Mechanism of NO-CO Reaction over Highly Dispersed Cuprous Oxide on γ-Alumina Catalyst Using Metal-Support Interfacial Site in the Presence of Oxygen: Similarity to and Difference from Biological Systems

Ryoichi Fukuda,[†‡*] Shogo Sakai,[†] Nozomi Takagi,[†] Masafuyu Matsui,[†] Masahiro Ehara,[†‖⊥] Saburo Hosokawa,[‡†] Tsunehiro Tanaka[‡†], Shigeyoshi Sakaki,[†§*]

[†]*Center for the Promotion of Interdisciplinary Education and Research, Elements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, 1-30 Goryo-Ohara, Nishikyo-ku, Kyoto 615-8245, Japan*

[‡]*Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, Kyoto-Daigaku-Katsura, Nishikyo-ku, Kyoto 615-8510, Japan*

[‖]*Research Center for Computational Science, 38 Nishigo-naka, Myodaiji, Okazaki, 444-8585, Japan*

[⊥]*Department of Theoretical and Computational Molecular Science, Institute for Molecular Science (IMS), 38 Nishigo-naka, Myodaiji, Okazaki, 444-8585, Japan*

[§]*Fukui Institute for Fundamental Chemistry (FIFC), Kyoto University, Takano-Nishihiraki-cho 34-4, Sakyou-ku, Kyoto 606-8103, Japan*
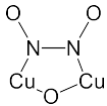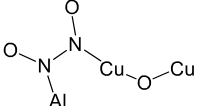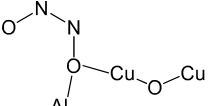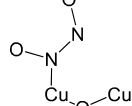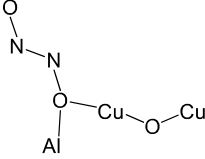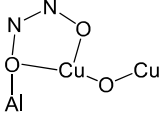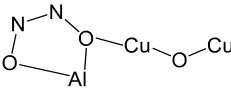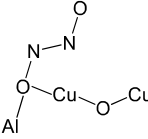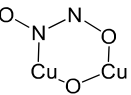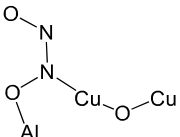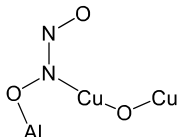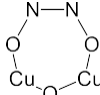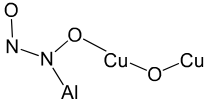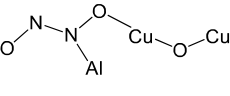
Supporting Information

·   Figure S1. Correlation between N-O bond lengths and bond order.

·   Table S1. Adsorption conformers of ONNO on **CAT**.

·   Table S2. Activation energies and heat of reactions for O-NNO bond cleavage initiated from 5 conformers.

·   Table S3. Temperature dependence of the Gibbs free-energy of activation for O-N_2 bond cleavage

·   Table S4. List of calculated models

·   Absorption energy of *cis*-ONNO molecule to **CAT**

·   Absorption energy of CO to **CAT**

·   Cartesian coordinates of the calculated models.
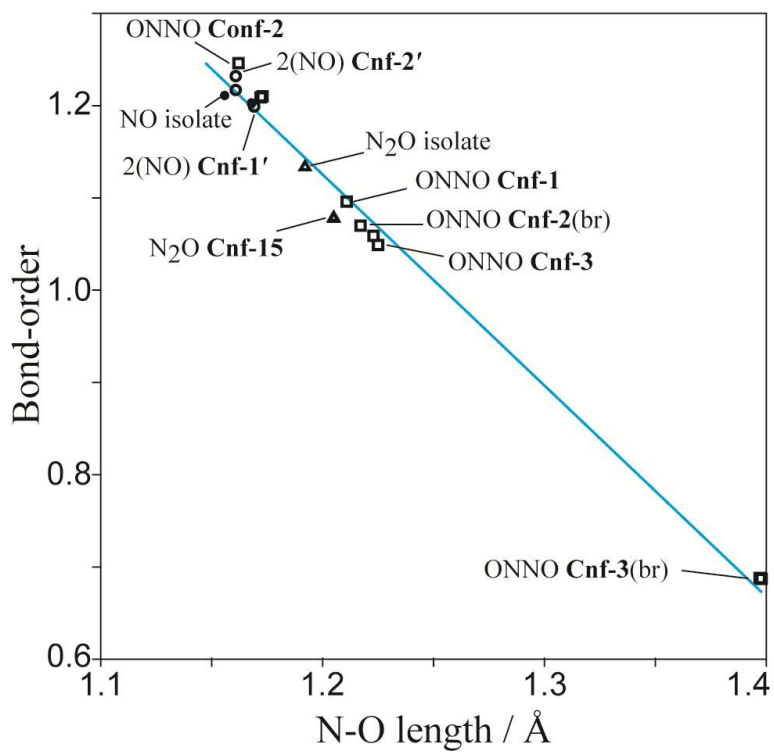
Figure S1. Correlation between N-O bond lengths and bond order. Values are given in Table 1.

Table S1. Adsorption conformers of ONNO on CAT. Relative energies (ΔE) with respect to **CAT** + 2(NO) and bond lengths are shown for singlet and triplet states.

	Cnf-1	Cnf-2	Cnf-3	Cnf-4
Structure				
Singlet				
ΔE/kcal·mol^{-1}	−17.0	−20.3	−16.7	−15.4
N-N/Å	1.886	1.820	1.230	1.863
N-O/Å	1.173, 1.173	1.172, 1.168	1.397, 1.225	1.177, 1.158
Triplet				
ΔE/kcal·mol^{-1}	−12.1	−20.5	−16.9	−11.7
N-N/Å	1.465	1.408	1.229	1.888
N-O/Å	1.211, 1.211	1.223, 1.217	1.398, 1.225	1.172, 1.163

	Cnf-5	Cnf-6	Cnf-7	Cnf-8
Structure				
Singlet				
ΔE/kcal·mol^{-1}	−20.1	−22.0	−24.5	−17.1
N-N/Å	1.244	1.343	1.345	1.220
N-O/Å	1.373, 1.219	1.278, 1.257	1.285, 1.260	1.296, 1.189
Triplet				
ΔE/kcal·mol^{-1}	−20.1	−21.9	−25.1	−19.4
N-N/Å	1.243	1.306	1.321	1.247
N-O/Å	1.375, 1.219	1.298, 1.275	1.304, 1.275	1.367, 1.218

	Cnf-9	Cnf-10	Cnf-11	Cnf-12
Structure				
Singlet				
ΔE/kcal·mol^{-1}	−12.6	−19.1	−22.8	−10.5
N-N/Å	1.269	1.415	1.360	1.242
N-O/Å	1.303, 1.259	1.265, 1.210	1.260, 1.233	1.329, 1.330
Triplet				
ΔE/kcal·mol^{-1}	−15.6	−17.8	−23.4	−11.1
N-N/Å	1.365	1.427	1.361	1.242
N-O/Å	1.251, 1.234	1.256, 1.207	1.258, 1.231	1.329, 1.329

	Cnf-13	Cnf-14
Structure		
Singlet		
ΔE/kcal·mol^{-1}	−15.0	−20.1
N-N/Å	1.411	1.335
N-O/Å	1.267, 1.212	1.261, 1.269
Triplet		
ΔE/kcal·mol^{-1}	−14.2	−20.2
N-N/Å	1.403	1.333
N-O/Å	1.274, 1.214	1.263, 1.269

Table S2. Activation energy (E_a), heat of reaction (ΔH), and N-O bond length at the transition state for the O-NNO cleavage.

Reactant	E_a/kcal· mol^{-1}	Δ/kcal· mol^{-1}	N-O/Å
Cnf-3, triplet	6.5	−10.5	1.663
Cnf-6, triplet	12.6	−9.3	1.662
Cnf-8, triplet	14.2	−5.3	1.652
Cnf-7, triplet	19.9	−4.9	1.685
Cnf-5, triplet	20.9	0.8	1.655

Table S3. Temperature dependence of the Gibbs free-energy of activation (G_a) for O-N_2 bond cleavage on **CAT:O** site in triplet state.

Temperature/K	G_a/kcal· mol^{-1}
300	22.3
350	22.6
400	23.0
450	23.3
500	23.7
550	24.1
600	24.5
650	24.9
700	25.3
750	25.7
800	26.2

Table S4. List of calculated models.

Model #	Spin multpl.	Total energy/E_h	Zero-point en./E_h	Description
01	1	-4746.09907276	0.132636	$Al_{26}O_{62}H_{46}$ cluster
02	1	-5213.80704180	0.137927	**CAT**, $Al_{26}O_{62}H_{46}(Cu_2O)$
03	1	-5327.10096019	0.145060	**CAT**(CO)
04	2	-5343.66423102	0.143630	**CAT**(NO) on-top site
05	2	-5343.66523215	0.144192	**CAT**(NO) bridge site
06	6	-5343.53314938	0.140940	**CAT**(N)(O); dissociative adsorption of NO
07	1	-5473.52522882	0.150022	**CAT**(NO)(NO), **Cnf-1′**
08	3	-5473.52523377	0.150018	**CAT**(NO)(NO), **Cnf-1′**
09	1	-5473.51140818	0.150706	**CAT**(NO)(NO), **Cnf-2′**
10	3	-5473.50778862	0.149990	**CAT**(NO)(NO), **Cnf-2′**
11	1	-5473.50327123	0.151614	TS for NO dimerization, 07 → 15
12	3	-5473.49392290	0.149628	TS for NO dimerization, 08 → 16
13	1	-5473.50233913	0.151993	TS for NO dimerization, 09 → 17
14	3	-5473.50031003	0.150220	TS for NO dimerization, 10 → 18
15	1	-5473.50577081	0.152176	**CAT**(ONNO), **Cnf-1**
16	3	-5473.49791120	0.151007	**CAT**(ONNO), **Cnf-1**
17	1	-5473.51101021	0.152632	**CAT**(ONNO), **Cnf-2**
18	3	-5473.51136023	0.152693	**CAT**(ONNO), **Cnf-2**
19	1	-5473.50535663	0.152733	**CAT**(ONNO), **Cnf-3**
20	3	-5473.50563803	0.152751	**CAT**(ONNO), **Cnf-3**
21	1	-5473.50320967	0.151813	**CAT**(ONNO), **Cnf-4**
22	3	-5473.49725676	0.150042	**CAT**(ONNO), **Cnf-4**
23	1	-5473.51065679	0.153032	**CAT**(ONNO), **Cnf-5**
24	3	-5473.51069501	0.153072	**CAT**(ONNO), **Cnf-5**
25	1	-5473.51376809	0.152177	**CAT**(ONNO), **Cnf-6**
26	3	-5473.51363030	0.151613	**CAT**(ONNO), **Cnf-6**
27	1	-5473.51766692	0.152258	**CAT**(ONNO), **Cnf-7**
28	3	-5473.51876045	0.152096	**CAT**(ONNO), **Cnf-7**
29	1	-5473.50593958	0.153747	**CAT**(ONNO), **Cnf-8**
30	3	-5473.50962235	0.152896	**CAT**(ONNO), **Cnf-8**
31	1	-5473.49873568	0.152027	**CAT**(ONNO), **Cnf-9**
32	3	-5473.50357580	0.151609	**CAT**(ONNO), **Cnf-9**
33	1	-5473.50917469	0.151512	**CAT**(ONNO), **Cnf-10**
34	3	-5473.50706222	0.151631	**CAT**(ONNO), **Cnf-10**
35	1	-5473.51498194	0.152304	**CAT**(ONNO), **Cnf-11**
36	3	-5473.51598816	0.152398	**CAT**(ONNO), **Cnf-11**
37	1	-5473.49545077	0.152308	**CAT**(ONNO), **Cnf-12**
38	3	-5473.49644070	0.152196	**CAT**(ONNO), **Cnf-12**
39	1	-5473.50257214	0.151365	**CAT**(ONNO), **Cnf-13**
40	3	-5473.50131269	0.151708	**CAT**(ONNO), **Cnf-13**
41	1	-5473.51075352	0.152453	**CAT**(ONNO), **Cnf-14**
42	3	-5473.51094984	0.152358	**CAT**(ONNO), **Cnf-14**
43	3	-5473.49533524	0.151121	TS for O-NNO dissociation from **Cnf-3**
44	3	-5473.49334431	0.151044	TS for O-NNO dissociation from **Cnf-6**
45	3	-5473.48706173	0.151078	TS for O-NNO dissociation from **Cnf-8**
46	3	-5473.48647116	0.150730	TS for O-NNO dissociation from **Cnf-7**
47	3	-5473.47746176	0.150275	TS for O-NNO dissociation from **Cnf-5**
48	1	-5288.91486849	0.140200	**CAT:O**
49	3	-5288.94042548	0.139549	**CAT:O**
50	1	-5473.48352302	0.150218	TS for **Cnf-2** to **Cnf-3**, 17 → 19
51	3	-5473.48295036	0.150246	TS for **Cnf-2** to **Cnf-3**, 18 → 20
52	1	-5473.50003562	0.151710	TS for **Cnf-1** to **Cnf-4**, 15 → 21
53	3	-5473.50085257	0.148611	TS for **Cnf-1** to **Cnf-4**, 16 → 22
54	1	-5473.49561474	0.150988	TS for **Cnf-4** to **Cnf-3**, 21 → 19
55	3	-5473.49459342	0.150184	TS for **Cnf-4** to **Cnf-3**, 22 → 20

56	1	-5398.40717677	0.150313	**CAT**(ON$_2$), **Cnf-16**
57	1	-5398.36663753	0.145989	TS for ON$_2$ decomposition on **CAT** (from 56)
58	3	-5398.35555920	0.145727	TS for ON$_2$ decomposition on **CAT** (from 56)
59	3	-5473.54142955	0.152024	**CAT:O**(ON$_2$), **Cnf-15**
60	3	-5473.50413464	0.147665	TS for ON$_2$ decomposition on **CAT:O** (from 59)
61	5	-5473.50024259	0.147510	TS for ON$_2$ decomposition on **CAT:O** (from 59)
62	3	-5364.07140207	0.141491	**CAT:OO**
63	5	-5364.07584427	0.141730	**CAT:OO**
64	5	-5477.34294726	0.147586	**CAT:OO**(CO)
65	5	-5477.33579277	0.147612	TS for CO oxidation on **CAT:OO**, 64 → 67
66	3	-5477.33363675	0.147422	TS for CO oxidation on **CAT:OO**, 64 → 68
67	5	-5477.39419733	0.150747	**CAT:O**(CO$_2$)
68	3	-5477.45580829	0.152340	**CAT:O**(CO$_2$)
69	3	-5402.20642388	0.145829	**CAT:O**(CO), **Cnf-17**
70	3	-5402.20068881	0.145780	TS for CO oxidation on CAT:O, 69 → 71
71	3	-5402.25633402	0.148559	**CAT**(CO$_2$)
72	1	-5402.32787516	0.150553	**CAT**(CO$_2$)
73	1	-5511.69726506	0.157545	**CAT**(N$_2$O)(CO)
74	1	-5511.61991468	0.155406	TS for N$_2$O-CO reaction (from 73)
75	3	-5364.07962528	0.143167	**CAT**(O$_2$), Cu-Al bridge
76	3	-5364.07973803	0.142526	**CAT**(O$_2$), Cu side-on
77	3	-5364.00074019	0.140858	TS for O$_2$ dissociation (from 76)
78	3	-5477.37733534	0.149801	**CAT**(O$_2$)(CO)
79	3	-5477.32504517	0.149828	TS for CO-O$_2$ reaction (from 78)
80	4	-5493.91427740	0.146323	**CAT:OO**(NO)
81	6	-5493.91506044	0.146292	**CAT:OO**(NO)
82	2	-129.833293	0.004605	NO molecule
83	1	-113.258297	0.005059	CO molecule
84	1	-188.504221	0.011453	N$_2$O molecule
85	1	-184.586087	0.011734	CO$_2$ molecule
86	3	-150.259271	0.003863	O$_2$ molecule
87	1	-109.474369	0.005633	N$_2$ molecule

Absorption energy of *cis*-ONNO molecule to CAT

We estimated the absorption energy of *cis*-ONNO molecule to **CAT**. It is very difficult to describe the accurate electronic structure of isolated *cis*-ONNO molecule with using DFT because of its multireference character.[1,2] Therefore, we used high-level *ab initio* calculation results available for isolated ONNO molecule (NO dimer). The binding energy of isolated NO dimer with respect to two NO monomer was calculated to be 3.46 kcal·mol^{-1} by the MRMP2 method for the *cis* conformer,[2] and the experimentally estimated binding energy is 2.8–3.8 kcal·mol^{-1} (Ref. 2). Using the binding energy of 3.46 kcal·mol^{-1}, we obtained the absorption energy of *cis*-ONNO to **CAT** as follows: 13.5 kcal·mol^{-1} to Cu_2O site in the singlet state (**Cnf-1**) and 16.8 kcal·mol^{-1} to Cu-Al interfacial site in the singlet state (**Cnf-2**). The adsorption energies of *cis*-ONNO are summarized in Table 1.

Absorption energy of CO to CAT

The adsorption energy of CO at site A is 4.1 kcal·mol^{-1}. Such a very weak binding energy indicates the coordination sphere of the Cu(II) site in **CAT:O** or **CAT:OO** is almost saturated already. The Cu-C distance of Cu-CO in **Cnf-17** is 2.190 Å. This bond distance is significantly longer than the Cu-C distance of non-oxidized **CAT**(CO) (1.846 Å) and is close to the adsorption distance of CO on CuO (110) surface predicted by the DV-Xα computation.[3] The calculated C-O stretching frequencies are 2223 cm^{-1} and 2240 cm^{-1} for **CAT:O**(CO) and **CAT:OO**(CO), respectively; they exhibit a slight blueshift in comparison with that of free CO molecule (2220cm^{-1}). These features are similar to those of the second-sphere CO observed in $Cu(CO)_n^+$ (n > 4) molecules,[4] where the first coordination sphere is saturated by four CO ligands.

References

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[2] J. Ivanic, M. W. Schmidt, B. Luke, *J. Chem. Phys.* **2012**, *137*, 214316.
[3] Y. Duan, K. Zhang, X. Xie, *Surf. Sci.* **1994**, *321*, L249–L254.
[4] A. D. Brathwaite, Z. D. Reed, M. A. Duncan, *J. Phys. Chem. A* **2011**, *115*, 10461–104690.

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Model #01      Cartesian coordinates in angstrom
               x            y             z            Relaxed/Frozen
Al             4.718090     6.298720      9.025530     F
Al             6.299120     6.298720      11.957100    F
Al             4.718090     14.697000     9.025530     F
Al             4.828310     11.950760     9.158180     F
Al             4.828310     9.044950      9.158180     F
Al             7.260470     8.998620      12.959550    F
Al             7.260470     11.997090     12.959550    F
Al             6.299120     14.697000     11.957100    F
Al             4.636030     10.497860     12.053020    F
O              3.286790     10.497860     13.239720    F
Al             6.284430     4.911620      6.956080     F
Al             6.284430     16.084100     6.956080     F
Al             7.604150     10.497860     2.473790     F
O              6.427200     10.497860     1.094350     F
Al             6.373450     6.298720      3.886400     F
O              4.781440     6.298720      2.980340     F
Al             6.373450     14.697000     3.886400     F
O              4.781440     14.697000     2.980340     F
O              3.454040     4.977000      9.235300     F
O              3.454040     7.620430      9.235300     F
O              6.249990     5.002880      13.162250    F
O              3.454040     16.018710     9.235300     F
O              3.454040     13.375290     9.235300     F
O              7.425510     9.104840      14.776050    F
O              7.425510     11.890870     14.776050    F
O              6.249990     15.992840     13.162250    F
O              4.962260     3.365420      7.283450     F
O              7.499840     3.492590      6.705350     F
O              4.962260     17.630300     7.283450     F
O              7.499840     17.503130     6.705350     F
O              7.704780     6.298720      2.777150     F
O              7.704780     14.697000     2.777150     F
Al             3.479000     10.497860     7.046730     F
O              1.926550     11.807730     6.890260     F
O              1.926550     9.187980      6.890260     F
O              3.361120     10.497860     5.169010     F
Al             2.050920     10.497860     10.125660    F
O              0.574780     10.497860     9.076090     F
O              2.097750     9.088320      11.188760    F
O              2.097750     11.907400     11.188760    F
Al             3.393320     6.298720      6.011420     F
O              1.956480     6.298720      7.179490     F
O              3.339460     7.715090      4.949250     F
O              3.339460     4.882340      4.949250     F
Al             3.393320     14.697000     6.011420     F
O              1.956480     14.697000     7.179490     F
O              3.339460     16.113380     4.949250     F
O              3.339460     13.280620     4.949250     F
H              3.439920     4.911170      10.243970    F
H              3.439230     7.689480      10.293370    F
H              6.818390     4.213070      13.048230    F
H              6.229200     4.955320      14.133900    F
H              3.439930     16.084520     10.243550    F
H              3.439220     13.306190     10.293980    F
H              6.776960     8.347650      14.909840    F
H              6.777010     12.648010     14.909830    F
H              6.229200     16.040400     14.133950    F
H              6.818390     16.782650     13.048230    F
H              4.227170     2.738070      7.166140     F
H              6.932390     2.747750      6.973660     F
H              7.409140     3.550970      5.707010     F
H              4.227170     18.257650     7.166140     F
H              6.932400     18.247960     6.973660     F
H              7.409130     17.444750     5.706960     F
H              7.521090     6.298720      1.832230     F
H              7.521090     14.697000     1.832230     F
H              3.346920     10.497860     14.197640    F
H              6.469070     10.497860     0.138110     F
H              0.036290     9.692190      9.043070     F
H              0.036300     11.303520     9.043070     F
H              2.008450     9.058200      12.145150    F
H              2.008450     11.937520     12.145160    F
```

H	4.786760	6.298720	2.000110	F
H	4.786760	14.697000	2.000090	F
H	6.866360	9.838780	15.040440	F
H	6.866350	11.156920	15.040450	F
H	4.132080	16.721550	9.197250	F
H	4.893480	17.534250	8.246090	F
H	4.893480	3.461470	8.246090	F
H	4.132060	4.274190	9.197250	F
H	2.690120	11.221850	5.059460	F
H	2.690120	9.773870	5.059460	F
H	1.278480	12.508620	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991770	6.298720	8.126700	F
H	1.991770	14.697000	8.126700	F
H	4.137960	13.968640	3.050500	F
H	4.137960	7.027070	3.050500	F
H	3.423390	4.865220	3.998930	F
H	3.423390	16.130500	3.998930	F
H	3.423050	7.732140	4.002720	F
H	3.423050	13.263570	4.002720	F
H	2.742680	6.961340	9.160660	F
H	2.742700	14.034350	9.160660	F
Al	6.283750	7.679370	6.968190	R
O	4.827320	6.295240	7.136480	R
O	7.524130	6.255060	7.424970	R
O	6.221350	7.620430	5.044300	R
Al	7.271770	6.152810	9.228040	R
O	6.496430	7.457910	13.302360	R
O	7.700430	5.957610	10.906910	R
O	5.996230	4.837970	8.850270	R
O	6.037020	7.597820	8.952080	R
Al	7.288260	9.026150	4.875580	R
Al	7.288260	11.969580	4.875580	R
Al	6.283770	13.316350	6.968200	R
Al	6.415720	10.497860	7.041150	R
O	4.827330	14.700490	7.136470	R
O	4.928760	11.806580	7.290990	R
O	4.928760	9.189110	7.290990	R
O	7.524130	14.740680	7.424980	R
O	6.296590	10.497860	4.994740	R
O	7.528050	11.961520	6.713020	R
O	7.528040	9.034200	6.713020	R
O	6.221350	13.375290	5.044310	R
Al	7.271760	14.842900	9.228050	R
Al	7.205660	10.497750	10.574610	R
O	6.188160	10.497860	13.151160	R
O	6.496480	13.537820	13.302350	R
O	6.310450	10.497860	9.019580	R
O	7.700440	15.038110	10.906920	R
O	6.037040	13.397890	8.952060	R
O	5.996210	16.157760	8.850280	R
O	8.019450	9.160370	11.425730	R
O	8.019320	11.835240	11.425680	R
O	4.797790	6.129510	10.950250	R
O	4.797810	14.866130	10.950240	R
O	4.991040	9.132530	10.971080	R
O	4.990740	11.863270	10.971090	R
O	6.336150	4.939010	5.084760	R
O	6.336170	16.056720	5.084740	R
O	8.078410	9.064240	3.304510	R
O	8.078410	11.931470	3.304510	R
O	3.506160	10.497820	9.032810	R

```
Model #02      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043066       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.242008	7.648509	6.975723	R
O	4.829275	6.291380	7.126012	R
O	7.532200	6.268269	7.418156	R
O	6.214926	7.629711	5.047416	R
Al	7.266579	6.138204	9.235811	R
O	6.471309	7.462140	13.288800	R
O	7.705453	5.945802	10.903596	R
O	6.004567	4.834884	8.828104	R
O	6.043255	7.590155	8.932233	R
Al	7.273681	9.018934	4.858291	R
Al	7.276597	11.977011	4.858563	R
Al	6.242620	13.347601	6.975887	R
Al	6.386657	10.498323	7.128647	R
O	4.829508	14.704356	7.125759	R
O	4.968249	11.814323	7.270088	R
O	4.968206	9.181980	7.270072	R
O	7.532384	14.728087	7.418462	R
O	6.328886	10.498846	5.078197	R
O	7.569486	12.003160	6.702585	R
O	7.568717	8.993292	6.702148	R
O	6.217029	13.365816	5.046899	R
Al	7.266496	14.858110	9.236107	R
Al	8.091799	10.498302	10.431930	R
O	6.186426	10.497811	13.135877	R
O	6.470818	13.533320	13.288544	R
O	6.398624	10.498097	9.054570	R
O	7.705305	15.051242	10.903873	R
O	6.043369	13.405885	8.932281	R
O	6.004241	16.161103	8.828145	R
O	8.215860	9.113896	11.553691	R
O	8.217324	11.881885	11.554672	R
O	4.824116	6.081764	10.927129	R
O	4.824127	14.913755	10.927085	R
O	4.788886	9.069774	10.960968	R
O	4.789177	11.925916	10.961011	R
O	6.341162	4.952358	5.086090	R
O	6.340990	16.043280	5.086049	R
O	8.073866	9.068156	3.306195	R
O	8.080428	11.924539	3.308270	R
O	3.499171	10.497831	8.967453	R
Cu	8.951961	11.760467	8.018135	R
Cu	8.952427	9.234016	8.017922	R
O	9.489941	10.497694	9.307602	R

```
Model #03        Cartesian coordinates in angstrom
                 x              y              z              Relaxed/Frozen
Al               4.718091       6.298715       9.025534       F
Al               6.299120       6.298715       11.957102      F
Al               4.718091       14.697002      9.025534       F
Al               4.828311       11.950763      9.158184       F
Al               4.828311       9.044955       9.158184       F
Al               7.260466       8.998624       12.959551      F
Al               7.260466       11.997093      12.959551      F
Al               6.299120       14.697002      11.957102      F
Al               4.636026       10.497859      12.053017      F
O                3.286788       10.497859      13.239718      F
Al               6.284430       4.911618       6.956078       F
Al               6.284430       16.084099      6.956078       F
Al               7.604152       10.497859      2.473791       F
O                6.427205       10.497859      1.094354       F
Al               6.373455       6.298715       3.886397       F
O                4.781442       6.298715       2.980335       F
Al               6.373455       14.697002      3.886397       F
O                4.781442       14.697002      2.980335       F
O                3.454035       4.977004       9.235301       F
O                3.454035       7.620427       9.235301       F
O                6.249989       5.002877       13.162247      F
O                3.454035       16.018713      9.235301       F
O                3.454035       13.375290      9.235301       F
O                7.425505       9.104843       14.776051      F
O                7.425505       11.890874      14.776051      F
O                6.249989       15.992841      13.162247      F
O                4.962264       3.365416       7.283451       F
O                7.499839       3.492587       6.705345       F
O                4.962264       17.630302      7.283451       F
O                7.499839       17.503130      6.705345       F
O                7.704784       6.298715       2.777154       F
O                7.704784       14.697002      2.777154       F
Al               3.478998       10.497859      7.046735       F
O                1.926548       11.807732      6.890259       F
O                1.926548       9.187985       6.890259       F
O                3.361122       10.497859      5.169014       F
Al               2.050923       10.497859      10.125656      F
O                0.574778       10.497859      9.076089       F
O                2.097749       9.088323       11.188759      F
O                2.097749       11.907395      11.188759      F
Al               3.393316       6.298715       6.011417       F
O                1.956477       6.298715       7.179493       F
O                3.339459       7.715095       4.949249       F
O                3.339459       4.882336       4.949249       F
Al               3.393316       14.697002      6.011417       F
O                1.956477       14.697002      7.179493       F
O                3.339459       16.113380      4.949249       F
O                3.339459       13.280622      4.949249       F
H                3.439923       4.911172       10.243970      F
H                3.439232       7.689483       10.293373      F
H                6.818393       4.213072       13.048228      F
H                6.229200       4.955319       14.133904      F
H                3.439929       16.084518      10.243550      F
H                3.439218       13.306190      10.293977      F
H                6.776962       8.347647       14.909841      F
H                6.777013       12.648010      14.909830      F
H                6.229199       16.040400      14.133948      F
H                6.818394       16.782646      13.048228      F
H                4.227165       2.738070       7.166136       F
H                6.932392       2.747750       6.973661       F
H                7.409135       3.550965       5.707009       F
H                4.227165       18.257647      7.166137       F
H                6.932397       18.247959      6.973659       F
H                7.409131       17.444750      5.706962       F
H                7.521090       6.298716       1.832227       F
H                7.521091       14.697002      1.832228       F
H                3.346923       10.497859      14.197637      F
H                6.469066       10.497859      0.138110       F
H                0.036291       9.692187       9.043065       F
H                0.036295       11.303524      9.043066       F
H                2.008448       9.058198       12.145152      F
H                2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.266408	7.665741	6.989932	R
O	4.837135	6.294648	7.125625	R
O	7.546936	6.266664	7.433283	R
O	6.255217	7.623876	5.063873	R
Al	7.258599	6.127451	9.248892	R
O	6.467706	7.459669	13.295581	R
O	7.707055	5.922672	10.910511	R
O	6.003128	4.830652	8.827239	R
O	6.048782	7.587950	8.940406	R
Al	7.294969	9.032421	4.890108	R
Al	7.248209	11.975960	4.843587	R
Al	6.241905	13.348677	6.974197	R
Al	6.390044	10.491688	7.131082	R
O	4.828129	14.705527	7.127147	R
O	4.971811	11.811845	7.271872	R
O	4.965234	9.178819	7.274415	R
O	7.529195	14.730048	7.416656	R
O	6.313025	10.493420	5.067248	R
O	7.561818	12.008683	6.679370	R
O	7.581702	9.038020	6.745088	R
O	6.198175	13.368873	5.044929	R
Al	7.266764	14.855555	9.233797	R
Al	7.993700	10.430435	10.377394	R
O	6.181978	10.496977	13.145598	R
O	6.488381	13.538482	13.288845	R
O	6.370159	10.494289	9.066546	R
O	7.707146	15.043105	10.902855	R
O	6.043669	13.404808	8.932054	R
O	6.004245	16.161155	8.830134	R
O	8.162813	9.057847	11.516084	R
O	8.178768	11.809827	11.525978	R
O	4.827493	6.080316	10.924138	R
O	4.824100	14.914180	10.929158	R
O	4.788167	9.069075	10.961751	R
O	4.787306	11.928239	10.963344	R
O	6.344118	4.949306	5.085590	R
O	6.342409	16.044964	5.085392	R
O	8.099892	9.088359	3.333084	R
O	8.055110	11.939601	3.294863	R
O	3.496845	10.498820	8.967972	R
Cu	8.924365	11.564505	7.922281	R
Cu	9.379654	8.850776	7.973430	R
O	9.344895	10.307995	9.205269	R
C	10.403297	7.432714	7.381917	R
O	11.068383	6.566894	7.051349	R

```
Model #04       Cartesian coordinates in angstrom
                x               y               z               Relaxed/Frozen
Al              4.718091        6.298715        9.025534        F
Al              6.299120        6.298715        11.957102       F
Al              4.718091        14.697002       9.025534        F
Al              4.828311        11.950763       9.158184        F
Al              4.828311        9.044955        9.158184        F
Al              7.260466        8.998624        12.959551       F
Al              7.260466        11.997093       12.959551       F
Al              6.299120        14.697002       11.957102       F
Al              4.636026        10.497859       12.053017       F
O               3.286788        10.497859       13.239718       F
Al              6.284430        4.911618        6.956078        F
Al              6.284430        16.084099       6.956078        F
Al              7.604152        10.497859       2.473791        F
O               6.427205        10.497859       1.094354        F
Al              6.373455        6.298715        3.886397        F
O               4.781442        6.298715        2.980335        F
Al              6.373455        14.697002       3.886397        F
O               4.781442        14.697002       2.980335        F
O               3.454035        4.977004        9.235301        F
O               3.454035        7.620427        9.235301        F
O               6.249989        5.002877        13.162247       F
O               3.454035        16.018713       9.235301        F
O               3.454035        13.375290       9.235301        F
O               7.425505        9.104843        14.776051       F
O               7.425505        11.890874       14.776051       F
O               6.249989        15.992841       13.162247       F
O               4.962264        3.365416        7.283451        F
O               7.499839        3.492587        6.705345        F
O               4.962264        17.630302       7.283451        F
O               7.499839        17.503130       6.705345        F
O               7.704784        6.298715        2.777154        F
O               7.704784        14.697002       2.777154        F
Al              3.478998        10.497859       7.046735        F
O               1.926548        11.807732       6.890259        F
O               1.926548        9.187985        6.890259        F
O               3.361122        10.497859       5.169014        F
Al              2.050923        10.497859       10.125656       F
O               0.574778        10.497859       9.076089        F
O               2.097749        9.088323        11.188759       F
O               2.097749        11.907395       11.188759       F
Al              3.393316        6.298715        6.011417        F
O               1.956477        6.298715        7.179493        F
O               3.339459        7.715095        4.949249        F
O               3.339459        4.882336        4.949249        F
Al              3.393316        14.697002       6.011417        F
O               1.956477        14.697002       7.179493        F
O               3.339459        16.113380       4.949249        F
O               3.339459        13.280622       4.949249        F
H               3.439923        4.911172        10.243970       F
H               3.439232        7.689483        10.293373       F
H               6.818393        4.213072        13.048228       F
H               6.229200        4.955319        14.133904       F
H               3.439929        16.084518       10.243550       F
H               3.439218        13.306190       10.293977       F
H               6.776962        8.347647        14.909841       F
H               6.777013        12.648010       14.909830       F
H               6.229199        16.040400       14.133948       F
H               6.818394        16.782646       13.048228       F
H               4.227165        2.738070        7.166136        F
H               6.932392        2.747750        6.973661        F
H               7.409135        3.550965        5.707009        F
H               4.227165        18.257647       7.166137        F
H               6.932397        18.247959       6.973659        F
H               7.409131        17.444750       5.706962        F
H               7.521090        6.298716        1.832227        F
H               7.521091        14.697002       1.832228        F
H               3.346923        10.497859       14.197637       F
H               6.469066        10.497859       0.138110        F
H               0.036291        9.692187        9.043066        F
H               0.036295        11.303524       9.043066        F
H               2.008448        9.058198        12.145152       F
H               2.008447        11.937518       12.145155       F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.254286	7.658728	6.986141	R
O	4.832373	6.295580	7.126030	R
O	7.535186	6.270963	7.423750	R
O	6.259500	7.628097	5.063591	R
Al	7.266720	6.128932	9.242582	R
O	6.467782	7.460823	13.294239	R
O	7.704238	5.927613	10.908297	R
O	6.004069	4.833072	8.826705	R
O	6.047953	7.590132	8.938434	R
Al	7.311072	9.026375	4.889111	R
Al	7.249854	11.975641	4.847559	R
Al	6.241884	13.350246	6.974671	R
Al	6.390396	10.495037	7.132381	R
O	4.828144	14.705250	7.127027	R
O	4.971899	11.811660	7.271510	R
O	4.969768	9.179855	7.271941	R
O	7.529337	14.729971	7.416814	R
O	6.327367	10.485082	5.081992	R
O	7.563436	12.010090	6.683151	R
O	7.592042	9.030307	6.754044	R
O	6.197597	13.366921	5.045192	R
Al	7.267044	14.855836	9.234297	R
Al	7.993773	10.444730	10.383714	R
O	6.182900	10.497526	13.143739	R
O	6.485248	13.537514	13.288862	R
O	6.375215	10.494429	9.064767	R
O	7.706658	15.045014	10.903019	R
O	6.043453	13.404367	8.931803	R
O	6.004093	16.160628	8.829725	R
O	8.165897	9.070966	11.518603	R
O	8.178563	11.825528	11.524535	R
O	4.824616	6.082444	10.925325	R
O	4.824054	14.913178	10.928562	R
O	4.788517	9.070964	10.960757	R
O	4.788238	11.927069	10.962108	R
O	6.337815	4.951252	5.085457	R
O	6.342168	16.043430	5.086021	R
O	8.106077	9.088931	3.329844	R
O	8.050030	11.939435	3.296488	R
O	3.498080	10.498003	8.966874	R
Cu	8.931854	11.585354	7.928235	R
Cu	9.205208	8.829406	8.018621	R
O	9.352441	10.330165	9.215004	R
N	10.512853	7.528697	8.077746	R
O	11.451494	6.927781	8.427865	R

Model #05   Cartesian coordinates in angstrom

	x	y	z	Relaxed/Frozen
Al	4.718091	6.298715	9.025534	F
Al	6.299120	6.298715	11.957102	F
Al	4.718091	14.697002	9.025534	F
Al	4.828311	11.950763	9.158184	F
Al	4.828311	9.044955	9.158184	F
Al	7.260466	8.998624	12.959551	F
Al	7.260466	11.997093	12.959551	F
Al	6.299120	14.697002	11.957102	F
Al	4.636026	10.497859	12.053017	F
O	3.286788	10.497859	13.239718	F
Al	6.284430	4.911618	6.956078	F
Al	6.284430	16.084099	6.956078	F
Al	7.604152	10.497859	2.473791	F
O	6.427205	10.497859	1.094354	F
Al	6.373455	6.298715	3.886397	F
O	4.781442	6.298715	2.980335	F
Al	6.373455	14.697002	3.886397	F
O	4.781442	14.697002	2.980335	F
O	3.454035	4.977004	9.235301	F
O	3.454035	7.620427	9.235301	F
O	6.249989	5.002877	13.162247	F
O	3.454035	16.018713	9.235301	F
O	3.454035	13.375290	9.235301	F
O	7.425505	9.104843	14.776051	F
O	7.425505	11.890874	14.776051	F
O	6.249989	15.992841	13.162247	F
O	4.962264	3.365416	7.283451	F
O	7.499839	3.492587	6.705345	F
O	4.962264	17.630302	7.283451	F
O	7.499839	17.503130	6.705345	F
O	7.704784	6.298715	2.777154	F
O	7.704784	14.697002	2.777154	F
Al	3.478998	10.497859	7.046735	F
O	1.926548	11.807732	6.890259	F
O	1.926548	9.187985	6.890259	F
O	3.361122	10.497859	5.169014	F
Al	2.050923	10.497859	10.125656	F
O	0.574778	10.497859	9.076089	F
O	2.097749	9.088323	11.188759	F
O	2.097749	11.907395	11.188759	F
Al	3.393316	6.298715	6.011417	F
O	1.956477	6.298715	7.179493	F
O	3.339459	7.715095	4.949249	F
O	3.339459	4.882336	4.949249	F
Al	3.393316	14.697002	6.011417	F
O	1.956477	14.697002	7.179493	F
O	3.339459	16.113380	4.949249	F
O	3.339459	13.280622	4.949249	F
H	3.439923	4.911172	10.243970	F
H	3.439232	7.689483	10.293373	F
H	6.818393	4.213072	13.048228	F
H	6.229200	4.955319	14.133904	F
H	3.439929	16.084518	10.243550	F
H	3.439218	13.306190	10.293977	F
H	6.776962	8.347647	14.909841	F
H	6.777013	12.648010	14.909830	F
H	6.229199	16.040400	14.133948	F
H	6.818394	16.782646	13.048228	F
H	4.227165	2.738070	7.166136	F
H	6.932392	2.747750	6.973661	F
H	7.409135	3.550965	5.707009	F
H	4.227165	18.257647	7.166137	F
H	6.932397	18.247959	6.973659	F
H	7.409131	17.444750	5.706962	F
H	7.521090	6.298716	1.832227	F
H	7.521091	14.697002	1.832228	F
H	3.346923	10.497859	14.197637	F
H	6.469066	10.497859	0.138110	F
H	0.036291	9.692187	9.043065	F
H	0.036295	11.303524	9.043066	F
H	2.008448	9.058198	12.145152	F
H	2.008447	11.937518	12.145155	F

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.236763	7.655337	6.970460	R
O	4.823002	6.298582	7.126874	R
O	7.507929	6.267527	7.379942	R
O	6.247603	7.636527	5.050877	R
Al	7.308153	6.149696	9.227874	R
O	6.472942	7.462120	13.292595	R
O	7.688788	5.912886	10.913325	R
O	6.016459	4.846371	8.825793	R
O	6.055606	7.595747	8.930027	R
Al	7.314254	9.025171	4.886428	R
Al	7.251885	11.976454	4.844926	R
Al	6.244744	13.350687	6.975201	R
Al	6.389427	10.495915	7.125822	R
O	4.828466	14.704681	7.127110	R
O	4.973585	11.812490	7.271354	R
O	4.967495	9.184677	7.271375	R
O	7.530146	14.730661	7.417460	R
O	6.330104	10.485419	5.078429	R
O	7.566521	12.008947	6.680211	R
O	7.589471	9.026479	6.749301	R
O	6.199396	13.367229	5.045763	R
Al	7.267033	14.857517	9.235175	R
Al	7.992778	10.485867	10.399035	R
O	6.185706	10.498703	13.140168	R
O	6.479723	13.536358	13.290486	R
O	6.386588	10.499902	9.063372	R
O	7.705844	15.049617	10.903602	R
O	6.044348	13.404876	8.932274	R
O	6.003675	16.161112	8.829481	R
O	8.175435	9.103027	11.525017	R
O	8.183600	11.863978	11.527354	R
O	4.813399	6.093417	10.930284	R
O	4.823742	14.912546	10.928163	R
O	4.793621	9.074785	10.959758	R
O	4.792458	11.926753	10.962134	R
O	6.330190	4.947849	5.079811	R
O	6.342174	16.043493	5.086064	R
O	8.113575	9.091343	3.329558	R
O	8.049827	11.941597	3.293036	R
O	3.499545	10.499599	8.967813	R
O	9.365719	10.370581	9.243219	R
Cu	8.935721	11.582604	7.920403	R
Cu	9.015926	8.790674	8.223626	R
N	9.588538	7.120237	8.871368	R
O	10.592176	6.573806	9.113501	R

```
Model #06      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043065       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.204344	7.647217	6.959271	R
O	4.791452	6.309603	7.129421	R
O	7.441320	6.289616	7.254279	R
O	6.223814	7.661019	5.029205	R
Al	7.436263	6.194533	9.199358	R
O	6.478954	7.470790	13.291190	R
O	7.648447	5.887003	10.931091	R
O	6.044582	4.884084	8.814920	R
O	6.045515	7.617760	8.911441	R
Al	7.332599	9.015527	4.905792	R
Al	7.268854	11.971548	4.870808	R
Al	6.250101	13.346133	6.986524	R
Al	6.391339	10.496045	7.132006	R
O	4.825000	14.703096	7.129661	R
O	4.955787	11.826842	7.267987	R
O	4.940949	9.205717	7.264520	R
O	7.529741	14.728638	7.426769	R
O	6.347787	10.482505	5.110463	R
O	7.574054	11.982951	6.732248	R
O	7.583411	9.026778	6.793010	R
O	6.221634	13.369285	5.063223	R
Al	7.263216	14.873268	9.243205	R
Al	7.838644	10.573035	10.364864	R
O	6.186148	10.505007	13.141490	R
O	6.479029	13.539254	13.297820	R
O	6.319217	10.526810	9.067629	R
O	7.703888	15.072874	10.907632	R
O	6.046982	13.406020	8.938004	R
O	5.998800	16.164847	8.828213	R
O	8.145633	9.215277	11.503486	R
O	8.104952	11.954132	11.462446	R
O	4.776300	6.120779	10.945683	R
O	4.823653	14.910877	10.925406	R
O	4.792839	9.093822	10.955074	R
O	4.784513	11.930379	10.961443	R
O	6.295063	4.938776	5.062196	R
O	6.333615	16.041833	5.087820	R
O	8.127594	9.106065	3.346231	R
O	8.034157	11.943948	3.302077	R
O	3.474061	10.507655	8.956353	R
O	9.084158	10.479812	9.041451	R
Cu	9.264659	11.895780	7.807605	R
Cu	8.881419	8.745956	8.405987	R
O	9.098179	6.937366	8.762886	R
N	10.554751	13.025437	7.160818	R

```
Model #07      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al     4.718091       6.298715       9.025534       F
Al     6.299120       6.298715       11.957102      F
Al     4.718091       14.697002      9.025534       F
Al     4.828311       11.950763      9.158184       F
Al     4.828311       9.044955       9.158184       F
Al     7.260466       8.998624       12.959551      F
Al     7.260466       11.997093      12.959551      F
Al     6.299120       14.697002      11.957102      F
Al     4.636026       10.497859      12.053017      F
O      3.286788       10.497859      13.239718      F
Al     6.284430       4.911618       6.956078       F
Al     6.284430       16.084099      6.956078       F
Al     7.604152       10.497859      2.473791       F
O      6.427205       10.497859      1.094354       F
Al     6.373455       6.298715       3.886397       F
O      4.781442       6.298715       2.980335       F
Al     6.373455       14.697002      3.886397       F
O      4.781442       14.697002      2.980335       F
O      3.454035       4.977004       9.235301       F
O      3.454035       7.620427       9.235301       F
O      6.249989       5.002877       13.162247      F
O      3.454035       16.018713      9.235301       F
O      3.454035       13.375290      9.235301       F
O      7.425505       9.104843       14.776051      F
O      7.425505       11.890874      14.776051      F
O      6.249989       15.992841      13.162247      F
O      4.962264       3.365416       7.283451       F
O      7.499839       3.492587       6.705345       F
O      4.962264       17.630302      7.283451       F
O      7.499839       17.503130      6.705345       F
O      7.704784       6.298715       2.777154       F
O      7.704784       14.697002      2.777154       F
Al     3.478998       10.497859      7.046735       F
O      1.926548       11.807732      6.890259       F
O      1.926548       9.187985       6.890259       F
O      3.361122       10.497859      5.169014       F
Al     2.050923       10.497859      10.125656      F
O      0.574778       10.497859      9.076089       F
O      2.097749       9.088323       11.188759      F
O      2.097749       11.907395      11.188759      F
Al     3.393316       6.298715       6.011417       F
O      1.956477       6.298715       7.179493       F
O      3.339459       7.715095       4.949249       F
O      3.339459       4.882336       4.949249       F
Al     3.393316       14.697002      6.011417       F
O      1.956477       14.697002      7.179493       F
O      3.339459       16.113380      4.949249       F
O      3.339459       13.280622      4.949249       F
H      3.439923       4.911172       10.243970      F
H      3.439232       7.689483       10.293373      F
H      6.818393       4.213072       13.048228      F
H      6.229200       4.955319       14.133904      F
H      3.439929       16.084518      10.243550      F
H      3.439218       13.306190      10.293977      F
H      6.776962       8.347647       14.909841      F
H      6.777013       12.648010      14.909830      F
H      6.229199       16.040400      14.133948      F
H      6.818394       16.782646      13.048228      F
H      4.227165       2.738070       7.166136       F
H      6.932392       2.747750       6.973661       F
H      7.409135       3.550965       5.707009       F
H      4.227165       18.257647      7.166137       F
H      6.932397       18.247959      6.973659       F
H      7.409131       17.444750      5.706962       F
H      7.521090       6.298716       1.832227       F
H      7.521091       14.697002      1.832228       F
H      3.346923       10.497859      14.197637      F
H      6.469066       10.497859      0.138110       F
H      0.036291       9.692187       9.043065       F
H      0.036295       11.303524      9.043066       F
H      2.008448       9.058198       12.145152      F
H      2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.248940	7.659598	6.985516	R
O	4.831529	6.292800	7.127675	R
O	7.534100	6.269757	7.423502	R
O	6.242522	7.625797	5.062801	R
Al	7.266166	6.128705	9.241136	R
O	6.486638	7.455845	13.294101	R
O	7.707104	5.935571	10.908021	R
O	6.004484	4.831740	8.828544	R
O	6.048965	7.589814	8.940279	R
Al	7.283994	9.030112	4.883931	R
Al	7.284438	11.965890	4.884418	R
Al	6.249576	13.336208	6.985810	R
Al	6.410819	10.497346	7.157277	R
O	4.831543	14.702641	7.127690	R
O	4.971374	11.816559	7.273213	R
O	4.971395	9.179091	7.273163	R
O	7.534105	14.726087	7.423579	R
O	6.325368	10.498172	5.090188	R
O	7.581275	11.970100	6.745667	R
O	7.580995	9.025770	6.745435	R
O	6.243304	13.370270	5.063026	R
Al	7.266129	14.866904	9.241162	R
Al	7.902635	10.498248	10.340664	R
O	6.182296	10.497864	13.149755	R
O	6.486587	13.539877	13.294156	R
O	6.311408	10.498021	9.080760	R
O	7.707066	15.060292	10.908000	R
O	6.048997	13.405949	8.940406	R
O	6.004362	16.163963	8.828459	R
O	8.139457	9.130220	11.492673	R
O	8.139305	11.866196	11.492544	R
O	4.825486	6.080004	10.927400	R
O	4.825495	14.915578	10.927412	R
O	4.786686	9.065699	10.966334	R
O	4.786533	11.930015	10.966376	R
O	6.339936	4.950054	5.085177	R
O	6.339861	16.045786	5.085113	R
O	8.078048	9.075757	3.323431	R
O	8.078599	11.919829	3.323405	R
O	3.491912	10.497859	8.967278	R
O	9.106672	10.498047	9.021188	R
Cu	9.212125	12.074043	7.964945	R
Cu	9.212024	8.922065	7.965084	R
N	10.426378	7.540277	7.968402	R
O	11.464552	7.128666	7.623497	R
N	10.429998	13.452705	7.972726	R
O	11.472045	13.860578	7.635005	R

```
Model #08        Cartesian coordinates in angstrom
                 x                y                z                Relaxed/Frozen
Al               4.718091         6.298715         9.025534         F
Al               6.299120         6.298715         11.957102        F
Al               4.718091         14.697002        9.025534         F
Al               4.828311         11.950763        9.158184         F
Al               4.828311         9.044955         9.158184         F
Al               7.260466         8.998624         12.959551        F
Al               7.260466         11.997093        12.959551        F
Al               6.299120         14.697002        11.957102        F
Al               4.636026         10.497859        12.053017        F
O                3.286788         10.497859        13.239718        F
Al               6.284430         4.911618         6.956078         F
Al               6.284430         16.084099        6.956078         F
Al               7.604152         10.497859        2.473791         F
O                6.427205         10.497859        1.094354         F
Al               6.373455         6.298715         3.886397         F
O                4.781442         6.298715         2.980335         F
Al               6.373455         14.697002        3.886397         F
O                4.781442         14.697002        2.980335         F
O                3.454035         4.977004         9.235301         F
O                3.454035         7.620427         9.235301         F
O                6.249989         5.002877         13.162247        F
O                3.454035         16.018713        9.235301         F
O                3.454035         13.375290        9.235301         F
O                7.425505         9.104843         14.776051        F
O                7.425505         11.890874        14.776051        F
O                6.249989         15.992841        13.162247        F
O                4.962264         3.365416         7.283451         F
O                7.499839         3.492587         6.705345         F
O                4.962264         17.630302        7.283451         F
O                7.499839         17.503130        6.705345         F
O                7.704784         6.298715         2.777154         F
O                7.704784         14.697002        2.777154         F
Al               3.478998         10.497859        7.046735         F
O                1.926548         11.807732        6.890259         F
O                1.926548         9.187985         6.890259         F
O                3.361122         10.497859        5.169014         F
Al               2.050923         10.497859        10.125656        F
O                0.574778         10.497859        9.076089         F
O                2.097749         9.088323         11.188759        F
O                2.097749         11.907395        11.188759        F
Al               3.393316         6.298715         6.011417         F
O                1.956477         6.298715         7.179493         F
O                3.339459         7.715095         4.949249         F
O                3.339459         4.882336         4.949249         F
Al               3.393316         14.697002        6.011417         F
O                1.956477         14.697002        7.179493         F
O                3.339459         16.113380        4.949249         F
O                3.339459         13.280622        4.949249         F
H                3.439923         4.911172         10.243970        F
H                3.439232         7.689483         10.293373        F
H                6.818393         4.213072         13.048228        F
H                6.229200         4.955319         14.133904        F
H                3.439929         16.084518        10.243550        F
H                3.439218         13.306190        10.293977        F
H                6.776962         8.347647         14.909841        F
H                6.777013         12.648010        14.909830        F
H                6.229199         16.040400        14.133948        F
H                6.818394         16.782646        13.048228        F
H                4.227165         2.738070         7.166136         F
H                6.932392         2.747750         6.973661         F
H                7.409135         3.550965         5.707009         F
H                4.227165         18.257647        7.166137         F
H                6.932397         18.247959        6.973659         F
H                7.409131         17.444750        5.706962         F
H                7.521090         6.298716         1.832227         F
H                7.521091         14.697002        1.832228         F
H                3.346923         10.497859        14.197637        F
H                6.469066         10.497859        0.138110         F
H                0.036291         9.692187         9.043065         F
H                0.036295         11.303524        9.043066         F
H                2.008448         9.058198         12.145152        F
H                2.008447         11.937518        12.145155        F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.248940	7.659598	6.985516	R
O	4.831529	6.292800	7.127675	R
O	7.534100	6.269757	7.423502	R
O	6.242522	7.625797	5.062801	R
Al	7.266166	6.128705	9.241136	R
O	6.486638	7.455845	13.294101	R
O	7.707104	5.935571	10.908021	R
O	6.004484	4.831740	8.828544	R
O	6.048965	7.589814	8.940279	R
Al	7.283994	9.030112	4.883931	R
Al	7.284438	11.965890	4.884418	R
Al	6.249576	13.336208	6.985810	R
Al	6.410819	10.497346	7.157277	R
O	4.831543	14.702641	7.127690	R
O	4.971374	11.816559	7.273213	R
O	4.971395	9.179091	7.273163	R
O	7.534105	14.726087	7.423579	R
O	6.325368	10.498172	5.090188	R
O	7.581275	11.970100	6.745667	R
O	7.580995	9.025770	6.745435	R
O	6.243304	13.370270	5.063026	R
Al	7.266129	14.866904	9.241162	R
Al	7.902635	10.498248	10.340664	R
O	6.182296	10.497864	13.149755	R
O	6.486587	13.539877	13.294156	R
O	6.311408	10.498021	9.080760	R
O	7.707066	15.060292	10.908000	R
O	6.048997	13.405949	8.940406	R
O	6.004362	16.163963	8.828459	R
O	8.139457	9.130220	11.492673	R
O	8.139305	11.866196	11.492544	R
O	4.825486	6.080004	10.927400	R
O	4.825495	14.915578	10.927412	R
O	4.786686	9.065699	10.966334	R
O	4.786533	11.930015	10.966376	R
O	6.339936	4.950054	5.085177	R
O	6.339861	16.045786	5.085113	R
O	8.078048	9.075757	3.323431	R
O	8.078599	11.919829	3.323405	R
O	3.491912	10.497859	8.967278	R
O	9.106672	10.498047	9.021188	R
Cu	9.212125	12.074043	7.964945	R
Cu	9.212024	8.922065	7.965084	R
N	10.426378	7.540277	7.968402	R
O	11.464552	7.128666	7.623497	R
N	10.429998	13.452705	7.972726	R
O	11.472045	13.860578	7.635005	R

