Supporting Information

For
pH-Dependent Transfer Hydrogenation or Dihydrogen Release
Catalyzed by \([\eta^6\text{-arene}RuCl(\kappa^2-N,N\text{-dmobpy})]^+\) Complex: A DFT
Mechanistic Understanding

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Figure S1. The free energy profiles along the hydride transfer step by path B.

Path B: In this pathway, the ketone substrate could be stabilized with formic acid through hydrogen bond. Firstly, the ketone stabilized with formic acid coordinates with metal hydride 5 to form intermediate 9. Then the hydride is transferred from Ru center to the carbon atom of ketone via TS9-10 with an energy barrier of 12.5 kcal/mol. Subsequently, intermediate 10 is formed, the free energy of complex 10 is -18.3 kcal/mol. The free energy profiles along path B are shown in Figure S1, in this pathway, the energy barrier is 12.5 kcal/mol from 9 to TS9-10. As a result, we can conclude that path B is less favorable than path A.
**Figure S2.** The free energy profiles along the hydride transfer step by path C.

**Path C:** In this pathway, the ketone substrate is coordinated to the Ru atom during the hydride transfer by inner-sphere mechanism. As shown in Figure S2, the oxygen atom of acetophenone forms the Ru-O bond with Ru center of complex 5 firstly, resulting in the dissociation of one 4-methylpyridine to form complex 11 with a high energy barrier of 22.5 kcal/mol. Subsequently, the hydride transfers to carbon atom of ketone through TS11-12, which owing an energy barrier of 5.3 kcal/mol. From 11 to TS11-12, the C-H distance decreases form 2.990 Å to 1.104 Å, indicating that the C-H bond is formed. Path C has an energy barrier of 27.8 kcal/mol, which is 22.9 kcal/mol higher than that of Path A. As a result, we can conclude that path C is less favorable than path A.
Figure S3. The free energy profiles along the hydride transfer step by path D.

Path D: In this pathway, the ketone substrate also coordinates to the Ru atom during the hydride transfer by inner-sphere mechanism. Meanwhile, the arene ring occurs the ring slippage from η⁶-coordination to η²-coordination to form complex 13. Then the hydride transfer to the carbon atom of ketone through TS13-12, which owing an energy barrier of 16.7 kcal/mol (see Figure S3). Obviously, Path A is more favorable than Path D.
Figure S4. The free energy profiles of hydrogen release pathway when hydrated proton is $\text{H}_7\text{O}_3^+$. 

Figure S4 shows the free energy profiles of dihydrogen release pathway and hydride transfer pathway mediated by $\text{H}_7\text{O}_3^+$, the energy barrier of the dihydrogen release pathway is 10.3 kcal/mol. Interestingly, the reaction along the hydride transfer pathway is 8.9 kcal/mol. In general, the dihydrogen release pathway driven by this cyclometallated TM single-site system is less favorable than the hydride transfer pathway under acidic condition. Obviously, the hydride transfer pathway via outer-sphere mechanism is more favorable than the hydrogen release pathway for the reaction mediated by hydrated proton $\text{H}_7\text{O}_3^+$. 
Figure S5. The free energy profiles of hydrogen release pathway when proton source is HCOOH.

As shown in Figure S5, **TS24-25** with formic acid as proton source has an activation energy barrier of 20.3 kcal/mol, 10.9 kcal/mol higher than that of **TS14-15** with the hydrated proton H$_5$O$_2^+$. The calculation results suggest that the hydrogen release pathway is more favorable along H$_5$O$_2^+$ as proton source than formic acid as proton source.
Figure S6. The free energy profiles of TH of ketones catalyzed by cyclometallated ruthenium single-site complex when chose different basis set to describe Ru.

When the effective core potential (ECP) of Ru with a double-ζ valence basis set (LANL2DZ) was chosen to describe Ru, the metal hydride formation is the rate-determining step with a free energy barrier of 14.1 kcal/mol. When the sdd basis set was chosen to describe Ru, the metal hydride formation is the rate-determining step with a free energy barrier of 15.5 kcal/mol (see Figure S6). The difference of calculated results between the two basis set is little which is only 1.4 kcal/mol.
Figure S7. The free energy profiles of the formation of metal hydride 5 when the dissociation of one 4-methylpyridine.

As shown in Figure S7, one 4-methylpyridine is dissociated to provide a vacant coordinate site to form complex 4c firstly, this process is exothermic by 23.3 kcal/mol. Subsequently, the hydride transfers to Ru through TS4c-5, which owes an energy barrier of 26.7 kcal/mol. This high energy barrier implies that this pathway is less favorable than the ion-pair mechanism.
Figure S8. The free energy profiles of the formation of PhMeCOH$_5$O$_2^+$ and PhMeCOH$_3$O$^+$. The reactions of PhMeCO + H$_5$O$_2^+$ -> PhMeCOH$_5$O$_2^+$ and PhMeCO + H$_3$O$^+$ -> PhMeCOH$_3$O$^+$ as shown in Figure S8, these processes are endergonic by 3.6 and 5.3 kcal/mol, respectively.
As shown in Figure S9, the APT charges of $C^1$ in complex 22, 6 and 16 are increasing in turn, however, the energy barriers of these pathways are decreasing in turn. It indicates that $H_3O^+$ hydrated proton contributes more charges to the carbon atom of ketone. The calculated results show that the hydride transfer pathway for the reaction mediated by $H_3O^+$ is more favorable than those mediated by $H_5O_2^+$ or $H_7O_3^+$. 

Figure S9. Relationship between APT charge of $C^1$ atom and free energy barriers of hydride transfer pathway.
As shown in Figure S10, the APT charges of $H^3$ in complex 20, 14 and 18 are increasing in turn, however, the energy barriers of these pathways are decreasing in turn. This means that $H_3O^+$ has stronger acidity. The calculated results show that the dihydrogen release pathway for the reaction mediated by $H_3O^+$ is more favorable than those mediated by $H_2O_2^+$ or $H_2O_3^+$.
Table S1. The APT charge of $H^1$ atom in hydrated protons $H_3O^+$, $H_5O_2^+$ and $H_7O_3^+$.

| Hydrated proton | APT charge of $H^1$ atom |
|-----------------|-------------------------|
| $H_3O^+$        | 0.51                    |
| $H_5O_2^+$      | 0.44                    |
| $H_7O_3^+$      | 0.40                    |
Table S2. The calculated electronic energies ($E$, in a. u.), free Gibbs energies ($G$, in a. u.), relative electronic energies ($\Delta E$, kcal/mol), and relative Gibbs energies ($\Delta G$, kcal/mol, 298K).

| Complex                  | $G$    | $E$    | $\Delta E$ | $\Delta G$ |
|--------------------------|--------|--------|------------|------------|
| CO$_2$           | -188.525108 | -188.51598911 | \   | \   |
| H$_2$O              | -76.407070   | -76.41101011   | \   | \   |
| H$_3$O$^+$           | -76.823038   | -76.83965507   | \   | \   |
| H$_2$O$_2$$^+$       | -153.244176  | -153.27668220  | \   | \   |
| H$_2$O$_3$$^+$       | -229.650596  | -229.70612822  | \   | \   |
| HCOO$^-$             | -189.691831  | -189.70231192  | \   | \   |
| HCOO$^-$             | -189.238205  | -189.23601139  | \   | \   |
| OH$^-$               | -75.880497   | -75.87298358   | \   | \   |
| H$_2$               | -1.173712    | -1.17238411    | \   | \   |
| PhCOCH$_3$          | -384.678258  | -384.78399771  | \   | \   |
| PhCOCH$_3$...HCOOH   | -574.356005  | -574.49112237  | \   | \   |
| PhCOCH$_3$...H$_3$O$^+$ | -461.509704  | -461.65022147  | \   | \   |
| PhCOCH$_3$...H$_2$O$_2$$^+$ | -537.916675  | -538.07962941  | \   | \   |
| PhCOCH$_3$...H$_2$O$_3$$^+$ | -614.325414  | -614.50620610  | \   | \   |
| Phenylethanol        | -385.859331  | -385.98929721  | \   | \   |
| 2                     | -1283.297302 | -1283.71544664 | 0.0 | 0.0 |
| 3                     | -1396.147723 | -1396.55992586 | -12.2 | -12.1 |
| 4a                    | -1396.127545 | -1396.53901329 | 0.9  | 0.6  |
| 4b                    | -1396.134620 | -1396.54505987 | -2.9  | -3.9  |
| TS4a-5               | -1396.125275 | -1396.53244412 | 5.0  | 2.0  |
| TS4b-5               | -1396.098258 | -1396.50673372 | 21.2  | 20.1  |
| 5                     | -1207.619209 | -1208.02037691 | 2.6  | -10.0 |
| 6                     | -1745.538164 | -1746.12596623 | -25.6  | -7.8  |
| TS6-7                | -1745.530284 | -1746.11695319 | -19.9  | -2.9  |
| 7                     | -1745.548222 | -1746.13852352 | -33.5  | -14.1 |
| 8                     | -1282.837906 | -1283.24155288 | 12.1  | 18.4  |
| 8'                   | -1282.837906 | -1283.24155288 | -40.2  | -42.1 |
| 9                     | -1781.995596 | -1782.55672512 | -25.8  | -22.8 |
| TS9-10               | -1781.975608 | -1782.53698596 | -13.1  | -10.3 |
| 10                    | -1781.988490 | -1782.55745103 | -26.3  | -18.3 |
| 11                    | -1592.261620 | -1592.79101903 | 11.0  | 12.5  |
| TS11-12              | -1592.253225 | -1592.78133189 | 17.1  | 17.8  |
| Complex       | Imaginary frequencies |
|---------------|-----------------------|
| TS4a-4        | 558.66i               |
| TS4b-4        | 254.59i               |
| TS6-7         | 416.93i               |
| TS9-10        | 542.38i               |
| TS11-12       | 507.19i               |
| TS13-12       | 188.50i               |
| TS14-15       | 920.23i               |
| TS16-17       | 337.70i               |
| TS18-19       | 997.06i               |
| TS20-21       | 672.18i               |
| TS22-23       | 455.20i               |
| TS24-25       | 44.44i                |

Table S3. Calculated imaginary frequencies of transition states at ωB97X-D/BSI level.
Figure S11. Typical geometric structure diagram.
### Atomic Cartesian coordinates of intermediates and transition states (unit: Å).

|   | X          | Y          | Z          |
|---|------------|------------|------------|
| 44| 0.948762000| -0.726993000| -0.458109000|
| 7 | 0.089909000| 1.203478000| -0.431265000|
| 7 | -1.097393000| -1.074573000| -0.073743000|
| 8 | -1.651000000| 4.923733000| -0.304185000|
| 8 | -5.100226000| -1.441541000| 0.794376000|
| 6 | 0.769913000| 2.319140000| -0.746314000|
| 1 | 1.799778000| 2.179952000| -1.045033000|
| 6 | 0.203064000| 3.570846000| -0.707986000|
| 1 | 0.782569000| 4.448999000| -0.964189000|
| 6 | -1.142745000| 3.688987000| -0.337745000|
| 6 | -1.865914000| 2.527097000| -0.048825000|
| 1 | -2.915300000| 2.571890000| 0.206626000|
| 6 | -1.216832000| 1.304838000| -0.115583000|
| 6 | -3.025759000| 5.086275000| 0.053210000|
| 1 | -3.675235000| 4.576097000| -0.663721000|
| 1 | -3.211643000| 6.158434000| 0.020405000|
| 1 | -3.209860000| 4.710922000| 1.063714000|
| 6 | -1.894130000| 0.009356000| 0.093201000|
| 6 | -3.235532000| -0.115093000| 0.387600000|
| 1 | -3.872226000| 0.749723000| 0.524871000|
| 6 | -3.797103000| -1.393147000| 0.505039000|
| 6 | -2.977977000| -2.507364000| 0.305144000|
| 1 | -3.347062000| -3.522298000| 0.367601000|
| 6 | -1.642077000| -2.293433000| 0.020110000|
| 1 | -0.979475000| -3.133424000| -0.144370000|
| 6 | -5.716414000| -2.725541000| 0.922079000|
| 1 | -5.646227000| -3.281874000| -0.016791000|
| 1 | -6.761598000| -2.527258000| 1.153537000|
| 1 | -5.257448000| -3.294194000| 1.735564000|
| 6 | 1.923766000| -0.940997000| 1.509981000|
| 1 | 1.516636000| -0.589093000| 2.450013000|
| 6 | 1.559331000| -2.224904000| 1.034168000|
| 1 | 0.855358000| -2.817792000| 1.609283000|
| 6 | 2.021904000| -2.720073000| -0.212396000|
| 6 | 2.807783000| -1.836878000| -0.992503000|
| 1 | 3.070541000| -2.123624000| -2.005628000|
### Coordinates (Angstroms)

|    | X               | Y               | Z               |
|----|-----------------|-----------------|-----------------|
| 44 | -0.976657000    | -0.677927000    | 0.217669000     |
| 7  | -0.020551000    | 1.199023000     | 0.293212000     |
| 7  | 1.039575000     | -1.122929000    | -0.193451000    |
| 8  | 1.937776000     | 4.814381000     | 0.358726000     |
| 8  | 5.045250000     | -1.693863000    | -0.919428000    |
| 6  | -0.638000000    | 2.337775000     | 0.648673000     |
| 1  | -1.681682000    | 2.249368000     | 0.919972000     |
| 6  | 0.002778000     | 3.554521000     | 0.678722000     |
| 1  | -0.528588000    | 4.453743000     | 0.964514000     |
| 6  | 1.358461000     | 3.609237000     | 0.332469000     |
| 6  | 2.016091000     | 2.422003000     | -0.000464000    |
| 1  | 3.069938000     | 2.415223000     | -0.241904000    |
| 6  | 1.294726000     | 1.237138000     | 0.000739000     |
| 6  | 3.317483000     | 4.914765000     | 0.001283000     |
| 1  | 3.942114000     | 4.340961000     | 0.691751000     |
| 1  | 3.563431000     | 5.972532000     | 0.077417000     |
| 1  | 3.478392000     | 4.572286000     | -1.024979000    |
| 6  | 1.903266000     | -0.083212000    | -0.264280000    |
| 6  | 3.246773300     | -0.274968000    | -0.515178000    |
| 1  | 3.941703000     | 0.553485000     | -0.572006000    |
### Coordinates (Angstroms)

|   | X             | Y             | Z             |
|---|---------------|---------------|---------------|
| 6 | 3.734276000   | -1.577514000  | -0.682311000  |
| 6 | 2.842533000   | -2.647832000  | -0.579460000  |
| 1 | 3.152946000   | -3.678980000  | -0.682311000  |
| 6 | 1.511246000   | -2.366790000  | -0.332258000  |
| 1 | 0.791074000   | -3.170011000  | -0.232530000  |
| 6 | 5.590951000   | -3.008222000  | -1.054827000  |
| 1  | 5.442038000 | -3.583327000 | -0.136528000 |
| 1  | 6.655656000 | -2.866768000 | -1.232463000 |
| 1  | 5.140783000 | -3.529866000 | -1.904156000 |
| 6  | -1.916683000 | -0.998245000 | -1.788420000 |
| 1  | -1.440433000 | -0.831076000 | -2.746212000 |
| 6  | -1.738212000 | -2.252530000 | -1.142771000 |
| 1  | -1.111374000 | -2.999051000 | -1.620017000 |
| 6  | -2.278694000 | -2.523361000 | 0.132546000   |
| 6  | -2.986098000 | -1.460266000 | 0.766256000   |
| 1  | -3.324054000 | -1.590858000 | 1.789305000   |
| 6  | -3.187014000 | -0.216440000 | 0.137879000   |
| 1  | -3.703616000 | 0.563975000  | 0.679955000   |
| 6  | -2.655427000 | 0.035956000  | -1.164010000  |
| 6  | -2.830014000 | 1.375355000  | -1.867929000  |
| 6  | -3.775440000 | 2.333468000  | -1.141414000  |
| 6  | -3.333883000 | 1.158172000  | -3.303035000  |
| 1  | -1.836544000 | 1.837260000  | -1.922684000  |
| 1  | -3.443101000 | 2.586192000  | -0.132102000  |
| 1  | -3.842748000 | 3.267365000  | -1.705607000  |
| 1  | -4.783077000 | 1.909686000  | -1.071380000  |
| 1  | -2.640908000 | 0.569159000  | -3.907946000  |
| 1  | -4.303230000 | 0.648895000  | -3.297826000  |
| 1  | -3.461904000 | 2.126922000  | -3.793940000  |
| 6  | -2.061680000 | -3.835358000 | 0.823774000   |
| 1  | -2.917899000 | -4.495555000 | 0.653333000   |
| 1  | -1.166990000 | -4.332007000 | 0.441576000   |
| 1  | -1.952369000 | -3.690191000 | 1.900953000   |
| 8  | -0.277036000 | -0.829657000 | 2.208775000   |
| 6  | -0.874294000 | -0.193578000 | 3.155506000   |
| 1  | -1.732620000 | 0.434600000  | 2.846393000   |
| 8  | -0.546748000 | -0.250648000 | 4.343732000   |
|   |          |          |            |          |          |          |
|---|----------|----------|-----------|----------|----------|----------|
| 8 | 3.534779000 | -3.968683000 | 0.456430000 |          |          |          |
| 8 | 3.825065000 | 3.329562000 | -0.070961000 |          |          |          |
| 6 | 0.178135000 | -2.817308000 | -0.043024000 |          |          |          |
| 1 | -0.825572000 | -3.208122000 | -0.150621000 |          |          |          |
| 6 | 1.247770000 | -3.660836000 | 0.140716000 |          |          |          |
| 1 | -1.103758000 | -4.732933000 | 0.187655000 |          |          |          |
| 6 | 2.529092000 | -3.109390000 | 0.270362000 |          |          |          |
| 6 | 2.675206000 | -1.721785000 | 0.198013000 |          |          |          |
| 1 | 3.646417000 | -1.256321000 | 0.287904000 |          |          |          |
| 6 | 1.544134000 | -0.941438000 | 0.011213000 |          |          |          |
| 6 | 4.859759000 | -3.450552000 | 0.597890000 |          |          |          |
| 1 | 5.163089000 | -2.910213000 | -0.303406000 |          |          |          |
| 1 | 5.500205000 | -4.319703000 | 0.737743000 |          |          |          |
| 1 | 4.929067000 | -2.797507000 | 1.472571000 |          |          |          |
| 6 | 1.579717000 | 0.532568000 | -0.079298000 |          |          |          |
| 6 | 2.738765000 | 1.276717000 | -0.024208000 |          |          |          |
| 1 | 3.709060000 | 0.814186000 | 0.102956000 |          |          |          |
| 6 | 2.664902000 | 2.670885000 | -0.140965000 |          |          |          |
| 6 | 1.413586000 | 3.264638000 | -0.324118000 |          |          |          |
| 1 | 1.283692000 | 4.332125000 | -0.438295000 |          |          |          |
| 6 | 0.300407000 | 2.445608000 | -0.366759000 |          |          |          |
| 1 | -0.683054000 | 2.870847000 | -0.521452000 |          |          |          |
| 6 | 3.803982000 | 4.755631000 | -0.171404000 |          |          |          |
| 1 | 3.413780000 | 5.070719000 | -1.143201000 |          |          |          |
| 1 | 4.840984000 | 5.071894000 | -0.071930000 |          |          |          |
| 1 | 3.205844000 | 5.190707000 | 0.634310000 |          |          |          |
| 6 | -2.734263000 | 1.303463000 | 0.627326000 |          |          |          |
| 1 | -2.585451000 | 2.374980000 | 0.708402000 |          |          |          |
| 6 | -3.350443000 | 0.779220000 | -0.511561000 |          |          |          |
| 1 | -3.666336000 | 1.444232000 | -1.306843000 |          |          |          |
| 6 | -3.489058000 | -0.639832000 | -0.684505000 |          |          |          |
| 6 | -3.004959000 | -1.486981000 | 0.325866000 |          |          |          |
| 1 | -3.061014000 | -2.561523000 | 0.197654000 |          |          |          |
| 6 | -2.326994000 | -0.946549000 | 1.459190000 |          |          |          |
| 1 | -1.868886000 | -1.633912000 | 2.160978000 |          |          |          |
| 6 | -2.173435000 | 0.450433000 | 1.634681000 |          |          |          |
| 6 | -1.451636000 | 1.067272000 | 2.810818000 |          |          |          |
| 6 | -0.331069000 | 0.190311000 | 3.365976000 |          |          |          |
| 6 | -2.481240000 | 1.419697000 | 3.892320000 |          |          |          |
| 1 | -1.006563000 | 1.998902000 | 2.442232000 |          |          |          |
| 1 | 0.376341000 | -0.098330000 | 2.582419000 |          |          |          |
| 1 | 0.218181000 | 0.741724000 | 4.134074000 |          |          |          |
| 1 | -0.721871000 | -0.719938000 | 3.832033000 |          |          |          |
| 1 | -3.254862000 | 2.088554000 | 3.502943000 |          |          |          |
|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| 1 | -2.967317000 | 0.514023000 | 4.270339000 |
| 1 | -1.989177000 | 1.920350000 | 4.731260000 |
| 6 | -4.067512000 | -1.172949000 | -1.957894000 |
| 1 | -5.147218000 | -0.994134000 | -1.971426000 |
| 1 | -3.628166000 | -0.654053000 | -2.813719000 |
| 1 | -3.885856000 | -2.244307000 | -2.056071000 |
| 8 | -1.398788000 | 0.772380000 | -3.642608000 |
| 6 | -0.506938000 | 0.174891000 | -3.032021000 |
| 1 | -0.911665000 | -0.412354000 | -2.076455000 |
| 8 | 0.701200000 | 0.010824000 | -3.215152000 |

