

Supporting Information

Interaction of Biologically Important Organic Molecules with the Unsaturated Copper Centers of the HKUST-1 Metal-Organic Framework.

- 1) Deformation energies of the MOF and the guest molecules upon adsorption.
- 2) Cartesian coordinates of all structures

1) Deformation energies of the MOF and the guest molecules upon adsorption.

Table S1: Deformation energies of the MOF ($\delta E(\text{MOF})$), the guest molecules $\delta E(\text{guest})$ upon adsorption . (kJ mol⁻¹)

	Binding mode	$\delta E(\text{MOF})$	$\delta E(\text{guest})$	$\delta E(\text{Total})$
Urea	($\eta^1\text{-N}$)-Cu	+6.7	+6.1	+12.8
	($\eta^1\text{-O}$)-Urea	+25.4	+7.9	+33.2
	LCW	+5.6	+4.8	+10.4
	SCW	+3.1	+0.9	+4.1
Glycine	($\eta^1\text{-N}$)-Cu	+8.3	+6.5	+14.8
	($\eta^1\text{-O}_\alpha$)-Cu	+14.2	+1.9	+16.0
	($\eta^1\text{-O}_\beta$)-Cu	+12.0	+11.8	+23.8
	LCW	+4.4	+8.4	+12.7
	SCW	+2.8	+7.2	+10.0
Caffeine	($\eta^1\text{-N}:\eta^1\text{-O}:\eta^1\text{-O}$)-Cu	+35.6	+6.2	+41.8
	LCW	+3.8	+2.7	+6.5
Niacin	($\eta^1\text{-N}:\eta^1\text{-O}$)-Cu	+22.4	+7.6	+30.0
	($\eta^1\text{-O}$)-Cu	+15.7	+8.2	+23.9
	LCW	+14.6	+3.3	+17.9
H ₂ O	($\eta^1\text{-O}$)-Cu	+4.9	+0.2	+5.1
	LCW	+0.9	+0	+0.9
	SCW	+3.9	+0.1	+4.0

${}^i\delta E(\text{MOF})$, $\delta E(\text{guest})$ are the deformation energies of the MOF and guest molecule respectively with respect to their isolated geometries.

2) Cartesian coordinates of all structures

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Energy = -53933.38787644 , Cu24

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 C -4.6944628 -8.6209180 2.9711306
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O	1.0143185	-7.2058151	-4.5256260	H	-3.6486873	2.8953259	-6.6858490
O	1.0085654	-8.8230859	-6.1249034	H	-3.3234556	9.9918907	-5.6728722
O	-1.8119493	-8.8160246	-6.1263543	H	-10.7574447	5.6355733	-2.5916795
O	-1.8032069	6.1149901	-8.1267311	H	-7.4196739	2.8943580	-2.9231171
O	1.0077134	8.1007223	-6.1286142	H	2.5174258	-10.7096301	6.3536934

H	5.6248449	-3.2843795	10.6991062	C	-0.9178636	1.2484977	4.3313231
H	9.9575443	-6.3654299	3.2578592	H	-0.2768820	2.2400047	6.1392807
H	2.5375304	-6.3611154	10.7107063	H	-1.9584721	2.5664070	5.7088280
H	6.6266486	-3.6165394	3.5958338	O	-1.4757038	0.1533394	4.8982797
H	2.8753016	-3.6241991	7.3698406	O	-0.4441858	1.2651894	3.2110910
H	5.5965350	-10.7126702	3.2690855	H	-1.3911190	-0.5807053	4.2404711
H	2.8560500	-7.3753635	3.6084779				418
H	9.9652049	-3.2790632	6.3353599				Energy = -54217.31446253 , Cu24 - Glycine(O)
H	2.4832848	5.6035662	10.6926601	C	-5.5653905	-10.2086744	3.7673897
H	5.5846962	9.9938234	3.2788393	C	-5.1146345	-8.9519668	3.3121596
H	9.9543414	2.5571693	6.3404992	C	-4.0240400	-8.3286116	3.9445723
H	2.5033199	9.9736001	6.3627586	C	-3.3972356	-8.9471253	5.0411945
H	2.8687111	6.6365778	3.6301203	C	-3.8518929	-10.2038379	5.4924754
H	5.5956182	2.5515266	10.6833050	C	-4.9274096	-10.8340019	4.8489966
H	2.8184685	2.8458344	7.3719332	C	-5.8143886	-8.2596846	2.1795868
H	9.9494181	5.6390403	3.2586284	O	-5.2892037	-7.1800128	1.7478524
H	6.6158638	2.8944287	3.6003452	Cu	-6.2015482	-6.1260385	0.3299802
H	2.5221309	-6.3613878	-10.0036383	O	-7.2615088	-5.2184453	-1.0862674
H	9.9438282	-3.2871386	-5.6566170	C	-8.3417662	-5.7452720	-1.5147515
H	2.5083926	-10.7190984	-5.6437326	O	-8.8765682	-6.8198747	-1.0768618
H	2.8533392	-7.3803633	-2.9052154	Cu	-7.9440497	-7.8680134	0.3349517
H	5.6015260	-3.2769138	-10.0035902	O	-8.8671868	-6.8061151	1.7446592
H	2.8587431	-3.6177345	-6.6680940	C	-8.3309324	-5.7301468	2.1771672
H	5.5877263	-10.7224695	-2.5593231	C	-9.0233351	-5.0300320	3.3097120
H	9.9406079	-6.3741627	-2.5799195	C	-10.2814115	-5.4801539	3.7617331
H	6.6151262	-3.6167317	-2.9042154	C	-10.9087344	-4.8430498	4.8426041
H	11.0981608	4.4856302	5.1854650	C	-10.2789810	-3.7690287	5.4886802
H	4.4292366	11.1448251	-4.4848996	C	-9.0206079	-3.3150030	5.0410533
H	-5.2547403	11.1363171	-4.5229746	C	-8.4000815	-3.9407623	3.9448034
H	11.1070915	-5.2105141	5.1830697	C	-8.3275997	-2.1881794	5.7489854
H	4.4704236	-5.2091317	11.8502004	O	-8.8705401	-1.7553216	6.8219728
H	4.4437854	-11.8570584	5.1987391	Cu	-7.9655226	-0.3391436	7.8836159
H	-5.2392445	4.4874994	-11.1657718	O	-6.9522618	1.0819651	8.8406596
H	-11.8751491	-5.2111924	-4.5019618	C	-5.8800100	1.5277776	8.3095434
H	-11.8821245	4.4792837	5.1853771	C	-5.1808964	2.6541267	9.0139111
H	-11.8979796	4.4819633	-4.5231262	C	-5.6341949	3.1134023	10.2673011
H	-5.2984023	4.5556197	11.9352470	C	-4.9839730	4.1853708	10.8981797
H	-5.2317192	-5.2046382	-11.1612933	C	-3.8926397	4.8119861	10.2785984
H	4.4310806	4.4726849	11.8298775	C	-3.4294756	4.3516871	9.0276195
H	11.0852159	-5.2221487	-4.5098596	C	-4.0754511	3.2705019	8.4018141
H	4.4601240	4.4912016	-11.1444877	C	-2.2845612	5.0382104	8.3464171
H	-5.1989357	-5.1668593	11.8778440	O	-1.9391684	6.1826553	8.7721706
H	-5.2395306	-11.8403995	5.1988451	Cu	-0.4301356	7.0799240	7.8099976
H	-11.8328233	-5.1640911	5.2239273	O	0.8852276	5.9663484	8.8013460
H	-5.2559100	-11.8427315	-4.4913282	C	1.4172192	4.9666633	8.2109975
H	4.4493747	-5.2060521	-11.1494369	O	1.0946020	4.5146241	7.0638187
H	4.4325715	-11.8682818	-4.4866335	Cu	-0.3931575	5.3193663	5.9987814
H	11.0820268	4.4984923	-4.4995064	O	-1.9249517	6.3382766	5.2345108
H	4.4254206	11.1312800	5.2081427	C	-2.2680651	7.4767160	5.6929198
H	-5.2936475	11.1102762	5.2168942	C	-3.3924354	8.1825022	4.9915903
N	-0.5272383	3.6927101	4.6354681	C	-3.8237926	9.4511163	5.4319673
H	0.3930921	3.5621453	4.1846848	C	-4.8958749	10.0903596	4.7912996
H	-1.1758653	3.9373884	3.8704968	C	-5.5510825	9.4644180	3.7205245
C	-0.9449506	2.4434853	5.2725827	C	-5.1212931	8.1972039	3.2741382

