1	-0.529755000	3.257163000	-0.542611000
1	-0.387478000	4.037761000	-2.100993000
6	0.310160000	5.246295000	-0.473603000
1	0.959720000	5.897810000	-1.069597000
1	-0.652179000	5.757009000	-0.358841000
1	0.756002000	5.158972000	0.522191000
6	1.889478000	2.564251000	0.936443000
1	2.030222000	1.679358000	1.566259000
1	0.927730000	3.007623000	1.256525000
6	3.025481000	3.541316000	1.238962000
1	3.974565000	3.045853000	1.006021000
1	2.959277000	4.416712000	0.582424000
6	3.002218000	3.999215000	2.694533000
1	3.076682000	3.146703000	3.379977000
1	3.831270000	4.678022000	2.916745000
1	2.070237000	4.527350000	2.928597000
1	-2.094151000	2.169178000	1.354039000
1	-0.726709000	1.227677000	-0.008277000
6	2.150657000	0.088177000	-1.832494000
1	1.661581000	-0.875057000	-2.007961000
1	2.025117000	0.678637000	-2.746054000
6	3.608564000	-0.116418000	-1.516269000
6	4.544788000	0.906252000	-1.700445000
6	4.048633000	-1.319346000	-0.958418000
6	5.878336000	0.727222000	-1.344959000
1	4.218371000	1.852483000	-2.121396000
6	5.380816000	-1.504081000	-0.597942000
1	3.334201000	-2.123556000	-0.807288000
6	6.302967000	-0.479586000	-0.791320000

1	6.590864000	1.532353000	-1.500349000
1	5.697236000	-2.450644000	-0.168380000
1	7.344427000	-0.619532000	-0.517174000
1	1.693117000	0.213779000	0.243002000

**TSA12-14**

Coordinates (Angstroms)

	X	Y	Z
44	0.662707000	-0.022228000	-1.063801000
6	-1.469461000	1.834232000	-2.052831000
6	-2.469995000	2.383972000	-2.849823000
6	-3.089742000	1.597094000	-3.811911000
6	-2.696354000	0.273132000	-3.953475000
6	-1.682513000	-0.208211000	-3.137539000
7	-1.077489000	0.547284000	-2.214087000
1	-3.871844000	2.014187000	-4.437131000
1	-2.767214000	3.416911000	-2.718580000
1	-3.156358000	-0.383257000	-4.682649000
1	-1.338182000	-1.232948000	-3.210132000
6	-0.820062000	2.575475000	-0.939730000
6	-1.188235000	3.843731000	-0.518568000
6	-0.585834000	4.352807000	0.634735000
6	0.336661000	3.597770000	1.333614000
6	0.687741000	2.323014000	0.857717000
7	0.113271000	1.871019000	-0.275240000
1	-0.859490000	5.340873000	0.991055000
1	-1.939221000	4.420755000	-1.042572000
1	0.791939000	3.972203000	2.243074000
6	1.571596000	1.381968000	1.559339000
15	2.494475000	0.324301000	0.382032000
6	1.183497000	-1.602493000	-1.909242000
8	1.537665000	-2.512398000	-2.531948000
6	3.295385000	-1.096570000	1.393705000
6	2.989134000	-2.395965000	0.632219000
6	4.817553000	-1.023592000	1.589608000
6	2.681436000	-1.155091000	2.802682000
1	3.373469000	-3.252073000	1.199772000
1	1.918208000	-2.540937000	0.482697000
1	3.465543000	-2.407265000	-0.353692000
1	5.112664000	-0.183469000	2.220846000
1	5.128846000	-1.937686000	2.109049000
1	5.378415000	-0.982798000	0.653781000
1	3.037591000	-2.068084000	3.295515000

1	3.016004000	-0.306079000	3.408922000
1	1.589554000	-1.145434000	2.815779000
6	3.840053000	1.403691000	-0.428403000
6	4.500437000	0.598302000	-1.557730000
6	3.175526000	2.644875000	-1.054717000
6	4.893992000	1.937119000	0.560381000
1	4.979975000	-0.317389000	-1.201654000
1	3.764411000	0.317358000	-2.316963000
1	5.273926000	1.206782000	-2.041707000
1	2.779616000	3.324254000	-0.294158000
1	3.939917000	3.195084000	-1.616241000
1	2.371964000	2.388759000	-1.747063000
1	5.392529000	2.805358000	0.114213000
1	4.442070000	2.273009000	1.500094000
1	5.670800000	1.210331000	0.789767000
6	-0.999162000	-0.856601000	1.641133000
8	-0.286016000	-0.201365000	2.583480000
7	-2.447466000	-0.567444000	1.659433000
6	-3.202411000	-1.172630000	2.754404000
1	-3.254409000	-2.253179000	2.568114000
1	-4.237170000	-0.825602000	2.668999000
6	-2.731201000	-0.963342000	4.203473000
1	-1.736197000	-1.401706000	4.326196000
1	-3.419114000	-1.532265000	4.845180000
6	-2.673231000	0.490946000	4.661893000
1	-3.608688000	1.024236000	4.451211000
1	-2.494779000	0.555344000	5.741158000
1	-1.850140000	0.995286000	4.151146000
6	-2.710242000	0.834141000	1.366566000
1	-2.236075000	1.022839000	0.399029000
1	-2.230352000	1.522011000	2.080658000
6	-4.186843000	1.198647000	1.228368000
1	-4.688388000	0.438968000	0.615735000
1	-4.680699000	1.193817000	2.206383000
6	-4.366042000	2.576303000	0.594616000
1	-3.972099000	2.592650000	-0.427733000
1	-5.422622000	2.858875000	0.549756000
1	-3.837137000	3.346436000	1.167301000
1	2.161811000	1.854676000	2.347770000
1	0.704364000	0.595702000	2.086827000
6	-0.747337000	-2.384844000	1.646883000
1	0.315157000	-2.516120000	1.860711000
1	-1.267845000	-2.842953000	2.495401000
6	-1.074019000	-3.132461000	0.372885000

6	-0.309438000	-4.248190000	0.011167000
6	-2.112386000	-2.742690000	-0.481715000
6	-0.567936000	-4.953381000	-1.160268000
1	0.505756000	-4.564846000	0.658032000
6	-2.371790000	-3.445751000	-1.656512000
1	-2.710493000	-1.880228000	-0.200789000
6	-1.601116000	-4.552300000	-2.003631000
1	0.044664000	-5.811886000	-1.420008000
1	-3.187039000	-3.127551000	-2.301702000
1	-1.802817000	-5.097539000	-2.921086000
1	-0.689986000	-0.533612000	0.588770000
1	1.485563000	0.647192000	-2.201039000

### TSA13-14

Coordinates (Angstroms)

	X	Y	Z
44	-0.646176000	-0.146424000	-0.904690000
6	1.088952000	-2.499874000	-1.496921000
6	2.002729000	-3.336122000	-2.133930000
6	2.834283000	-2.818229000	-3.116640000
6	2.731262000	-1.470697000	-3.439009000
6	1.786698000	-0.698376000	-2.779253000
7	0.979146000	-1.193143000	-1.833394000
1	3.554074000	-3.457113000	-3.616695000
1	2.076630000	-4.380626000	-1.857801000
1	3.364274000	-1.016981000	-4.192576000
1	1.660477000	0.354425000	-3.000692000
6	0.223660000	-2.951637000	-0.382847000
6	0.242898000	-4.231822000	0.161138000
6	-0.554473000	-4.498500000	1.268059000
6	-1.340731000	-3.490682000	1.809236000
6	-1.332988000	-2.231057000	1.214267000
7	-0.572956000	-1.996900000	0.132253000
1	-0.551487000	-5.487665000	1.713329000
1	0.870823000	-5.008322000	-0.257577000
1	-1.953356000	-3.669231000	2.685478000
6	-2.100690000	-1.058558000	1.753644000
15	-2.579979000	0.111028000	0.384390000
6	-0.769869000	1.377352000	-1.963168000
8	-0.892318000	2.264021000	-2.700474000
6	-3.025451000	1.768071000	1.230945000
6	-2.531866000	2.875716000	0.286034000
6	-4.512998000	2.020806000	1.509165000

6	-2.297204000	1.866482000	2.581174000
1	-2.735819000	3.855033000	0.735670000
1	-1.460709000	2.800534000	0.097826000
1	-3.041372000	2.839819000	-0.682778000
1	-4.938212000	1.290191000	2.200705000
1	-4.603652000	3.004829000	1.984518000
1	-5.117541000	2.048295000	0.599678000
1	-2.371686000	2.898972000	2.944419000
1	-2.774725000	1.226396000	3.331652000
1	-1.240501000	1.590416000	2.541408000
6	-4.136745000	-0.685692000	-0.372689000
6	-4.517909000	0.136022000	-1.612801000
6	-3.787751000	-2.119960000	-0.814305000
6	-5.343191000	-0.816435000	0.576543000
1	-4.766028000	1.173112000	-1.364610000
1	-3.700284000	0.146676000	-2.339592000
1	-5.399046000	-0.306527000	-2.092635000
1	-3.665136000	-2.789021000	0.043704000
1	-4.620919000	-2.509802000	-1.410981000
1	-2.886124000	-2.157942000	-1.427128000
1	-6.034441000	-1.560505000	0.163677000
1	-5.057252000	-1.166584000	1.574202000
1	-5.905385000	0.108486000	0.686768000
6	1.254906000	0.966649000	1.617190000
8	0.620558000	0.513013000	2.602672000
7	2.552235000	0.413467000	1.308897000
6	3.689516000	1.186912000	1.817433000
1	3.767999000	2.116746000	1.240821000
1	4.594646000	0.620520000	1.577354000
6	3.727871000	1.549582000	3.314081000
1	2.929884000	2.262873000	3.545455000
1	4.672076000	2.086327000	3.478334000
6	3.621457000	0.384614000	4.294507000
1	4.370593000	-0.389589000	4.090743000
1	3.776361000	0.732677000	5.321551000
1	2.626871000	-0.064245000	4.236974000
6	2.639863000	-1.030380000	1.476763000
1	1.656050000	-1.431545000	1.224785000
1	2.831069000	-1.331952000	2.515484000
6	3.693035000	-1.664811000	0.567901000
1	3.436608000	-1.456457000	-0.476443000
1	4.673375000	-1.205403000	0.738402000
6	3.819055000	-3.167712000	0.802438000
1	2.853002000	-3.671802000	0.693557000

1	4.520088000	-3.624469000	0.096565000
1	4.181320000	-3.377926000	1.814969000
1	-2.930385000	-1.377761000	2.390176000
1	-1.379025000	-0.496831000	2.363185000
6	1.133319000	2.471561000	1.312409000
1	0.101061000	2.732459000	1.546420000
1	1.735116000	3.001317000	2.062453000
6	1.473553000	3.033878000	-0.050524000
6	0.984163000	4.304464000	-0.371648000
6	2.263089000	2.375386000	-0.998015000
6	1.277274000	4.908513000	-1.590018000
1	0.357876000	4.827865000	0.347770000
6	2.562046000	2.979807000	-2.217013000
1	2.626909000	1.379636000	-0.765429000
6	2.073103000	4.246976000	-2.520796000
1	0.878843000	5.893949000	-1.813051000
1	3.185965000	2.453355000	-2.935308000
1	2.304078000	4.713030000	-3.473972000
1	0.460176000	0.517584000	0.359250000
1	-1.561858000	-0.833685000	-2.071503000

### TSA15-1

Coordinates (Angstroms)

	X	Y	Z
44	-0.372898000	-0.818740000	-0.105795000
6	-3.159398000	0.286289000	0.056849000
6	-4.524795000	0.368210000	0.324867000
6	-5.268094000	-0.796067000	0.447351000
6	-4.627717000	-2.020881000	0.296562000
6	-3.263610000	-2.031206000	0.051501000
7	-2.536532000	-0.911469000	-0.060288000
1	-6.331539000	-0.746705000	0.655973000
1	-4.997934000	1.335767000	0.443116000
1	-5.165840000	-2.958089000	0.376946000
1	-2.718489000	-2.961524000	-0.055314000
6	-2.304024000	1.473199000	-0.169150000
6	-2.771431000	2.757571000	-0.373448000
6	-1.842625000	3.748887000	-0.728190000
6	-0.516272000	3.428551000	-0.913660000
6	-0.084566000	2.099027000	-0.702025000
7	-0.991393000	1.182417000	-0.277158000
1	-2.180796000	4.768622000	-0.884164000
1	-3.825881000	2.992507000	-0.300353000

1	0.202844000	4.177392000	-1.226283000
6	1.206656000	1.568251000	-1.047223000
15	1.748582000	0.155026000	-0.027788000
6	0.137837000	-2.605504000	-0.044892000
8	0.443446000	-3.725782000	0.012920000
6	2.306954000	0.757323000	1.680488000
6	1.216365000	1.710926000	2.200178000
6	2.385513000	-0.438214000	2.645346000
6	3.637258000	1.520877000	1.675539000
1	1.184115000	2.644000000	1.631085000
1	0.226933000	1.247897000	2.170929000
1	1.439926000	1.964579000	3.243152000
1	3.171688000	-1.147651000	2.380562000
1	2.604291000	-0.068246000	3.654484000
1	1.435322000	-0.978232000	2.677360000
1	3.802110000	1.956522000	2.668486000
1	4.492160000	0.874308000	1.461473000
1	3.631587000	2.343339000	0.953060000
6	3.199538000	-0.588212000	-0.989015000
6	3.915495000	-1.630710000	-0.117541000
6	2.658402000	-1.309456000	-2.236151000
6	4.203198000	0.471191000	-1.471856000
1	4.477206000	-1.175001000	0.701467000
1	3.214842000	-2.359678000	0.302221000
1	4.633116000	-2.181699000	-0.736302000
1	2.155001000	-0.625319000	-2.922923000
1	3.506838000	-1.755272000	-2.769512000
1	1.958258000	-2.106952000	-1.981341000
1	5.021089000	-0.033219000	-2.000884000
1	3.742671000	1.167515000	-2.178372000
1	4.648384000	1.048007000	-0.660661000
1	0.575111000	0.497786000	-1.878606000
1	1.938210000	2.293599000	-1.400059000
1	-0.521749000	-0.911422000	1.481387000
1	-0.020893000	-0.314345000	-1.989539000

**TSA16-17**

Coordinates (Angstroms)

	X	Y	Z
44	-0.532203000	-1.274004000	-0.469743000
6	-3.195670000	-0.267569000	0.478730000
6	-4.573023000	-0.078165000	0.594774000
6	-5.431157000	-0.725640000	-0.280497000

6	-4.890170000	-1.551364000	-1.259757000
6	-3.513341000	-1.694473000	-1.321642000
7	-2.677679000	-1.072587000	-0.478857000
1	-6.503868000	-0.586256000	-0.198933000
1	-4.969966000	0.574622000	1.362464000
1	-5.517818000	-2.079947000	-1.967871000
1	-3.043956000	-2.326933000	-2.065599000
6	-2.212956000	0.416627000	1.353141000
6	-2.553091000	1.244271000	2.415127000
6	-1.514850000	1.839140000	3.141167000
6	-0.202626000	1.643183000	2.765488000
6	0.095440000	0.827492000	1.648093000
7	-0.930000000	0.198254000	1.014091000
1	-1.747927000	2.462776000	3.999038000
1	-3.585688000	1.412709000	2.692824000
1	0.611104000	2.113626000	3.306798000
6	1.399531000	0.705167000	1.045773000
15	1.644800000	-0.910877000	0.244852000
6	-0.190236000	-2.591538000	-1.723429000
8	0.023247000	-3.419612000	-2.515571000
6	2.256863000	-2.050979000	1.655249000
6	1.288330000	-1.863688000	2.837564000
6	2.181617000	-3.522995000	1.222054000
6	3.662113000	-1.705434000	2.167833000
1	1.392118000	-0.877245000	3.298249000
1	0.247941000	-2.005827000	2.533863000
1	1.522575000	-2.611045000	3.605462000
1	2.904718000	-3.778458000	0.445577000
1	2.389553000	-4.168414000	2.084761000
1	1.179604000	-3.758747000	0.851972000
1	3.875384000	-2.300655000	3.064537000
1	4.452788000	-1.921914000	1.446144000
1	3.737738000	-0.650979000	2.455314000
6	3.063611000	-0.694236000	-1.007018000
6	3.751832000	-2.034418000	-1.309684000
6	2.479083000	-0.212342000	-2.342910000
6	4.095748000	0.337564000	-0.527044000
1	4.326283000	-2.424482000	-0.468589000
1	3.026560000	-2.793693000	-1.617905000
1	4.453005000	-1.894344000	-2.141309000
1	1.923744000	0.718189000	-2.245735000
1	3.299510000	-0.041508000	-3.051717000
1	1.792671000	-0.944945000	-2.770451000
1	4.877902000	0.457444000	-1.287404000