4b Coordinates (Angstroms)

|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| 44 | -0.049221000 | -1.338121000 | 1.289378000 |
| 7 | -1.152904000 | 0.354822000 | 1.064307000 |
| 7 | 1.314693000 | -0.100572000 | 0.450384000 |
| 8 | -3.392121000 | 3.634697000 | 0.000847000 |
| 8 | 3.864208000 | 2.762936000 | -1.038179000 |
| 6 | -2.451676000 | 0.461723000 | 1.388973000 |
| 1 | -2.881162000 | -0.379346000 | 1.920805000 |
| 6 | -3.208401000 | 1.561894000 | 1.055127000 |
| 1 | -4.256287000 | 1.614674000 | 1.322751000 |
| 6 | -2.606848000 | 2.600930000 | 0.333634000 |
| 6 | -1.252191000 | 2.501584000 | 0.007053000 |
| 1 | -0.748266000 | 3.281644000 | -0.546963000 |
| 6 | -0.557166000 | 1.365877000 | 0.395396000 |
| 6 | -2.831892000 | 4.682212000 | -0.791437000 |
| 1 | -2.019548000 | 5.185285000 | -0.258492000 |
| 1 | -3.643813000 | 5.386210000 | -0.967033000 |
| 1 | -2.468777000 | 4.293306000 | -1.747558000 |
| 6 | 0.875843000 | 1.141432000 | 0.121337000 |
| 6 | 1.732259000 | 2.098479000 | -0.384199000 |
| 1 | 1.387154000 | 3.095339000 | -0.628886000 |
| 6 | 3.085592000 | 1.783213000 | -0.559749000 |
| 6 | 3.528444000 | 0.500671000 | -0.225328000 |
| 1 | 4.558646000 | 0.191509000 | -0.339304000 |
| 6 | 2.605835000 | -0.401782000 | 0.273550000 |
| 1 | 2.902504000 | -1.408044000 | 0.548599000 |
| 6 | 5.260653000 | 2.502109000 | -1.184374000 |
| 1 | 5.709116000 | 2.239590000 | -0.221910000 |
| 1 | 5.696883000 | 3.429933000 | -1.550944000 |
| 1 | 5.434454000 | 1.702450000 | -1.910459000 |
| 6 | -0.879347000 | -2.684811000 | -1.139305000 |
|    | X               | Y               | Z               |
|----|----------------|----------------|----------------|
| 44 | 1.187436000    | -0.486643000   | 0.294863000    |
| 7  | -0.595321000   | -1.505421000   | -0.127672000   |
| 7  | -0.256999000   | 1.038175000    | 0.324723000    |
| 8  | -4.135940000   | -3.363650000   | -1.095161000   |
| 8  | -3.306995000   | 3.795187000    | 0.169173000    |
| 6  | -0.681381000   | -2.838130000   | -0.290086000   |
| 1  | 0.235402000    | -3.398556000   | -0.153827000   |
| 6  | -1.859128000   | -3.471820000   | -0.609352000   |
| 1  | -1.891688000   | -4.546348000   | -0.740121000   |
| 6  | -3.019167000   | -2.702863000   | -0.768213000   |
| 6  | -2.941721000   | -1.322480000   | -0.573223000   |
| 1  | -3.815768000   | -0.693826000   | -0.670622000   |
| 6  | -1.713930000   | -0.762025000   | -0.247401000   |

**TS4a-5**

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**Coordinates (Angstroms)**

|    | X               | Y               | Z               |
|----|----------------|----------------|----------------|
| 44 | 1.187436000    | -0.486643000   | 0.294863000    |
| 7  | -0.595321000   | -1.505421000   | -0.127672000   |
| 7  | -0.256999000   | 1.038175000    | 0.324723000    |
| 8  | -4.135940000   | -3.363650000   | -1.095161000   |
| 8  | -3.306995000   | 3.795187000    | 0.169173000    |
| 6  | -0.681381000   | -2.838130000   | -0.290086000   |
| 1  | 0.235402000    | -3.398556000   | -0.153827000   |
| 6  | -1.859128000   | -3.471820000   | -0.609352000   |
| 1  | -1.891688000   | -4.546348000   | -0.740121000   |
| 6  | -3.019167000   | -2.702863000   | -0.768213000   |
| 6  | -2.941721000   | -1.322480000   | -0.573223000   |
| 1  | -3.815768000   | -0.693826000   | -0.670622000   |
| 6  | -1.713930000   | -0.762025000   | -0.247401000   |

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521
|   |       |       |       |
|---|-------|-------|-------|
| 1 | -5.337063000 | -2.616785000 | -1.296252000 |
| 1 | -5.636594000 | -2.106410000 | -0.376157000 |
| 1 | -6.094240000 | -3.345999000 | -1.572170000 |
| 1 | -5.213300000 | -1.891107000 | -2.105480000 |
| 6 | -1.525275000 | 0.681168000  | 0.008348000  |
| 6 | -2.547648000 | 1.607481000  | -0.041950000 |
| 1 | -3.563272000 | 1.325220000  | -0.287844000 |
| 6 | -2.271793000 | 2.950405000  | 0.240735000  |
| 6 | -0.965380000 | 3.112640000  | 0.579044000  |
| 1 | -0.684841000 | 4.328120000  | 0.817630000  |
| 6 | -0.001429000 | 2.320320000  | 0.615350000  |
| 1 | 1.020871000 | 2.556457000  | 0.881060000  |
| 6 | -3.071474000 | 5.175638000  | 0.452836000  |
| 1 | -2.708590000 | 5.306631000  | 1.476352000  |
| 1 | -4.036039000 | 5.667677000  | 0.339123000  |
| 1 | -2.355523000 | 5.999270000  | -0.257360000 |
| 6 | 3.120612000 | 0.665437000  | 0.208985000  |
| 1 | 3.305111000 | 1.630022000  | 0.668677000  |
| 6 | 3.313204000 | -0.506817000 | 0.958781000  |
| 1 | 3.632437000 | -0.430169000 | 1.992424000  |
| 6 | 3.016173000 | -1.795443000 | 0.409887000  |
| 6 | 2.509245000 | -1.827749000 | -0.906313000 |
| 1 | 2.204744000 | -2.780138000 | -1.327729000 |
| 6 | 2.335934000 | -0.647147000 | -1.688260000 |
| 1 | 1.922255000 | -0.733946000 | -2.685142000 |
| 6 | 2.618524000 | 0.612840000  | -1.133210000 |
| 6 | 2.414820000 | 1.904114000  | -1.894022000 |
| 6 | 1.202170000 | 1.889105000  | -2.824630000 |
| 6 | 3.704208000 | 2.227989000  | -2.662013000 |
| 1 | 2.263590000 | 2.690252000  | -1.145923000 |
| 1 | 0.284681000 | 1.628511000  | -2.288140000 |
| 1 | 1.068065000 | 2.880806000  | -3.265780000 |
| 1 | 1.332561000 | 1.178522000  | -3.646880000 |
| 1 | 4.565510000 | 2.280533000  | -1.989158000 |
| 1 | 3.905080000 | 1.461794000  | -3.418454000 |
| 1 | 3.606103000 | 3.192735000  | -3.168240000 |
| 6 | 3.207308000 | -3.049106000 | 1.210412000  |
| 1 | 4.226651000 | -3.426228000 | 1.079253000  |
| 1 | 3.048157000 | -2.859229000 | 2.273982000  |
| 1 | 2.512096000 | -3.825718000 | 0.883030000  |
| 8 | 0.995633000 | 0.490803000  | 3.589190000  |
| 6 | 0.106566000 | -0.109816000 | 3.063133000  |
| 1 | 0.746652000 | -0.815171000 | 1.859086000  |
| 8 | -1.032852000 | -0.467522000 | 3.039572000  |
|      | X           | Y           | Z           |
|------|-------------|-------------|-------------|
| 44   | -0.186824000| -1.532787000| -1.210212000|
| 7    | 1.245946000 | 0.079422000 | -1.185292000|
| 7    | -1.346050000| 0.079158000 | -0.714582000|
| 8    | 3.853555000 | 3.177887000 | -0.507404000|
| 8    | -3.371282000| 3.471409000 | 0.435335000 |
| 6    | 2.562670000 | -0.041278000| -1.408381000|
| 1    | 2.900276000 | -1.007580000| -1.766203000|
| 6    | 3.449741000 | 0.990479000 | -1.190330000|
| 1    | 4.508989000 | 0.861575000 | -1.383094000|
| 6    | 2.954546000 | 2.209074000 | -0.719253000|
| 6    | 1.581462000 | 2.342426000 | -0.489643000|
| 1    | 1.167134000 | 3.268311000 | -0.117287000|
| 6    | 0.761943000 | 1.249940000 | -0.736622000|
| 6    | 3.396234000 | 4.433060000 | -0.001130000|
| 1    | 2.694953000 | 4.901188000 | -0.697945000|
| 1    | 4.286597000 | 5.052461000 | 0.093854000 |
| 1    | 2.928328000 | 4.308258000 | 0.979815000 |
| 6    | -0.703333000| 1.265683000 | -0.519912000|
| 6    | -1.394133000| 2.397566000 | -0.141516000|
| 1    | -0.891486000| 3.344376000 | 0.006871000 |
| 6    | -2.778266000| 2.334007000 | 0.064714000 |
| 6    | -3.426549000| 1.111416000 | -0.118823000|
| 1    | -4.489727000| 0.983297000 | 0.032352000 |
| 6    | -2.669249000| 0.020368000 | -0.501329000|
| 1    | -3.139767000| -0.943519000| -0.647824000|
| 6    | -4.776875000| 3.448327000 | 0.695928000 |
| 1    | -5.332672000| 3.174695000 | -0.205363000|
| 1    | -5.034954000| 4.463421000 | 0.993097000 |
| 1    | -5.007409000| 2.753206000 | 1.508100000|
| 6    | 0.657317000 | -2.492854000| 1.638015000 |
| 1    | 0.025143000 | -3.367232000| 1.504392000 |
| 6    | 2.004422000 | -2.567354000| 1.291941000 |
| 1    | 2.398759000 | -3.491947000| 0.877657000 |
| 6    | 2.859434000 | -1.476881000| 1.483264000 |
| 6    | 2.310337000 | -0.307338000| 2.009059000 |
| 1    | 2.946794000 | 0.561762000 | 2.152533000 |
| 6    | 0.957915000 | -0.223239000| 2.338581000 |
| 1    | 0.577730000 | 0.711628000 | 2.736866000 |
| 6    | 0.101517000 | -1.312886000| 2.164063000 |
| 6    | -1.369749000| -1.289436000| 2.555813000 |
|   | X           | Y           | Z           |
|---|-------------|-------------|-------------|
| 6 | -1.875901000| 0.092692000 | 2.965226000 |
| 6 | -1.646900000| -2.299416000| 3.678971000 |
| 1 | -1.939087000| -1.612262000| 1.673782000 |
| 1 | -1.656538000| 0.852912000 | 2.211482000 |
| 1 | -2.959606000| 0.066320000 | 3.112781000 |
| 1 | -1.419058000| 0.414824000 | 3.907829000 |
| 1 | -1.364691000| -1.317109000| 3.394182000 |
| 1 | -1.087556000| -2.032002000| 4.582553000 |
| 1 | -2.712826000| -2.305283000| 3.929438000 |
| 6 | 4.318335000 | -1.569223000| 1.121630000 |
| 1 | 4.838326000 | -2.285253000| 1.767195000 |
| 1 | 4.449029000 | -1.910968000| 0.089771000 |
| 1 | 4.814838000 | -0.600977000| 1.224739000 |
| 8 | -0.796120000| -1.670026000| -3.214358000|
| 6 | -1.674296000| -2.164591000| -2.445870000|
| 1 | -1.179356000| -2.791771000| -0.996532000|
| 8 | -2.811766000| -2.556849000| -2.559916000|

5

Coordinates (Angstroms)

|   | X           | Y           | Z           |
|---|-------------|-------------|-------------|
| 44| 0.980597000 | -0.708956000| -0.585022000|
| 7 | 0.022830000 | 1.170290000 | -0.641129000|
| 7 | -1.023751000| -1.161676000| -0.128706000|
| 8 | -1.906745000| 4.804820000 | -0.408735000|
| 8 | -5.008016000| -1.710897000| 0.762450000 |
| 6 | 0.639873000 | 2.330525000 | -0.927774000|
| 1 | 1.674029000 | 2.253560000 | -1.237154000|
| 6 | 0.012091000 | 3.552336000 | -0.851670000|
| 1 | 0.545763000 | 4.465010000 | -1.086688000|
| 6 | -1.335082000| 3.594349000 | -0.472499000|
| 6 | -1.990483000| 2.393915000 | -0.195555000|
| 1 | -3.033602000| 2.380389000 | 0.088050000 |
| 6 | -1.279209000| 1.204082000 | -0.289814000|
| 6 | -3.283753000| 4.885145000 | -0.038937000|
| 1 | -3.912364000| 4.356874000 | -0.761891000|
| 1 | -3.528442000| 5.946117000 | -0.045871000|
| 1 | -3.442659000| 4.477807000 | 0.963968000 |
| 6 | -1.882909000| -0.118890000| -0.028502000|
| 6 | -3.218851000| -0.305464000| 0.272964000 |
| 1 | -3.908569000| 0.525776000 | 0.348972000 |
| 6 | -3.703307000| -1.601988000| 0.475673000 |
| 6 | -2.816550000| -2.674965000| 0.360986000 |
| 1 | -3.123073000| -3.703487000| 0.497405000 |
## Coordinates (Angstroms)

|   | X       | Y       | Z       |
|---|---------|---------|---------|
| 44| 1.1707820000 | 0.4155640000 | 0.6151790000 |
| 7 | -0.1562130000 | 0.9989990000 | -0.8971820000 |
| 7 | -0.7188580000 | 0.1547790000 | 1.4990320000 |
| 8 | -2.8582060000 | 2.3297290000 | -3.7094020000 |
| 8 | -4.5723750000 | -0.2162590000 | 2.9083990000 |
| 6 | 0.2145460000 | 1.3359580000 | 2.4245910000 |
| 1 | 1.2686740000 | 1.2403100000 | -2.3742780000 |
| 6 | -0.6761140000 | 1.7766340000 | -3.0966170000 |
| 1 | -0.3391610000 | 2.0300470000 | -4.0942150000 |
| X         | Y         | Z         |
|-----------|-----------|-----------|
| 3.281782000 | -2.398944000 | 0.692588000 |
| -3.032625000 | -1.689364000 | -1.980571000 |
| -1.676512000 | -1.924496000 | -2.186167000 |
| -0.935464000 | -2.623334000 | -1.227058000 |
| -1.560931000 | -3.064074000 | -0.051476000 |
| -2.908055000 | -2.810554000 | 0.157959000  |
| -3.646610000 | -2.127266000 | -0.810367000 |
| -3.047888000 | -1.152568000 | -2.730102000 |
| -1.206032000 | -1.566533000 | -3.095770000 |
| -0.978906000 | -3.594353000 | 0.694411000  |
| -3.385466000 | -3.137728000 | 1.075673000  |
| -4.700865000 | -1.929411000 | -0.645016000 |
| 0.502748000  | -2.916542000 | -1.428666000 |
| 1.051300000 | -3.753233000 | -0.695724000 |
| 1.263368000  | -2.242589000 | -2.527986000 |
| 1.034062000  | -2.750521000 | -3.472056000 |
| 0.976330000  | -1.195728000 | -2.634040000 |
| 2.335404000  | -2.311565000 | -2.342419000 |
| 3.453924000  | -4.423655000 | -0.963215000 |
| 4.024716000  | -3.604571000 | -1.248988000 |
| 2.463025000  | -4.124992000 | -0.869017000 |
| 3.761030000  | -4.703013000 | -0.087887000 |
| 4.796839000  | -2.411016000 | -1.630312000 |
| 5.502535000  | -2.628149000 | -2.252436000 |
| 5.241857000  | -2.077073000 | -0.840736000 |

