

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

Chenguang Luo,^a Longfei Li,^b Xin Yue,^a Pengjie Li,^a Lin Zhang,^a Zuoyin Yang,^a Min Pu,^a Zexing

Cao^{c,*}, Ming Lei^{a,c,*}

^a State Key Laboratory of Chemical Resource Engineering, Institute of Computational Chemistry, College of Chemistry, Beijing University of Chemical Technology, Beijing, 100029, China

^b College of Pharmaceutical Science, Hebei University, Baoding, 071002, China

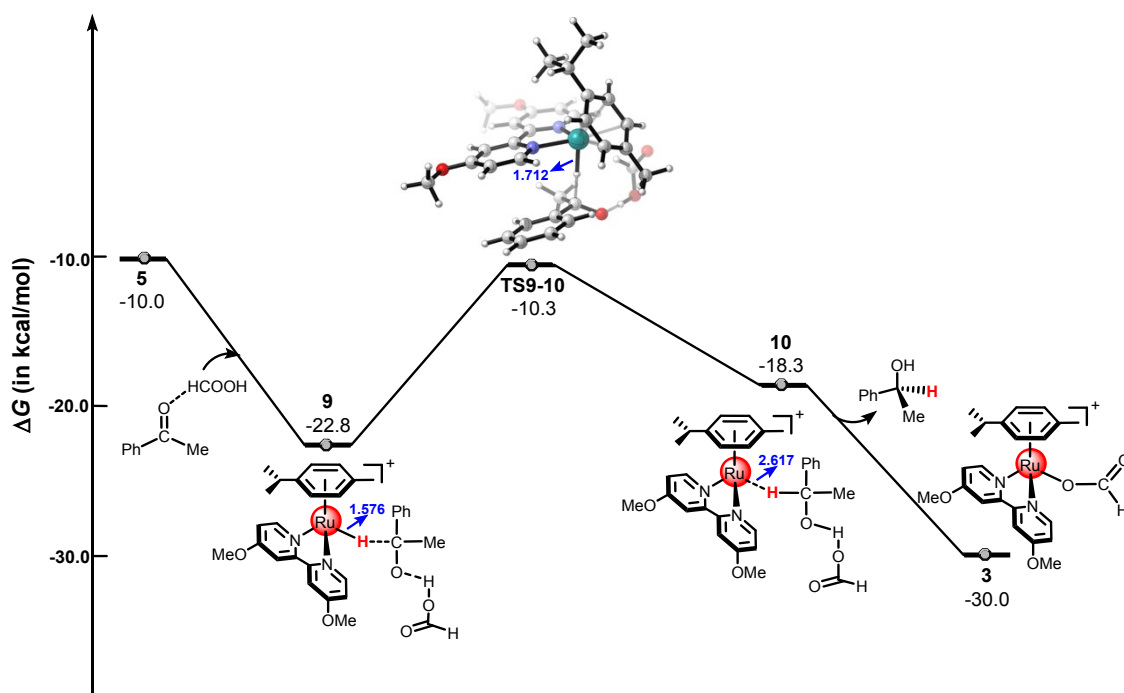
^c State Key Laboratory of Physical Chemistry of Solid Surfaces, Xiamen University, Xiamen 361005, China

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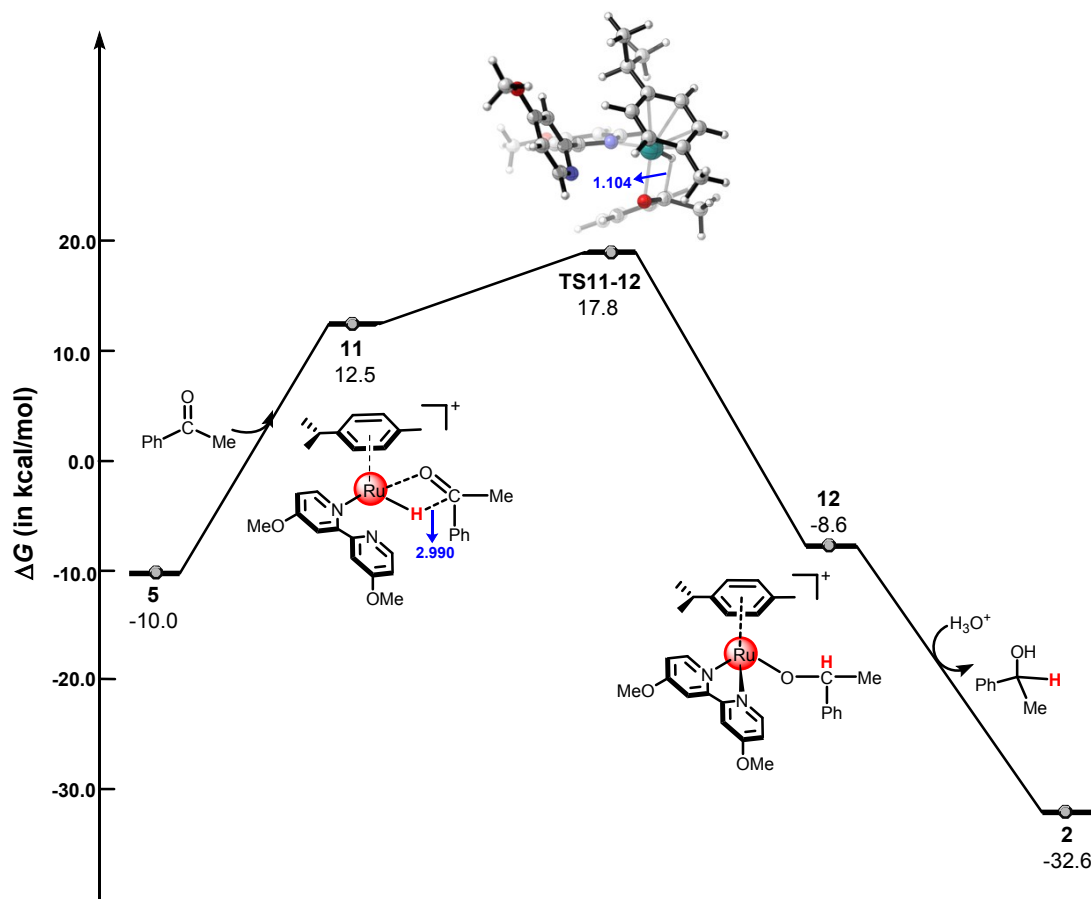
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Figure S1. The free energy profiles along the hydride transfer step by path B.



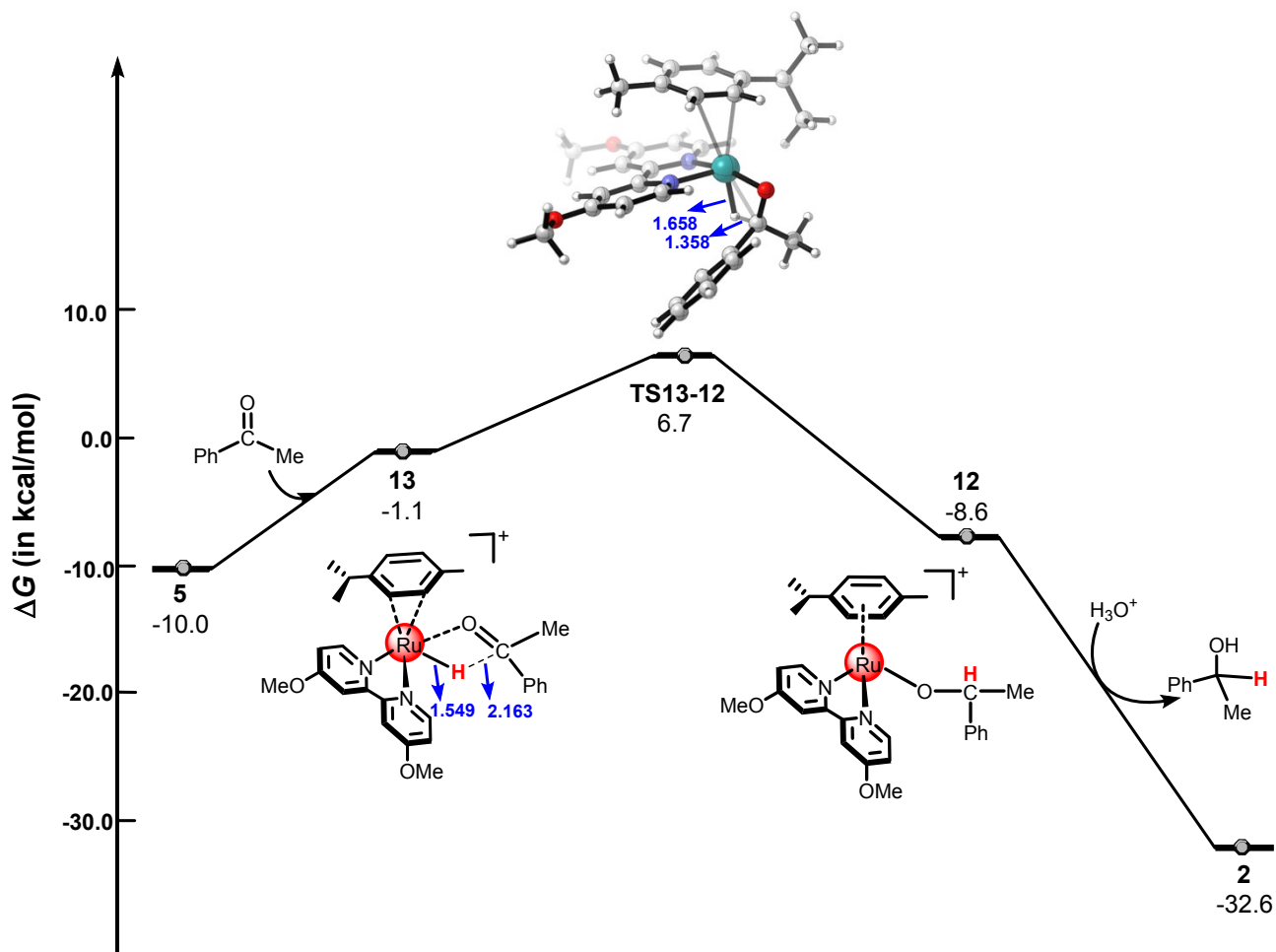
Path B: In this pathway, the ketone substrate could be stabilized with formic acid through hydrogen bond. Firstly, the ketone stabilized with formic acid coordinates with metal hydride **5** to form intermediate **9**. Then the hydride is transferred from Ru center to the carbon atom of ketone via **TS9-10** 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 from 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 η^6 -coordination to η^2 -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 H_7O_3^+ .