1	3.633297000	1.317018000	-0.368532000
1	4.586570000	0.046185000	0.403758000
1	0.998158000	1.738884000	-0.067490000
1	2.216955000	1.078434000	1.666221000
1	-0.749059000	-2.441606000	0.713973000
1	-0.405515000	-0.044487000	-1.667914000
7	0.548606000	2.452818000	-0.921645000
6	-0.689621000	3.167334000	-0.499083000
1	-0.832618000	3.008843000	0.571922000
1	-0.540830000	4.241041000	-0.653645000
6	-1.910415000	2.686378000	-1.275520000
1	-1.773271000	2.918418000	-2.339059000
1	-1.964396000	1.595743000	-1.199919000
6	-3.197814000	3.319245000	-0.759639000
1	-4.063876000	2.933342000	-1.304355000
1	-3.343449000	3.095016000	0.302551000
1	-3.188095000	4.409008000	-0.874626000
6	1.626828000	3.329719000	-1.422130000
1	2.365119000	2.695749000	-1.920193000
1	1.217429000	4.015461000	-2.173448000
6	2.295139000	4.097482000	-0.286414000
1	2.659725000	3.379955000	0.457183000
1	1.558312000	4.729750000	0.222339000
6	3.449478000	4.956541000	-0.792968000
1	3.922028000	5.499353000	0.030192000
1	4.219261000	4.341867000	-1.271778000
1	3.105980000	5.694121000	-1.526216000
1	0.282913000	1.736967000	-1.610636000

### TSA17-18

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
44	0.084647000	-0.990915000	-0.747250000
6	-2.694928000	-1.475051000	0.267785000
6	-4.020895000	-1.903403000	0.336439000
6	-4.621595000	-2.465285000	-0.779789000
6	-3.882236000	-2.590755000	-1.949965000
6	-2.566649000	-2.154142000	-1.949697000
7	-1.982505000	-1.608063000	-0.875498000
1	-5.652460000	-2.800607000	-0.734659000
1	-4.578804000	-1.799972000	1.258432000
1	-4.307241000	-3.023233000	-2.848149000
1	-1.944141000	-2.239207000	-2.832630000

6	-1.997176000	-0.819809000	1.405707000
6	-2.606621000	-0.543930000	2.616582000
6	-1.841092000	0.140690000	3.585639000
6	-0.551706000	0.514366000	3.324937000
6	0.060668000	0.195245000	2.063825000
7	-0.724481000	-0.468620000	1.143487000
1	-2.286635000	0.372168000	4.548958000
1	-3.629472000	-0.827623000	2.824378000
1	0.037902000	1.037586000	4.070550000
6	1.372663000	0.521248000	1.720941000
15	2.065056000	-0.332242000	0.314341000
6	0.814602000	-1.525892000	-2.368873000
8	1.271059000	-1.888450000	-3.375898000
6	3.072555000	-1.792682000	1.027428000
6	2.185675000	-2.472621000	2.085463000
6	3.391277000	-2.822524000	-0.066955000
6	4.366254000	-1.362922000	1.732175000
1	2.016070000	-1.820262000	2.946465000
1	1.214372000	-2.762540000	1.677148000
1	2.689696000	-3.379938000	2.440714000
1	4.049147000	-2.428105000	-0.844775000
1	3.899336000	-3.684965000	0.383123000
1	2.476056000	-3.181853000	-0.544021000
1	4.802292000	-2.230289000	2.243349000
1	5.122940000	-0.987988000	1.038681000
1	4.177156000	-0.598143000	2.492901000
6	3.260216000	0.877152000	-0.526206000
6	4.187540000	0.151869000	-1.510701000
6	2.402968000	1.864925000	-1.326135000
6	4.082682000	1.705750000	0.473766000
1	4.934694000	-0.466362000	-1.007713000
1	3.623870000	-0.481527000	-2.202867000
1	4.731357000	0.892633000	-2.109806000
1	1.722325000	2.396030000	-0.658255000
1	3.051096000	2.609948000	-1.804547000
1	1.810306000	1.366631000	-2.096317000
1	4.709135000	2.416739000	-0.079657000
1	3.429351000	2.286686000	1.132266000
1	4.746139000	1.104320000	1.095689000
1	-0.162575000	2.379424000	0.611299000
1	2.011189000	0.949659000	2.488903000
1	0.366630000	-2.479886000	-0.202108000
1	-0.375052000	0.636861000	-1.435616000
7	-0.889001000	2.459884000	-0.105347000

6	-2.225072000	2.460292000	0.517886000
1	-2.175434000	1.830602000	1.407813000
1	-2.482240000	3.475471000	0.849677000
6	-3.288250000	1.921311000	-0.435468000
1	-3.398679000	2.592445000	-1.295594000
1	-2.946035000	0.960229000	-0.832093000
6	-4.633702000	1.748303000	0.261153000
1	-5.382627000	1.348034000	-0.428188000
1	-4.545775000	1.054853000	1.104225000
1	-5.011117000	2.700613000	0.650312000
6	-0.614015000	3.606631000	-0.988717000
1	0.043646000	3.260045000	-1.793459000
1	-1.555075000	3.905930000	-1.459125000
6	0.017724000	4.785884000	-0.256532000
1	0.933525000	4.443507000	0.242605000
1	-0.660929000	5.132995000	0.532147000
6	0.350455000	5.934258000	-1.204316000
1	0.803483000	6.771142000	-0.665535000
1	1.057607000	5.612763000	-1.976248000
1	-0.547715000	6.308378000	-1.707282000
1	-0.642241000	1.362425000	-0.786646000

### TSB2-6

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
44	0.670268000	-0.844885000	-0.311653000
6	-2.044529000	-0.135353000	-1.360744000
6	-3.337265000	-0.265486000	-1.870353000
6	-3.944762000	-1.510568000	-1.895950000
6	-3.244903000	-2.614676000	-1.417124000
6	-1.956516000	-2.423002000	-0.946850000
7	-1.363245000	-1.219096000	-0.917739000
1	-4.950824000	-1.619284000	-2.287540000
1	-3.866261000	0.604475000	-2.238059000
1	-3.678786000	-3.607864000	-1.419768000
1	-1.356028000	-3.248762000	-0.582329000
6	-1.347804000	1.170547000	-1.237354000
6	-1.945842000	2.378452000	-1.547967000
6	-1.167505000	3.547522000	-1.364978000
6	0.125280000	3.466482000	-0.937200000
6	0.732288000	2.186110000	-0.659629000
7	-0.092848000	1.079305000	-0.762933000
1	-1.606264000	4.518887000	-1.576863000

1	-2.959358000	2.442463000	-1.920522000
1	0.725322000	4.361819000	-0.810906000
6	2.055035000	2.014384000	-0.300342000
1	2.691306000	2.887418000	-0.192473000
15	2.636856000	0.369853000	0.062770000
6	1.382668000	-2.541092000	-0.091555000
8	1.830631000	-3.613086000	-0.001682000
6	3.255830000	0.394347000	1.867158000
6	2.211392000	1.171335000	2.684330000
6	3.294719000	-1.044836000	2.406186000
6	4.613670000	1.073900000	2.082984000
1	2.155135000	2.221100000	2.383203000
1	1.231622000	0.703602000	2.567591000
1	2.490467000	1.131882000	3.745850000
1	3.958758000	-1.696870000	1.832670000
1	3.657741000	-1.035672000	3.442513000
1	2.290874000	-1.477515000	2.399090000
1	4.807591000	1.140528000	3.161272000
1	5.446343000	0.520820000	1.641732000
1	4.624989000	2.095275000	1.688418000
6	4.115854000	0.066682000	-1.096448000
6	4.894739000	-1.189799000	-0.683856000
6	3.564556000	-0.158440000	-2.514112000
6	5.057454000	1.280585000	-1.174150000
1	5.432081000	-1.063142000	0.259729000
1	4.232636000	-2.056456000	-0.588566000
1	5.639954000	-1.426940000	-1.453433000
1	2.874463000	0.637739000	-2.810217000
1	4.400604000	-0.167596000	-3.225352000
1	3.034187000	-1.108793000	-2.595633000
1	5.850892000	1.071560000	-1.902599000
1	4.522014000	2.170011000	-1.519676000
1	5.543510000	1.518001000	-0.228252000
6	-1.138625000	0.050918000	2.152850000
6	-2.430527000	-0.597545000	1.881466000
8	-0.107090000	-0.750502000	1.839985000
1	-2.411524000	-1.674058000	2.051110000
1	1.099231000	-0.912206000	-1.835523000
6	-3.646678000	-0.032100000	1.446631000
6	-3.776023000	1.349651000	1.155861000
6	-4.781494000	-0.872899000	1.331337000
6	-5.007445000	1.865170000	0.797227000
1	-2.907209000	1.996043000	1.193745000
6	-6.007464000	-0.347271000	0.968408000

1	-4.672704000	-1.933464000	1.537004000
6	-6.116967000	1.020033000	0.704039000
1	-5.109286000	2.921588000	0.574774000
1	-6.876800000	-0.990043000	0.885284000
1	-7.078035000	1.432711000	0.412798000
1	-1.099575000	1.064692000	1.704540000
1	-1.232190000	0.274125000	3.256663000

**TSB8-9**

Coordinates (Angstroms)

	X	Y	Z
7	2.577859000	-0.035786000	-0.435017000
6	3.604346000	0.911007000	0.043434000
1	3.615039000	1.777582000	-0.623719000
1	4.588904000	0.436614000	-0.042188000
6	3.034834000	-1.436405000	-0.493242000
1	4.047352000	-1.447911000	-0.918817000
1	3.115606000	-1.838264000	0.524574000
6	-1.634652000	0.610618000	-1.757535000
1	-1.725490000	0.244294000	-2.785207000
1	-1.624090000	1.703084000	-1.820275000
6	-0.234258000	0.096906000	-1.313223000
8	0.721164000	0.451272000	-2.162641000
1	-0.345546000	-1.000057000	-1.170091000
7	0.141968000	0.554787000	0.149588000
1	1.456995000	0.199723000	0.067626000
6	-0.048916000	2.003069000	0.373524000
1	-1.126210000	2.222794000	0.374574000
1	0.298193000	2.221917000	1.392399000
6	-0.483628000	-0.161004000	1.284109000
1	-1.561510000	0.035802000	1.316126000
1	-0.058284000	0.281446000	2.195333000
1	2.124433000	0.228911000	-1.368379000
6	-0.242177000	-1.664420000	1.347601000
1	0.833918000	-1.870355000	1.298129000
1	-0.705624000	-2.164034000	0.492514000
6	-0.820014000	-2.245811000	2.635285000
1	-0.651995000	-3.325216000	2.690286000
1	-0.361363000	-1.790746000	3.520338000
1	-1.899848000	-2.071486000	2.690491000
6	0.657763000	2.947863000	-0.594730000
1	1.741061000	2.837807000	-0.486765000
1	0.435452000	2.666097000	-1.624563000

6	0.264594000	4.394454000	-0.307794000
1	0.485237000	4.674869000	0.729170000
1	0.805849000	5.085259000	-0.960702000
1	-0.807046000	4.554518000	-0.472682000
6	3.382621000	1.373017000	1.484176000
1	4.225720000	2.016018000	1.762100000
1	2.488659000	2.004910000	1.527751000
6	3.245692000	0.236813000	2.493659000
1	4.129208000	-0.411124000	2.492930000
1	3.122454000	0.631288000	3.506560000
1	2.371731000	-0.386646000	2.276981000
6	2.142075000	-2.328238000	-1.350504000
1	1.951281000	-1.827687000	-2.304849000
1	1.167884000	-2.450325000	-0.871128000
6	2.776685000	-3.698696000	-1.565550000
1	2.130676000	-4.337583000	-2.174396000
1	3.740412000	-3.615234000	-2.079802000
1	2.950260000	-4.213000000	-0.613434000
6	-2.803400000	0.134130000	-0.935459000
6	-3.090044000	-1.233162000	-0.838777000
6	-3.599790000	1.023252000	-0.207993000
6	-4.104999000	-1.697946000	-0.008894000
1	-2.501815000	-1.940935000	-1.417165000
6	-4.621826000	0.564996000	0.619335000
1	-3.408837000	2.090894000	-0.285547000
6	-4.870301000	-0.799947000	0.732383000
1	-4.301037000	-2.764022000	0.059109000
1	-5.222799000	1.275283000	1.179525000
1	-5.660569000	-1.160626000	1.383499000

### TSC7-13

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
44	-0.165399000	-1.096351000	-0.901772000
6	0.450199000	-3.217012000	1.116297000
6	0.993497000	-4.351489000	1.716578000
6	2.026062000	-5.032486000	1.087678000
6	2.494304000	-4.564314000	-0.132872000
6	1.896083000	-3.440358000	-0.683219000
7	0.899019000	-2.782647000	-0.083099000
1	2.458258000	-5.915362000	1.546633000
1	0.612820000	-4.703207000	2.667580000
1	3.303715000	-5.057299000	-0.658531000

1	2.216865000	-3.044253000	-1.639730000
6	-0.617974000	-2.402728000	1.754224000
6	-1.107112000	-2.620832000	3.034171000
6	-2.078540000	-1.741396000	3.524786000
6	-2.478954000	-0.657599000	2.772168000
6	-1.910140000	-0.445565000	1.498380000
7	-1.056442000	-1.374527000	1.009446000
1	-2.503399000	-1.904475000	4.510481000
1	-0.754639000	-3.441925000	3.645026000
1	-3.205154000	0.052332000	3.152930000
6	-2.091846000	0.762668000	0.701690000
15	-2.029049000	0.331228000	-1.068230000
6	0.619444000	-0.876329000	-2.564519000
8	1.103162000	-0.793736000	-3.619428000
6	-2.079938000	1.951637000	-2.072647000
6	-1.324401000	3.025105000	-1.286888000
6	-1.343110000	1.708080000	-3.399823000
6	-3.469314000	2.531216000	-2.370080000
1	-1.858043000	3.313779000	-0.376925000
1	-0.330872000	2.684054000	-1.015654000
1	-1.209134000	3.920271000	-1.910199000
1	-1.749591000	0.859762000	-3.956742000
1	-1.430270000	2.598774000	-4.033722000
1	-0.280548000	1.519119000	-3.235035000
1	-3.335066000	3.506446000	-2.854070000
1	-4.054291000	1.915764000	-3.055354000
1	-4.049741000	2.697836000	-1.458923000
6	-3.646838000	-0.639096000	-1.452386000
6	-3.668649000	-0.994966000	-2.945906000
6	-3.677429000	-1.956907000	-0.651034000
6	-4.933174000	0.108442000	-1.048612000
1	-3.746306000	-0.113959000	-3.588794000
1	-2.767532000	-1.549023000	-3.229114000
1	-4.536771000	-1.629793000	-3.162040000
1	-3.801591000	-1.779319000	0.420503000
1	-4.546820000	-2.536409000	-0.985309000
1	-2.785757000	-2.563999000	-0.803930000
1	-5.758095000	-0.612133000	-1.004738000
1	-4.845491000	0.556430000	-0.053056000
1	-5.230685000	0.883654000	-1.751490000
6	1.546065000	1.196930000	0.713116000
8	1.292728000	-0.091574000	0.526056000
1	-1.088336000	-2.151650000	-1.655195000
1	-2.936387000	1.373876000	1.032641000