TS6-7 Coordinates (Angstroms)

| X         | Y         | Z         |
|-----------|-----------|-----------|
| 1.165988000 | 0.222110000 | 0.576591000 |
| -0.108569000 | 1.160539000 | -0.785214000 |
| -0.737318000 | -0.206381000 | 1.334439000 |
| -2.727413000 | 3.085012000 | -3.312551000 |
| -4.608606000 | -0.705589000 | 2.640646000 |
| 0.302678000  | 1.773215000 | -1.906000000 |
| 1.365264000  | 1.734791000 | -2.114767000 |
| -0.560249000 | 2.416495000 | -2.765909000 |
| -0.192613000 | 2.895692000 | -3.664671000 |
| -1.925392000 | 2.444007000 | -2.452768000 |
| -2.360446000 | 1.803504000 | -1.292557000 |
| -3.407756000 | 1.779436000 | -1.026388000 |
| -1.423879000 | 1.161246000 | -0.492865000 |
| -4.127805000 | 3.120434000 | -3.033691000 |
| -4.544670000 | 2.109087000 | -3.006466000 |
|   |      |       |       |
|---|------|-------|-------|
| 1 | -4.577619000 | 3.679438000 | -3.852511000 |
| 1 | -4.321964000 | 3.631705000 | -2.086248000 |
| 6 | -1.784898000 | 0.384457000 | 0.709585000 |
| 6 | -3.080271000 | 0.226177000 | 1.157902000 |
| 1 | -3.917465000 | 0.696954000 | 0.659296000 |
| 6 | -3.327326000 | -0.583927000 | 2.271659000 |
| 6 | -2.248335000 | -1.207554000 | 2.900902000 |
| 1 | -2.367708000 | -1.857320000 | 3.754888000 |
| 6 | -0.980170000 | -0.983250000 | 2.392780000 |
| 6 | -0.118277000 | -1.457969000 | 2.850639000 |
| 1 | -0.112410000 | -1.177808000 | 4.662619000 |
| 6 | 2.030717000 | 1.143049000 | 2.510508000 |
| 1 | 1.482178000 | 1.453491000 | 3.393723000 |
| 6 | 2.423504000 | -0.225714000 | 2.385796000 |
| 1 | 2.172670000 | -0.925588000 | 3.174899000 |
| 6 | 3.122156000 | -0.683566000 | 1.253321000 |
| 6 | 3.367807000 | 0.251014000 | 0.194077000 |
| 1 | 3.857318000 | -0.082042000 | -0.713609000 |
| 6 | 2.926106000 | 1.580526000 | 0.307162000 |
| 1 | 3.074472000 | 2.252885000 | -0.531833000 |
| 6 | 2.929748000 | 2.073680000 | 1.497741000 |
| 1 | 0.912952000 | -1.070007000 | -0.399207000 |
| 6 | 1.934950000 | 3.536597000 | 1.653590000 |
| 6 | 0.987310000 | 4.049783000 | 0.566495000 |
| 6 | 3.224656000 | 4.367402000 | 1.695206000 |
| 1 | 1.429816000 | 3.638850000 | 2.619924000 |
| 1 | 0.035837000 | 3.511060000 | 0.581444000 |
| 1 | 0.781746000 | 5.111934000 | 0.730140000 |
| 1 | 1.427271000 | 3.945224000 | -0.430704000 |
| 1 | 3.900324000 | 4.018366000 | 2.481848000 |
| 1 | 3.754913000 | 4.308368000 | 0.738399000 |
| 1 | 2.990874000 | 5.418900000 | 1.886709000 |
| 6 | 3.579214000 | -2.105421000 | 1.146285000 |
| 1 | 4.619604000 | -2.180710000 | 1.479880000 |
| 1 | 2.969750000 | -2.759534000 | 1.773500000 |
| 1 | 3.529302000 | -2.456609000 | 0.116576000 |
| 6 | -3.057748000 | -1.460358000 | -2.094175000 |
| 6 | -1.672642000 | -1.462669000 | -2.225261000 |
| 6 | -0.889852000 | -2.231839000 | -1.357564000 |
| 6 | -1.507938000 | -2.981368000 | -0.345182000 |
| 6 | -2.887159000 | -2.963220000 | -0.210817000 |
### Coordinates (Angstroms)

|   | X (Angstroms) | Y (Angstroms) | Z (Angstroms) |
|---|---------------|---------------|---------------|
| 6 | -3.665299000  | -2.204126000  | -1.087577000 |
| 1 | -3.658738000  | -0.861471000  | -2.770227000 |
| 1 | -1.214114000  | -0.864738000  | -3.005128000 |
| 1 | -0.901807000  | -3.567085000  | 0.336714000  |
| 1 | -3.359698000  | -3.531063000  | 0.583673000  |
| 1 | -4.744625000  | -2.187924000  | -0.976176000 |
| 6 | 0.576658000   | -2.299167000  | -1.520216000 |
| 8 | 1.144860000   | -3.325203000  | -0.974441000 |
| 6 | 1.274329000   | -1.623446000  | -2.659467000 |
| 1 | 1.123410000   | -2.246247000  | -3.549154000 |
| 1 | 0.874632000   | -0.630818000  | -2.852746000 |
| 1 | 2.342889000   | -1.547280000  | -2.459143000 |
| 8 | 3.430410000   | -3.956618000  | -1.839622000 |
| 1 | 4.018547000   | -3.173508000  | -1.968226000 |
| 1 | 2.103784000   | -3.508120000  | -1.313890000 |
| 1 | 3.850439000   | -4.467597000  | -1.137218000 |
| 8 | 4.948935000   | -1.741274000  | -2.064654000 |
| 1 | 5.638546000   | -1.800073000  | -2.735890000 |
| 1 | 5.424439000   | -1.715300000  | -1.225761000 |

### 7

Coordinates (Angstroms)
|   | x   | y   | z   |
|---|-----|-----|-----|
| 6 | -2.199451000 | -1.028331000 | 2.921070000 |
| 1 | -2.334987000 | -1.648819000 | 3.796324000 |
| 6 | -0.921476000 | -0.814406000 | 2.438773000 |
| 1 | -0.066227000 | -1.258964000 | 2.932725000 |
| 6 | -4.881664000 | -1.403612000 | 3.691525000 |
| 1 | -4.550697000 | -2.432119000 | 3.521572000 |
| 1 | -5.966941000 | -1.374418000 | 3.771710000 |
| 1 | -4.433429000 | -1.007948000 | 4.607142000 |
| 6 | 2.052053000 | 0.988479000 | 2.437365000 |
| 1 | 1.438837000 | 1.230463000 | 3.299219000 |
| 6 | 2.578493000 | -0.323280000 | 2.308749000 |
| 1 | 2.363433000 | -1.069460000 | 3.066822000 |
| 6 | 3.260631000 | -0.694469000 | 1.136382000 |
| 6 | 3.469447000 | 0.288992000 | 0.113586000 |
| 1 | 3.942580000 | -0.009957000 | -0.815254000 |
| 6 | 2.998654000 | 1.597054000 | 0.275362000 |
| 1 | 3.117400000 | 2.305049000 | -0.537663000 |
| 6 | 2.252460000 | 1.977961000 | 1.436892000 |
| 1 | 0.704555000 | -1.422923000 | -0.402853000 |
| 6 | 1.779525000 | 3.396905000 | 1.661991000 |
| 6 | 1.084380000 | 4.035715000 | 0.459756000 |
| 6 | 2.999673000 | 4.219987000 | 2.102560000 |
| 1 | 1.066563000 | 3.367150000 | 2.492519000 |
| 1 | 0.144736000 | 3.529463000 | 0.225920000 |
| 1 | 0.855457000 | 5.080229000 | 0.689886000 |
| 1 | 1.715856000 | 4.027373000 | -0.434510000 |
| 1 | 3.476720000 | 3.785225000 | 2.986540000 |
| 1 | 3.743942000 | 4.269620000 | 1.300219000 |
| 1 | 2.694948000 | 5.242079000 | 2.344527000 |
| 6 | 3.704228000 | -2.103352000 | 0.911954000 |
| 1 | 4.794527000 | -2.154456000 | 1.000447000 |
| 1 | 3.261709000 | -2.779347000 | 1.645024000 |
| 1 | 3.435338000 | -2.436751000 | -0.090100000 |
| 6 | -3.236490000 | -1.496930000 | -2.016361000 |
| 6 | -1.844233000 | -1.510086000 | -2.091069000 |
| 6 | -1.089310000 | -2.233066000 | -1.164990000 |
| 6 | -1.757214000 | -2.940784000 | -0.158907000 |
| 6 | -3.145142000 | -2.926963000 | -0.082853000 |
| 6 | -3.891395000 | -2.202016000 | -1.011969000 |
| 1 | -3.805021000 | -0.923084000 | -2.741796000 |
| 1 | -1.356740000 | -0.937822000 | -2.873536000 |
| 1 | -1.184278000 | -3.490027000 | 0.573790000 |
| 1 | -3.646126000 | -3.471119000 | 0.712113000 |
| 1 | -4.974715000 | -2.183426000 | -0.946581000 |
| n  | X            | Y            | Z             |
|----|--------------|--------------|---------------|
| 6  | 0.429000000 | -2.212892000 | -1.172940000  |
| 8  | 0.923136000 | -3.433218000 | -0.693812000  |
| 6  | 1.076306000 | -1.799422000 | -2.482846000  |
| 1  | 0.840647000 | -2.529707000 | -3.262542000  |
| 1  | 0.736459000 | -0.815998000 | -2.810431000  |
| 1  | 2.159662000 | -1.748948000 | -2.356936000  |
| 8  | 3.289413000 | -4.174706000 | -1.846374000  |
| 1  | 3.790021000 | -3.365930000 | -2.084132000  |
| 1  | 1.791014000 | -3.626369000 | -1.115370000  |
| 8  | 3.775297000 | -4.535102000 | -1.095833000  |
| 1  | 4.648118000 | -1.814135000 | -2.327516000  |
| 1  | 5.139616000 | -1.819444000 | -3.156606000  |
| 1  | 5.325512000 | -1.825563000 | -1.641231000  |

Coordinates (Angstroms)

| n  | X            | Y            | Z             |
|----|--------------|--------------|---------------|
| 44 | -1.285152000 | 0.127470000  | -0.574865000  |
| 7  | 0.265856000 | -1.308480000 | -0.498999000  |
| 7  | 0.465284000 | 1.283214000  | -0.295145000  |
| 8  | 3.352318000 | -0.401878900 | -0.289581000  |
| 8  | 4.026308000 | 3.245356000  | 0.322440000   |
| 6  | 0.063089000 | -2.629677000 | -0.627746000  |
| 1  | -0.959269000 | -2.945316000 | -0.797383000  |
| 6  | 1.084517000 | -3.549359000 | -0.560852000  |
| 1  | 0.886637000 | -4.608141000 | -0.672796000  |
| 6  | 2.390229000 | -3.089209000 | -0.349519000  |
| 6  | 2.607722000 | -1.716018000 | -0.219083000  |
| 1  | 3.601516000 | -1.321347000 | -0.058783000  |
| 6  | 1.518848000 | -0.857467000 | -0.303200000  |
| 6  | 4.702049000 | -3.590792000 | -0.101500000  |
| 1  | 5.023219000 | -2.942018000 | -0.921547000  |
| 1  | 5.300135000 | -4.500832000 | -0.098896000  |
| 1  | 4.816878000 | -3.073426000 | 0.855362000   |
| 6  | 1.635585000 | 0.613106000  | -0.186934000  |
| 6  | 2.831565000 | 1.274052000  | 0.013762000   |
| 1  | 3.771017000 | 0.744004000  | 0.102278000   |
| 6  | 2.835666000 | 2.670854000  | 0.111104000   |
| 6  | 1.626422000 | 3.358164000  | -0.018538000  |
| 1  | 1.557898000 | 4.436272000  | 0.037140000   |
| 6  | 0.475305000 | 2.618120000  | -0.221827000  |
| 1  | -0.481913000 | 3.113491000  | -0.333465000  |
| 6  | 4.075809000 | 4.666890000  | 0.455720000   |
| 1  | 3.726730000 | 5.156071000  | -0.457974000  |
|   | X               | Y               | Z               |
|---|-----------------|-----------------|-----------------|
| 1 | 5.123800000     | 4.908114000     | 0.625802000     |
| 1 | 3.478266000     | 4.996941000     | 1.310637000     |
| 6 | -2.398851000    | 1.282315000     | 0.938818000     |
| 1 | -1.992034000    | 2.136235000     | 1.471960000     |
| 6 | -3.037248000    | 1.502984000     | -0.314355000    |
| 1 | -3.126025000    | 2.509289000     | -0.706073000    |
| 6 | -3.487258000    | 0.402089000     | -1.081441000    |
| 6 | -3.275170000    | -0.909156000    | -0.578561000    |
| 1 | -3.551084000    | -1.769651000    | -1.176270000    |
| 6 | -2.638500000    | -1.098341000    | 0.676514000     |
| 1 | -2.429867000    | -2.113639000    | 0.996344000     |
| 6 | -2.231130000    | -0.010995000    | 1.492112000     |
| 6 | -1.609137000    | -0.202873000    | 2.858753000     |
| 6 | -0.539473000    | -1.296604000    | 2.896938000     |
| 6 | -2.720281000    | -0.474647000    | 3.880929000     |
| 1 | -1.128897000    | 0.746884000     | 3.119305000     |
| 1 | 0.283031000     | -1.071512000    | 2.212506000     |
| 1 | -0.128712000    | -1.375414000    | 3.907968000     |
| 1 | -0.948124000    | -2.277285000    | 2.631724000     |
| 1 | -3.469314000    | 0.322865000     | 3.874010000     |
| 1 | -3.226407000    | -1.420593000    | 3.657661000     |
| 1 | -2.301027000    | -0.544651000    | 4.889224000     |
| 6 | -4.098257000    | 0.610731000     | -2.432798000    |
| 1 | -5.182229000    | 0.718423000     | -2.324447000    |
| 1 | -3.712629000    | 1.518343000     | -2.901642000    |
| 1 | -3.907147000    | -0.243108000    | -3.086932000    |
| 8 | -0.742375000    | 0.260211000     | -2.559727000    |
| 1 | -1.554754000    | 0.128953000     | -3.057921000    |

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Coordinates (Angstroms)

| X            | Y            | Z            |
|--------------|--------------|--------------|
| -0.997818000 | -0.810484000 | -0.494369000 |
| -0.843058000 | 1.258172000  | -0.124402000 |
| 0.927488000  | -0.331077000 | -1.199159000 |
| -0.326947000 | 5.270278000  | 0.675510000  |
| 4.684295000  | 0.913722000  | -2.342436000 |
| -1.788073000 | 1.998811000  | 0.481995000  |
| -2.703228000 | 1.486807000  | 0.751813000  |
| -1.630989000 | 3.337257000  | 0.758026000  |
| -2.417887000 | 3.894918000  | 1.250663000  |
| -0.436128000 | 3.965711000  | 0.389612000  |
| 0.552209000  | 3.207156000  | -0.237925000 |
| 1.491849000  | 3.652970000  | -0.531720000 |
|   | x1   | y1   | z1   |
|---|------|------|------|
| 6 | 0.314807000 | 1.857183000 | -0.471914000 |
| 6 | 0.883860000 | 5.941953000 | 0.327341000 |
| 1 | 1.738381000 | 5.499520000 | 0.847899000 |
| 1 | 0.751986000 | 6.972843000 | 0.652059000 |
| 1 | 1.048489000 | 5.915492000 | -0.753963000 |
| 6 | 1.318236000 | 0.960892000 | -1.082157000 |
| 6 | 2.573187000 | 1.380285000 | -1.482692000 |
| 1 | 2.895813000 | 2.407690000 | -1.372350000 |
| 6 | 3.469286000 | 0.450000000 | -2.015942000 |
| 6 | 3.059576000 | -0.877826000 | -2.146751000 |
| 1 | 3.704887000 | -1.651706000 | -2.539695000 |
| 6 | 1.791935000 | -1.215776000 | -1.711292000 |
| 1 | 1.452898000 | -2.242466000 | -1.766374000 |
| 6 | 5.657029000 | -0.024541000 | -2.803489000 |
| 1 | 5.846017000 | -0.790860000 | -2.045158000 |
| 1 | 6.564960000 | 0.551175000 | -2.975977000 |
| 1 | 5.335970000 | -0.493450000 | -3.738125000 |
| 6 | -1.979712000 | -1.876981000 | -2.389787000 |
| 1 | -1.695917000 | -1.839902000 | -3.436372000 |
| 6 | -1.293461000 | -2.780529000 | -1.513083000 |
| 1 | -0.502858000 | -3.405697000 | -1.913871000 |
| 6 | -1.647341000 | -2.912745000 | -0.154762000 |
| 6 | -2.649858000 | -2.022010000 | 0.349143000 |
| 1 | -2.925812000 | -2.063839000 | 1.396042000 |
| 6 | -3.222940000 | -1.048845000 | -0.489822000 |
| 1 | -3.928838000 | -0.346522000 | -0.058511000 |
| 6 | -2.950229000 | -1.005260000 | -1.902600000 |
| 1 | -0.245771000 | -0.887073000 | 0.888428000 |
| 6 | -3.692244000 | -0.049573000 | -2.812236000 |
| 6 | -3.549530000 | 1.413352000 | -2.383762000 |
| 6 | -5.169543000 | -0.455322000 | -2.890899000 |
| 1 | -3.252524000 | -0.155596000 | -3.810099000 |
| 1 | -2.500273000 | 1.721678000 | -2.365060000 |
| 1 | -4.085351000 | 2.059382000 | -3.085855000 |
| 1 | -3.973893000 | 1.582129000 | -1.388438000 |
| 1 | -5.282530000 | -1.489026000 | -3.231265000 |
| 1 | -5.651628000 | -0.362635000 | -1.911353000 |
| 1 | -5.703793000 | 0.194955000 | -3.590266000 |
| 6 | -0.984308000 | -3.915946000 | 0.743767000 |
| 1 | -1.566781000 | -4.842828000 | 0.770196000 |
| 1 | 0.020053000 | -4.152197000 | 0.384241000 |
| 1 | -0.910091000 | -3.528592000 | 1.762854000 |
| 6 | 4.348103000 | -0.698941000 | 0.987374000 |
| 6 | 3.290276000 | -0.144808000 | 1.701096000 |
|        | X       | Y       | Z       |
|--------|---------|---------|---------|
| 6      | 2.280598 | -0.96948 | 2.211175|
| 6      | 2.328036 | -2.34884 | 1.969418|
| 6      | 3.375875 | -2.89637 | 1.241104|
| 6      | 4.392179 | -0.701886| 0.757817|
| 1      | 5.129108 | -0.055234| 0.595749|
| 1      | 3.262469 | 0.927395 | 1.862884|
| 1      | 1.536829 | -2.983901| 2.353139|
| 1      | 3.404427 | -3.964579| 1.052574|
| 6      | 5.213832 | -2.499353| 0.191723|
| 6      | 1.150575 | -0.417426| 3.004535|
| 8      | 0.391149 | -1.188743| 3.598149|
| 6      | 0.962686 | 1.068651 | 3.082846|
| 1      | 1.802417 | 1.511825 | 3.628677|
| 1      | 0.956070 | 1.514061 | 2.084668|
| 1      | 0.035711 | 1.305808 | 3.603994|
| 1      | -1.780052| -0.024037| 2.300960|
| 6      | -2.526677| -0.006924| 3.108829|
| 8      | -2.071487| -0.425393| 4.278626|
| 1      | -1.120511| -0.688855| 4.161201|
| 8      | -3.676504| 0.354416 | 2.945487|