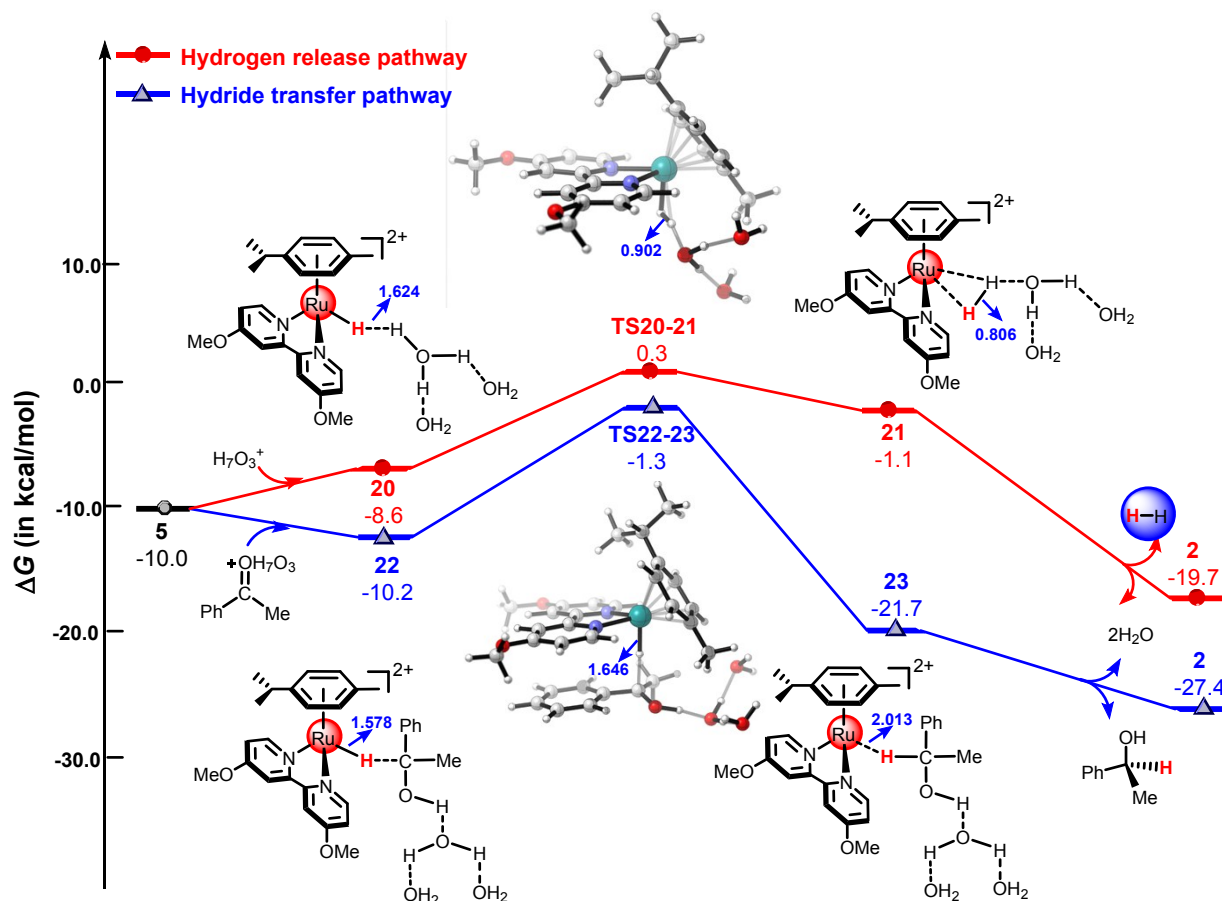
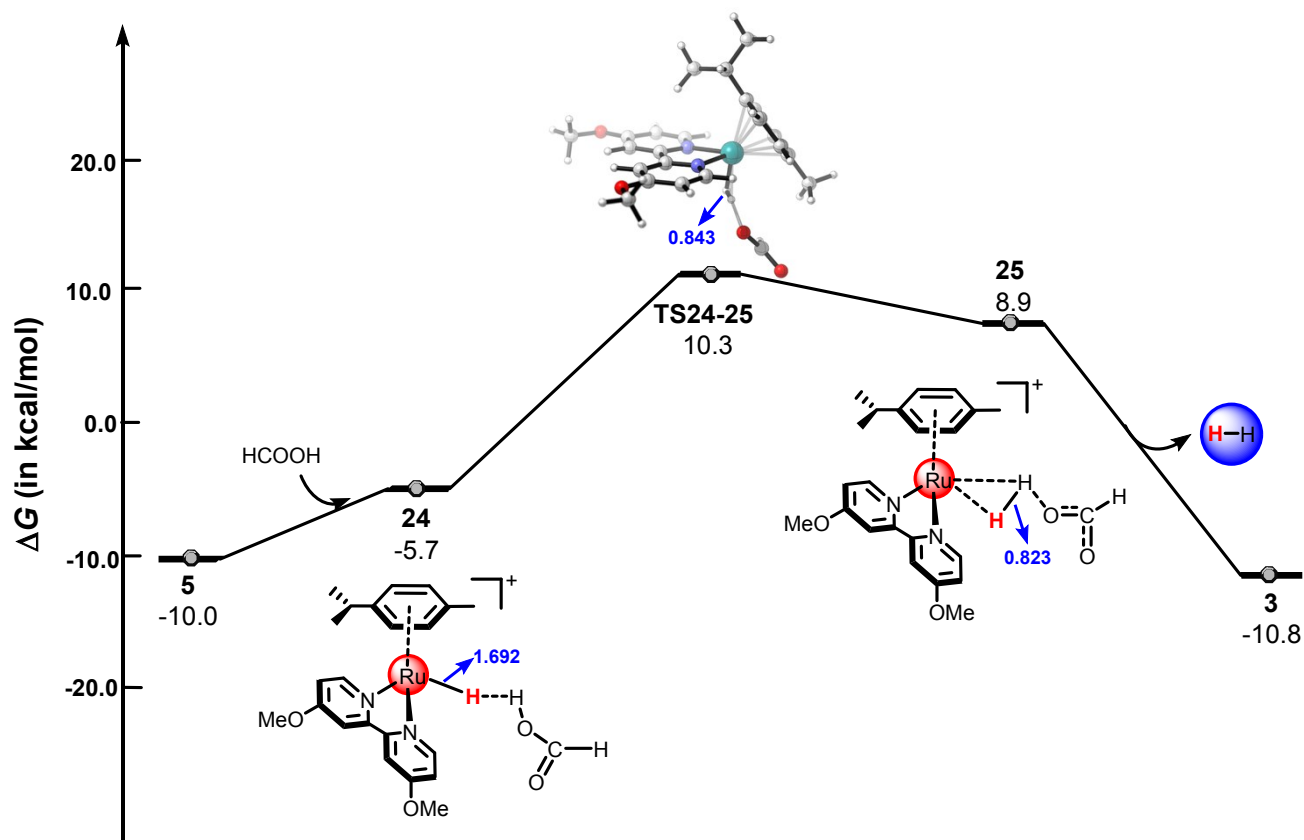


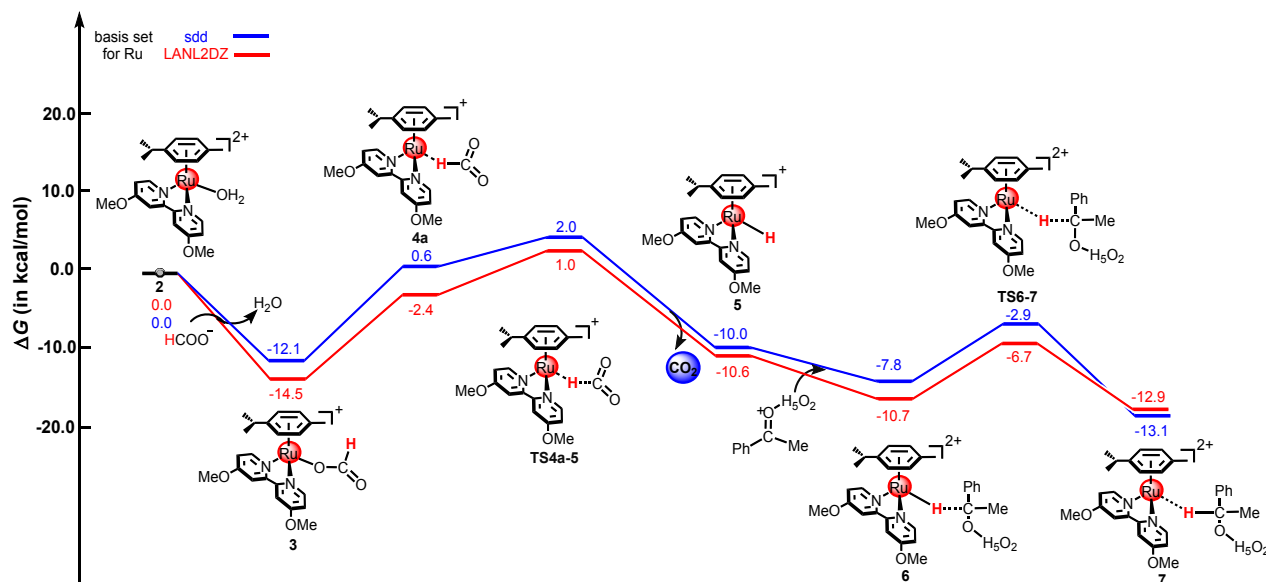
Figure S4 shows the free energy profiles of dihydrogen release pathway and hydride transfer pathway mediated by H_7O_3^+ , the energy barrier of the dihydrogen release pathway is 10.3 kcal/mol. Interestingly, the reaction along the hydride transfer pathway is 8.9 kcal/mol. In general, the dihydrogen 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 H_7O_3^+ .

Figure S5. The free energy profiles of hydrogen release pathway when proton source is HCOOH.