C -4.0369094 7.5627265 3.9064255
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Cu -6.2397474 5.3864350 0.2988682
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O -6.9131401 8.0702601 -1.0997199
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C 1.4172041 7.5631388 -5.0567090
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C	-5.5423406	-3.7953893	-9.5668602	Cu	5.3811575	-0.3655251	-5.4349979
C	-4.8963658	-4.8718532	-10.1928747	O	6.4408640	-1.7787665	-4.5219461
C	-3.8198243	-5.5115378	-9.5605531	C	7.5208457	-2.2091448	-5.0475926
O	-5.2897488	-7.1866488	-1.0817249	C	8.2128247	-3.3432956	-4.3498346
O	-7.2516407	-5.2050209	1.7445526	C	9.4695873	-3.7983126	-4.8006726
O	-7.2993791	4.4821682	-1.1148136	C	10.0938090	-4.8817064	-4.1645386
O	-7.3013708	4.4781557	1.7149346	C	9.4626814	-5.5271871	-3.0907075
O	-8.8948011	1.0635332	6.8141541	C	8.2060053	-5.0760973	-2.6359321
O	-6.8892091	-1.7376705	8.8116604	C	7.5886139	-3.9777422	-3.2609346
C	-5.8052884	-2.1586838	8.2822841	C	7.5080391	-5.7807456	-1.5099168
O	-5.2779623	-1.7189829	7.2065647	O	6.4289462	-5.2532345	-1.0791250
C	-5.0971386	-3.2846654	8.9764316	Cu	5.3774135	-6.1624409	0.3383527
C	-4.0073928	-3.9164636	8.3504244	O	4.4569123	-7.2209046	-1.0717218
C	-3.3748876	-5.0091388	8.9702093	C	4.9764562	-8.3046145	-1.4997876
C	-3.8215718	-5.4552671	10.2316421	O	6.0513065	-8.8429919	-1.0666254
C	-4.8951531	-4.8115414	10.8648478	Cu	7.1111295	-7.9133512	0.3367864
C	-5.5400673	-3.7352669	10.2375624	O	6.0493290	-8.8286034	1.7541380
O	0.9968003	-6.8169935	8.8000512	C	4.9762821	-8.2872822	2.1875312
C	1.4365050	-5.7449819	8.2618148	C	4.2699820	-8.9772586	3.3176760
O	1.0065205	-5.2185357	7.1818557	C	4.7148384	-10.2354982	3.7742929
C	2.5737934	-5.0503252	8.9510852	C	4.0698632	-10.8596005	4.8524798
C	3.2149826	-3.9691668	8.3206152	C	2.9931487	-10.2267228	5.4912463
C	4.3144641	-3.3447635	8.9361459	C	2.5442049	-8.9683608	5.0386700
C	4.7604937	-3.7927025	10.1970745	C	3.1780341	-8.3511178	3.9453057
C	4.1089744	-4.8595096	10.8339340	O	4.5078884	-1.8088573	7.1424944
C	3.0239853	-5.4949456	10.2117599	O	4.4798259	1.0124493	7.1488121
C	5.0240377	-2.2254098	8.2326209	C	5.0006161	1.4478518	8.2297392
O	6.0956566	-1.7851169	8.7709709	C	4.2779733	2.5594338	8.9305534
Cu	7.1509083	-0.3772820	7.8374649	C	4.6929763	2.9912944	10.2076212
O	8.0851508	-1.7917261	6.7913871	C	4.0230142	4.0477579	10.8425785
C	7.5567586	-2.2214068	5.7105003	C	2.9514235	4.6892769	10.2029173
O	6.4828308	-1.7850086	5.1770294	C	2.5363663	4.2642738	8.9238859
Cu	5.4133035	-0.3848581	6.0916960	C	3.1952831	3.1930768	8.2954752
O	6.4549235	1.0444458	5.1870097	O	6.0858459	1.0311241	8.7595934
C	7.5380209	1.4720171	5.7090620	O	8.0786777	1.0316046	6.7796573
C	8.2276963	2.6066156	5.0103726	O	8.0448251	6.1239590	1.7408868
C	9.4881254	3.0583339	5.4541001	O	8.0173826	6.1408986	-1.0775615
C	10.1107055	4.1409674	4.8150767	O	8.0481680	1.0497013	-6.1148780
C	9.4742458	4.7890444	3.7459427	Cu	7.1262841	-0.3627564	-7.1742853
C	8.2135219	4.3416213	3.2987767	O	6.0731754	1.0456865	-8.1069894
C	7.5979632	3.2439194	3.9263193	C	4.9949700	1.4778441	-7.5747850
C	7.5090751	5.0502688	2.1791594	C	4.2934346	2.6064908	-8.2717297
O	6.4201686	4.5323783	1.7616641	C	4.7449602	3.0593602	-9.5290090
Cu	5.3603187	5.4458384	0.3503459	C	4.1043437	4.1367968	-10.1588669
O	6.4138473	4.5278953	-1.0648917	C	3.0254873	4.7786294	-9.5326778
C	7.4890205	5.0577239	-1.5020674	C	2.5700686	4.3297252	-8.2754168
C	8.1869774	4.3529211	-2.6282498	C	3.1994818	3.2371109	-7.6524475
C	7.5716339	3.2534857	-3.2534266	C	1.4393086	5.0319856	-7.5827573
C	8.1975009	2.6203111	-4.3423392	O	1.0060427	6.1077445	-8.1188871
C	9.4536966	3.0774459	-4.7926156	Cu	-0.4123702	7.1593200	-7.1974768
C	10.0758849	4.1617733	-4.1562459	O	-1.8317073	8.0820220	-6.1479868
C	9.4430880	4.8060585	-3.0827706	C	-2.2679733	7.5453772	-5.0737465
C	7.5089270	1.4849028	-5.0413774	C	-3.4006234	8.2378129	-4.3743657
O	6.4287428	1.0522695	-4.5178570	C	-4.0362539	7.6121514	-3.2869647