**TS9-10**

Coordinates (Angstroms)

|        | X       | Y       | Z       |
|--------|---------|---------|---------|
| 44     | 0.803490| -0.620610| 0.635351|
| 7      | 1.040075| 1.277505 | -0.213757|
| 7      | -1.108634| 0.206429 | 0.782104|
| 8      | 1.366735| 5.046300 | -1.832468|
| 8      | -4.821403| 1.965786 | 0.611331|
| 6      | 2.207706| 1.757819 | -0.676702|
| 1      | 3.065242| 1.099862 | -0.604126|
| 6      | 2.331179| 3.014604 | -1.221368|
| 1      | 3.287230| 3.367770 | -1.587197|
| 6      | 1.196675| 3.832748 | -1.295289|
| 6      | -0.018024| 3.341970 | -0.812603|
| 1      | -0.917255| 3.940779 | -0.842329|
| 6      | -0.056092| 2.058955 | -0.283411|
| 6      | 0.237737| 5.916627 | -1.926251|
| 1      | -0.540954| 5.476261 | -2.555680|
| 1      | 0.609582| 6.829670 | -2.388157|
| 1      | -0.164594| 6.141327 | -0.934265|
| 6      | -1.288621| 1.435207 | 0.241766|
| 6      | -2.535759| 2.025096 | 0.183226|
| 1      | -2.688816| 2.993294 | -0.276483|
|   | x         | y         | z       |
|---|-----------|-----------|---------|
| 6 | -3.637903000 | 1.349667000 | 0.720194000 |
| 6 | -3.439186000 | 0.101330000 | 1.312871000 |
| 1 | -4.245379000 | -0.475649000 | 1.744588000 |
| 6 | -2.164257000 | -1.418544000 | 2.212291000 |
| 1 | -1.982860000 | 1.970461000 | 0.936433000 |
| 6 | -5.973915000 | 1.303482000 | 1.134717000 |
| 1 | -6.134439000 | 0.347069000 | 0.627790000 |
| 6 | -6.811344000 | 1.970461000 | 0.936433000 |
| 1 | -5.874357000 | 1.144977000 | 2.643050000 |
| 6 | 0.698164000 | -1.577350000 | 2.643050000 |
| 1 | -0.180993000 | -1.567702000 | 3.281585000 |
| 6 | 0.839839000 | -2.616417000 | 1.694253000 |
| 1 | 0.087487000 | -3.930640000 | 1.628715000 |
| 6 | 1.941546000 | -2.617741000 | 0.796515000 |
| 6 | 2.865046000 | -1.544724000 | 0.863535000 |
| 1 | 3.691908000 | -1.498163000 | 0.165012000 |
| 6 | 2.693593000 | -0.506765000 | 1.814077000 |
| 1 | 3.853866000 | 0.329133000 | 1.793268000 |
| 6 | 1.634216000 | -0.513969000 | 2.755425000 |
| 1 | 0.235942000 | -1.025050000 | -0.928901000 |
| 6 | 1.478777000 | 0.571764000 | 3.799444000 |
| 6 | 1.487862000 | 1.979147000 | 3.196240000 |
| 6 | 2.568622000 | 0.414202000 | 4.866923000 |
| 1 | 0.504836000 | 0.415356000 | 4.276255000 |
| 1 | 0.661640000 | 2.110816000 | 2.491743000 |
| 1 | 1.382407000 | 2.724286000 | 3.990518000 |
| 1 | 2.424174000 | 2.187580000 | 2.667641000 |
| 1 | 2.538905000 | -0.580650000 | 5.321255000 |
| 1 | 3.562034000 | 0.561883000 | 4.429018000 |
| 1 | 2.434165000 | 1.156461000 | 5.659554000 |
| 6 | 2.106548000 | -3.699437000 | -0.224785000 |
| 1 | 3.080940000 | -4.179082000 | -0.956520000 |
| 1 | 1.325883000 | -4.455789000 | -0.124789000 |
| 1 | 2.059759000 | -3.289938000 | -1.236394000 |
| 6 | -4.085726000 | -1.621497000 | -1.483677000 |
| 6 | -2.851236000 | -1.158816000 | -1.941126000 |
| 6 | -1.686566000 | -1.873262000 | -1.661588000 |
| 6 | -1.771158000 | -3.051412000 | -0.912665000 |
| 6 | -2.997786000 | -3.504111000 | -0.444411000 |
| 6 | -4.162455000 | -2.790186000 | -0.733779000 |
| 1 | -4.986183000 | -1.058898000 | -1.710481000 |
| 1 | -2.812149000 | -0.240898000 | -2.517796000 |
| 1 | -0.862364000 | -3.602372000 | -0.688372000 |
| 1 | -3.048636000 | -4.415017000 | 0.144060000 |
|   | X             | Y             | Z             |
|---|---------------|---------------|---------------|
| 1 | -5.122098000  | -3.143906000  | -0.369942000  |
| 6 | -0.331048000  | -1.439522000  | -2.182904000  |
| 8 | 0.408899000   | -2.390534000  | -2.634831000  |
| 6 | -0.258317000  | -0.102625000  | -2.899872000  |
| 1 | -0.717102000  | -0.229635000  | -3.886749000  |
| 1 | -0.786461000  | 0.692538000   | -2.374328000  |
| 1 | 0.781464000   | 0.194537000   | -3.043649000  |
| 1 | 2.547517000   | -0.836982000  | -1.756249000  |
| 6 | 3.224884000   | -1.081110000  | -2.591001000  |
| 8 | 2.679901000   | -1.825521000  | -3.523417000  |
| 1 | 1.706973000   | -2.043916000  | -3.222970000  |
| 8 | 4.379721000   | -0.688046000  | -2.627910000  |

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Coordinates (Angstroms)

|   | X             | Y             | Z             |
|---|---------------|---------------|---------------|
| 44| -1.102234000  | -0.843255000  | -0.417987000  |
| 7 | -1.246757000  | 1.177848000   | 0.125089000   |
| 7 | 0.675559000   | -0.017934000  | -1.177676000  |
| 8 | -1.367072000  | 5.141965000   | 1.181153000   |
| 8 | 4.293617000   | 1.743347000   | -1.983535000  |
| 6 | -2.306307000  | 1.711696000   | 0.760999000   |
| 1 | -3.118184000  | 1.036211000   | 0.999392000   |
| 6 | -2.357815000  | 3.035761000   | 1.123996000   |
| 1 | -3.222720000  | 3.435960000   | 1.637739000   |
| 6 | -1.269438000  | 3.863157000   | 0.815351000   |
| 6 | -0.165787000  | 3.311210000   | 0.155824000   |
| 1 | 0.690990000   | 3.917218000   | -0.103763000  |
| 6 | -0.190629000  | 1.965004000   | -0.167839000  |
| 6 | -0.275963000  | 6.023359000   | 0.901105000   |
| 1 | 0.636770000   | 5.677936000   | 1.394331000   |
| 1 | -0.569946000  | 6.989482000   | 1.307377000   |
| 1 | -0.113893000  | 6.109295000   | -0.176936000  |
| 6 | 0.924885000   | 1.274738000   | -0.852352000  |
| 6 | 2.136745000   | 1.868061000   | -1.127942000  |
| 1 | 2.349327000   | 2.890757000   | -0.844723000  |
| 6 | 3.131682000   | 1.122190000   | -1.777694000  |
| 6 | 2.853164000   | -0.194270000  | -2.150559000  |
| 1 | 3.574787000   | -0.821921000  | -2.654686000  |
| 6 | 1.623553000   | -0.722235000  | -1.809835000  |
| 1 | 1.390504000   | -1.753126000  | -2.045209000  |
| 6 | 5.338519000   | 1.028345000   | -2.649077000  |
| 1 | 5.614608000   | 0.130747000   | -2.088489000  |
| 1 | 6.182856000   | 1.714556000   | -2.685422000  |
|   | 5.036008000 | 0.760881000 | -3.665468000 |
|---|-------------|-------------|---------------|
| 6 | -1.490549000 | -2.135392000 | -2.128402000  |
| 1 | -0.902239000 | -2.124760000 | -3.040201000  |
| 6 | -1.104650000 | -2.986667000 | -1.069573000  |
| 1 | -0.225714000 | -3.611773000 | -1.174616000  |
| 6 | -1.752679000 | -2.891645000 | 0.187032000   |
| 6 | -2.873993000 | -2.016628000 | 0.321272000   |
| 1 | -3.341282000 | -1.890450000 | 1.290779000   |
| 6 | -3.263534000 | -1.191265000 | -0.744993000  |
| 6 | -0.407225000 | -0.459628000 | -1.194170000  |
| 6 | -2.558830000 | -1.199147000 | -1.988964000  |
| 1 | 0.562429000  | -0.726536000 | 1.597504000   |
| 6 | -2.960114000 | -0.307549000 | -3.141576000  |
| 6 | -3.174685000 | 1.153153000  | -2.741574000  |
| 6 | -4.217669000 | -0.904742000 | -3.788641000  |
| 1 | -2.144288000 | -0.345603000 | -3.871359000  |
| 1 | -2.256391000 | 1.596749000  | -2.346796000  |
| 1 | -3.480243000 | 1.727412000  | -3.620933000  |
| 1 | -3.960661000 | 1.260225000  | -1.986843000  |
| 1 | -4.054107000 | -1.943991000 | -4.089129000  |
| 6 | -5.060702000 | -0.877457000 | -3.089726000  |
| 6 | -4.492541000 | -0.329641000 | -4.677448000  |
| 6 | -1.234778000 | -3.625922000 | 1.383745000   |
| 1 | -1.979985000 | -4.358630000 | 1.708301000   |
| 1 | -0.303219000 | -4.146313000 | 1.156728000   |
| 1 | -1.064584000 | -2.936635000 | 2.215543000   |
| 6 | 4.868893000  | -0.601354000 | 0.650256000   |
| 6 | 3.745934000  | -0.186278000 | 1.367457000   |
| 6 | 2.651538000  | -1.035263000 | 1.530142000   |
| 6 | 2.699245000  | -2.308559000 | 0.948457000   |
| 6 | 3.818364000  | -2.728105000 | 0.238024000   |
| 6 | 4.911299000  | -1.873150000 | 0.088434000   |
| 1 | 5.708473000  | 0.076818000  | 0.529801000   |
| 1 | 3.733928000  | 0.809751000  | 1.797260000   |
| 1 | 1.845574000  | -2.973772000 | 1.054161000   |
| 1 | 3.836973000  | -3.718848000 | -0.205679000  |
| 1 | 5.785728000  | -2.195993000 | -0.468280000  |
| 6 | 1.405472000  | -0.642243000 | 2.302651000   |
| 8 | 1.210384000  | -1.590509000 | 3.341249000   |
| 6 | 1.404399000  | 0.779417000  | 2.849191000   |
| 1 | 2.205914000  | 0.915358000  | 3.582187000   |
| 1 | 1.528255000  | 1.521065000  | 2.054235000   |
| 1 | 0.449500000  | 0.973482000  | 3.346189000   |
| 1 | -1.450059000 | -0.327610000 | 2.367690000   |
11

Coordinates (Angstroms)

|   |   |   |   |
|---|---|---|---|
|   |   |   |   |
| 44 | -0.823883000 | -1.621671000 | 0.165325000 |
| 7  | 0.497668000  | -0.065299000 | 1.011387000 |
| 7  | -0.280549000 | 1.310369000  | -1.757811000 |
| 8  | 3.832395000  | 2.196530000  | 1.987601000  |
| 8  | -3.082477000 | 4.051012000  | -0.394563000 |
| 6  | 1.415301000  | -0.457487000 | 1.925521000  |
| 1  | 1.253246000  | -1.427916000 | 2.375224000  |
| 6  | 2.516983000  | 0.286211000  | 2.281340000  |
| 1  | 3.229447000  | -0.095458000 | 3.002353000  |
| 6  | 2.714816000  | 1.528569000  | 1.671866000  |
| 6  | 1.738340000  | 1.983845000  | 0.786585000  |
| 1  | 1.809810000  | 2.948574000  | 0.301799000  |
| 6  | 0.660691000  | 1.161663000  | 0.478666000  |
| 6  | 4.079581000  | 3.436080000  | 1.323089000  |
| 1  | 4.126357000  | 3.291804000  | 0.239486000  |
| 1  | 5.045559000  | 3.781165000  | 1.688765000  |
| 1  | 3.309544000  | 4.172077000  | 1.571590000  |
| 6  | -0.353301000 | 1.704794000  | -0.477480000 |
| 6  | -1.265476000 | 2.635737000  | -0.007680000 |
| 1  | -1.268414000 | 2.943817000  | 1.031813000  |
| 6  | -2.203417000 | 3.166116000  | -0.900464000 |
| 6  | -2.167869000 | 2.741479000  | -2.229905000 |
| 1  | -2.863950000 | 3.104473000  | -2.975056000 |
| 6  | -1.186806000 | 1.824969000  | -2.591971000 |
| 1  | -1.128670000 | 1.492133000  | -3.624876000 |
| 6  | -4.062706000 | 4.593834000  | -1.276700000 |
| 1  | -3.591041000 | 5.153045000  | -2.090365000 |
| 1  | -4.666396000 | 5.267848000  | -0.670353000 |
| 1  | -4.699844000 | 3.804644000  | -1.687698000 |
| 6  | -2.870840000 | -0.445467000 | -0.434351000 |
| 1  | -3.080787000 | 0.602145000  | -0.617093000 |
| 6  | -2.590837000 | -1.287631000 | -1.488213000 |
| 1  | -2.565099000 | -0.904695000 | -2.502910000 |
| 6  | -2.225698000 | -2.661316000 | -1.240477000 |
| 6  | -2.364668000 | -3.184823000 | 0.061841000  |
| 1  | -2.179343000 | -4.236982000 | 0.243598000  |
### Coordinates (Angstroms)

|   |     X     |     Y     |     Z     |
|---|----------|----------|----------|
| 6 | -2.61772300 | -2.30394600 | 1.15629600 |
| 1 | -2.64124000 | -2.69981400 | 2.16384000 |
| 6 | -2.75794200 | -0.91072100 | 0.92673900 |
| 6 | -3.00187100 | 0.07292600  | 2.05297100 |
| 6 | -2.31190700 | -0.30475500 | 3.36286700 |
| 6 | -4.51253100 | 0.24918100  | 4.08353500 |
| 1 | -2.59087200 | 1.03128700  | 1.71710900 |
| 1 | -1.24477900 | -0.49370400 | 3.21058200 |
| 1 | -2.41574200 | 0.51155400  | 4.08353500 |
| 1 | -2.75830700 | -1.19681300 | 3.81471800 |
| 1 | -5.00147700 | 0.56703300  | 1.32405900 |
| 1 | -4.97111100 | -0.69197900 | 2.57362200 |
| 1 | -4.71132100 | 1.00590900  | 3.01550000 |
| 6 | -1.81279900 | -3.53894900 | -2.38633100 |
| 1 | -2.69584900 | -3.85584000 | -2.95124500 |
| 1 | -1.15355500 | -2.97014000 | -3.06869500 |
| 1 | -1.29456400 | -4.43095000 | -2.02798300 |
| 6 |  4.02702400 |  1.02508100 | -1.72852200 |
| 6 |  3.02951500 |  0.06157400 | -1.65794400 |
| 6 |  3.25845500 | -1.14050600 | -0.97633100 |
| 6 |  4.50176100 | -1.36687400 | -0.36906600 |
| 6 |  5.49036700 | -0.39237900 | -0.42647700 |
| 6 |  5.25380500 |  0.80336700 | -1.10432300 |
| 1 |  3.84275700 |  1.95812300 | -2.25085200 |
| 1 |  2.05467800 |  0.24402800 | -2.09745200 |
| 1 |  4.69312100 | -2.29039800 |  0.16663300 |
| 1 |  6.44528700 | -0.56273200 |  0.05914600 |
| 1 |  6.02647400 |  1.56465000 | -1.14299400 |
| 6 |  2.13280400 | -2.08598600 | -0.79851200 |
| 8 |  1.00559300 | -1.75144300 | -1.18904500 |
| 6 |  2.35256900 | -3.39579100 | -0.10974800 |
| 1 |  3.20667400 | -3.92013500 | -0.54663400 |
| 1 |  2.57557200 | -3.21984200 |  0.94794700 |
| 1 |  1.45155100 | -4.00394900 | -0.18796800 |
| 1 | -0.05448900 | -2.53962000 |  1.18863000 |