```
Model #09      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al      4.718091       6.298715       9.025534       F
Al      6.299120       6.298715       11.957102      F
Al      4.718091       14.697002      9.025534       F
Al      4.828311       11.950763      9.158184       F
Al      4.828311       9.044955       9.158184       F
Al      7.260466       8.998624       12.959551      F
Al      7.260466       11.997093      12.959551      F
Al      6.299120       14.697002      11.957102      F
Al      4.636026       10.497859      12.053017      F
O       3.286788       10.497859      13.239718      F
Al      6.284430       4.911618       6.956078       F
Al      6.284430       16.084099      6.956078       F
Al      7.604152       10.497859      2.473791       F
O       6.427205       10.497859      1.094354       F
Al      6.373455       6.298715       3.886397       F
O       4.781442       6.298715       2.980335       F
Al      6.373455       14.697002      3.886397       F
O       4.781442       14.697002      2.980335       F
O       3.454035       4.977004       9.235301       F
O       3.454035       7.620427       9.235301       F
O       6.249989       5.002877       13.162247      F
O       3.454035       16.018713      9.235301       F
O       3.454035       13.375290      9.235301       F
O       7.425505       9.104843       14.776051      F
O       7.425505       11.890874      14.776051      F
O       6.249989       15.992841      13.162247      F
O       4.962264       3.365416       7.283451       F
O       7.499839       3.492587       6.705345       F
O       4.962264       17.630302      7.283451       F
O       7.499839       17.503130      6.705345       F
O       7.704784       6.298715       2.777154       F
O       7.704784       14.697002      2.777154       F
Al      3.478998       10.497859      7.046735       F
O       1.926548       11.807732      6.890259       F
O       1.926548       9.187985       6.890259       F
O       3.361122       10.497859      5.169014       F
Al      2.050923       10.497859      10.125656      F
O       0.574778       10.497859      9.076089       F
O       2.097749       9.088323       11.188759      F
O       2.097749       11.907395      11.188759      F
Al      3.393316       6.298715       6.011417       F
O       1.956477       6.298715       7.179493       F
O       3.339459       7.715095       4.949249       F
O       3.339459       4.882336       4.949249       F
Al      3.393316       14.697002      6.011417       F
O       1.956477       14.697002      7.179493       F
O       3.339459       16.113380      4.949249       F
O       3.339459       13.280622      4.949249       F
H       3.439923       4.911172       10.243970      F
H       3.439232       7.689483       10.293373      F
H       6.818393       4.213072       13.048228      F
H       6.229200       4.955319       14.133904      F
H       3.439929       16.084518      10.243550      F
H       3.439218       13.306190      10.293977      F
H       6.776962       8.347647       14.909841      F
H       6.777013       12.648010      14.909830      F
H       6.229199       16.040400      14.133948      F
H       6.818394       16.782646      13.048228      F
H       4.227165       2.738070       7.166136       F
H       6.932392       2.747750       6.973661       F
H       7.409135       3.550965       5.707009       F
H       4.227165       18.257647      7.166137       F
H       6.932397       18.247959      6.973659       F
H       7.409131       17.444750      5.706962       F
H       7.521090       6.298716       1.832227       F
H       7.521091       14.697002      1.832228       F
H       3.346923       10.497859      14.197637      F
H       6.469066       10.497859      0.138110       F
H       0.036291       9.692187       9.043065       F
H       0.036295       11.303524      9.043066       F
H       2.008448       9.058198       12.145152      F
H       2.008447       11.937518      12.145155      F
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H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.246938	7.657513	6.976517	R
O	4.824826	6.300205	7.126025	R
O	7.512564	6.268559	7.375314	R
O	6.245623	7.634611	5.052449	R
Al	7.311316	6.163992	9.232532	R
O	6.472271	7.461994	13.295352	R
O	7.680007	5.891777	10.920384	R
O	6.019009	4.851932	8.824469	R
O	6.055253	7.597270	8.931883	R
Al	7.302488	9.028484	4.886319	R
Al	7.248641	11.977240	4.843792	R
Al	6.238421	13.350252	6.972800	R
Al	6.390253	10.494581	7.128454	R
O	4.827938	14.706041	7.127093	R
O	4.972380	11.813444	7.272449	R
O	4.967171	9.186412	7.272422	R
O	7.529697	14.729007	7.416732	R
O	6.322160	10.490331	5.075174	R
O	7.560270	12.011485	6.680480	R
O	7.585879	9.032689	6.747213	R
O	6.196109	13.368103	5.044199	R
Al	7.266426	14.856258	9.234237	R
Al	7.982745	10.459374	10.384345	R
O	6.184975	10.497825	13.142217	R
O	6.484543	13.537547	13.289292	R
O	6.386197	10.500226	9.064055	R
O	7.706970	15.044723	10.902836	R
O	6.043673	13.405160	8.931830	R
O	6.004457	16.160976	8.829468	R
O	8.161660	9.073695	11.509217	R
O	8.183615	11.830636	11.530629	R
O	4.810134	6.097618	10.931184	R
O	4.824408	14.914303	10.928414	R
O	4.793742	9.077205	10.959205	R
O	4.792360	11.928670	10.962862	R
O	6.332038	4.945452	5.078113	R
O	6.342850	16.043749	5.086152	R
O	8.108709	9.091449	3.331942	R
O	8.050614	11.941554	3.293708	R
O	3.499395	10.500721	8.968301	R
O	9.368017	10.394215	9.236367	R
Cu	8.915172	11.642541	7.952974	R
Cu	9.270413	8.912218	7.995344	R
N	9.406690	7.101135	8.982806	R
O	10.397279	6.557275	9.250283	R
N	10.980374	8.490310	7.151242	R
O	11.851871	7.832189	7.543966	R

```
Model #10      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043065       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.248644	7.654632	6.980401	R
O	4.824329	6.298947	7.127313	R
O	7.518639	6.274701	7.377691	R
O	6.240241	7.633194	5.053892	R
Al	7.319273	6.156741	9.218517	R
O	6.477453	7.458828	13.295113	R
O	7.674240	5.872674	10.917777	R
O	6.020817	4.850326	8.823537	R
O	6.055589	7.594562	8.935502	R
Al	7.289134	9.029879	4.880616	R
Al	7.248700	11.977669	4.844832	R
Al	6.237289	13.350814	6.972528	R
Al	6.385973	10.496602	7.129769	R
O	4.827964	14.706514	7.127157	R
O	4.970137	11.814566	7.272453	R
O	4.966239	9.185195	7.272317	R
O	7.529968	14.728701	7.416766	R
O	6.315786	10.494506	5.073456	R
O	7.557878	12.011786	6.682536	R
O	7.577592	9.036860	6.740420	R
O	6.196536	13.368818	5.044270	R
Al	7.266230	14.855737	9.233866	R
Al	7.993220	10.434971	10.374948	R
O	6.183959	10.496460	13.143896	R
O	6.488259	13.537943	13.287773	R
O	6.382912	10.498033	9.062491	R
O	7.707929	15.040392	10.902649	R
O	6.043379	13.405209	8.931547	R
O	6.004908	16.160841	8.829753	R
O	8.161180	9.053095	11.508573	R
O	8.186538	11.803631	11.533193	R
O	4.812243	6.094873	10.932344	R
O	4.824876	14.914884	10.928685	R
O	4.794114	9.076047	10.960254	R
O	4.791398	11.929382	10.963339	R
O	6.331768	4.946144	5.078762	R
O	6.342873	16.043784	5.086308	R
O	8.100752	9.088577	3.330270	R
O	8.053912	11.939244	3.296405	R
O	3.499168	10.500533	8.968666	R
O	9.362303	10.363866	9.209749	R
Cu	8.917595	11.655600	7.959793	R
Cu	9.311296	8.994439	7.850959	R
N	9.351853	7.123122	9.546044	R
O	10.371586	6.664151	9.846502	R
N	10.818147	8.157091	7.104312	R
O	11.612103	7.316436	7.246702	R

```
Model #11      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043065       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.252906	7.654737	6.988605	R
O	4.832484	6.292682	7.127011	R
O	7.540022	6.271986	7.425956	R
O	6.232505	7.623596	5.062424	R
Al	7.265026	6.133743	9.242394	R
O	6.482019	7.456821	13.293464	R
O	7.707085	5.935889	10.907644	R
O	6.005158	4.834156	8.827362	R
O	6.046226	7.590297	8.938434	R
Al	7.266813	9.027734	4.873183	R
Al	7.267074	11.967995	4.873242	R
Al	6.252844	13.340911	6.988603	R
Al	6.394900	10.497854	7.147858	R
O	4.832497	14.703032	7.126982	R
O	4.970873	11.816261	7.272315	R
O	4.970861	9.179441	7.272330	R
O	7.539996	14.723721	7.425956	R
O	6.312135	10.497927	5.084453	R
O	7.574361	11.973524	6.729522	R
O	7.574225	9.022134	6.729453	R
O	6.232717	13.372124	5.062447	R
Al	7.265017	14.861958	9.242390	R
Al	7.930893	10.497864	10.346800	R
O	6.180215	10.497868	13.150105	R
O	6.482037	13.538903	13.293479	R
O	6.340994	10.497868	9.068543	R
O	7.707072	15.059895	10.907636	R
O	6.046235	13.405400	8.938427	R
O	6.005115	16.161556	8.827337	R
O	8.141390	9.126558	11.498073	R
O	8.141165	11.869331	11.497897	R
O	4.825741	6.080844	10.926315	R
O	4.825766	14.914795	10.926302	R
O	4.786307	9.068419	10.962674	R
O	4.786093	11.927343	10.962684	R
O	6.341607	4.950995	5.085881	R
O	6.341588	16.044745	5.085860	R
O	8.071485	9.073870	3.320784	R
O	8.071710	11.921758	3.320819	R
O	3.495162	10.497828	8.966228	R
Cu	9.292631	11.844514	7.733168	R
Cu	9.292349	9.150934	7.733205	R
O	9.228200	10.497741	9.121328	R
O	12.172590	11.765657	7.947233	R
O	12.172071	9.230125	7.947624	R
N	11.157328	11.573162	7.400586	R
N	11.157095	9.423010	7.400561	R

```
Model #12        Cartesian coordinates in angstrom
                 x               y               z               Relaxed/Frozen
Al               4.718091        6.298715        9.025534        F
Al               6.299120        6.298715        11.957102       F
Al               4.718091        14.697002       9.025534        F
Al               4.828311        11.950763       9.158184        F
Al               4.828311        9.044955        9.158184        F
Al               7.260466        8.998624        12.959551       F
Al               7.260466        11.997093       12.959551       F
Al               6.299120        14.697002       11.957102       F
Al               4.636026        10.497859       12.053017       F
O                3.286788        10.497859       13.239718       F
Al               6.284430        4.911618        6.956078        F
Al               6.284430        16.084099       6.956078        F
Al               7.604152        10.497859       2.473791        F
O                6.427205        10.497859       1.094354        F
Al               6.373455        6.298715        3.886397        F
O                4.781442        6.298715        2.980335        F
Al               6.373455        14.697002       3.886397        F
O                4.781442        14.697002       2.980335        F
O                3.454035        4.977004        9.235301        F
O                3.454035        7.620427        9.235301        F
O                6.249989        5.002877        13.162247       F
O                3.454035        16.018713       9.235301        F
O                3.454035        13.375290       9.235301        F
O                7.425505        9.104843        14.776051       F
O                7.425505        11.890874       14.776051       F
O                6.249989        15.992841       13.162247       F
O                4.962264        3.365416        7.283451        F
O                7.499839        3.492587        6.705345        F
O                4.962264        17.630302       7.283451        F
O                7.499839        17.503130       6.705345        F
O                7.704784        6.298715        2.777154        F
O                7.704784        14.697002       2.777154        F
Al               3.478998        10.497859       7.046735        F
O                1.926548        11.807732       6.890259        F
O                1.926548        9.187985        6.890259        F
O                3.361122        10.497859       5.169014        F
Al               2.050923        10.497859       10.125656       F
O                0.574778        10.497859       9.076089        F
O                2.097749        9.088323        11.188759       F
O                2.097749        11.907395       11.188759       F
Al               3.393316        6.298715        6.011417        F
O                1.956477        6.298715        7.179493        F
O                3.339459        7.715095        4.949249        F
O                3.339459        4.882336        4.949249        F
Al               3.393316        14.697002       6.011417        F
O                1.956477        14.697002       7.179493        F
O                3.339459        16.113380       4.949249        F
O                3.339459        13.280622       4.949249        F
H                3.439923        4.911172        10.243970       F
H                3.439232        7.689483        10.293373       F
H                6.818393        4.213072        13.048228       F
H                6.229200        4.955319        14.133904       F
H                3.439929        16.084518       10.243550       F
H                3.439218        13.306190       10.293977       F
H                6.776962        8.347647        14.909841       F
H                6.777013        12.648010       14.909830       F
H                6.229199        16.040400       14.133948       F
H                6.818394        16.782646       13.048228       F
H                4.227165        2.738070        7.166136        F
H                6.932392        2.747750        6.973661        F
H                7.409135        3.550965        5.707009        F
H                4.227165        18.257647       7.166137        F
H                6.932397        18.247959       6.973659        F
H                7.409131        17.444750       5.706962        F
H                7.521090        6.298716        1.832227        F
H                7.521091        14.697002       1.832228        F
H                3.346923        10.497859       14.197637       F
H                6.469066        10.497859       0.138110        F
H                0.036291        9.692187        9.043065        F
H                0.036295        11.303524       9.043066        F
H                2.008448        9.058198        12.145152       F
H                2.008447        11.937518       12.145155       F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.251027	7.653822	6.984153	R
O	4.831977	6.292427	7.126808	R
O	7.539522	6.271403	7.424845	R
O	6.224281	7.624496	5.056888	R
Al	7.264757	6.135378	9.241014	R
O	6.478777	7.458175	13.292409	R
O	7.706788	5.938414	10.906667	R
O	6.005016	4.834541	8.827578	R
O	6.045290	7.590473	8.936787	R
Al	7.265594	9.025231	4.868264	R
Al	7.264235	11.969171	4.867133	R
Al	6.249794	13.341517	6.985883	R
Al	6.394187	10.494883	7.141823	R
O	4.832210	14.703508	7.126783	R
O	4.971239	11.815284	7.272796	R
O	4.968847	9.181038	7.273524	R
O	7.540118	14.724013	7.425885	R
O	6.311616	10.498210	5.080105	R
O	7.571355	11.980742	6.720024	R
O	7.567910	9.014443	6.717327	R
O	6.227204	13.371805	5.059181	R
Al	7.263808	14.862379	9.242106	R
Al	7.967368	10.500226	10.365607	R
O	6.181068	10.497990	13.147346	R
O	6.478415	13.537856	13.292914	R
O	6.364485	10.499813	9.064206	R
O	7.707052	15.059818	10.907060	R
O	6.045881	13.406016	8.937288	R
O	6.004778	16.162031	8.827158	R
O	8.157888	9.125726	11.511726	R
O	8.154669	11.877231	11.509053	R
O	4.825314	6.081347	10.926542	R
O	4.826068	14.914963	10.925862	R
O	4.787483	9.069789	10.961442	R
O	4.786863	11.926825	10.961717	R
O	6.342269	4.951121	5.086267	R
O	6.342620	16.044581	5.086223	R
O	8.069047	9.071732	3.315913	R
O	8.070641	11.924151	3.316620	R
O	3.496919	10.498573	8.966961	R
Cu	9.233222	11.799961	7.793710	R
Cu	9.254248	9.160434	7.785115	R
O	9.304772	10.494424	9.186401	R
O	12.127862	11.825344	7.456045	R
O	12.101983	9.037838	7.059347	R
N	11.079662	11.459183	7.095568	R
N	11.048616	9.508030	6.829537	R

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Model #13      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043065       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
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H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.239848	7.651472	6.976982	R
O	4.820048	6.300396	7.127027	R
O	7.503730	6.274971	7.361801	R
O	6.242151	7.637551	5.051097	R
Al	7.337079	6.154940	9.225115	R
O	6.469886	7.464250	13.295382	R
O	7.669952	5.887380	10.925151	R
O	6.023899	4.852938	8.822542	R
O	6.058298	7.598100	8.930348	R
Al	7.299860	9.027370	4.881673	R
Al	7.250370	11.978219	4.844971	R
Al	6.239087	13.351758	6.973656	R
Al	6.384954	10.498665	7.125758	R
O	4.828381	14.706195	7.126927	R
O	4.971817	11.815283	7.271976	R
O	4.968114	9.188920	7.270948	R
O	7.530745	14.729238	7.417639	R
O	6.323762	10.491045	5.077829	R
O	7.561296	12.011887	6.682621	R
O	7.584109	9.035288	6.746152	R
O	6.197371	13.368171	5.044985	R
Al	7.265937	14.857583	9.235180	R
Al	7.972881	10.455849	10.383825	R
O	6.185537	10.498964	13.141628	R
O	6.486294	13.538216	13.289385	R
O	6.389749	10.502393	9.060956	R
O	7.707318	15.045996	10.903208	R
O	6.044062	13.405469	8.931571	R
O	6.004298	16.161179	8.829182	R
O	8.165437	9.077776	11.512419	R
O	8.175823	11.833217	11.522160	R
O	4.803119	6.101290	10.933497	R
O	4.824995	14.914227	10.927930	R
O	4.797577	9.081019	10.957956	R
O	4.792567	11.929127	10.962270	R
O	6.328454	4.945024	5.076097	R
O	6.343068	16.043161	5.086464	R
O	8.109104	9.091385	3.330682	R
O	8.051769	11.940476	3.295145	R
O	3.500407	10.501350	8.967880	R
Cu	8.922918	11.652394	7.954622	R
Cu	9.199288	8.952226	7.963444	R
O	9.363240	10.381833	9.230491	R
N	9.509025	6.820490	9.054492	R
O	10.407114	6.286982	9.558829	R
O	11.790672	7.671599	8.362540	R
N	10.851139	8.080727	7.824472	R

```
Model #14        Cartesian coordinates in angstrom
                 x              y              z              Relaxed/Frozen
Al       4.718091       6.298715       9.025534       F
Al       6.299120       6.298715       11.957102      F
Al       4.718091       14.697002      9.025534       F
Al       4.828311       11.950763      9.158184       F
Al       4.828311       9.044955       9.158184       F
Al       7.260466       8.998624       12.959551      F
Al       7.260466       11.997093      12.959551      F
Al       6.299120       14.697002      11.957102      F
Al       4.636026       10.497859      12.053017      F
O        3.286788       10.497859      13.239718      F
Al       6.284430       4.911618       6.956078       F
Al       6.284430       16.084099      6.956078       F
Al       7.604152       10.497859      2.473791       F
O        6.427205       10.497859      1.094354       F
Al       6.373455       6.298715       3.886397       F
O        4.781442       6.298715       2.980335       F
Al       6.373455       14.697002      3.886397       F
O        4.781442       14.697002      2.980335       F
O        3.454035       4.977004       9.235301       F
O        3.454035       7.620427       9.235301       F
O        6.249989       5.002877       13.162247      F
O        3.454035       16.018713      9.235301       F
O        3.454035       13.375290      9.235301       F
O        7.425505       9.104843       14.776051      F
O        7.425505       11.890874      14.776051      F
O        6.249989       15.992841      13.162247      F
O        4.962264       3.365416       7.283451       F
O        7.499839       3.492587       6.705345       F
O        4.962264       17.630302      7.283451       F
O        7.499839       17.503130      6.705345       F
O        7.704784       6.298715       2.777154       F
O        7.704784       14.697002      2.777154       F
Al       3.478998       10.497859      7.046735       F
O        1.926548       11.807732      6.890259       F
O        1.926548       9.187985       6.890259       F
O        3.361122       10.497859      5.169014       F
Al       2.050923       10.497859      10.125656      F
O        0.574778       10.497859      9.076089       F
O        2.097749       9.088323       11.188759      F
O        2.097749       11.907395      11.188759      F
Al       3.393316       6.298715       6.011417       F
O        1.956477       6.298715       7.179493       F
O        3.339459       7.715095       4.949249       F
O        3.339459       4.882336       4.949249       F
Al       3.393316       14.697002      6.011417       F
O        1.956477       14.697002      7.179493       F
O        3.339459       16.113380      4.949249       F
O        3.339459       13.280622      4.949249       F
H        3.439923       4.911172       10.243970      F
H        3.439232       7.689483       10.293373      F
H        6.818393       4.213072       13.048228      F
H        6.229200       4.955319       14.133904      F
H        3.439929       16.084518      10.243550      F
H        3.439218       13.306190      10.293977      F
H        6.776962       8.347647       14.909841      F
H        6.777013       12.648010      14.909830      F
H        6.229199       16.040400      14.133948      F
H        6.818394       16.782646      13.048228      F
H        4.227165       2.738070       7.166136       F
H        6.932392       2.747750       6.973661       F
H        7.409135       3.550965       5.707009       F
H        4.227165       18.257647      7.166137       F
H        6.932397       18.247959      6.973659       F
H        7.409131       17.444750      5.706962       F
H        7.521090       6.298716       1.832227       F
H        7.521091       14.697002      1.832228       F
H        3.346923       10.497859      14.197637      F
H        6.469066       10.497859      0.138110       F
H        0.036291       9.692187       9.043065       F
H        0.036295       11.303524      9.043066       F
H        2.008448       9.058198       12.145152      F
H        2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.223839	7.654432	6.977385	R
O	4.820009	6.291860	7.127870	R
O	7.506232	6.300046	7.375354	R
O	6.228691	7.636191	5.049120	R
Al	7.338599	6.109415	9.221458	R
O	6.462786	7.465898	13.294920	R
O	7.680531	5.926713	10.923013	R
O	6.026834	4.839091	8.820229	R
O	6.051619	7.592220	8.931382	R
Al	7.287840	9.024600	4.875604	R
Al	7.259349	11.976954	4.847868	R
Al	6.246867	13.351420	6.976391	R
Al	6.381488	10.499021	7.123454	R
O	4.829385	14.704893	7.126745	R
O	4.973263	11.814956	7.270996	R
O	4.964014	9.186960	7.268512	R
O	7.531522	14.730693	7.418291	R
O	6.322362	10.494131	5.076607	R
O	7.570189	12.005298	6.685819	R
O	7.575176	9.029187	6.736055	R
O	6.207097	13.367610	5.047800	R
Al	7.266580	14.858166	9.235736	R
Al	7.983090	10.446868	10.389307	R
O	6.185290	10.499553	13.140842	R
O	6.487072	13.538261	13.289147	R
O	6.385596	10.496603	9.059096	R
O	7.707304	15.046832	10.903823	R
O	6.044942	13.404924	8.931974	R
O	6.004065	16.161217	8.829550	R
O	8.177927	9.080229	11.526437	R
O	8.173230	11.834596	11.516420	R
O	4.808080	6.085940	10.931351	R
O	4.824795	14.913384	10.927987	R
O	4.794617	9.078381	10.958862	R
O	4.791417	11.928196	10.961604	R
O	6.334111	4.948986	5.081041	R
O	6.341908	16.043269	5.086103	R
O	8.098295	9.085304	3.326377	R
O	8.061072	11.935825	3.297932	R
O	3.500032	10.500891	8.967002	R
Cu	8.934642	11.552117	7.927488	R
Cu	9.054622	8.778145	8.061526	R
O	9.352767	10.295783	9.219418	R
N	9.730963	5.742224	9.018855	R
O	10.486770	5.213999	9.734783	R
O	11.472226	7.690059	9.070628	R
N	10.417968	7.556235	8.595207	R

```
Model #15      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043065       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.252924	7.654449	6.988709	R
O	4.832536	6.292778	7.126912	R
O	7.540187	6.271794	7.426195	R
O	6.233040	7.623781	5.062283	R
Al	7.264859	6.133489	9.242554	R
O	6.481862	7.456866	13.293429	R
O	7.707004	5.935607	10.907686	R
O	6.004933	4.834153	8.827281	R
O	6.046112	7.590244	8.938315	R
Al	7.268581	9.027145	4.873199	R
Al	7.267551	11.968403	4.873025	R
Al	6.253049	13.341608	6.988624	R
Al	6.393933	10.497866	7.146105	R
O	4.832494	14.702947	7.127003	R
O	4.970770	11.816074	7.272307	R
O	4.970771	9.179568	7.272355	R
O	7.540317	14.723975	7.426242	R
O	6.313554	10.497570	5.084775	R
O	7.573836	11.974834	6.729192	R
O	7.574103	9.021212	6.729470	R
O	6.232419	13.371961	5.062214	R
Al	7.264879	14.862182	9.242630	R
Al	7.931347	10.498274	10.346541	R
O	6.180105	10.497844	13.150180	R
O	6.481757	13.538825	13.293436	R
O	6.344141	10.497970	9.067023	R
O	7.707064	15.060013	10.907730	R
O	6.046123	13.405457	8.938295	R
O	6.004989	16.161537	8.827344	R
O	8.139981	9.126304	11.497240	R
O	8.140303	11.869795	11.497572	R
O	4.825724	6.081103	10.926244	R
O	4.825771	14.914594	10.926216	R
O	4.786423	9.068844	10.962270	R
O	4.786287	11.926964	10.962300	R
O	6.341537	4.951179	5.085981	R
O	6.341621	16.044473	5.086039	R
O	8.072439	9.074028	3.320521	R
O	8.071750	11.921885	3.320514	R
O	3.495535	10.497789	8.966237	R
Cu	9.292562	11.833495	7.724418	R
Cu	9.292543	9.165569	7.724164	R
O	9.240046	10.499448	9.131968	R
N	11.169126	11.442344	7.423078	R
N	11.168905	9.556773	7.423254	R
O	12.174467	11.734370	7.952057	R
O	12.174438	9.264614	7.952084	R

```
Model #16      Cartesian coordinates in angstrom
               x             y             z             Relaxed/Frozen
Al      4.718091      6.298715      9.025534      F
Al      6.299120      6.298715      11.957102     F
Al      4.718091      14.697002     9.025534      F
Al      4.828311      11.950763     9.158184      F
Al      4.828311      9.044955      9.158184      F
Al      7.260466      8.998624      12.959551     F
Al      7.260466      11.997093     12.959551     F
Al      6.299120      14.697002     11.957102     F
Al      4.636026      10.497859     12.053017     F
O       3.286788      10.497859     13.239718     F
Al      6.284430      4.911618      6.956078      F
Al      6.284430      16.084099     6.956078      F
Al      7.604152      10.497859     2.473791      F
O       6.427205      10.497859     1.094354      F
Al      6.373455      6.298715      3.886397      F
O       4.781442      6.298715      2.980335      F
Al      6.373455      14.697002     3.886397      F
O       4.781442      14.697002     2.980335      F
O       3.454035      4.977004      9.235301      F
O       3.454035      7.620427      9.235301      F
O       6.249989      5.002877      13.162247     F
O       3.454035      16.018713     9.235301      F
O       3.454035      13.375290     9.235301      F
O       7.425505      9.104843      14.776051     F
O       7.425505      11.890874     14.776051     F
O       6.249989      15.992841     13.162247     F
O       4.962264      3.365416      7.283451      F
O       7.499839      3.492587      6.705345      F
O       4.962264      17.630302     7.283451      F
O       7.499839      17.503130     6.705345      F
O       7.704784      6.298715      2.777154      F
O       7.704784      14.697002     2.777154      F
Al      3.478998      10.497859     7.046735      F
O       1.926548      11.807732     6.890259      F
O       1.926548      9.187985      6.890259      F
O       3.361122      10.497859     5.169014      F
Al      2.050923      10.497859     10.125656     F
O       0.574778      10.497859     9.076089      F
O       2.097749      9.088323      11.188759     F
O       2.097749      11.907395     11.188759     F
Al      3.393316      6.298715      6.011417      F
O       1.956477      6.298715      7.179493      F
O       3.339459      7.715095      4.949249      F
O       3.339459      4.882336      4.949249      F
Al      3.393316      14.697002     6.011417      F
O       1.956477      14.697002     7.179493      F
O       3.339459      16.113380     4.949249      F
O       3.339459      13.280622     4.949249      F
H       3.439923      4.911172      10.243970     F
H       3.439232      7.689483      10.293373     F
H       6.818393      4.213072      13.048228     F
H       6.229200      4.955319      14.133904     F
H       3.439929      16.084518     10.243550     F
H       3.439218      13.306190     10.293977     F
H       6.776962      8.347647      14.909841     F
H       6.777013      12.648010     14.909830     F
H       6.229199      16.040400     14.133948     F
H       6.818394      16.782646     13.048228     F
H       4.227165      2.738070      7.166136      F
H       6.932392      2.747750      6.973661      F
H       7.409135      3.550965      5.707009      F
H       4.227165      18.257647     7.166137      F
H       6.932397      18.247959     6.973659      F
H       7.409131      17.444750     5.706962      F
H       7.521090      6.298716      1.832227      F
H       7.521091      14.697002     1.832228      F
H       3.346923      10.497859     14.197637     F
H       6.469066      10.497859     0.138110      F
H       0.036291      9.692187      9.043065      F
H       0.036295      11.303524     9.043066      F
H       2.008448      9.058198      12.145152     F
H       2.008447      11.937518     12.145155     F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.252899	7.652945	6.990303	R
O	4.832508	6.293577	7.127841	R
O	7.541846	6.272059	7.428715	R
O	6.235251	7.623849	5.065481	R
Al	7.264553	6.131248	9.243888	R
O	6.482915	7.457022	13.293171	R
O	7.707598	5.936279	10.908625	R
O	6.004446	4.834405	8.827539	R
O	6.046353	7.590757	8.939249	R
Al	7.271785	9.026201	4.876974	R
Al	7.272918	11.969521	4.877423	R
Al	6.253760	13.342927	6.990271	R
Al	6.392666	10.497879	7.140759	R
O	4.832600	14.701998	7.127865	R
O	4.971626	11.815127	7.273897	R
O	4.971518	9.180509	7.273838	R
O	7.542084	14.723763	7.428851	R
O	6.318935	10.498126	5.097707	R
O	7.577643	11.977891	6.738099	R
O	7.577346	9.017416	6.737556	R
O	6.236021	13.371761	5.065515	R
Al	7.264514	14.864349	9.244065	R
Al	7.904367	10.497441	10.341633	R
O	6.180457	10.497874	13.150429	R
O	6.482963	13.538669	13.293074	R
O	6.350804	10.497726	9.064725	R
O	7.707710	15.059356	10.908745	R
O	6.046421	13.404952	8.939274	R
O	6.004536	16.161279	8.827694	R
O	8.130047	9.126906	11.489410	R
O	8.130386	11.867907	11.489632	R
O	4.825859	6.082715	10.926105	R
O	4.825926	14.912934	10.926088	R
O	4.790230	9.070860	10.961292	R
O	4.790250	11.924934	10.961318	R
O	6.340075	4.952944	5.087585	R
O	6.340069	16.042699	5.087631	R
O	8.066997	9.073757	3.321974	R
O	8.068212	11.921364	3.322418	R
O	3.497342	10.497846	8.967085	R
Cu	9.306515	11.821381	7.735793	R
Cu	9.306057	9.175374	7.734154	R
O	9.250833	10.497176	9.144499	R
N	11.147725	11.231065	7.069409	R
N	11.147376	9.765913	7.068974	R
O	12.179868	11.782632	6.756622	R
O	12.178999	9.213775	6.755451	R

```
Model #17      Cartesian coordinates in angstrom
               x                y                z              Relaxed/Frozen
Al             4.718091         6.298715         9.025534       F
Al             6.299120         6.298715         11.957102      F
Al             4.718091         14.697002        9.025534       F
Al             4.828311         11.950763        9.158184       F
Al             4.828311         9.044955         9.158184       F
Al             7.260466         8.998624         12.959551      F
Al             7.260466         11.997093        12.959551      F
Al             6.299120         14.697002        11.957102      F
Al             4.636026         10.497859        12.053017      F
O              3.286788         10.497859        13.239718      F
Al             6.284430         4.911618         6.956078       F
Al             6.284430         16.084099        6.956078       F
Al             7.604152         10.497859        2.473791       F
O              6.427205         10.497859        1.094354       F
Al             6.373455         6.298715         3.886397       F
O              4.781442         6.298715         2.980335       F
Al             6.373455         14.697002        3.886397       F
O              4.781442         14.697002        2.980335       F
O              3.454035         4.977004         9.235301       F
O              3.454035         7.620427         9.235301       F
O              6.249989         5.002877         13.162247      F
O              3.454035         16.018713        9.235301       F
O              3.454035         13.375290        9.235301       F
O              7.425505         9.104843         14.776051      F
O              7.425505         11.890874        14.776051      F
O              6.249989         15.992841        13.162247      F
O              4.962264         3.365416         7.283451       F
O              7.499839         3.492587         6.705345       F
O              4.962264         17.630302        7.283451       F
O              7.499839         17.503130        6.705345       F
O              7.704784         6.298715         2.777154       F
O              7.704784         14.697002        2.777154       F
Al             3.478998         10.497859        7.046735       F
O              1.926548         11.807732        6.890259       F
O              1.926548         9.187985         6.890259       F
O              3.361122         10.497859        5.169014       F
Al             2.050923         10.497859        10.125656      F
O              0.574778         10.497859        9.076089       F
O              2.097749         9.088323         11.188759      F
O              2.097749         11.907395        11.188759      F
Al             3.393316         6.298715         6.011417       F
O              1.956477         6.298715         7.179493       F
O              3.339459         7.715095         4.949249       F
O              3.339459         4.882336         4.949249       F
Al             3.393316         14.697002        6.011417       F
O              1.956477         14.697002        7.179493       F
O              3.339459         16.113380        4.949249       F
O              3.339459         13.280622        4.949249       F
H              3.439923         4.911172         10.243970      F
H              3.439232         7.689483         10.293373      F
H              6.818393         4.213072         13.048228      F
H              6.229200         4.955319         14.133904      F
H              3.439929         16.084518        10.243550      F
H              3.439218         13.306190        10.293977      F
H              6.776962         8.347647         14.909841      F
H              6.777013         12.648010        14.909830      F
H              6.229199         16.040400        14.133948      F
H              6.818394         16.782646        13.048228      F
H              4.227165         2.738070         7.166136       F
H              6.932392         2.747750         6.973661       F
H              7.409135         3.550965         5.707009       F
H              4.227165         18.257647        7.166137       F
H              6.932397         18.247959        6.973659       F
H              7.409131         17.444750        5.706962       F
H              7.521090         6.298716         1.832227       F
H              7.521091         14.697002        1.832228       F
H              3.346923         10.497859        14.197637      F
H              6.469066         10.497859        0.138110       F
H              0.036291         9.692187         9.043065       F
H              0.036295         11.303524        9.043066       F
H              2.008448         9.058198         12.145152      F
H              2.008447         11.937518        12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.240024	7.664024	6.980860	R
O	4.825609	6.293548	7.127739	R
O	7.510252	6.282621	7.369336	R
O	6.244877	7.634582	5.055014	R
Al	7.331760	6.106161	9.236275	R
O	6.461921	7.465481	13.295919	R
O	7.685945	5.916674	10.934302	R
O	6.027869	4.836403	8.821589	R
O	6.060509	7.586441	8.932036	R
Al	7.297888	9.030726	4.883384	R
Al	7.248202	11.977652	4.843558	R
Al	6.241029	13.351956	6.973524	R
Al	6.386321	10.499465	7.128113	R
O	4.828236	14.705984	7.126975	R
O	4.970948	11.814126	7.270825	R
O	4.966451	9.183591	7.270806	R
O	7.530152	14.730040	7.417196	R
O	6.317913	10.492270	5.072905	R
O	7.561690	12.011710	6.679736	R
O	7.584430	9.043442	6.744782	R
O	6.196841	13.368678	5.044792	R
Al	7.266323	14.856867	9.234722	R
Al	7.978616	10.444329	10.381613	R
O	6.184087	10.498966	13.142572	R
O	6.487660	13.538632	13.289377	R
O	6.375132	10.499040	9.062600	R
O	7.707145	15.045467	10.903033	R
O	6.043883	13.404954	8.931145	R
O	6.004144	16.161036	8.829542	R
O	8.169224	9.074026	11.518863	R
O	8.172639	11.826915	11.518809	R
O	4.812400	6.084875	10.928303	R
O	4.824707	14.913787	10.928243	R
O	4.792978	9.075148	10.959210	R
O	4.788827	11.928524	10.962366	R
O	6.335453	4.945645	5.079553	R
O	6.342815	16.043641	5.086136	R
O	8.105315	9.089679	3.330673	R
O	8.052599	11.940070	3.294949	R
O	3.498556	10.499422	8.966911	R
Cu	8.926987	11.596650	7.930226	R
Cu	9.217767	8.850099	8.002555	R
O	9.337613	10.326132	9.206520	R
N	9.525159	5.899372	8.761768	R
O	10.278123	5.019020	8.677386	R
O	11.308416	6.909463	7.487451	R
N	10.271675	7.299947	7.871191	R

```
Model #18      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043065       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.190627	7.653036	6.975729	R
O	4.813304	6.289991	7.127688	R
O	7.502984	6.336802	7.347281	R
O	6.222075	7.643690	5.047799	R
Al	7.413729	6.067033	9.227277	R
O	6.448330	7.474114	13.296138	R
O	7.654436	5.880441	10.950830	R
O	6.048825	4.849446	8.808228	R
O	6.052201	7.601532	8.921703	R
Al	7.280233	9.026939	4.869767	R
Al	7.263961	11.979330	4.848755	R
Al	6.251626	13.356028	6.978549	R
Al	6.362698	10.508353	7.111896	R
O	4.830589	14.705354	7.126994	R
O	4.971785	11.820970	7.268518	R
O	4.957291	9.193924	7.260682	R
O	7.533883	14.731708	7.419947	R
O	6.320206	10.498533	5.078798	R
O	7.576127	12.002701	6.688749	R
O	7.567434	9.050573	6.741897	R
O	6.212873	13.368248	5.051658	R
Al	7.265931	14.860578	9.236799	R
Al	7.919866	10.393134	10.370580	R
O	6.186230	10.502442	13.141394	R
O	6.501594	13.541502	13.286697	R
O	6.375648	10.500477	9.051312	R
O	7.710169	15.040419	10.904283	R
O	6.046476	13.404615	8.931070	R
O	6.004514	16.161263	8.830068	R
O	8.155279	9.046460	11.510926	R
O	8.147940	11.790911	11.489060	R
O	4.794084	6.096579	10.930224	R
O	4.826761	14.913266	10.927560	R
O	4.803230	9.088960	10.955105	R
O	4.793464	11.930482	10.961378	R
O	6.329325	4.953655	5.081815	R
O	6.341752	16.041389	5.087159	R
O	8.096965	9.086043	3.327867	R
O	8.064283	11.933543	3.300180	R
O	3.501599	10.503249	8.965743	R
Cu	8.933021	11.434731	7.892132	R
Cu	8.914554	8.543694	8.054573	R
O	9.265033	10.113640	9.138885	R
N	10.180739	7.237736	8.776282	R
N	9.566817	6.017148	9.115685	R
O	11.397836	7.322804	8.856260	R
O	10.302450	5.106097	9.447566	R

```
Model #19      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043066       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.174334	7.649761	6.961340	R
O	4.804747	6.298922	7.125742	R
O	7.483526	6.339101	7.327281	R
O	6.220329	7.651740	5.037853	R
Al	7.430743	6.134555	9.235392	R
O	6.453955	7.472680	13.298146	R
O	7.632653	5.814746	10.951441	R
O	6.049337	4.874552	8.805275	R
O	6.052487	7.615011	8.917623	R
Al	7.292874	9.024325	4.865406	R
Al	7.267454	11.979725	4.847344	R
Al	6.254418	13.356679	6.978634	R
Al	6.360034	10.510166	7.105053	R
O	4.831209	14.705849	7.126993	R
O	4.972684	11.823494	7.266437	R
O	4.957732	9.197826	7.256043	R
O	7.534934	14.732818	7.420306	R
O	6.328470	10.495582	5.074667	R
O	7.579654	12.002513	6.688425	R
O	7.576747	9.056431	6.735793	R
O	6.215431	13.367911	5.052158	R
Al	7.265557	14.861182	9.237007	R
Al	7.896708	10.387516	10.367457	R
O	6.185646	10.503915	13.144059	R
O	6.505591	13.542774	13.286424	R
O	6.373374	10.504109	9.046885	R
O	7.711035	15.039282	10.904417	R
O	6.047195	13.405236	8.931067	R
O	6.004818	16.161907	8.830502	R
O	8.127962	9.038120	11.497278	R
O	8.147638	11.782430	11.486762	R
O	4.784641	6.118923	10.933370	R
O	4.827224	14.914187	10.927700	R
O	4.806162	9.095877	10.953153	R
O	4.796512	11.932626	10.962051	R
O	6.321412	4.952914	5.077679	R
O	6.342049	16.041411	5.087118	R
O	8.110137	9.088663	3.324309	R
O	8.064660	11.935588	3.297305	R
O	3.502423	10.504883	8.965152	R
Cu	8.930484	11.400260	7.882847	R
Cu	8.793061	8.465954	8.127429	R
O	9.223162	10.054423	9.114513	R
O	9.288522	6.846797	9.067587	R
N	10.538588	5.767634	10.471259	R
O	10.280653	4.621252	10.124224	R
N	10.198928	6.897786	10.125483	R

```
Model #20      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043066       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.174496	7.649923	6.961442	R
O	4.804966	6.298856	7.125712	R
O	7.484276	6.339135	7.327826	R
O	6.220246	7.651601	5.037866	R
Al	7.430672	6.135032	9.235390	R
O	6.454052	7.472531	13.298215	R
O	7.633194	5.815152	10.951261	R
O	6.049466	4.874636	8.805200	R
O	6.052563	7.614994	8.917607	R
Al	7.292947	9.024242	4.865299	R
Al	7.267127	11.979568	4.847202	R
Al	6.254848	13.356555	6.978471	R
Al	6.359806	10.510035	7.105140	R
O	4.831275	14.705871	7.127047	R
O	4.972582	11.823518	7.266405	R
O	4.957651	9.197673	7.255954	R
O	7.534978	14.732776	7.420224	R
O	6.328283	10.495407	5.074193	R
O	7.579457	12.002111	6.688282	R
O	7.576369	9.056227	6.735289	R
O	6.215396	13.367969	5.052140	R
Al	7.265625	14.861128	9.236956	R
Al	7.897091	10.386963	10.367331	R
O	6.185576	10.503861	13.144143	R
O	6.505623	13.542775	13.286413	R
O	6.373029	10.503887	9.046893	R
O	7.711012	15.039227	10.904414	R
O	6.047228	13.405207	8.931158	R
O	6.004939	16.161901	8.830569	R
O	8.127899	9.037518	11.497342	R
O	8.147626	11.781902	11.486891	R
O	4.784891	6.118650	10.933278	R
O	4.827106	14.914364	10.927798	R
O	4.806182	9.095661	10.953215	R
O	4.796362	11.932592	10.962067	R
O	6.321664	4.952876	5.077825	R
O	6.342099	16.041450	5.087088	R
O	8.110032	9.088477	3.324074	R
O	8.064675	11.935558	3.297312	R
O	3.502397	10.504888	8.965162	R
Cu	8.930317	11.399357	7.882801	R
Cu	8.793134	8.466018	8.127137	R
O	9.223370	10.053767	9.115150	R
O	9.289475	6.850754	9.067777	R
N	10.541205	5.773537	10.471820	R
O	10.286701	4.626072	10.126801	R
N	10.201591	6.902753	10.125565	R