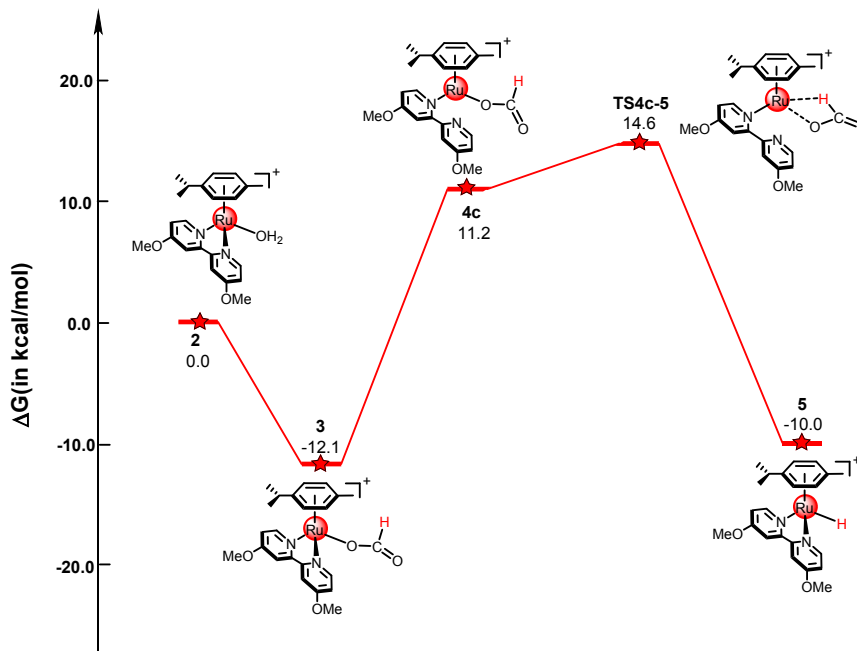
As shown in Figure S5, **TS24-25** with formic acid as proton source has an activation energy barrier of 20.3 kcal/mol, 10.9 kcal/mol higher than that of **TS14-15** with the hydrated proton H_3O_2^+ . The calculation results suggest that the hydrogen release pathway is more favorable along H_3O_2^+ 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.



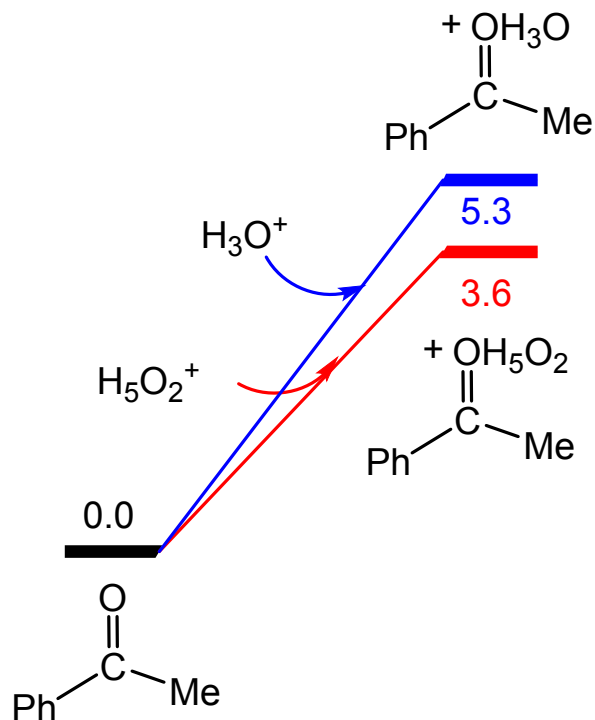
When the effective core potential (ECP) of Ru with a double- ζ valence basis set (LANL2DZ) was chosen to describe Ru, the metal hydride formation is the rate-determining step with a free energy barrier of 14.1 kcal/mol. When the sdd basis set was chosen to describe Ru, the metal hydride formation is 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.



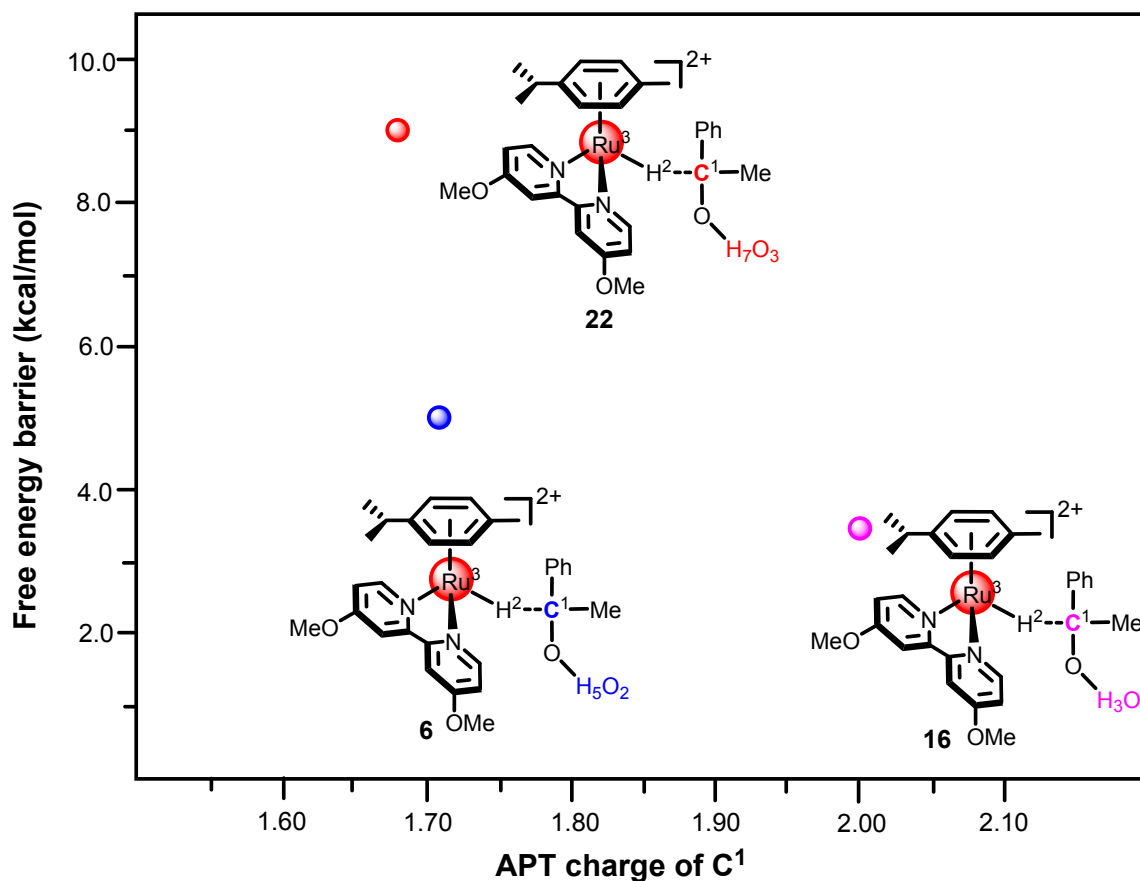
As shown in Figure S7, one 4-methylpyridine is dissociated to provide a vacant coordinate site to form complex **4c** firstly, this process is exothermic by 23.3 kcal/mol. Subsequently, the hydride transfers to Ru through **TS4c-5**, which owes an energy barrier of 26.7 kcal/mol. This high energy barrier implies that this pathway is less favorable than the ion-pair mechanism.

Figure S8. The free energy profiles of the formation of $\text{PhMeCOH}_5\text{O}_2^+$ and $\text{PhMeCOH}_3\text{O}^+$.



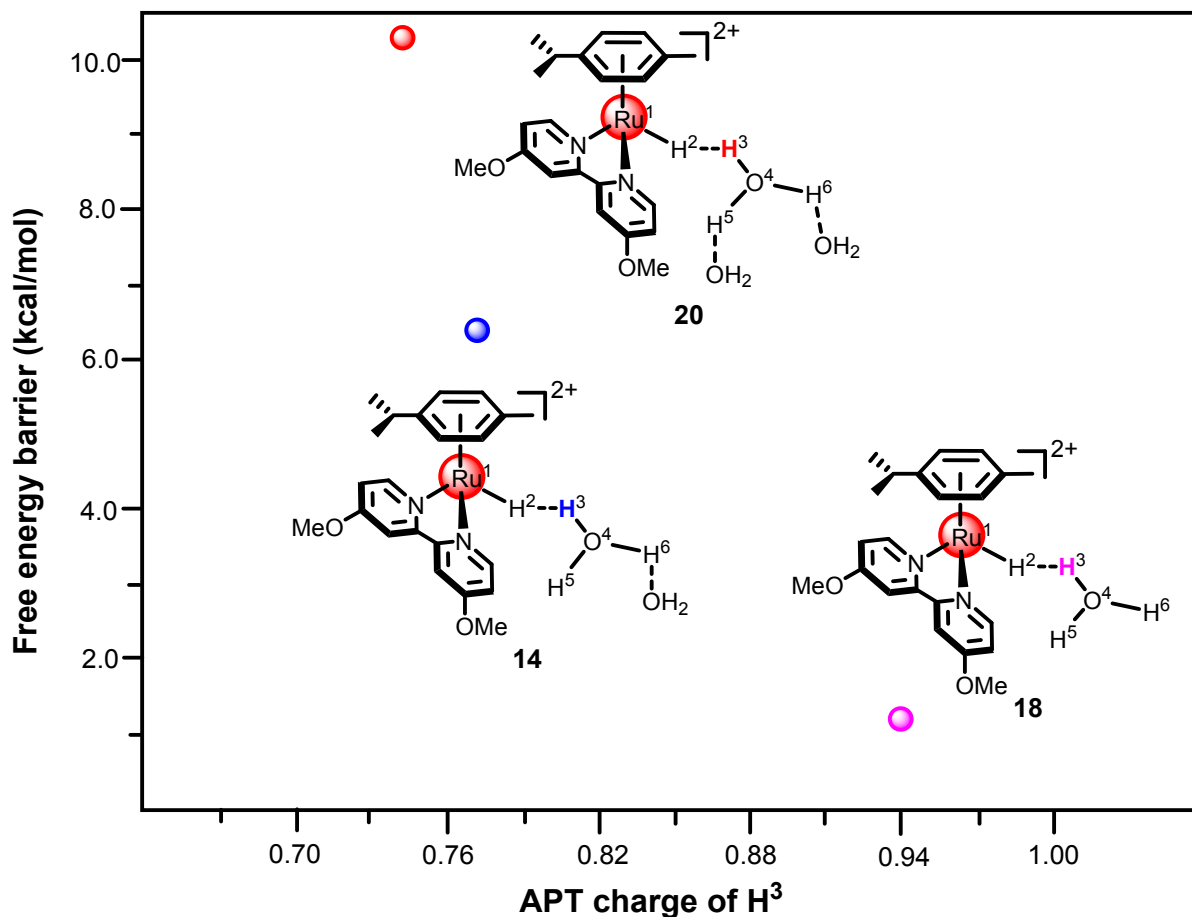
The reactions of $\text{PhMeCO} + \text{H}_5\text{O}_2^+ \rightarrow \text{PhMeCOH}_5\text{O}_2^+$ and $\text{PhMeCO} + \text{H}_3\text{O}^+ \rightarrow \text{PhMeCOH}_3\text{O}^+$ as shown in Figure S8, these processes are endergonic by 3.6 and 5.3 kcal/mol, respectively.

Figure S9. Relationship between APT charge of C¹ atom and free energy barriers of hydride transfer pathway.