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**TS11-12**

Coordinates (Angstroms)

|   |     X     |     Y     |     Z     |
|---|----------|----------|----------|
| 44|  0.00482200 | -1.51987800 |  0.10407100 |
| 7 |  0.62157600 |  0.53768600 |  0.42976400 |
| 7 | -1.16763500 |  0.87078000 | -2.10613900 |
| 8 |  2.39434600 |  4.22857200 |  1.05267000 |
| 8 | -4.57228000 |  2.60968500 | -0.48715900 |
| x   | y         | z         |
|-----|-----------|-----------|
| 6   | 1.654224000 | 0.728948000 | 1.281910000 |
| 1   | 2.029277000 | -0.154121000 | 1.781730000 |
| 6   | 2.238797000 | 1.948069000 | 1.525575000 |
| 1   | 3.073003000 | 2.030230000 | 2.211163000 |
| 6   | 1.761735000 | 3.067912000 | 0.839101000 |
| 6   | 0.657722000 | 2.901736000 | 0.002182000 |
| 1   | 0.203748000 | 3.735657000 | -0.517230000 |
| 6   | 0.107016000 | 1.634841000 | 0.012585000 |
| 1   | 0.947557000 | 5.642651000 | 0.539759000 |
| 1   | -0.811631000 | -0.180165000 | 3.782622000 |
| 6   | -0.771950000 | 0.721353000 | 2.080091000 |
| 1   | -1.593441000 | -1.337868000 | 1.662054000 |
| 6   | -1.797098000 | -0.210030000 | 2.652020000 |
| 6   | -0.724912000 | -0.288674000 | 3.209350000 |
| 1   | -0.287622000 | -0.517230000 | 3.403901000 |
| 1   | 0.015254000 | -4.325610000 | 1.131743000 |
| 6   | -0.811631000 | -2.479881000 | 1.933336000 |
| 1   | -0.287622000 | -2.578120000 | 2.875256000 |
| 6   | -1.593441000 | -1.337868000 | 1.662054000 |
| 6   | -1.797098000 | -0.210030000 | 2.652020000 |
| 6   | -0.771950000 | 0.721353000 | 2.080091000 |
| 1   | -3.224912000 | -0.288674000 | 3.209350000 |
| 1   | -3.727330000 | -1.225755000 | 3.756865000 |
| 1   | -3.404968000 | 0.541329000 | 3.898899000 |
|   | X             | Y             | Z             |
|---|---------------|---------------|---------------|
| 6 | -1.064056000  | -4.399872000  | -1.401980000  |
| 1 | -2.007924000  | -4.923535000  | -1.582914000  |
| 1 | -0.759387000  | -3.924820000  | -2.338370000  |
| 1 | -0.311627000  | -5.136354000  | -1.114755000  |
| 6 | 4.057738000   | 1.339734000   | -1.483185000  |
| 6 | 3.080601000   | 0.360971000   | -1.630735000  |
| 6 | 3.136196000   | -0.810044000  | -0.871909000  |
| 6 | 4.185500000   | -0.995394000  | 0.031840000   |
| 6 | 5.160188000   | -0.014405000  | 0.181715000   |
| 6 | 5.097848000   | 1.155257000   | -0.574271000  |
| 1 | 4.003100000   | 2.249541000   | -2.072560000  |
| 1 | 2.260520000   | 0.503187000   | -2.325167000  |
| 1 | 4.228188000   | -1.890947000  | 0.644188000   |
| 1 | 5.964913000   | -0.158928000  | 0.895407000   |
| 1 | 5.856766000   | 1.921838000   | -0.453353000  |
| 6 | 2.056334000   | -1.847449000  | -1.054621000  |
| 8 | 1.040883000   | -1.515622000  | -1.781500000  |
| 6 | 2.492435000   | -3.298816000  | -1.057258000  |
| 1 | 3.135732000   | -3.444139000  | -1.932118000  |
| 1 | 3.060611000   | -3.568923000  | -0.166473000  |
| 1 | 1.623284000   | -3.950254000  | -1.140640000  |
| 1 | 1.534646000   | -1.827836000  | 0.552494000   |

**12**

Coordinates (Angstroms)

|   | X             | Y             | Z             |
|---|---------------|---------------|---------------|
| 44| 1.413912000   | 0.618760000   | -0.107357000  |
| 7 | 0.116006000   | -0.811287000  | -0.932039000  |
| 7 | -0.463296000  | 1.574210000   | -0.086404000  |
| 8 | -2.567685000  | -3.592476000  | -2.334673000  |
| 8 | -4.238695000  | 3.194059000   | -0.229630000  |
| 6 | 0.487440000   | -2.064706000  | -1.239966000  |
| 1 | 1.527337000   | -2.314692000  | -1.065953000  |
| 6 | -0.393813000  | -3.000781000  | -1.731139000  |
| 1 | -0.065815000  | -4.009696000  | -1.948299000  |
| 6 | -1.732695000  | -2.635236000  | -1.910722000  |
| 6 | -2.117445000  | -1.324650000  | -1.622737000  |
| 1 | -3.142732000  | -1.005058000  | -1.743400000  |
| 6 | -1.168480000  | -0.448317000  | -1.119531000  |
| 6 | -3.957834000  | -3.281432000  | -2.441035000  |
| 1 | -4.356768000  | -2.951086000  | -1.477067000  |
| 1 | -4.444056000  | -4.208289000  | -2.741180000  |
| 1 | -4.129868000  | -2.514785000  | -3.202309000  |
|   | x       | y       | z       |
|---|---------|---------|---------|
| 6 | -1.494448000 | 0.919046000 | -0.664917000 |
| 6 | -2.757781000 | 1.471860000 | -0.138718000 |
| 1 | -3.585144000 | 0.955298000 | 0.513971000  |
| 6 | -2.989776000 | 2.718475000 | 0.507402000  |
| 6 | -1.935148000 | 3.613630000 | 0.102798000  |
| 1 | -2.051100000 | 4.312543000 | 1.463005000  |
| 6 | -0.694947000 | 2.748313000 | 0.507402000  |
| 1 | 0.1499939000 | 3.210796000 | 1.022794000  |
| 6 | -4.526525000 | 4.451314000 | 0.384397000  |
| 1 | -3.924164000 | 5.248291000 | -0.061097000 |
| 6 | 2.982519000  | 0.183169000 | -1.601134000 |
| 1 | 2.914723000  | -0.612576000 | -2.336946000 |
| 6 | 2.465343000  | 1.458949000 | -1.928318000 |
| 1 | 2.027510000  | 1.635081000 | -2.903693000 |
| 6 | 2.438103000  | 2.476551000 | -0.943714000 |
| 6 | 2.963664000  | 2.196766000 | 0.350679000  |
| 1 | 2.909500000  | 2.950188000 | 1.126935000  |
| 6 | 3.511722000  | 0.926394000 | 0.636555000  |
| 1 | 3.840752000  | 0.725151000 | 1.649830000  |
| 6 | 3.555366000  | -0.107900000 | -0.332107000 |
| 6 | 4.234084000  | -1.439336000 | -0.093427000 |
| 6 | 4.007901000  | -2.013269000 | 1.303768000  |
| 6 | 5.731965000  | -1.283693000 | -0.391452000 |
| 1 | 3.815512000  | -0.813524000 | -0.822417000 |
| 1 | 2.944337000  | -2.160280000 | 1.503173000  |
| 1 | 4.505988000  | -2.983564000 | 1.388414000  |
| 1 | 4.421322000  | -1.364730000 | 2.082909000  |
| 1 | 5.898343000  | -0.905854000 | -1.405250000 |
| 1 | 6.191150000  | -0.581814000 | 0.313789000  |
| 1 | 6.241729000  | -2.247097000 | -0.295041000 |
| 6 | 1.852478000  | 3.817715000 | -1.264070000 |
| 1 | 2.589235000  | 4.395466000 | -1.831643000 |
| 1 | 0.955998000  | 3.719640000 | -1.880213000 |
| 1 | 1.608775000  | 4.376433000 | -0.359140000 |
| 6 | -3.343235000 | -0.639931000 | 1.982796000  |
| 6 | -1.972989000 | -0.450300000 | 2.147169000  |
| 6 | -1.075099000 | -1.492838000 | 1.910011000  |
| 6 | -1.582462000 | -2.739426000 | 1.533658000  |
| 6 | -2.951134000 | -2.935981000 | 1.369059000  |
| 6 | -3.837814000 | -1.881520000 | 1.586053000  |
| 1 | -4.026361000 | 0.187381000 | 2.153163000  |
| 1 | -1.590108000 | 0.525441000 | 2.430998000  |
|   | X               | Y               | Z               |
|---|-----------------|-----------------|-----------------|
| 44| -0.229248000    | -1.189620000    | -0.411194000    |
| 7 | 1.230401000     | 0.051953000     | -1.223151000    |
| 7 | -0.867756000    | 0.643334000     | 0.207901000     |
| 8 | 4.167775000     | 2.656595000     | -2.438237000    |
| 8 | -1.815071000    | 4.488042000     | 1.339625000     |
| 6 | 2.320970000     | -0.367055000    | -1.884729000    |
| 1 | 2.390784000     | -1.432763000    | -2.067928000    |
| 6 | 3.307832000     | 0.493443000     | -2.307833000    |
| 1 | 4.180031000     | 0.123524000     | -2.832145000    |
| 6 | 3.173042000     | 1.859553000     | -2.030053000    |
| 6 | 2.034946000     | 2.302581000     | -1.350441000    |
| 1 | 1.895424000     | 3.348554000     | -1.116174000    |
| 6 | 1.087597000     | 1.366359000     | -0.962140000    |
| 6 | 4.087518000     | 4.051253000     | -2.138760000    |
| 1 | 3.217085000     | 4.503818000     | -2.622424000    |
| 1 | 4.999035000     | 4.491400000     | -2.539695000    |
| 1 | 4.044778000     | 4.213799000     | -1.057762000    |
| 6 | -0.121680000    | 1.709406000     | -0.183521000    |
| 6 | -0.451916000    | 2.997176000     | 0.184946000     |
| 1 | 0.135161000     | 3.847648000     | -0.136885000    |
| 6 | -1.553799000    | 3.213743000     | 1.020906000     |
| 6 | -2.275369000    | 2.108727000     | 1.475702000     |
| 1 | -3.115387000    | 2.196307000     | 2.151677000     |
| 6 | -1.892650000    | 0.852166000     | 1.041580000     |
| 1 | -2.420048000    | -0.030345000    | 1.377175000     |
| 6 | -2.922401000    | 4.752445000     | 2.202300000     |
| 1 | -3.856469000    | 4.403560000     | 1.752777000     |
| 1 | -2.952890000    | 5.834415000     | 2.320566000     |
| 1 | -2.775793000    | 4.280578000     | 3.178389000     |
| 6 | 3.495323000     | -0.991806000    | 1.073434000     |

Coordinates (Angstroms)
|   | 4.388774000 | -1.219761000 | 0.497505000 |
|---|-------------|--------------|--------------|
| 6 | 3.259582000 | 0.319987000  | 1.479309000  |
| 1 | 3.974034000 | 1.096256000  | 1.216563000  |
| 6 | 2.107586000 | 0.659707000  | 2.192182000  |
| 6 | 1.208583000 | -0.364821000 | 2.502478000  |
| 1 | 0.298924000 | -0.131109000 | 3.050175000  |
| 6 | 1.453749000 | -1.680651000 | 2.114709000  |
| 1 | 0.737617000 | -2.453938000 | 2.381834000  |
| 6 | 2.590736000 | -2.013921000 | 1.367120000  |
| 1 | -0.828230000| -0.921581000 | -1.814783000 |
| 6 | 2.817976000 | -3.429938000 | 0.869106000  |
| 6 | 1.677955000 | -3.892655000 | -0.049121000 |
| 6 | 3.006750000 | -4.416201000 | 2.027681000  |
| 1 | 3.741964000 | -3.420301000 | 0.278500000  |
| 1 | 1.513082000 | -3.179686000 | -0.868144000 |
| 1 | 1.906501000 | -4.866843000 | -0.493530000 |
| 1 | 0.739881000  | -3.990528000 | 0.507081000  |
| 1 | 3.842956000  | -4.122570000 | 2.669639000  |
| 1 | 2.104467000  | -4.465877000 | 2.647569000  |
| 1 | 3.205340000  | -5.422966000 | 1.646027000  |
| 6 | 1.842512000  | 2.081798000  | 2.611564000  |
| 1 | 2.145092000  | 2.785611000  | 1.829892000  |
| 1 | 0.780620000  | 2.239680000  | 2.820761000  |
| 1 | 2.402713000  | 2.338028000  | 3.518116000  |
| 6 | -4.770318000 | 0.061762000  | -2.062623000 |
| 6 | -3.605640000 | -0.690513000 | -1.953096000 |
| 6 | -3.332633000 | -1.407702000 | -0.784807000 |
| 6 | -4.258885000 | -1.379716000 | 0.260420000  |
| 6 | -5.428271000 | -0.630934000 | 0.149870000  |
| 6 | -5.684808000 | 0.095690000  | -1.009778000 |
| 1 | -4.964251000 | 0.624066000  | -2.970753000 |
| 1 | -2.889270000 | -0.703589000 | -2.769941000 |
| 1 | -4.053678000 | -1.938780000 | 1.168026000  |
| 1 | -6.138624000 | -0.615595000 | 0.970600000  |
| 1 | -6.593319000 | 0.683372000  | -1.095993000 |
| 6 | -2.080228000 | -2.229730000 | -0.632179000 |
| 8 | -1.625067000 | -2.429083000 | 0.575875000  |
| 6 | -1.890221000 | -3.340294000 | -1.647048000 |
| 1 | -2.620028000 | -4.134459000 | -1.447682000 |
| 1 | -2.046050000 | -2.980469000 | -2.666344000 |
| 1 | -0.885782000 | -3.766741000 | -1.564563000 |

**TS13-12**

Coordinates (Angstroms)
|   | X               | Y               | Z               |
|---|-----------------|-----------------|-----------------|
| 44| 0.370179000     | -1.187372000    | -0.190975000    |
| 7 | 1.205148000     | 0.570021000     | -0.963542000    |
| 7 | -0.962739000    | 0.222515000     | 0.416321000     |
| 8 | 2.763532000     | 4.182415000     | -2.192041000    |
| 8 | -3.625769000    | 3.231954000     | 1.292868000     |
| 6 | 2.377386000     | 0.660198000     | -1.613060000    |
| 1 | 2.898709000     | -0.273729000    | -1.786882000    |
| 6 | 2.961655000     | 1.857911000     | -2.039900000    |
| 1 | 3.856473000     | 1.890538000     | -2.558148000    |
| 6 | 2.200035000     | 3.037689000     | -1.778088000    |
| 6 | 0.975390000     | 2.954031000     | -1.113549000    |
| 1 | 0.394979000     | 3.839021000     | -0.892576000    |
| 6 | 0.513145000     | 1.702624000     | -0.727598000    |
| 6 | 2.082932000     | 5.408181000     | -1.923927000    |
| 1 | 1.112379000     | 5.434677000     | -2.428034000    |
| 1 | 2.723367000     | 6.192909000     | -2.323864000    |
| 1 | 1.950337000     | 5.557440000     | -0.847938000    |
| 6 | -0.750731000    | 1.498548000     | 0.007976000     |
| 6 | -1.645780000    | 2.507800000     | 0.305124000     |
| 1 | -1.487144000    | 3.523748000     | -0.033438000    |
| 6 | -2.784450000    | 2.214212000     | 1.063427000     |
| 6 | -2.962139000    | 0.911163000     | 1.535011000     |
| 1 | -3.802429000    | 0.620606000     | 2.151172000     |
| 6 | -2.022981000    | -0.042355000    | 1.188189000     |
| 1 | -2.120587000    | -1.065145000    | 1.527410000     |
| 6 | -4.815438000    | 2.961859000     | 2.035132000     |
| 1 | -5.420926000    | 2.200637000     | 1.534403000     |
| 1 | -5.362000000    | 3.903082000     | 2.067774000     |
| 1 | -4.575044000    | 2.641870000     | 3.053238000     |
| 6 | 3.701265000     | 0.081674000     | 1.128776000     |
| 1 | 4.644232000     | 0.308405000     | 0.638354000     |
| 6 | 2.966808000     | 1.118811000     | 1.714890000     |
| 1 | 3.355798000     | 2.132985000     | 1.673420000     |
| 6 | 1.733949000     | 0.882397000     | 2.311312000     |
| 6 | 1.265630000     | -0.442815000    | 2.338784000     |
| 1 | 0.332201000     | -0.667142000    | 2.847736000     |
| 6 | 2.002459000     | -1.484433000    | 1.768690000     |
| 1 | 1.663543000     | -2.508768000    | 1.897432000     |
| 6 | 3.229252000     | -1.224746000    | 1.123051000     |
| 1 | -0.539633000    | -1.486677000    | -1.543947000    |
| 6 | 3.981053000     | -2.337333000    | 0.420736000     |
| 6 | 3.062942000     | -3.133714000    | -0.517147000    |
| 6 | 4.666520000     | -3.268131000    | 1.428521000     |
| ID | X       | Y       | Z       |
|----|---------|---------|---------|
| 1  | 4.759258| -1.863947| -0.189601 |
| 1  | 2.500429| -2.467349| -1.187179 |
| 1  | 3.648529| -3.817027| -1.140086 |
| 1  | 2.339917| -3.732985| 0.046269  |
| 1  | 5.361241| -2.714873| 2.067724  |
| 1  | 3.925116| -3.753862| 2.072802  |
| 6  | 0.916858| 1.994503 | 2.913173  |
| 1  | 1.182128| 2.156607 | 3.964015  |
| 1  | 1.080716| 2.936459 | 2.381892  |
| 1  | -0.15199| 1.761843 | 2.877402  |
| 1  | 1.182128| 2.156607 | 3.964015  |
| 14 | -4.304565| -0.548530| -1.811621 |
| 1  | -0.300431| -1.037933| -1.882453 |
| 6  | -2.596577| -2.083723| -1.052231 |
| 6  | -3.515503| -2.657406| -0.174016 |
| 6  | -4.820236| -2.172782| -0.106590 |
| 6  | -5.214887| -1.111078| -0.916993 |
|   |   x         |   y         |   z         |
|---|------------|------------|------------|
| 6 | 1.814958000 | -0.264755000 | -0.611840000 |
| 6 | 5.627044000 | -1.798478000 | -1.482929000 |
| 1 | 5.668551000 | -0.850502000 | 0.156967000  |
| 6 | 2.165766000 | 3.141818000 | 1.002051000  |
| 6 | 0.817297000 | 3.378475000 | 1.278532000  |
| 1 | 0.470137000 | 4.280769000 | 1.764088000  |
| 6 | -0.103260000 | 2.413918000 | 0.911639000  |
| 1 | -1.158552000 | 2.562818000 | 1.106129000  |
| 6 | 2.848788000 | 5.207993000 | 1.951823000  |
| 1 | 3.800468000 | 5.714835000 | 2.103434000  |
| 1 | 2.372219000 | 5.022200000 | 2.918832000  |
| 6 | -2.000525000 | -0.498759000 | 1.957050000  |
| 1 | -1.633520000 | -0.031670000 | 2.865275000  |
| 6 | -2.888204000 | 0.241204000 | 1.114935000  |
| 1 | -3.194138000 | 1.239777000 | 1.407305000  |
| 6 | -3.380448000 | -0.310170000 | -0.085866000 |
| 6 | -2.899985000 | -1.599410000 | -0.478080000 |
| 1 | -3.221479000 | -2.034214000 | -1.416948000 |
| 6 | -1.972108000 | -2.281008000 | 0.332094000  |
| 1 | -1.577936000 | -3.228690000 | -0.020119000 |
| 6 | -1.544652000 | -1.773603000 | 1.603913000  |
| 1 | -1.190437000 | 0.389053000 | -1.641019000 |
| 6 | -0.647155000 | -2.579157000 | 2.518823000  |
| 6 | 0.642821000 | -3.049310000 | 1.841910000  |
| 6 | -1.438747000 | -3.764173000 | 3.086777000  |
| 1 | -0.371035000 | -1.921459000 | 3.350485000  |
| 1 | 1.242546000 | -2.202292000 | 1.496559000  |
| 1 | 1.243642000 | -3.625722000 | 2.552025000  |
| 1 | 0.437480000 | -3.696552000 | 0.982824000  |
| 1 | -2.346691000 | -3.426770000 | 3.595628000  |
| 1 | -1.731509000 | -4.454285000 | 2.287597000  |
| 1 | -0.828469000 | -4.320187000 | 3.804769000  |
| 6 | -4.377036000 | 0.420584000 | -0.934482000 |
| 1 | -5.380016000 | 0.037358000 | -0.720530000 |
| 1 | -4.367413000 | 1.491451000 | -0.722872000 |
| 1 | -4.175979000 | 0.263949000 | -1.996191000 |
| 8 | -2.126657000 | 2.749540000 | -1.636226000 |
| 1 | -2.556490000 | 3.047273000 | -0.819075000 |
|    | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 44 | -1.161821 | -0.205691 | -0.13091  |
| 7  | 0.599735  | -1.079830 | -0.847160 |
| 7  | 0.293123  | 1.249422  | 0.259078  |
| 8  | 4.163474  | -2.863598 | -1.853670 |
| 8  | 3.390194  | 3.849133  | 0.996234  |
| 6  | 0.650696  | -2.300948 | -1.407110 |
| 1  | -0.298421 | -2.794014 | -1.576136 |
| 6  | 1.835522  | -2.906703 | -1.753977 |
| 1  | 1.841543  | -3.894419 | -2.197521 |
| 6  | 3.037045  | -2.226857 | -1.518001 |
| 6  | 2.986533  | -0.947148 | -0.960140 |
| 1  | 3.889453  | -0.384288 | -0.769367 |
| 6  | 1.749514  | -0.407683 | -0.639745 |
| 6  | 5.413010  | -2.210516 | -1.619136 |
| 1  | 5.479963  | -1.281042 | -2.191650 |
| 1  | 6.175005  | -2.908308 | -1.962204 |
| 1  | 5.551355  | -2.008550 | -0.553026 |
| 6  | 1.575814  | 0.929949  | -0.038727 |
| 6  | 2.613536  | 1.805931  | 0.205472  |
| 1  | 3.639153  | 1.557224  | -0.036222 |
| 6  | 2.338341  | 3.053046  | 0.780856  |
| 6  | 1.012558  | 3.377200  | 1.081651  |
| 1  | 0.728056  | 4.322557  | 1.523297  |
| 6  | 0.030839  | 2.446505  | 0.796713  |
| 1  | -1.009882 | 2.661926  | 1.007270  |
| 6  | 3.161837  | 5.125177  | 1.598510  |
| 1  | 2.525479  | 5.746653  | 0.961852  |
| 1  | 4.144421  | 5.583874  | 1.695970  |
| 1  | 2.708854  | 5.010680  | 2.587322  |
| 6  | -2.056128 | -0.074386 | 1.948507  |
| 1  | -1.686253 | 0.572391  | 2.737702  |
| 6  | -3.004775 | 0.441329  | 1.028575  |
| 1  | -3.365636 | 1.457355  | 1.138535  |
| 6  | -3.448546 | -0.347544 | -0.058207 |
| 6  | -2.907802 | -1.656368 | -0.216987 |
|   | X               | Y               | Z               |
|---|----------------|----------------|----------------|
| 1 | -3.197602000   | -2.260181000   | -1.068389000   |
| 6 | -1.953292000   | -2.141450000   | 0.697057000    |
| 1 | -1.506586000   | -3.113915000   | 0.515295000    |
| 6 | -1.516681000   | -1.373092000   | 1.816162000    |
| 1 | -1.174092000   | 0.329455000    | -1.739526000   |
| 6 | -0.553736000   | -1.937826000   | 2.839262000    |
| 6 | 0.755489000    | -2.440583000   | 2.226433000    |
| 6 | -1.261711000   | -3.046265000   | 3.629011000    |
| 1 | -0.312972000   | -1.123939000   | 3.531273000    |
| 1 | 1.311969000    | -1.623479000   | 1.759505000    |
| 1 | 1.384850000    | -2.875005000   | 3.008718000    |
| 1 | 0.581417000    | -3.213819000   | 1.470542000    |
| 1 | -2.184624000   | -2.679510000   | 4.088193000    |
| 1 | -1.515387000   | -3.887937000   | 2.975147000    |
| 1 | -0.608372000   | -3.419758000   | 4.422974000    |
| 6 | -4.429230000   | 0.197049000    | -1.048876000   |
| 1 | -5.443501000   | -0.051478000   | -0.720315000   |
| 1 | -4.348516000   | 1.282391000    | -1.122351000   |
| 1 | -4.272323000   | -0.245080000   | -2.034992000   |
| 8 | -1.973058000   | 2.477909000    | -1.796572000   |
| 1 | -2.454006000   | 2.685646000    | -0.983786000   |
| 1 | -2.664161000   | 2.404340000    | -2.512533000   |
| 1 | -1.516013000   | 1.191102000    | -1.576907000   |
| 8 | -3.719448000   | 2.281387000    | -3.779551000   |
| 1 | -4.223205000   | 3.103372000    | -3.799784000   |
| 1 | -4.372139000   | 1.607479000    | -3.557603000   |