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Model #21      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043065       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.256879	7.659234	6.988502	R
O	4.832736	6.295432	7.126051	R
O	7.535312	6.271610	7.424367	R
O	6.259618	7.627332	5.064505	R
Al	7.269336	6.123248	9.243631	R
O	6.466732	7.461391	13.294618	R
O	7.702447	5.926442	10.910623	R
O	6.004109	4.831738	8.826640	R
O	6.048658	7.589440	8.939301	R
Al	7.307393	9.027769	4.888615	R
Al	7.248712	11.975662	4.846381	R
Al	6.241911	13.350840	6.974266	R
Al	6.389248	10.496255	7.132044	R
O	4.828127	14.705399	7.127070	R
O	4.971599	11.812295	7.271512	R
O	4.969691	9.180362	7.272249	R
O	7.529554	14.730072	7.416788	R
O	6.323869	10.486513	5.079004	R
O	7.562540	12.010226	6.682103	R
O	7.591019	9.035022	6.751867	R
O	6.197379	13.367388	5.045071	R
Al	7.266951	14.855876	9.234257	R
Al	7.991026	10.440576	10.382018	R
O	6.182962	10.497804	13.143766	R
O	6.486586	13.537959	13.288816	R
O	6.374667	10.494521	9.064804	R
O	7.706924	15.044428	10.902954	R
O	6.043616	13.404493	8.931605	R
O	6.004203	16.160668	8.829750	R
O	8.165516	9.068181	11.517966	R
O	8.178103	11.821562	11.523913	R
O	4.823388	6.082651	10.925699	R
O	4.824234	14.913401	10.928574	R
O	4.788929	9.071721	10.960638	R
O	4.788205	11.927582	10.962275	R
O	6.338828	4.950946	5.084997	R
O	6.342284	16.043494	5.086056	R
O	8.105433	9.089003	3.330540	R
O	8.050412	11.939584	3.296109	R
O	3.498041	10.498392	8.966949	R
Cu	8.928559	11.581595	7.928081	R
Cu	9.224744	8.826811	8.003962	R
O	9.348222	10.322438	9.210190	R
N	10.506155	7.444620	7.954012	R
O	12.816277	6.968654	7.410208	R
N	12.121046	7.847001	7.117170	R
O	10.694578	6.434496	8.527740	R

```
Model #22      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al       4.718091       6.298715       9.025534       F
Al       6.299120       6.298715      11.957102       F
Al       4.718091      14.697002       9.025534       F
Al       4.828311      11.950763       9.158184       F
Al       4.828311       9.044955       9.158184       F
Al       7.260466       8.998624      12.959551       F
Al       7.260466      11.997093      12.959551       F
Al       6.299120      14.697002      11.957102       F
Al       4.636026      10.497859      12.053017       F
O        3.286788      10.497859      13.239718       F
Al       6.284430       4.911618       6.956078       F
Al       6.284430      16.084099       6.956078       F
Al       7.604152      10.497859       2.473791       F
O        6.427205      10.497859       1.094354       F
Al       6.373455       6.298715       3.886397       F
O        4.781442       6.298715       2.980335       F
Al       6.373455      14.697002       3.886397       F
O        4.781442      14.697002       2.980335       F
O        3.454035       4.977004       9.235301       F
O        3.454035       7.620427       9.235301       F
O        6.249989       5.002877      13.162247       F
O        3.454035      16.018713       9.235301       F
O        3.454035      13.375290       9.235301       F
O        7.425505       9.104843      14.776051       F
O        7.425505      11.890874      14.776051       F
O        6.249989      15.992841      13.162247       F
O        4.962264       3.365416       7.283451       F
O        7.499839       3.492587       6.705345       F
O        4.962264      17.630302       7.283451       F
O        7.499839      17.503130       6.705345       F
O        7.704784       6.298715       2.777154       F
O        7.704784      14.697002       2.777154       F
Al       3.478998      10.497859       7.046735       F
O        1.926548      11.807732       6.890259       F
O        1.926548       9.187985       6.890259       F
O        3.361122      10.497859       5.169014       F
Al       2.050923      10.497859      10.125656       F
O        0.574778      10.497859       9.076089       F
O        2.097749       9.088323      11.188759       F
O        2.097749      11.907395      11.188759       F
Al       3.393316       6.298715       6.011417       F
O        1.956477       6.298715       7.179493       F
O        3.339459       7.715095       4.949249       F
O        3.339459       4.882336       4.949249       F
Al       3.393316      14.697002       6.011417       F
O        1.956477      14.697002       7.179493       F
O        3.339459      16.113380       4.949249       F
O        3.339459      13.280622       4.949249       F
H        3.439923       4.911172      10.243970       F
H        3.439232       7.689483      10.293373       F
H        6.818393       4.213072      13.048228       F
H        6.229200       4.955319      14.133904       F
H        3.439929      16.084518      10.243550       F
H        3.439218      13.306190      10.293977       F
H        6.776962       8.347647      14.909841       F
H        6.777013      12.648010      14.909830       F
H        6.229199      16.040400      14.133948       F
H        6.818394      16.782646      13.048228       F
H        4.227165       2.738070       7.166136       F
H        6.932392       2.747750       6.973661       F
H        7.409135       3.550965       5.707009       F
H        4.227165      18.257647       7.166137       F
H        6.932397      18.247959       6.973659       F
H        7.409131      17.444750       5.706962       F
H        7.521090       6.298716       1.832227       F
H        7.521091      14.697002       1.832228       F
H        3.346923      10.497859      14.197637       F
H        6.469066      10.497859       0.138110       F
H        0.036291       9.692187       9.043065       F
H        0.036295      11.303524       9.043066       F
H        2.008448       9.058198      12.145152       F
H        2.008447      11.937518      12.145155       F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.255520	7.657353	6.986348	R
O	4.833006	6.294811	7.126275	R
O	7.537923	6.270862	7.427681	R
O	6.250389	7.626683	5.062082	R
Al	7.263347	6.125553	9.244452	R
O	6.467724	7.461320	13.293302	R
O	7.704594	5.929389	10.909135	R
O	6.002874	4.831588	8.827046	R
O	6.047366	7.589316	8.938612	R
Al	7.299794	9.025259	4.881751	R
Al	7.254119	11.975486	4.848546	R
Al	6.241948	13.350077	6.974683	R
Al	6.389593	10.495218	7.131131	R
O	4.828337	14.704737	7.126930	R
O	4.971874	11.811505	7.272132	R
O	4.969592	9.180513	7.272922	R
O	7.530069	14.729265	7.417305	R
O	6.324245	10.489095	5.079244	R
O	7.564048	12.007967	6.686567	R
O	7.584810	9.026322	6.740647	R
O	6.201776	13.366977	5.045980	R
Al	7.266911	14.856491	9.234740	R
Al	8.010019	10.453239	10.391221	R
O	6.183485	10.497513	13.142321	R
O	6.482480	13.536707	13.288634	R
O	6.385648	10.493747	9.062698	R
O	7.706543	15.045700	10.903180	R
O	6.043616	13.404410	8.931842	R
O	6.004173	16.160551	8.829386	R
O	8.171545	9.075300	11.521344	R
O	8.185633	11.833111	11.531018	R
O	4.825133	6.082155	10.925185	R
O	4.824182	14.913034	10.928107	R
O	4.788476	9.071335	10.960345	R
O	4.789114	11.926443	10.961430	R
O	6.339586	4.951890	5.086357	R
O	6.341742	16.043192	5.086302	R
O	8.095528	9.083409	3.324148	R
O	8.056728	11.936363	3.298912	R
O	3.498870	10.498341	8.967182	R
Cu	8.929606	11.621567	7.950252	R
Cu	9.225011	8.941778	7.970807	R
O	9.385814	10.375310	9.239238	R
N	10.516674	7.546319	7.699139	R
O	12.320460	6.916932	6.038512	R
N	11.555808	7.787221	6.141319	R
O	10.811940	6.570052	8.275897	R

```
Model #23      Cartesian coordinates in angstrom
               x             y             z             Relaxed/Frozen
Al             4.718091      6.298715      9.025534      F
Al             6.299120      6.298715      11.957102     F
Al             4.718091      14.697002     9.025534      F
Al             4.828311      11.950763     9.158184      F
Al             4.828311      9.044955      9.158184      F
Al             7.260466      8.998624      12.959551     F
Al             7.260466      11.997093     12.959551     F
Al             6.299120      14.697002     11.957102     F
Al             4.636026      10.497859     12.053017     F
O              3.286788      10.497859     13.239718     F
Al             6.284430      4.911618      6.956078      F
Al             6.284430      16.084099     6.956078      F
Al             7.604152      10.497859     2.473791      F
O              6.427205      10.497859     1.094354      F
Al             6.373455      6.298715      3.886397      F
O              4.781442      6.298715      2.980335      F
Al             6.373455      14.697002     3.886397      F
O              4.781442      14.697002     2.980335      F
O              3.454035      4.977004      9.235301      F
O              3.454035      7.620427      9.235301      F
O              6.249989      5.002877      13.162247     F
O              3.454035      16.018713     9.235301      F
O              3.454035      13.375290     9.235301      F
O              7.425505      9.104843      14.776051     F
O              7.425505      11.890874     14.776051     F
O              6.249989      15.992841     13.162247     F
O              4.962264      3.365416      7.283451      F
O              7.499839      3.492587      6.705345      F
O              4.962264      17.630302     7.283451      F
O              7.499839      17.503130     6.705345      F
O              7.704784      6.298715      2.777154      F
O              7.704784      14.697002     2.777154      F
Al             3.478998      10.497859     7.046735      F
O              1.926548      11.807732     6.890259      F
O              1.926548      9.187985      6.890259      F
O              3.361122      10.497859     5.169014      F
Al             2.050923      10.497859     10.125656     F
O              0.574778      10.497859     9.076089      F
O              2.097749      9.088323      11.188759     F
O              2.097749      11.907395     11.188759     F
Al             3.393316      6.298715      6.011417      F
O              1.956477      6.298715      7.179493      F
O              3.339459      7.715095      4.949249      F
O              3.339459      4.882336      4.949249      F
Al             3.393316      14.697002     6.011417      F
O              1.956477      14.697002     7.179493      F
O              3.339459      16.113380     4.949249      F
O              3.339459      13.280622     4.949249      F
H              3.439923      4.911172      10.243970     F
H              3.439232      7.689483      10.293373     F
H              6.818393      4.213072      13.048228     F
H              6.229200      4.955319      14.133904     F
H              3.439929      16.084518     10.243550     F
H              3.439218      13.306190     10.293977     F
H              6.776962      8.347647      14.909841     F
H              6.777013      12.648010     14.909830     F
H              6.229199      16.040400     14.133948     F
H              6.818394      16.782646     13.048228     F
H              4.227165      2.738070      7.166136      F
H              6.932392      2.747750      6.973661      F
H              7.409135      3.550965      5.707009      F
H              4.227165      18.257647     7.166137      F
H              6.932397      18.247959     6.973659      F
H              7.409131      17.444750     5.706962      F
H              7.521090      6.298716      1.832227      F
H              7.521091      14.697002     1.832228      F
H              3.346923      10.497859     14.197637     F
H              6.469066      10.497859     0.138110      F
H              0.036291      9.692187      9.043065      F
H              0.036295      11.303524     9.043066      F
H              2.008448      9.058198      12.145152     F
H              2.008447      11.937518     12.145155     F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.177048	7.650272	6.958047	R
O	4.806697	6.300518	7.125051	R
O	7.491538	6.338956	7.330707	R
O	6.218769	7.651194	5.036734	R
Al	7.424028	6.152049	9.231842	R
O	6.456276	7.470734	13.296450	R
O	7.620895	5.786938	10.941689	R
O	6.049350	4.877445	8.803972	R
O	6.054079	7.614299	8.918018	R
Al	7.289033	9.026142	4.861941	R
Al	7.267581	11.980413	4.846640	R
Al	6.252618	13.355910	6.978017	R
Al	6.360421	10.510121	7.103757	R
O	4.830973	14.705807	7.127059	R
O	4.972017	11.822706	7.266146	R
O	4.958146	9.196009	7.256284	R
O	7.534221	14.731906	7.419464	R
O	6.325371	10.497545	5.070921	R
O	7.578203	12.002186	6.687430	R
O	7.574210	9.056411	6.728939	R
O	6.214695	13.367901	5.051459	R
Al	7.265927	14.860008	9.235850	R
Al	7.897874	10.380098	10.364595	R
O	6.185746	10.502898	13.143681	R
O	6.505839	13.542129	13.284839	R
O	6.371007	10.502185	9.046252	R
O	7.711322	15.034903	10.903694	R
O	6.046744	13.404545	8.930713	R
O	6.005213	16.161315	8.830608	R
O	8.108657	9.015634	11.482749	R
O	8.155392	11.764710	11.495809	R
O	4.788064	6.120132	10.931867	R
O	4.827175	14.914036	10.927830	R
O	4.803384	9.094478	10.952934	R
O	4.798004	11.932282	10.962252	R
O	6.323781	4.953323	5.079182	R
O	6.341784	16.041364	5.087205	R
O	8.107128	9.086415	3.321745	R
O	8.067093	11.934462	3.297867	R
O	3.502203	10.504632	8.965107	R
Cu	8.930722	11.403916	7.883213	R
Cu	8.796966	8.473079	8.117594	R
O	9.224008	10.058411	9.115703	R
N	10.169808	7.049573	10.157353	R
O	9.281665	6.900786	9.120969	R
N	10.172794	6.071260	10.925330	R
O	10.833403	5.883849	11.931997	R

```
Model #24      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al     4.718091       6.298715       9.025534       F
Al     6.299120       6.298715       11.957102      F
Al     4.718091       14.697002      9.025534       F
Al     4.828311       11.950763      9.158184       F
Al     4.828311       9.044955       9.158184       F
Al     7.260466       8.998624       12.959551      F
Al     7.260466       11.997093      12.959551      F
Al     6.299120       14.697002      11.957102      F
Al     4.636026       10.497859      12.053017      F
O      3.286788       10.497859      13.239718      F
Al     6.284430       4.911618       6.956078       F
Al     6.284430       16.084099      6.956078       F
Al     7.604152       10.497859      2.473791       F
O      6.427205       10.497859      1.094354       F
Al     6.373455       6.298715       3.886397       F
O      4.781442       6.298715       2.980335       F
Al     6.373455       14.697002      3.886397       F
O      4.781442       14.697002      2.980335       F
O      3.454035       4.977004       9.235301       F
O      3.454035       7.620427       9.235301       F
O      6.249989       5.002877       13.162247      F
O      3.454035       16.018713      9.235301       F
O      3.454035       13.375290      9.235301       F
O      7.425505       9.104843       14.776051      F
O      7.425505       11.890874      14.776051      F
O      6.249989       15.992841      13.162247      F
O      4.962264       3.365416       7.283451       F
O      7.499839       3.492587       6.705345       F
O      4.962264       17.630302      7.283451       F
O      7.499839       17.503130      6.705345       F
O      7.704784       6.298715       2.777154       F
O      7.704784       14.697002      2.777154       F
Al     3.478998       10.497859      7.046735       F
O      1.926548       11.807732      6.890259       F
O      1.926548       9.187985       6.890259       F
O      3.361122       10.497859      5.169014       F
Al     2.050923       10.497859      10.125656      F
O      0.574778       10.497859      9.076089       F
O      2.097749       9.088323       11.188759      F
O      2.097749       11.907395      11.188759      F
Al     3.393316       6.298715       6.011417       F
O      1.956477       6.298715       7.179493       F
O      3.339459       7.715095       4.949249       F
O      3.339459       4.882336       4.949249       F
Al     3.393316       14.697002      6.011417       F
O      1.956477       14.697002      7.179493       F
O      3.339459       16.113380      4.949249       F
O      3.339459       13.280622      4.949249       F
H      3.439923       4.911172       10.243970      F
H      3.439232       7.689483       10.293373      F
H      6.818393       4.213072       13.048228      F
H      6.229200       4.955319       14.133904      F
H      3.439929       16.084518      10.243550      F
H      3.439218       13.306190      10.293977      F
H      6.776962       8.347647       14.909841      F
H      6.777013       12.648010      14.909830      F
H      6.229199       16.040400      14.133948      F
H      6.818394       16.782646      13.048228      F
H      4.227165       2.738070       7.166136       F
H      6.932392       2.747750       6.973661       F
H      7.409135       3.550965       5.707009       F
H      4.227165       18.257647      7.166137       F
H      6.932397       18.247959      6.973659       F
H      7.409131       17.444750      5.706962       F
H      7.521090       6.298716       1.832227       F
H      7.521091       14.697002      1.832228       F
H      3.346923       10.497859      14.197637      F
H      6.469066       10.497859      0.138110       F
H      0.036291       9.692187       9.043065       F
H      0.036295       11.303524      9.043066       F
H      2.008448       9.058198       12.145152      F
H      2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.175750	7.651309	6.958202	R
O	4.806779	6.299902	7.124992	R
O	7.490192	6.339976	7.330051	R
O	6.218795	7.651167	5.036621	R
Al	7.425263	6.149939	9.231656	R
O	6.455887	7.470882	13.296682	R
O	7.621918	5.790282	10.942374	R
O	6.049849	4.876905	8.804145	R
O	6.053977	7.614611	8.918019	R
Al	7.289443	9.025869	4.861907	R
Al	7.268328	11.980274	4.846617	R
Al	6.253366	13.356171	6.977773	R
Al	6.360469	10.510261	7.103733	R
O	4.831033	14.705683	7.127054	R
O	4.972255	11.822606	7.266238	R
O	4.958067	9.196203	7.256214	R
O	7.534388	14.732188	7.419544	R
O	6.325850	10.497569	5.070841	R
O	7.578757	12.002263	6.687525	R
O	7.574447	9.056498	6.728601	R
O	6.215225	13.367762	5.051467	R
Al	7.265887	14.860196	9.235938	R
Al	7.897505	10.379307	10.365097	R
O	6.185802	10.503010	13.143587	R
O	6.505940	13.542140	13.284821	R
O	6.371018	10.502125	9.046677	R
O	7.711363	15.034953	10.903773	R
O	6.046869	13.404622	8.930643	R
O	6.005189	16.161429	8.830697	R
O	8.109932	9.015344	11.483523	R
O	8.155246	11.764406	11.495609	R
O	4.787995	6.119769	10.931860	R
O	4.827186	14.914021	10.927841	R
O	4.803548	9.094483	10.953029	R
O	4.798061	11.932319	10.962279	R
O	6.323792	4.952972	5.078979	R
O	6.341712	16.041342	5.087235	R
O	8.107198	9.086355	3.321515	R
O	8.067078	11.934686	3.297455	R
O	3.502268	10.504647	8.965135	R
Cu	8.930548	11.399971	7.882062	R
Cu	8.796274	8.471442	8.118306	R
O	9.222999	10.055251	9.116053	R
N	10.187718	7.035209	10.136157	R
O	9.284498	6.891307	9.109638	R
N	10.179327	6.059133	10.906008	R
O	10.851624	5.855036	11.901708	R

```
Model #25      Cartesian coordinates in angstrom
                x              y              z              Relaxed/Frozen
Al              4.718091       6.298715       9.025534       F
Al              6.299120       6.298715       11.957102      F
Al              4.718091       14.697002      9.025534       F
Al              4.828311       11.950763      9.158184       F
Al              4.828311       9.044955       9.158184       F
Al              7.260466       8.998624       12.959551      F
Al              7.260466       11.997093      12.959551      F
Al              6.299120       14.697002      11.957102      F
Al              4.636026       10.497859      12.053017      F
O               3.286788       10.497859      13.239718      F
Al              6.284430       4.911618       6.956078       F
Al              6.284430       16.084099      6.956078       F
Al              7.604152       10.497859      2.473791       F
O               6.427205       10.497859      1.094354       F
Al              6.373455       6.298715       3.886397       F
O               4.781442       6.298715       2.980335       F
Al              6.373455       14.697002      3.886397       F
O               4.781442       14.697002      2.980335       F
O               3.454035       4.977004       9.235301       F
O               3.454035       7.620427       9.235301       F
O               6.249989       5.002877       13.162247      F
O               3.454035       16.018713      9.235301       F
O               3.454035       13.375290      9.235301       F
O               7.425505       9.104843       14.776051      F
O               7.425505       11.890874      14.776051      F
O               6.249989       15.992841      13.162247      F
O               4.962264       3.365416       7.283451       F
O               7.499839       3.492587       6.705345       F
O               4.962264       17.630302      7.283451       F
O               7.499839       17.503130      6.705345       F
O               7.704784       6.298715       2.777154       F
O               7.704784       14.697002      2.777154       F
Al              3.478998       10.497859      7.046735       F
O               1.926548       11.807732      6.890259       F
O               1.926548       9.187985       6.890259       F
O               3.361122       10.497859      5.169014       F
Al              2.050923       10.497859      10.125656      F
O               0.574778       10.497859      9.076089       F
O               2.097749       9.088323       11.188759      F
O               2.097749       11.907395      11.188759      F
Al              3.393316       6.298715       6.011417       F
O               1.956477       6.298715       7.179493       F
O               3.339459       7.715095       4.949249       F
O               3.339459       4.882336       4.949249       F
Al              3.393316       14.697002      6.011417       F
O               1.956477       14.697002      7.179493       F
O               3.339459       16.113380      4.949249       F
O               3.339459       13.280622      4.949249       F
H               3.439923       4.911172       10.243970      F
H               3.439232       7.689483       10.293373      F
H               6.818393       4.213072       13.048228      F
H               6.229200       4.955319       14.133904      F
H               3.439929       16.084518      10.243550      F
H               3.439218       13.306190      10.293977      F
H               6.776962       8.347647       14.909841      F
H               6.777013       12.648010      14.909830      F
H               6.229199       16.040400      14.133948      F
H               6.818394       16.782646      13.048228      F
H               4.227165       2.738070       7.166136       F
H               6.932392       2.747750       6.973661       F
H               7.409135       3.550965       5.707009       F
H               4.227165       18.257647      7.166137       F
H               6.932397       18.247959      6.973659       F
H               7.409131       17.444750      5.706962       F
H               7.521090       6.298716       1.832227       F
H               7.521091       14.697002      1.832228       F
H               3.346923       10.497859      14.197637      F
H               6.469066       10.497859      0.138110       F
H               0.036291       9.692187       9.043065       F
H               0.036295       11.303524      9.043066       F
H               2.008448       9.058198       12.145152      F
H               2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.231535	7.641787	6.983930	R
O	4.809519	6.307734	7.128399	R
O	7.476723	6.281114	7.332687	R
O	6.270913	7.647806	5.058848	R
Al	7.384753	6.146844	9.224156	R
O	6.469142	7.470016	13.292495	R
O	7.646144	5.846819	10.935657	R
O	6.028997	4.862130	8.819288	R
O	6.061325	7.606498	8.930024	R
Al	7.341646	9.023249	4.894069	R
Al	7.244115	11.979175	4.843724	R
Al	6.233355	13.356086	6.972834	R
Al	6.382734	10.504607	7.120304	R
O	4.828619	14.707209	7.127415	R
O	4.972904	11.818892	7.270437	R
O	4.978315	9.196905	7.267963	R
O	7.534269	14.726821	7.421668	R
O	6.346484	10.476606	5.098761	R
O	7.560868	12.018121	6.682641	R
O	7.624543	9.055176	6.783632	R
O	6.190330	13.366560	5.045947	R
Al	7.262645	14.864103	9.238878	R
Al	7.889818	10.472415	10.378435	R
O	6.187163	10.502685	13.140955	R
O	6.490409	13.540099	13.290700	R
O	6.388130	10.516510	9.057325	R
O	7.708485	15.051063	10.904240	R
O	6.045452	13.405805	8.930517	R
O	6.003657	16.162017	8.827909	R
O	8.153568	9.115196	11.506639	R
O	8.139080	11.861564	11.485893	R
O	4.787198	6.119989	10.938159	R
O	4.827417	14.913255	10.925472	R
O	4.809641	9.094266	10.954041	R
O	4.797460	11.929968	10.961158	R
O	6.312184	4.946963	5.071444	R
O	6.344809	16.038941	5.089378	R
O	8.139475	9.107077	3.339861	R
O	8.031162	11.948954	3.290197	R
O	3.503419	10.502917	8.966447	R
Cu	8.931083	11.732369	7.959092	R
Cu	9.143178	8.854781	8.044178	R
O	9.275929	10.380755	9.163936	R
O	11.118379	8.252455	8.171879	R
O	9.220927	6.989694	9.032456	R
N	10.363484	6.441289	9.199176	R
N	11.389251	7.242436	8.870074	R

```
Model #26      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043065       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.233314	7.642911	6.975926	R
O	4.801662	6.313110	7.129913	R
O	7.464195	6.282833	7.320663	R
O	6.253776	7.650953	5.048644	R
Al	7.401315	6.169268	9.216618	R
O	6.464444	7.472265	13.293367	R
O	7.645644	5.864334	10.931736	R
O	6.029848	4.870476	8.819837	R
O	6.057585	7.613820	8.925270	R
Al	7.337639	9.019318	4.891385	R
Al	7.237035	11.975630	4.839803	R
Al	6.230741	13.355141	6.971254	R
Al	6.379098	10.498770	7.113977	R
O	4.825628	14.707422	7.127750	R
O	4.961316	11.822548	7.267480	R
O	4.960752	9.200558	7.264624	R
O	7.532648	14.725919	7.420629	R
O	6.336117	10.477763	5.088433	R
O	7.552823	12.016713	6.682235	R
O	7.610343	9.056297	6.767071	R
O	6.186641	13.367196	5.045630	R
Al	7.262392	14.862744	9.238212	R
Al	7.880199	10.466853	10.380886	R
O	6.185543	10.503896	13.140826	R
O	6.490173	13.540826	13.291353	R
O	6.367269	10.519099	9.055771	R
O	7.707547	15.052663	10.903217	R
O	6.043910	13.405430	8.928771	R
O	6.002965	16.161222	8.827188	R
O	8.159641	9.120985	11.515469	R
O	8.126416	11.866336	11.478346	R
O	4.781149	6.124750	10.941388	R
O	4.826852	14.913225	10.924832	R
O	4.804055	9.097756	10.952425	R
O	4.787894	11.931695	10.960070	R
O	6.304758	4.946299	5.070138	R
O	6.342512	16.039132	5.089679	R
O	8.134638	9.106437	3.336476	R
O	8.026986	11.952386	3.288170	R
O	3.489448	10.504771	8.960496	R
Cu	8.925573	11.733547	7.957266	R
Cu	9.214637	8.869500	7.997724	R
O	9.226080	10.355738	9.145798	R
N	10.160475	6.153111	8.514204	R
N	11.044401	6.691903	7.717606	R
O	9.267277	6.970460	8.980726	R
O	10.755677	7.825705	7.211055	R

```
Model #27     Cartesian coordinates in angstrom
              x              y              z              Relaxed/Frozen
Al            4.718091       6.298715       9.025534       F
Al            6.299120       6.298715       11.957102      F
Al            4.718091       14.697002      9.025534       F
Al            4.828311       11.950763      9.158184       F
Al            4.828311       9.044955       9.158184       F
Al            7.260466       8.998624       12.959551      F
Al            7.260466       11.997093      12.959551      F
Al            6.299120       14.697002      11.957102      F
Al            4.636026       10.497859      12.053017      F
O             3.286788       10.497859      13.239718      F
Al            6.284430       4.911618       6.956078       F
Al            6.284430       16.084099      6.956078       F
Al            7.604152       10.497859      2.473791       F
O             6.427205       10.497859      1.094354       F
Al            6.373455       6.298715       3.886397       F
O             4.781442       6.298715       2.980335       F
Al            6.373455       14.697002      3.886397       F
O             4.781442       14.697002      2.980335       F
O             3.454035       4.977004       9.235301       F
O             3.454035       7.620427       9.235301       F
O             6.249989       5.002877       13.162247      F
O             3.454035       16.018713      9.235301       F
O             3.454035       13.375290      9.235301       F
O             7.425505       9.104843       14.776051      F
O             7.425505       11.890874      14.776051      F
O             6.249989       15.992841      13.162247      F
O             4.962264       3.365416       7.283451       F
O             7.499839       3.492587       6.705345       F
O             4.962264       17.630302      7.283451       F
O             7.499839       17.503130      6.705345       F
O             7.704784       6.298715       2.777154       F
O             7.704784       14.697002      2.777154       F
Al            3.478998       10.497859      7.046735       F
O             1.926548       11.807732      6.890259       F
O             1.926548       9.187985       6.890259       F
O             3.361122       10.497859      5.169014       F
Al            2.050923       10.497859      10.125656      F
O             0.574778       10.497859      9.076089       F
O             2.097749       9.088323       11.188759      F
O             2.097749       11.907395      11.188759      F
Al            3.393316       6.298715       6.011417       F
O             1.956477       6.298715       7.179493       F
O             3.339459       7.715095       4.949249       F
O             3.339459       4.882336       4.949249       F
Al            3.393316       14.697002      6.011417       F
O             1.956477       14.697002      7.179493       F
O             3.339459       16.113380      4.949249       F
O             3.339459       13.280622      4.949249       F
H             3.439923       4.911172       10.243970      F
H             3.439232       7.689483       10.293373      F
H             6.818393       4.213072       13.048228      F
H             6.229200       4.955319       14.133904      F
H             3.439929       16.084518      10.243550      F
H             3.439218       13.306190      10.293977      F
H             6.776962       8.347647       14.909841      F
H             6.777013       12.648010      14.909830      F
H             6.229199       16.040400      14.133948      F
H             6.818394       16.782646      13.048228      F
H             4.227165       2.738070       7.166136       F
H             6.932392       2.747750       6.973661       F
H             7.409135       3.550965       5.707009       F
H             4.227165       18.257647      7.166137       F
H             6.932397       18.247959      6.973659       F
H             7.409131       17.444750      5.706962       F
H             7.521090       6.298716       1.832227       F
H             7.521091       14.697002      1.832228       F
H             3.346923       10.497859      14.197637      F
H             6.469066       10.497859      0.138110       F
H             0.036291       9.692187       9.043065       F
H             0.036295       11.303524      9.043066       F
H             2.008448       9.058198       12.145152      F
H             2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.224479	7.632719	7.002328	R
O	4.799464	6.297712	7.127288	R
O	7.463926	6.277522	7.316439	R
O	6.245660	7.645541	5.056016	R
Al	7.510741	5.948389	9.200192	R
O	6.462093	7.477875	13.291086	R
O	7.662534	5.912991	10.958215	R
O	6.019523	4.843993	8.821550	R
O	6.036713	7.619685	8.912979	R
Al	7.323501	9.014041	4.900874	R
Al	7.238772	11.974218	4.840950	R
Al	6.233672	13.355404	6.974332	R
Al	6.368656	10.499271	7.111963	R
O	4.825828	14.707963	7.127020	R
O	4.959645	11.830196	7.266735	R
O	4.945900	9.217213	7.260497	R
O	7.534286	14.726300	7.422012	R
O	6.333383	10.479033	5.093102	R
O	7.557171	12.011472	6.683272	R
O	7.592758	9.046993	6.783106	R
O	6.190665	13.367104	5.047194	R
Al	7.261833	14.866519	9.241233	R
Al	7.875420	10.533620	10.396748	R
O	6.187577	10.506825	13.136644	R
O	6.481568	13.540370	13.295822	R
O	6.378471	10.536712	9.054341	R
O	7.705377	15.067784	10.904648	R
O	6.045340	13.407596	8.929902	R
O	6.001909	16.162439	8.825587	R
O	8.186624	9.195110	11.538026	R
O	8.113211	11.940044	11.468021	R
O	4.775697	6.112521	10.949100	R
O	4.826407	14.913100	10.923368	R
O	4.802487	9.104930	10.951770	R
O	4.789113	11.932341	10.959179	R
O	6.305801	4.944265	5.064903	R
O	6.342396	16.039084	5.089159	R
O	8.130305	9.109948	3.348735	R
O	8.028841	11.951766	3.288564	R
O	3.485365	10.510901	8.959376	R
Cu	8.947653	11.746653	7.941601	R
Cu	8.925542	8.802522	8.272811	R
O	9.243636	10.419555	9.174023	R
N	10.374662	6.250827	8.715382	R
N	10.188252	4.926398	8.856434	R
O	8.994752	4.555672	9.019038	R
O	9.316817	6.945963	8.934968	R

```
Model #28        Cartesian coordinates in angstrom
                 x               y               z               Relaxed/Frozen
Al       4.718091        6.298715        9.025534        F
Al       6.299120        6.298715        11.957102       F
Al       4.718091        14.697002       9.025534        F
Al       4.828311        11.950763       9.158184        F
Al       4.828311        9.044955        9.158184        F
Al       7.260466        8.998624        12.959551       F
Al       7.260466        11.997093       12.959551       F
Al       6.299120        14.697002       11.957102       F
Al       4.636026        10.497859       12.053017       F
O        3.286788        10.497859       13.239718       F
Al       6.284430        4.911618        6.956078        F
Al       6.284430        16.084099       6.956078        F
Al       7.604152        10.497859       2.473791        F
O        6.427205        10.497859       1.094354        F
Al       6.373455        6.298715        3.886397        F
O        4.781442        6.298715        2.980335        F
Al       6.373455        14.697002       3.886397        F
O        4.781442        14.697002       2.980335        F
O        3.454035        4.977004        9.235301        F
O        3.454035        7.620427        9.235301        F
O        6.249989        5.002877        13.162247       F
O        3.454035        16.018713       9.235301        F
O        3.454035        13.375290       9.235301        F
O        7.425505        9.104843        14.776051       F
O        7.425505        11.890874       14.776051       F
O        6.249989        15.992841       13.162247       F
O        4.962264        3.365416        7.283451        F
O        7.499839        3.492587        6.705345        F
O        4.962264        17.630302       7.283451        F
O        7.499839        17.503130       6.705345        F
O        7.704784        6.298715        2.777154        F
O        7.704784        14.697002       2.777154        F
Al       3.478998        10.497859       7.046735        F
O        1.926548        11.807732       6.890259        F
O        1.926548        9.187985        6.890259        F
O        3.361122        10.497859       5.169014        F
Al       2.050923        10.497859       10.125656       F
O        0.574778        10.497859       9.076089        F
O        2.097749        9.088323        11.188759       F
O        2.097749        11.907395       11.188759       F
Al       3.393316        6.298715        6.011417        F
O        1.956477        6.298715        7.179493        F
O        3.339459        7.715095        4.949249        F
O        3.339459        4.882336        4.949249        F
Al       3.393316        14.697002       6.011417        F
O        1.956477        14.697002       7.179493        F
O        3.339459        16.113380       4.949249        F
O        3.339459        13.280622       4.949249        F
H        3.439923        4.911172        10.243970       F
H        3.439232        7.689483        10.293373       F
H        6.818393        4.213072        13.048228       F
H        6.229200        4.955319        14.133904       F
H        3.439929        16.084518       10.243550       F
H        3.439218        13.306190       10.293977       F
H        6.776962        8.347647        14.909841       F
H        6.777013        12.648010       14.909830       F
H        6.229199        16.040400       14.133948       F
H        6.818394        16.782646       13.048228       F
H        4.227165        2.738070        7.166136        F
H        6.932392        2.747750        6.973661        F
H        7.409135        3.550965        5.707009        F
H        4.227165        18.257647       7.166137        F
H        6.932397        18.247959       6.973659        F
H        7.409131        17.444750       5.706962        F
H        7.521090        6.298716        1.832227        F
H        7.521091        14.697002       1.832228        F
H        3.346923        10.497859       14.197637       F
H        6.469066        10.497859       0.138110        F
H        0.036291        9.692187        9.043066        F
H        0.036295        11.303524       9.043066        F
H        2.008448        9.058198        12.145152       F
H        2.008447        11.937518       12.145155       F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.226143	7.627236	7.009419	R
O	4.793824	6.296247	7.127047	R
O	7.458681	6.273779	7.317190	R
O	6.238923	7.645325	5.056351	R
Al	7.555208	5.896007	9.200839	R
O	6.457282	7.480935	13.289954	R
O	7.657459	5.896624	10.963699	R
O	6.018420	4.841285	8.822179	R
O	6.021427	7.631779	8.906317	R
Al	7.318832	9.012493	4.906632	R
Al	7.230980	11.972734	4.840033	R
Al	6.232408	13.355177	6.973735	R
Al	6.360792	10.496740	7.110481	R
O	4.821746	14.707977	7.127212	R
O	4.944561	11.834889	7.263926	R
O	4.926804	9.222999	7.254819	R
O	7.530492	14.726795	7.418968	R
O	6.324740	10.477979	5.093277	R
O	7.547810	12.011319	6.680583	R
O	7.584112	9.045932	6.788507	R
O	6.183413	13.367386	5.045620	R
Al	7.262755	14.864086	9.239428	R
Al	7.882309	10.530094	10.393030	R
O	6.185962	10.507958	13.136440	R
O	6.481203	13.540762	13.295856	R
O	6.360076	10.541922	9.051051	R
O	7.703562	15.068960	10.903003	R
O	6.043211	13.407399	8.927446	R
O	6.000833	16.161308	8.824837	R
O	8.189015	9.198621	11.542740	R
O	8.103183	11.942813	11.461126	R
O	4.768750	6.118415	10.951252	R
O	4.824915	14.912811	10.923074	R
O	4.792543	9.110330	10.949107	R
O	4.777093	11.934372	10.957314	R
O	6.299871	4.944564	5.062814	R
O	6.339423	16.039437	5.088724	R
O	8.127189	9.112873	3.354417	R
O	8.019435	11.954940	3.287036	R
O	3.468468	10.513474	8.951080	R
Cu	8.942564	11.701155	7.923106	R
Cu	8.917444	8.746894	8.294694	R
O	9.235371	10.389196	9.168881	R
N	10.379166	6.216897	8.671303	R
N	10.192861	4.913963	8.781400	R
O	8.997401	4.525569	8.992186	R
O	9.316506	6.924551	8.938431	R

```
Model #29      Cartesian coordinates in angstrom
               x               y               z               Relaxed/Frozen
Al             4.718091        6.298715        9.025534        F
Al             6.299120        6.298715        11.957102       F
Al             4.718091        14.697002       9.025534        F
Al             4.828311        11.950763       9.158184        F
Al             4.828311        9.044955        9.158184        F
Al             7.260466        8.998624        12.959551       F
Al             7.260466        11.997093       12.959551       F
Al             6.299120        14.697002       11.957102       F
Al             4.636026        10.497859       12.053017       F
O              3.286788        10.497859       13.239718       F
Al             6.284430        4.911618        6.956078        F
Al             6.284430        16.084099       6.956078        F
Al             7.604152        10.497859       2.473791        F
O              6.427205        10.497859       1.094354        F
Al             6.373455        6.298715        3.886397        F
O              4.781442        6.298715        2.980335        F
Al             6.373455        14.697002       3.886397        F
O              4.781442        14.697002       2.980335        F
O              3.454035        4.977004        9.235301        F
O              3.454035        7.620427        9.235301        F
O              6.249989        5.002877        13.162247       F
O              3.454035        16.018713       9.235301        F
O              3.454035        13.375290       9.235301        F
O              7.425505        9.104843        14.776051       F
O              7.425505        11.890874       14.776051       F
O              6.249989        15.992841       13.162247       F
O              4.962264        3.365416        7.283451        F
O              7.499839        3.492587        6.705345        F
O              4.962264        17.630302       7.283451        F
O              7.499839        17.503130       6.705345        F
O              7.704784        6.298715        2.777154        F
O              7.704784        14.697002       2.777154        F
Al             3.478998        10.497859       7.046735        F
O              1.926548        11.807732       6.890259        F
O              1.926548        9.187985        6.890259        F
O              3.361122        10.497859       5.169014        F
Al             2.050923        10.497859       10.125656       F
O              0.574778        10.497859       9.076089        F
O              2.097749        9.088323        11.188759       F
O              2.097749        11.907395       11.188759       F
Al             3.393316        6.298715        6.011417        F
O              1.956477        6.298715        7.179493        F
O              3.339459        7.715095        4.949249        F
O              3.339459        4.882336        4.949249        F
Al             3.393316        14.697002       6.011417        F
O              1.956477        14.697002       7.179493        F
O              3.339459        16.113380       4.949249        F
O              3.339459        13.280622       4.949249        F
H              3.439923        4.911172        10.243970       F
H              3.439232        7.689483        10.293373       F
H              6.818393        4.213072        13.048228       F
H              6.229200        4.955319        14.133904       F
H              3.439929        16.084518       10.243550       F
H              3.439218        13.306190       10.293977       F
H              6.776962        8.347647        14.909841       F
H              6.777013        12.648010       14.909830       F
H              6.229199        16.040400       14.133948       F
H              6.818394        16.782646       13.048228       F
H              4.227165        2.738070        7.166136        F
H              6.932392        2.747750        6.973661        F
H              7.409135        3.550965        5.707009        F
H              4.227165        18.257647       7.166137        F
H              6.932397        18.247959       6.973659        F
H              7.409131        17.444750       5.706962        F
H              7.521090        6.298716        1.832227        F
H              7.521091        14.697002       1.832228        F
H              3.346923        10.497859       14.197637       F
H              6.469066        10.497859       0.138110        F
H              0.036291        9.692187        9.043065        F
H              0.036295        11.303524       9.043066        F
H              2.008448        9.058198        12.145152       F
H              2.008447        11.937518       12.145155       F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.203157	7.636145	6.948000	R
O	4.803059	6.304312	7.126523	R
O	7.476505	6.295181	7.324341	R
O	6.162187	7.647838	5.014438	R
Al	7.402137	6.235453	9.201234	R
O	6.475878	7.466131	13.296668	R
O	7.664207	5.910142	10.917301	R
O	6.038089	4.884813	8.820754	R
O	6.042793	7.620268	8.912757	R
Al	7.229889	9.022516	4.832272	R
Al	7.302064	11.979514	4.853590	R
Al	6.263217	13.348113	6.983299	R
Al	6.371132	10.499386	7.092735	R
O	4.833732	14.702785	7.126472	R
O	4.983260	11.822528	7.272818	R
O	4.954561	9.210182	7.269084	R
O	7.539225	14.731390	7.425545	R
O	6.313271	10.525933	5.048512	R
O	7.600485	11.982810	6.707910	R
O	7.518626	9.013310	6.666723	R
O	6.249162	13.370375	5.060291	R
Al	7.264695	14.866359	9.241132	R
Al	7.930172	10.475880	10.393034	R
O	6.189342	10.500902	13.139040	R
O	6.486722	13.538325	13.290779	R
O	6.433069	10.516596	9.049501	R
O	7.708877	15.053622	10.907533	R
O	6.049414	13.407628	8.936678	R
O	6.003469	16.163670	8.829691	R
O	8.151782	9.108319	11.517494	R
O	8.154991	11.863210	11.500946	R
O	4.787938	6.118475	10.943966	R
O	4.825649	14.912988	10.927273	R
O	4.813588	9.095424	10.953817	R
O	4.804144	11.927709	10.960993	R
O	6.324397	4.946779	5.073494	R
O	6.339310	16.043594	5.086550	R
O	8.067651	9.067701	3.303170	R
O	8.104509	11.922347	3.303843	R
O	3.506315	10.509939	8.971249	R
Cu	8.992181	11.537269	7.966999	R
Cu	8.869679	9.038482	8.033322	R
O	9.436937	10.293247	9.337678	R
N	10.020637	7.436955	10.054198	R
N	10.414014	8.519140	10.457990	R
O	11.174054	8.972944	11.251713	R
O	9.228858	7.254300	9.044324	R

```
Model #30      Cartesian coordinates in angstrom
               x            y            z            Relaxed/Frozen
Al    4.718091     6.298715     9.025534     F
Al    6.299120     6.298715     11.957102    F
Al    4.718091     14.697002    9.025534     F
Al    4.828311     11.950763    9.158184     F
Al    4.828311     9.044955     9.158184     F
Al    7.260466     8.998624     12.959551    F
Al    7.260466     11.997093    12.959551    F
Al    6.299120     14.697002    11.957102    F
Al    4.636026     10.497859    12.053017    F
O     3.286788     10.497859    13.239718    F
Al    6.284430     4.911618     6.956078     F
Al    6.284430     16.084099    6.956078     F
Al    7.604152     10.497859    2.473791     F
O     6.427205     10.497859    1.094354     F
Al    6.373455     6.298715     3.886397     F
O     4.781442     6.298715     2.980335     F
Al    6.373455     14.697002    3.886397     F
O     4.781442     14.697002    2.980335     F
O     3.454035     4.977004     9.235301     F
O     3.454035     7.620427     9.235301     F
O     6.249989     5.002877     13.162247    F
O     3.454035     16.018713    9.235301     F
O     3.454035     13.375290    9.235301     F
O     7.425505     9.104843     14.776051    F
O     7.425505     11.890874    14.776051    F
O     6.249989     15.992841    13.162247    F
O     4.962264     3.365416     7.283451     F
O     7.499839     3.492587     6.705345     F
O     4.962264     17.630302    7.283451     F
O     7.499839     17.503130    6.705345     F
O     7.704784     6.298715     2.777154     F
O     7.704784     14.697002    2.777154     F
Al    3.478998     10.497859    7.046735     F
O     1.926548     11.807732    6.890259     F
O     1.926548     9.187985     6.890259     F
O     3.361122     10.497859    5.169014     F
Al    2.050923     10.497859    10.125656    F
O     0.574778     10.497859    9.076089     F
O     2.097749     9.088323     11.188759    F
O     2.097749     11.907395    11.188759    F
Al    3.393316     6.298715     6.011417     F
O     1.956477     6.298715     7.179493     F
O     3.339459     7.715095     4.949249     F
O     3.339459     4.882336     4.949249     F
Al    3.393316     14.697002    6.011417     F
O     1.956477     14.697002    7.179493     F
O     3.339459     16.113380    4.949249     F
O     3.339459     13.280622    4.949249     F
H     3.439923     4.911172     10.243970    F
H     3.439232     7.689483     10.293373    F
H     6.818393     4.213072     13.048228    F
H     6.229200     4.955319     14.133904    F
H     3.439929     16.084518    10.243550    F
H     3.439218     13.306190    10.293977    F
H     6.776962     8.347647     14.909841    F
H     6.777013     12.648010    14.909830    F
H     6.229199     16.040400    14.133948    F
H     6.818394     16.782646    13.048228    F
H     4.227165     2.738070     7.166136     F
H     6.932392     2.747750     6.973661     F
H     7.409135     3.550965     5.707009     F
H     4.227165     18.257647    7.166137     F
H     6.932397     18.247959    6.973659     F
H     7.409131     17.444750    5.706962     F
H     7.521090     6.298716     1.832227     F
H     7.521091     14.697002    1.832228     F
H     3.346923     10.497859    14.197637    F
H     6.469066     10.497859    0.138110     F
H     0.036291     9.692187     9.043066     F
H     0.036295     11.303524    9.043066     F
H     2.008448     9.058198     12.145152    F
H     2.008447     11.937518    12.145155    F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.174406	7.649852	6.958732	R
O	4.807048	6.300444	7.124298	R
O	7.494298	6.343335	7.337419	R
O	6.214864	7.649644	5.036219	R
Al	7.428342	6.145872	9.246615	R
O	6.453260	7.473499	13.295866	R
O	7.618810	5.776885	10.952348	R
O	6.049026	4.877319	8.803288	R
O	6.053075	7.615835	8.918016	R
Al	7.279557	9.027589	4.856204	R
Al	7.270781	11.980506	4.846440	R
Al	6.256386	13.355777	6.979840	R
Al	6.355880	10.511460	7.099941	R
O	4.831682	14.705682	7.126824	R
O	4.971495	11.823853	7.265707	R
O	4.955958	9.196908	7.255319	R
O	7.535222	14.732438	7.420514	R
O	6.320212	10.501892	5.064089	R
O	7.580158	11.998380	6.688787	R
O	7.564482	9.060385	6.719514	R
O	6.219317	13.368935	5.053264	R
Al	7.265980	14.861414	9.237086	R
Al	7.892231	10.382089	10.364547	R
O	6.186024	10.503247	13.143467	R
O	6.505695	13.542495	13.285964	R
O	6.370785	10.502675	9.044176	R
O	7.711109	15.038363	10.904606	R
O	6.047248	13.404741	8.930921	R
O	6.005065	16.161771	8.830671	R
O	8.129655	9.031915	11.496032	R
O	8.143819	11.775995	11.485191	R
O	4.782285	6.124692	10.932443	R
O	4.827289	14.913831	10.927576	R
O	4.808930	9.096439	10.953015	R
O	4.795999	11.932339	10.961847	R
O	6.326182	4.953879	5.080008	R
O	6.341783	16.041978	5.086842	R
O	8.101941	9.083403	3.318806	R
O	8.071967	11.932878	3.298430	R
O	3.502349	10.504353	8.965176	R
Cu	8.932615	11.387523	7.883308	R
Cu	8.776252	8.464631	8.100249	R
O	9.217881	10.036384	9.116574	R
N	10.084536	6.903967	10.223337	R
N	11.049316	7.679336	10.075567	R
O	11.970592	7.920330	10.834877	R
O	9.269731	6.908660	9.125284	R

```
Model #31      Cartesian coordinates in angstrom
               x               y               z               Relaxed/Frozen
Al             4.718091        6.298715        9.025534        F
Al             6.299120        6.298715        11.957102       F
Al             4.718091        14.697002       9.025534        F
Al             4.828311        11.950763       9.158184        F
Al             4.828311        9.044955        9.158184        F
Al             7.260466        8.998624        12.959551       F
Al             7.260466        11.997093       12.959551       F
Al             6.299120        14.697002       11.957102       F
Al             4.636026        10.497859       12.053017       F
O              3.286788        10.497859       13.239718       F
Al             6.284430        4.911618        6.956078        F
Al             6.284430        16.084099       6.956078        F
Al             7.604152        10.497859       2.473791        F
O              6.427205        10.497859       1.094354        F
Al             6.373455        6.298715        3.886397        F
O              4.781442        6.298715        2.980335        F
Al             6.373455        14.697002       3.886397        F
O              4.781442        14.697002       2.980335        F
O              3.454035        4.977004        9.235301        F
O              3.454035        7.620427        9.235301        F
O              6.249989        5.002877        13.162247       F
O              3.454035        16.018713       9.235301        F
O              3.454035        13.375290       9.235301        F
O              7.425505        9.104843        14.776051       F
O              7.425505        11.890874       14.776051       F
O              6.249989        15.992841       13.162247       F
O              4.962264        3.365416        7.283451        F
O              7.499839        3.492587        6.705345        F
O              4.962264        17.630302       7.283451        F
O              7.499839        17.503130       6.705345        F
O              7.704784        6.298715        2.777154        F
O              7.704784        14.697002       2.777154        F
Al             3.478998        10.497859       7.046735        F
O              1.926548        11.807732       6.890259        F
O              1.926548        9.187985        6.890259        F
O              3.361122        10.497859       5.169014        F
Al             2.050923        10.497859       10.125656       F
O              0.574778        10.497859       9.076089        F
O              2.097749        9.088323        11.188759       F
O              2.097749        11.907395       11.188759       F
Al             3.393316        6.298715        6.011417        F
O              1.956477        6.298715        7.179493        F
O              3.339459        7.715095        4.949249        F
O              3.339459        4.882336        4.949249        F
Al             3.393316        14.697002       6.011417        F
O              1.956477        14.697002       7.179493        F
O              3.339459        16.113380       4.949249        F
O              3.339459        13.280622       4.949249        F
H              3.439923        4.911172        10.243970       F
H              3.439232        7.689483        10.293373       F
H              6.818393        4.213072        13.048228       F
H              6.229200        4.955319        14.133904       F
H              3.439929        16.084518       10.243550       F
H              3.439218        13.306190       10.293977       F
H              6.776962        8.347647        14.909841       F
H              6.777013        12.648010       14.909830       F
H              6.229199        16.040400       14.133948       F
H              6.818394        16.782646       13.048228       F
H              4.227165        2.738070        7.166136        F
H              6.932392        2.747750        6.973661        F
H              7.409135        3.550965        5.707009        F
H              4.227165        18.257647       7.166137        F
H              6.932397        18.247959       6.973659        F
H              7.409131        17.444750       5.706962        F
H              7.521090        6.298716        1.832227        F
H              7.521091        14.697002       1.832228        F
H              3.346923        10.497859       14.197637       F
H              6.469066        10.497859       0.138110        F
H              0.036291        9.692187        9.043065        F
H              0.036295        11.303524       9.043066        F
H              2.008448        9.058198        12.145152       F
H              2.008447        11.937518       12.145155       F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.255505	7.649457	6.991047	R
O	4.831631	6.294023	7.129120	R
O	7.538792	6.270217	7.429368	R
O	6.233981	7.624999	5.066885	R
Al	7.264969	6.128666	9.243422	R
O	6.488100	7.456860	13.291836	R
O	7.708425	5.941826	10.909044	R
O	6.003439	4.833704	8.829419	R
O	6.046841	7.591500	8.940196	R
Al	7.276384	9.022331	4.881695	R
Al	7.284612	11.969450	4.882573	R
Al	6.251991	13.342781	6.995277	R
Al	6.396497	10.492255	7.147022	R
O	4.833226	14.701533	7.128243	R
O	4.977693	11.817293	7.272313	R
O	4.973486	9.180379	7.273364	R
O	7.544275	14.721350	7.432749	R
O	6.332152	10.501337	5.115791	R
O	7.595008	11.976607	6.758030	R
O	7.586037	9.013181	6.742804	R
O	6.250473	13.371857	5.073865	R
Al	7.263619	14.870252	9.247571	R
Al	7.873852	10.517653	10.339002	R
O	6.181905	10.498080	13.149857	R
O	6.482083	13.538628	13.294285	R
O	6.328046	10.500186	9.070495	R
O	7.707704	15.064756	10.910883	R
O	6.048007	13.405547	8.941669	R
O	6.004021	16.162239	8.826572	R
O	8.126177	9.148657	11.483287	R
O	8.116124	11.887299	11.477834	R
O	4.825514	6.083900	10.927192	R
O	4.827005	14.913210	10.924721	R
O	4.790565	9.070696	10.962715	R
O	4.790053	11.926098	10.962551	R
O	6.336908	4.954454	5.088464	R
O	6.338228	16.040889	5.088729	R
O	8.059838	9.073833	3.322487	R
O	8.069648	11.920712	3.324178	R
O	3.496002	10.499289	8.965882	R
Cu	9.320448	11.881053	7.739328	R
Cu	9.348891	9.204214	7.694242	R
O	9.151516	10.540820	9.064533	R
N	11.147191	9.672760	7.083190	R
N	11.811262	10.754038	7.045617	R
O	11.557749	8.540990	6.715904	R
O	11.194972	11.849993	7.389286	R

```
Model #32      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al     4.718091       6.298715       9.025534       F
Al     6.299120       6.298715       11.957102      F
Al     4.718091       14.697002      9.025534       F
Al     4.828311       11.950763      9.158184       F
Al     4.828311       9.044955       9.158184       F
Al     7.260466       8.998624       12.959551      F
Al     7.260466       11.997093      12.959551      F
Al     6.299120       14.697002      11.957102      F
Al     4.636026       10.497859      12.053017      F
O      3.286788       10.497859      13.239718      F
Al     6.284430       4.911618       6.956078       F
Al     6.284430       16.084099      6.956078       F
Al     7.604152       10.497859      2.473791       F
O      6.427205       10.497859      1.094354       F
Al     6.373455       6.298715       3.886397       F
O      4.781442       6.298715       2.980335       F
Al     6.373455       14.697002      3.886397       F
O      4.781442       14.697002      2.980335       F
O      3.454035       4.977004       9.235301       F
O      3.454035       7.620427       9.235301       F
O      6.249989       5.002877       13.162247      F
O      3.454035       16.018713      9.235301       F
O      3.454035       13.375290      9.235301       F
O      7.425505       9.104843       14.776051      F
O      7.425505       11.890874      14.776051      F
O      6.249989       15.992841      13.162247      F
O      4.962264       3.365416       7.283451       F
O      7.499839       3.492587       6.705345       F
O      4.962264       17.630302      7.283451       F
O      7.499839       17.503130      6.705345       F
O      7.704784       6.298715       2.777154       F
O      7.704784       14.697002      2.777154       F
Al     3.478998       10.497859      7.046735       F
O      1.926548       11.807732      6.890259       F
O      1.926548       9.187985       6.890259       F
O      3.361122       10.497859      5.169014       F
Al     2.050923       10.497859      10.125656      F
O      0.574778       10.497859      9.076089       F
O      2.097749       9.088323       11.188759      F
O      2.097749       11.907395      11.188759      F
Al     3.393316       6.298715       6.011417       F
O      1.956477       6.298715       7.179493       F
O      3.339459       7.715095       4.949249       F
O      3.339459       4.882336       4.949249       F
Al     3.393316       14.697002      6.011417       F
O      1.956477       14.697002      7.179493       F
O      3.339459       16.113380      4.949249       F
O      3.339459       13.280622      4.949249       F
H      3.439923       4.911172       10.243970      F
H      3.439232       7.689483       10.293373      F
H      6.818393       4.213072       13.048228      F
H      6.229200       4.955319       14.133904      F
H      3.439929       16.084518      10.243550      F
H      3.439218       13.306190      10.293977      F
H      6.776962       8.347647       14.909841      F
H      6.777013       12.648010      14.909830      F
H      6.229199       16.040400      14.133948      F
H      6.818394       16.782646      13.048228      F
H      4.227165       2.738070       7.166136       F
H      6.932392       2.747750       6.973661       F
H      7.409135       3.550965       5.707009       F
H      4.227165       18.257647      7.166137       F
H      6.932397       18.247959      6.973659       F
H      7.409131       17.444750      5.706962       F
H      7.521090       6.298716       1.832227       F
H      7.521091       14.697002      1.832228       F
H      3.346923       10.497859      14.197637      F
H      6.469066       10.497859      0.138110       F
H      0.036291       9.692187       9.043065       F
H      0.036295       11.303524      9.043066       F
H      2.008448       9.058198       12.145152      F
H      2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.254123	7.651641	6.992781	R
O	4.831985	6.294609	7.128030	R
O	7.539917	6.273438	7.427648	R
O	6.240822	7.624273	5.068837	R
Al	7.266518	6.130600	9.243847	R
O	6.481223	7.457662	13.293354	R
O	7.706576	5.935516	10.908967	R
O	6.004660	4.835049	8.827354	R
O	6.046725	7.591513	8.939432	R
Al	7.272709	9.027438	4.875951	R
Al	7.272820	11.970102	4.875963	R
Al	6.254214	13.343762	6.989782	R
Al	6.388762	10.501818	7.139180	R
O	4.832470	14.702087	7.127672	R
O	4.970585	11.815771	7.273231	R
O	4.973856	9.180741	7.272407	R
O	7.540799	14.723822	7.427499	R
O	6.318714	10.497105	5.096726	R
O	7.577365	11.975499	6.734372	R
O	7.582706	9.023718	6.742276	R
O	6.234918	13.371198	5.064911	R
Al	7.265333	14.863321	9.243197	R
Al	7.899617	10.492047	10.343290	R
O	6.180536	10.498137	13.150118	R
O	6.483737	13.538658	13.292568	R
O	6.350222	10.497046	9.063342	R
O	7.707478	15.057961	10.908274	R
O	6.046268	13.404292	8.938446	R
O	6.004696	16.160747	8.827721	R
O	8.127047	9.121875	11.487820	R
O	8.130089	11.863138	11.489079	R
O	4.825135	6.083746	10.925953	R
O	4.825697	14.912320	10.926151	R
O	4.790588	9.071718	10.960799	R
O	4.790419	11.924658	10.960951	R
O	6.337984	4.953893	5.087530	R
O	6.339895	16.042523	5.087467	R
O	8.070687	9.075191	3.323126	R
O	8.066972	11.922071	3.320801	R
O	3.497664	10.497376	8.966436	R
Cu	9.294300	11.806843	7.742308	R
Cu	9.307061	9.209276	7.697382	R
O	9.245156	10.488228	9.142455	R
N	11.260194	9.418966	7.336787	R
N	11.943681	10.587114	7.162278	R
O	11.952694	8.398040	7.381820	R
O	11.216845	11.604386	7.134274	R