As shown in Figure S9, the APT charges of C¹ in complex **22**, **6** and **16** are increasing in turn, however, the energy barriers of these pathways are decreasing in turn. It indicates that H₃O⁺ 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 H₃O⁺ is more favorable than those mediated by H₅O₂⁺ or H₇O₃⁺.

Figure S10. Relationship between APT charge of H³ atom and free energy barriers of hydrogen release pathway.



As shown in Figure S10, the APT charges of H³ in complex **20**, **14** and **18** are increasing in turn, however, the energy barriers of these pathways are decreasing in turn. This means that H₃O⁺ has stronger acidity. The calculated results show that the dihydrogen release pathway for the reaction mediated by H₃O⁺ is more favorable than those mediated by H₅O₂⁺ or H₇O₃⁺.

Table S1. The APT charge of H¹ atom in hydrated protons H₃O⁺, H₅O₂⁺ and H₇O₃⁺.

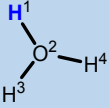
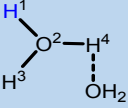
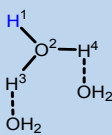
Hydrated proton			
APT charge of H ¹ atom	0.51	0.44	0.40

Table S2. The calculated electronic energies (E , in a. u.), free Gibbs energies (G , in a. u.), relative electronic energies (ΔE , kcal/mol), and relative Gibbs energies (ΔG , kcal/mol, 298K).

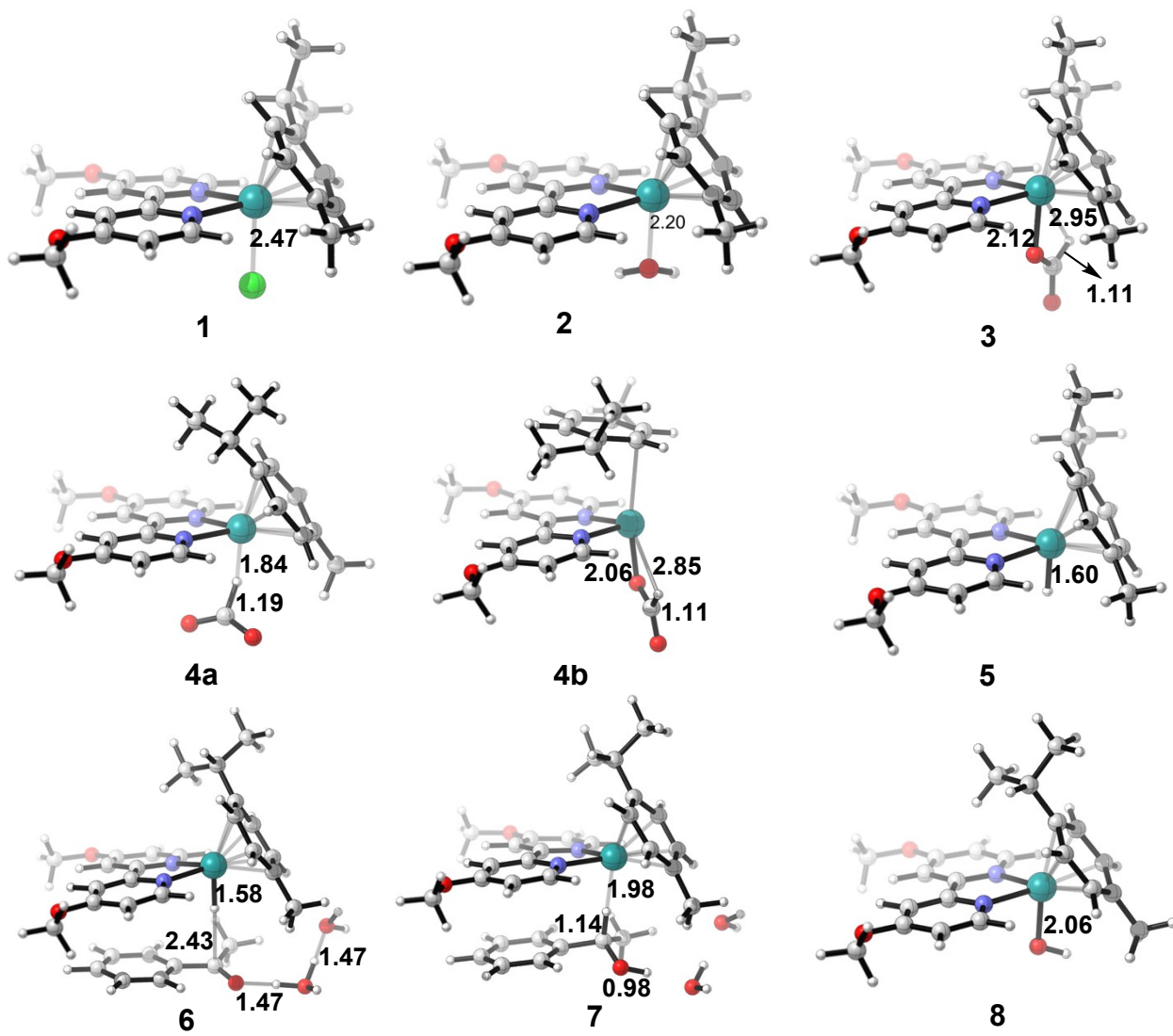
Complex	G	E	ΔE	ΔG
CO ₂	-188.525108	-188.51598911	\	\
H ₂ O	-76.407070	-76.41101011	\	\
H ₃ O ⁺	-76.823038	-76.83965507	\	\
H ₅ O ₂ ⁺	-153.244176	-153.27668220	\	\
H ₇ O ₃ ⁺	-229.650596	-229.70612822	\	\
HCOOH	-189.691831	-189.70231192	\	\
HCOO ⁻	-189.238205	-189.23601139	\	\
OH ⁻	-75.880497	-75.87298358	\	\
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 ₅ O ₂ ⁺	-537.916675	-538.07962941	\	\
PhCOCH ₃ ...H ₇ 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

12	-1592.295309	-1592.83277478	-15.2	-8.6
13	-1592.283316	-1592.81551942	-4.4	-1.1
TS13-12	-1592.270890	-1592.80000160	5.3	6.7
14	-1360.858805	-1361.31516122	-8.8	-7.1
TS14-15	-1360.848400	-1361.30291643	-1.1	-0.6
15	-1360.856080	-1361.30970441	-5.4	-5.4
16	-1669.130987	-1669.69517204	-29.5	-6.0
TS16-17	-1669.125403	-1669.69170204	-27.3	-2.5
17	-1669.148003	-1669.71865057	-44.2	-16.7
18	-1284.444144	-1284.88054613	-10.3	-11.2
TS18-19	-1284.446841	-1284.87630717	-9.9	-10.1
19	-1284.455409	-1284.88705326	-14.4	-18.2
20	-1437.267522	-1437.74786123	-23.4	-8.6
TS20-21	-1437.253417	-1437.72831119	-11.1	0.3
21	-1437.255509	-1437.73082754	-12.7	-1.1
22	-1821.944921	-1822.55320593	-14.1	-10.2
TS22-23	-1821.930703	-1822.54115003	-6.5	-1.3
24	-1397.313345	-1397.74679124	-12.5	-5.7
TS24-25	-1397.287870	-1397.71649807	6.5	10.3
25	-1397.290179	-1397.71664883	6.4	8.9

Table S3. Calculated imaginary frequencies of transition states at ω B97X-D/BSI level.

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

Figure S11. Typical geometric structure diagram.



Atomic Cartesian coordinates of intermediates and transition states (unit: Å).

2

Coordinates (Angstroms)			
	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	2.319114000	-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	2.527907000	-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	-3.209896000	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

6	3.217972000	-0.566037000	-0.516878000
1	3.818446000	0.064125000	-1.159075000
6	2.808816000	-0.112628000	0.759741000
6	3.241830000	1.220647000	1.341269000
6	4.186616000	2.017343000	0.443040000
6	3.911348000	0.977946000	2.704308000
1	2.329801000	1.805524000	1.512544000
1	3.772821000	2.221649000	-0.547310000
1	4.403277000	2.979352000	0.914537000
1	5.136028000	1.488179000	0.308912000
1	3.241760000	0.487318000	3.414683000
1	4.806081000	0.357878000	2.587322000
1	4.216084000	1.935168000	3.136022000
6	1.657523000	-4.085111000	-0.713417000
1	2.489645000	-4.773232000	-0.534492000
1	0.781658000	-4.477820000	-0.192823000
1	1.457796000	-4.066427000	-1.787121000
8	0.281936000	-0.705021000	-2.559496000
1	1.042066000	-0.478424000	-3.110846000
1	-0.355354000	0.005940000	-2.711406000

3

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	3.246773000	-0.274968000	-0.515178000
1	3.941703000	0.553485000	-0.572006000

6	3.734276000	-1.577514000	-0.682311000
6	2.842533000	-2.647832000	-0.579460000
1	3.152946000	-3.678980000	-0.682059000
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	0.679995000
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

4a

Coordinates (Angstroms)

	X	Y	Z
44	-1.294247000	-0.154450000	-0.295158000
7	0.312914000	-1.479613000	-0.102131000
7	0.366227000	1.115463000	-0.234791000

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

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	2.600993000	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

1	-0.299400000	-3.555086000	-0.839225000
6	-2.202074000	-2.560748000	-0.711269000
1	-2.621980000	-3.316795000	-0.052475000
6	-2.996078000	-1.484114000	-1.123530000
6	-2.412478000	-0.530475000	-1.956217000
1	-2.997502000	0.329902000	-2.271630000
6	-1.090188000	-0.648549000	-2.385803000
1	-0.681260000	0.120365000	-3.033309000
6	-0.300544000	-1.731136000	-1.996739000
6	1.123397000	-1.942084000	-2.484589000
6	1.747101000	-0.707654000	-3.133914000
6	1.181675000	-3.135400000	-3.449461000
1	1.724020000	-2.202755000	-1.603177000
1	1.658213000	0.180398000	-2.502212000
1	2.810467000	-0.882344000	-3.322928000
1	1.272155000	-0.484362000	-4.095824000
1	0.798085000	-4.048504000	-2.984690000
1	0.584716000	-2.934096000	-4.345918000
1	2.213599000	-3.323431000	-3.763254000
6	-4.430106000	-1.367839000	-0.679792000
1	-5.068771000	-2.061523000	-1.238014000
1	-4.539619000	-1.607002000	0.382293000
1	-4.814567000	-0.357502000	-0.842535000
8	0.552763000	-0.753710000	3.173371000
6	1.687624000	-1.192272000	3.602746000
1	2.250025000	-1.831514000	2.892703000
8	2.152337000	-0.949006000	4.717892000