1	2.392603000	1.357379000	1.414859000
7	0.344315000	1.856166000	1.478734000
1	-0.797741000	1.428812000	0.986076000
6	0.376217000	3.327535000	1.578959000
1	0.371194000	3.738608000	0.570539000
1	1.317312000	3.651495000	2.044345000
6	-0.816552000	3.919654000	2.329310000
1	-0.763465000	3.676357000	3.395887000
1	-1.739684000	3.467164000	1.949326000
6	-0.873193000	5.435294000	2.155844000
1	-0.992052000	5.706794000	1.101112000
1	-1.713306000	5.866041000	2.708177000
1	0.044040000	5.910331000	2.521041000
6	0.289883000	1.220541000	2.822347000
1	0.419084000	0.153557000	2.634756000
1	-0.718404000	1.368830000	3.221132000
6	1.310934000	1.675939000	3.864298000
1	2.327850000	1.573854000	3.472531000
1	1.171825000	2.733456000	4.115850000
6	1.939076000	1.935396000	-0.586903000
1	1.243096000	1.604251000	-1.365002000
1	1.879308000	3.024153000	-0.506099000
6	3.349584000	1.573763000	-0.997997000
6	3.716396000	0.240766000	-1.220456000
6	4.321367000	2.564249000	-1.159633000
6	5.014142000	-0.084525000	-1.599275000
1	2.968272000	-0.527631000	-1.060954000
6	5.622887000	2.240992000	-1.539299000
1	4.057728000	3.605396000	-0.987355000
6	5.973744000	0.913193000	-1.762765000
1	5.278601000	-1.124984000	-1.767889000
1	6.362374000	3.027864000	-1.658453000
1	6.986754000	0.657275000	-2.059493000
6	1.170245000	0.833736000	5.131223000
1	1.327948000	-0.228531000	4.916042000
1	1.898821000	1.135268000	5.889371000
1	0.170870000	0.938358000	5.569233000

**TSD7-8**

Coordinates (Angstroms)

	X	Y	Z
44	-1.391930000	0.227046000	-0.918475000
6	-3.556051000	-1.768191000	-0.362899000



6	-4.563689000	-2.706147000	-0.575741000
6	-4.632055000	-3.373617000	-1.790006000
6	-3.683517000	-3.089733000	-2.764697000
6	-2.716808000	-2.133194000	-2.493539000
7	-2.648012000	-1.478832000	-1.327032000
1	-5.411898000	-4.105997000	-1.969118000
1	-5.291376000	-2.909344000	0.200693000
1	-3.689996000	-3.589285000	-3.726281000
1	-1.968577000	-1.865920000	-3.230182000
6	-3.356997000	-1.077448000	0.934646000
6	-3.986266000	-1.424845000	2.123801000
6	-3.549398000	-0.811368000	3.299584000
6	-2.484968000	0.073275000	3.275114000
6	-1.882796000	0.386463000	2.046211000
7	-2.393017000	-0.146233000	0.913373000
1	-4.026591000	-1.057952000	4.242896000
1	-4.766562000	-2.174668000	2.152873000
1	-2.099825000	0.512703000	4.188207000
6	-0.634498000	1.128983000	1.862511000
15	-0.667043000	2.099818000	0.311634000
6	-0.576282000	0.505396000	-2.558444000
8	-0.116752000	0.665771000	-3.615133000
6	1.077550000	2.865055000	0.157328000
6	2.089030000	2.002578000	0.933034000
6	1.444778000	2.877595000	-1.335044000
6	1.236678000	4.291884000	0.703298000
1	1.963201000	2.115287000	2.013874000
1	2.030214000	0.941760000	0.703115000
1	3.099145000	2.349583000	0.681895000
1	0.713919000	3.430723000	-1.933249000
1	2.420159000	3.360843000	-1.471396000
1	1.511061000	1.869727000	-1.747847000
1	2.287896000	4.582855000	0.587500000
1	0.641796000	5.028290000	0.159968000
1	0.998744000	4.357178000	1.767799000
6	-1.961970000	3.490724000	0.458123000
6	-1.969883000	4.273424000	-0.864002000
6	-3.357539000	2.864642000	0.645299000
6	-1.752613000	4.425821000	1.663303000
1	-1.024015000	4.787105000	-1.058075000
1	-2.176658000	3.605561000	-1.706835000
1	-2.756204000	5.037245000	-0.835529000
1	-3.463871000	2.390965000	1.625431000
1	-4.101821000	3.668410000	0.591232000

1	-3.589531000	2.130316000	-0.126446000
1	-2.682166000	4.977417000	1.846698000
1	-1.526653000	3.863822000	2.576482000
1	-0.970217000	5.166967000	1.511033000
6	4.714604000	0.986221000	-1.529892000
8	5.117138000	1.267356000	-2.634253000
1	-0.256050000	1.605062000	2.767922000
1	3.640262000	0.786675000	-1.345300000
6	5.597111000	0.878570000	-0.302544000
1	6.642242000	0.877957000	-0.626089000
1	5.431628000	1.785264000	0.293272000
6	5.248391000	-0.344901000	0.512372000
6	5.469871000	-1.618135000	-0.020989000
6	4.659022000	-0.237656000	1.772996000
6	5.108796000	-2.758814000	0.689660000
1	5.928701000	-1.715193000	-1.002079000
6	4.302497000	-1.377036000	2.489683000
1	4.478204000	0.745413000	2.198854000
6	4.525330000	-2.640179000	1.948971000
1	5.281240000	-3.739839000	0.257898000
1	3.842496000	-1.276532000	3.467708000
1	4.240155000	-3.528567000	2.503922000
1	-2.610634000	1.083505000	-1.553408000
7	0.244024000	-0.900231000	0.272416000
1	0.073708000	0.157341000	1.302410000
6	1.472932000	-1.048601000	-0.503776000
1	1.667333000	-0.091331000	-0.996627000
6	-0.126591000	-2.159854000	0.906689000
1	-1.041585000	-2.008541000	1.487273000
1	2.351529000	-1.248531000	0.136797000
1	-0.377763000	-2.936842000	0.161816000
6	1.445373000	-2.119378000	-1.602369000
1	1.478215000	-3.120863000	-1.155686000
1	0.491169000	-2.044304000	-2.139066000
6	2.607243000	-1.959980000	-2.579012000
1	3.568262000	-2.014474000	-2.055452000
1	2.601516000	-2.741742000	-3.345637000
1	2.559950000	-0.992368000	-3.091056000
6	0.914264000	-2.733876000	1.875579000
1	1.821598000	-3.025036000	1.335459000
1	1.214362000	-1.941581000	2.573633000
6	0.375791000	-3.936473000	2.645870000
1	-0.505514000	-3.664306000	3.239329000
1	0.076845000	-4.740237000	1.962850000

1 1.124412000 -4.346987000 3.332001000  
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**TSD8-13**  
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Coordinates (Angstroms)

	X	Y	Z
44	-1.268142000	0.659896000	0.125956000
6	0.061315000	2.769390000	-1.558550000
6	0.412746000	4.011499000	-2.081114000
6	0.084399000	5.164985000	-1.381887000
6	-0.584093000	5.046650000	-0.171212000
6	-0.905632000	3.777285000	0.288054000
7	-0.596529000	2.662449000	-0.382920000
1	0.350573000	6.138581000	-1.778786000
1	0.936039000	4.084219000	-3.026170000
1	-0.858193000	5.916090000	0.414550000
1	-1.426034000	3.635324000	1.227578000
6	0.379145000	1.492696000	-2.247448000
6	1.101394000	1.407395000	-3.432964000
6	1.333824000	0.153884000	-3.986445000
6	0.825309000	-0.975938000	-3.362065000
6	0.103935000	-0.831171000	-2.179229000
7	-0.079973000	0.383892000	-1.635739000
1	1.898038000	0.062522000	-4.908349000
1	1.481159000	2.295491000	-3.921448000
1	0.977095000	-1.963684000	-3.781770000
6	-0.500369000	-2.006100000	-1.462090000
15	-1.954023000	-1.497164000	-0.420257000
6	-2.522201000	0.870640000	1.476248000
8	-3.383119000	0.968913000	2.249252000
6	-2.145662000	-2.910173000	0.824275000
6	-1.223896000	-2.578846000	2.001917000
6	-3.578653000	-2.961661000	1.377386000
6	-1.742918000	-4.281409000	0.258632000
1	-0.181006000	-2.398926000	1.735988000
1	-1.581743000	-1.693362000	2.528959000
1	-1.234846000	-3.414867000	2.711358000
1	-4.312999000	-3.321903000	0.654332000
1	-3.595187000	-3.653607000	2.227163000
1	-3.903653000	-1.985088000	1.749960000
1	-1.909953000	-5.040373000	1.031832000
1	-2.315605000	-4.580008000	-0.620966000
1	-0.678968000	-4.317614000	0.006171000
6	-3.394913000	-1.558036000	-1.668684000

6	-4.637162000	-0.879794000	-1.068447000
6	-2.994043000	-0.778555000	-2.935658000
6	-3.751089000	-2.983326000	-2.119630000
1	-5.020152000	-1.397599000	-0.187418000
1	-4.427059000	0.156855000	-0.793038000
1	-5.436765000	-0.873879000	-1.818659000
1	-2.182414000	-1.265914000	-3.484498000
1	-3.858200000	-0.742978000	-3.609098000
1	-2.702461000	0.250169000	-2.714002000
1	-4.515190000	-2.923031000	-2.903614000
1	-2.892553000	-3.508779000	-2.550120000
1	-4.164897000	-3.596973000	-1.318431000
6	2.122025000	-1.011286000	1.967358000
8	1.737295000	-1.825970000	2.819523000
1	-0.737944000	-2.808130000	-2.166753000
1	2.832903000	-0.214456000	2.266673000
6	2.303038000	-1.481578000	0.518178000
1	1.756005000	-2.427621000	0.447840000
1	1.872200000	-0.772145000	-0.186496000
6	3.754069000	-1.731432000	0.182563000
6	4.548655000	-2.524546000	1.018273000
6	4.337461000	-1.175873000	-0.959287000
6	5.884734000	-2.762420000	0.714385000
1	4.104294000	-2.947950000	1.914860000
6	5.675676000	-1.412244000	-1.266983000
1	3.732827000	-0.549221000	-1.611294000
6	6.453878000	-2.207880000	-0.431232000
1	6.486183000	-3.381102000	1.374230000
1	6.111805000	-0.970665000	-2.158719000
1	7.497951000	-2.391895000	-0.666422000
1	-2.454682000	1.042147000	-0.856577000
7	0.695655000	0.572559000	1.716305000
6	0.185903000	0.570960000	3.089901000
1	-0.556527000	-0.223925000	3.182378000
6	1.584623000	1.728197000	1.605426000
1	1.022054000	2.675849000	1.589210000
1	0.994559000	0.286274000	3.788739000
1	2.216116000	1.800920000	2.514985000
6	-0.426178000	1.868204000	3.642548000
1	0.352438000	2.627536000	3.781063000
1	-1.139148000	2.287683000	2.924469000
6	-1.130468000	1.626155000	4.974895000
1	-0.437631000	1.204258000	5.712076000
1	-1.538874000	2.552193000	5.393650000

1	-1.958738000	0.918917000	4.857523000
6	2.540914000	1.748222000	0.411636000
1	3.339663000	1.013522000	0.549817000
1	2.016107000	1.448702000	-0.496963000
6	3.168640000	3.125779000	0.218338000
1	2.405442000	3.889186000	0.026898000
1	3.720377000	3.433479000	1.114171000
1	3.873010000	3.134100000	-0.620348000
1	0.239277000	-2.400167000	-0.761009000

### **tBuOK**

Coordinates (Angstroms)			
	X	Y	Z
6	-1.068029000	-0.000140000	0.006649000
8	0.287719000	-0.001534000	0.111619000
6	-1.501539000	0.004019000	-1.480619000
1	-1.093527000	-0.881296000	-1.983228000
1	-2.590857000	0.006161000	-1.622662000
1	-1.090563000	0.890459000	-1.978797000
6	-1.672858000	-1.255934000	0.680723000
1	-2.767850000	-1.307480000	0.610904000
1	-1.257554000	-2.156874000	0.213224000
1	-1.396097000	-1.273537000	1.741709000
6	-1.670644000	1.253440000	0.686831000
1	-1.392039000	1.266579000	1.747342000
1	-1.255945000	2.156412000	0.222719000
1	-2.765768000	1.305798000	0.619490000
19	2.567730000	-0.000119000	0.009202000

### **C<sub>8</sub>H<sub>8</sub>O**

Coordinates (Angstroms)			
	X	Y	Z
6	-2.566803000	0.009782000	-0.745747000
6	-1.602456000	0.582057000	0.205045000
8	-2.479163000	-0.471146000	0.589292000
1	-3.477635000	0.555549000	-0.988633000
1	-2.203511000	-0.673140000	-1.512826000
1	-1.843817000	1.549967000	0.645375000
6	-0.146992000	0.266370000	0.122533000
6	0.785384000	1.302473000	0.057089000
6	0.296148000	-1.056877000	0.086420000
6	2.143219000	1.020649000	-0.058528000

1	0.446839000	2.334672000	0.098356000
6	1.653409000	-1.337683000	-0.026018000
1	-0.432450000	-1.858123000	0.161318000
6	2.580214000	-0.300531000	-0.102330000
1	2.861701000	1.833020000	-0.108155000
1	1.989845000	-2.369736000	-0.050652000
1	3.639596000	-0.520478000	-0.189906000

**NH(CH<sub>3</sub>CH<sub>3</sub>CH<sub>3</sub>)<sub>2</sub>**

Coordinates (Angstroms)

	X	Y	Z
7	0.000000000	0.437521000	-0.059491000
1	-0.000058000	1.102974000	0.709957000
6	1.214766000	-0.359720000	0.016647000
1	1.219344000	-1.052011000	-0.836002000
1	1.252069000	-0.991680000	0.925616000
6	-1.214765000	-0.359738000	0.016507000
1	-1.219400000	-1.051804000	-0.836327000
1	-1.252025000	-0.991937000	0.925314000
6	-2.460982000	0.516847000	-0.041158000
1	-2.444501000	1.224640000	0.798281000
1	-2.422874000	1.117290000	-0.956888000
6	2.460988000	0.516842000	-0.041313000
1	2.444525000	1.224892000	0.797906000
1	2.422850000	1.116998000	-0.957228000
6	3.749921000	-0.298259000	0.004040000
1	3.799698000	-1.005113000	-0.831395000
1	4.631206000	0.347382000	-0.053521000
1	3.822148000	-0.876412000	0.931823000
6	-3.749918000	-0.298260000	0.003991000
1	-4.631199000	0.347406000	-0.053370000
1	-3.799724000	-1.004886000	-0.831635000
1	-3.822126000	-0.876663000	0.931619000

**PhCH<sub>2</sub>CON(CH<sub>3</sub>CH<sub>3</sub>CH<sub>3</sub>)<sub>2</sub>**

Coordinates (Angstroms)

	X	Y	Z
6	-0.515381000	-0.352997000	-1.352946000
8	-0.760136000	-1.378817000	-1.983497000
7	-1.353769000	0.116039000	-0.388882000
6	-2.565686000	-0.642501000	-0.101718000
1	-2.919044000	-1.089151000	-1.033570000