```
Model #33      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043066       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.223779	7.642827	6.984672	R
O	4.801357	6.300455	7.133039	R
O	7.457002	6.295026	7.323582	R
O	6.253268	7.649566	5.051949	R
Al	7.425465	6.072404	9.203044	R
O	6.463397	7.473562	13.292969	R
O	7.657487	5.914089	10.936347	R
O	6.036587	4.845456	8.821390	R
O	6.054645	7.606535	8.926415	R
Al	7.339547	9.015548	4.899199	R
Al	7.243400	11.974779	4.843706	R
Al	6.234828	13.354980	6.974109	R
Al	6.380744	10.498384	7.117146	R
O	4.827446	14.706749	7.127661	R
O	4.967807	11.822065	7.268591	R
O	4.964871	9.202371	7.266957	R
O	7.534875	14.726573	7.422503	R
O	6.343980	10.475637	5.098638	R
O	7.561752	12.013119	6.687145	R
O	7.613027	9.048133	6.781326	R
O	6.193917	13.366375	5.048532	R
Al	7.261818	14.865415	9.240042	R
Al	7.870679	10.489912	10.384112	R
O	6.187700	10.504237	13.138769	R
O	6.488188	13.540362	13.292458	R
O	6.374860	10.525945	9.057962	R
O	7.707837	15.056404	10.904513	R
O	6.045542	13.406443	8.930644	R
O	6.002905	16.162287	8.827126	R
O	8.167219	9.143137	11.517860	R
O	8.125282	11.887051	11.475379	R
O	4.784414	6.106844	10.941590	R
O	4.827315	14.913002	10.924599	R
O	4.807311	9.096684	10.954008	R
O	4.793269	11.930787	10.960833	R
O	6.308986	4.946216	5.070667	R
O	6.343214	16.038697	5.089684	R
O	8.136851	9.109112	3.343544	R
O	8.028868	11.950974	3.289463	R
O	3.495379	10.505636	8.963654	R
Cu	8.951578	11.725934	7.941944	R
Cu	9.074116	8.766262	8.153351	R
O	9.218126	10.357117	9.139478	R
N	9.962734	7.021984	8.436484	R
N	11.316864	6.908458	8.040674	R
O	9.449933	5.992740	8.962625	R
O	11.846631	5.867907	8.358487	R

```
Model #34      Cartesian coordinates in angstrom
               x               y               z               Relaxed/Frozen
Al             4.718091        6.298715        9.025534        F
Al             6.299120        6.298715        11.957102       F
Al             4.718091        14.697002       9.025534        F
Al             4.828311        11.950763       9.158184        F
Al             4.828311        9.044955        9.158184        F
Al             7.260466        8.998624        12.959551       F
Al             7.260466        11.997093       12.959551       F
Al             6.299120        14.697002       11.957102       F
Al             4.636026        10.497859       12.053017       F
O              3.286788        10.497859       13.239718       F
Al             6.284430        4.911618        6.956078        F
Al             6.284430        16.084099       6.956078        F
Al             7.604152        10.497859       2.473791        F
O              6.427205        10.497859       1.094354        F
Al             6.373455        6.298715        3.886397        F
O              4.781442        6.298715        2.980335        F
Al             6.373455        14.697002       3.886397        F
O              4.781442        14.697002       2.980335        F
O              3.454035        4.977004        9.235301        F
O              3.454035        7.620427        9.235301        F
O              6.249989        5.002877        13.162247       F
O              3.454035        16.018713       9.235301        F
O              3.454035        13.375290       9.235301        F
O              7.425505        9.104843        14.776051       F
O              7.425505        11.890874       14.776051       F
O              6.249989        15.992841       13.162247       F
O              4.962264        3.365416        7.283451        F
O              7.499839        3.492587        6.705345        F
O              4.962264        17.630302       7.283451        F
O              7.499839        17.503130       6.705345        F
O              7.704784        6.298715        2.777154        F
O              7.704784        14.697002       2.777154        F
Al             3.478998        10.497859       7.046735        F
O              1.926548        11.807732       6.890259        F
O              1.926548        9.187985        6.890259        F
O              3.361122        10.497859       5.169014        F
Al             2.050923        10.497859       10.125656       F
O              0.574778        10.497859       9.076089        F
O              2.097749        9.088323        11.188759       F
O              2.097749        11.907395       11.188759       F
Al             3.393316        6.298715        6.011417        F
O              1.956477        6.298715        7.179493        F
O              3.339459        7.715095        4.949249        F
O              3.339459        4.882336        4.949249        F
Al             3.393316        14.697002       6.011417        F
O              1.956477        14.697002       7.179493        F
O              3.339459        16.113380       4.949249        F
O              3.339459        13.280622       4.949249        F
H              3.439923        4.911172        10.243970       F
H              3.439232        7.689483        10.293373       F
H              6.818393        4.213072        13.048228       F
H              6.229200        4.955319        14.133904       F
H              3.439929        16.084518       10.243550       F
H              3.439218        13.306190       10.293977       F
H              6.776962        8.347647        14.909841       F
H              6.777013        12.648010       14.909830       F
H              6.229199        16.040400       14.133948       F
H              6.818394        16.782646       13.048228       F
H              4.227165        2.738070        7.166136        F
H              6.932392        2.747750        6.973661        F
H              7.409135        3.550965        5.707009        F
H              4.227165        18.257647       7.166137        F
H              6.932397        18.247959       6.973659        F
H              7.409131        17.444750       5.706962        F
H              7.521090        6.298716        1.832227        F
H              7.521091        14.697002       1.832228        F
H              3.346923        10.497859       14.197637       F
H              6.469066        10.497859       0.138110        F
H              0.036291        9.692187        9.043065        F
H              0.036295        11.303524       9.043066        F
H              2.008448        9.058198        12.145152       F
H              2.008447        11.937518       12.145155       F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.219808	7.636261	6.970744	R
O	4.801308	6.303463	7.130690	R
O	7.467648	6.292388	7.321294	R
O	6.209953	7.648321	5.036145	R
Al	7.414373	6.123792	9.202756	R
O	6.459579	7.475114	13.290003	R
O	7.645021	5.889909	10.930520	R
O	6.034925	4.859546	8.817810	R
O	6.056807	7.609796	8.918961	R
Al	7.285516	9.018544	4.866608	R
Al	7.255418	11.978678	4.840116	R
Al	6.241528	13.354919	6.974676	R
Al	6.365876	10.498391	7.102019	R
O	4.827466	14.704538	7.126937	R
O	4.965628	11.820951	7.268918	R
O	4.954478	9.202895	7.266049	R
O	7.533495	14.726949	7.421162	R
O	6.320171	10.496013	5.074067	R
O	7.565514	12.004720	6.682408	R
O	7.572495	9.031163	6.723473	R
O	6.203275	13.367637	5.049000	R
Al	7.263678	14.865342	9.239037	R
Al	7.965049	10.496834	10.416019	R
O	6.188813	10.503612	13.133559	R
O	6.478106	13.536786	13.290439	R
O	6.419372	10.517368	9.045799	R
O	7.706067	15.056589	10.904088	R
O	6.045496	13.405257	8.929167	R
O	6.002567	16.161542	8.826848	R
O	8.189358	9.132989	11.535882	R
O	8.155027	11.899604	11.501212	R
O	4.781823	6.116427	10.940304	R
O	4.826116	14.911606	10.924095	R
O	4.802579	9.097518	10.950309	R
O	4.792015	11.928059	10.957025	R
O	6.313034	4.947057	5.071803	R
O	6.340787	16.039563	5.088950	R
O	8.105644	9.091299	3.326485	R
O	8.054647	11.941516	3.293068	R
O	3.494938	10.506494	8.961964	R
Cu	8.910167	11.628292	7.956506	R
Cu	9.010958	9.006654	8.092321	R
O	9.390334	10.433422	9.272661	R
N	9.961543	7.368831	8.619301	R
N	11.379914	7.392802	8.460292	R
O	9.454135	6.313965	9.074538	R
O	11.926906	6.376379	8.812455	R

```
Model #35      Cartesian coordinates in angstrom
               x               y               z               Relaxed/Frozen
Al             4.718091        6.298715        9.025534        F
Al             6.299120        6.298715        11.957102       F
Al             4.718091        14.697002       9.025534        F
Al             4.828311        11.950763       9.158184        F
Al             4.828311        9.044955        9.158184        F
Al             7.260466        8.998624        12.959551       F
Al             7.260466        11.997093       12.959551       F
Al             6.299120        14.697002       11.957102       F
Al             4.636026        10.497859       12.053017       F
O              3.286788        10.497859       13.239718       F
Al             6.284430        4.911618        6.956078        F
Al             6.284430        16.084099       6.956078        F
Al             7.604152        10.497859       2.473791        F
O              6.427205        10.497859       1.094354        F
Al             6.373455        6.298715        3.886397        F
O              4.781442        6.298715        2.980335        F
Al             6.373455        14.697002       3.886397        F
O              4.781442        14.697002       2.980335        F
O              3.454035        4.977004        9.235301        F
O              3.454035        7.620427        9.235301        F
O              6.249989        5.002877        13.162247       F
O              3.454035        16.018713       9.235301        F
O              3.454035        13.375290       9.235301        F
O              7.425505        9.104843        14.776051       F
O              7.425505        11.890874       14.776051       F
O              6.249989        15.992841       13.162247       F
O              4.962264        3.365416        7.283451        F
O              7.499839        3.492587        6.705345        F
O              4.962264        17.630302       7.283451        F
O              7.499839        17.503130       6.705345        F
O              7.704784        6.298715        2.777154        F
O              7.704784        14.697002       2.777154        F
Al             3.478998        10.497859       7.046735        F
O              1.926548        11.807732       6.890259        F
O              1.926548        9.187985        6.890259        F
O              3.361122        10.497859       5.169014        F
Al             2.050923        10.497859       10.125656       F
O              0.574778        10.497859       9.076089        F
O              2.097749        9.088323        11.188759       F
O              2.097749        11.907395       11.188759       F
Al             3.393316        6.298715        6.011417        F
O              1.956477        6.298715        7.179493        F
O              3.339459        7.715095        4.949249        F
O              3.339459        4.882336        4.949249        F
Al             3.393316        14.697002       6.011417        F
O              1.956477        14.697002       7.179493        F
O              3.339459        16.113380       4.949249        F
O              3.339459        13.280622       4.949249        F
H              3.439923        4.911172        10.243970       F
H              3.439232        7.689483        10.293373       F
H              6.818393        4.213072        13.048228       F
H              6.229200        4.955319        14.133904       F
H              3.439929        16.084518       10.243550       F
H              3.439218        13.306190       10.293977       F
H              6.776962        8.347647        14.909841       F
H              6.777013        12.648010       14.909830       F
H              6.229199        16.040400       14.133948       F
H              6.818394        16.782646       13.048228       F
H              4.227165        2.738070        7.166136        F
H              6.932392        2.747750        6.973661        F
H              7.409135        3.550965        5.707009        F
H              4.227165        18.257647       7.166137        F
H              6.932397        18.247959       6.973659        F
H              7.409131        17.444750       5.706962        F
H              7.521090        6.298716        1.832227        F
H              7.521091        14.697002       1.832228        F
H              3.346923        10.497859       14.197637       F
H              6.469066        10.497859       0.138110        F
H              0.036291        9.692187        9.043065        F
H              0.036295        11.303524       9.043066        F
H              2.008448        9.058198        12.145152       F
H              2.008447        11.937518       12.145155       F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.225198	7.636932	6.972509	R
O	4.801663	6.303689	7.131067	R
O	7.467312	6.289503	7.323945	R
O	6.209181	7.647163	5.037228	R
Al	7.412189	6.122782	9.205509	R
O	6.459753	7.474650	13.290699	R
O	7.646975	5.889291	10.932483	R
O	6.033921	4.858034	8.819424	R
O	6.056817	7.609110	8.920759	R
Al	7.281939	9.019840	4.865337	R
Al	7.252624	11.977707	4.839392	R
Al	6.239330	13.354569	6.973739	R
Al	6.366178	10.497310	7.102139	R
O	4.826790	14.704845	7.127257	R
O	4.964401	11.821057	7.268912	R
O	4.954363	9.202588	7.266904	R
O	7.533157	14.726175	7.421233	R
O	6.315383	10.497176	5.072015	R
O	7.563390	12.004760	6.682742	R
O	7.572689	9.034578	6.718713	R
O	6.201988	13.368115	5.048943	R
Al	7.263232	14.865217	9.238981	R
Al	7.961380	10.490057	10.413824	R
O	6.188497	10.503274	13.134152	R
O	6.479013	13.537112	13.290521	R
O	6.415995	10.518648	9.046556	R
O	7.706158	15.055916	10.903968	R
O	6.045197	13.405275	8.929071	R
O	6.002536	16.161528	8.826808	R
O	8.188510	9.127357	11.534559	R
O	8.151694	11.893855	11.500086	R
O	4.782456	6.115973	10.940556	R
O	4.826228	14.911778	10.924030	R
O	4.802452	9.097385	10.950560	R
O	4.790259	11.928439	10.957276	R
O	6.313539	4.946193	5.071789	R
O	6.340563	16.039555	5.089217	R
O	8.101005	9.089785	3.324791	R
O	8.052700	11.942041	3.293036	R
O	3.493420	10.506231	8.961614	R
Cu	8.905742	11.644164	7.965177	R
Cu	9.066075	9.053503	8.041401	R
O	9.388672	10.442501	9.275088	R
N	9.919867	7.298108	8.483517	R
N	11.250491	7.236719	8.209558	R
O	9.461840	6.277895	9.064659	R
O	11.605771	8.270426	7.639403	R

```
Model #36      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043065       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.224931	7.636932	6.973476	R
O	4.802963	6.303308	7.131022	R
O	7.468207	6.288913	7.326070	R
O	6.213249	7.646701	5.038822	R
Al	7.407765	6.124839	9.207065	R
O	6.461185	7.474164	13.290310	R
O	7.648532	5.889148	10.932344	R
O	6.033718	4.857691	8.820071	R
O	6.057698	7.608420	8.922079	R
Al	7.286999	9.017856	4.864256	R
Al	7.257160	11.978553	4.840776	R
Al	6.239182	13.354649	6.974094	R
Al	6.368339	10.499719	7.102071	R
O	4.828035	14.705226	7.126890	R
O	4.967771	11.820416	7.269504	R
O	4.960619	9.202261	7.267159	R
O	7.533999	14.726340	7.421975	R
O	6.322712	10.495788	5.075742	R
O	7.566845	12.006608	6.684404	R
O	7.579410	9.031582	6.718748	R
O	6.204294	13.367279	5.048940	R
Al	7.263055	14.866154	9.239378	R
Al	7.965144	10.496042	10.417383	R
O	6.189074	10.503107	13.133535	R
O	6.477721	13.536596	13.290432	R
O	6.425259	10.518578	9.046398	R
O	7.706441	15.056065	10.904318	R
O	6.045554	13.405539	8.929599	R
O	6.002671	16.161912	8.826939	R
O	8.190511	9.130687	11.535562	R
O	8.157174	11.897880	11.504000	R
O	4.783901	6.115509	10.940277	R
O	4.826542	14.911855	10.924004	R
O	4.804152	9.096990	10.950828	R
O	4.792984	11.927772	10.957310	R
O	6.314668	4.946245	5.072017	R
O	6.341241	16.039205	5.089309	R
O	8.102645	9.088838	3.322579	R
O	8.055817	11.940611	3.293814	R
O	3.497870	10.505666	8.963158	R
Cu	8.908444	11.661436	7.972928	R
Cu	9.045061	9.083343	8.042392	R
O	9.397399	10.456151	9.281527	R
N	9.913880	7.335833	8.502617	R
N	11.240288	7.285943	8.201469	R
O	11.575311	8.314111	7.612517	R
O	9.462700	6.300698	9.056694	R

```
Model #37      Cartesian coordinates in angstrom
               x                y                z              Relaxed/Frozen
Al             4.718091         6.298715         9.025534       F
Al             6.299120         6.298715         11.957102      F
Al             4.718091         14.697002        9.025534       F
Al             4.828311         11.950763        9.158184       F
Al             4.828311         9.044955         9.158184       F
Al             7.260466         8.998624         12.959551      F
Al             7.260466         11.997093        12.959551      F
Al             6.299120         14.697002        11.957102      F
Al             4.636026         10.497859        12.053017      F
O              3.286788         10.497859        13.239718      F
Al             6.284430         4.911618         6.956078       F
Al             6.284430         16.084099        6.956078       F
Al             7.604152         10.497859        2.473791       F
O              6.427205         10.497859        1.094354       F
Al             6.373455         6.298715         3.886397       F
O              4.781442         6.298715         2.980335       F
Al             6.373455         14.697002        3.886397       F
O              4.781442         14.697002        2.980335       F
O              3.454035         4.977004         9.235301       F
O              3.454035         7.620427         9.235301       F
O              6.249989         5.002877         13.162247      F
O              3.454035         16.018713        9.235301       F
O              3.454035         13.375290        9.235301       F
O              7.425505         9.104843         14.776051      F
O              7.425505         11.890874        14.776051      F
O              6.249989         15.992841        13.162247      F
O              4.962264         3.365416         7.283451       F
O              7.499839         3.492587         6.705345       F
O              4.962264         17.630302        7.283451       F
O              7.499839         17.503130        6.705345       F
O              7.704784         6.298715         2.777154       F
O              7.704784         14.697002        2.777154       F
Al             3.478998         10.497859        7.046735       F
O              1.926548         11.807732        6.890259       F
O              1.926548         9.187985         6.890259       F
O              3.361122         10.497859        5.169014       F
Al             2.050923         10.497859        10.125656      F
O              0.574778         10.497859        9.076089       F
O              2.097749         9.088323         11.188759      F
O              2.097749         11.907395        11.188759      F
Al             3.393316         6.298715         6.011417       F
O              1.956477         6.298715         7.179493       F
O              3.339459         7.715095         4.949249       F
O              3.339459         4.882336         4.949249       F
Al             3.393316         14.697002        6.011417       F
O              1.956477         14.697002        7.179493       F
O              3.339459         16.113380        4.949249       F
O              3.339459         13.280622        4.949249       F
H              3.439923         4.911172         10.243970      F
H              3.439232         7.689483         10.293373      F
H              6.818393         4.213072         13.048228      F
H              6.229200         4.955319         14.133904      F
H              3.439929         16.084518        10.243550      F
H              3.439218         13.306190        10.293977      F
H              6.776962         8.347647         14.909841      F
H              6.777013         12.648010        14.909830      F
H              6.229199         16.040400        14.133948      F
H              6.818394         16.782646        13.048228      F
H              4.227165         2.738070         7.166136       F
H              6.932392         2.747750         6.973661       F
H              7.409135         3.550965         5.707009       F
H              4.227165         18.257647        7.166137       F
H              6.932397         18.247959        6.973659       F
H              7.409131         17.444750        5.706962       F
H              7.521090         6.298716         1.832227       F
H              7.521091         14.697002        1.832228       F
H              3.346923         10.497859        14.197637      F
H              6.469066         10.497859        0.138110       F
H              0.036291         9.692187         9.043065       F
H              0.036295         11.303524        9.043066       F
H              2.008448         9.058198         12.145152      F
H              2.008447         11.937518        12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.256122	7.649912	6.996930	R
O	4.832648	6.294335	7.128831	R
O	7.541673	6.271991	7.430682	R
O	6.248111	7.624148	5.075151	R
Al	7.265806	6.126999	9.246074	R
O	6.487077	7.456428	13.293294	R
O	7.708108	5.935534	10.910602	R
O	6.004261	4.834045	8.827775	R
O	6.048294	7.591011	8.941617	R
Al	7.281336	9.025513	4.884661	R
Al	7.281863	11.970381	4.884910	R
Al	6.255942	13.345648	6.996860	R
Al	6.396960	10.497857	7.154996	R
O	4.832675	14.701425	7.128787	R
O	4.978635	11.818213	7.270816	R
O	4.978612	9.177525	7.270810	R
O	7.541645	14.723601	7.430644	R
O	6.334757	10.498039	5.124726	R
O	7.600794	11.975012	6.757837	R
O	7.600775	9.020506	6.757625	R
O	6.248387	13.371575	5.075161	R
Al	7.265773	14.868713	9.246025	R
Al	7.851239	10.497982	10.331118	R
O	6.181710	10.497851	13.151008	R
O	6.486951	13.539229	13.293251	R
O	6.303324	10.497882	9.074885	R
O	7.708092	15.060182	10.910568	R
O	6.048289	13.404690	8.941601	R
O	6.004270	16.161671	8.827765	R
O	8.111930	9.130807	11.472788	R
O	8.112330	11.864861	11.473058	R
O	4.826357	6.083192	10.925751	R
O	4.826389	14.912471	10.925723	R
O	4.788448	9.068985	10.963641	R
O	4.788645	11.926801	10.963701	R
O	6.336822	4.955099	5.088371	R
O	6.336841	16.040604	5.088363	R
O	8.063284	9.075244	3.325615	R
O	8.063647	11.920302	3.325753	R
O	3.494029	10.497925	8.963995	R
Cu	9.359839	11.824387	7.664149	R
Cu	9.359967	9.172485	7.663662	R
O	9.067558	10.498247	8.995118	R
O	11.194067	9.142800	7.378292	R
O	11.193370	11.855377	7.376155	R
N	11.935922	9.877794	6.555488	R
N	11.935652	11.119571	6.554606	R

```
Model #38      Cartesian coordinates in angstrom
                x              y              z              Relaxed/Frozen
Al              4.718091       6.298715       9.025534       F
Al              6.299120       6.298715       11.957102      F
Al              4.718091       14.697002      9.025534       F
Al              4.828311       11.950763      9.158184       F
Al              4.828311       9.044955       9.158184       F
Al              7.260466       8.998624       12.959551      F
Al              7.260466       11.997093      12.959551      F
Al              6.299120       14.697002      11.957102      F
Al              4.636026       10.497859      12.053017      F
O               3.286788       10.497859      13.239718      F
Al              6.284430       4.911618       6.956078       F
Al              6.284430       16.084099      6.956078       F
Al              7.604152       10.497859      2.473791       F
O               6.427205       10.497859      1.094354       F
Al              6.373455       6.298715       3.886397       F
O               4.781442       6.298715       2.980335       F
Al              6.373455       14.697002      3.886397       F
O               4.781442       14.697002      2.980335       F
O               3.454035       4.977004       9.235301       F
O               3.454035       7.620427       9.235301       F
O               6.249989       5.002877       13.162247      F
O               3.454035       16.018713      9.235301       F
O               3.454035       13.375290      9.235301       F
O               7.425505       9.104843       14.776051      F
O               7.425505       11.890874      14.776051      F
O               6.249989       15.992841      13.162247      F
O               4.962264       3.365416       7.283451       F
O               7.499839       3.492587       6.705345       F
O               4.962264       17.630302      7.283451       F
O               7.499839       17.503130      6.705345       F
O               7.704784       6.298715       2.777154       F
O               7.704784       14.697002      2.777154       F
Al              3.478998       10.497859      7.046735       F
O               1.926548       11.807732      6.890259       F
O               1.926548       9.187985       6.890259       F
O               3.361122       10.497859      5.169014       F
Al              2.050923       10.497859      10.125656      F
O               0.574778       10.497859      9.076089       F
O               2.097749       9.088323       11.188759      F
O               2.097749       11.907395      11.188759      F
Al              3.393316       6.298715       6.011417       F
O               1.956477       6.298715       7.179493       F
O               3.339459       7.715095       4.949249       F
O               3.339459       4.882336       4.949249       F
Al              3.393316       14.697002      6.011417       F
O               1.956477       14.697002      7.179493       F
O               3.339459       16.113380      4.949249       F
O               3.339459       13.280622      4.949249       F
H               3.439923       4.911172       10.243970      F
H               3.439232       7.689483       10.293373      F
H               6.818393       4.213072       13.048228      F
H               6.229200       4.955319       14.133904      F
H               3.439929       16.084518      10.243550      F
H               3.439218       13.306190      10.293977      F
H               6.776962       8.347647       14.909841      F
H               6.777013       12.648010      14.909830      F
H               6.229199       16.040400      14.133948      F
H               6.818394       16.782646      13.048228      F
H               4.227165       2.738070       7.166136       F
H               6.932392       2.747750       6.973661       F
H               7.409135       3.550965       5.707009       F
H               4.227165       18.257647      7.166137       F
H               6.932397       18.247959      6.973659       F
H               7.409131       17.444750      5.706962       F
H               7.521090       6.298716       1.832227       F
H               7.521091       14.697002      1.832228       F
H               3.346923       10.497859      14.197637      F
H               6.469066       10.497859      0.138110       F
H               0.036291       9.692187       9.043065       F
H               0.036295       11.303524      9.043066       F
H               2.008448       9.058198       12.145152      F
H               2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.255500	7.649786	6.996990	R
O	4.832528	6.294195	7.128931	R
O	7.541328	6.272308	7.430646	R
O	6.246492	7.624305	5.075182	R
Al	7.265884	6.126997	9.246063	R
O	6.486669	7.456575	13.293298	R
O	7.707971	5.935344	10.910610	R
O	6.004274	4.834106	8.827792	R
O	6.048185	7.591298	8.941657	R
Al	7.278839	9.026058	4.884303	R
Al	7.283170	11.970271	4.885507	R
Al	6.255976	13.345446	6.997449	R
Al	6.397112	10.497656	7.154888	R
O	4.832672	14.701257	7.128745	R
O	4.979067	11.817838	7.271296	R
O	4.978375	9.178019	7.271452	R
O	7.541339	14.723501	7.430576	R
O	6.333634	10.499217	5.124552	R
O	7.601290	11.973654	6.758675	R
O	7.599040	9.021005	6.757633	R
O	6.249782	13.371669	5.075811	R
Al	7.266091	14.868321	9.245873	R
Al	7.850891	10.496984	10.331139	R
O	6.181780	10.497858	13.150867	R
O	6.487108	13.539206	13.293121	R
O	6.306289	10.498067	9.075536	R
O	7.708047	15.059907	10.910533	R
O	6.048182	13.404487	8.941845	R
O	6.004247	16.161397	8.827883	R
O	8.111301	9.129642	11.472335	R
O	8.112736	11.863527	11.473263	R
O	4.826252	6.083380	10.925743	R
O	4.826212	14.912222	10.925878	R
O	4.788592	9.069337	10.963375	R
O	4.789145	11.926614	10.963599	R
O	6.336841	4.955244	5.088464	R
O	6.336514	16.040723	5.088321	R
O	8.061247	9.074681	3.325561	R
O	8.064540	11.919859	3.326092	R
O	3.494435	10.498247	8.964159	R
Cu	9.361635	11.813601	7.660609	R
Cu	9.357484	9.169181	7.665367	R
O	9.078529	10.494474	9.002619	R
O	11.190968	9.126257	7.372909	R
O	11.194711	11.839610	7.361421	R
N	11.930849	9.857569	6.546376	R
N	11.932399	11.099347	6.541118	R

```
Model #39      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043065       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.208867	7.643025	6.982891	R
O	4.803229	6.297033	7.130739	R
O	7.468888	6.308103	7.327063	R
O	6.238530	7.648570	5.050154	R
Al	7.428428	6.065597	9.211757	R
O	6.454715	7.475399	13.294177	R
O	7.651425	5.887474	10.945016	R
O	6.038999	4.848158	8.816272	R
O	6.053567	7.606182	8.922920	R
Al	7.311358	9.020668	4.883515	R
Al	7.251565	11.978686	4.845082	R
Al	6.242034	13.356802	6.976068	R
Al	6.369258	10.504134	7.113171	R
O	4.828119	14.706328	7.127015	R
O	4.966805	11.822401	7.267464	R
O	4.959595	9.199009	7.261436	R
O	7.533120	14.729517	7.420592	R
O	6.332971	10.486712	5.089626	R
O	7.566636	12.011431	6.685951	R
O	7.594197	9.052638	6.763813	R
O	6.199643	13.367185	5.048763	R
Al	7.263954	14.862822	9.237967	R
Al	7.892614	10.443048	10.378623	R
O	6.186923	10.503852	13.139215	R
O	6.494437	13.540600	13.289293	R
O	6.374154	10.514813	9.052789	R
O	7.708897	15.047735	10.903768	R
O	6.045437	13.405567	8.929790	R
O	6.003459	16.161705	8.828518	R
O	8.158863	9.094746	11.512016	R
O	8.136708	11.840468	11.481948	R
O	4.786109	6.107532	10.937197	R
O	4.826860	14.913108	10.925894	R
O	4.804354	9.096003	10.953144	R
O	4.791144	11.931072	10.960470	R
O	6.314283	4.948655	5.073293	R
O	6.342481	16.039733	5.088501	R
O	8.121041	9.099454	3.336319	R
O	8.045104	11.943734	3.293894	R
O	3.495683	10.504375	8.962473	R
Cu	8.933331	11.590926	7.929529	R
Cu	9.014801	8.689835	8.077285	R
O	9.245834	10.242930	9.145634	R
O	10.130480	7.122452	8.503085	R
N	9.518911	6.151820	9.040551	R
N	10.324134	5.084139	9.491819	R
O	11.514779	5.279024	9.379601	R

```
Model #40      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043065       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.191235	7.647763	6.977069	R
O	4.809865	6.293232	7.128626	R
O	7.495868	6.333083	7.340724	R
O	6.229045	7.646162	5.049465	R
Al	7.425132	6.064294	9.226746	R
O	6.450592	7.474462	13.295694	R
O	7.646242	5.856579	10.953334	R
O	6.047168	4.852241	8.808309	R
O	6.055384	7.604798	8.921770	R
Al	7.290298	9.025185	4.870934	R
Al	7.262830	11.980039	4.848601	R
Al	6.249239	13.357592	6.977917	R
Al	6.361890	10.510675	7.111416	R
O	4.830471	14.705877	7.127046	R
O	4.971401	11.822261	7.267943	R
O	4.960694	9.195842	7.259804	R
O	7.534211	14.731471	7.420205	R
O	6.327199	10.494418	5.083830	R
O	7.574622	12.006186	6.688736	R
O	7.577627	9.054590	6.748540	R
O	6.210084	13.367460	5.050910	R
Al	7.265296	14.861562	9.237105	R
Al	7.904409	10.398914	10.368976	R
O	6.186683	10.503096	13.141459	R
O	6.501997	13.541666	13.286580	R
O	6.376727	10.504232	9.049770	R
O	7.710479	15.040452	10.904165	R
O	6.046608	13.404753	8.930575	R
O	6.004493	16.161394	8.829897	R
O	8.144493	9.049577	11.502847	R
O	8.145811	11.794044	11.486538	R
O	4.790615	6.104518	10.931409	R
O	4.827273	14.913175	10.927040	R
O	4.805256	9.092528	10.953938	R
O	4.795530	11.930940	10.961263	R
O	6.323985	4.953919	5.079935	R
O	6.342231	16.040372	5.087756	R
O	8.105425	9.089434	3.328981	R
O	8.060236	11.935288	3.299273	R
O	3.502401	10.503798	8.965383	R
Cu	8.931777	11.467538	7.902855	R
Cu	8.913282	8.555852	8.051905	R
O	9.250927	10.124530	9.127066	R
O	10.153079	7.278088	8.839302	R
N	9.534706	6.204126	9.136028	R
N	10.327815	5.110973	9.516006	R
O	11.523380	5.318371	9.483058	R

```
Model #41      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043065       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.240464	7.632645	7.012044	R
O	4.802995	6.296231	7.127673	R
O	7.466966	6.270230	7.331222	R
O	6.258238	7.642678	5.063997	R
Al	7.491116	5.941663	9.210972	R
O	6.461708	7.477548	13.292100	R
O	7.675668	5.938709	10.960615	R
O	6.014255	4.836090	8.825910	R
O	6.035832	7.614141	8.918464	R
Al	7.327274	9.016057	4.900206	R
Al	7.237220	11.974935	4.841149	R
Al	6.226218	13.353833	6.971581	R
Al	6.374763	10.501059	7.115921	R
O	4.826387	14.708944	7.126731	R
O	4.959669	11.830113	7.267409	R
O	4.956935	9.215716	7.260951	R
O	7.536915	14.722258	7.424017	R
O	6.334950	10.478603	5.094099	R
O	7.551889	12.013506	6.685115	R
O	7.613894	9.054526	6.779606	R
O	6.187787	13.367329	5.045654	R
Al	7.259771	14.867700	9.242834	R
Al	7.865047	10.528621	10.392461	R
O	6.187006	10.506343	13.137770	R
O	6.482179	13.541186	13.296544	R
O	6.375845	10.537182	9.055345	R
O	7.706233	15.068911	10.905016	R
O	6.044951	13.408231	8.929349	R
O	6.002705	16.162725	8.824532	R
O	8.190251	9.197238	11.538701	R
O	8.103479	11.938876	11.463652	R
O	4.779935	6.106175	10.949211	R
O	4.828069	14.914473	10.922305	R
O	4.805146	9.103957	10.952918	R
O	4.787951	11.932927	10.959344	R
O	6.308473	4.944157	5.065492	R
O	6.344553	16.038395	5.090149	R
O	8.133672	9.111089	3.347695	R
O	8.026443	11.952834	3.288494	R
O	3.488114	10.508799	8.960247	R
Cu	8.929125	11.876434	7.988185	R
Cu	9.126002	8.962843	8.094488	R
O	9.231403	10.493012	9.166365	R
O	10.323657	7.329328	8.271380	R
N	9.573935	6.445321	8.767093	R
N	10.059810	5.201688	8.760317	R
O	9.070361	4.461182	9.045051	R

```
Model #42      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043065       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.226645	7.633442	7.009725	R
O	4.804788	6.293635	7.126501	R
O	7.479674	6.281582	7.338730	R
O	6.248623	7.640460	5.064344	R
Al	7.488051	5.938013	9.214642	R
O	6.454746	7.477896	13.293125	R
O	7.668429	5.909612	10.964645	R
O	6.016973	4.836095	8.820870	R
O	6.036363	7.613166	8.916371	R
Al	7.305250	9.020926	4.889081	R
Al	7.242403	11.977912	4.841332	R
Al	6.234911	13.357480	6.973670	R
Al	6.361087	10.507519	7.112722	R
O	4.825428	14.708221	7.126722	R
O	4.957113	11.829662	7.266636	R
O	4.950639	9.211991	7.257681	R
O	7.532069	14.727919	7.419541	R
O	6.325499	10.486082	5.086768	R
O	7.554939	12.014234	6.680956	R
O	7.593177	9.059091	6.769233	R
O	6.190107	13.367302	5.045082	R
Al	7.263442	14.863423	9.238713	R
Al	7.906956	10.483346	10.388568	R
O	6.186706	10.505745	13.137757	R
O	6.487029	13.540567	13.292198	R
O	6.379663	10.525747	9.050750	R
O	7.706332	15.058355	10.903525	R
O	6.044407	13.406734	8.928333	R
O	6.002562	16.161596	8.826542	R
O	8.183793	9.144399	11.533237	R
O	8.127190	11.889927	11.476402	R
O	4.781466	6.105691	10.944691	R
O	4.826273	14.913554	10.924326	R
O	4.799046	9.101794	10.952021	R
O	4.785713	11.932642	10.958728	R
O	6.312671	4.946385	5.068416	R
O	6.342011	16.039622	5.088469	R
O	8.117993	9.101806	3.341951	R
O	8.038918	11.946321	3.291930	R
O	3.486974	10.508138	8.958569	R
Cu	8.916842	11.673360	7.952097	R
Cu	9.037159	8.822916	8.076414	R
O	9.288496	10.358488	9.184937	R
O	10.392881	7.433172	8.681118	R
N	9.590429	6.498662	8.962370	R
N	10.099536	5.267005	8.975408	R
O	9.097769	4.495632	9.081872	R

```
Model #43      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043066       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.166563	7.653426	6.954002	R
O	4.804156	6.298081	7.125184	R
O	7.483688	6.348037	7.312982	R
O	6.207304	7.653956	5.030797	R
Al	7.439021	6.155058	9.240804	R
O	6.455655	7.471437	13.299368	R
O	7.631925	5.805644	10.956865	R
O	6.057224	4.882022	8.803842	R
O	6.050825	7.616105	8.914943	R
Al	7.280042	9.027247	4.858941	R
Al	7.270594	11.980431	4.847560	R
Al	6.255534	13.355242	6.979272	R
Al	6.359367	10.510212	7.103965	R
O	4.831366	14.706064	7.126938	R
O	4.972171	11.823866	7.266467	R
O	4.954215	9.197856	7.254510	R
O	7.534483	14.733099	7.419968	R
O	6.321371	10.501851	5.067347	R
O	7.581049	12.000229	6.688775	R
O	7.567311	9.057848	6.723205	R
O	6.218549	13.368970	5.052776	R
Al	7.266026	14.859940	9.236345	R
Al	7.907544	10.369762	10.362301	R
O	6.185087	10.502974	13.145125	R
O	6.508055	13.543191	13.286079	R
O	6.369276	10.501442	9.046804	R
O	7.711310	15.037036	10.904366	R
O	6.046909	13.405275	8.931593	R
O	6.005036	16.161886	8.830997	R
O	8.135864	9.025275	11.503225	R
O	8.149616	11.765574	11.489176	R
O	4.784975	6.118906	10.933128	R
O	4.826937	14.914743	10.928532	R
O	4.807155	9.094226	10.954382	R
O	4.794607	11.933204	10.962736	R
O	6.322613	4.951944	5.077808	R
O	6.341690	16.042606	5.086472	R
O	8.102953	9.084882	3.320884	R
O	8.070529	11.933517	3.298218	R
O	3.501751	10.504437	8.965588	R
Cu	8.928771	11.359397	7.871430	R
Cu	8.780017	8.427904	8.106861	R
O	9.221240	10.014931	9.109111	R
O	9.258201	6.829286	9.026986	R
N	10.458380	6.023397	10.886604	R
O	10.493570	4.831253	11.044334	R
N	10.194789	7.048851	10.383715	R

```
Model #44        Cartesian coordinates in angstrom
                 x               y               z               Relaxed/Frozen
Al      4.718091        6.298715        9.025534        F
Al      6.299120        6.298715        11.957102       F
Al      4.718091        14.697002       9.025534        F
Al      4.828311        11.950763       9.158184        F
Al      4.828311        9.044955        9.158184        F
Al      7.260466        8.998624        12.959551       F
Al      7.260466        11.997093       12.959551       F
Al      6.299120        14.697002       11.957102       F
Al      4.636026        10.497859       12.053017       F
O       3.286788        10.497859       13.239718       F
Al      6.284430        4.911618        6.956078        F
Al      6.284430        16.084099       6.956078        F
Al      7.604152        10.497859       2.473791        F
O       6.427205        10.497859       1.094354        F
Al      6.373455        6.298715        3.886397        F
O       4.781442        6.298715        2.980335        F
Al      6.373455        14.697002       3.886397        F
O       4.781442        14.697002       2.980335        F
O       3.454035        4.977004        9.235301        F
O       3.454035        7.620427        9.235301        F
O       6.249989        5.002877        13.162247       F
O       3.454035        16.018713       9.235301        F
O       3.454035        13.375290       9.235301        F
O       7.425505        9.104843        14.776051       F
O       7.425505        11.890874       14.776051       F
O       6.249989        15.992841       13.162247       F
O       4.962264        3.365416        7.283451        F
O       7.499839        3.492587        6.705345        F
O       4.962264        17.630302       7.283451        F
O       7.499839        17.503130       6.705345        F
O       7.704784        6.298715        2.777154        F
O       7.704784        14.697002       2.777154        F
Al      3.478998        10.497859       7.046735        F
O       1.926548        11.807732       6.890259        F
O       1.926548        9.187985        6.890259        F
O       3.361122        10.497859       5.169014        F
Al      2.050923        10.497859       10.125656       F
O       0.574778        10.497859       9.076089        F
O       2.097749        9.088323        11.188759       F
O       2.097749        11.907395       11.188759       F
Al      3.393316        6.298715        6.011417        F
O       1.956477        6.298715        7.179493        F
O       3.339459        7.715095        4.949249        F
O       3.339459        4.882336        4.949249        F
Al      3.393316        14.697002       6.011417        F
O       1.956477        14.697002       7.179493        F
O       3.339459        16.113380       4.949249        F
O       3.339459        13.280622       4.949249        F
H       3.439923        4.911172        10.243970       F
H       3.439232        7.689483        10.293373       F
H       6.818393        4.213072        13.048228       F
H       6.229200        4.955319        14.133904       F
H       3.439929        16.084518       10.243550       F
H       3.439218        13.306190       10.293977       F
H       6.776962        8.347647        14.909841       F
H       6.777013        12.648010       14.909830       F
H       6.229199        16.040400       14.133948       F
H       6.818394        16.782646       13.048228       F
H       4.227165        2.738070        7.166136        F
H       6.932392        2.747750        6.973661        F
H       7.409135        3.550965        5.707009        F
H       4.227165        18.257647       7.166137        F
H       6.932397        18.247959       6.973659        F
H       7.409131        17.444750       5.706962        F
H       7.521090        6.298716        1.832227        F
H       7.521091        14.697002       1.832228        F
H       3.346923        10.497859       14.197637       F
H       6.469066        10.497859       0.138110        F
H       0.036291        9.692187        9.043065        F
H       0.036295        11.303524       9.043066        F
H       2.008448        9.058198        12.145152       F
H       2.008447        11.937518       12.145155       F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.163066	7.654003	6.954218	R
O	4.805052	6.298452	7.124062	R
O	7.490103	6.353725	7.318124	R
O	6.201430	7.652503	5.030391	R
Al	7.446766	6.151282	9.251970	R
O	6.451780	7.474413	13.296301	R
O	7.619293	5.774531	10.960133	R
O	6.057811	4.883148	8.800611	R
O	6.050714	7.617308	8.914621	R
Al	7.269023	9.028559	4.852886	R
Al	7.274750	11.980830	4.848152	R
Al	6.257551	13.355425	6.979871	R
Al	6.355087	10.512855	7.100474	R
O	4.831743	14.705912	7.126733	R
O	4.971072	11.825242	7.265815	R
O	4.951881	9.198670	7.253640	R
O	7.534961	14.733205	7.420229	R
O	6.316617	10.506505	5.061634	R
O	7.582416	11.996855	6.690634	R
O	7.557302	9.061493	6.713798	R
O	6.222758	13.369384	5.053683	R
Al	7.266373	14.859957	9.236737	R
Al	7.898427	10.369590	10.359604	R
O	6.185299	10.503252	13.144964	R
O	6.508728	13.543641	13.286851	R
O	6.366642	10.501408	9.044756	R
O	7.711155	15.038492	10.904704	R
O	6.047129	13.405091	8.931582	R
O	6.005033	16.161719	8.830937	R
O	8.149616	9.036144	11.511375	R
O	8.140833	11.770216	11.481655	R
O	4.780079	6.124109	10.933181	R
O	4.826841	14.914540	10.928539	R
O	4.811591	9.095958	10.954199	R
O	4.793993	11.933323	10.962607	R
O	6.325672	4.952743	5.079245	R
O	6.341236	16.042798	5.086328	R
O	8.094858	9.080597	3.317219	R
O	8.077018	11.930678	3.299889	R
O	3.501650	10.504583	8.965759	R
Cu	8.931441	11.343463	7.871280	R
Cu	8.756065	8.416978	8.086223	R
O	9.210916	9.992192	9.110100	R
N	10.168564	7.056254	10.436906	R
N	11.163593	7.615054	10.168802	R
O	11.981166	8.156541	9.470629	R
O	9.253486	6.857167	9.039787	R