TS4a-5

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

6	-5.337063000	-2.616785000	-1.296252000
1	-5.636594000	-2.106641000	-0.376157000
1	-6.094240000	-3.348599000	-1.572170000
1	-5.213330000	-1.891107000	-2.105448000
6	-1.525275000	0.681168000	0.008348000
6	-2.547648000	1.607481000	-0.041950000
1	-3.563272000	1.325252000	-0.287844000
6	-2.271793000	2.950405000	0.240735000
6	-0.965380000	3.311264000	0.579044000
1	-0.684841000	4.328192000	0.817603000
6	-0.001429000	2.320302000	0.611535000
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	5.599527000	-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	-0.647174000	-1.688266000
1	1.922255000	-0.733946000	-2.685142000
6	2.618542000	0.612840000	-1.133261000
6	2.414820000	1.904114000	-1.894092000
6	1.202137000	1.889105000	-2.824463000
6	3.704208000	2.227989000	-2.662013000
1	2.263590000	2.690252000	-1.145923000
1	0.284681000	1.628511000	-2.288141000
1	1.068065000	2.880806000	-3.265780000
1	1.332561000	1.178522000	-3.646880000
1	4.565551000	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

TS4b-5

Coordinates (Angstroms)

	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	-1.199033000
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	-0.117278000
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	-0.307738000	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

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	-3.317109000	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

6	-1.495318000	-2.400717000	0.056590000
1	-0.779651000	-3.207158000	-0.052630000
6	-5.550894000	-3.020940000	0.934426000
1	-5.425924000	-3.613347000	0.023366000
1	-6.611168000	-2.875569000	1.135102000
1	-5.081241000	-3.529879000	1.781206000
6	2.181582000	-1.120754000	1.406206000
1	1.845930000	-1.032005000	2.431853000
6	1.874663000	-2.308764000	0.682089000
1	1.304617000	-3.088738000	1.177538000
6	2.302897000	-2.524781000	-0.649111000
6	2.953315000	-1.430836000	-1.293007000
1	3.248755000	-1.522407000	-2.332214000
6	3.179015000	-0.213694000	-0.616449000
1	3.645771000	0.597929000	-1.158385000
6	2.819835000	-0.047993000	0.762306000
1	0.458671000	-0.849341000	-2.088898000
6	3.068186000	1.260822000	1.505608000
6	3.941119000	2.253143000	0.734709000
6	3.694732000	0.996383000	2.882448000
1	2.085789000	1.724755000	1.662100000
1	3.499045000	2.560763000	-0.215553000
1	4.076560000	3.156134000	1.336250000
1	4.932196000	1.832159000	0.533398000
1	3.060987000	0.376614000	3.520923000
1	4.664213000	0.498388000	2.774486000
1	3.857066000	1.946033000	3.400440000
6	2.069396000	-3.831507000	-1.348142000
1	2.916118000	-4.505569000	-1.181261000
1	1.169890000	-4.320214000	-0.965076000
1	1.957466000	-3.684636000	-2.424591000

6

Coordinates (Angstroms)

	X	Y	Z
44	1.170782000	0.415564000	0.615179000
7	-0.156213000	0.998999000	-0.897182000
7	-0.718858000	0.154779000	1.499032000
8	-2.858206000	2.329729000	-3.709402000
8	-4.572375000	-0.216259000	2.908399000
6	0.214546000	1.335958000	-2.144900000
1	1.268674000	1.240431000	-2.374278000
6	-0.676114000	1.776634000	-3.096617000
1	-0.339161000	2.030047000	-4.094215000

6	-2.027525000	1.894465000	-2.751223000
6	-2.421592000	1.543332000	-1.460431000
1	-3.457155000	1.604823000	-1.157238000
6	-1.461194000	1.078751000	-0.570206000
6	-4.249435000	2.429105000	-3.406340000
1	-4.656976000	1.455136000	-3.119186000
1	-4.727140000	2.769119000	-4.323844000
1	-4.425200000	3.158403000	-2.609879000
6	-1.787735000	0.573976000	0.778255000
6	-3.077914000	0.463442000	1.260213000
1	-3.934075000	0.786377000	0.682183000
6	-3.295187000	-0.122474000	2.511190000
6	-2.194270000	-0.579733000	3.238532000
1	-2.290955000	-1.056837000	4.204366000
6	-0.934649000	-0.417281000	2.689254000
1	-0.054903000	-0.758835000	3.221274000
6	-4.840386000	-0.844850000	4.162109000
1	-4.498609000	-1.884113000	4.156269000
1	-5.922324000	-0.816432000	4.281948000
1	-4.366542000	-0.298566000	4.982902000
6	2.221753000	1.776020000	2.234334000
1	1.777006000	2.319357000	3.061777000
6	2.529418000	0.386095000	2.405143000
1	2.316138000	-0.091184000	3.355299000
6	3.126734000	-0.368945000	1.374243000
6	3.322797000	0.272234000	0.107559000
1	3.733139000	-0.284617000	-0.726466000
6	2.919621000	1.610669000	-0.069101000
1	3.021969000	2.055328000	-1.053797000
6	2.428574000	2.417864000	1.014068000
1	0.885169000	-1.035186000	0.063048000
6	2.121556000	3.887118000	0.813881000
6	1.075950000	4.124917000	-0.280255000
6	3.415670000	4.653431000	0.513184000
1	1.712844000	4.261052000	1.759305000
1	0.134305000	3.619108000	-0.046644000
1	0.876069000	5.196431000	-0.378249000
1	1.425912000	3.763026000	-1.252950000
1	4.155095000	4.515164000	1.307977000
1	3.859851000	4.313228000	-0.428869000
1	3.210436000	5.724187000	0.419963000
6	3.517078000	-1.803906000	1.576746000
1	4.594531000	-1.875755000	1.759283000
1	2.994790000	-2.231967000	2.435179000

1	3.281782000	-2.398944000	0.692588000
6	-3.032625000	-1.689364000	-1.980571000
6	-1.676512000	-1.924496000	-2.186167000
6	-0.935464000	-2.623334000	-1.227058000
6	-1.560931000	-3.064074000	-0.051476000
6	-2.908055000	-2.810554000	0.157959000
6	-3.646610000	-2.127266000	-0.810367000
1	-3.604788000	-1.152568000	-2.730102000
1	-1.206032000	-1.566533000	-3.095770000
1	-0.978906000	-3.594353000	0.694411000
1	-3.385466000	-3.137728000	1.075673000
1	-4.700865000	-1.929411000	-0.645016000
6	0.502748000	-2.916542000	-1.428666000
8	1.051300000	-3.753233000	-0.695724000
6	1.263368000	-2.242589000	-2.527986000
1	1.034062000	-2.750521000	-3.472056000
1	0.976330000	-1.195728000	-2.634040000
1	2.335404000	-2.311565000	-2.342419000
8	3.453924000	-4.423655000	-0.963215000
1	4.024716000	-3.604571000	-1.248988000
1	2.463025000	-4.124992000	-0.869017000
1	3.761030000	-4.703013000	-0.087887000
8	4.796839000	-2.411016000	-1.630312000
1	5.502535000	-2.628149000	-2.252436000
1	5.241857000	-2.077073000	-0.840736000

TS6-7

Coordinates (Angstroms)

	X	Y	Z
44	1.165988000	0.222110000	0.576591000
7	-0.108569000	1.160539000	-0.785214000
7	-0.737318000	-0.206381000	1.334439000
8	-2.727413000	3.085012000	-3.312551000
8	-4.608606000	-0.705589000	2.640646000
6	0.302678000	1.773215000	-1.909600000
1	1.365264000	1.734791000	-2.114767000
6	-0.560249000	2.416495000	-2.765909000
1	-0.192613000	2.895692000	-3.664671000
6	-1.925392000	2.444007000	-2.452768000
6	-2.360446000	1.803504000	-1.292557000
1	-3.407756000	1.779436000	-1.026388000
6	-1.423879000	1.161246000	-0.492865000
6	-4.127805000	3.120434000	-3.033691000
1	-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	3.757488000
6	-0.980170000	-0.988325000	2.392780000
1	-0.118277000	-1.457969000	2.850639000
6	-4.912202000	-1.539056000	3.759935000
1	-4.626746000	-2.576094000	3.560105000
1	-5.991195000	-1.474946000	3.891024000
1	-4.411241000	-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	-0.925558000	3.174889000
6	3.122156000	-0.683556000	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	2.292748000	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	3.579241000	-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

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
44	1.247387000	0.219976000	0.563140000
7	0.001588000	1.155567000	-0.828414000
7	-0.665954000	-0.071429000	1.355401000
8	-2.511126000	3.127886000	-3.407843000
8	-4.555032000	-0.578775000	2.570352000
6	0.448040000	1.710621000	-1.969858000
1	1.507544000	1.613726000	-2.171643000
6	-0.383359000	2.365359000	-2.846156000
1	0.006408000	2.799563000	-3.758096000
6	-1.745601000	2.471187000	-2.533442000
6	-2.214579000	1.886571000	-1.353561000
1	-3.260523000	1.927863000	-1.084247000
6	-1.312941000	1.223412000	-0.536772000
6	-3.907745000	3.258399000	-3.131234000
1	-4.384776000	2.276235000	-3.067063000
1	-4.321749000	3.813766000	-3.970853000
1	-4.066879000	3.815612000	-2.203777000
6	-1.701833000	0.494158000	0.686685000
6	-3.003457000	0.339456000	1.107375000
1	-3.833048000	0.779229000	0.569505000
6	-3.269035000	-0.443040000	2.239511000

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	-1.066946000	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	0.225902000
1	0.855457000	5.080229000	0.689886000
1	1.715856000	4.027373000	-0.434510000
1	3.475750000	3.785225000	2.986540000
1	3.743942000	4.266962000	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	-0.090010000
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	-3.499027000	0.573790000
1	-3.646126000	-3.471119000	0.712113000
1	-4.974715000	-2.183426000	-0.946581000

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	-3.365693000	-2.084132000
1	1.791014000	-3.626369000	-1.115370000
1	3.775297000	-4.535102000	-1.095833000
8	4.648118000	-1.814135000	-2.327516000
1	5.139616000	-1.819444000	-3.156606000
1	5.325512000	-1.825563000	-1.641231000

8

Coordinates (Angstroms)

	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	-4.018789000	-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

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	-1.081414000
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	2.896983000
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

9

Coordinates (Angstroms)

	X	Y	Z
44	-0.997818000	-0.810484000	-0.494369000
7	-0.843058000	1.258172000	-0.124402000
7	0.927488000	-0.331077000	-1.199159000
8	-0.326947000	5.270278000	0.675510000
8	4.684295000	0.913722000	-2.342436000
6	-1.788073000	1.998811000	0.481995000
1	-2.703228000	1.486807000	0.751813000
6	-1.630989000	3.337257000	0.758026000
1	-2.417887000	3.894918000	1.250663000
6	-0.436128000	3.965711000	0.389612000
6	0.552209000	3.207156000	-0.237925000
1	1.491849000	3.652970000	-0.531720000