C	-5.1318027	8.2313122	-2.6590399	H	6.5920158	2.8999593	-2.9019847
C	-5.5784941	9.4913325	-3.1090814	H	2.8473596	2.8869303	-6.6719086
C	-4.9320947	10.1235386	-4.1816667	H	5.5487902	10.0116043	-2.5577558
C	-3.8516426	9.4974798	-4.8209352	H	2.8239884	6.6620707	-2.9064175
O	6.0742202	-1.7745471	-8.1061205	H	9.9262426	2.5715646	-5.6482971
C	4.9978232	-2.2096136	-7.5728299	H	-3.3163884	-6.3139521	10.6994637
C	4.2969652	-3.3388087	-8.2697198	H	-3.3510371	-10.6705888	6.3542769
C	4.7491740	-3.7922236	-9.5265431	H	-3.6725295	-7.3484820	3.5926123
C	4.1091343	-4.8702104	-10.1560976	H	-6.3967799	-3.2309492	10.7099377
C	3.0298846	-5.5117775	-9.5302867	H	-3.6620127	-3.5683457	7.3667148
C	2.5735660	-5.0621639	-8.2736057	H	-6.4226232	-10.6791975	3.2622420
C	3.2026910	-3.9692759	-7.6507851	H	-10.7514152	-6.3363498	3.2543805
O	8.0571422	-1.7730359	-6.1221761	H	-10.7473813	-3.2686123	6.3497895
O	4.4718303	-1.7815352	-6.4919992	H	-7.4188617	-3.5897865	3.5951797
O	4.4681714	1.0472698	-6.4954438	H	-3.3072423	9.9196978	6.2834863
O	1.0076376	4.5073751	-6.5026785	H	-6.5020593	2.6202827	10.7312077
O	-1.8380673	6.4648587	-4.5485407	H	-10.8064585	5.6137772	3.2165212
O	-6.9085579	8.0479063	1.7196682	H	-3.3834712	5.6663747	10.7503697
O	8.0385243	-6.8602172	-1.0791462	H	-7.4646414	2.8813987	3.5734291
O	8.0583901	-6.8685253	1.7402065	H	-3.7419809	2.9035444	7.4210627
C	7.5318427	-5.7877849	2.1727665	H	-6.4042654	9.9432008	3.2162434
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Cu	5.2374611	-6.3113329	0.0937040	C	3.0575625	-4.1515736	-7.8868404
O	4.3286331	-7.3861624	-1.2990071	O	7.9299934	-1.9699473	-6.3786526
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O	5.9401532	-8.9912812	-1.2842888	O	4.3492288	0.8592814	-6.7292839
Cu	6.9994219	-8.0342590	0.1180267	O	0.8988808	4.2990026	-6.7142335
O	5.9850168	-8.9711080	1.5387166	O	-1.9333174	6.2590503	-4.7281018
C	4.9044685	-8.4439922	1.9719147	O	-6.7874248	7.8372156	1.5851128
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O	3.8011452	0.4607793	4.2942118
C	1.6016609	1.3178993	5.6306866
H	0.9938291	0.4461771	5.3037856
H	2.4512183	0.9616788	6.2422668
H	0.9694592	2.0209754	6.2037641
C	4.9524550	1.5654994	2.0549938
H	5.6139389	1.1025166	2.8114814
H	4.6091367	0.7871672	1.3386973
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C	2.4049342	4.8190626	0.9661704
C	0.2912901	5.5317628	2.1386792
H	-0.5995564	4.8774078	2.2236641
H	0.3733053	6.1321924	3.0672133
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432

Energy = -54612.59124635 , Cu24- Caffeine

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C	-4.9817862	-10.9179582	4.7340863
C	-5.8755428	-8.3608709	2.0484021
O	-5.3471845	-7.2857159	1.6088924
Cu	-6.2588249	-6.2322136	0.1914664
O	-7.3101246	-5.3190702	-1.2263228
C	-8.3900487	-5.8458393	-1.6557276
O	-8.9227607	-6.9229795	-1.2212748
Cu	-8.0016627	-7.9729889	0.1984898
O	-8.9397659	-6.9115384	1.5989252

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C	-10.9777238	-4.9165786	4.6894895
C	-10.3457401	-3.8348407	5.3213216
C	-9.0882543	-3.3880424	4.8650509
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C	-8.3843608	-2.2554897	5.5535990
O	-8.9092978	-1.8039549	6.6263424
Cu	-7.9469841	-0.3940686	7.6701986
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C	-5.7304746	1.4088175	7.9809561
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C	-5.4006307	2.9528292	9.9437011
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C	-3.8828734	3.1223840	8.0402995
C	-2.0857718	4.8976160	7.9770209
O	-1.6945871	5.9890981	8.5137264
Cu	-0.2970438	7.1109128	7.6734958
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Cu	-0.1585873	5.3085981	5.8927763
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C	-2.0478408	7.4109452	5.4255507
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Cu	-0.4540262	-7.8944277	7.7117755	C	-8.4723282	3.1508787	-3.4458376
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Cu	-0.4830544	-6.1846073	5.9375493	C	-10.3552940	2.9822384	-4.9836896
O	-1.8971067	-5.2870262	7.0154653	C	-8.3803827	4.9429104	-1.6870531
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O	-1.8658693	-6.8676540	8.6509610	O	-7.3157541	-1.8654291	-4.6980480
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C	-9.0910434	-3.4246254	-4.5112790	O	-6.9537219	-1.8732988	-8.2838426
C	-10.3505839	-3.8779266	-4.9559977	O	-6.9543539	-8.8950134	1.6203921
C	-10.9777223	-4.9540996	-4.3106396	O	-6.9394740	-8.9099965	-1.2026580
C	-10.3466472	-5.5943393	-3.2337098	C	-5.8658270	-8.3747549	-1.6420451
C	-8.3976305	-2.2972223	-5.2186305	C	-5.1645962	-9.0735815	-2.7699891
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C	-8.4067738	1.3915797	-5.2392545	C	-3.4463664	-9.0761540	-4.4987145
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Cu	-6.2661170	-0.4529364	-5.6223912	C	-2.3206405	-8.3810724	-5.2066252
O	-5.3563648	0.9565188	-6.6884332	O	-1.8906535	-7.2984682	-4.6857281
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C	-5.1822964	2.5100651	-8.4692698	O	0.9332786	-5.3371278	-6.6679241
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C	-3.4547756	4.2297811	-8.4767143	O	-1.8876284	-6.9378097	-8.2737499
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C	3.9512777	10.0285396	-4.2380711	O	-7.3180666	-5.3169684	1.6013122
C	4.5783701	9.4077627	-3.1479947	O	-7.3019052	4.4044949	-1.2667431
C	4.1359743	8.1448616	-2.7006196	O	-7.2881586	4.4360811	1.5612592
C	3.0635410	7.5090001	-3.3512145	O	-8.8857761	1.0189508	6.6464136
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O	5.9283596	8.0043090	-1.1636202	C	-5.8617074	-2.2551450	8.0847935
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C	4.7961486	9.7508828	3.6862420	C	-3.8825936	-5.5324970	10.0697228
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C	3.3514548	7.8144139	3.9580896	C	1.3567663	-5.6871582	8.0226488
C	1.6063251	7.6867474	5.7369128	O	0.9202961	-5.1988014	6.9273509
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O	-1.8891878	-8.9174561	-6.2830772	H	-10.8072273	5.5631682	-2.7588496
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432