1	-3.330788000	0.062093000	0.244082000
6	-1.093550000	1.293486000	0.428775000
1	-1.513167000	1.103307000	1.423037000
1	-0.018149000	1.412568000	0.579531000
6	0.781568000	0.409700000	-1.610077000
1	0.633093000	1.492213000	-1.585309000
1	1.078212000	0.140573000	-2.626907000
6	1.871319000	0.011631000	-0.632951000
6	2.625609000	0.979056000	0.033086000
6	2.139553000	-1.338314000	-0.388342000
6	3.628906000	0.608184000	0.925413000
1	2.427907000	2.032574000	-0.149991000
6	3.139593000	-1.709787000	0.502971000
1	1.554203000	-2.095192000	-0.902325000
6	3.887836000	-0.737530000	1.163632000
1	4.206093000	1.373409000	1.435543000
1	3.335181000	-2.762514000	0.682590000
1	4.667323000	-1.028897000	1.860600000
6	-1.695984000	2.575613000	-0.146293000
1	-2.775226000	2.437130000	-0.280234000
1	-1.280042000	2.748002000	-1.146009000
6	-1.427683000	3.782065000	0.747645000
1	-1.852847000	4.694097000	0.319465000
1	-1.867573000	3.645614000	1.741590000
1	-0.352659000	3.946294000	0.881320000
6	-2.337194000	-1.734206000	0.943280000
1	-1.928364000	-1.283405000	1.856042000
1	-1.576358000	-2.421295000	0.558634000
6	-3.618305000	-2.495757000	1.267389000
1	-3.436454000	-3.278968000	2.008992000
1	-4.387392000	-1.827690000	1.671393000
1	-4.030097000	-2.974368000	0.372487000

## H<sub>2</sub>

-----			
Coordinates (Angstroms)			
	X	Y	Z
1	0.000000000	0.000000000	0.371384000
1	0.000000000	0.000000000	-0.371384000

## TSB3-5

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			

6	3.522411000	-0.241650000	-0.785332000
6	4.731548000	-0.873085000	-1.089464000
6	4.917050000	-1.444821000	-2.336881000
6	3.892206000	-1.366031000	-3.276157000
6	2.716863000	-0.732907000	-2.910255000
7	2.521680000	-0.204555000	-1.692939000
1	5.852948000	-1.938343000	-2.577331000
1	5.518300000	-0.920342000	-0.347799000
1	3.998550000	-1.781071000	-4.271645000
1	1.889689000	-0.636535000	-3.605253000
6	3.256064000	0.414070000	0.519160000
6	4.212406000	0.534971000	1.503276000
6	3.836579000	1.196226000	2.696626000
6	2.577802000	1.695521000	2.848148000
6	1.603668000	1.569893000	1.792678000
7	2.001275000	0.892832000	0.656219000
1	4.564760000	1.308543000	3.495028000
1	5.213585000	0.144707000	1.382920000
1	2.289608000	2.214845000	3.756210000
6	0.325995000	2.098053000	1.861705000
15	-0.673060000	2.061099000	0.400630000
6	-0.404570000	0.682298000	-2.483916000
8	-1.099104000	0.637820000	-3.424268000
6	-0.831307000	3.857997000	-0.215106000
6	0.559265000	4.504647000	-0.100936000
6	-1.271872000	3.897155000	-1.685553000
6	-1.803243000	4.700539000	0.622200000
1	0.865679000	4.614332000	0.942600000
1	1.327596000	3.923919000	-0.618448000
1	0.524686000	5.502120000	-0.556425000
1	-2.235980000	3.408211000	-1.848694000
1	-1.378974000	4.942079000	-2.003155000
1	-0.531160000	3.424914000	-2.335553000
1	-1.678468000	5.758127000	0.359207000
1	-2.846853000	4.442077000	0.425790000
1	-1.614359000	4.606748000	1.696227000
6	-2.369429000	1.395271000	0.914329000
6	-3.323472000	1.415152000	-0.296660000
6	-2.121834000	-0.049799000	1.399764000
6	-3.036686000	2.119205000	2.096471000
1	-3.806926000	2.391168000	-0.406420000
1	-2.798702000	1.231785000	-1.241668000
1	-4.101867000	0.649164000	-0.181516000
1	-1.775778000	-0.046070000	2.438143000



1	-3.051540000	-0.629022000	1.323832000
1	-1.353967000	-0.563667000	0.818314000
1	-3.877995000	1.505582000	2.441225000
1	-2.346705000	2.231718000	2.939064000
1	-3.437153000	3.099422000	1.840120000
1	0.027020000	2.654665000	2.744251000
6	0.650767000	-2.564718000	-0.134512000
6	0.895489000	-3.272648000	-1.382440000
1	0.951024000	-2.688754000	-2.296905000
1	-0.123710000	-3.322380000	0.217864000
8	-0.034609000	-1.472859000	-0.500509000
1	0.748392000	-4.347618000	-1.473511000
6	1.677373000	-2.527983000	0.972372000
6	1.340346000	-1.858752000	2.148706000
6	2.908801000	-3.173548000	0.860215000
6	2.236232000	-1.835263000	3.210191000
1	0.388679000	-1.340852000	2.219265000
6	3.798643000	-3.158129000	1.929532000
1	3.180900000	-3.667843000	-0.069156000
6	3.461844000	-2.490245000	3.104078000
1	1.981410000	-1.298372000	4.117377000
1	4.760588000	-3.653118000	1.839311000
1	4.161854000	-2.468340000	3.933528000
1	1.253898000	2.088332000	-1.490368000
44	0.689415000	0.713997000	-0.995721000
19	-2.550686000	-1.449631000	-1.497257000
8	-4.488339000	-1.799544000	-0.212642000
6	-5.620873000	-2.178101000	0.442814000
6	-6.664869000	-2.750032000	-0.547488000
6	-5.308779000	-3.269619000	1.496211000
6	-6.262181000	-0.974031000	1.175839000
1	-6.900322000	-1.994680000	-1.306510000
1	-6.242346000	-3.621691000	-1.062605000
1	-7.603019000	-3.058782000	-0.066074000
1	-4.578984000	-2.885490000	2.219252000
1	-6.194219000	-3.610279000	2.050475000
1	-4.861582000	-4.141085000	1.001791000
1	-7.183265000	-1.230730000	1.716998000
1	-5.547760000	-0.559402000	1.897862000
1	-6.500559000	-0.186453000	0.451225000

**B16**

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Coordinates (Angstroms)  
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	X	Y	Z
44	-0.448668000	-0.331483000	-0.624275000
6	1.658358000	1.746110000	-1.015578000
6	2.831175000	2.377309000	-1.429700000
6	3.815476000	1.639919000	-2.069890000
6	3.597201000	0.285908000	-2.293055000
6	2.405265000	-0.275600000	-1.865556000
7	1.455718000	0.426042000	-1.232008000
1	4.735566000	2.116335000	-2.390512000
1	2.977330000	3.435620000	-1.251231000
1	4.335449000	-0.336998000	-2.783151000
1	2.192100000	-1.324506000	-2.022843000
6	0.578178000	2.451328000	-0.291090000
6	0.616287000	3.798593000	0.062894000
6	-0.442640000	4.332301000	0.784178000
6	-1.496763000	3.510321000	1.164843000
6	-1.478355000	2.169007000	0.795573000
7	-0.469340000	1.678864000	0.054223000
1	-0.438529000	5.381475000	1.060096000
1	1.453258000	4.425709000	-0.217581000
1	-2.322666000	3.895790000	1.752176000
6	-2.518748000	1.186267000	1.262575000
15	-2.608108000	-0.329765000	0.175233000
6	-0.343935000	-2.101974000	-1.155204000
8	-0.248798000	-3.220028000	-1.466833000
6	-3.968241000	0.111989000	-1.075487000
6	-3.636766000	1.511460000	-1.625366000
6	-3.915371000	-0.884241000	-2.244557000
6	-5.389068000	0.160806000	-0.499584000
1	-3.784710000	2.295721000	-0.875521000
1	-2.610979000	1.561726000	-2.001000000
1	-4.313776000	1.731919000	-2.458907000
1	-4.170849000	-1.903151000	-1.942741000
1	-4.637805000	-0.577182000	-3.010438000
1	-2.920018000	-0.898268000	-2.695453000
1	-6.070262000	0.546829000	-1.267608000
1	-5.760929000	-0.824805000	-0.209989000
1	-5.465176000	0.830504000	0.363728000
6	-3.228176000	-1.666051000	1.370350000
6	-3.729112000	-2.872481000	0.561583000
6	-2.033466000	-2.135452000	2.217796000
6	-4.325084000	-1.187447000	2.336385000
1	-4.676111000	-2.674194000	0.053549000
1	-2.995225000	-3.192227000	-0.184854000

1	-3.895603000	-3.715300000	1.242709000
1	-1.564393000	-1.317196000	2.772323000
1	-2.389492000	-2.876059000	2.944424000
1	-1.256712000	-2.592012000	1.602440000
1	-4.608204000	-2.022316000	2.988625000
1	-3.974923000	-0.380187000	2.987544000
1	-5.230855000	-0.849930000	1.833453000
1	-2.191183000	0.821371000	2.243613000
1	-3.488030000	1.672038000	1.407635000
1	-0.979098000	0.172097000	-2.151287000
1	0.119614000	-0.724663000	0.916055000
6	2.664843000	1.344382000	2.129941000
8	3.398113000	0.723117000	3.177138000
6	2.708711000	-0.117293000	2.250048000
1	1.823180000	-0.605421000	2.652543000
1	1.765619000	1.879352000	2.434477000
1	3.269885000	1.829311000	1.364375000
6	3.539507000	-0.961062000	1.344454000
6	2.986236000	-2.106981000	0.770255000
6	4.860539000	-0.617801000	1.050575000
6	3.741044000	-2.893165000	-0.096005000
1	1.951401000	-2.359529000	0.981177000
6	5.613916000	-1.402967000	0.183635000
1	5.298126000	0.258095000	1.520550000
6	5.055824000	-2.542752000	-0.393610000
1	3.296927000	-3.779019000	-0.540455000
1	6.642919000	-1.131837000	-0.034110000
1	5.647003000	-3.159010000	-1.064571000

### TSB16-17

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
44	-0.123904000	-1.053268000	-0.625842000
6	-2.766620000	-1.423823000	0.716840000
6	-4.093315000	-1.784149000	0.943995000
6	-4.861579000	-2.261735000	-0.107845000
6	-4.283116000	-2.368440000	-1.366632000
6	-2.955531000	-2.001659000	-1.522712000
7	-2.206897000	-1.542828000	-0.510719000
1	-5.897283000	-2.539839000	0.053809000
1	-4.527675000	-1.687510000	1.931128000
1	-4.843848000	-2.728619000	-2.220977000
1	-2.460617000	-2.072950000	-2.483625000

6	-1.892242000	-0.854793000	1.768737000
6	-2.302175000	-0.584532000	3.071365000
6	-1.405285000	0.019906000	3.943650000
6	-0.140461000	0.373504000	3.492549000
6	0.213180000	0.091420000	2.176088000
7	-0.645707000	-0.544913000	1.361732000
1	-1.700105000	0.230826000	4.966092000
1	-3.302400000	-0.831276000	3.404841000
1	0.564388000	0.879434000	4.142436000
6	1.509103000	0.553632000	1.569886000
15	1.992415000	-0.470246000	0.088356000
6	0.302431000	-1.468239000	-2.384323000
8	0.567562000	-1.729773000	-3.485068000
6	3.030791000	-1.870512000	0.839422000
6	2.226294000	-2.459956000	2.012664000
6	3.225583000	-2.974819000	-0.211711000
6	4.395421000	-1.427891000	1.384411000
1	2.161943000	-1.767412000	2.858114000
1	1.215283000	-2.743735000	1.709187000
1	2.736505000	-3.361290000	2.371235000
1	3.837271000	-2.648219000	-1.055683000
1	3.736386000	-3.826546000	0.253280000
1	2.263711000	-3.322425000	-0.598057000
1	4.860280000	-2.275731000	1.901601000
1	5.084922000	-1.117455000	0.596368000
1	4.310776000	-0.614448000	2.112841000
6	3.087582000	0.696709000	-0.921559000
6	3.911305000	-0.113997000	-1.933532000
6	2.156197000	1.628944000	-1.710483000
6	4.012295000	1.572666000	-0.061431000
1	4.713920000	-0.687160000	-1.463561000
1	3.283784000	-0.800036000	-2.511367000
1	4.378728000	0.577887000	-2.643627000
1	1.497980000	2.203446000	-1.055394000
1	2.767230000	2.340162000	-2.279630000
1	1.525743000	1.076122000	-2.408752000
1	4.622587000	2.198308000	-0.723352000
1	3.443356000	2.250168000	0.582538000
1	4.695862000	0.997735000	0.563756000
1	1.324880000	1.565087000	1.183723000
1	2.297735000	0.628097000	2.323849000
1	0.163420000	-2.621968000	-0.196859000
1	-0.520610000	0.625195000	-0.999893000
6	-1.617156000	1.731845000	-1.395761000

8	-2.551986000	2.738681000	-2.678122000
6	-1.505518000	1.882494000	-2.847664000
1	-0.549376000	2.308441000	-3.209256000
1	-2.439258000	1.108449000	-1.067190000
6	-1.164589000	2.776275000	-0.441447000
6	-1.465114000	2.641653000	0.916533000
6	-0.404203000	3.878682000	-0.847617000
6	-0.988562000	3.556117000	1.852148000
1	-2.080830000	1.808709000	1.243402000
6	0.072528000	4.793231000	0.084127000
1	-0.203553000	4.027725000	-1.902708000
6	-0.206738000	4.631699000	1.441068000
1	-1.231633000	3.425076000	2.902661000
1	0.661475000	5.641714000	-0.251662000
1	0.166608000	5.348343000	2.166389000
1	-1.691440000	0.940677000	-3.400132000

#### TSC16-17

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
44	-0.253963000	-0.029295000	-0.637247000
6	1.575364000	2.330027000	-0.521097000
6	2.674305000	3.161001000	-0.728181000
6	3.786820000	2.668307000	-1.395142000
6	3.776494000	1.350244000	-1.832006000
6	2.649477000	0.578010000	-1.596056000
7	1.568014000	1.050623000	-0.965398000
1	4.650812000	3.302797000	-1.560659000
1	2.667346000	4.180812000	-0.363538000
1	4.627831000	0.909087000	-2.335702000
1	2.605177000	-0.459834000	-1.901031000
6	0.370210000	2.758946000	0.226602000
6	0.202141000	4.022497000	0.787603000
6	-0.954955000	4.287144000	1.506951000
6	-1.900552000	3.283851000	1.680810000
6	-1.677447000	2.035794000	1.108020000
7	-0.576740000	1.811739000	0.368973000
1	-1.109976000	5.266838000	1.946079000
1	0.956818000	4.789636000	0.667953000
1	-2.799288000	3.457728000	2.261747000
6	-2.591537000	0.861775000	1.340990000
15	-2.422107000	-0.444699000	0.018675000
6	0.040086000	-1.633471000	-1.520013000