6	0.314807000	1.857183000	-0.471914000
6	0.883860000	5.941953000	0.327341000
1	1.738381000	5.499552000	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	-2.365606000
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

6	2.280598000	-0.969480000	2.211175000
6	2.328036000	-2.348884000	1.969418000
6	3.375875000	-2.896370000	1.241104000
6	4.392179000	-2.071886000	0.757817000
1	5.129108000	-0.055234000	0.595749000
1	3.262469000	0.927395000	1.862884000
1	1.536829000	-2.983901000	2.353139000
1	3.404427000	-3.964579000	1.052574000
1	5.213832000	-2.499353000	0.191723000
6	1.150575000	-0.417426000	3.004535000
8	0.391149000	-1.188743000	3.598149000
6	0.962686000	1.068651000	3.082846000
1	1.802417000	1.511825000	3.628677000
1	0.956070000	1.514061000	2.084668000
1	0.035711000	1.305808000	3.603994000
1	-1.780052000	-0.024037000	2.300906000
6	-2.526677000	-0.006924000	3.108829000
8	-2.071487000	-0.425393000	4.278626000
1	-1.120511000	-0.688855000	4.161201000
8	-3.676504000	0.354416000	2.945487000

TS9-10

Coordinates (Angstroms)

	X	Y	Z
44	0.803490000	-0.620610000	0.635351000
7	1.040075000	1.277505000	-0.213757000
7	-1.108634000	0.206429000	0.782104000
8	1.366735000	5.046300000	-1.832468000
8	-4.821403000	1.965786000	0.611331000
6	2.207706000	1.757819000	-0.676702000
1	3.065242000	1.099862000	-0.604126000
6	2.331179000	3.014604000	-1.221368000
1	3.287230000	3.367770000	-1.587197000
6	1.196675000	3.832748000	-1.295289000
6	-0.018024000	3.341497000	-0.812603000
1	-0.917255000	3.940779000	-0.842329000
6	-0.056092000	2.058955000	-0.283411000
6	0.237737000	5.916627000	-1.926251000
1	-0.540954000	5.476261000	-2.555680000
1	0.609582000	6.829670000	-2.388157000
1	-0.164594000	6.141327000	-0.934265000
6	-1.288621000	1.435207000	0.241766000
6	-2.535759000	2.025096000	0.183226000
1	-2.688816000	2.993294000	-0.276483000

6	-3.637903000	1.349667000	0.720194000
6	-3.439186000	0.101330000	1.312871000
1	-4.245379000	-0.475649000	1.744588000
6	-2.164257000	-0.432091000	1.299911000
1	-1.982860000	-1.418544000	1.707378000
6	-5.973915000	1.303482000	1.134717000
1	-6.134439000	0.347069000	0.627790000
1	-6.811344000	1.970461000	0.936433000
1	-5.874357000	1.144977000	2.212291000
6	0.698164000	-1.577350000	2.644305000
1	-0.180993000	-1.567702000	3.281585000
6	0.839839000	-2.616417000	1.694253000
1	0.087487000	-3.393064000	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	3.385386000	0.329313000	1.793268000
6	1.634216000	-0.513969000	2.755425000
1	0.235942000	-1.025050000	-0.928901000
6	1.478770000	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	-3.699473000	-0.224785000
1	3.080940000	-4.179082000	-0.095562000
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

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	2.678901000	-1.825521000	-3.523417000
1	1.706973000	-2.043916000	-3.222970000
8	4.379721000	-0.688046000	-2.627910000

10

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

1	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	1.290797000
6	-3.263534000	-1.191265000	-0.744993000
1	-4.047225000	-0.459628000	-0.582019000
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
1	-5.060702000	-0.877457000	-3.089726000
1	-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

6	-1.994617000	-0.597717000	3.300003000
8	-1.302045000	-1.133577000	4.213394000
1	0.303682000	-1.426914000	3.700654000
8	-3.220077000	-0.351005000	3.338722000

11

Coordinates (Angstroms)

	X	Y	Z
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

6	-2.617723000	-2.303946000	1.156296000
1	-2.641240000	-2.699814000	2.163840000
6	-2.757942000	-0.910721000	0.926739000
6	-3.001871000	0.072926000	2.052971000
6	-2.311907000	-0.304755000	3.362687000
6	-4.512531000	0.249181000	2.250376000
1	-2.590872000	1.031287000	1.717109000
1	-1.244779000	-0.493704000	3.210582000
1	-2.415742000	0.511554000	4.083535000
1	-2.758307000	-1.196813000	3.814718000
1	-5.001477000	0.567033000	1.324059000
1	-4.971111000	-0.691979000	2.573622000
1	-4.711321000	1.005909000	3.015500000
6	-1.812799000	-3.538949000	-2.386331000
1	-2.695849000	-3.855840000	-2.951245000
1	-1.153555000	-2.997014000	-3.068695000
1	-1.294564000	-4.430950000	-2.027983000
6	4.027024000	1.025081000	-1.728522000
6	3.029515000	0.061574000	-1.657944000
6	3.258455000	-1.140506000	-0.976331000
6	4.501761000	-1.366874000	-0.369066000
6	5.490367000	-0.392379000	-0.426477000
6	5.253805000	0.803367000	-1.104323000
1	3.842757000	1.958123000	-2.250852000
1	2.054678000	0.244028000	-2.097452000
1	4.693121000	-2.290398000	0.166663000
1	6.445287000	-0.562732000	0.059146000
1	6.026474000	1.564650000	-1.142994000
6	2.132804000	-2.085986000	-0.798512000
8	1.005593000	-1.751443000	-1.189045000
6	2.352569000	-3.395791000	-0.109748000
1	3.206674000	-3.920135000	-0.546634000
1	2.575572000	-3.219842000	0.947947000
1	1.451551000	-4.003949000	-0.187968000
1	-0.054489000	-2.539620000	1.188630000

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Coordinates (Angstroms)			
	X	Y	Z

44	0.004822000	-1.519878000	0.104071000
7	0.621576000	0.537686000	0.429764000
7	-1.167635000	0.870780000	-2.106139000
8	2.394346000	4.228572000	1.052670000
8	-4.572280000	2.609685000	-0.487159000

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	-0.161830000
6	1.980277000	5.371328000	0.302776000
1	2.083178000	5.186705000	-0.770579000
1	2.648497000	6.177356000	0.601930000
1	0.947557000	5.642651000	0.539759000
6	-1.165032000	1.532858000	-0.940690000
6	-2.285928000	2.145699000	-0.399727000
1	-2.232992000	2.681826000	0.541099000
6	-3.509329000	2.021753000	-1.066944000
6	-3.541895000	1.295039000	-2.258002000
1	-4.453308000	1.146199000	-2.822669000
6	-2.346154000	0.759522000	-2.723536000
1	-2.344411000	0.210731000	-3.661422000
6	-5.847495000	2.439606000	-1.102974000
1	-5.860124000	2.870955000	-2.108398000
1	-6.555696000	2.972181000	-0.469670000
1	-6.119379000	1.380555000	-1.148999000
6	-2.284413000	-1.265863000	0.401348000
1	-2.893331000	-0.397057000	0.184294000
6	-2.112245000	-2.244305000	-0.568150000
1	-2.576137000	-2.126049000	-1.541909000
6	-1.258422000	-3.372339000	-0.327017000
6	-0.644691000	-3.487934000	0.935241000
1	0.015254000	-4.325610000	1.131743000
6	-0.811631000	-2.479881000	1.933336000
1	-0.287622000	-2.578812000	2.875256000
6	-1.593441000	-1.337868000	1.662054000
6	-1.797098000	-0.210030000	2.652020000
6	-0.771950000	-0.180165000	3.782622000
6	-3.224912000	-0.288674000	3.209350000
1	-1.708993000	0.721353000	2.080098000
1	0.253710000	-0.192366000	3.403901000
1	-0.904489000	0.732921000	4.369257000
1	-0.897703000	-1.031338000	4.460280000
1	-3.973216000	-0.235510000	2.412851000
1	-3.372733000	-1.225755000	3.756865000
1	-3.404968000	0.541329000	3.898899000

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	2.260502000	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	2.056534000	-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

6	-1.494448000	0.919046000	-0.664917000
6	-2.757781000	1.471860000	-0.730945000
1	-3.585144000	0.955298000	-1.199975000
6	-2.989776000	2.718475000	-0.138718000
6	-1.935148000	3.361363000	0.513971000
1	-2.051100000	4.312543000	1.015734000
6	-0.694947000	2.748313000	0.507402000
1	0.149939000	3.210796000	1.002798000
6	-4.526525000	4.451314000	0.384397000
1	-4.350245000	4.405963000	1.463005000
1	-5.582151000	4.637271000	0.192974000
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	2.950518000	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	-0.391454000
1	3.815512000	-2.143524000	-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	-1.405025000
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	-0.450530000	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

1	-0.891865000	-3.558121000	1.344374000
1	-3.325848000	-3.905464000	1.053157000
1	-4.904569000	-2.027318000	1.445791000
6	0.430557000	-1.298457000	2.077009000
8	0.873550000	-0.002255000	1.813501000
6	0.834993000	-1.668003000	3.510256000
1	0.353850000	-0.989198000	4.223212000
1	0.540154000	-2.693444000	3.756562000
1	1.920140000	-1.579686000	3.627186000
1	0.908975000	-2.032966000	1.405528000

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Coordinates (Angstroms)

	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	2.320907000	-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

1	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	3.205534000	-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

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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	2.906165000	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	5.555744000	-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

1	4.759258000	-1.863947000	-0.189601000
1	2.500429000	-2.467349000	-1.187179000
1	3.648529000	-3.817027000	-1.140086000
1	2.339917000	-3.732985000	0.046269000
1	5.361241000	-2.714873000	2.067724000
1	3.925116000	-3.753862000	2.072802000
1	5.227900000	-4.052426000	0.910205000
6	0.916858000	1.994503000	2.913173000
1	1.080716000	2.936459000	2.381892000
1	-0.151990000	1.761843000	2.877402000
1	1.182128000	2.156607000	3.964015000
6	-4.304565000	-0.548530000	-1.811621000
6	-3.004431000	-1.037933000	-1.882453000
6	-2.596577000	-2.083723000	-1.052231000
6	-3.515503000	-2.657406000	-0.174016000
6	-4.820236000	-2.172782000	-0.106590000
6	-5.214887000	-1.111078000	-0.916993000
1	-4.604435000	0.280132000	-2.445487000
1	-2.287548000	-0.577416000	-2.558443000
1	-3.198365000	-3.463471000	0.479821000
1	-5.524262000	-2.616376000	0.590643000
1	-6.225642000	-0.720771000	-0.850961000
6	-1.161393000	-2.590464000	-1.055811000
8	-0.692287000	-3.002540000	0.124227000
6	-0.816265000	-3.493269000	-2.237864000
1	-1.356444000	-4.437885000	-2.119512000
1	-1.106272000	-3.039285000	-3.188744000
1	0.258453000	-3.695491000	-2.245505000