```
Model #45        Cartesian coordinates in angstrom
                 x              y              z              Relaxed/Frozen
Al               4.718091       6.298715       9.025534       F
Al               6.299120       6.298715       11.957102      F
Al               4.718091       14.697002      9.025534       F
Al               4.828311       11.950763      9.158184       F
Al               4.828311       9.044955       9.158184       F
Al               7.260466       8.998624       12.959551      F
Al               7.260466       11.997093      12.959551      F
Al               6.299120       14.697002      11.957102      F
Al               4.636026       10.497859      12.053017      F
O                3.286788       10.497859      13.239718      F
Al               6.284430       4.911618       6.956078       F
Al               6.284430       16.084099      6.956078       F
Al               7.604152       10.497859      2.473791       F
O                6.427205       10.497859      1.094354       F
Al               6.373455       6.298715       3.886397       F
O                4.781442       6.298715       2.980335       F
Al               6.373455       14.697002      3.886397       F
O                4.781442       14.697002      2.980335       F
O                3.454035       4.977004       9.235301       F
O                3.454035       7.620427       9.235301       F
O                6.249989       5.002877       13.162247      F
O                3.454035       16.018713      9.235301       F
O                3.454035       13.375290      9.235301       F
O                7.425505       9.104843       14.776051      F
O                7.425505       11.890874      14.776051      F
O                6.249989       15.992841      13.162247      F
O                4.962264       3.365416       7.283451       F
O                7.499839       3.492587       6.705345       F
O                4.962264       17.630302      7.283451       F
O                7.499839       17.503130      6.705345       F
O                7.704784       6.298715       2.777154       F
O                7.704784       14.697002      2.777154       F
Al               3.478998       10.497859      7.046735       F
O                1.926548       11.807732      6.890259       F
O                1.926548       9.187985       6.890259       F
O                3.361122       10.497859      5.169014       F
Al               2.050923       10.497859      10.125656      F
O                0.574778       10.497859      9.076089       F
O                2.097749       9.088323       11.188759      F
O                2.097749       11.907395      11.188759      F
Al               3.393316       6.298715       6.011417       F
O                1.956477       6.298715       7.179493       F
O                3.339459       7.715095       4.949249       F
O                3.339459       4.882336       4.949249       F
Al               3.393316       14.697002      6.011417       F
O                1.956477       14.697002      7.179493       F
O                3.339459       16.113380      4.949249       F
O                3.339459       13.280622      4.949249       F
H                3.439923       4.911172       10.243970      F
H                3.439232       7.689483       10.293373      F
H                6.818393       4.213072       13.048228      F
H                6.229200       4.955319       14.133904      F
H                3.439929       16.084518      10.243550      F
H                3.439218       13.306190      10.293977      F
H                6.776962       8.347647       14.909841      F
H                6.777013       12.648010      14.909830      F
H                6.229199       16.040400      14.133948      F
H                6.818394       16.782646      13.048228      F
H                4.227165       2.738070       7.166136       F
H                6.932392       2.747750       6.973661       F
H                7.409135       3.550965       5.707009       F
H                4.227165       18.257647      7.166137       F
H                6.932397       18.247959      6.973659       F
H                7.409131       17.444750      5.706962       F
H                7.521090       6.298716       1.832227       F
H                7.521091       14.697002      1.832228       F
H                3.346923       10.497859      14.197637      F
H                6.469066       10.497859      0.138110       F
H                0.036291       9.692187       9.043065       F
H                0.036295       11.303524      9.043066       F
H                2.008448       9.058198       12.145152      F
H                2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.164033	7.652509	6.955344	R
O	4.803219	6.298258	7.124907	R
O	7.484475	6.350105	7.315752	R
O	6.205188	7.652931	5.030955	R
Al	7.451944	6.148216	9.245209	R
O	6.457165	7.472759	13.297130	R
O	7.619882	5.778460	10.959504	R
O	6.057091	4.881639	8.802430	R
O	6.050003	7.617761	8.915022	R
Al	7.275906	9.026866	4.856792	R
Al	7.273458	11.980581	4.847743	R
Al	6.256950	13.355574	6.979309	R
Al	6.356912	10.511798	7.100735	R
O	4.831592	14.705930	7.126878	R
O	4.971700	11.824907	7.266224	R
O	4.953066	9.199557	7.253859	R
O	7.534849	14.733328	7.420186	R
O	6.320376	10.503746	5.064590	R
O	7.581939	11.998821	6.689998	R
O	7.563269	9.060279	6.719327	R
O	6.221047	13.369012	5.053160	R
Al	7.266239	14.860006	9.236645	R
Al	7.893730	10.373631	10.359157	R
O	6.186779	10.502006	13.143488	R
O	6.507911	13.543039	13.286599	R
O	6.367511	10.502732	9.045935	R
O	7.711231	15.037476	10.904676	R
O	6.047128	13.405183	8.931698	R
O	6.005030	16.161791	8.831050	R
O	8.147474	9.030540	11.506253	R
O	8.139459	11.768194	11.482967	R
O	4.779391	6.124881	10.935001	R
O	4.826821	14.914530	10.928607	R
O	4.813969	9.096591	10.954896	R
O	4.794583	11.933290	10.962939	R
O	6.323356	4.951304	5.077328	R
O	6.341436	16.042605	5.086477	R
O	8.100594	9.083661	3.319865	R
O	8.073525	11.932669	3.298401	R
O	3.502015	10.504542	8.966315	R
Cu	8.931690	11.354970	7.872503	R
Cu	8.758852	8.423098	8.104392	R
O	9.210228	10.004655	9.112400	R
O	9.251814	6.872648	9.067959	R
N	10.139043	6.882782	10.461443	R
N	10.639117	7.931097	10.634139	R
O	11.341341	8.734782	11.183950	R

```
Model #46        Cartesian coordinates in angstrom
                 x               y               z               Relaxed/Frozen
Al      4.718091        6.298715        9.025534        F
Al      6.299120        6.298715        11.957102       F
Al      4.718091        14.697002       9.025534        F
Al      4.828311        11.950763       9.158184        F
Al      4.828311        9.044955        9.158184        F
Al      7.260466        8.998624        12.959551       F
Al      7.260466        11.997093       12.959551       F
Al      6.299120        14.697002       11.957102       F
Al      4.636026        10.497859       12.053017       F
O       3.286788        10.497859       13.239718       F
Al      6.284430        4.911618        6.956078        F
Al      6.284430        16.084099       6.956078        F
Al      7.604152        10.497859       2.473791        F
O       6.427205        10.497859       1.094354        F
Al      6.373455        6.298715        3.886397        F
O       4.781442        6.298715        2.980335        F
Al      6.373455        14.697002       3.886397        F
O       4.781442        14.697002       2.980335        F
O       3.454035        4.977004        9.235301        F
O       3.454035        7.620427        9.235301        F
O       6.249989        5.002877        13.162247       F
O       3.454035        16.018713       9.235301        F
O       3.454035        13.375290       9.235301        F
O       7.425505        9.104843        14.776051       F
O       7.425505        11.890874       14.776051       F
O       6.249989        15.992841       13.162247       F
O       4.962264        3.365416        7.283451        F
O       7.499839        3.492587        6.705345        F
O       4.962264        17.630302       7.283451        F
O       7.499839        17.503130       6.705345        F
O       7.704784        6.298715        2.777154        F
O       7.704784        14.697002       2.777154        F
Al      3.478998        10.497859       7.046735        F
O       1.926548        11.807732       6.890259        F
O       1.926548        9.187985        6.890259        F
O       3.361122        10.497859       5.169014        F
Al      2.050923        10.497859       10.125656       F
O       0.574778        10.497859       9.076089        F
O       2.097749        9.088323        11.188759       F
O       2.097749        11.907395       11.188759       F
Al      3.393316        6.298715        6.011417        F
O       1.956477        6.298715        7.179493        F
O       3.339459        7.715095        4.949249        F
O       3.339459        4.882336        4.949249        F
Al      3.393316        14.697002       6.011417        F
O       1.956477        14.697002       7.179493        F
O       3.339459        16.113380       4.949249        F
O       3.339459        13.280622       4.949249        F
H       3.439923        4.911172        10.243970       F
H       3.439232        7.689483        10.293373       F
H       6.818393        4.213072        13.048228       F
H       6.229200        4.955319        14.133904       F
H       3.439929        16.084518       10.243550       F
H       3.439218        13.306190       10.293977       F
H       6.776962        8.347647        14.909841       F
H       6.777013        12.648010       14.909830       F
H       6.229199        16.040400       14.133948       F
H       6.818394        16.782646       13.048228       F
H       4.227165        2.738070        7.166136        F
H       6.932392        2.747750        6.973661        F
H       7.409135        3.550965        5.707009        F
H       4.227165        18.257647       7.166137        F
H       6.932397        18.247959       6.973659        F
H       7.409131        17.444750       5.706962        F
H       7.521090        6.298716        1.832227        F
H       7.521091        14.697002       1.832228        F
H       3.346923        10.497859       14.197637       F
H       6.469066        10.497859       0.138110        F
H       0.036291        9.692187        9.043065        F
H       0.036295        11.303524       9.043066        F
H       2.008448        9.058198        12.145152       F
H       2.008447        11.937518       12.145155       F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.183161	7.645911	6.958218	R
O	4.805291	6.301628	7.125404	R
O	7.485524	6.316682	7.315968	R
O	6.228231	7.652154	5.038291	R
Al	7.435127	6.156562	9.224411	R
O	6.457347	7.471953	13.295543	R
O	7.634440	5.820327	10.942855	R
O	6.048860	4.878135	8.807983	R
O	6.058113	7.614580	8.914033	R
Al	7.302756	9.025753	4.871913	R
Al	7.263662	11.980337	4.845867	R
Al	6.252044	13.356049	6.978320	R
Al	6.361440	10.508737	7.106116	R
O	4.830746	14.706054	7.126991	R
O	4.972363	11.822721	7.267126	R
O	4.958001	9.197417	7.258410	R
O	7.534028	14.732667	7.420210	R
O	6.330788	10.493134	5.075530	R
O	7.576725	12.004798	6.685499	R
O	7.577143	9.054541	6.745739	R
O	6.210923	13.368122	5.051003	R
Al	7.265538	14.861503	9.237092	R
Al	7.908200	10.415736	10.378873	R
O	6.186179	10.503844	13.142502	R
O	6.500191	13.541742	13.288035	R
O	6.376812	10.505243	9.050270	R
O	7.709818	15.043525	10.904461	R
O	6.046792	13.405339	8.931379	R
O	6.004211	16.162098	8.830203	R
O	8.145052	9.065233	11.509763	R
O	8.150448	11.812152	11.488944	R
O	4.784874	6.119509	10.935174	R
O	4.826586	14.913657	10.927625	R
O	4.807154	9.093131	10.953941	R
O	4.796575	11.931561	10.962141	R
O	6.319221	4.949852	5.074396	R
O	6.342411	16.041816	5.086931	R
O	8.116092	9.092096	3.327568	R
O	8.059134	11.938621	3.294753	R
O	3.502182	10.504627	8.966145	R
Cu	8.930983	11.424460	7.884139	R
Cu	8.767715	8.516159	8.202795	R
O	9.245290	10.111076	9.144707	R
N	10.338088	6.424677	8.066709	R
N	10.457880	5.255685	8.103255	R
O	10.225023	4.167043	8.566058	R
O	9.266180	6.969724	9.246510	R

```
Model #47      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043066       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.219040	7.636966	6.970099	R
O	4.798082	6.310520	7.129913	R
O	7.449677	6.272986	7.283476	R
O	6.267001	7.656752	5.045074	R
Al	7.442542	6.174967	9.187762	R
O	6.478525	7.469768	13.292437	R
O	7.644328	5.882869	10.922535	R
O	6.041602	4.873190	8.818154	R
O	6.062063	7.615695	8.918585	R
Al	7.372283	9.011720	4.916111	R
Al	7.245138	11.975435	4.845490	R
Al	6.236422	13.353068	6.976651	R
Al	6.389079	10.495655	7.121314	R
O	4.829255	14.706850	7.127791	R
O	4.977310	11.820757	7.270611	R
O	4.969274	9.205296	7.270215	R
O	7.535743	14.728360	7.424154	R
O	6.367072	10.465582	5.112464	R
O	7.569097	12.016303	6.686589	R
O	7.620645	9.032477	6.817951	R
O	6.194520	13.366090	5.049586	R
Al	7.261656	14.868825	9.241267	R
Al	7.861546	10.552507	10.397714	R
O	6.189520	10.505101	13.138544	R
O	6.480947	13.538950	13.295183	R
O	6.388656	10.533250	9.063580	R
O	7.706940	15.063645	10.905746	R
O	6.047192	13.407942	8.933950	R
O	6.002223	16.164196	8.827488	R
O	8.154704	9.184647	11.511467	R
O	8.138619	11.935400	11.485319	R
O	4.777058	6.123336	10.946270	R
O	4.826830	14.912870	10.924971	R
O	4.813611	9.097353	10.954312	R
O	4.804463	11.929909	10.962749	R
O	6.303003	4.939222	5.061751	R
O	6.345048	16.039558	5.089018	R
O	8.160763	9.120737	3.353379	R
O	8.018564	11.956350	3.284491	R
O	3.502432	10.507165	8.968732	R
Cu	8.971158	11.746497	7.928609	R
Cu	8.887876	8.744416	8.424653	R
O	9.226893	10.412115	9.167049	R
N	10.213312	6.357974	7.794728	R
N	10.339910	5.195525	7.891771	R
O	9.259699	6.942023	9.014897	R
O	10.734467	4.087759	7.634868	R

```
Model #48      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al      4.718091       6.298715       9.025534       F
Al      6.299120       6.298715       11.957102      F
Al      4.718091       14.697002      9.025534       F
Al      4.828311       11.950763      9.158184       F
Al      4.828311       9.044955       9.158184       F
Al      7.260466       8.998624       12.959551      F
Al      7.260466       11.997093      12.959551      F
Al      6.299120       14.697002      11.957102      F
Al      4.636026       10.497859      12.053017      F
O       3.286788       10.497859      13.239718      F
Al      6.284430       4.911618       6.956078       F
Al      6.284430       16.084099      6.956078       F
Al      7.604152       10.497859      2.473791       F
O       6.427205       10.497859      1.094354       F
Al      6.373455       6.298715       3.886397       F
O       4.781442       6.298715       2.980335       F
Al      6.373455       14.697002      3.886397       F
O       4.781442       14.697002      2.980335       F
O       3.454035       4.977004       9.235301       F
O       3.454035       7.620427       9.235301       F
O       6.249989       5.002877       13.162247      F
O       3.454035       16.018713      9.235301       F
O       3.454035       13.375290      9.235301       F
O       7.425505       9.104843       14.776051      F
O       7.425505       11.890874      14.776051      F
O       6.249989       15.992841      13.162247      F
O       4.962264       3.365416       7.283451       F
O       7.499839       3.492587       6.705345       F
O       4.962264       17.630302      7.283451       F
O       7.499839       17.503130      6.705345       F
O       7.704784       6.298715       2.777154       F
O       7.704784       14.697002      2.777154       F
Al      3.478998       10.497859      7.046735       F
O       1.926548       11.807732      6.890259       F
O       1.926548       9.187985       6.890259       F
O       3.361122       10.497859      5.169014       F
Al      2.050923       10.497859      10.125656      F
O       0.574778       10.497859      9.076089       F
O       2.097749       9.088323       11.188759      F
O       2.097749       11.907395      11.188759      F
Al      3.393316       6.298715       6.011417       F
O       1.956477       6.298715       7.179493       F
O       3.339459       7.715095       4.949249       F
O       3.339459       4.882336       4.949249       F
Al      3.393316       14.697002      6.011417       F
O       1.956477       14.697002      7.179493       F
O       3.339459       16.113380      4.949249       F
O       3.339459       13.280622      4.949249       F
H       3.439923       4.911172       10.243970      F
H       3.439232       7.689483       10.293373      F
H       6.818393       4.213072       13.048228      F
H       6.229200       4.955319       14.133904      F
H       3.439929       16.084518      10.243550      F
H       3.439218       13.306190      10.293977      F
H       6.776962       8.347647       14.909841      F
H       6.777013       12.648010      14.909830      F
H       6.229199       16.040400      14.133948      F
H       6.818394       16.782646      13.048228      F
H       4.227165       2.738070       7.166136       F
H       6.932392       2.747750       6.973661       F
H       7.409135       3.550965       5.707009       F
H       4.227165       18.257647      7.166137       F
H       6.932397       18.247959      6.973659       F
H       7.409131       17.444750      5.706962       F
H       7.521090       6.298716       1.832227       F
H       7.521091       14.697002      1.832228       F
H       3.346923       10.497859      14.197637      F
H       6.469066       10.497859      0.138110       F
H       0.036291       9.692187       9.043066       F
H       0.036295       11.303524      9.043066       F
H       2.008448       9.058198       12.145152      F
H       2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.203398	7.655425	6.962026	R
O	4.796856	6.307204	7.126452	R
O	7.450031	6.297848	7.234162	R
O	6.245556	7.663620	5.033865	R
Al	7.437664	6.183887	9.211500	R
O	6.463240	7.473250	13.291120	R
O	7.641784	5.845855	10.938005	R
O	6.052940	4.886116	8.809526	R
O	6.046290	7.612634	8.909532	R
Al	7.353243	9.019586	4.902785	R
Al	7.238630	11.978136	4.840326	R
Al	6.237436	13.356514	6.973824	R
Al	6.378514	10.504822	7.119218	R
O	4.825271	14.707453	7.127330	R
O	4.960988	11.822886	7.266760	R
O	4.951902	9.203523	7.260053	R
O	7.529386	14.731616	7.418399	R
O	6.346590	10.473221	5.093873	R
O	7.558128	12.022422	6.676017	R
O	7.604596	9.053087	6.794220	R
O	6.184042	13.367204	5.044783	R
Al	7.264916	14.861646	9.236773	R
Al	7.914117	10.490802	10.385115	R
O	6.185612	10.504643	13.140133	R
O	6.487275	13.540100	13.292416	R
O	6.364197	10.520062	9.058814	R
O	7.705622	15.056173	10.903171	R
O	6.043714	13.405790	8.929498	R
O	6.001604	16.161536	8.828553	R
O	8.169143	9.141167	11.526218	R
O	8.136873	11.888177	11.482264	R
O	4.781507	6.117474	10.940541	R
O	4.824549	14.912099	10.926345	R
O	4.799270	9.093493	10.953377	R
O	4.784741	11.930948	10.960328	R
O	6.294478	4.940454	5.064237	R
O	6.341470	16.041141	5.087646	R
O	8.151627	9.114550	3.345912	R
O	8.022275	11.955230	3.284156	R
O	3.487151	10.504235	8.959707	R
Cu	8.937741	11.579227	7.890844	R
Cu	8.893396	8.628002	8.352790	R
O	9.252467	10.289657	9.157282	R
O	9.066971	6.917592	8.792000	R

```
Model #49      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043065       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.210321	7.648503	6.964465	R
O	4.797141	6.309791	7.128961	R
O	7.445172	6.289114	7.256758	R
O	6.243442	7.661420	5.033891	R
Al	7.433746	6.182201	9.204511	R
O	6.471552	7.472949	13.291634	R
O	7.650169	5.881844	10.935456	R
O	6.045764	4.880941	8.816074	R
O	6.049795	7.616024	8.915009	R
Al	7.355295	9.012476	4.910852	R
Al	7.248364	11.975482	4.844974	R
Al	6.238691	13.352197	6.977574	R
Al	6.386985	10.495051	7.117713	R
O	4.828343	14.706272	7.127828	R
O	4.974058	11.822823	7.270104	R
O	4.958065	9.208952	7.268367	R
O	7.535603	14.728776	7.424256	R
O	6.356026	10.473986	5.103742	R
O	7.569990	12.013118	6.689297	R
O	7.602557	9.034425	6.801082	R
O	6.199575	13.368079	5.051857	R
Al	7.261531	14.868692	9.241421	R
Al	7.867642	10.538668	10.393371	R
O	6.188945	10.505232	13.138034	R
O	6.482221	13.539506	13.295303	R
O	6.382564	10.531412	9.062184	R
O	7.706813	15.064073	10.905778	R
O	6.046985	13.408330	8.933897	R
O	6.001813	16.164211	8.827299	R
O	8.168878	9.182654	11.521141	R
O	8.128661	11.930085	11.477922	R
O	4.778384	6.121815	10.944768	R
O	4.826470	14.913536	10.924999	R
O	4.811421	9.098259	10.953938	R
O	4.798623	11.931003	10.962060	R
O	6.297917	4.938557	5.062025	R
O	6.343156	16.040526	5.088687	R
O	8.151728	9.118451	3.351971	R
O	8.022255	11.956404	3.283968	R
O	3.496512	10.508133	8.966087	R
Cu	8.983780	11.727232	7.918440	R
Cu	8.910574	8.719707	8.417269	R
O	9.222928	10.388691	9.156589	R
O	9.105118	6.892096	8.746770	R

```
Model #50      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718090       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043065       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.261724	7.654571	6.992672	R
O	4.831308	6.300412	7.128695	R
O	7.533459	6.274458	7.432998	R
O	6.272100	7.629939	5.071947	R
Al	7.268305	6.120618	9.247586	R
O	6.465161	7.463086	13.294821	R
O	7.702601	5.926823	10.913252	R
O	6.000807	4.833385	8.828492	R
O	6.047893	7.593309	8.942638	R
Al	7.330551	9.018903	4.887482	R
Al	7.251756	11.975547	4.849046	R
Al	6.238126	13.352836	6.973872	R
Al	6.390313	10.498523	7.126846	R
O	4.828411	14.705606	7.127690	R
O	4.972632	11.812929	7.271966	R
O	4.977850	9.183951	7.272690	R
O	7.531849	14.728953	7.419987	R
O	6.341519	10.478976	5.092444	R
O	7.563644	12.014653	6.690964	R
O	7.607824	9.040944	6.760193	R
O	6.198022	13.365760	5.046912	R
Al	7.264343	14.860029	9.236257	R
Al	7.942804	10.429383	10.376867	R
O	6.183839	10.498898	13.143492	R
O	6.490902	13.538881	13.288077	R
O	6.378774	10.499868	9.063715	R
O	7.708695	15.042995	10.903535	R
O	6.044279	13.404603	8.931659	R
O	6.003770	16.161288	8.829609	R
O	8.150904	9.064330	11.508109	R
O	8.161810	11.814757	11.508734	R
O	4.822092	6.087845	10.926487	R
O	4.826013	14.912835	10.927434	R
O	4.794769	9.077419	10.958912	R
O	4.791396	11.927480	10.961660	R
O	6.325852	4.957371	5.089606	R
O	6.342513	16.040620	5.088360	R
O	8.110841	9.091138	3.325045	R
O	8.045879	11.941299	3.297362	R
O	3.500415	10.498634	8.966840	R
Cu	9.310178	8.950696	7.870793	R
Cu	8.925713	11.669599	7.972087	R
O	9.292038	10.298021	9.175292	R
N	11.010040	5.568693	7.331869	R
O	10.886289	5.362950	6.164532	R
O	10.316240	7.697341	6.795946	R
N	10.756440	7.002544	7.741380	R

```
Model #51       Cartesian coordinates in angstrom
                x              y              z              Relaxed/Frozen
Al              4.718090       6.298715       9.025534       F
Al              6.299120       6.298715       11.957102      F
Al              4.718091       14.697002      9.025534       F
Al              4.828311       11.950763      9.158184       F
Al              4.828311       9.044955       9.158184       F
Al              7.260466       8.998624       12.959551      F
Al              7.260466       11.997093      12.959551      F
Al              6.299120       14.697002      11.957102      F
Al              4.636026       10.497859      12.053017      F
O               3.286788       10.497859      13.239718      F
Al              6.284430       4.911618       6.956078       F
Al              6.284430       16.084099      6.956078       F
Al              7.604152       10.497859      2.473791       F
O               6.427205       10.497859      1.094354       F
Al              6.373455       6.298715       3.886397       F
O               4.781442       6.298715       2.980335       F
Al              6.373455       14.697002      3.886397       F
O               4.781442       14.697002      2.980335       F
O               3.454035       4.977004       9.235301       F
O               3.454035       7.620427       9.235301       F
O               6.249989       5.002877       13.162247      F
O               3.454035       16.018713      9.235301       F
O               3.454035       13.375290      9.235301       F
O               7.425505       9.104843       14.776051      F
O               7.425505       11.890874      14.776051      F
O               6.249989       15.992841      13.162247      F
O               4.962264       3.365416       7.283451       F
O               7.499839       3.492587       6.705345       F
O               4.962264       17.630302      7.283451       F
O               7.499839       17.503130      6.705345       F
O               7.704784       6.298715       2.777154       F
O               7.704784       14.697002      2.777154       F
Al              3.478998       10.497859      7.046735       F
O               1.926548       11.807732      6.890259       F
O               1.926548       9.187985       6.890259       F
O               3.361122       10.497859      5.169014       F
Al              2.050923       10.497859      10.125656      F
O               0.574778       10.497859      9.076089       F
O               2.097749       9.088323       11.188759      F
O               2.097749       11.907395      11.188759      F
Al              3.393316       6.298715       6.011417       F
O               1.956477       6.298715       7.179493       F
O               3.339459       7.715095       4.949249       F
O               3.339459       4.882336       4.949249       F
Al              3.393316       14.697002      6.011417       F
O               1.956477       14.697002      7.179493       F
O               3.339459       16.113380      4.949249       F
O               3.339459       13.280622      4.949249       F
H               3.439923       4.911172       10.243970      F
H               3.439232       7.689483       10.293373      F
H               6.818393       4.213072       13.048228      F
H               6.229200       4.955319       14.133904      F
H               3.439929       16.084518      10.243550      F
H               3.439218       13.306190      10.293977      F
H               6.776962       8.347647       14.909841      F
H               6.777013       12.648010      14.909830      F
H               6.229199       16.040400      14.133948      F
H               6.818394       16.782646      13.048228      F
H               4.227165       2.738070       7.166136       F
H               6.932392       2.747750       6.973661       F
H               7.409135       3.550965       5.707009       F
H               4.227165       18.257647      7.166137       F
H               6.932397       18.247959      6.973659       F
H               7.409131       17.444750      5.706962       F
H               7.521090       6.298716       1.832227       F
H               7.521091       14.697002      1.832228       F
H               3.346923       10.497859      14.197637      F
H               6.469066       10.497859      0.138110       F
H               0.036291       9.692187       9.043066       F
H               0.036295       11.303524      9.043066       F
H               2.008448       9.058198       12.145152      F
H               2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.267962	7.658533	7.034574	R
O	4.831727	6.300025	7.134900	R
O	7.534562	6.270395	7.446200	R
O	6.279519	7.617279	5.090716	R
Al	7.268720	6.105473	9.256167	R
O	6.467620	7.462558	13.294221	R
O	7.706626	5.920216	10.920559	R
O	5.998937	4.827064	8.831978	R
O	6.049753	7.590771	8.958778	R
Al	7.333526	9.005499	4.891871	R
Al	7.253736	11.977005	4.845281	R
Al	6.233440	13.350184	6.974124	R
Al	6.395153	10.498180	7.102525	R
O	4.827839	14.705047	7.127861	R
O	4.972776	11.810796	7.268325	R
O	4.979801	9.180720	7.276096	R
O	7.531106	14.726548	7.420389	R
O	6.348584	10.474822	5.091965	R
O	7.564075	12.016668	6.688308	R
O	7.610621	9.039964	6.766757	R
O	6.196683	13.364544	5.045360	R
Al	7.264054	14.859893	9.236144	R
Al	7.931712	10.433490	10.372443	R
O	6.183786	10.498459	13.144057	R
O	6.490371	13.538879	13.288624	R
O	6.381980	10.499702	9.056350	R
O	7.708379	15.043472	10.903204	R
O	6.042969	13.403904	8.931249	R
O	6.003624	16.160813	8.829360	R
O	8.148980	9.069180	11.505429	R
O	8.154231	11.818873	11.504123	R
O	4.823410	6.086774	10.926664	R
O	4.825988	14.911995	10.927237	R
O	4.794940	9.078296	10.958668	R
O	4.792555	11.926154	10.961027	R
O	6.330387	4.951284	5.087919	R
O	6.342364	16.039942	5.089060	R
O	8.099695	9.086217	3.322811	R
O	8.047742	11.941685	3.295075	R
O	3.500613	10.498834	8.966531	R
O	9.293098	10.325413	9.178045	R
Cu	8.922958	11.710360	7.985473	R
Cu	9.337835	9.009941	7.853557	R
N	11.978800	6.302180	6.501060	R
O	12.245760	6.816373	5.453636	R
O	10.370004	7.922638	6.648733	R
N	10.901343	6.977805	7.277457	R

```
Model #52        Cartesian coordinates in angstrom
                 x              y              z              Relaxed/Frozen
Al        4.718091       6.298715       9.025534       F
Al        6.299120       6.298715       11.957102      F
Al        4.718091       14.697002      9.025534       F
Al        4.828311       11.950763      9.158184       F
Al        4.828311       9.044955       9.158184       F
Al        7.260466       8.998624       12.959551      F
Al        7.260466       11.997093      12.959551      F
Al        6.299120       14.697002      11.957102      F
Al        4.636026       10.497859      12.053017      F
O         3.286788       10.497859      13.239718      F
Al        6.284430       4.911618       6.956078       F
Al        6.284430       16.084099      6.956078       F
Al        7.604152       10.497859      2.473791       F
O         6.427205       10.497859      1.094354       F
Al        6.373455       6.298715       3.886397       F
O         4.781442       6.298715       2.980335       F
Al        6.373455       14.697002      3.886397       F
O         4.781442       14.697002      2.980335       F
O         3.454035       4.977004       9.235301       F
O         3.454035       7.620427       9.235301       F
O         6.249989       5.002877       13.162247      F
O         3.454035       16.018713      9.235301       F
O         3.454035       13.375290      9.235301       F
O         7.425505       9.104843       14.776051      F
O         7.425505       11.890874      14.776051      F
O         6.249989       15.992841      13.162247      F
O         4.962264       3.365416       7.283451       F
O         7.499839       3.492587       6.705345       F
O         4.962264       17.630302      7.283451       F
O         7.499839       17.503130      6.705345       F
O         7.704784       6.298715       2.777154       F
O         7.704784       14.697002      2.777154       F
Al        3.478998       10.497859      7.046735       F
O         1.926548       11.807732      6.890259       F
O         1.926548       9.187985       6.890259       F
O         3.361122       10.497859      5.169014       F
Al        2.050923       10.497859      10.125656      F
O         0.574778       10.497859      9.076089       F
O         2.097749       9.088323       11.188759      F
O         2.097749       11.907395      11.188759      F
Al        3.393316       6.298715       6.011417       F
O         1.956477       6.298715       7.179493       F
O         3.339459       7.715095       4.949249       F
O         3.339459       4.882336       4.949249       F
Al        3.393316       14.697002      6.011417       F
O         1.956477       14.697002      7.179493       F
O         3.339459       16.113380      4.949249       F
O         3.339459       13.280622      4.949249       F
H         3.439923       4.911172       10.243970      F
H         3.439232       7.689483       10.293373      F
H         6.818393       4.213072       13.048228      F
H         6.229200       4.955319       14.133904      F
H         3.439929       16.084518      10.243550      F
H         3.439218       13.306190      10.293977      F
H         6.776962       8.347647       14.909841      F
H         6.777013       12.648010      14.909830      F
H         6.229199       16.040400      14.133948      F
H         6.818394       16.782646      13.048228      F
H         4.227165       2.738070       7.166136       F
H         6.932392       2.747750       6.973661       F
H         7.409135       3.550965       5.707009       F
H         4.227165       18.257647      7.166137       F
H         6.932397       18.247959      6.973659       F
H         7.409131       17.444750      5.706962       F
H         7.521090       6.298716       1.832227       F
H         7.521091       14.697002      1.832228       F
H         3.346923       10.497859      14.197637      F
H         6.469066       10.497859      0.138110       F
H         0.036291       9.692187       9.043065       F
H         0.036295       11.303524      9.043066       F
H         2.008448       9.058198       12.145152      F
H         2.008447       11.937518      12.145155      F
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H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.250888	7.656379	6.987906	R
O	4.832730	6.294634	7.126163	R
O	7.540812	6.274951	7.427428	R
O	6.243480	7.626207	5.062408	R
Al	7.265139	6.130932	9.243815	R
O	6.468915	7.460336	13.294373	R
O	7.704613	5.928612	10.908279	R
O	6.004441	4.834417	8.825742	R
O	6.045772	7.590452	8.938135	R
Al	7.287467	9.025956	4.877799	R
Al	7.260297	11.975553	4.853452	R
Al	6.245977	13.349205	6.976736	R
Al	6.389770	10.499526	7.133219	R
O	4.829408	14.704123	7.126816	R
O	4.971911	11.812803	7.272592	R
O	4.969296	9.181706	7.272857	R
O	7.532442	14.728556	7.418874	R
O	6.322001	10.493058	5.080638	R
O	7.567847	12.001674	6.693619	R
O	7.575017	9.024926	6.739265	R
O	6.208309	13.367569	5.048428	R
Al	7.266767	14.857091	9.236151	R
Al	7.982842	10.451087	10.377686	R
O	6.182016	10.497599	13.145003	R
O	6.483985	13.537494	13.289139	R
O	6.381224	10.494125	9.061947	R
O	7.706888	15.047257	10.904000	R
O	6.044482	13.404277	8.932698	R
O	6.004442	16.160345	8.829091	R
O	8.154511	9.074846	11.510341	R
O	8.171411	11.830372	11.520966	R
O	4.825069	6.082326	10.924933	R
O	4.824426	14.912899	10.927786	R
O	4.788369	9.071930	10.959722	R
O	4.789087	11.925981	10.960980	R
O	6.339832	4.952365	5.086774	R
O	6.341478	16.043125	5.086439	R
O	8.088783	9.080768	3.323923	R
O	8.061687	11.932816	3.302599	R
O	3.498833	10.498531	8.966972	R
Cu	9.239795	8.999961	7.841209	R
Cu	9.001788	11.664073	7.929803	R
O	9.362876	10.377824	9.231348	R
N	11.545286	10.708659	7.530901	R
N	11.145666	8.895931	7.759149	R
O	12.505647	10.862940	8.160863	R
O	12.006056	8.477321	8.443958	R

```
Model #53      Cartesian coordinates in angstrom
               x               y               z               Relaxed/Frozen
Al             4.718091        6.298715        9.025534        F
Al             6.299120        6.298715        11.957102       F
Al             4.718091        14.697002       9.025534        F
Al             4.828311        11.950763       9.158184        F
Al             4.828311        9.044955        9.158184        F
Al             7.260466        8.998624        12.959551       F
Al             7.260466        11.997093       12.959551       F
Al             6.299120        14.697002       11.957102       F
Al             4.636026        10.497859       12.053017       F
O              3.286788        10.497859       13.239718       F
Al             6.284430        4.911618        6.956078        F
Al             6.284430        16.084099       6.956078        F
Al             7.604152        10.497859       2.473791        F
O              6.427205        10.497859       1.094354        F
Al             6.373455        6.298715        3.886397        F
O              4.781442        6.298715        2.980335        F
Al             6.373455        14.697002       3.886397        F
O              4.781442        14.697002       2.980335        F
O              3.454035        4.977004        9.235301        F
O              3.454035        7.620427        9.235301        F
O              6.249989        5.002877        13.162247       F
O              3.454035        16.018713       9.235301        F
O              3.454035        13.375290       9.235301        F
O              7.425505        9.104843        14.776051       F
O              7.425505        11.890874       14.776051       F
O              6.249989        15.992841       13.162247       F
O              4.962264        3.365416        7.283451        F
O              7.499839        3.492587        6.705345        F
O              4.962264        17.630302       7.283451        F
O              7.499839        17.503130       6.705345        F
O              7.704784        6.298715        2.777154        F
O              7.704784        14.697002       2.777154        F
Al             3.478998        10.497859       7.046735        F
O              1.926548        11.807732       6.890259        F
O              1.926548        9.187985        6.890259        F
O              3.361122        10.497859       5.169014        F
Al             2.050923        10.497859       10.125656       F
O              0.574778        10.497859       9.076089        F
O              2.097749        9.088323        11.188759       F
O              2.097749        11.907395       11.188759       F
Al             3.393316        6.298715        6.011417        F
O              1.956477        6.298715        7.179493        F
O              3.339459        7.715095        4.949249        F
O              3.339459        4.882336        4.949249        F
Al             3.393316        14.697002       6.011417        F
O              1.956477        14.697002       7.179493        F
O              3.339459        16.113380       4.949249        F
O              3.339459        13.280622       4.949249        F
H              3.439923        4.911172        10.243970       F
H              3.439232        7.689483        10.293373       F
H              6.818393        4.213072        13.048228       F
H              6.229200        4.955319        14.133904       F
H              3.439929        16.084518       10.243550       F
H              3.439218        13.306190       10.293977       F
H              6.776962        8.347647        14.909841       F
H              6.777013        12.648010       14.909830       F
H              6.229199        16.040400       14.133948       F
H              6.818394        16.782646       13.048228       F
H              4.227165        2.738070        7.166136        F
H              6.932392        2.747750        6.973661        F
H              7.409135        3.550965        5.707009        F
H              4.227165        18.257647       7.166137        F
H              6.932397        18.247959       6.973659        F
H              7.409131        17.444750       5.706962        F
H              7.521090        6.298716        1.832227        F
H              7.521091        14.697002       1.832228        F
H              3.346923        10.497859       14.197637       F
H              6.469066        10.497859       0.138110        F
H              0.036291        9.692187        9.043065        F
H              0.036295        11.303524       9.043066        F
H              2.008448        9.058198        12.145152       F
H              2.008447        11.937518       12.145155       F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.254951	7.661272	6.991328	R
O	4.832879	6.296269	7.126140	R
O	7.535652	6.270044	7.426441	R
O	6.271466	7.626202	5.067525	R
Al	7.264935	6.127653	9.243857	R
O	6.464529	7.462752	13.292280	R
O	7.704682	5.927479	10.909048	R
O	6.003151	4.831963	8.827251	R
O	6.047724	7.589098	8.940539	R
Al	7.329840	9.020370	4.892786	R
Al	7.245648	11.976310	4.843803	R
Al	6.233804	13.351365	6.972648	R
Al	6.392189	10.495981	7.122997	R
O	4.826297	14.706561	7.127612	R
O	4.970641	11.811778	7.268341	R
O	4.970796	9.179282	7.270744	R
O	7.525794	14.731238	7.415059	R
O	6.337886	10.477381	5.084168	R
O	7.561868	12.023243	6.674330	R
O	7.599403	9.030086	6.759030	R
O	6.185888	13.363299	5.039543	R
Al	7.266105	14.855052	9.231888	R
Al	8.054722	10.441357	10.412057	R
O	6.186248	10.497490	13.137121	R
O	6.483266	13.535393	13.286111	R
O	6.380725	10.498097	9.060075	R
O	7.706953	15.037294	10.901519	R
O	6.041998	13.404885	8.930669	R
O	6.003790	16.161468	8.830668	R
O	8.196009	9.062247	11.537159	R
O	8.220157	11.817451	11.553218	R
O	4.825041	6.082776	10.925377	R
O	4.823959	14.914320	10.929222	R
O	4.787813	9.070567	10.961404	R
O	4.790681	11.929197	10.964036	R
O	6.336787	4.949932	5.085129	R
O	6.342017	16.042533	5.086273	R
O	8.109550	9.088236	3.325805	R
O	8.045688	11.942063	3.293119	R
O	3.497601	10.498530	8.967084	R
Cu	9.226259	8.832264	8.003454	R
Cu	8.881374	11.558264	7.938608	R
O	9.378124	10.321970	9.214185	R
N	11.465895	9.748932	6.061216	R
N	10.480163	7.483683	8.063079	R
O	12.558029	9.958674	6.374343	R
O	11.371796	6.814993	8.409556	R

```
Model #54        Cartesian coordinates in angstrom
                 x              y              z              Relaxed/Frozen
Al               4.718110       6.298736       9.025543       F
Al               6.299091       6.298738       11.957117      F
Al               4.718083       14.696998      9.025536       F
Al               4.828307       11.950750      9.158168       F
Al               4.828314       9.044957       9.158170       F
Al               7.260411       8.998622       12.959493      F
Al               7.260465       11.997032      12.959510      F
Al               6.299132       14.697001      11.957102      F
Al               4.636020       10.497859      12.053020      F
O                3.286790       10.497858      13.239720      F
Al               6.284454       4.911652       6.956091       F
Al               6.284411       16.084088      6.956080       F
Al               7.604197       10.497864      2.473808       F
O                6.427207       10.497857      1.094352       F
Al               6.373418       6.298719       3.886415       F
O                4.781437       6.298719       2.980344       F
Al               6.373413       14.696991      3.886426       F
O                4.781439       14.697000      2.980340       F
O                3.454039       4.977000       9.235298       F
O                3.454039       7.620429       9.235305       F
O                6.249991       5.002874       13.162244      F
O                3.454038       16.018715      9.235305       F
O                3.454036       13.375294      9.235298       F
O                7.425529       9.104824       14.776050      F
O                7.425515       11.890868      14.776050      F
O                6.249991       15.992840      13.162249      F
O                4.962269       3.365415       7.283468       F
O                7.499838       3.492584       6.705356       F
O                4.962263       17.630301      7.283453       F
O                7.499841       17.503129      6.705346       F
O                7.704787       6.298714       2.777157       F
O                7.704790       14.697002      2.777161       F
Al               3.479000       10.497855      7.046721       F
O                1.926547       11.807732      6.890265       F
O                1.926549       9.187985       6.890247       F
O                3.361122       10.497864      5.169014       F
Al               2.050924       10.497856      10.125651      F
O                0.574778       10.497860      9.076089       F
O                2.097748       9.088324       11.188760      F
O                2.097749       11.907394      11.188760      F
Al               3.393319       6.298723       6.011417       F
O                1.956477       6.298712       7.179493       F
O                3.339458       7.715094       4.949248       F
O                3.339459       4.882335       4.949251       F
Al               3.393314       14.697000      6.011419       F
O                1.956477       14.697003      7.179493       F
O                3.339460       16.113380      4.949248       F
O                3.339459       13.280622      4.949249       F
H                3.439924       4.911171       10.243970      F
H                3.439231       7.689479       10.293373      F
H                6.818395       4.213073       13.048230      F
H                6.229207       4.955319       14.133904      F
H                3.439932       16.084521      10.243550      F
H                3.439222       13.306193      10.293977      F
H                6.776956       8.347652       14.909841      F
H                6.777027       12.648022      14.909829      F
H                6.229199       16.040400      14.133948      F
H                6.818390       16.782648      13.048225      F
H                4.227167       2.738068       7.166134       F
H                6.932392       2.747750       6.973660       F
H                7.409130       3.550961       5.707009       F
H                4.227167       18.257650      7.166135       F
H                6.932398       18.247959      6.973661       F
H                7.409132       17.444749      5.706962       F
H                7.521090       6.298714       1.832227       F
H                7.521091       14.697004      1.832228       F
H                3.346923       10.497860      14.197637      F
H                6.469066       10.497866      0.138110       F
H                0.036291       9.692187       9.043066       F
H                0.036295       11.303524      9.043066       F
H                2.008449       9.058198       12.145152      F
H                2.008447       11.937518      12.145155      F
```

H	4.786758	6.298708	2.000110	F
H	4.786758	14.697008	2.000090	F
H	6.866368	9.838794	15.040441	F
H	6.866338	11.156934	15.040447	F
H	4.132076	16.721548	9.197254	F
H	4.893484	17.534252	8.246089	F
H	4.893480	3.461469	8.246093	F
H	4.132058	4.274188	9.197258	F
H	2.690120	11.221847	5.059459	F
H	2.690117	9.773873	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137968	13.968639	3.050495	F
H	4.137968	7.027079	3.050495	F
H	3.423386	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423054	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160661	F
Al	6.268245	7.662391	6.989741	R
O	4.835752	6.294777	7.125569	R
O	7.541052	6.268497	7.432734	R
O	6.243898	7.624263	5.060197	R
Al	7.261765	6.131518	9.247097	R
O	6.466421	7.460448	13.295373	R
O	7.705525	5.923544	10.910113	R
O	6.003222	4.831369	8.827955	R
O	6.046806	7.589843	8.940279	R
Al	7.278642	9.033156	4.880178	R
Al	7.250691	11.976601	4.843851	R
Al	6.239740	13.348816	6.973435	R
Al	6.390187	10.492035	7.130742	R
O	4.828141	14.705516	7.126882	R
O	4.971770	11.812366	7.271762	R
O	4.967964	9.180655	7.272889	R
O	7.529607	14.728453	7.416791	R
O	6.307154	10.498926	5.060978	R
O	7.560921	12.007218	6.681771	R
O	7.581221	9.037324	6.726893	R
O	6.200694	13.369104	5.044916	R
Al	7.266423	14.855606	9.234127	R
Al	7.998210	10.429040	10.380877	R
O	6.181943	10.497069	13.144997	R
O	6.487299	13.538233	13.288529	R
O	6.376551	10.493986	9.063999	R
O	7.707167	15.043486	10.902723	R
O	6.043489	13.404728	8.931737	R
O	6.004520	16.160792	8.829511	R
O	8.165756	9.057656	11.518267	R
O	8.178705	11.811149	11.526879	R
O	4.825689	6.082000	10.925167	R
O	4.824485	14.914407	10.928568	R
O	4.788137	9.071113	10.960872	R
O	4.787018	11.928120	10.962476	R
O	6.343788	4.948338	5.084383	R
O	6.342201	16.044483	5.085703	R
O	8.095725	9.084784	3.330005	R
O	8.061911	11.936320	3.297301	R
O	3.497537	10.498969	8.967387	R
Cu	9.419234	9.003910	7.845838	R
Cu	8.915696	11.605948	7.951944	R
O	9.360475	10.335065	9.219418	R
N	10.620571	7.856236	6.897140	R
O	11.140580	6.137035	5.242178	R
N	10.134226	6.440687	5.711797	R
O	11.767919	8.018304	6.688540	R

```
Model #55      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718110       6.298736       9.025543       F
Al             6.299091       6.298738       11.957117      F
Al             4.718083       14.696998      9.025536       F
Al             4.828307       11.950750      9.158168       F
Al             4.828314       9.044957       9.158170       F
Al             7.260411       8.998622       12.959493      F
Al             7.260465       11.997032      12.959510      F
Al             6.299132       14.697001      11.957102      F
Al             4.636020       10.497859      12.053020      F
O              3.286790       10.497858      13.239720      F
Al             6.284454       4.911652       6.956091       F
Al             6.284411       16.084088      6.956080       F
Al             7.604197       10.497864      2.473808       F
O              6.427207       10.497857      1.094352       F
Al             6.373418       6.298719       3.886415       F
O              4.781437       6.298719       2.980344       F
Al             6.373413       14.696991      3.886426       F
O              4.781439       14.697000      2.980340       F
O              3.454039       4.977000       9.235298       F
O              3.454039       7.620429       9.235305       F
O              6.249991       5.002874       13.162244      F
O              3.454038       16.018715      9.235305       F
O              3.454036       13.375294      9.235298       F
O              7.425529       9.104824       14.776050      F
O              7.425515       11.890868      14.776050      F
O              6.249991       15.992840      13.162249      F
O              4.962269       3.365415       7.283468       F
O              7.499838       3.492584       6.705356       F
O              4.962263       17.630301      7.283453       F
O              7.499841       17.503129      6.705346       F
O              7.704787       6.298714       2.777157       F
O              7.704790       14.697002      2.777161       F
Al             3.479000       10.497855      7.046721       F
O              1.926547       11.807732      6.890265       F
O              1.926549       9.187985       6.890247       F
O              3.361122       10.497864      5.169014       F
Al             2.050924       10.497856      10.125651      F
O              0.574778       10.497860      9.076089       F
O              2.097748       9.088324       11.188760      F
O              2.097749       11.907394      11.188760      F
Al             3.393319       6.298723       6.011417       F
O              1.956477       6.298712       7.179493       F
O              3.339458       7.715094       4.949248       F
O              3.339459       4.882335       4.949251       F
Al             3.393314       14.697000      6.011419       F
O              1.956477       14.697003      7.179493       F
O              3.339460       16.113380      4.949248       F
O              3.339459       13.280622      4.949249       F
H              3.439924       4.911171       10.243970      F
H              3.439231       7.689479       10.293373      F
H              6.818395       4.213073       13.048230      F
H              6.229207       4.955319       14.133904      F
H              3.439932       16.084521      10.243550      F
H              3.439222       13.306193      10.293977      F
H              6.776956       8.347652       14.909841      F
H              6.777027       12.648022      14.909829      F
H              6.229199       16.040400      14.133948      F
H              6.818390       16.782648      13.048225      F
H              4.227167       2.738068       7.166134       F
H              6.932392       2.747750       6.973660       F
H              7.409130       3.550961       5.707009       F
H              4.227167       18.257650      7.166135       F
H              6.932398       18.247959      6.973661       F
H              7.409132       17.444749      5.706962       F
H              7.521090       6.298714       1.832227       F
H              7.521091       14.697004      1.832228       F
H              3.346923       10.497860      14.197637      F
H              6.469066       10.497866      0.138110       F
H              0.036291       9.692187       9.043066       F
H              0.036295       11.303524      9.043066       F
H              2.008449       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298708	2.000110	F
H	4.786758	14.697008	2.000090	F
H	6.866368	9.838794	15.040441	F
H	6.866338	11.156934	15.040447	F
H	4.132076	16.721548	9.197254	F
H	4.893484	17.534252	8.246089	F
H	4.893480	3.461469	8.246093	F
H	4.132058	4.274188	9.197258	F
H	2.690120	11.221847	5.059459	F
H	2.690117	9.773873	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137968	13.968639	3.050495	F
H	4.137968	7.027079	3.050495	F
H	3.423386	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423054	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160661	F
Al	6.259807	7.656933	6.988533	R
O	4.832909	6.295641	7.126754	R
O	7.535829	6.271394	7.430602	R
O	6.250591	7.626844	5.062742	R
Al	7.261714	6.128435	9.245278	R
O	6.467646	7.460944	13.294017	R
O	7.705697	5.928182	10.909103	R
O	6.002062	4.831677	8.828075	R
O	6.046224	7.590348	8.940460	R
Al	7.298174	9.025175	4.880068	R
Al	7.252369	11.975694	4.848742	R
Al	6.239299	13.350064	6.974042	R
Al	6.392400	10.495100	7.132986	R
O	4.828087	14.705182	7.126951	R
O	4.971554	11.811649	7.272161	R
O	4.973043	9.180559	7.272278	R
O	7.530045	14.728642	7.417237	R
O	6.323783	10.488929	5.079537	R
O	7.561718	12.009627	6.687229	R
O	7.592426	9.027017	6.737118	R
O	6.199856	13.367031	5.045293	R
Al	7.266492	14.856367	9.234691	R
Al	8.001758	10.444233	10.386556	R
O	6.182799	10.497394	13.143375	R
O	6.484196	13.537280	13.288549	R
O	6.381988	10.494302	9.063171	R
O	7.706864	15.045089	10.902970	R
O	6.043420	13.404588	8.931668	R
O	6.004308	16.160551	8.829226	R
O	8.169755	9.070094	11.520469	R
O	8.181287	11.825447	11.528170	R
O	4.825311	6.082603	10.925590	R
O	4.824496	14.913533	10.928043	R
O	4.788679	9.071918	10.960479	R
O	4.788157	11.927040	10.961541	R
O	6.337604	4.952253	5.086580	R
O	6.342074	16.043031	5.086448	R
O	8.098831	9.085011	3.325132	R
O	8.055803	11.936606	3.299420	R
O	3.498676	10.497811	8.966767	R
Cu	9.303392	8.996028	7.876029	R
Cu	8.927196	11.651523	7.962310	R
O	9.360139	10.361312	9.219797	R
N	10.588174	7.784099	7.076957	R
O	13.040497	7.712605	6.731464	R
N	12.295061	8.435318	7.253875	R
O	10.570707	6.768017	6.484216	R