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C	-2.3089927	-5.8461807	8.4550579	O	-8.9003308	6.0788828	-0.8679092
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Cu	-6.2533636	-0.4369453	-5.1664922	C	-2.2953727	-8.3377815	-4.8418039
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C	-4.9720993	2.4677391	-7.9594333	O	0.9182923	-5.1775226	-6.1735973
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C	-3.8855745	3.0955893	-7.3213464	C	-2.3182244	-5.8039943	-7.3556702
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O	1.1454584	6.6402087	-4.4106644	C	-5.6182353	-3.8306940	-9.3076972
C	1.5511079	7.7017425	-4.9937351	C	-4.9689246	-4.8992952	-9.9439267
C	2.6718638	8.4364059	-4.3243644	C	-3.8913541	-5.5428822	-9.3170369
C	3.0855915	9.7173582	-4.7434172	O	-5.3507222	-7.2815832	-0.8806369
C	4.1502519	10.3549860	-4.0853946	O	-7.3155171	-5.3203527	1.9554963
C	4.8119724	9.7212552	-3.0202359	O	-7.3261700	4.4367771	-0.8415239
C	4.3979458	8.4406382	-2.6016985	O	-7.3097294	4.4196324	1.9859202
C	3.3327958	7.8085147	-3.2588127	O	-8.9588858	0.9387224	7.0111756
C	5.0729500	7.7083015	-1.4801586	O	-6.9291373	-1.8435735	9.0128189
O	6.1607748	8.1916873	-1.0261586	C	-5.8670887	-2.2928752	8.4627720
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C	4.8226798	7.4001866	2.1822829	C	-4.0706870	-4.0523611	8.5315526
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C	3.9138041	9.9939017	4.8231397	C	-4.9529954	-4.9411383	11.0496925
C	2.8695113	9.3505246	5.5023422	C	-5.5990526	-3.8661158	10.4212501
C	2.4369444	8.0742830	5.0856606	O	0.9490343	-6.9348240	8.9947616
C	3.0529215	7.4478682	3.9853646	C	1.3795867	-5.8558865	8.4627773
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C	2.5117469	-5.1546576	9.1540760	C	4.0460497	-10.9463985	5.0269921
C	3.1334919	-4.0574037	8.5320838	C	2.9681869	-10.3216309	5.6720711
C	4.2303159	-3.4259967	9.1452484	C	2.5093295	-9.0652722	5.2240186
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C	2.9780840	-5.6079128	10.4058016	O	4.3973408	0.9667636	7.3630864
C	4.9200940	-2.2930029	8.4433708	C	4.9348787	1.3970833	8.4368198
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Cu	7.0415531	-0.4358327	8.0036787	C	4.7124352	2.9931060	10.3840588
O	7.9965731	-1.8382758	6.9806913	C	4.0791147	4.0755142	11.0130068
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O	6.3505542	-1.8974837	5.4117504	C	2.5186474	4.2485094	9.1497079
Cu	5.2692658	-0.4698574	6.2913986	C	3.1404469	3.1515334	8.5282142
O	6.2570812	0.9184961	5.2861430	O	6.0160319	0.9622016	8.9612029
C	7.3450125	1.3661695	5.7807818	O	7.8916410	0.9707826	6.8662354
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O	7.9210934	6.0784662	1.8104677
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H	-10.8149036	-6.3806582	3.3290284	H	5.5611352	-10.9491683	-2.6988302
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O	-8.4881552	-1.4099068	-6.4778039
Cu	-7.5612839	0.0036892	-7.5331132
O	-8.5084623	1.4106981	-6.4911138
C	-7.9892350	1.8426425	-5.4066748
O	-6.9131360	1.4161851	-4.8699127
Cu	-5.8323830	0.0164555	-5.7780312

432

Energy = -54612.53804424 , Caffeine @ LCW

C	-5.1856398	-9.8389437	3.4603724
C	-4.7428173	-8.5777547	3.0097906
C	-3.6530542	-7.9521898	3.6416465
C	-3.0184403	-8.5732249	4.7323876
C	-3.4651410	-9.8345790	5.1787466
C	-4.5404639	-10.4664017	4.5364979
C	-5.4481234	-7.8846116	1.8810568
O	-4.9316237	-6.7977753	1.4565122
Cu	-5.8436341	-5.7530324	0.0333671
O	-6.8914408	-4.8489389	-1.3922325
C	-7.9665567	-5.3806466	-1.8277355
O	-8.4998599	-6.4570860	-1.3927091
Cu	-7.5737686	-7.5070677	0.0248507
O	-8.5202299	-6.4624259	1.4303888
C	-7.9953044	-5.3824124	1.8665608
C	-8.6954923	-4.6901731	2.9989618
C	-9.9476075	-5.1529579	3.4546891
C	-10.5780833	-4.5214987	4.5372623
C	-9.9577232	-3.4403617	5.1809982
C	-8.7057722	-2.9736165	4.7289142
C	-8.0822361	-3.5941645	3.6316458
C	-8.0187604	-1.8399763	5.4316490
O	-8.5533837	-1.4138119	6.5110774
Cu	-7.6435728	0.0181932	7.5531153
O	-6.6082815	1.4519737	8.4686807
C	-5.5285573	1.8835424	7.9392893
C	-4.8353919	3.0214990	8.6296089

O	-4.9242927	1.4431526	-6.8208202	C	-2.9694665	-4.6632890	-8.5834260
C	-5.4394406	1.8642272	-7.9096484	C	-3.6112282	-3.5723759	-7.9704946
C	-4.7380732	2.9969450	-8.6003657	C	-4.7027978	-2.9501386	-8.6021816
C	-5.1772775	3.4441962	-9.8639639	C	-5.1398564	-3.4097889	-9.8620706
C	-4.5359599	4.5243812	-10.4885080	C	-4.4869191	-4.4856510	-10.4819243
C	-3.4684022	5.1741767	-9.8512628	C	-3.4101384	-5.1189974	-9.8434361
C	-3.0252085	4.7307875	-8.5877462	O	-4.9121764	-6.8076991	-1.3707856
C	-3.6555812	3.6359611	-7.9696420	O	-6.9194807	-4.8466107	1.4381586
C	-1.9062746	5.4404986	-7.8836855	O	-6.9625334	4.8616119	-1.4030229
O	-1.4860549	4.9207773	-6.7965099	O	-6.9710893	4.8691845	1.4262641
Cu	-0.0747019	5.8363083	-5.7438906	O	-8.5908107	1.4048513	6.4822839
O	1.3360268	6.8805317	-4.8158470	O	-6.5726421	-1.3703602	8.4970229
C	1.7478418	7.9781169	-5.3197732	C	-5.4987226	-1.8076751	7.9605250
C	2.8641134	8.6790751	-4.6020612	O	-4.9779079	-1.3841233	6.8754049
C	3.2953653	9.9533128	-5.0259827	C	-4.7954732	-2.9348379	8.6577514
C	4.3613823	10.5879221	-4.3710276	C	-3.6993293	-3.5622984	8.0391599
C	5.0132933	9.9501917	-3.3051964	C	-3.0696443	-4.6556555	8.6603478
C	4.5859922	8.6757584	-2.8772669	C	-3.5273527	-5.1087913	9.9152415
C	3.5046961	8.0475251	-3.5209544	C	-4.6080302	-4.4696336	10.5410830
C	5.3037102	7.9700009	-1.7648192	C	-5.2486166	-3.3910939	9.9131362
O	6.3701558	8.5144120	-1.3208118	O	1.3033519	-6.3886472	8.5450810
Cu	7.4655850	7.5484218	0.0407902	C	1.7422145	-5.3159841	8.0079608
O	6.4334782	8.4230251	1.4904625	O	1.3338423	-4.8057637	6.9121074
C	5.3559105	7.8804872	1.9121869	C	2.8508191	-4.5977025	8.7202220
C	4.6369292	8.5794989	3.0285333	C	3.4887978	-3.5102577	8.0976243
C	5.0850930	9.8391924	3.4792018	C	4.5599081	-2.8601995	8.7364381
C	4.4270528	10.4821541	4.5378147	C	4.9805539	-3.2891422	10.0125896
C	3.3326370	9.8669934	5.1633097	C	4.3329548	-4.3636530	10.6403698
C	2.8799823	8.6077283	4.7171622	C	3.2765472	-5.0243121	9.9954557
C	3.5277439	7.9708175	3.6430242	C	5.2701674	-1.7378708	8.0394587
C	1.7331966	7.9291861	5.4075451	O	6.3039991	-1.2532556	8.6115583
O	1.2855231	8.4813522	6.4690636	Cu	7.4168828	0.0879289	7.6366955
C	-8.6975707	2.9664252	-4.7089310	O	8.3151505	-1.3897474	6.6698945
C	-8.0899316	3.5959119	-3.6079582	C	7.8353052	-1.7899973	5.5548088
C	-8.7211341	4.6852588	-2.9813638	O	6.8013021	-1.3096725	4.9745250
C	-9.9755843	5.1319450	-3.4466644	Cu	5.6904917	0.0667823	5.8820534
C	-10.5905577	4.4908055	-4.5324141	O	6.7147422	1.4856573	4.9460725
C	-9.9521713	3.4166575	-5.1702586	C	7.8405697	1.8554272	5.4246890
C	-8.0381008	5.3872208	-1.8447792	C	8.5840099	2.9064938	4.6551519
O	-8.5762655	6.4644336	-1.4176512	C	9.9062575	3.2528752	5.0014599
O	-6.8768734	-1.4102413	-4.8725905	C	10.5791091	4.2547739	4.2854959
O	-4.8993048	-1.3854644	-6.8336175	C	9.9336073	4.9291769	3.2380990
C	-5.4167071	-1.8240648	-7.9142901	C	8.6122195	4.5837341	2.8868203
O	-6.4951391	-1.4019125	-8.4541643	C	7.9453756	3.5671471	3.5913436
O	-6.5181638	-8.4273890	1.4418949	C	7.8921662	5.3178243	1.7956909
O	-6.5056221	-8.4306429	-1.3779739	O	6.8079896	4.7920244	1.3661121
C	-5.4284995	-7.8910695	-1.8039015	Cu	5.7447660	5.7865826	0.0103678
C	-4.7153217	-8.5833775	-2.9277613	O	6.8233888	4.9408500	-1.4344247
C	-5.1550144	-9.8442344	-3.3821943	C	7.8788375	5.5099940	-1.8787823
C	-4.5040676	-10.4696275	-4.4559582	C	8.5567004	4.8685325	-3.0484694
C	-3.4266566	-9.8355132	-5.0923895	C	7.9478966	3.7719918	-3.6806213
C	-2.9829111	-8.5746583	-4.6417176	C	8.5477503	3.1885586	-4.8084967
C	-3.6226036	-7.9561171	-3.5527218	C	9.7728003	3.6911060	-5.2941386
C	-1.8540030	-7.8738369	-5.3390810	C	10.3898145	4.7750830	-4.6513669
O	-1.4306391	-6.7914702	-4.8127637	C	9.7824007	5.3693059	-3.5345190
Cu	-0.0178311	-5.7224559	-5.7197077	C	7.8744043	2.0303542	-5.4776875
O	1.3973692	-4.8035010	-6.7729109	O	6.7814232	1.6237947	-4.9605080
C	1.8431448	-5.3386637	-7.8418246	Cu	5.7477091	0.1347609	-5.7709968
O	1.4265279	-6.4273228	-8.3653658	O	6.8205898	-1.2099360	-4.7820852
Cu	0.0076504	-7.4775180	-7.4485725	C	7.8654533	-1.6906539	-5.3354068
O	-1.3935030	-6.4292908	-8.4036082	C	8.5312897	-2.8484534	-4.6585856
C	-1.8424582	-5.3563907	-7.8753680	C	9.7317794	-3.3762949	-5.1768376