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Coordinates (Angstroms)

	X	Y	Z
44	-1.117855000	-0.273402000	-0.175008000
7	0.718843000	-0.992815000	-0.903663000
7	0.231925000	1.266172000	0.308935000
8	4.435440000	-2.517615000	-1.803427000
8	3.167899000	3.978858000	1.297537000
6	0.875289000	-2.177210000	-1.520355000
1	-0.032433000	-2.717201000	-1.759800000
6	2.109985000	-2.696742000	-1.834034000
1	2.198589000	-3.659915000	-2.320929000
6	3.254716000	-1.961172000	-1.503510000
6	3.098152000	-0.714151000	-0.896194000
1	3.954818000	-0.107664000	-0.637620000

6	1.814958000	-0.264755000	-0.611840000
6	5.627044000	-1.798478000	-1.482929000
1	5.668551000	-0.850502000	-2.027199000
1	6.449752000	-2.438316000	-1.798362000
1	5.695927000	-1.617210000	-0.406166000
6	1.540344000	1.031200000	0.042926000
6	2.522944000	1.945354000	0.370556000
1	3.567974000	1.760509000	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	2.198888000	5.825211000	1.324463000
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	-2.888804000	0.241204000	1.114935000
1	-3.194138000	1.239777000	1.407305000
6	-3.380448000	-0.310017000	-0.085886000
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	-3.049431000	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	-0.722827000
1	-4.175979000	0.263949000	-1.996191000
8	-2.126657000	2.749540000	-1.636226000
1	-2.556490000	3.047273000	-0.819075000

1	-2.871803000	2.691225000	-2.426085000
1	-1.783544000	1.831525000	-1.454558000
8	-3.763214000	2.601939000	-3.443726000
1	-3.802791000	3.442411000	-3.918920000
1	-4.646563000	2.471798000	-3.074140000

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Coordinates (Angstroms)

	X	Y	Z
44	-1.161821000	-0.205691000	-0.130910000
7	0.599735000	-1.079830000	-0.847160000
7	0.293123000	1.249422000	0.259078000
8	4.163474000	-2.863598000	-1.853670000
8	3.390194000	3.849133000	0.996234000
6	0.650696000	-2.300948000	-1.407110000
1	-0.298421000	-2.794014000	-1.576136000
6	1.835522000	-2.906703000	-1.753977000
1	1.841543000	-3.894419000	-2.197521000
6	3.037045000	-2.226857000	-1.518001000
6	2.986533000	-0.947148000	-0.960140000
1	3.889453000	-0.384288000	-0.769367000
6	1.749514000	-0.407683000	-0.639745000
6	5.413010000	-2.210516000	-1.619136000
1	5.479963000	-1.281042000	-2.191650000
1	6.175005000	-2.908308000	-1.962204000
1	5.551355000	-2.008550000	-0.553026000
6	1.575814000	0.929949000	-0.038727000
6	2.613536000	1.805931000	0.205472000
1	3.639153000	1.557224000	-0.036222000
6	2.338341000	3.053046000	0.780856000
6	1.012558000	3.377200000	1.081651000
1	0.728056000	4.322557000	1.523297000
6	0.030839000	2.446505000	0.796713000
1	-1.009882000	2.661926000	1.007270000
6	3.161837000	5.125177000	1.598510000
1	2.525479000	5.746653000	0.961852000
1	4.144421000	5.583874000	1.695970000
1	2.708854000	5.010680000	2.587322000
6	-2.056128000	-0.074386000	1.948507000
1	-1.686253000	0.572391000	2.737702000
6	-3.004775000	0.441329000	1.028575000
1	-3.365636000	1.457355000	1.138535000
6	-3.448546000	-0.347544000	-0.058207000
6	-2.907802000	-1.656368000	-0.216987000

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

15

Coordinates (Angstroms)

	X	Y	Z
44	-1.199237000	-0.215954000	-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	5.326428000	-2.530342000	-1.322567000

1	5.396833000	-1.710882000	-2.043619000
1	6.072920000	-3.288168000	-1.552929000
1	5.481411000	-2.155182000	-0.307126000
6	1.541008000	0.888637000	-0.246887000
6	2.586531000	1.775011000	-0.103461000
1	3.616637000	1.468151000	-0.233104000
6	2.313000000	3.111357000	0.218825000
6	0.981547000	3.509190000	0.372304000
1	0.700766000	4.526426000	0.608999000
6	-0.008221000	2.557239000	0.218118000
1	-1.052394000	2.818165000	0.338539000
6	3.151708000	5.282899000	0.693918000
1	2.586804000	5.790652000	-0.092797000
1	4.141918000	5.726998000	0.780673000
1	2.627312000	5.365124000	1.649931000
6	-1.925162000	0.382112000	1.877897000
1	-1.525177000	1.228613000	2.427695000
6	-3.010603000	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	-1.275003000	-2.897934000	1.184802000
6	-1.266310000	-0.872983000	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	2.341486000	-1.311063000
1	-2.934209000	1.932924000	-2.779674000
1	-1.504891000	0.573598000	-1.796174000

8	-3.557432000	0.621405000	-3.861604000
1	-4.493251000	0.575803000	-3.634542000
1	-3.181598000	-0.154455000	-3.429606000

16

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
1	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	-3.835866000	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	-3.887369000	0.985861000
1	-4.143186000	-4.042525000	-0.648071000
1	-3.767974000	-5.260601000	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

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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	0.381496000	1.647053000	-2.104944000
1	1.388904000	1.485587000	-2.468976000
6	-0.526055000	2.376740000	-2.837105000
1	-0.250632000	2.804814000	-3.792899000
6	-1.816745000	2.558156000	-2.323099000
6	-2.136256000	1.984569000	-1.093054000
1	-3.124518000	2.088597000	-0.668465000
6	-1.165533000	1.246932000	-0.428114000
6	-4.007456000	3.433979000	-2.605485000
1	-4.497567000	2.462177000	-2.491473000
1	-4.517835000	4.013618000	-3.373086000
1	-4.028898000	3.979655000	-1.657698000
6	-1.421023000	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
1	0.358479000	-1.426059000	2.776762000
6	-4.263121000	-1.071769000	4.321102000
1	-4.069247000	-2.127865000	4.111252000
1	-5.313849000	-0.933357000	4.570703000
1	-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
1	2.927629000	-1.533901000	2.373055000
6	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

1	1.563508000	3.781796000	-0.234246000
1	4.596987000	3.517103000	2.096624000
1	4.096569000	4.076021000	0.490183000
1	3.593661000	4.969213000	1.934733000
6	3.802974000	-2.374238000	-0.087009000
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	-1.188909000	-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	-3.006633000	0.986971000
1	-4.935406000	-1.538387000	-0.520421000
6	0.215980000	-2.514492000	-1.551461000
8	0.678094000	-3.567660000	-0.961450000
6	0.889347000	-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

17

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	-0.889906000	0.910887000
6	-4.301238000	-1.296997000	3.783373000
1	-4.635457000	-0.424059000	3.214882000
1	-4.849167000	-1.356987000	4.722040000
1	-4.460304000	-2.210816000	3.204674000
6	-1.482083000	-0.829500000	-0.551196000
6	-2.711519000	-0.956273000	-1.157363000
1	-3.613204000	-1.149391000	-0.591026000
6	-2.812549000	-0.783826000	-2.545107000
6	-1.656222000	-0.507201000	-3.278148000
1	-1.667262000	-0.350999000	-4.348435000
6	-0.456143000	-0.425925000	-2.596234000
1	0.464803000	-0.214632000	-3.126206000
6	-4.211893000	-0.633210000	-4.456722000
1	-3.913001000	0.390265000	-4.700713000
1	-5.275935000	-0.762696000	-4.646824000
1	-3.641123000	-1.347786000	-5.055928000
6	2.638081000	-1.464019000	-1.666326000
1	2.246638000	-1.859947000	-2.597815000
6	3.142993000	-0.151197000	-1.634086000
1	3.145306000	0.449263000	-2.536019000
6	3.531152000	0.434754000	-0.397033000
6	3.456725000	-0.340389000	0.788777000
1	3.695575000	0.114335000	1.742635000
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	-1.535005000
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	-5.659098000	-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

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	2.474886000	-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	4.739346000	-0.604144000

18

Coordinates (Angstroms)

	X	Y	Z
44	-1.227031000	0.170242000	-0.475322000
7	0.331238000	-1.208254000	-0.743217000
7	0.502160000	1.294880000	-0.047424000
8	3.435503000	-3.900528000	-0.976420000
8	4.031114000	3.111316000	1.041587000
6	0.145914000	-2.480537000	-1.136091000
1	-0.868686000	-2.761305000	-1.389193000
6	1.172492000	-3.392055000	-1.217018000
1	0.984285000	-4.411255000	-1.530818000
6	2.468934000	-2.978164000	-0.887358000
6	2.672351000	-1.652384000	-0.500263000
1	3.659876000	-1.290500000	-0.250534000
6	1.578655000	-0.797882000	-0.439447000
6	4.771166000	-3.522218000	-0.639219000
1	5.135462000	-2.741209000	-1.313039000
1	5.370311000	-4.422539000	-0.764735000
1	4.830810000	-3.182463000	0.398763000
6	1.678751000	0.621484000	-0.040058000
6	2.861554000	1.234830000	0.324095000
1	3.803202000	0.701072000	0.335117000

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	0.396721000
1	-2.849015000	2.549023000	0.453893000
6	-3.383758000	0.835594000	-0.747923000
6	-3.307332000	-0.591604000	-0.821514000
1	-3.657560000	-1.106586000	-1.707973000
6	-2.734104000	-1.321563000	0.236566000
1	-2.635571000	-2.396696000	0.128196000
6	-2.287001000	-0.695856000	1.446846000
1	-0.915024000	0.441732000	-2.042443000
6	-1.782467000	-1.509702000	2.619396000
6	-0.642745000	-2.461391000	2.246575000
6	-2.954164000	-2.271381000	3.252683000
1	-1.399995000	-0.796215000	3.357448000
1	0.220373000	-1.914587000	1.856502000
1	-0.322853000	-3.018043000	3.132669000
1	-0.955953000	-3.190111000	1.491811000
1	-3.761118000	-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	-3.627551000	2.652349000	-1.871492000
1	-3.806092000	1.162493000	-2.829332000
8	-0.997232000	2.760868000	-2.708661000
1	-1.198049000	3.420828000	-2.021380000
1	-1.710586000	2.795190000	-3.371170000
1	-1.012642000	1.833517000	-2.270311000