```
Model #56      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.717996       6.298635       9.025588       F
Al             6.299191       6.298979       11.957050      F
Al             4.718014       14.696931      9.025564       F
Al             4.828266       11.950610      9.158207       F
Al             4.828039       9.044839       9.158173       F
Al             7.260523       8.998662       12.959451      F
Al             7.260557       11.996884      12.959405      F
Al             6.299113       14.697042      11.957131      F
Al             4.636091       10.497818      12.053037      F
O              3.286786       10.497864      13.239716      F
Al             6.284122       4.912053       6.956134       F
Al             6.284446       16.083975      6.956192       F
Al             7.604080       10.497775      2.473921       F
O              6.427246       10.497874      1.094320       F
Al             6.373521       6.298812       3.886468       F
O              4.781448       6.298705       2.980326       F
Al             6.373532       14.696959      3.886458       F
O              4.781443       14.697008      2.980334       F
O              3.454056       4.976988       9.235326       F
O              3.454036       7.620428       9.235343       F
O              6.250043       5.002859       13.162230      F
O              3.454040       16.018719      9.235295       F
O              3.454024       13.375270      9.235304       F
O              7.425500       9.104830       14.776052      F
O              7.425500       11.890907      14.776054      F
O              6.249988       15.992850      13.162237      F
O              4.962364       3.365368       7.283628       F
O              7.499843       3.492595       6.705317       F
O              4.962257       17.630295      7.283457       F
O              7.499816       17.503151      6.705359       F
O              7.704772       6.298700       2.777140       F
O              7.704758       14.697015      2.777123       F
Al             3.478979       10.497849      7.046760       F
O              1.926558       11.807743      6.890260       F
O              1.926552       9.187978       6.890260       F
O              3.361166       10.497853      5.169011       F
Al             2.051007       10.497926      10.125658      F
O              0.574784       10.497857      9.076081       F
O              2.097764       9.088323       11.188758      F
O              2.097758       11.907396      11.188758      F
Al             3.393416       6.298670       6.011337       F
O              1.956483       6.298720       7.179501       F
O              3.339466       7.715105       4.949261       F
O              3.339462       4.882337       4.949248       F
Al             3.393402       14.697092      6.011319       F
O              1.956481       14.697000      7.179498       F
O              3.339448       16.113384      4.949254       F
O              3.339446       13.280604      4.949274       F
H              3.439929       4.911167       10.243970      F
H              3.439265       7.689470       10.293375      F
H              6.818394       4.213072       13.048228      F
H              6.229163       4.955320       14.133903      F
H              3.439934       16.084522      10.243550      F
H              3.439239       13.306202      10.293979      F
H              6.776964       8.347645       14.909841      F
H              6.777031       12.648025      14.909830      F
H              6.229194       16.040400      14.133948      F
H              6.818393       16.782646      13.048228      F
H              4.227300       2.737932       7.166029       F
H              6.932384       2.747747       6.973636       F
H              7.409113       3.550946       5.707010       F
H              4.227188       18.257670      7.166119       F
H              6.932385       18.247963      6.973623       F
H              7.409126       17.444753      5.706962       F
H              7.521090       6.298703       1.832227       F
H              7.521091       14.697004      1.832228       F
H              3.346923       10.497865      14.197637      F
H              6.469066       10.497863      0.138110       F
H              0.036294       9.692186       9.043062       F
H              0.036291       11.303521      9.043071       F
H              2.008439       9.058197       12.145151      F
H              2.008437       11.937519      12.145154      F
```

H	4.786758	6.298714	2.000110	F
H	4.786758	14.697000	2.000090	F
H	6.866328	9.838762	15.040445	F
H	6.866303	11.156964	15.040452	F
H	4.132075	16.721548	9.197247	F
H	4.893475	17.534246	8.246088	F
H	4.893410	3.461526	8.246082	F
H	4.132054	4.274187	9.197222	F
H	2.690124	11.221851	5.059459	F
H	2.690115	9.773877	5.059460	F
H	1.278479	12.508616	6.923338	F
H	1.278489	8.487091	6.923332	F
H	1.991769	6.298720	8.126704	F
H	1.991769	14.696996	8.126702	F
H	4.137962	13.968645	3.050505	F
H	4.137960	7.027072	3.050508	F
H	3.423379	4.865219	3.998926	F
H	3.423381	16.130498	3.998927	F
H	3.423045	7.732142	4.002715	F
H	3.423046	13.263575	4.002714	F
H	2.742665	6.961361	9.160613	F
H	2.742718	14.034373	9.160643	F
Al	6.235382	7.645311	6.968164	R
O	4.821090	6.294895	7.127698	R
O	7.510314	6.271294	7.382898	R
O	6.203057	7.634823	5.038021	R
Al	7.312768	6.161537	9.218968	R
O	6.483539	7.458744	13.292526	R
O	7.684570	5.910791	10.913892	R
O	6.018102	4.848438	8.827847	R
O	6.049651	7.595523	8.931311	R
Al	7.266030	9.020586	4.853931	R
Al	7.276710	11.978025	4.854736	R
Al	6.244407	13.347113	6.975266	R
Al	6.388541	10.497370	7.123399	R
O	4.829553	14.704293	7.126222	R
O	4.971457	11.814105	7.271970	R
O	4.966362	9.187946	7.272463	R
O	7.532457	14.728530	7.418157	R
O	6.323742	10.503777	5.068575	R
O	7.571129	12.002614	6.699074	R
O	7.557458	8.999065	6.694627	R
O	6.217551	13.367095	5.047474	R
Al	7.267181	14.856718	9.235267	R
Al	8.053410	10.496283	10.408640	R
O	6.187802	10.495959	13.137191	R
O	6.473576	13.533396	13.288007	R
O	6.406420	10.503623	9.058844	R
O	7.706287	15.046469	10.903936	R
O	6.043655	13.406009	8.933192	R
O	6.004795	16.160795	8.829001	R
O	8.187290	9.091110	11.523820	R
O	8.218116	11.856162	11.560213	R
O	4.812672	6.093483	10.934029	R
O	4.823855	14.914431	10.928122	R
O	4.792979	9.074981	10.960584	R
O	4.794528	11.927177	10.962590	R
O	6.334644	4.947985	5.080716	R
O	6.340767	16.044040	5.086019	R
O	8.077915	9.070436	3.307355	R
O	8.080439	11.927445	3.304213	R
O	3.500402	10.500631	8.969332	R
Cu	8.961452	9.215577	8.004293	R
Cu	8.955555	11.737487	8.008026	R
O	9.478614	10.490408	9.314589	R
O	9.517155	7.062057	9.244198	R
N	10.598435	7.237949	11.295846	R
N	10.051157	7.155330	10.320366	R

```
Model #57        Cartesian coordinates in angstrom
                 x                y                z                Relaxed/Frozen
Al               4.717996         6.298635         9.025588         F
Al               6.299191         6.298979         11.957050        F
Al               4.718014         14.696931        9.025564         F
Al               4.828266         11.950610        9.158207         F
Al               4.828039         9.044839         9.158173         F
Al               7.260523         8.998662         12.959451        F
Al               7.260557         11.996884        12.959405        F
Al               6.299113         14.697042        11.957131        F
Al               4.636091         10.497818        12.053037        F
O                3.286786         10.497864        13.239716        F
Al               6.284122         4.912053         6.956134         F
Al               6.284446         16.083975        6.956192         F
Al               7.604080         10.497775        2.473921         F
O                6.427246         10.497874        1.094320         F
Al               6.373521         6.298812         3.886468         F
O                4.781448         6.298705         2.980326         F
Al               6.373532         14.696959        3.886458         F
O                4.781443         14.697008        2.980334         F
O                3.454056         4.976988         9.235326         F
O                3.454036         7.620428         9.235343         F
O                6.250043         5.002859         13.162230        F
O                3.454040         16.018719        9.235295         F
O                3.454024         13.375270        9.235304         F
O                7.425500         9.104830         14.776052        F
O                7.425500         11.890907        14.776054        F
O                6.249988         15.992850        13.162237        F
O                4.962364         3.365368         7.283628         F
O                7.499843         3.492595         6.705317         F
O                4.962257         17.630295        7.283457         F
O                7.499816         17.503151        6.705359         F
O                7.704772         6.298700         2.777140         F
O                7.704758         14.697015        2.777123         F
Al               3.478979         10.497849        7.046760         F
O                1.926558         11.807743        6.890260         F
O                1.926552         9.187978         6.890260         F
O                3.361166         10.497853        5.169011         F
Al               2.051007         10.497926        10.125658        F
O                0.574784         10.497857        9.076081         F
O                2.097764         9.088323         11.188758        F
O                2.097758         11.907396        11.188758        F
Al               3.393416         6.298670         6.011337         F
O                1.956483         6.298720         7.179501         F
O                3.339466         7.715105         4.949261         F
O                3.339462         4.882337         4.949248         F
Al               3.393402         14.697092        6.011319         F
O                1.956481         14.697000        7.179498         F
O                3.339448         16.113384        4.949254         F
O                3.339446         13.280604        4.949274         F
H                3.439929         4.911167         10.243970        F
H                3.439265         7.689470         10.293375        F
H                6.818394         4.213072         13.048228        F
H                6.229163         4.955320         14.133903        F
H                3.439934         16.084522        10.243550        F
H                3.439239         13.306202        10.293979        F
H                6.776964         8.347645         14.909841        F
H                6.777031         12.648025        14.909830        F
H                6.229194         16.040400        14.133948        F
H                6.818393         16.782646        13.048228        F
H                4.227300         2.737932         7.166029         F
H                6.932384         2.747747         6.973636         F
H                7.409113         3.550946         5.707010         F
H                4.227188         18.257670        7.166119         F
H                6.932385         18.247963        6.973623         F
H                7.409126         17.444753        5.706962         F
H                7.521090         6.298703         1.832227         F
H                7.521091         14.697004        1.832228         F
H                3.346923         10.497865        14.197637        F
H                6.469066         10.497863        0.138110         F
H                0.036294         9.692186         9.043062         F
H                0.036291         11.303521        9.043071         F
H                2.008439         9.058197         12.145151        F
H                2.008437         11.937519        12.145154        F
```

H	4.786758	6.298714	2.000110	F
H	4.786758	14.697000	2.000090	F
H	6.866328	9.838762	15.040445	F
H	6.866303	11.156964	15.040452	F
H	4.132075	16.721548	9.197247	F
H	4.893475	17.534246	8.246088	F
H	4.893410	3.461526	8.246082	F
H	4.132054	4.274187	9.197222	F
H	2.690124	11.221851	5.059459	F
H	2.690115	9.773877	5.059460	F
H	1.278479	12.508616	6.923338	F
H	1.278489	8.487091	6.923332	F
H	1.991769	6.298720	8.126704	F
H	1.991769	14.696996	8.126702	F
H	4.137962	13.968645	3.050505	F
H	4.137960	7.027072	3.050508	F
H	3.423379	4.865219	3.998926	F
H	3.423381	16.130498	3.998927	F
H	3.423045	7.732142	4.002715	F
H	3.423046	13.263575	4.002714	F
H	2.742665	6.961361	9.160613	F
H	2.742718	14.034373	9.160643	F
Al	6.212226	7.651923	6.958055	R
O	4.805333	6.303002	7.128777	R
O	7.468858	6.289847	7.300904	R
O	6.235132	7.651976	5.034760	R
Al	7.391717	6.189398	9.187532	R
O	6.489918	7.458917	13.292049	R
O	7.651818	5.841216	10.922584	R
O	6.039742	4.872025	8.818815	R
O	6.050923	7.604453	8.923924	R
Al	7.328167	9.019775	4.888828	R
Al	7.248163	11.976492	4.843804	R
Al	6.242065	13.351651	6.974119	R
Al	6.388552	10.498477	7.122985	R
O	4.827488	14.706016	7.127712	R
O	4.970280	11.816812	7.270775	R
O	4.960827	9.194657	7.267546	R
O	7.530041	14.730620	7.417433	R
O	6.338767	10.480103	5.085124	R
O	7.563873	12.012825	6.680007	R
O	7.589576	9.028835	6.761565	R
O	6.194560	13.367046	5.045551	R
Al	7.266596	14.857614	9.234769	R
Al	7.969629	10.492538	10.384149	R
O	6.187803	10.497429	13.139623	R
O	6.481295	13.535914	13.289620	R
O	6.381786	10.510006	9.062779	R
O	7.706591	15.045989	10.903438	R
O	6.044064	13.405646	8.932480	R
O	6.003863	16.161237	8.829917	R
O	8.168197	9.099713	11.512044	R
O	8.186067	11.852644	11.529771	R
O	4.800998	6.105378	10.939783	R
O	4.823773	14.913038	10.928492	R
O	4.798221	9.081291	10.960187	R
O	4.794503	11.928670	10.963456	R
O	6.311600	4.942111	5.070218	R
O	6.342095	16.042800	5.086814	R
O	8.130662	9.100382	3.334230	R
O	8.038227	11.947702	3.288916	R
O	3.496854	10.501907	8.967543	R
Cu	8.911014	8.725417	8.273227	R
Cu	8.953500	11.615270	7.909659	R
O	9.323204	10.362702	9.203444	R
O	9.155117	6.998720	8.988764	R
N	10.781973	7.040999	10.997984	R
N	9.789193	6.935405	10.499079	R

```
Model #58      Cartesian coordinates in angstrom
               x                y                z                Relaxed/Frozen
Al             4.717996         6.298635         9.025588         F
Al             6.299191         6.298979         11.957050        F
Al             4.718014         14.696931        9.025564         F
Al             4.828266         11.950610        9.158207         F
Al             4.828039         9.044839         9.158173         F
Al             7.260523         8.998662         12.959451        F
Al             7.260557         11.996884        12.959405        F
Al             6.299113         14.697042        11.957131        F
Al             4.636091         10.497818        12.053037        F
O              3.286786         10.497864        13.239716        F
Al             6.284122         4.912053         6.956134         F
Al             6.284446         16.083975        6.956192         F
Al             7.604080         10.497775        2.473921         F
O              6.427246         10.497874        1.094320         F
Al             6.373521         6.298812         3.886468         F
O              4.781448         6.298705         2.980326         F
Al             6.373532         14.696959        3.886458         F
O              4.781443         14.697008        2.980334         F
O              3.454056         4.976988         9.235326         F
O              3.454036         7.620428         9.235343         F
O              6.250043         5.002859         13.162230        F
O              3.454040         16.018719        9.235295         F
O              3.454024         13.375270        9.235304         F
O              7.425500         9.104830         14.776052        F
O              7.425500         11.890907        14.776054        F
O              6.249988         15.992850        13.162237        F
O              4.962364         3.365368         7.283628         F
O              7.499843         3.492595         6.705317         F
O              4.962257         17.630295        7.283457         F
O              7.499816         17.503151        6.705359         F
O              7.704772         6.298700         2.777140         F
O              7.704758         14.697015        2.777123         F
Al             3.478979         10.497849        7.046760         F
O              1.926558         11.807743        6.890260         F
O              1.926552         9.187978         6.890260         F
O              3.361166         10.497853        5.169011         F
Al             2.051007         10.497926        10.125658        F
O              0.574784         10.497857        9.076081         F
O              2.097764         9.088323         11.188758        F
O              2.097758         11.907396        11.188758        F
Al             3.393416         6.298670         6.011337         F
O              1.956483         6.298720         7.179501         F
O              3.339466         7.715105         4.949261         F
O              3.339462         4.882337         4.949248         F
Al             3.393402         14.697092        6.011319         F
O              1.956481         14.697000        7.179498         F
O              3.339448         16.113384        4.949254         F
O              3.339446         13.280604        4.949274         F
H              3.439929         4.911167         10.243970        F
H              3.439265         7.689470         10.293375        F
H              6.818394         4.213072         13.048228        F
H              6.229163         4.955320         14.133903        F
H              3.439934         16.084522        10.243550        F
H              3.439239         13.306202        10.293979        F
H              6.776964         8.347645         14.909841        F
H              6.777031         12.648025        14.909830        F
H              6.229194         16.040400        14.133948        F
H              6.818393         16.782646        13.048228        F
H              4.227300         2.737932         7.166029         F
H              6.932384         2.747747         6.973636         F
H              7.409113         3.550946         5.707010         F
H              4.227188         18.257670        7.166119         F
H              6.932385         18.247963        6.973623         F
H              7.409126         17.444753        5.706962         F
H              7.521090         6.298703         1.832227         F
H              7.521091         14.697004        1.832228         F
H              3.346923         10.497865        14.197637        F
H              6.469066         10.497863        0.138110         F
H              0.036294         9.692186         9.043062         F
H              0.036291         11.303521        9.043071         F
H              2.008439         9.058197         12.145151        F
H              2.008437         11.937519        12.145154        F
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H	4.786758	6.298714	2.000110	F
H	4.786758	14.697000	2.000090	F
H	6.866328	9.838762	15.040445	F
H	6.866303	11.156964	15.040452	F
H	4.132075	16.721548	9.197247	F
H	4.893475	17.534246	8.246088	F
H	4.893410	3.461526	8.246082	F
H	4.132054	4.274187	9.197222	F
H	2.690124	11.221851	5.059459	F
H	2.690115	9.773877	5.059460	F
H	1.278479	12.508616	6.923338	F
H	1.278489	8.487091	6.923332	F
H	1.991769	6.298720	8.126704	F
H	1.991769	14.696996	8.126702	F
H	4.137962	13.968645	3.050505	F
H	4.137960	7.027072	3.050508	F
H	3.423379	4.865219	3.998926	F
H	3.423381	16.130498	3.998927	F
H	3.423045	7.732142	4.002715	F
H	3.423046	13.263575	4.002714	F
H	2.742665	6.961361	9.160613	F
H	2.742718	14.034373	9.160643	F
Al	6.212226	7.651923	6.958055	R
O	4.805333	6.303002	7.128777	R
O	7.468858	6.289847	7.300904	R
O	6.235132	7.651976	5.034760	R
Al	7.391717	6.189398	9.187532	R
O	6.489918	7.458917	13.292049	R
O	7.651818	5.841216	10.922584	R
O	6.039742	4.872025	8.818815	R
O	6.050923	7.604453	8.923924	R
Al	7.328167	9.019775	4.888828	R
Al	7.248163	11.976492	4.843804	R
Al	6.242065	13.351651	6.974119	R
Al	6.388552	10.498477	7.122985	R
O	4.827488	14.706016	7.127712	R
O	4.970280	11.816812	7.270775	R
O	4.960827	9.194657	7.267546	R
O	7.530041	14.730620	7.417433	R
O	6.338767	10.480103	5.085124	R
O	7.563873	12.012825	6.680007	R
O	7.589576	9.028835	6.761565	R
O	6.194560	13.367046	5.045551	R
Al	7.266596	14.857614	9.234769	R
Al	7.969629	10.492538	10.384149	R
O	6.187803	10.497429	13.139623	R
O	6.481295	13.535914	13.289620	R
O	6.381786	10.510006	9.062779	R
O	7.706591	15.045989	10.903438	R
O	6.044064	13.405646	8.932480	R
O	6.003863	16.161237	8.829917	R
O	8.168197	9.099713	11.512044	R
O	8.186067	11.852644	11.529771	R
O	4.800998	6.105378	10.939783	R
O	4.823773	14.913038	10.928492	R
O	4.798221	9.081291	10.960187	R
O	4.794503	11.928670	10.963456	R
O	6.311600	4.942111	5.070218	R
O	6.342095	16.042800	5.086814	R
O	8.130662	9.100382	3.334230	R
O	8.038227	11.947702	3.288916	R
O	3.496854	10.501907	8.967543	R
Cu	8.911014	8.725417	8.273227	R
Cu	8.953500	11.615270	7.909659	R
O	9.323204	10.362702	9.203444	R
O	9.155117	6.998720	8.988764	R
N	10.781973	7.040999	10.997984	R
N	9.789193	6.935405	10.499079	R

```
Model #59        Cartesian coordinates in angstrom
                 x               y               z              Relaxed/Frozen
Al       4.718134        6.298787        9.025575        F
Al       6.299199        6.298691        11.957091       F
Al       4.718050        14.696869       9.025064        F
Al       4.828239        11.950999       9.158196        F
Al       4.828346        9.045211        9.158193        F
Al       7.260465        8.998778        12.959355       F
Al       7.260416        11.997151       12.959495       F
Al       6.298917        14.696556       11.956997       F
Al       4.636052        10.497867       12.053046       F
O        3.286790        10.497863       13.239721       F
Al       6.284441        4.911766        6.956115        F
Al       6.284246        16.083659       6.956355        F
Al       7.604203        10.497770       2.473871        F
O        6.427181        10.497846       1.094374        F
Al       6.373519        6.298761        3.886463        F
O        4.781441        6.298715        2.980337        F
Al       6.373513        14.696932       3.886400        F
O        4.781433        14.697010       2.980352        F
O        3.454055        4.976986        9.235307        F
O        3.454090        7.620352        9.235338        F
O        6.250003        5.002880        13.162251       F
O        3.454040        16.018735       9.235196        F
O        3.453918        13.375343       9.235438        F
O        7.425522        9.104830        14.776050       F
O        7.425531        11.890947       14.776053       F
O        6.250142        15.992894       13.162196       F
O        4.962261        3.365418        7.283450        F
O        7.499823        3.492575        6.705337        F
O        4.962370        17.630340       7.283698        F
O        7.499856        17.503122       6.705383        F
O        7.704777        6.298704        2.777146        F
O        7.704776        14.697000       2.777144        F
Al       3.478896        10.498106       7.046857        F
O        1.926542        11.807724       6.890244        F
O        1.926577        9.187947        6.890283        F
O        3.361158        10.497868       5.169012        F
Al       2.050936        10.497850       10.125677       F
O        0.574780        10.497852       9.076087        F
O        2.097756        9.088319        11.188754       F
O        2.097751        11.907394       11.188761       F
Al       3.393314        6.298723        6.011419        F
O        1.956476        6.298708        7.179492        F
O        3.339456        7.715092        4.949245        F
O        3.339456        4.882336        4.949249        F
Al       3.393285        14.697035       6.011428        F
O        1.956480        14.697008       7.179496        F
O        3.339467        16.113375       4.949242        F
O        3.339472        13.280617       4.949256        F
H        3.439919        4.911176        10.243970       F
H        3.439245        7.689448        10.293376       F
H        6.818377        4.213062        13.048216       F
H        6.229159        4.955320        14.133903       F
H        3.439935        16.084524       10.243550       F
H        3.439267        13.306167       10.293976       F
H        6.776980        8.347631        14.909840       F
H        6.776976        12.647978       14.909831       F
H        6.229167        16.040399       14.133947       F
H        6.818424        16.782628       13.048249       F
H        4.227193        2.738041        7.166114        F
H        6.932387        2.747748        6.973645        F
H        7.409114        3.550947        5.707010        F
H        4.227420        18.257907       7.165935        F
H        6.932387        18.247962       6.973629        F
H        7.409089        17.444786       5.706964        F
H        7.521090        6.298720        1.832227        F
H        7.521091        14.697009       1.832228        F
H        3.346923        10.497850       14.197637       F
H        6.469066        10.497890       0.138110        F
H        0.036291        9.692187        9.043065        F
H        0.036295        11.303524       9.043065        F
H        2.008439        9.058197        12.145151       F
H        2.008448        11.937518       12.145155       F
```

H	4.786758	6.298712	2.000110	F
H	4.786758	14.696994	2.000090	F
H	6.866326	9.838760	15.040446	F
H	6.866396	11.156887	15.040439	F
H	4.132085	16.721544	9.197336	F
H	4.893274	17.534080	8.246057	F
H	4.893460	3.461485	8.246090	F
H	4.132056	4.274187	9.197234	F
H	2.690104	11.221832	5.059460	F
H	2.690145	9.773848	5.059458	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298716	8.126704	F
H	1.991769	14.697001	8.126702	F
H	4.137960	13.968647	3.050509	F
H	4.137967	7.027078	3.050497	F
H	3.423388	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423057	7.732143	4.002716	F
H	3.423048	13.263574	4.002715	F
H	2.742679	6.961343	9.160652	F
H	2.742701	14.034360	9.160700	F
Al	6.208211	7.649164	6.959888	R
O	4.798331	6.308976	7.128667	R
O	7.446624	6.291253	7.257061	R
O	6.240273	7.661625	5.031390	R
Al	7.435034	6.199094	9.199897	R
O	6.475831	7.472977	13.291240	R
O	7.653677	5.898656	10.932497	R
O	6.048267	4.884632	8.816805	R
O	6.048563	7.618181	8.914513	R
Al	7.349926	9.013264	4.903141	R
Al	7.258296	11.974256	4.849004	R
Al	6.229806	13.349355	6.971772	R
Al	6.388971	10.496768	7.113737	R
O	4.824541	14.704981	7.129431	R
O	4.973758	11.822588	7.271049	R
O	4.962960	9.210133	7.267965	R
O	7.521730	14.722969	7.398444	R
O	6.356177	10.476734	5.095326	R
O	7.566407	11.999831	6.700617	R
O	7.599273	9.035207	6.791651	R
O	6.204460	13.364331	5.048280	R
Al	7.293875	14.850300	9.227327	R
Al	7.832569	10.543394	10.385438	R
O	6.191730	10.508021	13.138014	R
O	6.498513	13.544831	13.298817	R
O	6.375198	10.529475	9.063337	R
O	7.694551	15.085940	10.913147	R
O	6.054080	13.404273	8.935219	R
O	6.014674	16.153964	8.827937	R
O	8.181627	9.216345	11.534655	R
O	8.112744	11.953090	11.458026	R
O	4.778315	6.120371	10.947121	R
O	4.820418	14.906094	10.929965	R
O	4.824548	9.096898	10.958200	R
O	4.809993	11.929465	10.965333	R
O	6.300150	4.938689	5.062508	R
O	6.339349	16.044239	5.085136	R
O	8.148468	9.112615	3.345291	R
O	8.038625	11.950174	3.289614	R
O	3.502627	10.507374	8.972785	R
Cu	8.895695	8.766076	8.390524	R
Cu	8.981160	11.890309	7.991936	R
O	9.184981	10.431094	9.136014	R
O	9.097995	6.943625	8.748898	R
N	10.565238	13.746820	11.391047	R
N	10.063269	13.785285	10.388883	R
O	9.574500	13.843005	9.289070	R

```
Model #60      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718141       6.298811       9.025583       F
Al             6.299236       6.298645       11.957119      F
Al             4.718033       14.696905      9.024978       F
Al             4.828281       11.951046      9.158253       F
Al             4.828338       9.045302       9.158122       F
Al             7.260363       8.998800       12.959316      F
Al             7.260407       11.997196      12.959575      F
Al             6.298930       14.696562      11.956940      F
Al             4.636080       10.497839      12.053049      F
O              3.286787       10.497868      13.239718      F
Al             6.284433       4.911793       6.956116       F
Al             6.284135       16.083312      6.956424       F
Al             7.604224       10.497817      2.473857       F
O              6.427170       10.497825      1.094384       F
Al             6.373534       6.298746       3.886461       F
O              4.781439       6.298714       2.980341       F
Al             6.373529       14.696991      3.886383       F
O              4.781442       14.697018      2.980337       F
O              3.454060       4.976981       9.235311       F
O              3.454113       7.620317       9.235346       F
O              6.250009       5.002883       13.162254      F
O              3.454054       16.018739      9.235256       F
O              3.453922       13.375347      9.235431       F
O              7.425554       9.104823       14.776047      F
O              7.425555       11.890913      14.776049      F
O              6.250216       15.992889      13.162204      F
O              4.962261       3.365419       7.283454       F
O              7.499815       3.492568       6.705336       F
O              4.962391       17.630328      7.283841       F
O              7.499818       17.503148      6.705347       F
O              7.704775       6.298700       2.777144       F
O              7.704777       14.697012      2.777145       F
Al             3.478864       10.498170      7.046842       F
O              1.926538       11.807720      6.890245       F
O              1.926589       9.187932       6.890290       F
O              3.361175       10.497860      5.169011       F
Al             2.050943       10.497837      10.125679      F
O              0.574780       10.497851      9.076088       F
O              2.097754       9.088319       11.188754      F
O              2.097751       11.907395      11.188760      F
Al             3.393312       6.298718       6.011420       F
O              1.956476       6.298710       7.179492       F
O              3.339457       7.715092       4.949245       F
O              3.339455       4.882336       4.949249       F
Al             3.393303       14.697073      6.011421       F
O              1.956480       14.696993      7.179496       F
O              3.339461       16.113374      4.949241       F
O              3.339478       13.280615      4.949258       F
H              3.439915       4.911180       10.243970      F
H              3.439237       7.689458       10.293375      F
H              6.818376       4.213061       13.048215      F
H              6.229155       4.955320       14.133903      F
H              3.439934       16.084523      10.243550      F
H              3.439262       13.306155      10.293375      F
H              6.776982       8.347629       14.909840      F
H              6.776979       12.647980      14.909831      F
H              6.229116       16.040398      14.133946      F
H              6.818416       16.782633      13.048243      F
H              4.227196       2.738038       7.166111       F
H              6.932387       2.747748       6.973645       F
H              7.409115       3.550948       5.707010       F
H              4.227516       18.258005      7.165859       F
H              6.932382       18.247964      6.973615       F
H              7.409086       17.444789      5.706964       F
H              7.521090       6.298724       1.832227       F
H              7.521091       14.696995      1.832228       F
H              3.346923       10.497848      14.197637      F
H              6.469066       10.497891      0.138110       F
H              0.036290       9.692187       9.043066       F
H              0.036296       11.303524      9.043064       F
H              2.008439       9.058197       12.145151      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298712	2.000110	F
H	4.786758	14.696976	2.000090	F
H	6.866325	9.838759	15.040446	F
H	6.866375	11.156904	15.040442	F
H	4.132082	16.721545	9.197312	F
H	4.893218	17.534034	8.246048	F
H	4.893460	3.461485	8.246090	F
H	4.132056	4.274187	9.197231	F
H	2.690098	11.221826	5.059460	F
H	2.690145	9.773848	5.059458	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697009	8.126702	F
H	4.137952	13.968655	3.050523	F
H	4.137967	7.027078	3.050496	F
H	3.423389	4.865219	3.998926	F
H	3.423390	16.130499	3.998927	F
H	3.423057	7.732143	4.002716	F
H	3.423043	13.263574	4.002715	F
H	2.742679	6.961343	9.160652	F
H	2.742701	14.034360	9.160701	F
Al	6.201331	7.640525	6.954410	R
O	4.781298	6.310181	7.130051	R
O	7.436990	6.288989	7.252496	R
O	6.196365	7.661414	5.022196	R
Al	7.447620	6.212663	9.193144	R
O	6.474481	7.471039	13.293218	R
O	7.643013	5.885873	10.924648	R
O	6.041164	4.889363	8.813081	R
O	6.038124	7.621919	8.903961	R
Al	7.306138	9.017306	4.896219	R
Al	7.288019	11.977124	4.880704	R
Al	6.197642	13.359498	6.958305	R
Al	6.369822	10.494054	7.111640	R
O	4.783330	14.688052	7.130552	R
O	4.910259	11.808900	7.253851	R
O	4.904986	9.194499	7.254095	R
O	7.446250	14.702195	7.291538	R
O	6.338873	10.495933	5.101526	R
O	7.547345	11.978541	6.759392	R
O	7.548741	9.022664	6.776507	R
O	6.192815	13.341560	5.028870	R
Al	7.432164	14.796152	9.192604	R
Al	7.784447	10.521508	10.368756	R
O	6.187550	10.499917	13.137367	R
O	6.477304	13.529263	13.297018	R
O	6.285945	10.504100	9.052945	R
O	7.630174	15.151369	10.922181	R
O	6.045155	13.377378	8.911147	R
O	6.033035	16.116168	8.812727	R
O	8.122491	9.166097	11.482380	R
O	8.089181	11.904493	11.453552	R
O	4.770615	6.124713	10.946034	R
O	4.772990	14.868643	10.942863	R
O	4.782695	9.091574	10.951504	R
O	4.778581	11.906183	10.951687	R
O	6.289846	4.939124	5.061533	R
O	6.298966	16.052420	5.067070	R
O	8.094568	9.087715	3.334123	R
O	8.073177	11.923975	3.319645	R
O	3.441226	10.499726	8.940409	R
Cu	8.888717	8.771319	8.367296	R
Cu	8.913613	12.182911	8.224462	R
O	9.049057	10.493180	9.035788	R
O	9.113526	6.980830	8.810255	R
N	11.121581	13.802082	10.370892	R
N	10.017680	14.043095	10.234477	R
O	9.214264	14.050663	8.949548	R

```
Model #61       Cartesian coordinates in angstrom
                x               y               z               Relaxed/Frozen
Al              4.718141        6.298811        9.025583        F
Al              6.299236        6.298645        11.957119       F
Al              4.718033        14.696905       9.024978        F
Al              4.828281        11.951046       9.158253        F
Al              4.828338        9.045302        9.158122        F
Al              7.260363        8.998800        12.959316       F
Al              7.260407        11.997196       12.959575       F
Al              6.298930        14.696562       11.956940       F
Al              4.636080        10.497839       12.053049       F
O               3.286787        10.497868       13.239718       F
Al              6.284433        4.911793        6.956116        F
Al              6.284135        16.083312       6.956424        F
Al              7.604224        10.497817       2.473857        F
O               6.427170        10.497825       1.094384        F
Al              6.373534        6.298746        3.886461        F
O               4.781439        6.298714        2.980341        F
Al              6.373529        14.696991       3.886383        F
O               4.781442        14.697018       2.980337        F
O               3.454060        4.976981        9.235311        F
O               3.454113        7.620317        9.235346        F
O               6.250009        5.002883        13.162254       F
O               3.454054        16.018739       9.235256        F
O               3.453922        13.375347       9.235431        F
O               7.425554        9.104823        14.776047       F
O               7.425555        11.890913       14.776049       F
O               6.250216        15.992889       13.162204       F
O               4.962261        3.365419        7.283454        F
O               7.499815        3.492568        6.705336        F
O               4.962391        17.630328       7.283841        F
O               7.499818        17.503148       6.705347        F
O               7.704775        6.298700        2.777144        F
O               7.704777        14.697012       2.777145        F
Al              3.478864        10.498170       7.046842        F
O               1.926538        11.807720       6.890245        F
O               1.926589        9.187932        6.890290        F
O               3.361175        10.497860       5.169011        F
Al              2.050943        10.497837       10.125679       F
O               0.574780        10.497851       9.076088        F
O               2.097754        9.088319        11.188754       F
O               2.097751        11.907395       11.188760       F
Al              3.393312        6.298718        6.011420        F
O               1.956476        6.298710        7.179492        F
O               3.339457        7.715092        4.949245        F
O               3.339455        4.882336        4.949249        F
Al              3.393303        14.697073       6.011421        F
O               1.956480        14.696993       7.179496        F
O               3.339461        16.113374       4.949241        F
O               3.339478        13.280615       4.949258        F
H               3.439915        4.911180        10.243970       F
H               3.439237        7.689458        10.293375       F
H               6.818376        4.213061        13.048215       F
H               6.229155        4.955320        14.133903       F
H               3.439934        16.084523       10.243550       F
H               3.439262        13.306155       10.293375       F
H               6.776982        8.347629        14.909840       F
H               6.776979        12.647980       14.909831       F
H               6.229116        16.040398       14.133946       F
H               6.818416        16.782633       13.048243       F
H               4.227196        2.738038        7.166111        F
H               6.932387        2.747748        6.973645        F
H               7.409115        3.550948        5.707010        F
H               4.227516        18.258005       7.165859        F
H               6.932382        18.247964       6.973615        F
H               7.409086        17.444789       5.706964        F
H               7.521090        6.298724        1.832227        F
H               7.521091        14.696995       1.832228        F
H               3.346923        10.497848       14.197637       F
H               6.469066        10.497891       0.138110        F
H               0.036290        9.692187        9.043066        F
H               0.036296        11.303524       9.043064        F
H               2.008439        9.058197        12.145151       F
H               2.008447        11.937518       12.145155       F
```

H	4.786758	6.298712	2.000110	F
H	4.786758	14.696976	2.000090	F
H	6.866325	9.838759	15.040446	F
H	6.866375	11.156904	15.040442	F
H	4.132082	16.721545	9.197312	F
H	4.893218	17.534034	8.246048	F
H	4.893460	3.461485	8.246090	F
H	4.132056	4.274187	9.197231	F
H	2.690098	11.221826	5.059460	F
H	2.690145	9.773848	5.059458	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697009	8.126702	F
H	4.137952	13.968655	3.050523	F
H	4.137967	7.027078	3.050496	F
H	3.423389	4.865219	3.998926	F
H	3.423390	16.130499	3.998927	F
H	3.423057	7.732143	4.002716	F
H	3.423043	13.263574	4.002715	F
H	2.742679	6.961343	9.160652	F
H	2.742701	14.034360	9.160701	F
Al	6.201331	7.640525	6.954410	R
O	4.781298	6.310181	7.130051	R
O	7.436990	6.288989	7.252496	R
O	6.196365	7.661414	5.022196	R
Al	7.447620	6.212663	9.193144	R
O	6.474481	7.471039	13.293218	R
O	7.643013	5.885873	10.924648	R
O	6.041164	4.889363	8.813081	R
O	6.038124	7.621919	8.903961	R
Al	7.306138	9.017306	4.896219	R
Al	7.288019	11.977124	4.880704	R
Al	6.197642	13.359498	6.958305	R
Al	6.369822	10.494054	7.111640	R
O	4.783330	14.688052	7.130552	R
O	4.910259	11.808900	7.253851	R
O	4.904986	9.194499	7.254095	R
O	7.446250	14.702195	7.291538	R
O	6.338873	10.495933	5.101526	R
O	7.547345	11.978541	6.759392	R
O	7.548741	9.022664	6.776507	R
O	6.192815	13.341560	5.028870	R
Al	7.432164	14.796152	9.192604	R
Al	7.784447	10.521508	10.368756	R
O	6.187550	10.499917	13.137367	R
O	6.477304	13.529263	13.297018	R
O	6.285945	10.504100	9.052945	R
O	7.630174	15.151369	10.922181	R
O	6.045155	13.377378	8.911147	R
O	6.033035	16.116168	8.812727	R
O	8.122491	9.166097	11.482380	R
O	8.089181	11.904493	11.453552	R
O	4.770615	6.124713	10.946034	R
O	4.772990	14.868643	10.942863	R
O	4.782695	9.091574	10.951504	R
O	4.778581	11.906183	10.951687	R
O	6.289846	4.939124	5.061533	R
O	6.298966	16.052420	5.067070	R
O	8.094568	9.087715	3.334123	R
O	8.073177	11.923975	3.319645	R
O	3.441226	10.499726	8.940409	R
Cu	8.913613	12.182911	8.224462	R
Cu	8.888717	8.771319	8.367296	R
O	9.049057	10.493180	9.035788	R
O	9.113526	6.980830	8.810255	R
N	11.121581	13.802082	10.370892	R
N	10.017680	14.043095	10.234477	R
O	9.214264	14.050663	8.949548	R

```
Model #62      Cartesian coordinates in angstrom
               x             y             z             Relaxed/Frozen
Al             4.718173      6.298911      9.025576      F
Al             6.299261      6.298761      11.957069     F
Al             4.718048      14.696800     9.025016      F
Al             4.828110      11.950989     9.158277      F
Al             4.828296      9.045501      9.158060      F
Al             7.260436      8.999298      12.958900     F
Al             7.260294      11.997700     12.959250     F
Al             6.298524      14.695997     11.957207     F
Al             4.636051      10.497892     12.053108     F
O              3.286798      10.497866     13.239730     F
Al             6.284442      4.911970      6.956137      F
Al             6.283918      16.082286     6.956934      F
Al             7.604237      10.497807     2.473992      F
O              6.427189      10.497839     1.094367      F
Al             6.373539      6.298801      3.886506      F
O              4.781440      6.298721      2.980339      F
Al             6.373400      14.696718     3.886501      F
O              4.781448      14.697025     2.980327      F
O              3.454100      4.976948      9.235332      F
O              3.454127      7.620267      9.235322      F
O              6.250027      5.002872      13.162244     F
O              3.454188      16.018922     9.234915      F
O              3.453920      13.375344     9.235529      F
O              7.425646      9.104791      14.776041     F
O              7.425714      11.891039     14.776041     F
O              6.250265      15.993050     13.162033     F
O              4.962267      3.365421      7.283490      F
O              7.499821      3.492574      6.705334      F
O              4.962539      17.630401     7.284092      F
O              7.499884      17.503123     6.705521      F
O              7.704782      6.298701      2.777153      F
O              7.704785      14.696992     2.777155      F
Al             3.478768      10.498243     7.046873      F
O              1.926554      11.807737     6.890236      F
O              1.926609      9.187906      6.890301      F
O              3.361183      10.497911     5.169010      F
Al             2.050945      10.497865     10.125628     F
O              0.574781      10.497850     9.076086      F
O              2.097764      9.088327      11.188763     F
O              2.097751      11.907385     11.188773     F
Al             3.393312      6.298744      6.011434      F
O              1.956476      6.298698      7.179492      F
O              3.339453      7.715090      4.949242      F
O              3.339457      4.882336      4.949249      F
Al             3.393322      14.697031     6.011457      F
O              1.956481      14.697051     7.179497      F
O              3.339471      16.113372     4.949239      F
O              3.339466      13.280637     4.949230      F
H              3.439931      4.911165      10.243969     F
H              3.439254      7.689420      10.293378     F
H              6.818347      4.213044      13.048195     F
H              6.229114      4.955321      14.133902     F
H              3.439931      16.084520     10.243550     F
H              3.439295      13.306236     10.293981     F
H              6.777056      8.347565      14.909837     F
H              6.776834      12.647855     14.909836     F
H              6.229100      16.040398     14.133946     F
H              6.818526      16.782564     13.048321     F
H              4.227219      2.738015      7.166094      F
H              6.932384      2.747748      6.973636      F
H              7.409073      3.550911      5.707011      F
H              4.227815      18.258310     7.165622      F
H              6.932337      18.247978     6.973478      F
H              7.409017      17.444848     5.706967      F
H              7.521090      6.298711      1.832227      F
H              7.521091      14.697047     1.832228      F
H              3.346923      10.497845     14.197637     F
H              6.469066      10.497903     0.138110      F
H              0.036292      9.692186      9.043064      F
H              0.036293      11.303523     9.043067      F
H              2.008442      9.058197      12.145151     F
H              2.008458      11.937517     12.145156     F
```

H	4.786758	6.298708	2.000110	F
H	4.786758	14.697015	2.000090	F
H	6.866247	9.838695	15.040457	F
H	6.866528	11.156780	15.040421	F
H	4.132090	16.721542	9.197382	F
H	4.893041	17.533889	8.246021	F
H	4.893450	3.461494	8.246089	F
H	4.132055	4.274186	9.197223	F
H	2.690109	11.221837	5.059460	F
H	2.690182	9.773813	5.059456	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298719	8.126704	F
H	1.991769	14.696984	8.126702	F
H	4.137971	13.968635	3.050490	F
H	4.137968	7.027079	3.050495	F
H	3.423387	4.865219	3.998926	F
H	3.423383	16.130499	3.998927	F
H	3.423062	7.732143	4.002716	F
H	3.423067	13.263572	4.002716	F
H	2.742679	6.961341	9.160667	F
H	2.742700	14.034350	9.160628	F
Al	6.203530	7.640655	6.954874	R
O	4.774524	6.311717	7.132741	R
O	7.430958	6.286776	7.255504	R
O	6.183471	7.657951	5.021790	R
Al	7.459686	6.215552	9.191694	R
O	6.464781	7.473782	13.293618	R
O	7.632177	5.868636	10.924257	R
O	6.033824	4.889759	8.816139	R
O	6.033219	7.623194	8.907662	R
Al	7.289202	9.020199	4.893417	R
Al	7.287544	11.974521	4.893747	R
Al	6.205996	13.355144	6.955329	R
Al	6.374146	10.498433	7.110648	R
O	4.774429	14.682952	7.132578	R
O	4.886987	11.803187	7.257103	R
O	4.887421	9.191598	7.256869	R
O	7.431124	14.708818	7.255930	R
O	6.321285	10.496557	5.094874	R
O	7.533606	11.972984	6.768427	R
O	7.534422	9.021159	6.769286	R
O	6.182561	13.337165	5.021341	R
Al	7.462745	14.779254	9.191236	R
Al	7.793032	10.499778	10.363687	R
O	6.182124	10.498091	13.136612	R
O	6.462536	13.521713	13.294654	R
O	6.264222	10.497503	9.060324	R
O	7.630570	15.126710	10.924861	R
O	6.032933	13.372226	8.907875	R
O	6.033482	16.105200	8.816565	R
O	8.099737	9.130979	11.467750	R
O	8.101242	11.866130	11.469656	R
O	4.760013	6.143664	10.950952	R
O	4.758178	14.851145	10.951570	R
O	4.769285	9.096596	10.950299	R
O	4.769389	11.899359	10.950454	R
O	6.285942	4.937182	5.060946	R
O	6.285638	16.058088	5.061064	R
O	8.076575	9.078703	3.329552	R
O	8.075510	11.916602	3.330010	R
O	3.424100	10.497733	8.937909	R
Cu	8.903408	12.243942	8.354163	R
Cu	8.898168	8.761585	8.351297	R
O	9.014363	10.499471	8.995214	R
O	9.123788	6.969509	8.805790	R
O	9.130145	14.029851	8.816172	R

```
Model #63      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718167       6.298904       9.025575       F
Al             6.299282       6.298771       11.957065      F
Al             4.718020       14.696828      9.025000       F
Al             4.828077       11.951010      9.158300       F
Al             4.828273       9.045486       9.158069       F
Al             7.260421       8.999335       12.958867      F
Al             7.260238       11.997733      12.959220      F
Al             6.298544       14.695964      11.957264      F
Al             4.636050       10.497901      12.053111      F
O              3.286800       10.497866      13.239733      F
Al             6.284451       4.911960       6.956124       F
Al             6.283896       16.082230      6.956959       F
Al             7.604228       10.497817      2.473988       F
O              6.427193       10.497844      1.094363       F
Al             6.373557       6.298804       3.886506       F
O              4.781441       6.298721       2.980336       F
Al             6.373398       14.696691      3.886514       F
O              4.781448       14.697021      2.980327       F
O              3.454101       4.976948       9.235338       F
O              3.454133       7.620263       9.235320       F
O              6.250036       5.002873       13.162246      F
O              3.454195       16.018936      9.234868       F
O              3.453912       13.375339      9.235544       F
O              7.425656       9.104793       14.776040      F
O              7.425725       11.891059      14.776042      F
O              6.250297       15.993039      13.162046      F
O              4.962266       3.365421       7.283486       F
O              7.499822       3.492575       6.705335       F
O              4.962541       17.630401      7.284103       F
O              7.499894       17.503117      6.705539       F
O              7.704782       6.298702       2.777153       F
O              7.704786       14.696990      2.777157       F
Al             3.478761       10.498247      7.046871       F
O              1.926554       11.807737      6.890238       F
O              1.926610       9.187905       6.890296       F
O              3.361184       10.497915      5.169010       F
Al             2.050945       10.497863      10.125634      F
O              0.574782       10.497852      9.076085       F
O              2.097766       9.088327       11.188764      F
O              2.097754       11.907385      11.188773      F
Al             3.393315       6.298742       6.011430       F
O              1.956476       6.298700       7.179492       F
O              3.339454       7.715091       4.949244       F
O              3.339458       4.882336       4.949249       F
Al             3.393323       14.697012      6.011458       F
O              1.956482       14.697054      7.179498       F
O              3.339473       16.113373      4.949240       F
O              3.339465       13.280638      4.949229       F
H              3.439933       4.911164       10.243969      F
H              3.439259       7.689421       10.293378      F
H              6.818343       4.213042       13.048192      F
H              6.229115       4.955321       14.133902      F
H              3.439933       16.084522      10.243550      F
H              3.439286       13.306240      10.293981      F
H              6.777063       8.347559       14.909836      F
H              6.776829       12.647850      14.909836      F
H              6.229104       16.040398      14.133946      F
H              6.818529       16.782562      13.048323      F
H              4.227215       2.738019       7.166097       F
H              6.932385       2.747748       6.973639       F
H              7.409074       3.550912       5.707011       F
H              4.227831       18.258326      7.165610       F
H              6.932336       18.247978      6.973476       F
H              7.409025       17.444841      5.706966       F
H              7.521090       6.298708       1.832227       F
H              7.521091       14.697052      1.832228       F
H              3.346923       10.497843      14.197637      F
H              6.469066       10.497903      0.138110       F
H              0.036292       9.692186       9.043064       F
H              0.036293       11.303523      9.043067       F
H              2.008443       9.058197       12.145151      F
H              2.008458       11.937517      12.145156      F
```

H	4.786758	6.298710	2.000110	F
H	4.786758	14.697020	2.000090	F
H	6.866242	9.838692	15.040458	F
H	6.866542	11.156768	15.040419	F
H	4.132088	16.721542	9.197369	F
H	4.893034	17.533883	8.246020	F
H	4.893449	3.461494	8.246089	F
H	4.132055	4.274186	9.197223	F
H	2.690111	11.221838	5.059460	F
H	2.690182	9.773813	5.059456	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298720	8.126704	F
H	1.991769	14.696983	8.126702	F
H	4.137973	13.968634	3.050487	F
H	4.137967	7.027078	3.050497	F
H	3.423386	4.865219	3.998926	F
H	3.423382	16.130499	3.998927	F
H	3.423061	7.732143	4.002716	F
H	3.423069	13.263572	4.002716	F
H	2.742679	6.961341	9.160667	F
H	2.742699	14.034348	9.160614	F
Al	6.199584	7.641686	6.955309	R
O	4.780314	6.309426	7.130742	R
O	7.436055	6.288552	7.252444	R
O	6.195409	7.660796	5.024031	R
Al	7.444549	6.205755	9.195634	R
O	6.473128	7.470581	13.295430	R
O	7.642069	5.878177	10.925661	R
O	6.040115	4.887688	8.812755	R
O	6.038816	7.620231	8.905168	R
Al	7.306914	9.016577	4.897104	R
Al	7.304396	11.978115	4.896355	R
Al	6.200550	13.353476	6.955374	R
Al	6.376854	10.497600	7.115463	R
O	4.780395	14.685973	7.130723	R
O	4.902863	11.804007	7.254582	R
O	4.902945	9.191626	7.254507	R
O	7.436281	14.706509	7.252691	R
O	6.347164	10.496746	5.109976	R
O	7.549689	11.977814	6.780929	R
O	7.550465	9.016915	6.781697	R
O	6.194157	13.334546	5.023908	R
Al	7.444446	14.789590	9.196222	R
Al	7.771747	10.498469	10.370966	R
O	6.187636	10.498218	13.136765	R
O	6.471508	13.525369	13.296670	R
O	6.277939	10.498024	9.056660	R
O	7.641843	15.115982	10.926404	R
O	6.038828	13.375477	8.905108	R
O	6.040224	16.107406	8.813165	R
O	8.104378	9.130274	11.466054	R
O	8.103180	11.867278	11.465805	R
O	4.770699	6.124763	10.945107	R
O	4.770135	14.871108	10.945051	R
O	4.778870	9.091303	10.951247	R
O	4.778637	11.904999	10.951435	R
O	6.288951	4.939213	5.062054	R
O	6.288730	16.055971	5.062423	R
O	8.085876	9.081233	3.330030	R
O	8.083353	11.915455	3.329316	R
O	3.435518	10.498064	8.938659	R
Cu	8.880572	12.233652	8.357461	R
Cu	8.881130	8.763529	8.357550	R
O	9.010654	10.498434	9.005156	R
O	9.106589	6.956904	8.767600	R
O	9.107399	14.039705	8.768938	R