C	10.3212857	-4.4983182	-4.5800236	O	4.8750869	-1.3507512	-6.7668923
C	9.7109753	-5.1063323	-3.4757885	O	4.7824698	1.4717076	-6.8777012
C	8.5155540	-4.5764741	-2.9452530	O	1.3400044	4.9425831	-6.8208434
C	7.9319159	-3.4404627	-3.5322220	O	-1.4934117	6.8882265	-4.8250912
C	7.8512528	-5.2452660	-1.7808001	O	-6.6162132	8.4403637	1.4260830
O	6.8565707	-4.6509670	-1.2463868	O	8.3337048	-6.3726833	-1.4172661
Cu	5.7649762	-5.6353345	0.1006436	O	8.5142853	-6.2345419	1.3916715
O	4.9131417	-6.6429817	-1.3884868	C	7.8980148	-5.2620625	1.9507462
C	5.3695212	-7.7873997	-1.7213560	O	6.7509778	-4.8176497	1.6128511
O	6.3838614	-8.3679820	-1.2059042	C	8.5664905	-4.6072256	3.1181703
Cu	7.5133100	-7.3629887	0.0944613	C	9.8201842	-5.0571975	3.5756778
O	6.5397358	-8.2258500	1.6014048	C	10.4305404	-4.4370120	4.6776584
C	5.3969941	-7.7776907	1.9475577	C	9.7904234	-3.3739641	5.3302672
C	4.7025389	-8.4681319	3.0805389	C	8.5358987	-2.9191989	4.8698936
C	5.1903563	-9.7001229	3.5643923	C	7.9297138	-3.5356863	3.7637132
C	4.5566854	-10.3312392	4.6451371	O	4.8007396	-6.7695620	1.4286730
C	3.4503174	-9.7286390	5.2620412	O	-1.4806374	-6.7801347	4.9246033
C	2.9600195	-8.4951777	4.7842441	C	4.6590585	-8.5068154	-2.8305479
C	3.5805658	-7.8737079	3.6853310	C	5.0842841	-9.7891064	-3.2360872
O	4.7933256	-1.3631834	6.9157008	C	4.4367787	-10.4416391	-4.2958429
O	4.7581162	1.4691501	6.9417610	C	3.3747944	-9.8154918	-4.9651399
C	5.3050712	1.9479229	7.9905522	C	2.9435108	-8.5347039	-4.5612749
C	4.5950575	3.0773240	8.6758172	C	3.5818277	-7.8869804	-3.4884137
C	5.0489450	3.5521448	9.9241718	C	1.8271778	-7.8452619	-5.2883252
C	4.3970634	4.6277766	10.5452880	O	1.3968770	-6.7541620	-4.7855789
C	3.3059860	5.2474229	9.9177850	O	1.4022710	-8.3950372	-6.3605785
C	2.8494674	4.7773199	8.6686470	O	-1.4144433	-8.4070068	-6.4137882
C	3.4885523	3.6847630	8.0561059	O	-1.4708699	6.5165091	-8.4170691
O	6.4100325	1.5611015	8.5029659	O	1.3068427	8.5256990	-6.3861764
O	8.3827573	1.4169137	6.4922711	O	4.8021162	6.8683186	-1.3587786
O	8.4059143	6.4127114	1.3937351	O	4.8450329	6.7956971	1.4752758
O	8.3936963	6.5859033	-1.4211817	O	1.3052162	6.8440255	4.8903432
O	8.4416781	1.5399069	-6.5131178	O	-1.5477815	4.9148809	6.8588813
Cu	7.4831313	0.1199036	-7.5194021	O	-1.5378530	8.4947599	6.4726807
O	6.4239345	1.5309838	-8.4512884	O	-1.4305690	-4.8267871	-6.7899029
C	5.3266359	1.9329513	-7.9356806	O	-6.5050467	1.4189505	-8.4559890
C	4.6240877	3.0682260	-8.6204328	O	-6.9443577	-1.3985170	4.9035267
C	5.0801740	3.5443209	-9.8673053	H	2.7841665	10.4300043	-5.8762061
C	4.4428986	4.6346840	-10.4782540	H	5.9417502	3.0494404	-10.3408307
C	3.3637032	5.2666174	-9.8425681	H	10.2450117	6.2289307	-3.0260106
C	2.9041320	4.7944015	-8.5953104	H	2.8646254	6.1358579	-10.2972901
C	3.5293081	3.6884618	-7.9924597	H	7.0003298	3.3718885	-3.2989808
C	1.7752565	5.4862866	-7.8899709	H	3.1747420	3.3210384	-7.0192037
O	1.3467614	6.5741647	-8.4054777	H	5.8639938	10.4243424	-2.7924447
Cu	-0.0818209	7.5921499	-7.4723438	H	3.1718615	7.0531509	-3.1915686
O	-1.5116868	8.4984024	-6.4316139	H	10.2277742	3.2175569	-6.1775763
C	-1.9379252	7.9610007	-5.3534060	H	-3.0247396	-5.9683668	10.3842399
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C	-4.6242228	10.5180875	-4.4698647	H	-6.0421616	-10.3114593	2.9558740
C	-3.5367019	9.9002374	-5.1048998	H	-10.4104378	-6.0143894	2.9495485
O	6.4225900	-1.2919627	-8.4324728	H	-10.4285427	-2.9444662	6.0434743
C	5.3752729	-1.7582040	-7.8675614	H	-7.1055879	-3.2337964	3.2790954
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C	3.4223347	-5.0857793	-9.7960678	H	-3.0811341	6.0718290	10.3438183
C	2.9692285	-4.6336356	-8.5390856	H	-7.1442466	3.2534281	3.2671108
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H 6.5231908 1.1629474 1.9857171
H 6.4691898 -0.6288574 1.6943839
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422