8	0.209680000	-2.636272000	-2.083693000
6	-3.774560000	0.019293000	-1.227424000
6	-3.628410000	1.525137000	-1.513534000
6	-3.529556000	-0.743931000	-2.538747000
6	-5.207009000	-0.232682000	-0.740346000
1	-3.915665000	2.140864000	-0.654641000
1	-2.607569000	1.780980000	-1.809652000
1	-4.297273000	1.793353000	-2.339434000
1	-3.638067000	-1.824959000	-2.421489000
1	-4.263499000	-0.418638000	-3.285684000
1	-2.529424000	-0.538019000	-2.928237000
1	-5.909330000	0.182486000	-1.472996000
1	-5.435280000	-1.296812000	-0.644760000
1	-5.412818000	0.255445000	0.218053000
6	-2.874702000	-2.041964000	0.933535000
6	-3.159341000	-3.149132000	-0.092977000
6	-1.648986000	-2.467777000	1.759616000
6	-4.063728000	-1.901339000	1.898337000
1	-4.100856000	-2.993491000	-0.625761000
1	-2.354032000	-3.238627000	-0.828571000
1	-3.236597000	-4.110145000	0.428589000
1	-1.350904000	-1.707474000	2.487261000
1	-1.899412000	-3.378601000	2.316578000
1	-0.783905000	-2.672691000	1.126772000
1	-4.219962000	-2.861770000	2.403248000
1	-3.874499000	-1.157942000	2.679142000
1	-4.997912000	-1.642326000	1.400358000
1	-2.269610000	0.386341000	2.275439000
1	-3.625022000	1.186508000	1.491699000
1	-0.786657000	0.625010000	-2.062469000
1	0.379781000	-0.589342000	0.894725000
6	1.309818000	-0.313695000	2.155301000
8	2.589910000	-0.684373000	3.376264000
6	2.216970000	-1.455765000	2.307807000
1	1.710717000	-2.409731000	2.540403000
1	0.455148000	-0.239109000	2.814720000
1	1.727009000	0.596023000	1.745625000
6	3.225988000	-1.655103000	1.200469000
6	2.983880000	-2.547018000	0.153893000
6	4.410005000	-0.919654000	1.207901000
6	3.911580000	-2.698818000	-0.873922000
1	2.063068000	-3.123817000	0.143701000
6	5.342157000	-1.072241000	0.184757000
1	4.578135000	-0.241571000	2.038989000

6	5.095623000	-1.961899000	-0.860025000
1	3.711668000	-3.396146000	-1.682493000
1	6.267292000	-0.502452000	0.204676000
1	5.826248000	-2.087544000	-1.654204000

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**B17**

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Coordinates (Angstroms)			
	X	Y	Z
44	0.404420000	-0.408632000	0.751442000
6	-2.156651000	1.058339000	1.214665000
6	-3.456986000	1.356820000	1.606037000
6	-4.175577000	0.426303000	2.345582000
6	-3.574945000	-0.778421000	2.677179000
6	-2.277655000	-1.015920000	2.245190000
7	-1.583335000	-0.126007000	1.528508000
1	-5.196045000	0.639370000	2.644419000
1	-3.919723000	2.291358000	1.317291000
1	-4.097401000	-1.538913000	3.244697000
1	-1.777557000	-1.952474000	2.456747000
6	-1.333861000	1.984084000	0.397759000
6	-1.719882000	3.274947000	0.053849000
6	-0.888197000	4.027349000	-0.764768000
6	0.298095000	3.479081000	-1.234545000
6	0.642342000	2.186591000	-0.850013000
7	-0.160015000	1.483280000	-0.032213000
1	-1.169517000	5.037890000	-1.041496000
1	-2.651157000	3.692758000	0.413415000
1	0.952854000	4.040930000	-1.890763000
6	1.875607000	1.491936000	-1.364907000
15	2.440950000	0.122406000	-0.231007000
6	0.930838000	-2.014974000	1.552053000
8	1.285926000	-2.967707000	2.101471000
6	3.678400000	0.967773000	0.921394000
6	3.033142000	2.268871000	1.434242000
6	3.953693000	0.054925000	2.127646000
6	5.002764000	1.333481000	0.238549000
1	2.922668000	3.018326000	0.644091000
1	2.055577000	2.096505000	1.892421000
1	3.686807000	2.702389000	2.199357000
1	4.394666000	-0.902311000	1.840376000
1	4.660620000	0.555209000	2.799650000
1	3.038879000	-0.147125000	2.690076000
1	5.599593000	1.946146000	0.924043000

1	5.599817000	0.452444000	-0.008004000
1	4.851824000	1.919865000	-0.673570000
6	3.289307000	-1.094642000	-1.399343000
6	4.104156000	-2.104986000	-0.578513000
6	2.167529000	-1.859702000	-2.120809000
6	4.184241000	-0.436736000	-2.461934000
1	4.996429000	-1.658240000	-0.132191000
1	3.506817000	-2.562816000	0.215994000
1	4.438994000	-2.911664000	-1.239970000
1	1.508319000	-1.201701000	-2.695608000
1	2.618161000	-2.563804000	-2.829119000
1	1.548507000	-2.436396000	-1.428630000
1	4.565891000	-1.219539000	-3.127531000
1	3.632600000	0.270186000	-3.089097000
1	5.047733000	0.078266000	-2.040765000
1	1.609572000	1.012076000	-2.314517000
1	2.670189000	2.209957000	-1.587453000
1	0.940981000	0.290624000	2.032338000
1	-0.432149000	-1.105250000	-1.125504000
6	-1.267288000	-1.727617000	-1.544364000
8	-2.298407000	-3.886138000	-1.234215000
6	-1.387125000	-3.071463000	-0.757012000
1	-0.317615000	-3.468448000	-0.733501000
1	-0.942073000	-1.955969000	-2.569159000
6	-2.514366000	-0.875630000	-1.593582000
6	-2.477684000	0.415684000	-2.130800000
6	-3.733046000	-1.353665000	-1.095979000
6	-3.612447000	1.223704000	-2.153401000
1	-1.541928000	0.798087000	-2.535684000
6	-4.865864000	-0.544102000	-1.110121000
1	-3.749124000	-2.393236000	-0.769982000
6	-4.813167000	0.747677000	-1.633155000
1	-3.555721000	2.222645000	-2.578053000
1	-5.803323000	-0.930762000	-0.718567000
1	-5.703654000	1.370463000	-1.650516000
1	-1.528197000	-2.741501000	0.328916000

## C17

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
44	-0.202878000	-0.035120000	-0.566672000
6	1.533784000	2.394486000	-0.535054000
6	2.601518000	3.256965000	-0.754905000



6	3.745212000	2.779543000	-1.384572000
6	3.795695000	1.448343000	-1.767223000
6	2.691861000	0.641879000	-1.523257000
7	1.583371000	1.101433000	-0.936146000
1	4.587991000	3.440343000	-1.555752000
1	2.555599000	4.287226000	-0.424650000
1	4.674462000	1.018486000	-2.231647000
1	2.701334000	-0.411287000	-1.777203000
6	0.308490000	2.799836000	0.198308000
6	0.080126000	4.077590000	0.696444000
6	-1.086414000	4.318786000	1.411883000
6	-1.986297000	3.285403000	1.634197000
6	-1.704284000	2.023101000	1.120119000
7	-0.590011000	1.816099000	0.399341000
1	-1.284546000	5.309721000	1.805982000
1	0.794517000	4.874531000	0.535427000
1	-2.893110000	3.446054000	2.205750000
6	-2.578206000	0.824898000	1.381651000
15	-2.396093000	-0.473845000	0.055565000
6	0.067515000	-1.602256000	-1.546657000
8	0.176993000	-2.543789000	-2.210079000
6	-3.700483000	0.002408000	-1.227862000
6	-3.549284000	1.508476000	-1.510971000
6	-3.434037000	-0.762512000	-2.534625000
6	-5.140889000	-0.250549000	-0.763656000
1	-3.838427000	2.124502000	-0.653609000
1	-2.529695000	1.772872000	-1.803622000
1	-4.214811000	1.776785000	-2.339075000
1	-3.521990000	-1.844604000	-2.415632000
1	-4.171595000	-0.453113000	-3.284037000
1	-2.439577000	-0.541690000	-2.930594000
1	-5.831572000	0.163788000	-1.507117000
1	-5.368176000	-1.314799000	-0.670024000
1	-5.360579000	0.237311000	0.191470000
6	-2.840424000	-2.083618000	0.938630000
6	-3.115768000	-3.181459000	-0.100048000
6	-1.606335000	-2.502122000	1.756260000
6	-4.031740000	-1.955085000	1.901054000
1	-4.055129000	-3.025222000	-0.636248000
1	-2.306069000	-3.265286000	-0.831674000
1	-3.192002000	-4.145410000	0.415238000
1	-1.302922000	-1.746472000	2.485945000
1	-1.843705000	-3.416488000	2.311508000
1	-0.746711000	-2.713890000	1.115953000

1	-4.188272000	-2.921711000	2.393020000
1	-3.844724000	-1.221497000	2.691150000
1	-4.963916000	-1.690214000	1.401185000
1	-2.225816000	0.360653000	2.310885000
1	-3.618474000	1.119655000	1.546028000
1	-0.772913000	0.537521000	-1.901072000
1	0.621446000	-0.868513000	1.197910000
6	1.193165000	-0.347927000	2.005528000
8	3.095189000	-0.544363000	3.411808000
6	2.413412000	-1.208240000	2.509155000
1	1.941175000	-2.187199000	2.847177000
1	0.503807000	-0.150913000	2.833343000
1	1.600646000	0.601992000	1.655620000
6	3.208967000	-1.604458000	1.234810000
6	2.740695000	-2.510200000	0.278700000
6	4.457805000	-1.019398000	1.036824000
6	3.492449000	-2.814727000	-0.855473000
1	1.781094000	-3.001843000	0.434598000
6	5.217181000	-1.314172000	-0.093514000
1	4.792029000	-0.346632000	1.822921000
6	4.736572000	-2.211427000	-1.048199000
1	3.112579000	-3.525602000	-1.584876000
1	6.192722000	-0.852242000	-0.229780000
1	5.330666000	-2.452748000	-1.925867000

## B18

Coordinates (Angstroms)

	X	Y	Z
44	-0.454723000	0.598341000	0.617455000
6	2.135185000	-0.759211000	1.263243000
6	3.394325000	-1.015747000	1.800712000
6	4.065988000	-0.008577000	2.476926000
6	3.455544000	1.231413000	2.611363000
6	2.200595000	1.416586000	2.052914000
7	1.554316000	0.455090000	1.383660000
1	5.050530000	-0.191371000	2.893437000
1	3.851016000	-1.990552000	1.688342000
1	3.937223000	2.049360000	3.134133000
1	1.684438000	2.365882000	2.134992000
6	1.359953000	-1.775203000	0.510742000
6	1.846807000	-3.029321000	0.154957000
6	1.044708000	-3.859435000	-0.618461000
6	-0.194496000	-3.410084000	-1.054948000

6	-0.621515000	-2.138218000	-0.680259000
7	0.134231000	-1.382828000	0.128780000
1	1.399565000	-4.844645000	-0.902938000
1	2.837793000	-3.349702000	0.450280000
1	-0.818861000	-4.023356000	-1.694932000
6	-1.873762000	-1.509636000	-1.228387000
15	-2.512092000	-0.133617000	-0.149410000
6	-0.924208000	2.340824000	1.024929000
8	-1.210589000	3.435807000	1.293971000
6	-3.600947000	-1.011947000	1.128143000
6	-2.769991000	-2.159760000	1.729653000
6	-3.952351000	-0.031034000	2.258400000
6	-4.886247000	-1.618675000	0.548776000
1	-2.568958000	-2.949624000	0.998605000
1	-1.818915000	-1.803209000	2.132806000
1	-3.337623000	-2.613352000	2.550507000
1	-4.613280000	0.772023000	1.925319000
1	-4.473544000	-0.573912000	3.056242000
1	-3.050703000	0.417902000	2.683655000
1	-5.392600000	-2.190991000	1.335394000
1	-5.591890000	-0.861917000	0.199264000
1	-4.683432000	-2.311553000	-0.274676000
6	-3.570144000	0.896218000	-1.330133000
6	-4.544738000	1.784655000	-0.542793000
6	-2.611996000	1.820803000	-2.100606000
6	-4.339616000	0.039948000	-2.348076000
1	-5.369207000	1.225192000	-0.094016000
1	-4.033579000	2.345220000	0.246483000
1	-4.984276000	2.516561000	-1.230630000
1	-1.758754000	1.282236000	-2.518420000
1	-3.169381000	2.319802000	-2.902905000
1	-2.199481000	2.591052000	-1.443759000
1	-4.953669000	0.699695000	-2.972601000
1	-3.661802000	-0.496265000	-3.018726000
1	-5.009098000	-0.686863000	-1.885154000
1	-2.623089000	-2.261004000	-1.490761000
1	-0.867900000	0.210117000	2.132634000
6	0.792405000	1.838860000	-2.022990000
6	2.136209000	2.206912000	-1.374038000
1	0.164442000	2.756950000	-1.965735000
1	0.986166000	1.691366000	-3.108175000
1	2.534834000	3.107494000	-1.863478000
6	3.204275000	1.133475000	-1.393684000
6	4.474386000	1.410972000	-0.873385000

6	2.974155000	-0.144417000	-1.914623000
6	5.481749000	0.451440000	-0.869495000
1	4.671769000	2.397331000	-0.458653000
6	3.983704000	-1.105026000	-1.921074000
1	1.974008000	-0.383793000	-2.260177000
6	5.240487000	-0.815877000	-1.397107000
1	6.456857000	0.692946000	-0.455165000
1	3.780416000	-2.090148000	-2.332900000
1	6.025073000	-1.567278000	-1.401188000
1	-1.558131000	-0.990806000	-2.141721000
1	1.944390000	2.490480000	-0.331553000
8	0.173871000	0.731757000	-1.502966000

### C18

#### Coordinates (Angstroms)

	X	Y	Z
44	-0.175587000	-0.089924000	-0.642765000
6	1.946279000	2.002254000	-0.412764000
6	3.109992000	2.732336000	-0.640740000
6	4.087166000	2.215307000	-1.479658000
6	3.876413000	0.977333000	-2.070480000
6	2.696063000	0.302474000	-1.797240000
7	1.752669000	0.794299000	-0.988348000
1	4.999643000	2.771741000	-1.665434000
1	3.253776000	3.698637000	-0.173432000
1	4.611507000	0.527621000	-2.726881000
1	2.495102000	-0.671284000	-2.225524000
6	0.855300000	2.480282000	0.471639000
6	0.911565000	3.643775000	1.233464000
6	-0.163693000	3.954853000	2.057227000
6	-1.243709000	3.086718000	2.137725000
6	-1.237018000	1.928089000	1.363813000
7	-0.224054000	1.682018000	0.521950000
1	-0.146861000	4.863326000	2.650180000
1	1.773007000	4.298565000	1.195401000
1	-2.076254000	3.289061000	2.801952000
6	-2.296301000	0.866144000	1.484924000
15	-2.403127000	-0.201686000	-0.037282000
6	-0.107331000	-1.630795000	-1.667493000
8	-0.067679000	-2.586529000	-2.329203000
6	-3.607595000	0.730781000	-1.164721000
6	-3.130780000	2.192637000	-1.246903000
6	-3.552718000	0.128232000	-2.577782000