```
Model #64     Cartesian coordinates in angstrom
              x              y              z              Relaxed/Frozen
Al            4.718144       6.298915       9.025586       F
Al            6.299260       6.298778       11.957061      F
Al            4.718014       14.696822      9.024996       F
Al            4.828072       11.951002      9.158309       F
Al            4.828265       9.045485       9.158086       F
Al            7.260408       8.999308       12.958819      F
Al            7.260227       11.997703      12.959170      F
Al            6.298543       14.695952      11.957252      F
Al            4.636033       10.497894      12.053111      F
O             3.286798       10.497866      13.239731      F
Al            6.284435       4.911986       6.956130       F
Al            6.283897       16.082221      6.956957       F
Al            7.604249       10.497821      2.474009       F
O             6.427192       10.497847      1.094364       F
Al            6.373567       6.298821       3.886518       F
O             4.781440       6.298726       2.980338       F
Al            6.373409       14.696684      3.886520       F
O             4.781449       14.697019      2.980325       F
O             3.454087       4.976961       9.235337       F
O             3.454123       7.620259       9.235334       F
O             6.250053       5.002880       13.162254      F
O             3.454190       16.018932      9.234861       F
O             3.453904       13.375334      9.235545       F
O             7.425659       9.104790       14.776040      F
O             7.425737       11.891055      14.776041      F
O             6.250304       15.993040      13.162045      F
O             4.962266       3.365421       7.283486       F
O             7.499841       3.492593       6.705325       F
O             4.962541       17.630401      7.284103       F
O             7.499898       17.503114      6.705540       F
O             7.704784       6.298703       2.777155       F
O             7.704790       14.696990      2.777162       F
Al            3.478764       10.498244      7.046885       F
O             1.926553       11.807736      6.890239       F
O             1.926611       9.187904       6.890298       F
O             3.361190       10.497913      5.169010       F
Al            2.050941       10.497861      10.125638      F
O             0.574782       10.497851      9.076085       F
O             2.097766       9.088327       11.188764      F
O             2.097754       11.907385      11.188773      F
Al            3.393314       6.298746       6.011433       F
O             1.956476       6.298699       7.179492       F
O             3.339452       7.715091       4.949244       F
O             3.339458       4.882336       4.949249       F
Al            3.393323       14.697008      6.011452       F
O             1.956482       14.697055      7.179498       F
O             3.339474       16.113372      4.949239       F
O             3.339464       13.280638      4.949229       F
H             3.439924       4.911172       10.243969      F
H             3.439251       7.689419       10.293378      F
H             6.818356       4.213050       13.048201      F
H             6.229137       4.955321       14.133902      F
H             3.439930       16.084519      10.243550      F
H             3.439279       13.306238      10.293981      F
H             6.777063       8.347559       14.909836      F
H             6.776840       12.647859      14.909836      F
H             6.229112       16.040398      14.133946      F
H             6.818531       16.782561      13.048324      F
H             4.227215       2.738019       7.166097       F
H             6.932385       2.747748       6.973638       F
H             7.409086       3.550922       5.707011       F
H             4.227831       18.258326      7.165610       F
H             6.932336       18.247978      6.973476       F
H             7.409029       17.444838      5.706966       F
H             7.521090       6.298710       1.832227       F
H             7.521091       14.697052      1.832228       F
H             3.346923       10.497843      14.197637      F
H             6.469066       10.497905      0.138110       F
H             0.036292       9.692186       9.043064       F
H             0.036293       11.303523      9.043067       F
H             2.008443       9.058197       12.145151      F
H             2.008458       11.937517      12.145156      F
```

H	4.786758	6.298710	2.000110	F
H	4.786758	14.697020	2.000090	F
H	6.866244	9.838694	15.040458	F
H	6.866539	11.156770	15.040419	F
H	4.132088	16.721542	9.197365	F
H	4.893034	17.533883	8.246020	F
H	4.893449	3.461494	8.246089	F
H	4.132055	4.274186	9.197224	F
H	2.690113	11.221840	5.059460	F
H	2.690184	9.773810	5.059456	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298720	8.126704	F
H	1.991769	14.696983	8.126702	F
H	4.137973	13.968634	3.050486	F
H	4.137967	7.027078	3.050497	F
H	3.423387	4.865219	3.998926	F
H	3.423382	16.130499	3.998927	F
H	3.423062	7.732143	4.002716	F
H	3.423069	13.263572	4.002716	F
H	2.742679	6.961340	9.160674	F
H	2.742699	14.034348	9.160612	F
Al	6.205979	7.642531	6.957296	R
O	4.780673	6.310213	7.129727	R
O	7.438898	6.288375	7.251821	R
O	6.184983	7.659245	5.020512	R
Al	7.447448	6.213753	9.197469	R
O	6.469300	7.471940	13.295641	R
O	7.638173	5.871918	10.927710	R
O	6.039184	4.889089	8.812174	R
O	6.037736	7.620566	8.905586	R
Al	7.287060	9.021730	4.894112	R
Al	7.304643	11.978424	4.894643	R
Al	6.198569	13.351077	6.954781	R
Al	6.377308	10.493882	7.116146	R
O	4.780864	14.686954	7.130407	R
O	4.903436	11.805454	7.256392	R
O	4.898896	9.193628	7.256283	R
O	7.436146	14.705550	7.251420	R
O	6.334329	10.506590	5.101959	R
O	7.551314	11.976820	6.779396	R
O	7.541676	9.021457	6.765932	R
O	6.196089	13.336402	5.024042	R
Al	7.440389	14.790305	9.197514	R
Al	7.780619	10.477336	10.364300	R
O	6.186101	10.498364	13.138108	R
O	6.474456	13.526877	13.296768	R
O	6.277860	10.497252	9.056631	R
O	7.642619	15.116541	10.926380	R
O	6.039322	13.376732	8.905471	R
O	6.040521	16.108091	8.812791	R
O	8.117124	9.124091	11.475500	R
O	8.094034	11.857027	11.459909	R
O	4.767989	6.127139	10.946219	R
O	4.771254	14.872397	10.944445	R
O	4.778938	9.092799	10.950817	R
O	4.772649	11.906786	10.951170	R
O	6.291653	4.937069	5.060234	R
O	6.288866	16.056773	5.062358	R
O	8.078886	9.080539	3.331855	R
O	8.089283	11.914135	3.329688	R
O	3.433184	10.499393	8.937849	R
Cu	8.866042	12.224932	8.363804	R
Cu	8.995197	8.758917	8.272744	R
O	9.018571	10.504338	9.004138	R
O	9.117834	6.944255	8.810965	R
O	9.097572	14.036109	8.756587	R
C	11.066348	8.432078	7.231130	R
O	12.067685	7.928952	7.051929	R

```
Model #65      Cartesian coordinates in angstrom
               x             y             z             Relaxed/Frozen
Al             4.718157      6.298926      9.025576      F
Al             6.299235      6.298770      11.957085     F
Al             4.718017      14.696822     9.024991      F
Al             4.828078      11.951000     9.158307      F
Al             4.828293      9.045507      9.158051      F
Al             7.260409      8.999296      12.958862     F
Al             7.260262      11.997700     12.959208     F
Al             6.298555      14.695955     11.957250     F
Al             4.636051      10.497899     12.053102     F
O              3.286799      10.497868     13.239732     F
Al             6.284445      4.911994      6.956121      F
Al             6.283890      16.082223     6.956951      F
Al             7.604243      10.497820     2.473978      F
O              6.427186      10.497848     1.094369      F
Al             6.373578      6.298815      3.886501      F
O              4.781441      6.298725      2.980336      F
Al             6.373405      14.696694     3.886502      F
O              4.781448      14.697020     2.980326      F
O              3.454091      4.976957      9.235337      F
O              3.454132      7.620261      9.235310      F
O              6.250032      5.002899      13.162273     F
O              3.454189      16.018930     9.234865      F
O              3.453903      13.375330     9.235554      F
O              7.425635      9.104791      14.776042     F
O              7.425723      11.891047     14.776042     F
O              6.250305      15.993035     13.162050     F
O              4.962266      3.365421      7.283486      F
O              7.499837      3.492590      6.705321      F
O              4.962541      17.630401     7.284103      F
O              7.499898      17.503112     6.705531      F
O              7.704778      6.298704      2.777147      F
O              7.704783      14.696991     2.777154      F
Al             3.478765      10.498235     7.046882      F
O              1.926546      11.807727     6.890238      F
O              1.926615      9.187899      6.890301      F
O              3.361191      10.497908     5.169010      F
Al             2.050941      10.497848     10.125676     F
O              0.574779      10.497848     9.076090      F
O              2.097762      9.088332      11.188771     F
O              2.097754      11.907381     11.188778     F
Al             3.393317      6.298747      6.011432      F
O              1.956476      6.298701      7.179493      F
O              3.339454      7.715091      4.949244      F
O              3.339458      4.882335      4.949250      F
Al             3.393318      14.697006     6.011452      F
O              1.956482      14.697054     7.179498      F
O              3.339473      16.113372     4.949239      F
O              3.339464      13.280638     4.949229      F
H              3.439923      4.911173      10.243969     F
H              3.439260      7.689417      10.293378     F
H              6.818352      4.213047      13.048198     F
H              6.229134      4.955321      14.133902     F
H              3.439930      16.084519     10.243550     F
H              3.439282      13.306237     10.293981     F
H              6.777046      8.347574      14.909837     F
H              6.776832      12.647852     14.909836     F
H              6.229113      16.040398     14.133946     F
H              6.818531      16.782561     13.048324     F
H              4.227215      2.738019      7.166097      F
H              6.932383      2.747747      6.973632      F
H              7.409085      3.550921      5.707011      F
H              4.227831      18.258326     7.165610      F
H              6.932335      18.247978     6.973474      F
H              7.409027      17.444839     5.706966      F
H              7.521090      6.298712      1.832227      F
H              7.521091      14.697052     1.832228      F
H              3.346923      10.497843     14.197637     F
H              6.469066      10.497903     0.138110      F
H              0.036290      9.692187      9.043066      F
H              0.036295      11.303524     9.043065      F
H              2.008451      9.058198      12.145152     F
H              2.008464      11.937516     12.145157     F
```

H	4.786758	6.298710	2.000110	F
H	4.786758	14.697021	2.000090	F
H	6.866246	9.838696	15.040458	F
H	6.866536	11.156773	15.040419	F
H	4.132088	16.721542	9.197365	F
H	4.893034	17.533883	8.246020	F
H	4.893449	3.461494	8.246089	F
H	4.132056	4.274186	9.197229	F
H	2.690113	11.221840	5.059460	F
H	2.690186	9.773808	5.059456	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298720	8.126704	F
H	1.991769	14.696983	8.126702	F
H	4.137973	13.968634	3.050486	F
H	4.137966	7.027077	3.050498	F
H	3.423386	4.865219	3.998926	F
H	3.423382	16.130499	3.998927	F
H	3.423061	7.732143	4.002716	F
H	3.423069	13.263572	4.002716	F
H	2.742679	6.961342	9.160662	F
H	2.742699	14.034349	9.160618	F
Al	6.205098	7.640427	6.957144	R
O	4.782508	6.311894	7.126673	R
O	7.454861	6.297397	7.270735	R
O	6.169319	7.654425	5.019752	R
Al	7.464878	6.238463	9.199319	R
O	6.461831	7.473085	13.294881	R
O	7.620102	5.822812	10.926892	R
O	6.038727	4.896429	8.807874	R
O	6.035256	7.625748	8.902447	R
Al	7.244576	9.032076	4.871161	R
Al	7.294527	11.978208	4.882722	R
Al	6.192970	13.353086	6.950017	R
Al	6.355481	10.493897	7.105492	R
O	4.781513	14.687383	7.128584	R
O	4.897711	11.808035	7.252107	R
O	4.892803	9.192233	7.249662	R
O	7.440406	14.701021	7.253254	R
O	6.301950	10.521197	5.074275	R
O	7.537484	11.969794	6.768551	R
O	7.520354	9.042770	6.726913	R
O	6.193554	13.338976	5.022467	R
Al	7.438112	14.760618	9.194360	R
Al	7.793590	10.415867	10.365080	R
O	6.183115	10.498545	13.140871	R
O	6.482738	13.529581	13.295038	R
O	6.277375	10.495087	9.047773	R
O	7.646494	15.099871	10.919546	R
O	6.034619	13.372955	8.900121	R
O	6.042748	16.100702	8.811968	R
O	8.128937	9.087925	11.491843	R
O	8.081621	11.818380	11.450510	R
O	4.766065	6.134964	10.945904	R
O	4.773056	14.873260	10.944490	R
O	4.784256	9.094873	10.949870	R
O	4.766084	11.908359	10.950193	R
O	6.301493	4.940122	5.062982	R
O	6.291332	16.055470	5.063797	R
O	8.058544	9.072326	3.323599	R
O	8.099674	11.910200	3.330383	R
O	3.433921	10.498382	8.937387	R
Cu	8.827322	12.121210	8.342827	R
Cu	9.084898	8.722212	8.068211	R
O	9.017759	10.410638	8.993774	R
O	9.146560	7.046093	9.199485	R
O	9.067840	13.925159	8.753939	R
C	10.072571	7.142683	7.327107	R
O	10.702678	6.270031	6.947956	R

```
Model #66       Cartesian coordinates in angstrom
                x            y            z            Relaxed/Frozen
Al              4.718157     6.298926     9.025576     F
Al              6.299235     6.298770     11.957085    F
Al              4.718017     14.696822    9.024991     F
Al              4.828078     11.951000    9.158307     F
Al              4.828293     9.045507     9.158051     F
Al              7.260409     8.999296     12.958862    F
Al              7.260262     11.997700    12.959208    F
Al              6.298555     14.695955    11.957250    F
Al              4.636051     10.497899    12.053102    F
O               3.286799     10.497868    13.239732    F
Al              6.284445     4.911994     6.956121     F
Al              6.283890     16.082223    6.956951     F
Al              7.604243     10.497820    2.473978     F
O               6.427186     10.497848    1.094369     F
Al              6.373578     6.298815     3.886501     F
O               4.781441     6.298725     2.980336     F
Al              6.373405     14.696694    3.886502     F
O               4.781448     14.697020    2.980326     F
O               3.454091     4.976957     9.235337     F
O               3.454132     7.620261     9.235310     F
O               6.250032     5.002899     13.162273    F
O               3.454189     16.018930    9.234865     F
O               3.453903     13.375330    9.235554     F
O               7.425635     9.104791     14.776042    F
O               7.425723     11.891047    14.776042    F
O               6.250305     15.993035    13.162050    F
O               4.962266     3.365421     7.283486     F
O               7.499837     3.492590     6.705321     F
O               4.962541     17.630401    7.284103     F
O               7.499898     17.503112    6.705531     F
O               7.704778     6.298704     2.777147     F
O               7.704783     14.696991    2.777154     F
Al              3.478765     10.498235    7.046882     F
O               1.926546     11.807727    6.890238     F
O               1.926615     9.187899     6.890301     F
O               3.361191     10.497908    5.169010     F
Al              2.050941     10.497848    10.125676    F
O               0.574779     10.497848    9.076090     F
O               2.097762     9.088332     11.188771    F
O               2.097754     11.907381    11.188778    F
Al              3.393317     6.298747     6.011432     F
O               1.956476     6.298701     7.179493     F
O               3.339454     7.715091     4.949244     F
O               3.339458     4.882335     4.949250     F
Al              3.393318     14.697006    6.011452     F
O               1.956482     14.697054    7.179498     F
O               3.339473     16.113372    4.949239     F
O               3.339464     13.280638    4.949229     F
H               3.439923     4.911173     10.243969    F
H               3.439260     7.689417     10.293378    F
H               6.818352     4.213047     13.048198    F
H               6.229134     4.955321     14.133902    F
H               3.439930     16.084519    10.243550    F
H               3.439282     13.306237    10.293981    F
H               6.777046     8.347574     14.909837    F
H               6.776832     12.647852    14.909836    F
H               6.229113     16.040398    14.133946    F
H               6.818531     16.782561    13.048324    F
H               4.227215     2.738019     7.166097     F
H               6.932383     2.747747     6.973632     F
H               7.409085     3.550921     5.707011     F
H               4.227831     18.258326    7.165610     F
H               6.932335     18.247978    6.973474     F
H               7.409027     17.444839    5.706966     F
H               7.521090     6.298712     1.832227     F
H               7.521091     14.697052    1.832228     F
H               3.346923     10.497843    14.197637    F
H               6.469066     10.497903    0.138110     F
H               0.036290     9.692187     9.043066     F
H               0.036295     11.303524    9.043065     F
H               2.008451     9.058198     12.145152    F
H               2.008464     11.937516    12.145157    F
```

H	4.786758	6.298710	2.000110	F
H	4.786758	14.697021	2.000090	F
H	6.866246	9.838696	15.040458	F
H	6.866536	11.156773	15.040419	F
H	4.132088	16.721542	9.197365	F
H	4.893034	17.533883	8.246020	F
H	4.893449	3.461494	8.246089	F
H	4.132056	4.274186	9.197229	F
H	2.690113	11.221840	5.059460	F
H	2.690186	9.773808	5.059456	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298720	8.126704	F
H	1.991769	14.696983	8.126702	F
H	4.137973	13.968634	3.050486	F
H	4.137966	7.027077	3.050498	F
H	3.423386	4.865219	3.998926	F
H	3.423382	16.130499	3.998927	F
H	3.423061	7.732143	4.002716	F
H	3.423069	13.263572	4.002716	F
H	2.742679	6.961342	9.160662	F
H	2.742699	14.034349	9.160618	F
Al	6.205098	7.640427	6.957144	R
O	4.782508	6.311894	7.126673	R
O	7.454861	6.297397	7.270735	R
O	6.169319	7.654425	5.019752	R
Al	7.464878	6.238463	9.199319	R
O	6.461831	7.473085	13.294881	R
O	7.620102	5.822812	10.926892	R
O	6.038727	4.896429	8.807874	R
O	6.035256	7.625748	8.902447	R
Al	7.244576	9.032076	4.871161	R
Al	7.294527	11.978208	4.882722	R
Al	6.192970	13.353086	6.950071	R
Al	6.355481	10.493897	7.105492	R
O	4.781513	14.687383	7.128584	R
O	4.897711	11.808035	7.252107	R
O	4.892803	9.192233	7.249662	R
O	7.440406	14.701021	7.253254	R
O	6.301950	10.521197	5.074275	R
O	7.537484	11.969794	6.768551	R
O	7.520354	9.042770	6.726913	R
O	6.193554	13.338976	5.022467	R
Al	7.438112	14.760618	9.194360	R
Al	7.793590	10.415867	10.365080	R
O	6.183115	10.498545	13.140871	R
O	6.482738	13.529581	13.295038	R
O	6.277375	10.495087	9.047773	R
O	7.646494	15.099871	10.919544	R
O	6.034619	13.372955	8.900121	R
O	6.042748	16.100702	8.811968	R
O	8.128937	9.087925	11.491843	R
O	8.081621	11.818380	11.450510	R
O	4.766065	6.134964	10.945904	R
O	4.773056	14.873260	10.944490	R
O	4.784256	9.094873	10.949870	R
O	4.766084	11.908359	10.950193	R
O	6.301493	4.940122	5.062982	R
O	6.291332	16.055470	5.063797	R
O	8.058544	9.072326	3.323599	R
O	8.099674	11.910200	3.330383	R
O	3.433921	10.498382	8.937387	R
Cu	8.827322	12.121210	8.342827	R
Cu	9.084898	8.722212	8.068211	R
O	9.017759	10.410638	8.993774	R
O	9.146560	7.046093	9.199485	R
O	9.067840	13.925159	8.753939	R
C	10.072571	7.142683	7.327107	R
O	10.702678	6.270031	6.947956	R

```
Model #67        Cartesian coordinates in angstrom
                 x              y              z              Relaxed/Frozen
Al               4.718081       6.298892       9.025614       F
Al               6.299269       6.298805       11.956926      F
Al               4.718013       14.696817      9.025000       F
Al               4.828065       11.950999      9.158313       F
Al               4.828225       9.045445       9.158108       F
Al               7.260412       8.999320       12.958748      F
Al               7.260223       11.997705      12.959155      F
Al               6.298536       14.695946      11.957256      F
Al               4.636019       10.497891      12.053110      F
O                3.286796       10.497865      13.239729      F
Al               6.284426       4.912013       6.956143       F
Al               6.283907       16.082216      6.956964       F
Al               7.604263       10.497804      2.474052       F
O                6.427193       10.497843      1.094363       F
Al               6.373556       6.298831       3.886558       F
O                4.781439       6.298727       2.980340       F
Al               6.373425       14.696679      3.886534       F
O                4.781451       14.697019      2.980322       F
O                3.454075       4.976973       9.235338       F
O                3.454102       7.620243       9.235338       F
O                6.250076       5.002914       13.162291      F
O                3.454189       16.018931      9.234860       F
O                3.453906       13.375335      9.235539       F
O                7.425673       9.104779       14.776039      F
O                7.425737       11.891055      14.776041      F
O                6.250301       15.993040      13.162045      F
O                4.962266       3.365421       7.283486       F
O                7.499839       3.492589       6.705342       F
O                4.962541       17.630401      7.284103       F
O                7.499901       17.503112      6.705547       F
O                7.704796       6.298702       2.777169       F
O                7.704796       14.696991      2.777169       F
Al               3.478762       10.498245      7.046890       F
O                1.926564       11.807749      6.890233       F
O                1.926605       9.187911       6.890297       F
O                3.361187       10.497909      5.169010       F
Al               2.050940       10.497868      10.125624      F
O                0.574783       10.497854      9.076083       F
O                2.097767       9.088325       11.188761      F
O                2.097755       11.907386      11.188772      F
Al               3.393325       6.298753       6.011475       F
O                1.956473       6.298693       7.179488       F
O                3.339443       7.715090       4.949243       F
O                3.339457       4.882343       4.949240       F
Al               3.393324       14.697003      6.011451       F
O                1.956482       14.697055      7.179498       F
O                3.339475       16.113371      4.949238       F
O                3.339463       13.280638      4.949230       F
H                3.439919       4.911177       10.243969      F
H                3.439235       7.689414       10.293378      F
H                6.818349       4.213046       13.048196      F
H                6.229205       4.955320       14.133903      F
H                3.439929       16.084518      10.243550      F
H                3.439277       13.306239      10.293981      F
H                6.777071       8.347552       14.909836      F
H                6.776839       12.647859      14.909836      F
H                6.229111       16.040398      14.133946      F
H                6.818531       16.782561      13.048324      F
H                4.227215       2.738019       7.166097       F
H                6.932377       2.747745       6.973612       F
H                7.409110       3.550943       5.707010       F
H                4.227831       18.258326      7.165610       F
H                6.932336       18.247978      6.973477       F
H                7.409032       17.444835      5.706966       F
H                7.521090       6.298709       1.832227       F
H                7.521091       14.697051      1.832228       F
H                3.346923       10.497843      14.197637      F
H                6.469066       10.497902      0.138110       F
H                0.036292       9.692186       9.043064       F
H                0.036293       11.303523      9.043068       F
H                2.008440       9.058197       12.145151      F
H                2.008456       11.937517      12.145156      F
```

H	4.786758	6.298705	2.000110	F
H	4.786758	14.697019	2.000090	F
H	6.866243	9.838693	15.040458	F
H	6.866540	11.156769	15.040419	F
H	4.132088	16.721542	9.197365	F
H	4.893034	17.533883	8.246020	F
H	4.893449	3.461494	8.246089	F
H	4.132055	4.274186	9.197224	F
H	2.690113	11.221840	5.059460	F
H	2.690183	9.773811	5.059456	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298719	8.126704	F
H	1.991769	14.696983	8.126702	F
H	4.137973	13.968634	3.050486	F
H	4.137970	7.027082	3.050491	F
H	3.423397	4.865218	3.998927	F
H	3.423382	16.130499	3.998927	F
H	3.423072	7.732144	4.002717	F
H	3.423069	13.263572	4.002716	F
H	2.742679	6.961340	9.160672	F
H	2.742699	14.034347	9.160607	F
Al	6.215604	7.637357	6.976931	R
O	4.776848	6.303689	7.136405	R
O	7.437246	6.293664	7.297104	R
O	6.172455	7.647997	5.032686	R
Al	7.488819	6.095634	9.191457	R
O	6.453373	7.477730	13.294042	R
O	7.620260	5.858399	10.936038	R
O	6.033689	4.863945	8.818822	R
O	6.038333	7.619551	8.915438	R
Al	7.253433	9.022409	4.880177	R
Al	7.286819	11.974536	4.886525	R
Al	6.196120	13.354172	6.950127	R
Al	6.361817	10.495415	7.106903	R
O	4.776618	14.685104	7.131796	R
O	4.888009	11.807602	7.255677	R
O	4.885553	9.193531	7.256435	R
O	7.433668	14.704360	7.255427	R
O	6.302754	10.510770	5.086650	R
O	7.531621	11.974445	6.766897	R
O	7.522840	9.035077	6.739841	R
O	6.185017	13.338286	5.021552	R
Al	7.445689	14.774010	9.193111	R
Al	7.809416	10.448199	10.360487	R
O	6.181790	10.498056	13.135446	R
O	6.468444	13.523615	13.291413	R
O	6.271757	10.497585	9.054100	R
O	7.638151	15.111025	10.921800	R
O	6.033445	13.372897	8.904531	R
O	6.036803	16.103170	8.815413	R
O	8.103539	9.088002	11.467511	R
O	8.100265	11.825746	11.470737	R
O	4.754933	6.141896	10.950557	R
O	4.764895	14.856669	10.947587	R
O	4.767228	9.100191	10.948606	R
O	4.766255	11.901929	10.949468	R
O	6.294377	4.941614	5.066569	R
O	6.286967	16.055290	5.064346	R
O	8.049788	9.071074	3.323972	R
O	8.085960	11.912888	3.331557	R
O	3.425675	10.500880	8.936942	R
Cu	8.860872	12.194506	8.336780	R
Cu	9.106113	8.845061	8.038935	R
O	9.045748	10.500808	9.014651	R
O	9.424101	6.150055	9.013839	R
O	9.098061	13.991957	8.770727	R
C	10.035703	7.046335	8.360460	R
O	11.167502	7.135110	7.921976	R

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Model #68      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.716446       6.297334       9.024942       F
Al             6.301552       6.299709       11.957767      F
Al             4.718114       14.696826      9.025006       F
Al             4.828254       11.951348      9.158229       F
Al             4.827965       9.044900       9.158011       F
Al             7.260216       8.999020       12.958756      F
Al             7.259998       11.997953      12.959264      F
Al             6.298866       14.696132      11.957198      F
Al             4.635996       10.498020      12.053008      F
O              3.286825       10.497877      13.239762      F
Al             6.283176       4.911823       6.955793       F
Al             6.283990       16.082389      6.956837       F
Al             7.604394       10.498037      2.473868       F
O              6.427122       10.497861      1.094423       F
Al             6.374248       6.299114       3.886412       F
O              4.781378       6.298764       2.980448       F
Al             6.373440       14.696777      3.886595       F
O              4.781435       14.697034      2.980350       F
O              3.454024       4.977039       9.235448       F
O              3.454186       7.620424       9.235393       F
O              6.250272       5.002977       13.162367      F
O              3.454146       16.018885      9.234891       F
O              3.453901       13.375372      9.235696       F
O              7.425246       9.104791       14.776077      F
O              7.425680       11.890954      14.776040      F
O              6.250273       15.992980      13.162109      F
O              4.962468       3.365287       7.283668       F
O              7.499801       3.492537       6.705450       F
O              4.962530       17.630396      7.284085       F
O              7.499870       17.503135      6.705529       F
O              7.704796       6.298707       2.777168       F
O              7.704768       14.697007      2.777135       F
Al             3.478925       10.498105      7.046571       F
O              1.926562       11.807766      6.890395       F
O              1.926588       9.187924       6.890358       F
O              3.361213       10.498057      5.169008       F
Al             2.050973       10.497855      10.125770      F
O              0.574794       10.497856      9.076067       F
O              2.097799       9.088324       11.188758      F
O              2.097766       11.907404      11.188748      F
Al             3.393553       6.298879       6.011355       F
O              1.956481       6.298711       7.179498       F
O              3.339468       7.715110       4.949268       F
O              3.339494       4.882304       4.949291       F
Al             3.393275       14.697004      6.011505       F
O              1.956480       14.697033      7.179495       F
O              3.339464       16.113360      4.949225       F
O              3.339459       13.280643      4.949224       F
H              3.439934       4.911163       10.243968      F
H              3.439399       7.689548       10.293372      F
H              6.818034       4.212852       13.047974      F
H              6.228872       4.955326       14.133896      F
H              3.439901       16.084491      10.243551      F
H              3.439225       13.306171      10.293976      F
H              6.777077       8.347548       14.909836      F
H              6.776854       12.647872      14.909835      F
H              6.229138       16.040398      14.133947      F
H              6.818498       16.782582      13.048301      F
H              4.227230       2.738004       7.166085       F
H              6.932385       2.747747       6.973636       F
H              7.409348       3.551150       5.707001       F
H              4.227777       18.258271      7.165653       F
H              6.932343       18.247976      6.973498       F
H              7.409064       17.444808      5.706965       F
H              7.521090       6.298672       1.832227       F
H              7.521091       14.697004      1.832228       F
H              3.346923       10.497824      14.197637      F
H              6.469066       10.497820      0.138110       F
H              0.036292       9.692186       9.043064       F
H              0.036290       11.303521      9.043073       F
H              2.008412       9.058194       12.145148      F
H              2.008430       11.937519      12.145154      F
```

H	4.786758	6.298653	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866333	9.838766	15.040446	F
H	6.866536	11.156772	15.040420	F
H	4.132087	16.721543	9.197355	F
H	4.893057	17.533902	8.246024	F
H	4.893427	3.461513	8.246086	F
H	4.132055	4.274186	9.197227	F
H	2.690056	11.221788	5.059463	F
H	2.690193	9.773801	5.059456	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298712	8.126704	F
H	1.991769	14.696994	8.126702	F
H	4.137982	13.968625	3.050471	F
H	4.137968	7.027081	3.050494	F
H	3.423348	4.865223	3.998922	F
H	3.423398	16.130501	3.998929	F
H	3.423028	7.732140	4.002713	F
H	3.423077	13.263571	4.002716	F
H	2.742681	6.961330	9.160746	F
H	2.742698	14.034343	9.160576	F
Al	6.239630	7.659766	6.983715	R
O	4.837368	6.288067	7.125844	R
O	7.558326	6.267691	7.433934	R
O	6.221862	7.622780	5.061270	R
Al	7.252981	6.126490	9.253959	R
O	6.485158	7.453378	13.298936	R
O	7.712359	5.918975	10.910585	R
O	6.005926	4.831494	8.823379	R
O	6.051688	7.582405	8.935680	R
Al	7.248843	9.032773	4.857857	R
Al	7.342773	11.983307	4.904271	R
Al	6.206860	13.347575	6.959866	R
Al	6.395926	10.501403	7.125975	R
O	4.797441	14.685956	7.128246	R
O	4.962542	11.782873	7.268898	R
O	4.976513	9.166157	7.271362	R
O	7.445953	14.703731	7.257683	R
O	6.344292	10.522043	5.096759	R
O	7.594301	11.962063	6.786670	R
O	7.574519	9.003658	6.710488	R
O	6.234693	13.334784	5.029171	R
Al	7.438528	14.794226	9.199541	R
Al	7.833659	10.431741	10.379866	R
O	6.187896	10.489219	13.141813	R
O	6.477564	13.524210	13.292384	R
O	6.361743	10.458863	9.066072	R
O	7.651935	15.099562	10.932632	R
O	6.047757	13.376267	8.913850	R
O	6.047479	16.109886	8.816823	R
O	8.104724	9.036011	11.459075	R
O	8.168112	11.773579	11.522685	R
O	4.835084	6.076977	10.920247	R
O	4.777166	14.874044	10.947448	R
O	4.801852	9.059491	10.964892	R
O	4.817537	11.897663	10.957113	R
O	6.352003	4.956628	5.090632	R
O	6.300404	16.057085	5.061951	R
O	8.033174	9.045765	3.298276	R
O	8.147467	11.880589	3.348414	R
O	3.500757	10.485068	8.970717	R
Cu	8.887354	12.230112	8.391593	R
Cu	9.128156	9.091104	7.924075	R
O	9.146640	10.539993	9.089218	R
O	10.184242	5.379743	6.042169	R
O	9.104203	14.047022	8.765160	R
C	10.211573	6.377287	6.633437	R
O	10.351656	7.387561	7.220486	R

```
Model #69      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043065       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.211275	7.651366	6.961437	R
O	4.805745	6.305864	7.122894	R
O	7.484896	6.304374	7.289078	R
O	6.201766	7.650549	5.027642	R
Al	7.425976	6.215285	9.223547	R
O	6.453937	7.473963	13.295523	R
O	7.637144	5.833252	10.940889	R
O	6.048786	4.890148	8.809539	R
O	6.046363	7.616296	8.910634	R
Al	7.254499	9.039399	4.866544	R
Al	7.254732	11.980356	4.837440	R
Al	6.248282	13.352864	6.976864	R
Al	6.357196	10.497563	7.104250	R
O	4.828780	14.706518	7.126991	R
O	4.966199	11.825171	7.267053	R
O	4.943263	9.201431	7.259391	R
O	7.532926	14.730123	7.419481	R
O	6.292817	10.514147	5.048531	R
O	7.569760	11.999336	6.677369	R
O	7.554603	9.060805	6.717119	R
O	6.209766	13.373140	5.051173	R
Al	7.264700	14.860907	9.236940	R
Al	7.917384	10.410308	10.381213	R
O	6.185076	10.503772	13.142082	R
O	6.499221	13.542485	13.289318	R
O	6.373398	10.512552	9.050988	R
O	7.709059	15.046526	10.903855	R
O	6.046084	13.406143	8.930767	R
O	6.004048	16.162288	8.829082	R
O	8.169030	9.072850	11.526372	R
O	8.139039	11.818410	11.484250	R
O	4.781772	6.121721	10.939081	R
O	4.826488	14.915161	10.927138	R
O	4.804581	9.095691	10.953008	R
O	4.786308	11.933443	10.961748	R
O	6.322647	4.942240	5.067352	R
O	6.341695	16.044233	5.086043	R
O	8.101702	9.092895	3.335972	R
O	8.064196	11.939932	3.292280	R
O	3.492958	10.507506	8.963489	R
Cu	8.907531	11.438134	7.892930	R
Cu	9.101874	8.626531	8.084854	R
O	9.278433	10.171812	9.176018	R
O	9.145869	6.986020	9.091963	R
O	10.671547	6.499901	6.097285	R
C	10.135468	7.324822	6.659054	R

```
Model #70      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043066       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.211439	7.647672	6.961168	R
O	4.793970	6.311610	7.126087	R
O	7.458668	6.296129	7.277175	R
O	6.211207	7.655583	5.027193	R
Al	7.453781	6.208887	9.203530	R
O	6.457328	7.474557	13.291843	R
O	7.627930	5.826398	10.933134	R
O	6.044418	4.889055	8.810108	R
O	6.046076	7.619584	8.909208	R
Al	7.289597	9.030708	4.883602	R
Al	7.235637	11.976719	4.835222	R
Al	6.240923	13.353602	6.973545	R
Al	6.360265	10.495013	7.107547	R
O	4.823244	14.706906	7.127390	R
O	4.949146	11.826565	7.263808	R
O	4.929206	9.202699	7.257547	R
O	7.528626	14.729582	7.416792	R
O	6.300686	10.496191	5.061850	R
O	7.552436	12.007567	6.672895	R
O	7.563259	9.055898	6.743994	R
O	6.188701	13.370946	5.046230	R
Al	7.265341	14.858407	9.235789	R
Al	7.921750	10.445815	10.381370	R
O	6.182746	10.504785	13.141798	R
O	6.491525	13.541569	13.291378	R
O	6.348734	10.518358	9.050881	R
O	7.705407	15.054187	10.902211	R
O	6.042652	13.405100	8.927253	R
O	6.002173	16.160452	8.827784	R
O	8.177483	9.116641	11.537577	R
O	8.122902	11.860580	11.473178	R
O	4.775205	6.126310	10.943583	R
O	4.824266	14.913067	10.926061	R
O	4.793673	9.097766	10.951033	R
O	4.774009	11.933525	10.959040	R
O	6.306998	4.940213	5.063700	R
O	6.339303	16.042998	5.086797	R
O	8.118725	9.103663	3.342308	R
O	8.036642	11.950560	3.286883	R
O	3.473798	10.507392	8.954056	R
Cu	8.909828	11.504701	7.892030	R
Cu	9.094776	8.623697	8.163312	R
O	9.259022	10.230072	9.166818	R
O	9.197425	6.920771	9.180960	R
O	10.555488	6.054392	6.948754	R
C	9.950938	6.944083	7.339591	R

```
Model #71        Cartesian coordinates in angstrom
                 x              y              z              Relaxed/Frozen
Al               4.718091       6.298715       9.025534       F
Al               6.299120       6.298715       11.957102      F
Al               4.718091       14.697002      9.025534       F
Al               4.828311       11.950763      9.158184       F
Al               4.828311       9.044955       9.158184       F
Al               7.260466       8.998624       12.959551      F
Al               7.260466       11.997093      12.959551      F
Al               6.299120       14.697002      11.957102      F
Al               4.636026       10.497859      12.053017      F
O                3.286788       10.497859      13.239718      F
Al               6.284430       4.911618       6.956078       F
Al               6.284430       16.084099      6.956078       F
Al               7.604152       10.497859      2.473791       F
O                6.427205       10.497859      1.094354       F
Al               6.373455       6.298715       3.886397       F
O                4.781442       6.298715       2.980335       F
Al               6.373455       14.697002      3.886397       F
O                4.781442       14.697002      2.980335       F
O                3.454035       4.977004       9.235301       F
O                3.454035       7.620427       9.235301       F
O                6.249989       5.002877       13.162247      F
O                3.454035       16.018713      9.235301       F
O                3.454035       13.375290      9.235301       F
O                7.425505       9.104843       14.776051      F
O                7.425505       11.890874      14.776051      F
O                6.249989       15.992841      13.162247      F
O                4.962264       3.365416       7.283451       F
O                7.499839       3.492587       6.705345       F
O                4.962264       17.630302      7.283451       F
O                7.499839       17.503130      6.705345       F
O                7.704784       6.298715       2.777154       F
O                7.704784       14.697002      2.777154       F
Al               3.478998       10.497859      7.046735       F
O                1.926548       11.807732      6.890259       F
O                1.926548       9.187985       6.890259       F
O                3.361122       10.497859      5.169014       F
Al               2.050923       10.497859      10.125656      F
O                0.574778       10.497859      9.076089       F
O                2.097749       9.088323       11.188759      F
O                2.097749       11.907395      11.188759      F
Al               3.393316       6.298715       6.011417       F
O                1.956477       6.298715       7.179493       F
O                3.339459       7.715095       4.949249       F
O                3.339459       4.882336       4.949249       F
Al               3.393316       14.697002      6.011417       F
O                1.956477       14.697002      7.179493       F
O                3.339459       16.113380      4.949249       F
O                3.339459       13.280622      4.949249       F
H                3.439923       4.911172       10.243970      F
H                3.439232       7.689483       10.293373      F
H                6.818393       4.213072       13.048228      F
H                6.229200       4.955319       14.133904      F
H                3.439929       16.084518      10.243550      F
H                3.439218       13.306190      10.293977      F
H                6.776962       8.347647       14.909841      F
H                6.777013       12.648010      14.909830      F
H                6.229199       16.040400      14.133948      F
H                6.818394       16.782646      13.048228      F
H                4.227165       2.738070       7.166136       F
H                6.932392       2.747750       6.973661       F
H                7.409135       3.550965       5.707009       F
H                4.227165       18.257647      7.166137       F
H                6.932397       18.247959      6.973659       F
H                7.409131       17.444750      5.706962       F
H                7.521090       6.298716       1.832227       F
H                7.521091       14.697002      1.832228       F
H                3.346923       10.497859      14.197637      F
H                6.469066       10.497859      0.138110       F
H                0.036291       9.692187       9.043065       F
H                0.036295       11.303524      9.043066       F
H                2.008448       9.058198       12.145152      F
H                2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.215837	7.640464	6.985838	R
O	4.791996	6.298643	7.132633	R
O	7.448379	6.301672	7.307539	R
O	6.218213	7.650296	5.041785	R
Al	7.482519	6.051609	9.197657	R
O	6.453749	7.478793	13.292440	R
O	7.642463	5.896859	10.944006	R
O	6.044413	4.850979	8.817809	R
O	6.041520	7.616512	8.916170	R
Al	7.301342	9.017757	4.890286	R
Al	7.238603	11.973245	4.839093	R
Al	6.236405	13.353945	6.974047	R
Al	6.363189	10.495349	7.107900	R
O	4.823637	14.706532	7.127501	R
O	4.951683	11.827830	7.264564	R
O	4.932347	9.208458	7.259756	R
O	7.531669	14.726285	7.419698	R
O	6.314605	10.488362	5.080267	R
O	7.555192	12.006625	6.683250	R
O	7.569992	9.052108	6.758967	R
O	6.193016	13.368732	5.048911	R
Al	7.263227	14.862609	9.238600	R
Al	7.889123	10.475988	10.381752	R
O	6.185321	10.505830	13.138449	R
O	6.488037	13.541095	13.292360	R
O	6.360454	10.527163	9.049627	R
O	7.705801	15.058580	10.903119	R
O	6.043612	13.405583	8.927707	R
O	6.002122	16.160776	8.826241	R
O	8.178384	9.144014	11.530285	R
O	8.112015	11.886975	11.466482	R
O	4.770569	6.114946	10.945287	R
O	4.825774	14.912890	10.923979	R
O	4.796116	9.104127	10.949793	R
O	4.778734	11.933176	10.957951	R
O	6.304586	4.943304	5.067020	R
O	6.339228	16.040026	5.088863	R
O	8.115567	9.104255	3.343219	R
O	8.032412	11.950809	3.289055	R
O	3.475889	10.510123	8.954151	R
Cu	8.941785	11.652843	7.924294	R
Cu	9.064884	8.729008	8.113053	R
O	9.240718	10.330995	9.152055	R
O	9.434144	5.941928	8.985307	R
O	11.165866	7.020443	7.951262	R
C	10.041708	6.871871	8.388578	R

```
Model #72      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.718091       6.298715       9.025534       F
Al             6.299120       6.298715       11.957102      F
Al             4.718091       14.697002      9.025534       F
Al             4.828311       11.950763      9.158184       F
Al             4.828311       9.044955       9.158184       F
Al             7.260466       8.998624       12.959551      F
Al             7.260466       11.997093      12.959551      F
Al             6.299120       14.697002      11.957102      F
Al             4.636026       10.497859      12.053017      F
O              3.286788       10.497859      13.239718      F
Al             6.284430       4.911618       6.956078       F
Al             6.284430       16.084099      6.956078       F
Al             7.604152       10.497859      2.473791       F
O              6.427205       10.497859      1.094354       F
Al             6.373455       6.298715       3.886397       F
O              4.781442       6.298715       2.980335       F
Al             6.373455       14.697002      3.886397       F
O              4.781442       14.697002      2.980335       F
O              3.454035       4.977004       9.235301       F
O              3.454035       7.620427       9.235301       F
O              6.249989       5.002877       13.162247      F
O              3.454035       16.018713      9.235301       F
O              3.454035       13.375290      9.235301       F
O              7.425505       9.104843       14.776051      F
O              7.425505       11.890874      14.776051      F
O              6.249989       15.992841      13.162247      F
O              4.962264       3.365416       7.283451       F
O              7.499839       3.492587       6.705345       F
O              4.962264       17.630302      7.283451       F
O              7.499839       17.503130      6.705345       F
O              7.704784       6.298715       2.777154       F
O              7.704784       14.697002      2.777154       F
Al             3.478998       10.497859      7.046735       F
O              1.926548       11.807732      6.890259       F
O              1.926548       9.187985       6.890259       F
O              3.361122       10.497859      5.169014       F
Al             2.050923       10.497859      10.125656      F
O              0.574778       10.497859      9.076089       F
O              2.097749       9.088323       11.188759      F
O              2.097749       11.907395      11.188759      F
Al             3.393316       6.298715       6.011417       F
O              1.956477       6.298715       7.179493       F
O              3.339459       7.715095       4.949249       F
O              3.339459       4.882336       4.949249       F
Al             3.393316       14.697002      6.011417       F
O              1.956477       14.697002      7.179493       F
O              3.339459       16.113380      4.949249       F
O              3.339459       13.280622      4.949249       F
H              3.439923       4.911172       10.243970      F
H              3.439232       7.689483       10.293373      F
H              6.818393       4.213072       13.048228      F
H              6.229200       4.955319       14.133904      F
H              3.439929       16.084518      10.243550      F
H              3.439218       13.306190      10.293977      F
H              6.776962       8.347647       14.909841      F
H              6.777013       12.648010      14.909830      F
H              6.229199       16.040400      14.133948      F
H              6.818394       16.782646      13.048228      F
H              4.227165       2.738070       7.166136       F
H              6.932392       2.747750       6.973661       F
H              7.409135       3.550965       5.707009       F
H              4.227165       18.257647      7.166137       F
H              6.932397       18.247959      6.973659       F
H              7.409131       17.444750      5.706962       F
H              7.521090       6.298716       1.832227       F
H              7.521091       14.697002      1.832228       F
H              3.346923       10.497859      14.197637      F
H              6.469066       10.497859      0.138110       F
H              0.036291       9.692187       9.043065       F
H              0.036295       11.303524      9.043066       F
H              2.008448       9.058198       12.145152      F
H              2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.236936	7.645635	6.965057	R
O	4.820076	6.297225	7.128297	R
O	7.509131	6.271497	7.373404	R
O	6.202497	7.636296	5.036179	R
Al	7.322968	6.177144	9.209421	R
O	6.490672	7.456008	13.293130	R
O	7.678138	5.886324	10.917570	R
O	6.022525	4.855337	8.827789	R
O	6.051875	7.597337	8.932265	R
Al	7.267405	9.020885	4.852938	R
Al	7.274641	11.978860	4.853199	R
Al	6.241442	13.346642	6.973458	R
Al	6.390986	10.496693	7.120818	R
O	4.828806	14.704694	7.126593	R
O	4.971446	11.813607	7.272141	R
O	4.967614	9.189026	7.273474	R
O	7.531040	14.727104	7.416212	R
O	6.323379	10.504002	5.067225	R
O	7.568924	12.004562	6.696801	R
O	7.559109	9.001189	6.693388	R
O	6.213514	13.366886	5.046074	R
Al	7.267896	14.853845	9.232806	R
Al	8.038986	10.490901	10.392467	R
O	6.188984	10.493696	13.136769	R
O	6.475234	13.532719	13.285867	R
O	6.406874	10.504948	9.059304	R
O	7.707058	15.037437	10.902625	R
O	6.042746	13.405174	8.932841	R
O	6.005973	16.159800	8.829633	R
O	8.152556	9.058923	11.488861	R
O	8.230657	11.821029	11.576678	R
O	4.813588	6.097403	10.934571	R
O	4.823639	14.914557	10.928852	R
O	4.792220	9.075974	10.960390	R
O	4.798979	11.927416	10.963594	R
O	6.332241	4.947300	5.079827	R
O	6.340719	16.044159	5.086147	R
O	8.080265	9.071450	3.307102	R
O	8.078140	11.928982	3.302989	R
O	3.501122	10.501592	8.970172	R
Cu	8.955608	11.747413	8.004784	R
Cu	8.979380	9.223496	7.992787	R
O	9.473174	10.505381	9.313480	R
O	9.333326	7.201421	9.424590	R
O	10.312003	7.112538	11.545209	R
C	9.720140	7.175069	10.552021	R

```
Model #73      Cartesian coordinates in angstrom
               x            y            z           Relaxed/Frozen
Al             4.718091     6.298715     9.025534    F
Al             6.299120     6.298715     11.957102   F
Al             4.718091     14.697002    9.025534    F
Al             4.828311     11.950763    9.158184    F
Al             4.828311     9.044955     9.158184    F
Al             7.260466     8.998624     12.959551   F
Al             7.260466     11.997093    12.959551   F
Al             6.299120     14.697002    11.957102   F
Al             4.636026     10.497859    12.053017   F
O              3.286788     10.497859    13.239718   F
Al             6.284430     4.911618     6.956078    F
Al             6.284430     16.084099    6.956078    F
Al             7.604152     10.497859    2.473791    F
O              6.427205     10.497859    1.094354    F
Al             6.373455     6.298715     3.886397    F
O              4.781442     6.298715     2.980335    F
Al             6.373455     14.697002    3.886397    F
O              4.781442     14.697002    2.980335    F
O              3.454035     4.977004     9.235301    F
O              3.454035     7.620427     9.235301    F
O              6.249989     5.002877     13.162247   F
O              3.454035     16.018713    9.235301    F
O              3.454035     13.375290    9.235301    F
O              7.425505     9.104843     14.776051   F
O              7.425505     11.890874    14.776051   F
O              6.249989     15.992841    13.162247   F
O              4.962264     3.365416     7.283451    F
O              7.499839     3.492587     6.705345    F
O              4.962264     17.630302    7.283451    F
O              7.499839     17.503130    6.705345    F
O              7.704784     6.298715     2.777154    F
O              7.704784     14.697002    2.777154    F
Al             3.478998     10.497859    7.046735    F
O              1.926548     11.807732    6.890259    F
O              1.926548     9.187985     6.890259    F
O              3.361122     10.497859    5.169014    F
Al             2.050923     10.497859    10.125656   F
O              0.574778     10.497859    9.076089    F
O              2.097749     9.088323     11.188759   F
O              2.097749     11.907395    11.188759   F
Al             3.393316     6.298715     6.011417    F
O              1.956477     6.298715     7.179493    F
O              3.339459     7.715095     4.949249    F
O              3.339459     4.882336     4.949249    F
Al             3.393316     14.697002    6.011417    F
O              1.956477     14.697002    7.179493    F
O              3.339459     16.113380    4.949249    F
O              3.339459     13.280622    4.949249    F
H              3.439923     4.911172     10.243970   F
H              3.439232     7.689483     10.293373   F
H              6.818393     4.213072     13.048228   F
H              6.229200     4.955319     14.133904   F
H              3.439929     16.084518    10.243550   F
H              3.439218     13.306190    10.293977   F
H              6.776962     8.347647     14.909841   F
H              6.777013     12.648010    14.909830   F
H              6.229199     16.040400    14.133948   F
H              6.818394     16.782646    13.048228   F
H              4.227165     2.738070     7.166136    F
H              6.932392     2.747750     6.973661    F
H              7.409135     3.550965     5.707009    F
H              4.227165     18.257647    7.166137    F
H              6.932397     18.247959    6.973659    F
H              7.409131     17.444750    5.706962    F
H              7.521090     6.298716     1.832227    F
H              7.521091     14.697002    1.832228    F
H              3.346923     10.497859    14.197637   F
H              6.469066     10.497859    0.138110    F
H              0.036291     9.692187     9.043065    F
H              0.036295     11.303524    9.043066    F
H              2.008448     9.058198     12.145152   F
H              2.008447     11.937518    12.145155   F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.263635	7.656758	6.985912	R
O	4.827742	6.298568	7.127364	R
O	7.524041	6.270011	7.394726	R
O	6.239504	7.629279	5.056002	R
Al	7.312176	6.151791	9.230772	R
O	6.481463	7.456503	13.299413	R
O	7.676168	5.874819	10.923756	R
O	6.016955	4.846017	8.826800	R
O	6.055070	7.594053	8.939795	R
Al	7.277516	9.034541	4.881711	R
Al	7.249089	11.978359	4.843251	R
Al	6.236010	13.348316	6.972231	R
Al	6.386720	10.493714	7.128933	R
O	4.828096	14.707683	7.127219	R
O	4.969582	11.815625	7.272208	R
O	4.964770	9.185121	7.274356	R
O	7.529359	14.728767	7.416399	R
O	6.306175	10.501583	5.062454	R
O	7.557459	12.011776	6.681965	R
O	7.573462	9.045022	6.732748	R
O	6.197539	13.370342	5.044090	R
Al	7.266068	14.855072	9.232740	R
Al	7.982787	10.420721	10.358887	R
O	6.183722	10.495158	13.145790	R
O	6.492303	13.538768	13.287121	R
O	6.374726	10.502170	9.064331	R
O	7.708834	15.035873	10.902241	R
O	6.043090	13.405828	8.932189	R
O	6.005336	16.161452	8.830603	R
O	8.141415	9.029480	11.491033	R
O	8.190991	11.775455	11.540171	R
O	4.811663	6.096263	10.932985	R
O	4.824884	14.916469	10.929678	R
O	4.793083	9.076484	10.960944	R
O	4.791944	11.931408	10.965318	R
O	6.336604	4.945052	5.079200	R
O	6.343108	16.045309	5.085562	R
O	8.096953	9.088528	3.332992	R
O	8.059095	11.938820	3.296004	R
O	3.498020	10.501868	8.969518	R
Cu	8.912164	11.638633	7.964222	R
Cu	9.451323	9.064057	7.716191	R
O	9.347241	10.325800	9.196963	R
N	10.005118	7.113084	10.420289	R
N	10.528236	7.195068	11.408707	R
O	11.703868	7.726858	6.268675	R
O	9.508549	7.012042	9.328586	R
C	10.823138	8.230230	6.793009	R