Energy = -54369.47230522 , Niacine @ LCW

C -5.1101313 -9.8007819 3.4018673
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C -3.5659492 -7.9205820 3.5567187
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C -3.3638776 -9.8029101 5.0927363
C -4.4514909 -10.4307769 4.4682787
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Cu -5.8254882 -5.7159992 -0.0098878
O -6.9071714 -4.8314417 -1.4239535
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Cu -7.5410300 -7.4846898 -0.0053064
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C -7.9614580 -5.3614199 1.8408883
C -8.6553965 -4.6689502 2.9768863
C -9.9063468 -5.1274815 3.4397349
C -10.5293974 -4.4917643 4.5244114
C -9.9023168 -3.4117737 5.1637193
C -8.6509308 -2.9503370 4.7050677
C -8.0356413 -3.5741576 3.6051478
C -7.9514661 -1.8215210 5.4032925
O -8.4756965 -1.3894382 6.4854177
Cu -7.5255289 0.0134461 7.5303057
O -6.4563240 1.4143007 8.4565857
C -5.3833266 1.8460438 7.9138482
C -4.6650794 2.9633870 8.6120260

C	-5.1007579	3.4123348	9.8761310	O	-4.9188798	1.4125910	-6.8178447
C	-4.4422715	4.4778185	10.5082362	C	-5.4264695	1.8397341	-7.9077372
C	-3.3617245	5.1119177	9.8771749	C	-4.6951589	2.9465477	-8.6083126
C	-2.9227623	4.6672657	8.6125744	C	-5.1250718	3.3966019	-9.8739981
C	-3.5694539	3.5860776	7.9876484	C	-4.4529881	4.4513909	-10.5092411
C	-1.7937142	5.3648864	7.9127595	C	-3.3643315	5.0734770	-9.8802077
O	-1.3594182	6.4435386	8.4420586	C	-2.9309020	4.6275807	-8.6139457
Cu	0.0498892	7.4904927	7.5024588	C	-3.5916109	3.5570554	-7.9856791
O	1.4542075	6.4319556	8.4298804	C	-1.7935785	5.3140162	-7.9159366
C	1.8895780	5.3560895	7.8958827	O	-1.3799271	4.7905669	-6.8281960
O	1.4648325	4.8317908	6.8131406	Cu	0.0388666	5.6851122	-5.7580794
Cu	0.0420004	5.7444777	5.7638051	O	1.4599612	6.7312737	-4.8390654
O	-1.3771757	6.8028705	4.8579221	C	1.8922456	7.8121359	-5.3608468
C	-1.8010001	7.8861511	5.3822928	C	3.0279485	8.5009331	-4.6625458
C	-2.9319949	8.5843724	4.6864503	C	3.4740071	9.7631015	-5.1070398
C	-3.3822791	9.8406395	5.1436286	C	4.5589679	10.3878246	-4.4745062
C	-4.4623802	10.4726892	4.5099276	C	5.2145194	9.7511995	-3.4104025
C	-5.1086018	9.8500242	3.4318063	C	4.7724420	8.4889587	-2.9616190
C	-4.6622327	8.5938177	2.9708260	C	3.6724808	7.8704866	-3.5829084
C	-3.5676143	7.9681145	3.5938549	C	5.4900412	7.7930751	-1.8429313
C	-5.3713533	7.9050628	1.8420990	O	6.5691561	8.3338207	-1.4226065
O	-4.8594815	6.8178632	1.4139821	Cu	7.6169808	7.4413731	0.0081657
Cu	-5.7910012	5.7690452	0.0038665	O	6.5390365	8.3855405	1.3903514
O	-4.8562856	6.7986368	-1.4120349	C	5.4728207	7.8399508	1.8345294
C	-5.3663354	7.8848322	-1.8455487	C	4.7569021	8.5466879	2.9472880
O	-6.4346773	8.4363881	-1.4130685	C	5.1964994	9.8135530	3.3849993
Cu	-7.5095364	7.5351515	0.0024278	C	4.5435062	10.4544652	4.4481680
O	-8.4520178	6.4975447	1.4193505	C	3.4638441	9.8302032	5.0906008
C	-7.9281935	5.4165687	1.8541648	C	3.0198801	8.5636677	4.6562801
C	-8.6245927	4.7239350	2.9883281	C	3.6619895	7.9291827	3.5778943
C	-8.0082554	3.6269307	3.6161490	C	1.8891189	7.8730809	5.3609386
C	-8.6280527	3.0009583	4.7122589	O	1.4612170	8.4097929	6.4384522
C	-9.8803139	3.4631963	5.1679175	C	-8.6638337	3.0021401	-4.6918697
C	-10.5036012	4.5459531	4.5293634	C	-8.0376293	3.6244388	-3.5972824
C	-9.8763911	5.1832857	3.4483248	C	-8.6473263	4.7234996	-2.9668836
C	-7.9338519	1.8671373	5.4081236	C	-9.8993683	5.1877447	-3.4217834
O	-6.8601850	1.4335463	4.8718243	C	-10.5329873	4.5536486	-4.5010512
Cu	-5.8010840	0.0155198	5.7704781	C	-9.9159439	3.4694989	-5.1426980
O	-4.8732288	1.4233827	6.8234945	C	-7.9436179	5.4159313	-1.8371053
C	-1.7816830	-7.8508277	5.3288261	O	-8.4630239	6.4996134	-1.4034480
O	-1.3367524	-8.3950817	6.3959905	O	-6.9240123	-1.3973154	-4.8734684
Cu	0.0649390	-7.4658593	7.4457125	O	-4.9646263	-1.4098191	-6.8503407
O	1.4841517	-8.3407239	6.3522306	C	-5.4894406	-1.8352064	-7.9327825
C	1.9177951	-7.7830382	5.2870017	O	-6.5645769	-1.3982033	-8.4669231
O	1.4731547	-6.7018741	4.7754664	O	-6.4649381	-8.3929283	1.4009650
Cu	0.0528742	-5.6985472	5.7277101	O	-6.4651863	-8.3946795	-1.4147495
O	-1.3639444	-4.8081696	6.7947072	C	-5.3943803	-7.8459869	-1.8443091
C	-1.7908413	-5.3476643	7.8697717	C	-4.6707979	-8.5381239	-2.9613755
O	-1.3531382	-6.4279083	8.3917161	C	-5.0984755	-9.8044533	-3.4118308
C	-8.6825822	-4.6832015	-2.9845679	C	-4.4364862	-10.4301113	-4.4785756
C	-8.0715328	-3.5832572	-3.6123107	C	-3.3600490	-9.7911247	-5.1116541
C	-8.6954634	-2.9583223	-4.7067268	C	-2.9284312	-8.5242664	-4.6649852
C	-9.9460979	-3.4246719	-5.1617128	C	-3.5792513	-7.9054498	-3.5831186
C	-10.5641499	-4.5107647	-4.5236973	C	-1.8061975	-7.8154867	-5.3652591
C	-9.9331567	-5.1466237	-3.4436016	O	-1.4030648	-6.7170134	-4.8579071
C	-8.0044795	-1.8229961	-5.4024405	Cu	-0.0271288	-5.6118844	-5.7968776
O	-8.5382895	-1.3818304	-6.4758872	O	1.3690610	-4.7256416	-6.9194381
Cu	-7.5936861	0.0242412	-7.5281411	C	1.8105148	-5.2804293	-7.9798754
O	-8.5093471	1.4433003	-6.4750581	O	1.3788324	-6.3682911	-8.4927697
C	-7.9769242	1.8681152	-5.3940364	Cu	0.0142757	-7.4000541	-7.4925295
O	-6.9036641	1.4266422	-4.8639775	O	-1.4406609	-6.4122788	-8.4458419
Cu	-5.8573524	0.0072195	-5.7795554	C	-1.8922144	-5.3345742	-7.9316465