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15

Coordinates (Angstroms)

|   | X               | Y               | Z               |
|---|----------------|----------------|----------------|
| 44| -1.199237000   | -0.215934000   | -0.148469000   |
| 7 | 0.538645000    | -1.204895000   | -0.738630000   |
| 7 | 0.254391000    | 1.278310000    | -0.074994000   |
| 8 | 4.062475000    | -3.190308000   | -1.432333000   |
| 8 | 3.373034000    | 3.912015000    | 0.352725000    |
| 6 | 0.561915000    | -2.497510000   | -1.108988000   |
| 1 | -0.398436000   | -2.987390000   | -1.211035000   |
| 6 | 1.736055000    | -3.171879000   | -1.344719000   |
| 1 | 1.724603000    | -4.214106000   | -1.637821000   |
| 6 | 2.951067000    | -2.488724000   | -1.199249000   |
| 6 | 2.926748000    | -1.138713000   | -0.834341000   |
| 1 | 3.840387000    | -0.571692000   | -0.723977000   |
| 6 | 1.700481000    | -0.531699000   | -0.614838000   |
| 6 | 5.236428000    | -2.530342000   | -1.322567000   |
| I  |       X       |       Y       |       Z       |
| ---|---------------|---------------|---------------|
| 1  | 5.396833000   | -1.710882000  | -2.043619000  |
| 1  | 6.072920000   | -3.288168000  | -1.552929000  |
| 1  | 5.481411000   | -2.155182000  | -0.307126000  |
| 1  | 0.700766000   |  4.526426000  |  0.608999000  |
| 1  | -1.052394000  |  2.818165000  |  0.338539000  |
| 6  |  1.541008000  |  0.888637000  |  0.218118000  |
| 6  |  2.586531000  |  1.775011000  | -0.103461000  |
| 6  |  3.616637000  |  1.468151000  | -0.233104000  |
| 6  |  0.981547000  |  3.509190000  |  0.372304000  |
| 6  | -0.008221000  |  2.557239000  |  0.218118000  |
| 1  | -1.525177000  |  1.228613000  |  2.427695000  |
| 6  | -3.010630000  |  0.587396000  |  1.002353000  |
| 1  | -3.451760000  |  1.572606000  |  0.909002000  |
| 6  | -3.476090000  | -0.472435000  |  0.185160000  |
| 6  | -2.853328000  | -1.747102000  |  0.296218000  |
| 1  | -3.175203000  | -2.559360000  | -0.344052000  |
| 6  | -1.778501000  | -1.937681000  |  1.183293000  |
| 1  | -1.266310000  | -0.872938000  |  1.981346000  |
| 1  | -1.357109000  | -0.198208000  | -1.968014000  |
| 6  | -0.132508000  | -1.037521000  |  2.970875000  |
| 6  |  0.828478000  | -2.179128000  |  2.644194000  |
| 6  | -0.736584000  | -1.214443000  |  4.370969000  |
| 1  |  0.430871000  | -0.097574000  |  2.954417000  |
| 1  |  1.267396000  | -2.076714000  |  1.648067000  |
| 1  |  1.644356000  | -2.178463000  |  3.372049000  |
| 1  |  0.334700000  | -3.154092000  |  2.708627000  |
| 1  | -1.395596000  | -0.380717000  |  4.631451000  |
| 1  | -1.318856000  | -2.140914000  |  4.422824000  |
| 1  |  0.058607000  | -1.267933000  |  5.119942000  |
| 6  | -4.579890000  | -0.247015000  | -0.798089000  |
| 1  | -5.538333000  | -0.390649000  | -0.288491000  |
| 1  | -4.551205000  |  0.770257000  | -1.191460000  |
| 1  | -4.520556000  | -0.959259000  | -1.623083000  |
| 8  | -2.530751000  |  2.597009000  | -2.185593000  |
| 1  | -2.842010000  |  2.341848600  | -1.311063000  |
| 1  | -2.934209000  |  1.932924000  | -2.779674000  |
| 1  | -1.504891000  |  0.573598000  | -1.796174000  |
### Coordinates (Angstroms)

|   | X            | Y            | Z            |
|---|--------------|--------------|--------------|
| 44| -1.494087000 | -0.092935000 | 0.243527000  |
|  7| -0.058327000 | -0.853040000 | -1.076695000 |
|  7| 0.247234000  | -0.161261000 | 1.408649000  |
|  8| 2.791256000  | -2.579217000 | -3.496748000 |
|  8| 3.791737000  | -0.599809000 | 3.458935000  |
|  6| -0.277654000 | -1.088010000 | -2.381867000 |
|  1| -1.249571000 | -0.800450000 | -2.764771000 |
|  6| 0.666055000  | -1.661132000 | -3.203962000 |
|  1| 0.458415000  | -1.829735000 | -4.253372000 |
|  6| 1.903343000  | -2.025490000 | -2.658743000 |
|  6| 2.139623000  | -1.779028000 | -1.306713000 |
|  1| 3.088573000  | -2.023382000 | -0.850868000 |
|  6| 1.140916000  | -1.174760000 | -0.553645000 |
|  6| 4.078988000  | -2.924862000 | -2.985776000 |
|  1| 4.595546000  | -2.038546000 | -2.605133000 |
|  6| 4.629563000  | -3.335936000 | -3.830361000 |
|  1| 3.997887000  | -3.679711000 | -2.197948000 |
|  6| 1.321107000  | -0.775301000 | 0.855631000  |
|  6| 2.501432000  | -0.942929000 | 1.553675000  |
|  1| 3.361356000  | -1.430715000 | 1.113330000  |
|  6| 2.609717000  | -0.429544000 | 2.849829000  |
|  6| 1.511591000  | 0.231076000  | 3.405203000  |
|  1| 1.530603000  | 0.662518000  | 4.397081000  |
|  6| 0.358595000  | 0.333613000  | 2.647005000  |
|  1| -0.519130000 | 0.830443000  | 3.042735000  |
|  6| 3.957827000  | -0.047872000 | 4.765394000  |
|  1| 3.812242000  | 1.036332000  | 4.750123000  |
|  1| 4.983102000  | -0.274941000 | 5.053127000  |
|  1| 3.265248000  | -0.508877000 | 5.475598000  |
|  6| -2.894737000 | -1.034307000 | 1.806336000  |
|  1| -2.608239000 | -1.424247000 | 2.778442000  |
|  6| -3.156128000 | 0.364385000  | 1.682862000  |
|  1| -3.088852000 | 1.002645000  | 2.556075000  |
|  6| -3.486451000 | 0.924390000  | 0.425338000  |
|  6| -3.511008000 | 0.063643000  | -0.711630000 |
|  1| -3.716257000 | 0.470910000  | -1.694395000 |
|  6| -3.189390000 | -1.305627000 | -0.565647000 |
1       -3.135470000     -1.917730000     -1.460959000
6       -2.951295000     -1.907695000      0.706381000
1       -0.932085000      1.318078000     -0.215144000
6       -2.690849000     -3.393622000      0.839026000
6       -1.454479000     -3.858660000      0.048472000
6       -3.930369000     -4.191172000      0.416375000
1       -2.502318000     -3.589369000      1.900417000
1       -0.558500000     -3.314725000      0.398246000
1       -1.294990000     -4.911773000      0.169970000
1       -1.570344000     -3.632090000     -1.022006000
1       -4.814061000     -3.873690000      0.985861000
1       -4.143186000     -4.042525000     -0.648071000
1       -3.767974000     -5.260610000      0.581346000
6       -3.774536000     2.388727000      0.272595000
1       -4.836414000     2.578637000      0.458897000
1       -3.189189000     2.980965000      0.978657000
1       -3.542462000     2.711093000     -0.744812000
6       3.296597000     1.256179000     -1.718051000
6       2.047077000     1.810115000     -1.961846000
6       1.407034000     2.553628000     -0.958868000
6       2.019265000     2.714460000      0.297247000
6       3.258947000     2.145494000      0.535594000
6       3.899294000     1.421830000     -0.473068000
1       3.794945000     0.686960000     -2.494966000
1       1.579149000     1.668265000     -2.929644000
1       1.514320000     3.272964000      1.077023000
1       3.728078000     2.256425000      1.507061000
1       4.869996000     0.975845000     -0.281889000
6       0.122920000     3.186385000     -1.223273000
8       -0.308006000     4.001073000     -0.351642000
6       -0.629501000     2.955678000     -2.483095000
1       -0.082528000     3.431883000     -3.304702000
1       -0.692735000     1.886036000     -2.694877000
1       -1.628880000     3.383907000     -2.424097000
8       -2.315225000     5.382102000     -0.860977000
1       -2.078517000     5.924687000     -1.624547000
1       -1.194134000     4.508138000     -0.594430000
1       -3.087406000     4.877727000     -1.147067000

TS16-17

Coordinates (Angstroms)

|        | X       | Y       | Z       |
|--------|---------|---------|---------|
| 44     | 1.441716000 | 0.045189000 | 0.269057000 |
| 7      | 0.080207000  | 1.093305000  | -0.916768000 |
|   |       |       |              |       |       |       |
|---|-------|-------|-------------|-------|-------|-------|
| 7 | -0.355185000 | -0.150105000 | 1.325310000 | 8     | -2.667012000 | 3.273305000 | -3.071455000 |
| 8 | -4.037452000 | -0.274454000 | 3.158045000 | 6     | -0.526055000 | 2.376740000 | -2.837105000 |
| 6 | 0.381496000 | 1.647053000 | -2.104944000 | 1     | 1.388904000 | 1.485587000 | -2.468976000 |
| 8 | -4.037452000 | -0.274454000 | 3.158045000 | 6     | -0.526055000 | 2.376740000 | -2.837105000 |
| 6 | -2.136256000 | 1.984569000 | -1.093054000 | 1     | -3.124518000 | 2.088597000 | -0.668465000 |
| 6 | -1.165533000 | 1.246932000 | -0.428114000 | 6     | -0.007456000 | 3.433979000 | -2.605485000 |
| 1 | -0.250632000 | 2.804814000 | -3.792899000 | 1     | -4.497567000 | 2.462177000 | -2.491473000 |
| 1 | -4.517835000 | 4.013618000 | -3.373086000 | 1     | -4.028898000 | 3.979655000 | -1.657698000 |
| 6 | -4.210230000 | 0.529959000 | 0.836278000  | 6     | -2.649865000 | 0.500227000 | 1.463480000  |
| 1 | -3.504424000 | 1.035376000 | 1.070160000  | 6     | -2.811812000 | -0.271637000 | 2.619095000  |
| 6 | -1.716138000 | -0.983805000 | 3.111270000  | 1     | -1.772719000 | -1.605841000 | 3.994642000  |
| 6 | -0.515847000 | -0.888956000 | 2.428775000  | 6     | 0.358479000  | -1.426059000 | 2.776762000  |
| 1 | -4.263121000 | -1.071769000 | 4.321102000  | 6     | -4.069247000 | -2.127865000 | 4.111252000  |
| 1 | -5.313849000 | -0.933357000 | 4.570703000  | 6     | -3.638315000 | -0.732808000 | 5.152488000  |
| 6 | 2.703260000  | 0.609066000  | 2.065384000  | 1     | 2.331406000  | 0.772916000  | 3.072035000  |
| 6 | 3.029487000  | -0.719233000 | 1.665702000  | 6     | 2.927629000  | -1.533901000 | 2.373055000  |
| 1 | 3.453236000  | -0.984854000 | 0.344087000  | 6     | 3.508941000  | 0.097880000  | -0.583833000 |
| 1 | 3.775789000  | -0.088125000 | -1.617297000 | 6     | 3.155677000  | 1.400619000  | -0.167422000 |
| 1 | 3.139150000  | 2.193481000  | -0.908970000 | 6     | 2.800927000  | 1.702274000  | 1.182327000  |
| 1 | 0.871745000  | -1.239408000 | -0.560626000 | 6     | 2.501723000  | 3.118616000  | 1.625600000  |
| 6 | 1.351175000  | 3.754065000  | 0.839982000  | 6     | 3.775237000  | 3.968194000  | 1.532100000  |
| 1 | 2.203972000  | 3.064773000  | 2.678522000  | 1     | 0.419687000  | 3.200460000  | 0.988941000  |
| 1 | 1.193994000  | 4.783327000  | 1.176795000  |
|    | X                  | Y                  | Z                  |
|----|--------------------|--------------------|--------------------|
| 1  | 1.563508000        | 3.781796000        | -0.234246000       |
| 1  | 4.596987000        | 3.517103000        | 2.096624000        |
| 1  | 4.096569000        | 4.076021000        | 0.490183000        |
| 1  | 3.593611000        | 4.969213000        | 1.934733000        |
| 6  | 3.802974000        | -2.374238000       | -0.087090000       |
| 1  | 4.861937000        | -2.561110000       | 0.119981000        |
| 1  | 3.212047000        | -3.114950000       | 0.455376000        |
| 1  | 3.641006000        | -2.499055000       | -1.158270000       |
| 6  | -3.276285000       | -1.124475000       | -1.823080000       |
| 6  | -1.928228000       | -1.349175000       | -2.082247000       |
| 6  | -1.188990000       | -2.194367000       | -1.246860000       |
| 6  | -1.807164000       | -2.791494000       | -0.136810000       |
| 6  | -3.147417000       | -2.553945000       | 0.121219000        |
| 6  | -3.885794000       | -1.723282000       | -0.724684000       |
| 1  | -3.845607000       | -0.470557000       | -2.475089000       |
| 1  | -1.463809000       | -0.865467000       | -2.934745000       |
| 1  | -1.230232000       | -3.432084000       | 0.520292000        |
| 1  | -3.619043000       | -3.006330000       | 0.986971000        |
| 1  | -4.935406000       | -1.538370000       | -0.520421000       |
| 6  | 0.215980000        | -2.514492000       | -1.551461000       |
| 8  | 0.678094000        | -3.567660000       | -0.961450000       |
| 6  | 0.883477000        | -2.039102000       | -2.798841000       |
| 1  | 0.507072000        | -2.646595000       | -3.627970000       |
| 1  | 0.681147000        | -0.990331000       | -3.001967000       |
| 1  | 1.966812000        | -2.186605000       | -2.721834000       |
| 8  | 2.668765000        | -4.776967000       | -2.009714000       |
| 1  | 3.127950000        | -4.222920000       | -2.653180000       |
| 1  | 1.536557000        | -3.940014000       | -1.368272000       |
| 1  | 3.331432000        | -4.952369000       | -1.329850000       |