6	-5.056769000	0.739834000	-0.660233000
1	-3.243042000	2.717133000	-0.292348000
1	-2.088395000	2.263798000	-1.567292000
1	-3.747915000	2.723169000	-1.981367000
1	-3.943789000	-0.890904000	-2.615358000
1	-4.165811000	0.739023000	-3.251402000
1	-2.528994000	0.118614000	-2.960804000
1	-5.657094000	1.384813000	-1.313140000
1	-5.516677000	-0.250565000	-0.678321000
1	-5.140412000	1.143414000	0.354372000
6	-3.192936000	-1.794257000	0.604257000
6	-3.775133000	-2.609678000	-0.559365000
6	-2.055771000	-2.616028000	1.232365000
6	-4.268922000	-1.558987000	1.676763000
1	-4.687694000	-2.173428000	-0.973145000
1	-3.048310000	-2.731591000	-1.368948000
1	-4.027572000	-3.612293000	-0.194632000
1	-1.439354000	-2.020645000	1.909248000
1	-2.484324000	-3.469899000	1.770661000
1	-1.381671000	-3.000644000	0.462984000
1	-4.685534000	-2.528084000	1.975775000
1	-3.850373000	-1.100854000	2.577939000
1	-5.099161000	-0.940581000	1.332221000
1	-3.254844000	1.287163000	1.801169000
1	-0.608326000	0.692480000	-1.992833000
6	1.218913000	-1.928045000	1.457693000
1	0.806290000	-2.786085000	0.880450000
8	0.442916000	-0.802870000	1.350169000
6	2.648534000	-1.733102000	0.945106000
6	3.406593000	-0.645118000	1.390657000
6	3.234216000	-2.622988000	0.046069000
6	4.715633000	-0.461743000	0.963036000
1	2.943302000	0.064314000	2.070680000
6	4.547381000	-2.444093000	-0.392421000
1	2.653282000	-3.468093000	-0.317604000
6	5.293967000	-1.364306000	0.067717000
1	5.288972000	0.389722000	1.320146000
1	4.984093000	-3.149918000	-1.094033000
1	6.317061000	-1.221671000	-0.268777000
6	1.281315000	-2.387257000	2.926354000
1	0.272583000	-2.607340000	3.291554000
1	1.898123000	-3.285184000	3.051928000
1	1.699992000	-1.590211000	3.551271000
1	-1.947742000	0.181663000	2.267250000

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**E1**  
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Coordinates (Angstroms)

	X	Y	Z
6	-3.131049000	0.307723000	-0.190920000
6	-4.524227000	0.367467000	-0.175247000
6	-5.253825000	-0.810996000	-0.153334000
6	-4.568036000	-2.020930000	-0.152229000
6	-3.182425000	-2.002861000	-0.164299000
7	-2.467581000	-0.868929000	-0.180385000
1	-6.338275000	-0.785094000	-0.139819000
1	-5.033439000	1.323574000	-0.185283000
1	-5.091558000	-2.969831000	-0.140019000
1	-2.609352000	-2.922185000	-0.157968000
6	-2.259368000	1.494373000	-0.268458000
6	-2.714191000	2.810212000	-0.318018000
6	-1.787153000	3.829366000	-0.482980000
6	-0.445998000	3.505472000	-0.647555000
6	-0.056343000	2.170782000	-0.594193000
7	-0.947663000	1.195761000	-0.342709000
1	-2.110382000	4.864678000	-0.510202000
1	-3.769268000	3.037695000	-0.229064000
1	0.297814000	4.273798000	-0.827273000
6	1.342888000	1.725295000	-0.904596000
15	1.694422000	0.064698000	-0.145153000
6	-0.014715000	-2.453071000	-0.191941000
8	0.273739000	-3.570425000	-0.358877000
6	2.562932000	0.547084000	1.481169000
6	1.653341000	1.580653000	2.174049000
6	2.678530000	-0.690316000	2.386421000
6	3.950595000	1.185254000	1.335186000
1	1.677629000	2.550360000	1.666888000
1	0.613848000	1.252204000	2.235338000
1	2.010474000	1.741724000	3.197898000
1	3.354244000	-1.444403000	1.976555000
1	3.080257000	-0.387525000	3.361186000
1	1.711406000	-1.164140000	2.559205000
1	4.272441000	1.566778000	2.312188000
1	4.706496000	0.467278000	1.008652000
1	3.951611000	2.031778000	0.640901000
6	2.980120000	-0.659118000	-1.349276000
6	3.691927000	-1.845960000	-0.681436000
6	2.236465000	-1.196418000	-2.584147000

6	4.023563000	0.353144000	-1.852590000
1	4.386457000	-1.530572000	0.101315000
1	2.979851000	-2.558023000	-0.252402000
1	4.278561000	-2.384368000	-1.435393000
1	1.649750000	-0.424378000	-3.090267000
1	2.978090000	-1.574939000	-3.298732000
1	1.556063000	-2.008890000	-2.329661000
1	4.677229000	-0.148125000	-2.576536000
1	3.561867000	1.198462000	-2.372499000
1	4.662379000	0.747302000	-1.063338000
1	1.386927000	1.573452000	-1.990008000
1	2.078213000	2.495656000	-0.657312000
1	-0.361648000	-0.837471000	-1.629922000
25	-0.433825000	-0.749284000	-0.033135000
6	-0.624513000	-0.839384000	1.736669000
8	-0.845337000	-1.011777000	2.868784000

## E2

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
6	1.686843000	1.740171000	-0.919084000
6	2.880784000	2.357063000	-1.291588000
6	3.830045000	1.628610000	-1.991685000
6	3.556182000	0.301394000	-2.302400000
6	2.342254000	-0.239661000	-1.910962000
7	1.418810000	0.454149000	-1.230924000
1	4.767347000	2.088160000	-2.286216000
1	3.066822000	3.393202000	-1.034652000
1	4.268556000	-0.315728000	-2.836429000
1	2.090022000	-1.267442000	-2.137321000
6	0.651921000	2.389860000	-0.095223000
6	0.752178000	3.678185000	0.425176000
6	-0.229986000	4.123253000	1.298166000
6	-1.254254000	3.257174000	1.662839000
6	-1.299405000	1.982179000	1.106445000
7	-0.388249000	1.585980000	0.199903000
1	-0.181163000	5.123941000	1.714201000
1	1.585229000	4.319111000	0.163734000
1	-2.009662000	3.556138000	2.381068000
6	-2.287747000	0.942188000	1.549558000
15	-2.484886000	-0.376854000	0.252029000
6	-0.289076000	-1.896388000	-1.220224000
8	-0.159932000	-3.031933000	-1.456190000

6	-4.021790000	0.224829000	-0.699568000
6	-3.743949000	1.691225000	-1.085128000
6	-4.181658000	-0.599583000	-1.987204000
6	-5.346837000	0.195441000	0.073226000
1	-3.794618000	2.359099000	-0.219004000
1	-2.769513000	1.822398000	-1.560811000
1	-4.507361000	2.025783000	-1.797273000
1	-4.439057000	-1.641165000	-1.784760000
1	-4.991922000	-0.172974000	-2.590895000
1	-3.275355000	-0.591882000	-2.594204000
1	-6.115741000	0.707166000	-0.518755000
1	-5.704705000	-0.822011000	0.248036000
1	-5.283730000	0.713623000	1.035727000
6	-2.947108000	-1.901061000	1.294178000
6	-3.544941000	-2.977600000	0.374798000
6	-1.661430000	-2.474566000	1.915696000
6	-3.919440000	-1.612765000	2.450182000
1	-4.559897000	-2.729978000	0.053291000
1	-2.928012000	-3.144239000	-0.513798000
1	-3.601387000	-3.927627000	0.919497000
1	-1.133538000	-1.743325000	2.534735000
1	-1.933812000	-3.321086000	2.558178000
1	-0.963778000	-2.829384000	1.157117000
1	-4.107494000	-2.547644000	2.991898000
1	-3.502016000	-0.904181000	3.172461000
1	-4.884833000	-1.231452000	2.120178000
1	-1.846123000	0.442645000	2.420434000
1	-3.228305000	1.391262000	1.880152000
1	0.104876000	-0.777558000	0.611799000
6	2.487876000	1.211006000	2.307239000
8	3.170280000	0.478955000	3.314752000
6	2.496537000	-0.256601000	2.291590000
1	1.588733000	-0.759249000	2.621000000
1	1.592485000	1.740190000	2.633009000
1	3.127710000	1.751338000	1.610092000
6	3.344317000	-1.044570000	1.351797000
6	2.810875000	-2.169423000	0.721005000
6	4.667548000	-0.679862000	1.094171000
6	3.586014000	-2.915576000	-0.162211000
1	1.778536000	-2.445580000	0.909911000
6	5.441617000	-1.424374000	0.209806000
1	5.093198000	0.177201000	1.607974000
6	4.902756000	-2.544403000	-0.421575000
1	3.156725000	-3.787374000	-0.646597000



1	6.471931000	-1.137385000	0.020827000
1	5.510379000	-3.130110000	-1.105012000
25	-0.455427000	-0.205024000	-0.762932000
6	-0.970922000	0.316121000	-2.388211000
8	-1.189186000	0.590483000	-3.500366000

**E3**

Coordinates (Angstroms)

	X	Y	Z
6	1.545452000	2.372134000	-0.262257000
6	2.636687000	3.223492000	-0.386003000
6	3.764247000	2.783707000	-1.069793000
6	3.771027000	1.503227000	-1.602608000
6	2.639757000	0.712300000	-1.452594000
7	1.548710000	1.134469000	-0.807076000
1	4.628704000	3.431226000	-1.168153000
1	2.619366000	4.211565000	0.057438000
1	4.635896000	1.101122000	-2.115328000
1	2.608554000	-0.298108000	-1.841164000
6	0.338419000	2.694565000	0.532540000
6	0.146401000	3.883716000	1.224107000
6	-0.982664000	4.013672000	2.024407000
6	-1.863061000	2.948220000	2.144542000
6	-1.614016000	1.779701000	1.428742000
7	-0.558687000	1.690380000	0.603542000
1	-1.159297000	4.934990000	2.569039000
1	0.866616000	4.689029000	1.157638000
1	-2.726700000	3.005110000	2.797171000
6	-2.447809000	0.539869000	1.597202000
15	-2.335407000	-0.546966000	0.095173000
6	0.134302000	-1.374788000	-1.579114000
8	0.277805000	-2.313378000	-2.239041000
6	-3.810055000	0.032815000	-0.951449000
6	-3.744486000	1.570629000	-1.032256000
6	-3.703129000	-0.551017000	-2.370131000
6	-5.182457000	-0.332664000	-0.368193000
1	-3.977778000	2.040716000	-0.072304000
1	-2.776706000	1.947629000	-1.367108000
1	-4.494034000	1.916838000	-1.752349000
1	-3.826439000	-1.635476000	-2.382623000
1	-4.498280000	-0.124645000	-2.992495000
1	-2.752024000	-0.318254000	-2.851096000
1	-5.959913000	0.165185000	-0.959703000

1	-5.383352000	-1.405086000	-0.413191000
1	-5.301335000	0.001874000	0.667382000
6	-2.656567000	-2.286599000	0.772705000
6	-3.007437000	-3.230629000	-0.387756000
6	-1.347141000	-2.787614000	1.403050000
6	-3.747933000	-2.347071000	1.852887000
1	-4.002400000	-3.043337000	-0.798167000
1	-2.276122000	-3.168040000	-1.200088000
1	-2.997270000	-4.262683000	-0.019607000
1	-1.014893000	-2.163904000	2.235815000
1	-1.508143000	-3.796628000	1.798550000
1	-0.535003000	-2.842197000	0.675242000
1	-3.829313000	-3.379763000	2.211158000
1	-3.499683000	-1.729226000	2.721152000
1	-4.732262000	-2.050399000	1.491542000
1	-2.012745000	-0.028898000	2.428534000
1	-3.475446000	0.782113000	1.880563000
1	0.615288000	-0.911276000	0.799486000
6	1.082337000	-0.537895000	1.752943000
8	2.690976000	-1.053699000	3.390296000
6	2.171176000	-1.543851000	2.290268000
1	1.631640000	-2.538736000	2.381169000
1	0.299640000	-0.412972000	2.504816000
1	1.585643000	0.415310000	1.604337000
6	3.161220000	-1.749903000	1.114750000
6	2.873369000	-2.535948000	-0.003292000
6	4.390440000	-1.095958000	1.170601000
6	3.783672000	-2.652992000	-1.053303000
1	1.929852000	-3.077743000	-0.045261000
6	5.305792000	-1.203234000	0.126657000
1	4.585731000	-0.528219000	2.077018000
6	5.004162000	-1.979428000	-0.993847000
1	3.545083000	-3.274330000	-1.912988000
1	6.263986000	-0.692247000	0.187199000
1	5.722802000	-2.075912000	-1.803537000
6	-0.699190000	0.892861000	-2.124247000
8	-0.869407000	1.430895000	-3.135061000
25	-0.205952000	0.103498000	-0.618954000

#### E4

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
6	-2.440538000	1.654354000	0.731072000

6	-3.671614000	2.245428000	1.002200000
6	-4.164528000	3.211935000	0.135616000
6	-3.414352000	3.558904000	-0.980430000
6	-2.185840000	2.942069000	-1.173661000
7	-1.701191000	2.016882000	-0.340023000
1	-5.122415000	3.683187000	0.328241000
1	-4.241991000	1.954670000	1.876197000
1	-3.763200000	4.298901000	-1.691013000
1	-1.557687000	3.192354000	-2.020446000
6	-1.869084000	0.539218000	1.522225000
6	-2.536174000	-0.119925000	2.548936000
6	-1.938013000	-1.238960000	3.116646000
6	-0.726057000	-1.691568000	2.618203000
6	-0.109735000	-0.985692000	1.585769000
7	-0.658923000	0.135629000	1.099059000
1	-2.433983000	-1.771816000	3.921099000
1	-3.508211000	0.213476000	2.890969000
1	-0.264176000	-2.593647000	3.002923000
6	1.133955000	-1.477974000	0.906303000
15	2.072401000	-0.086497000	0.117790000
6	0.820579000	1.975153000	-1.897854000
8	1.205418000	2.455554000	-2.880291000
6	3.118264000	-0.961007000	-1.206432000
6	2.272250000	-1.020983000	-2.492445000
6	4.384518000	-0.155302000	-1.535875000
6	3.503485000	-2.396113000	-0.811160000
1	1.223172000	-1.260761000	-2.299522000
1	2.268826000	-0.052262000	-2.999035000
1	2.716434000	-1.752677000	-3.179006000
1	5.139478000	-0.189813000	-0.746936000
1	4.839537000	-0.578103000	-2.439490000
1	4.152588000	0.893023000	-1.751669000
1	4.163908000	-2.810165000	-1.582662000
1	4.035352000	-2.458156000	0.140438000
1	2.627302000	-3.049350000	-0.756019000
6	3.201750000	0.473676000	1.542744000
6	3.925114000	1.777656000	1.165511000
6	2.303205000	0.756170000	2.762868000
6	4.238396000	-0.571458000	1.980754000
1	4.659351000	1.635743000	0.370865000
1	3.227901000	2.555097000	0.847318000
1	4.462907000	2.157552000	2.042468000
1	1.876017000	-0.160956000	3.179324000
1	2.911292000	1.215488000	3.550993000

1	1.484415000	1.441250000	2.536923000
1	4.760846000	-0.201645000	2.871450000
1	3.775353000	-1.525241000	2.253358000
1	4.996363000	-0.763395000	1.218862000
6	-1.737704000	-0.810014000	-1.649881000
8	-0.442584000	-0.368363000	-1.544901000
1	1.732310000	-2.109213000	1.568372000
1	0.786767000	-2.093079000	0.070148000
6	-2.170283000	-0.853271000	-3.125297000
1	-2.090364000	0.151192000	-3.554515000
1	-1.505776000	-1.514005000	-3.693458000
1	-2.468400000	-0.153339000	-1.137416000
6	0.678369000	2.637492000	0.536223000
8	0.885771000	3.637285000	1.096493000
25	0.201979000	1.216247000	-0.408714000
6	-1.917570000	-2.191133000	-1.011583000
6	-2.982500000	-2.469696000	-0.155142000
6	-0.989467000	-3.207765000	-1.261863000
6	-3.112909000	-3.717931000	0.452941000
1	-3.713189000	-1.690534000	0.051979000
6	-1.111553000	-4.455448000	-0.659552000
1	-0.158038000	-3.002236000	-1.931016000
6	-2.173086000	-4.714508000	0.208262000
1	-3.944294000	-3.908357000	1.126391000
1	-0.376845000	-5.229545000	-0.864724000
1	-2.267573000	-5.686191000	0.684186000
1	-3.200772000	-1.209419000	-3.248825000

## E5

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Coordinates (Angstroms)