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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	-3.386354000	-1.195953000
1	0.972306000	-4.407368000	-1.504194000
6	2.455242000	-2.969822000	-0.866128000
6	2.659115000	-1.640554000	-0.487348000
1	3.646108000	-1.275563000	-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	-2.149001000	3.369759000
1	-1.243780000	-0.633117000	3.348426000
1	0.370161000	-1.783039000	1.887168000
1	-0.142363000	-2.862342000	3.193198000

1	-0.788911000	-3.085755000	1.563535000
1	-3.576500000	-1.474427000	3.651151000
1	-3.173412000	-2.930428000	2.721084000
1	-2.383815000	-2.627550000	4.277608000
6	-4.084555000	1.462426000	-1.873000000
1	-5.168730000	1.477219000	-1.721279000
1	-3.732433000	2.493620000	-1.935024000
1	-3.880799000	0.954620000	-2.817842000
8	-1.048529000	2.536586000	-2.736805000
1	-1.354560000	3.124191000	-2.028691000
1	-1.771317000	2.514224000	-3.382907000
1	-0.995205000	1.364416000	-2.213084000

19

Coordinates (Angstroms)

	X	Y	Z
44	-1.255857000	-0.021981000	-0.499445000
7	0.441146000	-1.230296000	-0.709565000
7	0.328455000	1.290897000	-0.107803000
8	3.814941000	-3.554729000	-0.949364000
8	3.623446000	3.555637000	0.839906000
6	0.382928000	-2.529088000	-1.052197000
1	-0.600086000	-2.931763000	-1.260808000
6	1.505335000	-3.318272000	-1.134769000
1	1.426607000	-4.362975000	-1.408030000
6	2.754915000	-2.748133000	-0.858880000
6	2.818047000	-1.394400000	-0.515485000
1	3.763287000	-0.914848000	-0.303335000
6	1.638654000	-0.668880000	-0.450948000
6	5.113624000	-3.007015000	-0.710151000
1	5.337148000	-2.213348000	-1.428657000
1	5.809974000	-3.832459000	-0.847807000
1	5.192914000	-2.624805000	0.311556000
6	1.577468000	0.763076000	-0.099571000
6	2.681742000	1.525321000	0.216455000
1	3.679194000	1.105081000	0.228437000
6	2.513125000	2.878863000	0.536585000
6	1.223948000	3.418432000	0.518729000
1	1.020229000	4.454710000	0.752224000
6	0.170177000	2.585949000	0.192118000
1	-0.842260000	2.969282000	0.178276000
6	3.499312000	4.935314000	1.194757000
1	3.072865000	5.509895000	0.368150000
1	4.512234000	5.278595000	1.397547000

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	-2.509146000	-1.643458000	0.480267000
1	-2.263609000	-2.699735000	0.496517000
6	-1.985430000	-0.778600000	1.493679000
1	-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

20

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

6	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

8	-2.598855000	1.896832000	-1.767074000
1	-3.254154000	2.110990000	-1.007126000
1	-3.143703000	1.615357000	-2.600587000
1	-2.047044000	1.118819000	-1.499227000
8	-3.911253000	1.213626000	-3.808048000
1	-4.512148000	1.931835000	-4.043708000
1	-4.490444000	0.483114000	-3.556185000
8	-4.284027000	2.520447000	0.027563000
1	-3.889444000	2.608095000	0.903902000
1	-4.932070000	1.811112000	0.122063000

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Coordinates (Angstroms)

	X	Y	Z
44	-0.891518000	-0.638629000	-0.128669000
7	1.057900000	-0.958219000	-0.835319000
7	0.086805000	1.158468000	0.307117000
8	4.989682000	-1.622051000	-1.830700000
8	2.259602000	4.567020000	1.031300000
6	1.461997000	-2.104785000	-1.408713000
1	0.695758000	-2.846230000	-1.597273000
6	2.773920000	-2.339239000	-1.748027000
1	3.066596000	-3.274298000	-2.208996000
6	3.727425000	-1.346743000	-1.488260000
6	3.309074000	-0.149341000	-0.901619000
1	4.013670000	0.639853000	-0.679468000
6	1.965820000	0.009066000	-0.595270000
6	5.989992000	-0.624311000	-1.613608000
1	5.757460000	0.288356000	-2.169741000
1	6.917468000	-1.054778000	-1.987490000
1	6.092042000	-0.402962000	-0.547351000
6	1.407601000	1.232302000	0.015423000
6	2.135003000	2.378965000	0.258924000
1	3.187739000	2.449740000	0.016669000
6	1.495176000	3.490986000	0.821788000
6	0.130769000	3.408381000	1.113991000
1	-0.424813000	4.231278000	1.543025000
6	-0.525785000	2.224825000	0.834371000
1	-1.585371000	2.120393000	1.033278000
6	1.647656000	5.735820000	1.580675000
1	0.857405000	6.104985000	0.920802000
1	2.441792000	6.477198000	1.651189000
1	1.242492000	5.532281000	2.575821000
6	-1.819885000	-0.783940000	1.924091000

1	-1.664451000	-0.058751000	2.716741000
6	-2.859135000	-0.559822000	0.989022000
1	-3.489636000	0.314223000	1.084169000
6	-3.024808000	-1.427542000	-0.118027000
6	-2.139478000	-2.536174000	-0.254450000
1	-2.225092000	-3.193502000	-1.111042000
6	-1.105134000	-2.732829000	0.680403000
1	-0.397918000	-3.537294000	0.506480000
6	-0.917268000	-1.866351000	1.796844000
1	-1.075150000	-0.116140000	-1.753772000
6	0.155731000	-2.119399000	2.835264000
6	1.554512000	-2.289733000	2.237552000
6	-0.243795000	-3.338733000	3.676576000
1	0.172025000	-1.242142000	3.491016000
1	1.884271000	-1.376972000	1.734478000
1	2.268861000	-2.513256000	3.035288000
1	1.594390000	-3.113635000	1.517401000
1	-1.231525000	-3.204957000	4.127886000
1	-0.267823000	-4.245413000	3.061726000
1	0.481729000	-3.494110000	4.480541000
6	-4.082591000	-1.156602000	-1.141305000
1	-5.032284000	-1.575925000	-0.794403000
1	-4.214153000	-0.082666000	-1.286870000
1	-3.829564000	-1.622638000	-2.095726000
8	-2.307152000	1.853005000	-1.889805000
1	-2.924751000	2.060409000	-1.152617000
1	-2.890318000	1.562950000	-2.632040000
1	-1.557969000	0.623549000	-1.571015000
8	-3.913941000	1.005640000	-3.907529000
1	-4.768005000	1.415547000	-3.727731000
1	-4.060280000	0.072891000	-3.712662000
8	-4.191833000	2.536222000	-0.022699000
1	-3.880290000	2.578996000	0.888487000
1	-4.852113000	1.833452000	-0.016338000

21

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
1	3.972070000	0.888772000	-0.746350000
6	1.976720000	0.115242000	-0.609643000
6	6.033766000	-0.286730000	-1.635111000
1	5.760271000	0.607022000	-2.203207000
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	3.060934000	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	6.556616000	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	0.034971000	-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

6	-4.054733000	-1.321512000	-0.977712000
1	-4.989885000	-1.721644000	-0.573378000
1	-4.183545000	-0.251664000	-1.154630000
1	-3.844442000	-1.823379000	-1.924161000
8	-2.629942000	1.883242000	-1.918982000
1	-3.254890000	2.005359000	-1.180125000
1	-3.145218000	1.403630000	-2.595095000
1	-1.375352000	0.226734000	-1.682249000
8	-4.101839000	0.584779000	-3.916339000
1	-4.842515000	1.198298000	-3.980481000
1	-4.486431000	-0.197279000	-3.505510000
8	-4.515038000	2.329407000	0.105372000
1	-4.094530000	2.419047000	0.967908000
1	-5.045253000	1.527864000	0.182215000

22

Coordinates (Angstroms)

	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	-2.056529000	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

1	-3.068411000	-1.973480000	1.311466000
8	-4.670336000	-2.926648000	-0.576015000
1	-4.808040000	-3.649896000	0.136270000
1	-3.666487000	-2.866101000	-0.712430000
1	-4.975718000	-2.043127000	-0.177627000
8	-4.895979000	-4.711652000	1.226617000
1	-4.891955000	-5.578152000	0.801856000
1	-5.760681000	-4.653538000	1.650851000
8	-5.375123000	-0.688877000	0.479360000
1	-6.203746000	-0.776008000	0.966009000
1	-5.562269000	-0.052244000	-0.221631000

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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	-3.065201000	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
6	2.981484000	1.340737000	0.104136000
1	3.504147000	1.190412000	-0.833603000
6	2.171731000	2.476102000	0.285472000
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	-0.318385000
1	2.446167000	5.046020000	2.522873000
1	2.146180000	5.330411000	0.797715000
1	1.125046000	6.112148000	2.014828000
6	3.913568000	-0.872787000	0.954696000
1	4.954551000	-0.634571000	1.199382000
1	3.582897000	-1.679670000	1.612237000
1	3.883855000	-1.221295000	-0.075869000
6	-2.734237000	-2.104849000	-2.116283000
6	-1.404900000	-1.713376000	-2.244968000
6	-0.434454000	-2.242797000	-1.388343000
6	-0.812599000	-3.151847000	-0.389170000
6	-2.140221000	-3.527618000	-0.257428000
6	-3.103686000	-3.007346000	-1.124482000
1	-3.480483000	-1.692003000	-2.787068000
1	-1.137309000	-0.998796000	-3.015371000
1	-0.063531000	-3.551025000	0.285624000
1	-2.430215000	-4.220765000	0.525117000
1	-4.142911000	-3.300676000	-1.016686000
6	0.995525000	-1.898461000	-1.554545000
8	1.828865000	-2.741465000	-1.040636000
6	1.467435000	-1.041364000	-2.689457000
1	1.493965000	-1.672102000	-3.586145000
1	0.804334000	-0.199484000	-2.872678000
1	2.473499000	-0.671371000	-2.491824000
8	4.143032000	-2.765112000	-1.947254000
1	4.698607000	-3.085000000	-1.197857000

1	2.810096000	-2.672875000	-1.419701000
1	4.473576000	-1.858215000	-2.139024000
8	5.568772000	-3.591215000	0.218324000
1	6.058717000	-2.806018000	0.490083000
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