```
Model #74        Cartesian coordinates in angstrom
                 x              y              z              Relaxed/Frozen
Al       4.718091       6.298715       9.025534       F
Al       6.299120       6.298715       11.957102      F
Al       4.718091       14.697002      9.025534       F
Al       4.828311       11.950763      9.158184       F
Al       4.828311       9.044955       9.158184       F
Al       7.260466       8.998624       12.959551      F
Al       7.260466       11.997093      12.959551      F
Al       6.299120       14.697002      11.957102      F
Al       4.636026       10.497859      12.053017      F
O        3.286788       10.497859      13.239718      F
Al       6.284430       4.911618       6.956078       F
Al       6.284430       16.084099      6.956078       F
Al       7.604152       10.497859      2.473791       F
O        6.427205       10.497859      1.094354       F
Al       6.373455       6.298715       3.886397       F
O        4.781442       6.298715       2.980335       F
Al       6.373455       14.697002      3.886397       F
O        4.781442       14.697002      2.980335       F
O        3.454035       4.977004       9.235301       F
O        3.454035       7.620427       9.235301       F
O        6.249989       5.002877       13.162247      F
O        3.454035       16.018713      9.235301       F
O        3.454035       13.375290      9.235301       F
O        7.425505       9.104843       14.776051      F
O        7.425505       11.890874      14.776051      F
O        6.249989       15.992841      13.162247      F
O        4.962264       3.365416       7.283451       F
O        7.499839       3.492587       6.705345       F
O        4.962264       17.630302      7.283451       F
O        7.499839       17.503130      6.705345       F
O        7.704784       6.298715       2.777154       F
O        7.704784       14.697002      2.777154       F
Al       3.478998       10.497859      7.046735       F
O        1.926548       11.807732      6.890259       F
O        1.926548       9.187985       6.890259       F
O        3.361122       10.497859      5.169014       F
Al       2.050923       10.497859      10.125656      F
O        0.574778       10.497859      9.076089       F
O        2.097749       9.088323       11.188759      F
O        2.097749       11.907395      11.188759      F
Al       3.393316       6.298715       6.011417       F
O        1.956477       6.298715       7.179493       F
O        3.339459       7.715095       4.949249       F
O        3.339459       4.882336       4.949249       F
Al       3.393316       14.697002      6.011417       F
O        1.956477       14.697002      7.179493       F
O        3.339459       16.113380      4.949249       F
O        3.339459       13.280622      4.949249       F
H        3.439923       4.911172       10.243970      F
H        3.439232       7.689483       10.293373      F
H        6.818393       4.213072       13.048228      F
H        6.229200       4.955319       14.133904      F
H        3.439929       16.084518      10.243550      F
H        3.439218       13.306190      10.293977      F
H        6.776962       8.347647       14.909841      F
H        6.777013       12.648010      14.909830      F
H        6.229199       16.040400      14.133948      F
H        6.818394       16.782646      13.048228      F
H        4.227165       2.738070       7.166136       F
H        6.932392       2.747750       6.973661       F
H        7.409135       3.550965       5.707009       F
H        4.227165       18.257647      7.166137       F
H        6.932397       18.247959      6.973659       F
H        7.409131       17.444750      5.706962       F
H        7.521090       6.298716       1.832227       F
H        7.521091       14.697002      1.832228       F
H        3.346923       10.497859      14.197637      F
H        6.469066       10.497859      0.138110       F
H        0.036291       9.692187       9.043065       F
H        0.036295       11.303524      9.043066       F
H        2.008448       9.058198       12.145152      F
H        2.008447       11.937518      12.145155      F
```

H	4.786758	6.298715	2.000110	F
H	4.786758	14.697002	2.000090	F
H	6.866357	9.838785	15.040442	F
H	6.866351	11.156924	15.040445	F
H	4.132076	16.721548	9.197253	F
H	4.893481	17.534250	8.246089	F
H	4.893481	3.461468	8.246093	F
H	4.132058	4.274188	9.197254	F
H	2.690119	11.221846	5.059459	F
H	2.690119	9.773872	5.059460	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298715	8.126704	F
H	1.991769	14.697002	8.126702	F
H	4.137964	13.968643	3.050502	F
H	4.137964	7.027075	3.050502	F
H	3.423387	4.865219	3.998926	F
H	3.423387	16.130499	3.998927	F
H	3.423053	7.732143	4.002716	F
H	3.423052	13.263574	4.002715	F
H	2.742679	6.961342	9.160657	F
H	2.742700	14.034354	9.160659	F
Al	6.233814	7.653955	6.976419	R
O	4.820910	6.295795	7.128420	R
O	7.507436	6.286843	7.377328	R
O	6.238100	7.635408	5.051272	R
Al	7.329601	6.134522	9.219499	R
O	6.473189	7.461117	13.295281	R
O	7.675484	5.896957	10.919635	R
O	6.024354	4.844023	8.822680	R
O	6.055760	7.593635	8.934459	R
Al	7.297065	9.025496	4.879261	R
Al	7.251938	11.976671	4.845226	R
Al	6.243400	13.351396	6.974351	R
Al	6.384350	10.498286	7.125219	R
O	4.828534	14.705230	7.127061	R
O	4.971987	11.813619	7.271290	R
O	4.966575	9.184735	7.270322	R
O	7.530344	14.729797	7.417067	R
O	6.322545	10.490050	5.076472	R
O	7.564374	12.008209	6.681523	R
O	7.581490	9.031341	6.740606	R
O	6.199977	13.367543	5.045664	R
Al	7.267034	14.856467	9.234536	R
Al	7.987054	10.451417	10.385962	R
O	6.185269	10.497610	13.141473	R
O	6.485208	13.537221	13.288578	R
O	6.383969	10.496801	9.060759	R
O	7.707082	15.043781	10.903196	R
O	6.044108	13.404495	8.931513	R
O	6.004481	16.160612	8.829697	R
O	8.167814	9.069529	11.514685	R
O	8.181838	11.826457	11.527375	R
O	4.809885	6.092067	10.931735	R
O	4.824398	14.913307	10.928321	R
O	4.794018	9.076739	10.959750	R
O	4.792211	11.927904	10.962259	R
O	6.331772	4.947548	5.080125	R
O	6.342189	16.043176	5.086322	R
O	8.104312	9.088002	3.327795	R
O	8.054118	11.938823	3.295819	R
O	3.499748	10.500066	8.967604	R
Cu	8.933104	11.586745	7.926836	R
Cu	9.104385	8.814973	8.035537	R
O	9.360527	10.346955	9.223540	R
N	10.318215	5.670208	10.176847	R
N	11.301475	5.768748	10.746952	R
O	11.625835	7.752281	9.072112	R
O	9.713292	6.357784	9.153393	R
C	10.520386	7.702262	8.695719	R

```
Model #75      Cartesian coordinates in angstrom
               x            y            z            Relaxed/Frozen
Al             4.718158     6.298867     9.025574     F
Al             6.299252     6.298745     11.957081    F
Al             4.718070     14.696821    9.025027     F
Al             4.828133     11.951019    9.158273     F
Al             4.828285     9.045458     9.158082     F
Al             7.260427     8.999260     12.958937    F
Al             7.260336     11.997661    12.959284    F
Al             6.298526     14.696062    11.957189    F
Al             4.636063     10.497898    12.053107    F
O              3.286795     10.497864    13.239727    F
Al             6.284443     4.911935     6.956112     F
Al             6.283921     16.082416    6.956901     F
Al             7.604223     10.497778    2.473974     F
O              6.427188     10.497844    1.094367     F
Al             6.373548     6.298791     3.886510     F
O              4.781445     6.298720     2.980330     F
Al             6.373423     14.696751    3.886479     F
O              4.781447     14.697024    2.980327     F
O              3.454092     4.976956     9.235336     F
O              3.454128     7.620278     9.235324     F
O              6.250021     5.002880     13.162252    F
O              3.454163     16.018890    9.234960     F
O              3.453922     13.375339    9.235502     F
O              7.425648     9.104793     14.776041    F
O              7.425704     11.891027    14.776041    F
O              6.250249     15.993037    13.162046    F
O              4.962264     3.365422     7.283481     F
O              7.499819     3.492572     6.705339     F
O              4.962530     17.630402    7.284053     F
O              7.499871     17.503132    6.705511     F
O              7.704779     6.298701     2.777148     F
O              7.704784     14.696995    2.777153     F
Al             3.478787     10.498245    7.046874     F
O              1.926554     11.807736    6.890232     F
O              1.926606     9.187911     6.890290     F
O              3.361185     10.497901    5.169010     F
Al             2.050948     10.497860    10.125639    F
O              0.574781     10.497850    9.076086     F
O              2.097763     9.088325     11.188761    F
O              2.097751     11.907387    11.188771    F
Al             3.393315     6.298738     6.011427     F
O              1.956476     6.298701     7.179492     F
O              3.339455     7.715091     4.949244     F
O              3.339457     4.882335     4.949250     F
Al             3.393319     14.697031    6.011447     F
O              1.956481     14.697046    7.179497     F
O              3.339470     16.113373    4.949241     F
O              3.339468     13.280635    4.949233     F
H              3.439929     4.911167     10.243969    F
H              3.439255     7.689425     10.293378    F
H              6.818345     4.213043     13.048193    F
H              6.229125     4.955321     14.133902    F
H              3.439933     16.084522    10.243550    F
H              3.439292     13.306227    10.293980    F
H              6.777049     8.347572     14.909837    F
H              6.776836     12.647857    14.909836    F
H              6.229110     16.040398    14.133946    F
H              6.818520     16.782568    13.048317    F
H              4.227214     2.738020     7.166097     F
H              6.932384     2.747748     6.973638     F
H              7.409081     3.550918     5.707011     F
H              4.227787     18.258281    7.165645     F
H              6.932340     18.247977    6.973488     F
H              7.409031     17.444836    5.706966     F
H              7.521090     6.298713     1.832227     F
H              7.521091     14.697040    1.832228     F
H              3.346923     10.497844    14.197637    F
H              6.469066     10.497901    0.138110     F
H              0.036292     9.692186     9.043064     F
H              0.036293     11.303523    9.043067     F
H              2.008441     9.058197     12.145151    F
H              2.008456     11.937517    12.145156    F
```

H	4.786758	6.298712	2.000110	F
H	4.786758	14.697011	2.000090	F
H	6.866252	9.838699	15.040456	F
H	6.866517	11.156789	15.040422	F
H	4.132089	16.721542	9.197377	F
H	4.893055	17.533900	8.246023	F
H	4.893451	3.461493	8.246089	F
H	4.132055	4.274186	9.197223	F
H	2.690107	11.221835	5.059460	F
H	2.690176	9.773819	5.059456	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298718	8.126704	F
H	1.991769	14.696987	8.126702	F
H	4.137969	13.968638	3.050494	F
H	4.137965	7.027076	3.050500	F
H	3.423387	4.865219	3.998926	F
H	3.423383	16.130499	3.998927	F
H	3.423060	7.732143	4.002716	F
H	3.423064	13.263572	4.002716	F
H	2.742679	6.961341	9.160666	F
H	2.742700	14.034351	9.160636	F
Al	6.200528	7.651585	6.970925	R
O	4.813616	6.296372	7.127540	R
O	7.501000	6.317740	7.352236	R
O	6.225154	7.642368	5.045913	R
Al	7.385011	6.115572	9.224784	R
O	6.458298	7.469811	13.295660	R
O	7.649889	5.859143	10.936468	R
O	6.038752	4.855573	8.811235	R
O	6.058810	7.602014	8.925412	R
Al	7.286106	9.025972	4.871293	R
Al	7.260753	11.978404	4.847595	R
Al	6.248793	13.353577	6.976964	R
Al	6.370142	10.506048	7.116920	R
O	4.829918	14.705029	7.126790	R
O	4.971599	11.819073	7.268763	R
O	4.960333	9.190843	7.263994	R
O	7.532770	14.730258	7.418902	R
O	6.322333	10.495093	5.077085	R
O	7.571272	12.004123	6.685863	R
O	7.571358	9.040409	6.739284	R
O	6.208535	13.367545	5.048897	R
Al	7.266329	14.858096	9.236172	R
Al	7.949865	10.420464	10.377302	R
O	6.185842	10.501991	13.141908	R
O	6.494985	13.540237	13.288216	R
O	6.378706	10.499382	9.053624	R
O	7.708562	15.041054	10.904126	R
O	6.045401	13.404518	8.931127	R
O	6.004699	16.160331	8.830068	R
O	8.149081	9.056199	11.506944	R
O	8.165224	11.808256	11.505320	R
O	4.795066	6.103088	10.931780	R
O	4.825563	14.913630	10.927683	R
O	4.797193	9.086195	10.955624	R
O	4.794038	11.930697	10.962140	R
O	6.327681	4.951016	5.079859	R
O	6.342001	16.041512	5.087229	R
O	8.100769	9.086262	3.326697	R
O	8.062191	11.935012	3.298667	R
O	3.500744	10.503534	8.965816	R
Cu	8.938443	11.491582	7.902794	R
Cu	8.927254	8.624503	8.101186	R
O	9.297958	10.192345	9.168482	R
O	10.144104	7.400132	8.942263	R
O	9.530823	6.291746	9.174099	R

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Model #76      Cartesian coordinates in angstrom
               x            y            z            Relaxed/Frozen
Al             4.718034     6.298578     9.025418     F
Al             6.299381     6.298797     11.957227    F
Al             4.717967     14.697088    9.024842     F
Al             4.828053     11.951185    9.158278     F
Al             4.828245     9.045253     9.158087     F
Al             7.260515     8.999090     12.958981    F
Al             7.260362     11.997818    12.959293    F
Al             6.298665     14.696056    11.957399    F
Al             4.636119     10.497915    12.053077    F
O              3.286795     10.497867    13.239727    F
Al             6.284552     4.912093     6.955911     F
Al             6.284076     16.082265    6.956670     F
Al             7.604173     10.497806    2.473964     F
O              6.427186     10.497829    1.094369     F
Al             6.373607     6.298658     3.886442     F
O              4.781439     6.298720     2.980340     F
Al             6.373463     14.696867    3.886432     F
O              4.781445     14.697024    2.980331     F
O              3.454065     4.976984     9.235352     F
O              3.454134     7.620308     9.235370     F
O              6.249964     5.002962     13.162338    F
O              3.454132     16.018855    9.234991     F
O              3.453926     13.375312    9.235552     F
O              7.425549     9.104806     14.776049    F
O              7.425626     11.891007    14.776047    F
O              6.250208     15.992957    13.162131    F
O              4.962275     3.365439     7.283607     F
O              7.499732     3.492497     6.705341     F
O              4.962540     17.630386    7.284172     F
O              7.499788     17.503205    6.705522     F
O              7.704776     6.298715     2.777145     F
O              7.704778     14.696980    2.777147     F
Al             3.478927     10.498224    7.046788     F
O              1.926538     11.807721    6.890264     F
O              1.926585     9.187932     6.890319     F
O              3.361125     10.497903    5.169014     F
Al             2.050944     10.497858    10.125656    F
O              0.574781     10.497851    9.076086     F
O              2.097764     9.088325     11.188760    F
O              2.097753     11.907389    11.188769    F
Al             3.393325     6.298772     6.011401     F
O              1.956477     6.298698     7.179493     F
O              3.339458     7.715092     4.949246     F
O              3.339459     4.882324     4.949265     F
Al             3.393316     14.696992    6.011430     F
O              1.956482     14.697052    7.179498     F
O              3.339473     16.113385    4.949255     F
O              3.339471     13.280635    4.949232     F
H              3.439914     4.911182     10.243970    F
H              3.439259     7.689465     10.293375    F
H              6.818244     4.212980     13.048122    F
H              6.229235     4.955319     14.133904    F
H              3.439921     16.084510    10.243551    F
H              3.439298     13.306198    10.293478    F
H              6.777020     8.347597     14.909838    F
H              6.776813     12.647836    14.909837    F
H              6.229209     16.040400    14.133948    F
H              6.818420     16.782630    13.048246    F
H              4.227237     2.737996     7.166079     F
H              6.932394     2.747751     6.973668     F
H              7.409120     3.550952     5.707009     F
H              4.227807     18.258302    7.165629     F
H              6.932352     18.247974    6.973522     F
H              7.409060     17.444811    5.706965     F
H              7.521090     6.298718     1.832227     F
H              7.521091     14.697038    1.832228     F
H              3.346923     10.497840    14.197637    F
H              6.469066     10.497906    0.138110     F
H              0.036292     9.692186     9.043064     F
H              0.036293     11.303523    9.043066     F
H              2.008440     9.058197     12.145151    F
H              2.008453     11.937517    12.145156    F
```

H	4.786758	6.298734	2.000110	F
H	4.786758	14.696990	2.000090	F
H	6.866278	9.838720	15.040453	F
H	6.866533	11.156776	15.040420	F
H	4.132089	16.721542	9.197377	F
H	4.893023	17.533874	8.246018	F
H	4.893423	3.461516	8.246085	F
H	4.132056	4.274186	9.197228	F
H	2.690114	11.221842	5.059459	F
H	2.690182	9.773813	5.059456	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298722	8.126704	F
H	1.991769	14.696981	8.126702	F
H	4.137960	13.968648	3.050510	F
H	4.137956	7.027067	3.050515	F
H	3.423379	4.865220	3.998925	F
H	3.423376	16.130498	3.998926	F
H	3.423056	7.732143	4.002716	F
H	3.423062	13.263572	4.002716	F
H	2.742679	6.961339	9.160681	F
H	2.742700	14.034353	9.160650	F
Al	6.261900	7.657463	6.993816	R
O	4.833610	6.297126	7.126831	R
O	7.537529	6.272765	7.434472	R
O	6.270486	7.626779	5.071553	R
Al	7.261930	6.121857	9.248791	R
O	6.465751	7.461526	13.295219	R
O	7.704599	5.921008	10.911686	R
O	6.000935	4.830728	8.827195	R
O	6.047637	7.590313	8.942572	R
Al	7.319379	9.024038	4.889068	R
Al	7.249158	11.975770	4.849852	R
Al	6.238225	13.351418	6.973527	R
Al	6.391293	10.498543	7.134177	R
O	4.827665	14.705339	7.127206	R
O	4.970414	11.812446	7.271461	R
O	4.976371	9.179852	7.271429	R
O	7.529821	14.728814	7.417723	R
O	6.333729	10.481276	5.090099	R
O	7.560558	12.014807	6.687244	R
O	7.606346	9.036933	6.759330	R
O	6.195217	13.365930	5.044599	R
Al	7.265852	14.855953	9.234908	R
Al	7.976589	10.425103	10.373714	R
O	6.182404	10.498116	13.144894	R
O	6.488752	13.538532	13.288637	R
O	6.371020	10.495217	9.064409	R
O	7.707446	15.040970	10.903208	R
O	6.043057	13.404206	8.931074	R
O	6.004130	16.159915	8.829869	R
O	8.152912	9.054593	11.508689	R
O	8.172124	11.806308	11.519366	R
O	4.825587	6.083451	10.924605	R
O	4.824713	14.913192	10.928074	R
O	4.788468	9.073000	10.959999	R
O	4.787979	11.927990	10.962114	R
O	6.334559	4.953230	5.087039	R
O	6.342007	16.041406	5.087471	R
O	8.106581	9.089000	3.327790	R
O	8.047419	11.939116	3.298746	R
O	3.498331	10.497573	8.965985	R
Cu	8.924805	11.632987	7.955673	R
Cu	9.311837	8.917448	7.862632	R
O	9.319663	10.303184	9.184549	R
O	10.467945	7.565359	6.869728	R
O	11.122726	7.927396	7.908071	R

```
Model #77        Cartesian coordinates in angstrom
                 x                y                z                Relaxed/Frozen
Al               4.718170         6.298910         9.025580         F
Al               6.299260         6.298760         11.957070        F
Al               4.718050         14.696800        9.025020         F
Al               4.828110         11.950990        9.158280         F
Al               4.828300         9.045500         9.158060         F
Al               7.260440         8.999300         12.958900        F
Al               7.260290         11.997700        12.959250        F
Al               6.298520         14.696000        11.957210        F
Al               4.636050         10.497890        12.053110        F
O                3.286800         10.497870        13.239730        F
Al               6.284440         4.911970         6.956140         F
Al               6.283920         16.082290        6.956930         F
Al               7.604240         10.497810        2.473990         F
O                6.427190         10.497840        1.094370         F
Al               6.373540         6.298800         3.886510         F
O                4.781440         6.298720         2.980340         F
Al               6.373400         14.696720        3.886500         F
O                4.781450         14.697030        2.980330         F
O                3.454100         4.976950         9.235330         F
O                3.454130         7.620270         9.235320         F
O                6.250030         5.002870         13.162240        F
O                3.454190         16.018920        9.234920         F
O                3.453920         13.375340        9.235530         F
O                7.425650         9.104790         14.776040        F
O                7.425710         11.891040        14.776040        F
O                6.250260         15.993050        13.162030        F
O                4.962270         3.365420         7.283490         F
O                7.499820         3.492570         6.705330         F
O                4.962540         17.630400        7.284090         F
O                7.499880         17.503120        6.705520         F
O                7.704780         6.298700         2.777150         F
O                7.704790         14.696990        2.777160         F
Al               3.478770         10.498240        7.046870         F
O                1.926550         11.807740        6.890240         F
O                1.926610         9.187910         6.890300         F
O                3.361180         10.497910        5.169010         F
Al               2.050950         10.497870        10.125630        F
O                0.574780         10.497850        9.076090         F
O                2.097760         9.088330         11.188760        F
O                2.097750         11.907380        11.188770        F
Al               3.393310         6.298740         6.011430         F
O                1.956480         6.298700         7.179490         F
O                3.339450         7.715090         4.949240         F
O                3.339460         4.882340         4.949250         F
Al               3.393320         14.697030        6.011460         F
O                1.956480         14.697050        7.179500         F
O                3.339470         16.113370        4.949240         F
O                3.339470         13.280640        4.949230         F
H                3.439930         4.911170         10.243970        F
H                3.439250         7.689420         10.293380        F
H                6.818350         4.213040         13.048190        F
H                6.229110         4.955320         14.133900        F
H                3.439930         16.084520        10.243550        F
H                3.439290         13.306240        10.293980        F
H                6.777060         8.347560         14.909840        F
H                6.776830         12.647850        14.909840        F
H                6.229100         16.040400        14.133950        F
H                6.818530         16.782560        13.048320        F
H                4.227220         2.738020         7.166090         F
H                6.932380         2.747750         6.973640         F
H                7.409070         3.550910         5.707010         F
H                4.227810         18.258310        7.165620         F
H                6.932340         18.247980        6.973480         F
H                7.409020         17.444850        5.706970         F
H                7.521090         6.298710         1.832230         F
H                7.521090         14.697050        1.832230         F
H                3.346920         10.497840        14.197640        F
H                6.469070         10.497900        0.138110         F
H                0.036290         9.692190         9.043060         F
H                0.036290         11.303520        9.043070         F
H                2.008440         9.058200         12.145150        F
H                2.008460         11.937520        12.145160        F
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H	4.786760	6.298710	2.000110	F
H	4.786760	14.697020	2.000090	F
H	6.866250	9.838690	15.040460	F
H	6.866530	11.156780	15.040420	F
H	4.132090	16.721540	9.197380	F
H	4.893040	17.533890	8.246020	F
H	4.893450	3.461490	8.246090	F
H	4.132060	4.274190	9.197220	F
H	2.690110	11.221840	5.059460	F
H	2.690180	9.773810	5.059460	F
H	1.278480	12.508620	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991770	6.298720	8.126700	F
H	1.991770	14.696980	8.126700	F
H	4.137970	13.968640	3.050490	F
H	4.137970	7.027080	3.050500	F
H	3.423390	4.865220	3.998930	F
H	3.423380	16.130500	3.998930	F
H	3.423060	7.732140	4.002720	F
H	3.423070	13.263570	4.002720	F
H	2.742680	6.961340	9.160670	F
H	2.742700	14.034350	9.160630	F
Al	6.258866	7.640845	6.978623	R
O	4.793610	6.314971	7.130835	R
O	7.464250	6.290349	7.275089	R
O	6.191195	7.649803	5.036244	R
Al	7.501947	6.182742	9.179276	R
O	6.466740	7.483872	13.284514	R
O	7.627096	5.916172	10.930496	R
O	6.048042	4.887786	8.817801	R
O	6.043947	7.635755	8.905039	R
Al	7.232964	9.036324	4.840453	R
Al	7.260519	11.961624	4.839342	R
Al	6.296619	13.336964	6.987949	R
Al	6.265471	10.503917	7.017045	R
O	4.829890	14.699944	7.128881	R
O	4.926127	11.839725	7.253875	R
O	4.904183	9.211458	7.251385	R
O	7.538860	14.725402	7.422280	R
O	6.241279	10.515925	4.976904	R
O	7.573871	11.896162	6.685202	R
O	7.526962	9.120903	6.682589	R
O	6.246064	13.376025	5.070985	R
Al	7.273165	14.855414	9.239235	R
Al	7.781706	10.532918	10.336809	R
O	6.200605	10.498484	13.124016	R
O	6.486679	13.538828	13.298480	R
O	6.328462	10.545628	9.027138	R
O	7.705154	15.054998	10.908056	R
O	6.047067	13.398666	8.931084	R
O	6.006486	16.156376	8.830594	R
O	8.232168	9.205864	11.556957	R
O	8.057041	11.907294	11.435597	R
O	4.757445	6.139732	10.954711	R
O	4.821744	14.904545	10.927167	R
O	4.845295	9.110289	10.954944	R
O	4.783659	11.928111	10.961249	R
O	6.298934	4.938985	5.061763	R
O	6.333696	16.044997	5.086364	R
O	8.090521	9.085057	3.320245	R
O	8.079285	11.933535	3.299114	R
O	3.474858	10.507706	8.961670	R
Cu	8.812467	10.466356	7.579909	R
Cu	9.553817	8.349792	10.177320	R
O	9.201965	10.058552	9.309761	R
O	9.275277	6.791638	8.982058	R
O	10.452953	6.919189	10.789097	R

```
Model #78      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al      4.717835       6.298612       9.025475       F
Al      6.299384       6.298646       11.957419      F
Al      4.717875       14.696836      9.025066       F
Al      4.827861       11.950745      9.158624       F
Al      4.828227       9.045282       9.158072       F
Al      7.260096       9.000421       12.957868      F
Al      7.260388       11.997822      12.958848      F
Al      6.298258       14.695803      11.957678      F
Al      4.636200       10.497831      12.053243      F
O       3.286795       10.497886      13.239727      F
Al      6.284524       4.912271       6.956042       F
Al      6.284109       16.081719      6.957020       F
Al      7.604163       10.497718      2.474360       F
O       6.427272       10.497890      1.094295       F
Al      6.373606       6.298664       3.886515       F
O       4.781481       6.298717       2.980266       F
Al      6.373583       14.696718      3.886690       F
O       4.781507       14.697060      2.980223       F
O       3.454156       4.976899       9.235359       F
O       3.454064       7.620378       9.235327       F
O       6.249989       5.002993       13.162372      F
O       3.454366       16.019083      9.234968       F
O       3.453937       13.375403      9.235510       F
O       7.425874       9.104716       14.776025      F
O       7.426002       11.891148      14.776021      F
O       6.250253       15.993036      13.162049      F
O       4.962211       3.365476       7.283519       F
O       7.499746       3.492493       6.705431       F
O       4.962466       17.630345      7.284069       F
O       7.499759       17.503233      6.705540       F
O       7.704744       6.298706       2.777107       F
O       7.704713       14.697037      2.777069       F
Al      3.478920       10.498125      7.047239       F
O       1.926579       11.807762      6.890203       F
O       1.926596       9.187946       6.890095       F
O       3.361164       10.497953      5.169011       F
Al      2.050993       10.497890      10.125643      F
O       0.574788       10.497849      9.076076       F
O       2.097779       9.088326       11.188760      F
O       2.097762       11.907391      11.188766      F
Al      3.393382       6.298768       6.011340       F
O       1.956482       6.298697       7.179498       F
O       3.339461       7.715099       4.949255       F
O       3.339463       4.882316       4.949275       F
Al      3.393374       14.697027      6.011361       F
O       1.956485       14.697083      7.179501       F
O       3.339466       16.113391      4.949264       F
O       3.339459       13.280637      4.949231       F
H       3.439924       4.911172       10.243969      F
H       3.439342       7.689450       10.293377      F
H       6.818202       4.212954       13.048092      F
H       6.229202       4.955320       14.133903      F
H       3.439908       16.084497      10.243552      F
H       3.439423       13.306277      10.293985      F
H       6.777216       8.347427       14.909830      F
H       6.776662       12.647705      14.909843      F
H       6.229197       16.040400      14.133948      F
H       6.818465       16.782602      13.048278      F
H       4.227277       2.737956       7.166048       F
H       6.932383       2.747747       6.973633       F
H       7.409122       3.550953       5.707009       F
H       4.227911       18.258408      7.165546       F
H       6.932318       18.247985      6.973421       F
H       7.409001       17.444862      5.706967       F
H       7.521090       6.298732       1.832227       F
H       7.521091       14.697013      1.832228       F
H       3.346923       10.497845      14.197637      F
H       6.469066       10.497934      0.138110       F
H       0.036293       9.692186       9.043063       F
H       0.036288       11.303520      9.043073       F
H       2.008434       9.058196       12.145150      F
H       2.008445       11.937518      12.145155      F
```

H	4.786758	6.298761	2.000110	F
H	4.786758	14.696959	2.000090	F
H	6.866030	9.838518	15.040487	F
H	6.866503	11.156801	15.040424	F
H	4.132082	16.721545	9.197311	F
H	4.892997	17.533853	8.246014	F
H	4.893418	3.461521	8.246085	F
H	4.132054	4.274185	9.197215	F
H	2.690130	11.221856	5.059458	F
H	2.690175	9.773820	5.059457	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298727	8.126704	F
H	1.991769	14.696961	8.126702	F
H	4.137938	13.968671	3.050548	F
H	4.137934	7.027044	3.050553	F
H	3.423368	4.865221	3.998924	F
H	3.423368	16.130497	3.998925	F
H	3.423048	7.732142	4.002715	F
H	3.423069	13.263571	4.002717	F
H	2.742679	6.961340	9.160671	F
H	2.742698	14.034343	9.160581	F
Al	6.254609	7.657858	6.992114	R
O	4.831470	6.293987	7.128773	R
O	7.533245	6.271437	7.430503	R
O	6.250933	7.623595	5.070233	R
Al	7.262375	6.125026	9.244501	R
O	6.486818	7.457304	13.293221	R
O	7.707951	5.935475	10.909679	R
O	6.002034	4.830133	8.829636	R
O	6.047583	7.590213	8.943658	R
Al	7.288222	9.026579	4.880485	R
Al	7.276595	11.962897	4.888702	R
Al	6.256227	13.331565	6.987224	R
Al	6.410462	10.504257	7.158576	R
O	4.835296	14.702818	7.127221	R
O	4.967763	11.818328	7.275186	R
O	4.977533	9.179759	7.272610	R
O	7.543912	14.728669	7.432972	R
O	6.323298	10.489572	5.090765	R
O	7.576572	11.969092	6.744044	R
O	7.592487	9.030976	6.749412	R
O	6.239607	13.371553	5.063075	R
Al	7.256429	14.867199	9.247418	R
Al	7.894414	10.495367	10.330485	R
O	6.181812	10.499504	13.150823	R
O	6.487959	13.540917	13.294757	R
O	6.306992	10.498357	9.081611	R
O	7.710104	15.059446	10.909828	R
O	6.048871	13.406878	8.941120	R
O	6.002820	16.164809	8.829330	R
O	8.133585	9.132231	11.487061	R
O	8.132711	11.865181	11.485315	R
O	4.825918	6.080512	10.927684	R
O	4.828430	14.916710	10.925825	R
O	4.785709	9.067181	10.966412	R
O	4.785578	11.932161	10.967006	R
O	6.336140	4.951114	5.086078	R
O	6.344439	16.044669	5.087049	R
O	8.079252	9.074491	3.319925	R
O	8.073899	11.918671	3.328689	R
O	3.491597	10.497118	8.967211	R
Cu	9.295686	12.101244	7.971453	R
Cu	9.291705	9.057379	7.808584	R
O	9.089681	10.509342	8.998731	R
O	10.517161	7.720797	6.953135	R
O	11.207925	8.273870	7.884804	R
C	10.443711	13.495073	7.633114	R
O	11.180013	14.344202	7.436686	R

```
Model #79      Cartesian coordinates in angstrom
               x              y              z              Relaxed/Frozen
Al             4.717974       6.298476       9.025386       F
Al             6.299312       6.298819       11.957195      F
Al             4.717953       14.696883      9.024927       F
Al             4.827881       11.950919      9.158479       F
Al             4.828107       9.045146       9.158100       F
Al             7.260143       9.000231       12.958261      F
Al             7.260090       11.997941      12.958975      F
Al             6.298418       14.695854      11.957623      F
Al             4.636148       10.497900      12.053169      F
O              3.286807       10.497853      13.239739      F
Al             6.284617       4.912027       6.955920       F
Al             6.284144       16.081880      6.956779       F
Al             7.604134       10.497888      2.474313       F
O              6.427272       10.497850      1.094295       F
Al             6.373628       6.298597       3.886413       F
O              4.781455       6.298718       2.980312       F
Al             6.373670       14.696802      3.886559       F
O              4.781461       14.697016      2.980304       F
O              3.454081       4.976967       9.235350       F
O              3.454054       7.620379       9.235338       F
O              6.250006       5.002962       13.162341      F
O              3.454255       16.018972      9.234990       F
O              3.453937       13.375365      9.235570       F
O              7.425849       9.104757       14.776025      F
O              7.426013       11.891120      14.776018      F
O              6.250244       15.992993      13.162093      F
O              4.962244       3.365450       7.283536       F
O              7.499739       3.492496       6.705384       F
O              4.962503       17.630359      7.284145       F
O              7.499797       17.503204      6.705558       F
O              7.704767       6.298706       2.777134       F
O              7.704766       14.696998      2.777133       F
Al             3.478843       10.498133      7.047190       F
O              1.926556       11.807738      6.890231       F
O              1.926598       9.187924       6.890261       F
O              3.361171       10.497878      5.169012       F
Al             2.050971       10.497886      10.125670      F
O              0.574785       10.497851      9.076080       F
O              2.097774       9.088324       11.188760      F
O              2.097764       11.907389      11.188768      F
Al             3.393366       6.298731       6.011329       F
O              1.956483       6.298722       7.179501       F
O              3.339466       7.715103       4.949260       F
O              3.339457       4.882321       4.949270       F
Al             3.393343       14.696953      6.011415       F
O              1.956483       14.697082      7.179498       F
O              3.339477       16.113388      4.949258       F
O              3.339455       13.280644      4.949221       F
H              3.439914       4.911182       10.243971      F
H              3.439266       7.689500       10.293374      F
H              6.818217       4.212964       13.048103      F
H              6.229252       4.955319       14.133904      F
H              3.439948       16.084537      10.243550      F
H              3.439353       13.306252      10.293982      F
H              6.777197       8.347445       14.909830      F
H              6.776751       12.647781      14.909840      F
H              6.229205       16.040400      14.133948      F
H              6.818441       16.782617      13.048262      F
H              4.227231       2.738003       7.166084       F
H              6.932395       2.747752       6.973670       F
H              7.409125       3.550957       5.707009       F
H              4.227859       18.258353      7.165589       F
H              6.932338       18.247978      6.973480       F
H              7.409022       17.444844      5.706967       F
H              7.521090       6.298732       1.832227       F
H              7.521091       14.697044      1.832228       F
H              3.346923       10.497852      14.197637      F
H              6.469066       10.497914      0.138110       F
H              0.036292       9.692186       9.043062       F
H              0.036293       11.303523      9.043067       F
H              2.008439       9.058197       12.145151      F
H              2.008447       11.937517      12.145156      F
```

H	4.786758	6.298753	2.000110	F
H	4.786758	14.696995	2.000090	F
H	6.866073	9.838553	15.040481	F
H	6.866550	11.156762	15.040418	F
H	4.132086	16.721543	9.197354	F
H	4.893014	17.533865	8.246016	F
H	4.893418	3.461521	8.246085	F
H	4.132058	4.274186	9.197242	F
H	2.690146	11.221872	5.059457	F
H	2.690165	9.773829	5.059456	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298719	8.126704	F
H	1.991769	14.696970	8.126702	F
H	4.137956	13.968652	3.050517	F
H	4.137944	7.027055	3.050534	F
H	3.423377	4.865220	3.998925	F
H	3.423369	16.130498	3.998926	F
H	3.423047	7.732142	4.002715	F
H	3.423076	13.263571	4.002717	F
H	2.742679	6.961339	9.160687	F
H	2.742699	14.034350	9.160627	F
Al	6.254453	7.651346	6.990240	R
O	4.832036	6.293494	7.127766	R
O	7.539866	6.271745	7.426210	R
O	6.231737	7.623934	5.065126	R
Al	7.266071	6.133415	9.242525	R
O	6.484252	7.458282	13.291131	R
O	7.707457	5.939135	10.907983	R
O	6.005126	4.835288	8.827713	R
O	6.046163	7.591613	8.938109	R
Al	7.265302	9.026894	4.873418	R
Al	7.277081	11.967963	4.877694	R
Al	6.251746	13.341311	6.991674	R
Al	6.389206	10.495172	7.142272	R
O	4.832566	14.700723	7.127309	R
O	4.972818	11.816437	7.272141	R
O	4.971211	9.180369	7.272548	R
O	7.541718	14.719238	7.428861	R
O	6.317010	10.501690	5.096485	R
O	7.583709	11.970387	6.743539	R
O	7.576575	9.020463	6.731271	R
O	6.243502	13.371073	5.068390	R
Al	7.265624	14.864931	9.245351	R
Al	7.905345	10.509230	10.344336	R
O	6.180727	10.498592	13.149688	R
O	6.478926	13.537911	13.294664	R
O	6.344132	10.499478	9.065168	R
O	7.705852	15.061107	10.909901	R
O	6.046794	13.403961	8.939173	R
O	6.005018	16.159762	8.826501	R
O	8.134853	9.139683	11.491533	R
O	8.124414	11.882573	11.485229	R
O	4.825659	6.082968	10.926322	R
O	4.825404	14.912421	10.925104	R
O	4.789766	9.070642	10.961512	R
O	4.788271	11.925270	10.961469	R
O	6.340229	4.952827	5.087034	R
O	6.338878	16.041166	5.088185	R
O	8.061270	9.071298	3.319467	R
O	8.074685	11.919134	3.324164	R
O	3.496740	10.498400	8.966082	R
Cu	9.293525	11.883216	7.742663	R
Cu	9.305767	9.238743	7.695503	R
O	9.225356	10.514947	9.122360	R
O	11.143136	9.444605	7.110952	R
O	11.932027	10.386928	7.535313	R
C	11.246850	11.929949	7.783018	R
O	12.072749	12.684020	8.120930	R

```
Model #80      Cartesian coordinates in angstrom
               x            y            z            Relaxed/Frozen
Al             4.718126     6.298940     9.025603     F
Al             6.299243     6.298805     11.957039    F
Al             4.718039     14.696795    9.024986     F
Al             4.828051     11.951034    9.158281     F
Al             4.828259     9.045471     9.158021     F
Al             7.260454     8.999375     12.958918    F
Al             7.260404     11.997796    12.959413    F
Al             6.298567     14.695902    11.957239    F
Al             4.636064     10.497864    12.053141    F
O              3.286801     10.497868    13.239735    F
Al             6.284428     4.911875     6.956085     F
Al             6.283928     16.082257    6.956937     F
Al             7.604178     10.497847    2.473942     F
O              6.427215     10.497815    1.094345     F
Al             6.373576     6.298788     3.886468     F
O              4.781425     6.298737     2.980363     F
Al             6.373391     14.696691    3.886489     F
O              4.781451     14.697022    2.980322     F
O              3.454060     4.976989     9.235352     F
O              3.454117     7.620269     9.235287     F
O              6.250027     5.002915     13.162290    F
O              3.454192     16.018933    9.234870     F
O              3.453893     13.375336    9.235523     F
O              7.425673     9.104755     14.776041    F
O              7.425582     11.891053    14.776055    F
O              6.250260     15.993040    13.162044    F
O              4.962272     3.365418     7.283497     F
O              7.499866     3.492611     6.705341     F
O              4.962547     17.630406    7.284106     F
O              7.499892     17.503118    6.705537     F
O              7.704781     6.298710     2.777152     F
O              7.704780     14.696984    2.777150     F
Al             3.478733     10.498224    7.046897     F
O              1.926564     11.807747    6.890225     F
O              1.926603     9.187917     6.890267     F
O              3.361187     10.497924    5.169010     F
Al             2.050944     10.497868    10.125620    F
O              0.574782     10.497851    9.076085     F
O              2.097767     9.088329     11.188767    F
O              2.097753     11.907382    11.188777    F
Al             3.393307     6.298748     6.011422     F
O              1.956477     6.298714     7.179494     F
O              3.339452     7.715094     4.949247     F
O              3.339459     4.882338     4.949246     F
Al             3.393326     14.697023    6.011448     F
O              1.956483     14.697056    7.179499     F
O              3.339474     16.113374    4.949241     F
O              3.339466     13.280636    4.949231     F
H              3.439953     4.911145     10.243968    F
H              3.439242     7.689413     10.293378    F
H              6.818339     4.213040     13.048189    F
H              6.229152     4.955320     14.133903    F
H              3.439938     16.084527    10.243550    F
H              3.439262     13.306231    10.293980    F
H              6.777092     8.347534     14.909835    F
H              6.776808     12.647832    14.909837    F
H              6.229092     16.040398    14.133946    F
H              6.818532     16.782560    13.048325    F
H              4.227195     2.738040     7.166113     F
H              6.932395     2.747751     6.973670     F
H              7.409082     3.550919     5.707011     F
H              4.227820     18.258315    7.165618     F
H              6.932339     18.247977    6.973486     F
H              7.409022     17.444844    5.706966     F
H              7.521090     6.298705     1.832227     F
H              7.521091     14.697054    1.832228     F
H              3.346923     10.497846    14.197637    F
H              6.469066     10.497890    0.138110     F
H              0.036293     9.692186     9.043063     F
H              0.036291     11.303522    9.043069     F
H              2.008445     9.058197     12.145151    F
H              2.008462     11.937517    12.145156    F
```

H	4.786758	6.298694	2.000110	F
H	4.786758	14.697018	2.000090	F
H	6.866264	9.838710	15.040455	F
H	6.866593	11.156726	15.040412	F
H	4.132087	16.721542	9.197364	F
H	4.893041	17.533889	8.246021	F
H	4.893465	3.461481	8.246091	F
H	4.132051	4.274184	9.197187	F
H	2.690117	11.221844	5.059460	F
H	2.690182	9.773813	5.059456	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298707	8.126704	F
H	1.991769	14.696981	8.126702	F
H	4.137971	13.968636	3.050491	F
H	4.137972	7.027083	3.050489	F
H	3.423390	4.865219	3.998926	F
H	3.423380	16.130499	3.998927	F
H	3.423061	7.732143	4.002716	F
H	3.423068	13.263572	4.002716	F
H	2.742679	6.961342	9.160661	F
H	2.742699	14.034347	9.160609	F
Al	6.196440	7.644538	6.956761	R
O	4.783361	6.307003	7.129801	R
O	7.441349	6.293753	7.253487	R
O	6.198256	7.659284	5.026365	R
Al	7.435590	6.200561	9.202564	R
O	6.471733	7.469911	13.296387	R
O	7.642614	5.869945	10.928855	R
O	6.041820	4.886751	8.811243	R
O	6.039532	7.617513	8.906051	R
Al	7.303593	9.018429	4.891776	R
Al	7.302738	11.978196	4.896163	R
Al	6.201799	13.355351	6.954999	R
Al	6.374188	10.501958	7.115908	R
O	4.780306	14.685370	7.130178	R
O	4.903419	11.801924	7.254322	R
O	4.906705	9.188772	7.253506	R
O	7.436358	14.707052	7.253110	R
O	6.344363	10.495523	5.106067	R
O	7.547815	11.976111	6.776232	R
O	7.551119	9.021047	6.779003	R
O	6.192697	13.334121	5.021985	R
Al	7.449757	14.783481	9.193804	R
Al	7.778983	10.485239	10.368476	R
O	6.187240	10.497603	13.137503	R
O	6.473484	13.525306	13.295643	R
O	6.279915	10.493807	9.055992	R
O	7.640853	15.114328	10.925493	R
O	6.037673	13.373861	8.904309	R
O	6.040235	16.106160	8.813391	R
O	8.098575	9.112500	11.461383	R
O	8.112295	11.848087	11.472908	R
O	4.773756	6.121811	10.942826	R
O	4.768943	14.869503	10.946233	R
O	4.777859	9.088816	10.951692	R
O	4.779699	11.903918	10.951506	R
O	6.292490	4.939790	5.063452	R
O	6.289294	16.056293	5.061600	R
O	8.085303	9.078748	3.326849	R
O	8.087186	11.912359	3.331447	R
O	3.438281	10.496137	8.939495	R
Cu	8.883830	12.230277	8.356500	R
Cu	8.897740	8.770803	8.301504	R
O	9.018705	10.481141	9.004449	R
O	9.096649	6.937811	8.770334	R
O	9.112176	14.020251	8.791621	R
N	11.049586	8.002497	6.939519	R
O	11.028053	7.383343	5.967185	R

```
Model #81      Cartesian coordinates in angstrom
               x               y               z               Relaxed/Frozen
Al             4.718175        6.298911        9.025582        F
Al             6.299309        6.298754        11.957060       F
Al             4.718012        14.696822       9.025000        F
Al             4.828064        11.951012       9.158303        F
Al             4.828272        9.045479        9.158067        F
Al             7.260388        8.999313        12.958868       F
Al             7.260274        11.997782       12.959219       F
Al             6.298564        14.695966       11.957258       F
Al             4.636045        10.497899       12.053109       F
O              3.286801        10.497866       13.239734       F
Al             6.284466        4.911929        6.956114        F
Al             6.283894        16.082229       6.956961        F
Al             7.604222        10.497831       2.473997        F
O              6.427197        10.497843       1.094359        F
Al             6.373556        6.298806        3.886504        F
O              4.781440        6.298723        2.980337        F
Al             6.373398        14.696692       3.886513        F
O              4.781449        14.697021       2.980326        F
O              3.454093        4.976957        9.235346        F
O              3.454131        7.620266        9.235316        F
O              6.250030        5.002878        13.162251       F
O              3.454195        16.018936       9.234867        F
O              3.453914        13.375342       9.235541        F
O              7.425654        9.104799        14.776040       F
O              7.425711        11.891046       14.776043       F
O              6.250292        15.993036       13.162049       F
O              4.962264        3.365421        7.283477        F
O              7.499822        3.492574        6.705340        F
O              4.962540        17.630401       7.284102        F
O              7.499894        17.503117       6.705540        F
O              7.704782        6.298703        2.777153        F
O              7.704786        14.696990       2.777157        F
Al             3.478752        10.498243       7.046882        F
O              1.926556        11.807739       6.890234        F
O              1.926610        9.187906        6.890293        F
O              3.361185        10.497915       5.169010        F
Al             2.050946        10.497865       10.125632       F
O              0.574782        10.497852       9.076085        F
O              2.097766        9.088327        11.188764       F
O              2.097754        11.907385       11.188773       F
Al             3.393313        6.298744        6.011431        F
O              1.956476        6.298701        7.179492        F
O              3.339453        7.715091        4.949244        F
O              3.339458        4.882336        4.949249        F
Al             3.393323        14.697013       6.011456        F
O              1.956482        14.697054       7.179498        F
O              3.339473        16.113373       4.949240        F
O              3.339465        13.280638       4.949229        F
H              3.439933        4.911164        10.243969       F
H              3.439255        7.689421        10.293378       F
H              6.818340        4.213040        13.048190       F
H              6.229120        4.955321        14.133902       F
H              3.439933        16.084522       10.243550       F
H              3.439285        13.306240       10.293981       F
H              6.777069        8.347554        14.909836       F
H              6.776826        12.647847       14.909836       F
H              6.229104        16.040398       14.133946       F
H              6.818528        16.782563       13.048322       F
H              4.227206        2.738028        7.166104        F
H              6.932386        2.747748        6.973643        F
H              7.409076        3.550914        5.707011        F
H              4.227832        18.258327       7.165609        F
H              6.932336        18.247978       6.973476        F
H              7.409025        17.444841       5.706966        F
H              7.521090        6.298707        1.832227        F
H              7.521091        14.697052       1.832228        F
H              3.346923        10.497843       14.197637       F
H              6.469066        10.497901       0.138110        F
H              0.036292        9.692186        9.043064        F
H              0.036293        11.303523       9.043067        F
H              2.008443        9.058197        12.145151       F
H              2.008458        11.937517       12.145156       F
```

H	4.786758	6.298708	2.000110	F
H	4.786758	14.697020	2.000090	F
H	6.866244	9.838693	15.040458	F
H	6.866542	11.156768	15.040419	F
H	4.132088	16.721542	9.197370	F
H	4.893034	17.533883	8.246020	F
H	4.893453	3.461491	8.246090	F
H	4.132054	4.274186	9.197218	F
H	2.690112	11.221839	5.059460	F
H	2.690182	9.773813	5.059456	F
H	1.278480	12.508617	6.923340	F
H	1.278480	8.487100	6.923340	F
H	1.991769	6.298719	8.126704	F
H	1.991769	14.696983	8.126702	F
H	4.137973	13.968634	3.050488	F
H	4.137968	7.027079	3.050496	F
H	3.423386	4.865219	3.998926	F
H	3.423382	16.130499	3.998927	F
H	3.423061	7.732143	4.002716	F
H	3.423069	13.263572	4.002716	F
H	2.742679	6.961341	9.160668	F
H	2.742699	14.034348	9.160613	F
Al	6.200317	7.642762	6.955898	R
O	4.781305	6.309079	7.130219	R
O	7.438107	6.289258	7.251527	R
O	6.193787	7.660164	5.023611	R
Al	7.442967	6.208057	9.198052	R
O	6.471697	7.470794	13.295664	R
O	7.641807	5.876235	10.926900	R
O	6.040770	4.888267	8.812209	R
O	6.038878	7.619583	8.905273	R
Al	7.302563	9.017760	4.895277	R
Al	7.305887	11.978349	4.896838	R
Al	6.200040	13.353100	6.955400	R
Al	6.377134	10.497482	7.116671	R
O	4.780670	14.686266	7.130515	R
O	4.903563	11.804182	7.254716	R
O	4.903121	9.191395	7.254461	R
O	7.436232	14.706381	7.252562	R
O	6.345522	10.498984	5.108255	R
O	7.550534	11.977954	6.781308	R
O	7.548362	9.017965	6.777933	R
O	6.195349	13.334632	5.023662	R
Al	7.444333	14.789945	9.196243	R
Al	7.775892	10.490774	10.368729	R
O	6.187269	10.498112	13.137168	R
O	6.472768	13.525869	13.296628	R
O	6.277997	10.497204	9.056852	R
O	7.642005	15.116037	10.926375	R
O	6.038861	13.375721	8.905278	R
O	6.040388	16.107669	8.813124	R
O	8.106994	9.125734	11.467853	R
O	8.101894	11.861822	11.465154	R
O	4.770941	6.124257	10.944756	R
O	4.770340	14.871234	10.945033	R
O	4.778728	9.090743	10.951364	R
O	4.776967	11.905306	10.951476	R
O	6.290741	4.938558	5.061875	R
O	6.288993	16.056098	5.062315	R
O	8.083337	9.080103	3.328943	R
O	8.087490	11.913645	3.330696	R
O	3.435961	10.497808	8.938750	R
Cu	8.879239	12.233316	8.360573	R
Cu	8.916773	8.767521	8.323181	R
O	9.014207	10.499325	9.005084	R
O	9.105897	6.948553	8.768984	R
O	9.106713	14.039890	8.767451	R
N	11.072503	8.116914	6.924871	R
O	11.001308	7.549084	5.923463	R