	X	Y	Z
6	2.102806000	-1.426334000	0.911485000
6	3.418951000	-1.848729000	1.097998000
6	4.001418000	-2.685274000	0.159316000
6	3.250155000	-3.071867000	-0.946427000
6	1.948599000	-2.611200000	-1.064896000
7	1.374116000	-1.806655000	-0.159194000
1	5.022720000	-3.027210000	0.287588000
1	3.981142000	-1.524919000	1.964108000
1	3.657966000	-3.727235000	-1.707595000
1	1.328889000	-2.890624000	-1.908377000
6	1.379863000	-0.561900000	1.859308000
6	1.956517000	0.041182000	2.974776000

6	1.154570000	0.811611000	3.804154000
6	-0.197027000	0.945867000	3.508603000
6	-0.711137000	0.329129000	2.372106000
7	0.079895000	-0.386849000	1.552083000
1	1.579304000	1.300402000	4.674656000
1	3.015450000	-0.063466000	3.173495000
1	-0.852810000	1.530448000	4.144563000
6	-2.164024000	0.405066000	1.991893000
15	-2.333430000	0.214602000	0.147312000
6	-0.820384000	-1.390065000	-1.965762000
8	-0.966535000	-1.508718000	-3.116945000
6	-2.210037000	2.016493000	-0.461089000
6	-0.968093000	2.640682000	0.202313000
6	-1.983892000	2.009155000	-1.981191000
6	-3.408124000	2.910928000	-0.118959000
1	-1.124752000	2.830182000	1.269288000
1	-0.090680000	2.003420000	0.069824000
1	-0.764459000	3.608825000	-0.271402000
1	-2.824471000	1.577532000	-2.529826000
1	-1.857527000	3.040754000	-2.333648000
1	-1.082250000	1.447215000	-2.233961000
1	-3.171890000	3.944772000	-0.400433000
1	-4.315416000	2.632780000	-0.659661000
1	-3.628509000	2.914156000	0.953808000
6	-4.135008000	-0.370476000	-0.042955000
6	-4.595490000	-0.164243000	-1.494167000
6	-4.156937000	-1.881719000	0.233851000
6	-5.132378000	0.290859000	0.922185000
1	-4.756557000	0.888343000	-1.738744000
1	-3.878819000	-0.580752000	-2.209542000
1	-5.550659000	-0.681436000	-1.645626000
1	-3.763262000	-2.133961000	1.223000000
1	-5.193910000	-2.236534000	0.191765000
1	-3.580675000	-2.433804000	-0.510611000
1	-6.124865000	-0.147505000	0.760204000
1	-4.871914000	0.108018000	1.969413000
1	-5.227842000	1.366531000	0.777592000
6	3.524523000	1.910090000	0.492782000
8	4.373625000	1.154917000	0.937994000
1	-2.675599000	-0.457169000	2.437656000
6	2.989026000	3.047910000	1.332912000
1	1.903428000	2.961836000	1.448394000
1	3.465233000	3.021779000	2.313248000
1	-2.634778000	1.305089000	2.398321000

1	0.131856000	0.175254000	-0.888171000
6	-1.156476000	-2.677833000	0.344536000
8	-1.457656000	-3.754334000	0.676859000
25	-0.532960000	-1.115672000	-0.247578000
6	2.969087000	1.718005000	-0.881493000
6	2.108386000	2.647568000	-1.472912000
6	3.298021000	0.551716000	-1.579084000
6	1.577005000	2.408134000	-2.734586000
1	1.840620000	3.559699000	-0.950272000
6	2.753132000	0.304449000	-2.830920000
1	3.971043000	-0.159622000	-1.113255000
6	1.887823000	1.230769000	-3.409082000
1	0.902791000	3.130954000	-3.182502000
1	2.992387000	-0.616648000	-3.353058000
1	1.449059000	1.032084000	-4.381879000
1	3.196378000	4.013388000	0.859751000

### F3

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
6	2.096595000	-1.127482000	1.061072000
6	3.405847000	-1.439368000	1.406022000
6	4.104024000	-0.580967000	2.245686000
6	3.470500000	0.555948000	2.724044000
6	2.163236000	0.806286000	2.329178000
7	1.490530000	-0.006940000	1.507183000
1	5.133160000	-0.796289000	2.511287000
1	3.888912000	-2.319201000	1.001608000
1	3.974688000	1.255999000	3.378958000
1	1.635859000	1.687593000	2.670492000
6	1.281841000	-1.947239000	0.138034000
6	1.675628000	-3.179152000	-0.369446000
6	0.866686000	-3.800388000	-1.311885000
6	-0.291561000	-3.167565000	-1.741553000
6	-0.642103000	-1.942393000	-1.180743000
7	0.115527000	-1.377694000	-0.225059000
1	1.150314000	-4.762878000	-1.723951000
1	2.597986000	-3.643848000	-0.046139000
1	-0.921770000	-3.609186000	-2.504794000
6	-1.822622000	-1.149849000	-1.665976000
15	-2.430270000	0.026775000	-0.363371000
6	-0.855691000	1.825624000	1.660525000
8	-1.199168000	2.767158000	2.232193000

6	-3.819961000	-0.946260000	0.482139000
6	-3.271876000	-2.349769000	0.805676000
6	-4.218705000	-0.236689000	1.786650000
6	-5.075416000	-1.135046000	-0.380144000
1	-3.151333000	-2.954891000	-0.098255000
1	-2.315108000	-2.331683000	1.329704000
1	-3.988193000	-2.869788000	1.451193000
1	-4.647466000	0.751476000	1.607015000
1	-4.980564000	-0.834947000	2.299765000
1	-3.380210000	-0.117239000	2.474005000
1	-5.754464000	-1.824259000	0.135402000
1	-5.620049000	-0.200631000	-0.531002000
1	-4.850012000	-1.572504000	-1.357830000
6	-3.136337000	1.453751000	-1.382467000
6	-4.000536000	2.348002000	-0.480928000
6	-1.933819000	2.277161000	-1.869424000
6	-3.940564000	1.022259000	-2.619641000
1	-4.949654000	1.875592000	-0.215100000
1	-3.479540000	2.628896000	0.439703000
1	-4.236301000	3.274306000	-1.016529000
1	-1.267674000	1.698027000	-2.515710000
1	-2.296934000	3.125999000	-2.459449000
1	-1.338370000	2.678885000	-1.046182000
1	-4.231113000	1.921884000	-3.174304000
1	-3.348066000	0.405583000	-3.302473000
1	-4.855950000	0.482431000	-2.378162000
1	-1.470032000	-0.536264000	-2.503939000
1	-2.606993000	-1.800545000	-2.061223000
1	0.587500000	1.117884000	-0.888556000
6	1.388704000	1.795302000	-1.289575000
8	2.384198000	3.948816000	-0.878188000
6	1.519931000	3.078156000	-0.409193000
1	0.448900000	3.447093000	-0.292240000
1	1.021497000	2.095172000	-2.280377000
6	2.652371000	0.982963000	-1.450421000
6	2.634767000	-0.249208000	-2.113290000
6	3.870834000	1.442378000	-0.934501000
6	3.786511000	-1.024477000	-2.230297000
1	1.701252000	-0.612307000	-2.540518000
6	5.021551000	0.667388000	-1.047261000
1	3.875042000	2.447802000	-0.516358000
6	4.986109000	-0.571073000	-1.687709000
1	3.745465000	-1.979809000	-2.746983000
1	5.958790000	1.040605000	-0.642638000

1	5.890249000	-1.166606000	-1.781187000
1	1.736694000	2.671944000	0.633803000
25	-0.427949000	0.270277000	0.844789000
6	-0.941717000	-0.576870000	2.305547000
8	-1.133968000	-1.107093000	3.316773000

**F4**

Coordinates (Angstroms)

	X	Y	Z
6	1.532855000	-2.109274000	-0.039226000
6	2.567813000	-3.033758000	-0.157690000
6	3.303657000	-3.080888000	-1.333757000
6	2.985290000	-2.199650000	-2.360167000
6	1.935549000	-1.311954000	-2.171533000
7	1.220124000	-1.260157000	-1.041326000
1	4.109850000	-3.797897000	-1.445855000
1	2.790888000	-3.714616000	0.654800000
1	3.532128000	-2.194976000	-3.295570000
1	1.642687000	-0.615830000	-2.948945000
6	0.717461000	-1.942118000	1.185305000
6	1.003587000	-2.543092000	2.407184000
6	0.225014000	-2.206455000	3.507388000
6	-0.772451000	-1.250863000	3.369861000
6	-0.999649000	-0.678786000	2.119138000
7	-0.301574000	-1.077764000	1.046534000
1	0.416104000	-2.665303000	4.471770000
1	1.825363000	-3.241759000	2.506571000
1	-1.363385000	-0.932516000	4.221495000
6	-1.958352000	0.458795000	1.918099000
15	-2.552423000	0.540940000	0.162342000
6	-0.566045000	0.750317000	-2.283590000
8	-0.540976000	1.408393000	-3.238267000
6	-3.150979000	2.336264000	-0.004197000
6	-1.931896000	3.201551000	-0.375630000
6	-4.169274000	2.465031000	-1.147125000
6	-3.754780000	2.891159000	1.296470000
1	-1.047820000	2.969020000	0.222789000
1	-1.643824000	3.043278000	-1.417586000
1	-2.201915000	4.258676000	-0.259688000
1	-5.144080000	2.034966000	-0.905090000
1	-4.327410000	3.529459000	-1.357266000
1	-3.802357000	2.001704000	-2.069233000
1	-4.129094000	3.904756000	1.108643000



1	-4.591037000	2.300826000	1.674613000
1	-3.004367000	2.969172000	2.088441000
6	-4.055632000	-0.625357000	0.182027000
6	-4.560673000	-0.862654000	-1.251460000
6	-3.584576000	-1.973474000	0.761079000
6	-5.228635000	-0.146432000	1.049664000
1	-5.017522000	0.028111000	-1.685062000
1	-3.765719000	-1.193991000	-1.921859000
1	-5.327544000	-1.646460000	-1.235765000
1	-3.351537000	-1.899998000	1.827673000
1	-4.393114000	-2.706481000	0.657350000
1	-2.708998000	-2.373363000	0.246769000
1	-5.991282000	-0.934171000	1.080184000
1	-4.928798000	0.052512000	2.083665000
1	-5.710327000	0.749284000	0.652202000
6	1.587437000	1.338679000	0.608338000
8	0.283307000	1.337043000	0.209035000
1	-2.751557000	0.458286000	2.669875000
1	-1.358378000	1.369024000	2.027796000
6	2.564107000	1.845378000	-0.479731000
1	2.394814000	1.251176000	-1.384212000
1	2.302458000	2.880901000	-0.722759000
6	3.998264000	1.741190000	-0.039617000
6	4.670076000	2.829251000	0.525361000
6	4.669933000	0.514777000	-0.105277000
6	5.973735000	2.701833000	0.999485000
1	4.163112000	3.788874000	0.591997000
6	5.972439000	0.381464000	0.365423000
1	4.160142000	-0.344075000	-0.535506000
6	6.630778000	1.476756000	0.921011000
1	6.476528000	3.562428000	1.431633000
1	6.475593000	-0.579177000	0.297370000
1	7.647565000	1.375698000	1.288968000
1	1.965177000	0.344594000	0.937206000
1	1.727806000	1.993395000	1.494279000
6	-1.278053000	-1.606365000	-1.654895000
8	-1.629860000	-2.522358000	-2.282187000
25	-0.563017000	-0.229071000	-0.796143000

**F5**

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
6	-1.592996000	-1.949928000	0.606685000

6	-2.889613000	-2.428019000	0.798163000
6	-3.556302000	-2.129709000	1.976734000
6	-2.902763000	-1.367365000	2.939233000
6	-1.615633000	-0.924611000	2.679494000
7	-0.968402000	-1.191719000	1.535401000
1	-4.567140000	-2.487788000	2.140141000
1	-3.379763000	-3.006943000	0.025858000
1	-3.378964000	-1.111367000	3.878477000
1	-1.073225000	-0.321326000	3.397332000
6	-0.802462000	-2.194480000	-0.613336000
6	-1.236249000	-2.954884000	-1.696567000
6	-0.389460000	-3.104944000	-2.785516000
6	0.862353000	-2.503982000	-2.760531000
6	1.237098000	-1.754675000	-1.649326000
7	0.405672000	-1.598057000	-0.604059000
1	-0.704659000	-3.685621000	-3.645914000
1	-2.221096000	-3.402441000	-1.704563000
1	1.550574000	-2.607033000	-3.592336000
6	2.582482000	-1.093904000	-1.537849000
15	2.480421000	0.342381000	-0.358777000
6	0.995373000	0.820515000	2.244241000
8	1.074877000	1.687468000	3.021117000
6	2.006113000	1.792383000	-1.502052000
6	0.799901000	1.347372000	-2.350796000
6	1.562097000	2.987931000	-0.643961000
6	3.109118000	2.237241000	-2.470947000
1	1.074452000	0.592362000	-3.094354000
1	-0.008045000	0.959764000	-1.725626000
1	0.416120000	2.216357000	-2.898246000
1	2.361559000	3.373435000	-0.007079000
1	1.241572000	3.804398000	-1.302593000
1	0.717256000	2.714841000	-0.007804000
1	2.695524000	2.977638000	-3.166721000
1	3.951738000	2.712214000	-1.963227000
1	3.489624000	1.407060000	-3.075217000
6	4.289426000	0.547506000	0.190223000
6	4.480126000	1.930572000	0.831646000
6	4.552180000	-0.504890000	1.279392000
6	5.330307000	0.338113000	-0.922239000
1	4.459054000	2.738984000	0.096865000
1	3.718936000	2.131962000	1.592323000
1	5.457907000	1.967205000	1.326794000
1	4.358186000	-1.525908000	0.936859000
1	5.606673000	-0.452930000	1.576545000

1	3.942560000	-0.324240000	2.166569000
1	6.333879000	0.436007000	-0.490398000
1	5.266954000	-0.662733000	-1.360474000
1	5.254186000	1.067764000	-1.728081000
6	-3.939840000	-0.517829000	-1.873023000
8	-4.185229000	-1.674090000	-2.136569000
1	3.277606000	-1.812651000	-1.086698000
6	-4.833683000	0.337106000	-0.999544000
1	-5.706317000	0.599750000	-1.612177000
1	-5.208288000	-0.305895000	-0.194559000
6	-4.174083000	1.578950000	-0.454733000
6	-4.763832000	2.836473000	-0.598882000
6	-2.952071000	1.484287000	0.215362000
6	-4.152841000	3.971345000	-0.071076000
1	-5.711940000	2.929034000	-1.122851000
6	-2.337196000	2.614998000	0.742805000
1	-2.462442000	0.521989000	0.327576000
6	-2.938684000	3.863085000	0.602759000
1	-4.626325000	4.941459000	-0.189587000
1	-1.387037000	2.505242000	1.256208000
1	-2.462609000	4.747443000	1.015112000
1	2.980662000	-0.838657000	-2.524351000
1	-0.053318000	0.700821000	0.338422000
1	-3.039638000	-0.019267000	-2.288866000
6	1.730307000	-1.679990000	1.914934000
8	2.216980000	-2.497012000	2.588339000
25	0.838421000	-0.427646000	1.009521000

### TSE2-3

Coordinates (Angstroms)

	X	Y	Z
6	1.553490000	2.319614000	-0.291974000
6	2.682917000	3.128440000	-0.393489000
6	3.788254000	2.662991000	-1.091165000
6	3.735340000	1.397196000	-1.661360000
6	2.578130000	0.646725000	-1.517984000
7	1.504341000	1.090876000	-0.853070000
1	4.679526000	3.275043000	-1.177686000
1	2.704290000	4.103837000	0.077385000
1	4.578548000	0.977642000	-2.196064000
1	2.501805000	-0.350326000	-1.933380000
6	0.352797000	2.683126000	0.488426000
6	0.184425000	3.887802000	1.164803000