Coordinates (Angstroms)

|    | X                  | Y                  | Z                  |
|----|--------------------|--------------------|--------------------|
| 44 | 1.436203000        | -0.368137000       | -0.190026000       |
| 7  | 0.000764000        | -0.707933000       | 1.306741000        |
| 7  | -0.359038000       | -0.588312000       | -1.271527000       |
| 8  | -2.925690000       | -1.162628000       | 4.151316000        |
| 8  | -4.039645000       | -0.884414000       | -3.059702000       |
| 6  | 0.280883000        | -0.695357000       | 2.622737000        |
| 1  | 1.318143000        | -0.544609000       | 2.895676000        |
| 6  | -0.687357000       | -0.847610000       | 3.586363000        |
| 1  | -0.431765000       | -0.818098000       | 4.638063000        |
| 6  | -2.016088000       | -1.035835000       | 3.182953000        |
| 6  | -2.307452000       | -1.071830000       | 1.816309000        |
|   |         |         |         |
|---|---------|---------|---------|
| 1 | -3.320665000 | -1.207642000 | 1.465196000 |
| 6 | -1.275662000 | -0.889060000 | 0.910887000 |
| 6 | -4.301238000 | -1.296977000 | 3.783373000 |
| 1 | -4.635457000 | -0.424059000 | 3.214882000 |
| 1 | -4.849167000 | -1.356987000 | 4.722040000 |
| 1 | -4.660304000 | -2.210816000 | 3.204674000 |
| 6 | -1.482083000 | -0.829500000 | -0.551196000 |
| 6 | -4.613204000 | -0.569270000 | -3.271848000 |
| 6 | -4.569135000 | -0.425820000 | -2.596234000 |
| 6 | -4.468030000 | -0.714632000 | -3.126206000 |
| 6 | -4.211893000 | -0.633210000 | -4.456722000 |
| 6 | -3.913001000 | 0.390265000 | -0.559280000 |
| 6 | -1.667262000 | -0.350999000 | -3.548350000 |
| 1 | -1.246638000 | -1.859947000 | -2.597815000 |
| 6 | -1.342993000 | -0.151197000 | -1.634086000 |
| 1 | -1.453060000 | 0.449263000 | -2.536019000 |
| 6 | -0.531152000 | 0.434754000 | -0.397033000 |
| 6 | 3.456725000 | -0.340389000 | -0.887770000 |
| 1 | 3.695575000 | 0.114335000 | -0.742635000 |
| 6 | 2.931959000 | -1.650390000 | 0.746510000 |
| 1 | 2.778504000 | -2.180196000 | 1.680768000 |
| 6 | 2.496380000 | -2.243762000 | -0.477494000 |
| 1 | -1.156900000 | 2.189285000 | -0.196516000 |
| 6 | 1.952819000 | -3.654137000 | -0.537751000 |
| 6 | 0.857551000 | -3.934804000 | 0.491965000 |
| 6 | 3.126993000 | -4.630783000 | -0.387828000 |
| 1 | 1.519202000 | -3.783807000 | -0.535005000 |
| 1 | -0.008522000 | -3.288124000 | 0.332841000 |
| 1 | 0.528123000 | -4.973324000 | 0.396168000 |
| 1 | 1.211283000 | -3.792218000 | 1.517931000 |
| 1 | 3.895181000 | -4.452140000 | -1.146153000 |
| 1 | 3.589382000 | -4.530726000 | 0.600144000 |
| 1 | 2.770769000 | -5.650988000 | -0.496434000 |
| 6 | 3.952458000 | 1.867621000 | -0.347882000 |
| 1 | 4.991721000 | 1.943062000 | -0.684721000 |
| 1 | 3.336914000 | 2.477634000 | -1.012491000 |
| 1 | 3.888899000 | 2.261010000 | 0.667099000 |
| 6 | -3.081426000 | 2.134349000 | 1.053951000 |
|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| 6 | -1.723535000 | 2.378987000 | 1.268194000 |
| 6 | -0.876196000 | 2.668058000 | 0.199412000 |
| 6 | -1.414890000 | 2.693336000 | -1.094397000 |
| 6 | -2.766203000 | 2.455571000 | -1.310527000 |
| 6 | -3.608285000 | 2.178625000 | -0.231611000 |
| 1 | -3.723368000 | 1.903289000 | 1.899040000 |
| 1 | -1.333263000 | 2.327788000 | 2.279792000 |
| 1 | -0.762231000 | 2.901532000 | -1.937729000 |
| 1 | -3.164470000 | 2.474866000 | -2.320629000 |
| 1 | -4.663578000 | 1.986826000 | -0.398607000 |
| 6 | 0.604563000 | 2.962443000 | 0.369695000 |
| 8 | 0.851088000 | 4.222269000 | -0.238916000 |
| 6 | 1.104937000 | 2.939016000 | 1.806320000 |
| 1 | 0.582676000 | 3.683906000 | 2.414626000 |
| 1 | 0.970994000 | 1.953439000 | 2.261263000 |
| 1 | 2.173064000 | 3.172307000 | 1.823921000 |
| 8 | 3.463323000 | 5.090071000 | 0.118428000 |
| 1 | 3.795903000 | 4.626785000 | 0.895828000 |
| 1 | 1.796977000 | 4.442807000 | -0.118001000 |
| 1 | 3.996228000 | 4.739336000 | -0.604144000 |
| 18 |                     |           |           |

Coordinates (Angstroms)
|    | X          | Y          | Z          |
|----|------------|------------|------------|
| 6  | 2.850568000 | 2.583880000 | 0.696327000 |
| 6  | 1.636484000 | 3.274552000 | 0.684275000 |
| 1  | 1.555496000 | 4.318442000 | 0.956342000 |
| 6  | 0.498683000 | 2.586807000 | 0.303613000 |
| 1  | -0.462129000 | 3.086790000 | 0.281833000 |
| 6  | 4.068197000 | 4.482560000 | 1.440498000 |
| 1  | 3.736441000 | 5.134705000 | 0.627461000 |
| 1  | 5.111067000 | 4.691155000 | 1.674000000 |
| 1  | 3.451207000 | 4.644703000 | 2.328813000 |
| 6  | -2.333918000 | 0.702561000 | 1.486475000 |
| 1  | -1.921257000 | 1.227405000 | 2.341952000 |
| 6  | -2.856299000 | 1.466380000 | 0.397210000 |
| 1  | -2.849015000 | 2.549023000 | 0.453893000 |
| 6  | -3.383758000 | 0.835340000 | -0.747923000 |
| 6  | -3.009010000 | -0.591014000 | 0.821540000 |
| 1  | -3.657560000 | -1.106586000 | -1.707973000 |
| 6  | -2.734104000 | -1.321530000 | 0.236566000 |
| 1  | -2.635571000 | -2.396960000 | 0.128196000 |
| 6  | -2.287001000 | -0.695856000 | 1.446846000 |
| 1  | -0.915024000 | 0.414732000 | -2.014430000 |
| 6  | -1.782467000 | -1.509720000 | 2.619360000 |
| 6  | -0.642745000 | -2.461391000 | 2.246575000 |
| 6  | -2.954164000 | -2.271381000 | 3.252683000 |
| 1  | -1.399955000 | -0.796215000 | 3.357448000 |
| 1  | 0.220373000  | -1.914587000 | 1.856502000 |
| 1  | -0.322853000 | -3.018043000 | 3.132669000 |
| 1  | -0.959535000 | -3.190111000 | 1.491811000 |
| 1  | -3.761180000 | -1.591258000 | 3.541127000 |
| 1  | -3.362209000 | -3.009526000 | 2.553179000 |
| 1  | -2.617999000 | -2.803249000 | 4.147758000 |
| 6  | -4.003006000 | 1.626798000  | -1.860721000 |
| 1  | -5.087494000 | 1.661584000  | -1.714603000 |
| 1  | -3.627510000 | 2.652349000  | -1.871492000 |
| 1  | -3.806092000 | 1.162493000  | -2.829320000 |
| 8  | -0.997232000 | 2.760868000  | -2.708661000 |
| 1  | -1.198094000 | 3.420828000  | -2.021380000 |
| 1  | -1.710586000 | 2.795190000  | -3.371170000 |
| 1  | -1.012642000 | 1.833517000  | -2.270311000 |

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**TS18-19**

Coordinates (Angstroms)

|    | X          | Y          | Z          |
|----|------------|------------|------------|
| 44 | -1.240157000 | 0.167533000 | -0.470901000 |
| 7  | 0.319355000  | -1.202679000 | -0.733775000 |
|   |   |   |
|---|---|---|
| 7 | 0.475704000 | 1.297162000 | -0.042263000 |
| 8 | 3.420120000 | -3.892105000 | -0.947142000 |
| 8 | 4.004031000 | 3.171020000 | 0.927997000 |
| 6 | 0.131861000 | -2.475945000 | -1.121220000 |
| 1 | -0.882507000 | -2.757180000 | -1.374295000 |
| 6 | 1.159350000 | -3.863540000 | -1.195953000 |
| 1 | 0.972306000 | -4.073680000 | -1.504194000 |
| 6 | 2.455242000 | -2.969822000 | -0.866128000 |
| 6 | 2.659115000 | -1.640554000 | -0.487348000 |
| 1 | 3.646108000 | -1.275630000 | -0.239437000 |
| 6 | 1.565581000 | -0.787467000 | -0.432761000 |
| 6 | 4.757386000 | -3.513472000 | -0.614517000 |
| 1 | 5.122400000 | -2.740874000 | -1.297382000 |
| 1 | 5.353443000 | -4.416982000 | -0.730917000 |
| 1 | 4.818008000 | -3.163021000 | 0.419701000 |
| 6 | 1.659139000 | 0.635840000 | -0.048385000 |
| 6 | 2.841408000 | 1.267781000 | 0.277955000 |
| 1 | 3.788200000 | 0.743267000 | 0.277013000 |
| 6 | 2.823045000 | 2.625269000 | 0.621155000 |
| 6 | 1.601508000 | 3.303512000 | 0.617902000 |
| 1 | 1.515649000 | 4.352912000 | 0.865938000 |
| 6 | 0.462638000 | 2.596765000 | 0.278207000 |
| 1 | -0.503244000 | 3.087110000 | 0.262847000 |
| 6 | 4.039680000 | 4.552234000 | 1.293359000 |
| 1 | 3.686238000 | 5.181067000 | 0.471248000 |
| 1 | 5.085814000 | 4.771916000 | 1.500217000 |
| 1 | 3.440194000 | 4.731669000 | 2.190172000 |
| 6 | -2.313381000 | 0.747110000 | 1.459648000 |
| 1 | -1.875916000 | 1.317989000 | 2.272143000 |
| 6 | -2.913808000 | 1.445079000 | 0.373040000 |
| 1 | -2.945300000 | 2.528517000 | 0.382890000 |
| 6 | -3.443759000 | 0.742236000 | -0.727364000 |
| 6 | -3.323862000 | -0.682609000 | -0.743990000 |
| 1 | -3.678385000 | -1.241775000 | -1.601424000 |
| 6 | -2.704015000 | -1.351759000 | 0.323756000 |
| 1 | -2.574402000 | -2.427041000 | 0.258097000 |
| 6 | -2.207654000 | -0.654465000 | 1.471227000 |
| 1 | -0.876141000 | 0.385986000 | -2.096982000 |
| 6 | -1.630928000 | -1.392809000 | 2.661071000 |
| 6 | -0.480597000 | -2.333849000 | 2.297006000 |
| 6 | -2.762445000 | -2.149010000 | 3.369759000 |
| 1 | -1.243780000 | -0.633117000 | 3.348426000 |
| 1 | 0.370161000 | -1.783039000 | 1.887168000 |
| 1 | -0.142363000 | -2.862342000 | 3.193198000 |
Coordinates (Angstroms)

| X            | Y            | Z            |
|--------------|--------------|--------------|
| -0.788911000 | -3.085755000 | 1.563535000  |
| -3.576500000 | -1.474427000 | 3.651151000  |
| -3.173412000 | -2.930428000 | 2.721084000  |
| -2.383815000 | -2.627550000 | 4.277608000  |
| -4.084555000 | 1.462426000  | -1.873000000 |
| -5.168730000 | 1.477219000  | -1.721279000 |
| -3.732433000 | 2.493620000  | -1.935024000 |
| -3.880799000 | 0.954620000  | -2.817842000 |
| -1.048529000 | 2.536586000  | -2.736805000 |
| -1.354560000 | 3.124191000  | -2.028691000 |
| -1.771317000 | 2.514224000  | -3.382907000 |
| -0.995205000 | 1.364416000  | -2.213084000 |

| X            | Y            | Z            |
|--------------|--------------|--------------|
| -1.255857000 | -0.021981000 | -0.499445000 |
| 0.441146000  | -1.230296000 | -0.709565000 |
| 0.328455000  | 1.290897000  | -0.107803000 |
| 3.814941000  | -3.554729000 | -0.949364000 |
| 3.623446000  | 3.555637000  | 0.839906000  |
| 0.382928000  | -2.529088000 | -1.052197000 |
| -0.600086000 | -2.931763000 | -1.260808000 |
| 1.505335000  | -3.318272000 | -1.134769000 |
| 1.426607000  | -4.362975000 | -1.408030000 |
| 2.754915000  | -2.748133000 | -0.858880000 |
| 2.818047000  | -1.394400000 | -0.515485000 |
| 3.763287000  | -0.914848000 | -0.303335000 |
| 1.638654000  | -0.668880000 | -0.450948000 |
| 5.113624000  | -3.007015000 | -0.710151000 |
| 5.337148000  | -2.213348000 | -1.428657000 |
| 5.809974000  | -3.832459000 | -0.847807000 |
| 5.192914000  | -2.624805000 | 0.311556000  |
| 1.577468000  | 0.763076000  | -0.099571000 |
| 2.681742000  | 1.525321000  | 0.216455000  |
| 3.679194000  | 1.105081000  | 0.228437000  |
| 2.513125000  | 2.878863000  | 0.536585000  |
| 1.223948000  | 3.418432000  | 0.518729000  |
| 1.020229000  | 4.454710000  | 0.752224000  |
| 0.170177000  | 2.585949000  | 0.192118000  |
| -0.842260000 | 2.969282000  | 0.178276000  |
| 3.499312000  | 4.935314000  | 1.194757000  |
| 3.072865000  | 5.509895000  | 0.368150000  |
| 4.512234000  | 5.278595000  | 1.397547000  |
|    | X             | Y             | Z             |
|----|---------------|---------------|---------------|
| 1  | 2.883951000   | 5.047915000   | 2.091687000   |
| 6  | -2.289316000  | 0.597724000   | 1.383945000   |
| 1  | -1.860404000  | 1.289581000   | 2.102120000   |
| 6  | -3.062036000  | 1.115704000   | 0.312654000   |
| 1  | -3.229389000  | 2.183715000   | 0.234636000   |
| 6  | -3.551139000  | 0.254660000   | -0.689589000  |
| 6  | -3.269300000  | -1.144151000  | -0.584039000  |
| 1  | -3.602396000  | -1.815102000  | -1.366913000  |
| 6  | -0.990707000  | -0.069887000  | -2.337526000  |
| 6  | -1.245227000  | -1.306860000  | 2.703108000   |
| 6  | -0.162538000  | -2.338204000  | 2.384651000   |
| 6  | -2.287956000  | -1.878340000  | 3.674525000   |
| 1  | -0.766018000  | -0.445571000  | 3.179935000   |
| 1  | 0.645053000   | -1.902167000  | 1.792274000   |
| 1  | 0.269226000   | -2.706924000  | 3.319510000   |
| 1  | -0.562452000  | -3.201978000  | 1.844148000   |
| 1  | -3.050673000  | -1.133913000  | 3.921286000   |
| 1  | -2.787181000  | -2.749603000  | 3.236358000   |
| 1  | -1.801996000  | -2.194516000  | 4.601824000   |
| 6  | -4.316162000  | 0.776756000   | -1.864250000  |
| 1  | -5.381929000  | 0.585331000   | -1.702770000  |
| 1  | -4.172069000  | 1.851271000   | -1.986439000  |
| 1  | -4.016206000  | 0.264262000   | -2.780528000  |
| 8  | -1.651557000  | 2.911802000   | -2.694569000  |
| 1  | -2.054713000  | 2.820508000   | -1.823958000  |
| 1  | -2.227536000  | 2.384598000   | -3.258960000  |
| 1  | -1.033355000  | 0.717722000   | -2.210961000  |