C -3.0370146 -4.6611111 -8.6294489
C -3.6812602 -3.5755535 -8.0102803
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C -5.2323648 -3.4256310 -9.8834546
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C 4.7759864 -2.9715630 8.6208130
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O 6.5701940 -1.4231367 8.4932328
Cu 7.6407958 0.0106582 7.6106391
O 8.6649006 -1.3692002 6.6226249
C 8.1732597 -1.8209157 5.5340499
O 7.0884104 -1.4297195 4.9836274
Cu 5.9521388 -0.0230825 5.8158463
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C 8.7727873 2.9386533 4.7248917
C 10.0437868 3.3761228 5.1519054
C 10.6750965 4.4427508 4.4940359
C 10.0368935 5.0898095 3.4248817
C 8.7662555 4.6539697 2.9954198
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Cu 5.8942918 5.6777818 0.0277706
O 6.9602674 4.7348961 -1.3496520
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C 8.0784386 1.7058365 -5.3232078
O 6.9795881 1.2944510 -4.8216146
Cu 5.9546788 -0.1131638 -5.7430179
O 7.1058647 -1.5031058 -4.8904288
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Cu 7.7592567 -7.2804126 0.0674237
O 6.7313365 -8.1430711 1.5190969
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C 3.6353210 -3.5577464 -8.0312018
O 8.6313528 -1.5286346 -6.5763221

O	5.0346281	-1.5181782	-6.7863907	H	-3.2196230	6.9880505	3.2380667
O	4.9944420	1.3029923	-6.7800242	H	-10.3492638	2.9627992	6.0287775
O	1.4578985	4.7536315	-6.7954075	H	-2.8418708	-10.2580709	-5.9629616
O	-1.3707728	6.7576152	-4.8524127	H	-6.0989670	-2.9350502	-10.3525140
O	-6.4413258	8.4523123	1.4079427	H	-10.3953031	-6.0114411	-2.9434635
O	8.7967165	-6.4552727	-1.4064761	H	-2.9743531	-5.9748444	-10.3528744
O	8.8618378	-6.3143888	1.4258631	H	-7.0957272	-3.2224713	-3.2585042
C	8.2866052	-5.3135669	1.9681438	H	-3.3320371	-3.2157655	-7.0324602
O	7.1525009	-4.8325305	1.6438263	H	-5.9568689	-10.2818902	-2.9151244
C	8.9813292	-4.6278415	3.1074105	H	-3.2463331	-6.9173874	-3.2351903
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C	10.8588377	-4.3821171	4.6379363	H	-2.8369704	5.9146651	-10.3552696
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C	8.9216524	-2.9198760	4.8442536	H	-10.3894160	2.9719409	-6.0027587
C	8.3246373	-3.5652122	3.7499399	H	-3.2160391	6.9548102	-3.2354692
O	5.0348052	-6.6421239	1.3284833	H	-5.9926495	2.9084658	-10.3435324
O	-1.3598066	-6.7646915	4.8099288	H	-3.2562262	3.2092315	-6.9984227
C	4.8304058	-8.1344302	-2.9372483	H	-2.8668674	10.2518468	-6.0230598
C	5.2802889	-9.4078975	-3.3484816	H	-10.3599203	6.0515674	-2.9187562
C	4.6260073	-10.0880858	-4.3846464	H	-7.0610668	3.2626263	-3.2457999
C	3.5244168	-9.5009338	-5.0226915	H	2.9954173	-10.2030312	5.8600778
C	3.0640782	-8.2321009	-4.6138327	H	6.0703152	-2.9502586	10.3590249
C	3.7156418	-7.5521118	-3.5669763	H	10.7548961	-5.8715315	3.0378301
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O	1.4283993	-6.5261313	-4.8167360	H	7.3306584	-3.2518809	3.4027039
O	1.4705555	-8.1881029	-6.3685900	H	3.3399977	-3.2221550	7.0045985
O	-1.3537504	-8.3597897	-6.4296806	H	6.1753608	-10.1008357	2.8834874
O	-1.3392648	6.3793523	-8.4551934	H	3.3724784	-6.8123400	3.1862227
O	1.4575137	8.3533780	-6.4335087	H	10.6501443	-2.8182650	6.1515344
O	4.9763382	6.7108482	-1.4039756	H	2.9323132	5.9587294	10.3286779
O	4.9697945	6.7396836	1.4275776	H	6.0571196	10.2793076	2.8811858
O	1.4534556	6.7941229	4.8374348	H	10.5215674	2.8697138	6.0045091
O	-1.3656339	4.8355711	6.8334496	H	2.9513283	10.3094066	5.9385840
O	-1.3597301	8.4222287	6.4549247	H	3.3193671	6.9412562	3.2391296
O	-1.4674390	-4.7789021	-6.8633082	H	6.0381433	2.9029726	10.3582715
O	-6.5055331	1.4196231	-8.4475417	H	3.3271498	3.2235757	6.9929575
O	-6.8756966	-1.3914691	4.8688719	H	10.5088603	5.9408494	2.9104734
H	2.9587028	10.2383937	-5.9555372	H	7.1476184	3.2419615	3.3131625
H	6.1374601	2.8808056	-10.2370092	H	2.8600910	-5.8879163	-10.4214236
H	10.4119975	5.9392450	-2.9062619	H	10.5270030	-3.0835891	-6.2055548
H	3.0070471	5.9116539	-10.2632745	H	3.0029151	-10.0120862	-5.8459061
H	7.2161969	3.0084694	-3.0953408	H	3.3548358	-6.5640853	-3.2465325
H	3.3369536	3.1485302	-6.9421791	H	6.0639541	-2.9326160	-10.3658356
H	6.0788289	10.2170683	-2.9132143	H	3.2996119	-3.2111176	-7.0438400
H	3.3278164	6.8857798	-3.2366256	H	6.1510225	-9.8476429	-2.8394813
H	10.4506738	2.8501321	-5.9775080	H	10.7134221	-6.0239810	-2.9919045
H	-2.8438759	-5.9637409	10.3004383	H	7.4290597	-3.2032039	-3.1835643
H	-2.8466396	-10.2721416	5.9434637	H	11.6708990	4.7799624	4.8246038
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H	-5.9640192	-2.9202836	10.3197008	H	-4.7996728	11.4140826	-4.8929215
H	-3.2303321	-3.2197143	6.9718203	H	11.8557913	-4.7000762	4.9838291
H	-5.9767574	-10.2692528	2.9113077	H	4.8826572	-4.8711094	11.4817744
H	-10.3745461	-5.9883465	2.9385691	H	4.9730541	-11.3038610	4.7456145
H	-10.3673541	-2.9134378	6.0280210	H	-4.7875586	4.7988799	-11.5001782
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H	-2.8746323	10.3050900	6.0026295	H	-11.4841131	4.9030093	4.8838913
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H	-3.2300098	3.2394072	7.0014330	H	11.7231516	-4.9827133	-5.0565775
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418