6	-0.950216000	4.059929000	1.945571000
6	-1.855343000	3.013414000	2.070896000
6	-1.629336000	1.832261000	1.370498000
7	-0.573372000	1.706186000	0.547835000
1	-1.113570000	4.993865000	2.472706000
1	0.923856000	4.675256000	1.088053000
1	-2.724463000	3.098533000	2.713540000
6	-2.478159000	0.605900000	1.555703000
15	-2.340992000	-0.526704000	0.086969000
6	0.110725000	-1.430591000	-1.468104000
8	0.318679000	-2.452776000	-1.984467000
6	-3.850676000	-0.030342000	-0.959677000
6	-3.807271000	1.503640000	-1.105091000
6	-3.735754000	-0.668396000	-2.353997000
6	-5.216491000	-0.392880000	-0.361604000
1	-4.052336000	2.008649000	-0.165540000
1	-2.838699000	1.872888000	-1.447698000
1	-4.556353000	1.812360000	-1.842977000
1	-3.854061000	-1.753440000	-2.322113000
1	-4.528767000	-0.272474000	-2.999540000
1	-2.780250000	-0.451052000	-2.833263000
1	-6.003476000	0.068307000	-0.970758000
1	-5.401356000	-1.469536000	-0.364362000
1	-5.339750000	-0.019450000	0.660287000
6	-2.636620000	-2.240086000	0.852216000
6	-2.948762000	-3.249223000	-0.263723000
6	-1.330800000	-2.682131000	1.533042000
6	-3.745690000	-2.280875000	1.916107000
1	-3.944631000	-3.105127000	-0.690049000
1	-2.213025000	-3.204111000	-1.072788000
1	-2.917639000	-4.263083000	0.151949000
1	-1.032078000	-2.002380000	2.335570000
1	-1.483437000	-3.670746000	1.982038000
1	-0.502174000	-2.748475000	0.826908000
1	-3.797543000	-3.293900000	2.332669000
1	-3.540102000	-1.604586000	2.751540000
1	-4.732809000	-2.044024000	1.521144000
1	-2.055890000	0.056823000	2.406901000
1	-3.507126000	0.860893000	1.823617000
1	0.388294000	-0.586583000	0.709266000
6	1.252202000	-0.395177000	2.010785000
8	2.478461000	-0.823397000	3.282887000
6	2.149809000	-1.547369000	2.170296000
1	1.632905000	-2.508557000	2.342571000

1	0.376935000	-0.334294000	2.643963000
1	1.705478000	0.526081000	1.673943000
6	3.206352000	-1.710508000	1.101450000
6	3.003743000	-2.564569000	0.016817000
6	4.389201000	-0.977149000	1.179398000
6	3.963688000	-2.674764000	-0.985902000
1	2.085981000	-3.142749000	-0.046052000
6	5.355896000	-1.091787000	0.183796000
1	4.528546000	-0.331233000	2.041009000
6	5.144572000	-1.937698000	-0.904308000
1	3.791181000	-3.340016000	-1.827145000
1	6.280167000	-0.525003000	0.257681000
1	5.900284000	-2.030127000	-1.679350000
25	-0.267316000	0.101003000	-0.666351000
6	-0.750150000	0.839196000	-2.210614000
8	-0.919003000	1.310800000	-3.260667000

#### TSE4-5

-----			
Coordinates (Angstroms)			
	X	Y	Z
-----			
6	-2.297713000	1.376384000	0.481242000
6	-3.554270000	1.952481000	0.645216000
6	-4.183973000	2.528276000	-0.448166000
6	-3.540584000	2.504988000	-1.679640000
6	-2.280651000	1.931044000	-1.762350000
7	-1.661737000	1.381953000	-0.710025000
1	-5.162951000	2.982746000	-0.340602000
1	-4.037994000	1.945422000	1.613931000
1	-3.994833000	2.933145000	-2.565532000
1	-1.735708000	1.908131000	-2.698806000
6	-1.578351000	0.660382000	1.552532000
6	-2.098594000	0.399693000	2.815502000
6	-1.369069000	-0.408861000	3.677127000
6	-0.172418000	-0.962285000	3.242713000
6	0.300729000	-0.650239000	1.970244000
7	-0.376222000	0.191446000	1.173112000
1	-1.748222000	-0.630362000	4.669228000
1	-3.063273000	0.791453000	3.112566000
1	0.397933000	-1.633520000	3.874765000
6	1.535097000	-1.266473000	1.384092000
15	2.295064000	-0.126700000	0.136428000
6	0.716044000	0.906647000	-2.375358000
8	0.985517000	0.984343000	-3.503328000

6	3.42224000	-1.279872000	-0.865005000
6	4.507535000	-0.476740000	-1.596982000
6	4.069254000	-2.386539000	-0.016236000
6	2.547172000	-1.962422000	-1.925317000
1	4.991740000	-1.130582000	-2.331615000
1	4.086291000	0.373723000	-2.143592000
1	5.288768000	-0.109390000	-0.927133000
1	3.318280000	-3.062039000	0.403238000
1	4.716640000	-2.991676000	-0.662530000
1	4.686161000	-2.007332000	0.799195000
1	3.163429000	-2.684120000	-2.476611000
1	1.706346000	-2.503492000	-1.480904000
1	2.160422000	-1.240877000	-2.647979000
6	3.381862000	1.021578000	1.204352000
6	3.931463000	2.178263000	0.352024000
6	2.487645000	1.612669000	2.310894000
6	4.556811000	0.320916000	1.902101000
1	4.668773000	1.843954000	-0.379072000
1	3.144958000	2.711098000	-0.184023000
1	4.429471000	2.901605000	1.008888000
1	2.191696000	0.857028000	3.044394000
1	3.052376000	2.382509000	2.849753000
1	1.583005000	2.081875000	1.920142000
1	5.032326000	1.029045000	2.591777000
1	4.234784000	-0.540147000	2.496042000
1	5.325772000	-0.009485000	1.200857000
6	-0.877238000	-2.206212000	-1.202246000
8	-0.144912000	-3.039682000	-0.604206000
1	2.220130000	-1.618238000	2.160080000
1	1.182654000	-2.132220000	0.800738000
6	-0.877598000	-2.219356000	-2.733408000
1	0.140094000	-2.358225000	-3.097514000
1	-1.481165000	-3.071809000	-3.068319000
1	-0.250836000	-0.836075000	-1.068014000
6	0.669530000	2.459886000	-0.365706000
8	0.795078000	3.611526000	-0.264883000
25	0.286032000	0.751691000	-0.662318000
6	-2.236153000	-1.918435000	-0.564407000
6	-2.463160000	-2.409043000	0.721840000
6	-3.281753000	-1.267537000	-1.224886000
6	-3.692110000	-2.232634000	1.348345000
1	-1.650810000	-2.937819000	1.208507000
6	-4.516332000	-1.095496000	-0.605158000
1	-3.138665000	-0.882924000	-2.228955000

6	-4.725289000	-1.572266000	0.687047000
1	-3.846466000	-2.618413000	2.352256000
1	-5.316668000	-0.584572000	-1.132743000
1	-5.689376000	-1.439616000	1.169639000
1	-1.282252000	-1.306656000	-3.175243000

**TSF2-3**

Coordinates (Angstroms)

	X	Y	Z
6	-2.688139000	-1.385477000	0.733880000
6	-4.014873000	-1.744875000	0.958581000
6	-4.780752000	-2.207388000	-0.101850000
6	-4.197787000	-2.297729000	-1.360079000
6	-2.867154000	-1.936156000	-1.506281000
7	-2.119003000	-1.492085000	-0.487463000
1	-5.818025000	-2.484327000	0.051673000
1	-4.449426000	-1.654791000	1.946504000
1	-4.757631000	-2.641426000	-2.221748000
1	-2.371329000	-1.999130000	-2.467243000
6	-1.810718000	-0.793673000	1.763858000
6	-2.209914000	-0.495832000	3.063062000
6	-1.323655000	0.176953000	3.894901000
6	-0.092031000	0.575459000	3.394198000
6	0.246847000	0.252723000	2.082357000
7	-0.582941000	-0.470012000	1.311063000
1	-1.604200000	0.411948000	4.916121000
1	-3.194945000	-0.770585000	3.420037000
1	0.599614000	1.149552000	4.000349000
6	1.492776000	0.766155000	1.423264000
15	1.979796000	-0.327969000	0.005168000
6	0.180449000	-1.282643000	-2.306082000
8	0.389491000	-1.402597000	-3.443392000
6	3.166050000	-1.561706000	0.837972000
6	2.428427000	-2.145331000	2.058943000
6	3.497459000	-2.708491000	-0.131771000
6	4.477840000	-0.952076000	1.351379000
1	2.301906000	-1.402125000	2.852577000
1	1.445821000	-2.548863000	1.808619000
1	3.024898000	-2.965004000	2.475243000
1	4.126078000	-2.381220000	-0.961923000
1	4.049242000	-3.487729000	0.407659000
1	2.602270000	-3.170203000	-0.551061000
1	5.016393000	-1.708254000	1.935480000

1	5.141946000	-0.641436000	0.541871000
1	4.308320000	-0.094791000	2.010760000
6	2.975347000	0.835207000	-1.113217000
6	3.845716000	0.016457000	-2.078339000
6	1.969622000	1.639440000	-1.950322000
6	3.845623000	1.848252000	-0.350122000
1	4.709834000	-0.435847000	-1.585775000
1	3.273911000	-0.774172000	-2.575081000
1	4.231232000	0.682316000	-2.859157000
1	1.279574000	2.203591000	-1.321461000
1	2.519996000	2.359000000	-2.569157000
1	1.380154000	1.004018000	-2.612177000
1	4.393506000	2.459135000	-1.077604000
1	3.237845000	2.534516000	0.247561000
1	4.583835000	1.385953000	0.305238000
1	1.229471000	1.736282000	0.981718000
1	2.291513000	0.943219000	2.148801000
1	-0.536416000	0.527887000	-0.952297000
6	-1.706367000	1.560822000	-1.281500000
8	-2.838562000	2.448649000	-2.525225000
6	-1.760921000	1.648486000	-2.745187000
1	-0.871862000	2.104093000	-3.224521000
1	-2.466967000	0.925657000	-0.847441000
6	-1.265444000	2.698964000	-0.434875000
6	-1.535683000	2.677863000	0.935826000
6	-0.553929000	3.787354000	-0.954477000
6	-1.073403000	3.687448000	1.776447000
1	-2.119251000	1.860416000	1.348998000
6	-0.091929000	4.796399000	-0.118515000
1	-0.377924000	3.851377000	-2.022627000
6	-0.338035000	4.746292000	1.253783000
1	-1.292410000	3.643715000	2.839330000
1	0.457036000	5.632357000	-0.541654000
1	0.024881000	5.536126000	1.904540000
1	-1.939269000	0.668977000	-3.231060000
6	0.148033000	-2.805665000	-0.273981000
8	0.199936000	-3.961994000	-0.159634000
25	-0.120023000	-1.074475000	-0.570757000

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**TSF4-5**  
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Coordinates (Angstroms)

	X	Y	Z
6	-1.699353000	2.309854000	-0.259559000



6	-2.825204000	3.123968000	-0.356197000
6	-3.961404000	2.638145000	-0.988013000
6	-3.942273000	1.346690000	-1.498074000
6	-2.784944000	0.593791000	-1.366702000
7	-1.680876000	1.058357000	-0.770114000
1	-4.848491000	3.256866000	-1.072052000
1	-2.819572000	4.121881000	0.065020000
1	-4.808361000	0.912493000	-1.982692000
1	-2.733717000	-0.421788000	-1.739802000
6	-0.463124000	2.701299000	0.450142000
6	-0.276245000	3.924907000	1.083240000
6	0.902431000	4.134416000	1.788128000
6	1.826765000	3.105530000	1.885977000
6	1.572107000	1.896914000	1.240447000
7	0.474582000	1.735206000	0.486029000
1	1.082602000	5.084563000	2.279949000
1	-1.030339000	4.700296000	1.032035000
1	2.733697000	3.219829000	2.468890000
6	2.438821000	0.688855000	1.438643000
15	2.248446000	-0.503355000	0.030691000
6	-0.340285000	-1.384107000	-1.539685000
8	-0.639566000	-2.308028000	-2.179278000
6	2.541787000	-2.236564000	0.786519000
6	1.673588000	-3.222877000	-0.009360000
6	3.986801000	-2.748210000	0.767630000
6	2.069822000	-2.247623000	2.249039000
1	1.884184000	-4.245229000	0.327238000
1	0.612966000	-3.024422000	0.155202000
1	1.866556000	-3.179301000	-1.085826000
1	4.669740000	-2.087971000	1.306891000
1	4.011511000	-3.722027000	1.271536000
1	4.365152000	-2.900788000	-0.246421000
1	1.967844000	-3.289802000	2.575342000
1	2.803119000	-1.774213000	2.910908000
1	1.112801000	-1.745180000	2.405989000
6	3.705042000	-0.001947000	-1.089161000
6	3.594080000	-0.803687000	-2.394164000
6	3.545393000	1.505205000	-1.375970000
6	5.123706000	-0.163528000	-0.511330000
1	3.720958000	-1.877481000	-2.218968000
1	2.629387000	-0.654964000	-2.885788000
1	4.378391000	-0.490548000	-3.093638000
1	3.830945000	2.105851000	-0.505886000
1	4.217150000	1.783773000	-2.196158000

1	2.536270000	1.793559000	-1.665731000
1	5.809299000	0.454736000	-1.103187000
1	5.201280000	0.178174000	0.526099000
1	5.495577000	-1.185260000	-0.565334000
6	-1.046718000	-0.301614000	2.203444000
8	-0.172604000	-0.009641000	3.038485000
1	3.474867000	0.960919000	1.657150000
1	2.016458000	0.205989000	2.325388000
6	-1.778735000	-1.652940000	2.314954000
1	-1.045978000	-2.463248000	2.272415000
1	-2.202905000	-1.658008000	3.327355000
6	-2.874873000	-1.851199000	1.306958000
6	-2.742428000	-2.765047000	0.259907000
6	-4.058357000	-1.109446000	1.394154000
6	-3.759343000	-2.938187000	-0.675426000
1	-1.829121000	-3.346284000	0.176923000
6	-5.080416000	-1.280260000	0.464792000
1	-4.180694000	-0.395462000	2.205341000
6	-4.934498000	-2.197201000	-0.574508000
1	-3.632776000	-3.655688000	-1.480391000
1	-5.994690000	-0.700503000	0.554528000
1	-5.732039000	-2.336083000	-1.298626000
1	-0.395796000	-0.609949000	0.787330000
1	-1.685478000	0.494363000	1.767298000
6	0.522562000	0.793724000	-2.241776000
8	0.659121000	1.210872000	-3.319272000
25	0.114110000	0.087500000	-0.662955000

**PhCOCH<sub>3</sub>**

Coordinates (Angstroms)

	X	Y	Z
6	-1.696878000	-0.202772000	-0.000033000
8	-2.208180000	-1.307740000	-0.000014000
6	-0.203879000	-0.055787000	-0.000114000
6	0.428234000	1.191445000	-0.000064000
6	0.575304000	-1.217502000	-0.000008000
6	1.816919000	1.273976000	-0.000030000
1	-0.155649000	2.106379000	-0.000086000
6	1.960961000	-1.134858000	0.000033000
1	0.072068000	-2.178456000	0.000019000
6	2.583801000	0.112063000	0.000059000
1	2.300434000	2.245548000	0.000025000
1	2.557432000	-2.041734000	0.000078000

1	3.667466000	0.178575000	0.000126000
6	-2.547867000	1.046008000	0.000086000
1	-3.600108000	0.760850000	0.000269000
1	-2.337720000	1.657637000	0.883500000
1	-2.338058000	1.657674000	-0.883395000

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