Coordinates (Angstroms)

|    | X             | Y             | Z             |
|----|---------------|---------------|---------------|
| 44 | -0.838723000  | -0.685242000  | -0.159610000  |
| 7  | 1.134970000   | -0.935230000  | -0.823683000  |
| 7  | 0.060593000   | 1.171844000   | 0.266658000   |
| 8  | 5.085878000   | -1.390144000  | -1.888218000  |
| 8  | 2.193045000   | 4.552709000   | 1.253828000   |
| 6  | 1.595718000   | -2.059069000  | -1.400056000  |
| 1  | 0.867367000   | -2.841044000  | -1.576545000  |
| 6  | 2.912994000   | -2.225242000  | -1.759252000  |
| 1  | 3.249146000   | -3.145417000  | -2.220782000  |
| 6  | 3.814713000   | -1.180364000  | -1.521943000  |
|   | 3.341097000 | -0.006457000 | -0.934048000 |
|---|-------------|---------------|---------------|
| 1 | 4.002228000 | 0.826302000   | -0.738037000  |
| 6 | 1.995127000 | 0.077732000   | -0.599636000  |
| 6 | 6.040084000 | -0.350157000  | -1.669284000  |
| 1 | 5.767066000 | 0.553500000   | -2.222258000  |
| 1 | 6.985847000 | -0.737070000  | -2.045627000  |
| 1 | 6.133620000 | -0.126025000  | -0.602652000  |
| 6 | 1.390861000 | 1.271337000   | 0.027077000   |
| 6 | 2.103709000 | 2.408182000   | 0.356440000   |
| 1 | 3.167304000 | 2.488318000   | 0.170940000   |
| 6 | 1.440801000 | 3.486473000   | 0.953037000   |
| 6 | 0.068111000 | 3.381860000   | 1.191931000   |
| 1 | -0.507442000 | 4.176660000   | 1.647001000 |
| 6 | -0.569253000 | 2.209173000   | 0.831384000   |
| 1 | -1.631023000 | 2.086208000   | 1.004189000   |
| 6 | 1.554523000 | 5.678462000   | 1.858242000   |
| 1 | 0.790355000 | 6.093242000   | 1.194441000   |
| 1 | 2.341626000 | 6.414286000   | 2.015518000   |
| 1 | 1.109312000 | 5.405221000   | 2.819306000   |
| 6 | -1.814011000 | -0.938355000  | 1.914266000   |
| 1 | -1.690754000 | -0.277169000  | 2.766453000   |
| 6 | -2.804943000 | -0.615647000  | 0.938547000   |
| 1 | -3.426410000 | 0.260871000   | 1.075485000   |
| 6 | -2.978299000 | -1.420919000  | -0.209204000  |
| 6 | -2.095467000 | -2.528247000  | -0.393974000  |
| 1 | -2.170975000 | -3.138960000  | -1.285524000  |
| 6 | -1.083054000 | -2.786163000  | 0.555374000   |
| 1 | -0.379246000 | -3.587863000  | 0.353255000   |
| 6 | -0.958315000 | -2.041106000  | 1.769226000   |
| 1 | -1.031823000 | -0.138013000  | -1.659194000  |
| 6 | 0.081203000 | -2.397368000  | 2.811901000   |
| 6 | 1.509580000 | -2.335117000  | 2.260444000   |
| 6 | -0.220043000 | -3.778160000  | 3.406991000   |
| 1 | -0.004476000 | -1.653153000  | 3.611318000   |
| 1 | 1.757447000 | -1.326088000  | 1.919143000   |
| 1 | 2.223472000 | -2.617306000  | 3.040317000   |
| 1 | 1.644976000 | -3.023095000  | 1.418857000   |
| 1 | -1.230157000 | -3.821757000  | 3.825333000   |
| 1 | -0.133804000 | -4.559326000  | 2.643481000   |
| 1 | 0.491623000 | -4.008813000  | 4.205353000   |
| 6 | -4.056044000 | -1.126701000  | -1.208907000  |
| 1 | -4.948500000 | -1.710153000  | -0.960247000  |
| 1 | -4.325398000 | -0.069070000  | -1.194776000  |
| 1 | -3.740349000 | -1.401888000  | -2.217598000  |
|   | X           | Y           | Z           |
|---|-------------|-------------|-------------|
| 8 | -2.59885500 | 1.89683200  | -1.76707400 |
| 1 | -3.25415400 | 2.11099000  | -1.00712600 |
| 1 | -3.14370300 | 1.61535700  | -2.60058700 |
| 1 | -2.04704400 | 1.11819000  | -1.49922700 |
| 8 | -3.91125300 | 1.21362600  | -3.80804800 |
| 1 | -4.51214800 | 1.93183500  | -4.04370800 |
| 1 | -4.49044400 | 0.48311400  | -3.55618500 |
| 8 | -4.28402700 | 2.52044700  | 0.02756300  |
| 1 | -3.89444000 | 2.60809500  | 0.90390200  |
| 1 | -4.93207000 | 1.81111200  | 0.12206300  |

**TS20-21**

Coordinates (Angstroms)

|   | X             | Y             | Z             |
|---|---------------|---------------|---------------|
| 44| -0.89151800   | -0.63862900   | -0.12866900   |
| 7 | 1.05790000    | -0.95821900   | -0.83531900   |
| 7 | 0.08680500    | 1.15846800    | 0.30711700    |
| 8 | 4.98968200    | -1.62205100   | -1.83070000   |
| 8 | 2.25960200    | 4.56702000    | 1.03130000    |
| 6 | 1.46199700    | -2.10478500   | -1.40871300   |
| 1 | 0.69575800    | -2.84623000   | -1.59727300   |
| 6 | 2.77392000    | -2.33923900   | -1.74802700   |
| 1 | 3.06659600    | -3.27429800   | -2.20899600   |
| 6 | 3.72742500    | -1.34674300   | -1.48826000   |
| 6 | 3.30907400    | -0.14934100   | -0.90161900   |
| 1 | 4.01367000    | 0.63985300    | -0.67946800   |
| 6 | 1.96582000    | 0.00906600    | -0.59527000   |
| 6 | 5.98999200    | -0.62431100   | -1.61360800   |
| 1 | 5.75746000    | 0.28835600    | -2.16974100   |
| 6 | 6.91746800    | -1.05477800   | -1.98749000   |
| 1 | 6.09204200    | -0.40296200   | -0.54735100   |
| 6 | 1.40760100    | 1.23230200    | 0.01542300    |
| 6 | 2.13500300    | 2.37896500    | 0.25892400    |
| 1 | 3.18773900    | 2.44974000    | 0.01666900    |
| 6 | 1.49517600    | 3.49098600    | 0.82178800    |
| 6 | 0.13076900    | 3.40838100    | 1.11399100    |
| 1 | -0.42481300   | 4.23127800    | 1.54302500    |
| 6 | -0.52578500   | 2.22482500    | 0.83437100    |
| 1 | -1.58537100   | 2.12039300    | 1.03327800    |
| 6 | 1.64765600    | 5.73582000    | 1.58067500    |
| 1 | 0.85740500    | 6.10498500    | 0.92080200    |
| 1 | 2.44179200    | 6.47719800    | 1.65118900    |
| 1 | 1.24249200    | 5.53228100    | 2.57582100    |
| 6 | -1.81988500   | -0.78394000   | 1.92409100    |
## Coordinates (Angstroms)

|  | X                | Y                | Z                |
|---|-----------------|-----------------|-----------------|
| 44 | -0.830657000   | -0.709729000   | -0.142236000   |
| 7  | 1.137188000    | -0.918650000   | -0.816763000   |
| 7  | 0.007475000    | 1.173845000    | 0.208635000    |
| 8  | 5.086835000    | -1.336057000   | -1.850545000   |
| 8  | 1.993898000    | 4.667422000    | 1.049008000    |
| 6  | 1.608541000    | -2.047565000   | -1.373163000   |
|   |     |     |     |
|---|-----|-----|-----|
| 1 | 0.890481000 | -2.842197000 | -1.533127000 |
| 6 | 2.928308000 | -2.197546000 | -1.726464000 |
| 1 | 3.280249000 | -3.119168000 | -2.172565000 |
| 6 | 3.814572000 | -1.136527000 | -1.498377000 |
| 6 | 3.322991000 | 0.044053000 | -0.932609000 |
| 6 | 3.972070000 | 0.888772000 | -0.746350000 |
| 6 | 1.976720000 | 0.115242000 | -0.609634000 |
| 6 | 6.033766000 | -0.286730000 | -1.635111000 |
| 1 | 5.760271000 | 0.607022000 | -2.032070000 |
| 1 | 6.984596000 | -0.674367000 | -1.997048000 |
| 1 | 6.113715000 | -0.050133000 | -0.570431000 |
| 6 | 1.335708000 | 1.309592000 | -0.025254000 |
| 6 | 1.999874000 | 2.484548000 | 0.253954000 |
| 1 | 3.069340000 | 2.596349000 | 0.072145000 |
| 6 | 1.285626000 | 3.566398000 | 0.787014000 |
| 6 | -0.088557000 | 3.426316000 | 1.000395000 |
| 1 | -0.702679000 | 4.224857000 | 1.394196000 |
| 6 | -0.678945000 | 2.214600000 | 0.694890000 |
| 1 | -1.741135000 | 2.066054000 | 0.845392000 |
| 6 | 1.315066000 | 5.797187000 | 1.603074000 |
| 1 | 0.555067000 | 6.168591000 | 0.909955000 |
| 1 | 2.081427000 | 6.556166000 | 1.749203000 |
| 1 | 0.858677000 | 5.543799000 | 2.564045000 |
| 6 | -1.644652000 | -0.819250000 | 1.944989000 |
| 1 | -1.459144000 | -0.068467000 | 2.706309000 |
| 6 | -2.746618000 | -0.650363000 | 1.070070000 |
| 1 | -3.392595000 | 0.211268000 | 1.175363000 |
| 6 | -2.952893000 | -1.554972000 | 0.006995000 |
| 6 | -2.049918000 | -2.654171000 | -0.146315000 |
| 1 | -2.171899000 | -3.335651000 | -0.979443000 |
| 6 | -0.961610000 | -2.802467000 | 0.724088000 |
| 1 | -0.250153000 | -3.600216000 | 0.538694000 |
| 6 | -0.722145000 | -1.879334000 | 1.790837000 |
| 1 | -0.988308000 | -0.424495000 | -1.956143000 |
| 6 | 0.399391000 | -2.087424000 | 2.786719000 |
| 6 | 1.777146000 | -2.266835000 | 2.145899000 |
| 6 | 0.034971100 | -3.288430000 | 3.670731000 |
| 1 | 0.430984000 | -1.193501000 | 3.418483000 |
| 1 | 2.096599000 | -1.357906000 | 1.630256000 |
| 1 | 2.513056000 | -2.489351000 | 2.923817000 |
| 1 | 1.791728000 | -3.094194000 | 1.429116000 |
| 1 | -0.942428000 | -3.153608000 | 4.143525000 |
| 1 | 0.006928000 | -4.211641000 | 3.081358000 |
| 1 | 0.782942000 | -3.412904000 | 4.459105000 |
|    | X                | Y                | Z                |
|----|------------------|------------------|------------------|
| 44 | -0.721382000     | 1.130978000     | -0.523772000     |
|  7 | 0.403184000      | 0.713689000     | 1.196774000      |
|  7 | 1.125082000      | 0.490628000     | -1.296508000     |
|  8 | 2.780609000      | 0.019624000     | 4.489988000      |
|  8 | 4.890802000      | -0.715570000    | -2.451526000     |
|  6 | -0.075560000     | 0.777593000     | 2.451764000      |
|  1 | -1.125542000     | 1.023118000     | 2.554281000      |
|  6 | 0.704174000      | 0.544970000     | 3.561596000      |
|  1 | 0.280658000      | 0.605760000     | 4.556426000      |
|  6 | 2.056965000      | 0.232686000     | 3.381226000      |
|  6 | 2.558701000      | 0.152492000     | 2.082799000      |
|  1 | 3.592807000      | -0.102075000    | 1.899402000      |
|  6 | 1.698116000      | 0.388146000     | 1.017026000      |
|  6 | 4.158182000      | -0.323044000    | 4.338267000      |
|  1 | 4.266790000      | -1.259155000    | 3.782102000      |
|  1 | 4.544907000      | -0.451396000    | 5.348155000      |
|  1 | 4.706087000      | 0.479514000     | 3.835441000      |
|  6 | 2.108843000      | 0.253217000     | -0.394476000     |
|  6 | 3.375891000      | -0.132839000    | -0.786321000     |
|  1 | 4.161544000      | -0.327855000    | -0.068007000     |
|  6 | 3.648401000      | -0.315648000    | -2.145223000     |
|  6 | 2.627363000      | -0.092812000    | -3.070802000     |
|  1 | 2.765502000      | -0.227282000    | -4.135246000     |
|  6 | 1.390522000      | 0.306407000     | -2.595071000     |
|  1 | 0.572512000      | 0.487806000     | -3.281672000     |
|  6 | 5.211590000      | -0.912337000    | -3.828925000     |
|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 4.586845000 | -1.697192000 | -4.265488000 |
| 1 | 6.255093000 | -1.222852000 | -3.847391000 |
| 1 | 5.093905000 | 0.018724000  | -4.390850000 |
| 6 | -0.941888000 | 3.138456000  | -1.711546000 |
| 1 | -0.191597000 | 3.659816000  | -2.297465000 |
| 6 | -1.676526000 | 2.071759000  | -2.324534000 |
| 1 | -1.474577000 | 1.814011000  | -3.358274000 |
| 6 | -2.659047000 | 1.353299000  | -1.611629000 |
| 6 | -2.851729000 | 1.676648000  | -0.228954000 |
| 1 | -3.567833000 | 1.119478000  | 0.363417000  |
| 6 | -2.056299000 | 2.671258000  | 0.375480000  |
| 1 | -2.172675000 | 2.846295000  | 1.440414000  |
| 6 | -1.129029000 | 3.476206000  | -0.369619000 |
| 1 | -1.025815000 | -0.418240000 | -0.463590000 |
| 6 | -0.370219000 | 4.608613000  | 0.288710000  |
| 6 | 0.430539000  | 4.148470000  | 1.510705000  |
| 6 | -1.338788000 | 5.739727000  | 0.656258000  |
| 1 | 0.338537000  | 4.991846000  | -0.454028000 |
| 1 | 1.164228000  | 3.384566000  | 1.236989000  |
| 1 | 0.964286000  | 4.997806000  | 1.947987000  |
| 1 | -0.222441000 | 3.731806000  | 2.285083000  |
| 1 | -1.887192000 | 6.093407000  | -0.222050000 |
| 1 | -2.068249000 | 5.401178000  | 1.400467000  |
| 1 | -0.791765000 | 6.586575000  | 1.081646000  |
| 6 | -3.461945000 | 0.264900000  | -2.261977000 |
| 1 | -4.436324000 | 0.656805000  | -2.572467000 |
| 1 | -2.950787000 | -0.122105000 | -3.146128000 |
| 1 | -3.630689000 | -0.558969000 | -1.565521000 |
| 6 | 2.224836000  | -3.108494000 | 1.140072000  |
| 6 | 0.853067000  | -2.899158000 | 1.246107000  |
| 6 | 0.051772000  | -2.910175000 | 0.098729000  |
| 6 | 0.644277000  | -3.109394000 | -1.156601000 |
| 6 | 2.013740000  | -3.302048000 | -1.259994000 |
| 6 | 2.804910000  | -3.307667000 | -0.109487000 |
| 1 | 2.840290000  | -3.102576000 | 2.033825000  |
| 1 | 0.415377000  | -2.732428000 | 2.224750000  |
| 1 | 0.022192000  | -3.103407000 | -2.045087000 |
| 1 | 2.470429000  | -3.440606000 | -2.234457000 |
| 1 | 3.876681000  | -3.456929000 | -0.192945000 |
| 6 | -1.418580000 | -2.722165000 | 0.177808000  |
| 8 | -2.109909000 | -2.931362000 | -0.827392000 |
| 6 | -2.049708000 | -2.321048000 | 1.477630000  |
| 1 | -2.073366000 | -3.190895000 | 2.143652000  |
| 1 | -1.474093000 | -1.537452000 | 1.973579000  |
### TS22-23

Coordinates (Angstroms)

| X       | Y       | Z       |
|---------|---------|---------|
| 44      | 0.898541000 | 0.658793000 | 0.558901000 |
| 7       | -0.618969000 | 1.211583000 | -0.762697000 |
| 7       | -0.789765000 | -0.290624000 | 1.348248000 |
| 8       | -3.722740000 | 2.331648000 | -3.223858000 |
| 8       | -4.317107000 | -1.942134000 | 2.678653000 |
| 6       | -0.420566000 | 1.931091000 | -1.881598000 |
| 1       | 0.604947000  | 2.200442000 | -2.102301000 |
| 6       | -1.446413000 | 2.306044000 | -2.717060000 |
| 1       | -1.247203000 | 2.875806000 | -3.616172000 |
| 6       | -2.756969000 | 1.940759000 | -2.382582000 |
| 6       | -2.970497000 | 1.196163000 | -1.222619000 |
| 1       | -3.963526000 | 0.880186000 | -0.934909000 |
| 6       | -1.874041000 | 0.832995000 | -0.451114000 |
| 6       | -5.067834000 | 1.945383000 | -2.939489000 |
| 1       | -5.164157000 | 0.855624000 | -2.914969000 |
| 1       | -5.666835000 | 2.347269000 | -3.755090000 |
| 1       | -5.404488000 | 2.374963000 | -1.991470000 |
| 6       | -1.973151000 | -0.032875000 | 0.740189000 |
| 6       | -3.155687000 | -0.583479000 | 1.191072000 |
| 1       | -4.100133000 | -0.388401000 | 0.699977000 |
| 6       | -3.135834000 | -1.439094000 | 2.297974000 |
| 6       | -1.912495000 | -1.716045000 | 2.911117000 |
| 1       | -1.823332000 | -2.379587000 | 3.760721000 |
| 6       | -0.774358000 | -1.120520000 | 2.397733000 |
| 1       | 0.193625000  | -1.312567000 | 2.844025000 |
| 6       | -4.343853000 | -2.813903000 | 3.809739000 |
| 1       | -3.770722000 | -3.724436000 | 3.612023000 |
| 1       | -5.392304000 | -3.062010000 | 3.961999000 |
| 1       | -3.954646000 | -2.310252000 | 4.699131000 |
| 6  | 1.543087000 | 1.729441000 | 2.497985000 |
|----|-------------|-------------|-------------|
| 1  | 0.962993000 | 1.837418000 | 3.408550000 |
| 6  | 2.317485000 | 0.544407000 | 2.308688000 |
| 1  | 2.320581000 | -0.219958000 | 3.077436000 |
| 6  | 3.067649000 | 0.347904000 | 1.134525000 |
| 1  | 2.078506000 | 3.186674000 | -0.529477000 |
| 6  | 1.473292000 | 2.724929000 | 1.513930000 |
| 1  | 0.980073000 | -0.659482000 | -0.422776000 |
| 6  | 0.693110000 | 4.004086000 | 1.734946000 |
| 6  | -0.407180000 | 4.227314000 | 0.694030000 |
| 6  | 1.663937000 | 5.191541000 | 1.771628000 |
| 1  | 0.218058000 | 3.917901000 | 2.718134000 |
| 1  | -1.145833000 | 3.421228000 | 0.715537000 |
| 1  | -0.923530000 | 5.170029000 | 0.899227000 |
| 1  | 0.005479000 | 4.289257000 | -0.318350000 |
| 1  | 2.446167000 | 5.046020000 | 2.522873000 |
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| 1  | 1.125046000 | 6.112148000 | 2.014828000 |
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| 1  | 3.582897000 | -1.679670000 | 1.612237000 |
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| 1  | -3.480483000 | -1.692003000 | -2.787068000 |
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| 1 | 2.810096000 | -2.672875000 | -1.419701000 |
| 1 | 4.473576000  | -1.858215000  | -2.139024000  |
| 8 | 5.568772000  | -3.591215000  | 0.218324000   |
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| 1 | 4.872242000  | -3.667259000  | 0.881235000   |
| 8 | 4.977727000  | -0.189447000  | -2.295220000  |
| 1 | 5.650120000  | -0.094428000  | -2.979522000  |
| 1 | 5.449878000  | -0.037383000  | -1.467859000  |