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Cu -7.5409058 0.0105941 -7.5168894
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C -4.4886411 4.4900241 -10.5092558
C -3.4124073 5.1326436 -9.8791814
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Cu	-0.0046346	5.7860651	-5.7756747	O	-8.4747530	1.4323902	6.4786723
O	1.4098826	6.8380522	-4.8585121	O	-6.4628949	-1.3058252	8.5590689
C	1.8364148	7.9226950	-5.3778449	C	-5.3978879	-1.7554348	8.0146529
C	2.9613061	8.6193804	-4.6698527	O	-4.8914174	-1.3551406	6.9158136
C	3.4143239	9.8785175	-5.1159101	C	-4.6878300	-2.8764345	8.7164485
C	4.4893215	10.5073183	-4.4700747	C	-3.5683362	-3.4768602	8.1111574
C	5.1287455	9.8781925	-3.3915748	C	-2.9482003	-4.5811470	8.7251543
C	4.6792245	8.6193844	-2.9411133	C	-3.4322995	-5.0621722	9.9607432
C	3.5887804	7.9976181	-3.5753987	C	-4.5289387	-4.4421452	10.5764908
C	5.3798768	7.9232420	-1.8115809	C	-5.1653045	-3.3586477	9.9523266
O	6.4613580	8.4518155	-1.3834769	O	1.3992312	-6.4479459	8.6579174
Cu	7.5096999	7.5259170	0.0347105	C	1.8658353	-5.3936283	8.1098598
O	6.4568143	8.4665557	1.4364194	O	1.4764698	-4.8854539	7.0069509
C	5.3836991	7.9309119	1.8770131	C	2.9812981	-4.6773430	8.8101568
C	4.6870720	8.6282875	3.0083965	C	3.6231439	-3.6109474	8.1556624
C	5.1491100	9.8797325	3.4669308	C	4.6840705	-2.9383822	8.7874671
C	4.5157081	10.5089361	4.5489716	C	5.1048774	-3.3371150	10.0742446
C	3.4324345	9.8883650	5.1885924	C	4.4543964	-4.3931809	10.7287480
C	2.9654802	8.6377715	4.7330088	C	3.3965954	-5.0676495	10.0991151
C	3.5886245	8.0148079	3.6368554	C	5.3762118	-1.8180815	8.0793478
C	1.8290007	7.9525284	5.4327977	O	6.5334088	-1.4867207	8.4846328
O	1.4134883	8.4804439	6.5199003	Cu	7.4756634	0.0340670	7.6005791
C	-8.6324996	2.9940221	-4.6953134	O	8.4599244	-1.2783996	6.4639923
C	-8.0106716	3.6265852	-3.6039211	C	7.8548709	-1.8073325	5.4711719
C	-8.6296176	4.7233580	-2.9780351	O	6.6928891	-1.4878128	5.0489448
C	-9.8853238	5.1751598	-3.4350456	Cu	5.7160151	0.0220158	5.8743679
C	-10.5142006	4.5313811	-4.5112156	O	6.8486565	1.3473649	4.8971765
C	-9.8885866	3.4490176	-5.1478052	C	7.8590957	1.8679459	5.4755806
C	-7.9342155	5.4263674	-1.8493459	C	8.5547099	2.9920248	4.7663372
O	-8.4629882	6.5093399	-1.4247938	C	9.8016524	3.4604565	5.2312936
O	-6.8648231	-1.3891441	-4.8528239	C	10.4345128	4.5327240	4.5856839
O	-4.8906160	-1.4084332	-6.8170659	C	9.8185162	5.1576142	3.4912996
C	-5.4080981	-1.8337885	-7.9030076	C	8.5700307	4.6958091	3.0246891
O	-6.4796041	-1.3963987	-8.4443711	C	7.9466326	3.6039865	3.6555949
O	-6.4485218	-8.3596141	1.4818495	C	7.8856026	5.3902346	1.8840639
O	-6.4649506	-8.4123607	-1.3383882	O	6.8112284	4.8612665	1.4439906
C	-5.3936756	-7.8758194	-1.7822306	Cu	5.7632790	5.7876431	0.0327664
C	-4.6954059	-8.5777606	-2.9095709	O	6.8211051	4.8793354	-1.3856164
C	-5.1471671	-9.8379924	-3.3539599	C	7.9079478	5.3982383	-1.8068318
C	-4.5121742	-10.4712708	-4.4326632	C	8.6060599	4.6958844	-2.9340980
C	-3.4383740	-9.8458951	-5.0837668	C	7.9874904	3.6016263	-3.5647332
C	-2.9821595	-8.5862840	-4.6424694	C	8.6119232	2.9712050	-4.6558832
C	-3.6061753	-7.9595440	-3.5490157	C	9.8697008	3.4262910	-5.1036436
C	-1.8558753	-7.8947630	-5.3527140	C	10.4947106	4.5062192	-4.4624138
O	-1.4184299	-6.8162804	-4.8299277	C	9.8636927	5.1473843	-3.3860175
Cu	-0.0076871	-5.7641743	-5.7529232	C	7.9186728	1.8411791	-5.3587368
O	1.4034230	-4.8575895	-6.8180642	O	6.8319006	1.4183971	-4.8409387
C	1.8412815	-5.3948976	-7.8893420	Cu	5.7795328	0.0010209	-5.7534006
O	1.4140825	-6.4791441	-8.4130427	O	6.8306474	-1.4091209	-4.8288419
Cu	-0.0093802	-7.5168388	-7.4846604	C	7.9072986	-1.8485303	-5.3538444
O	-1.4079045	-6.4564489	-8.4277103	C	8.5934410	-2.9829092	-4.6511594
C	-1.8476415	-5.3822951	-7.8936808	C	9.8409172	-3.4553439	-5.1096565
C	-2.9758203	-4.6819916	-8.5927695	C	10.4586387	-4.5409042	-4.4710041
C	-3.6103630	-3.5909105	-7.9724039	C	9.8299957	-5.1705727	-3.3865002
C	-4.7023418	-2.9617773	-8.5966452	C	8.5830963	-4.7011262	-2.9230625
C	-5.1470500	-3.4148324	-9.8562236	C	7.9722211	-3.6009917	-3.5510156
C	-4.5016510	-4.4910652	-10.4832773	C	7.8876314	-5.3918575	-1.7868995
C	-3.4244579	-5.1311888	-9.8523648	O	6.8280393	-4.8435546	-1.3353439
O	-4.8727367	-6.7883374	-1.3653040	Cu	5.7457485	-5.7619100	0.0623499
O	-6.8475845	-4.7982088	1.4488493	O	4.8497136	-6.8044968	-1.3683626
O	-6.8600970	4.8956873	-1.4107011	C	5.3536059	-7.9077148	-1.7651343
O	-6.8439567	4.8930429	1.4176731	O	6.4097027	-8.4583551	-1.3032676

Cu	7.4910473	-7.5018182	0.0731508	C	9.8644610	-5.0280365	3.4239095
O	6.4687761	-8.4092803	1.5159551	C	10.5026384	-4.3649350	4.4826114
C	5.3732817	-7.8928489	1.9237147	C	9.8548200	-3.3134859	5.1476225
C	4.6789653	-8.5791529	3.0632626	C	8.5641589	-2.9114476	4.7445443
C	5.1306641	-9.8342319	3.5221171	C	7.9310842	-3.5637992	3.6712624
C	4.4984079	-10.4532937	4.6107050	O	4.8245948	-6.8383273	1.4612793
C	3.4290013	-9.8174768	5.2587557	O	-1.4205597	-6.6795830	4.9910296
C	2.9737455	-8.5623856	4.8037315	C	4.6494334	-8.6100296	-2.8887692
C	3.5932902	-7.9507203	3.6989377	C	5.0824376	-9.8814983	-3.3191712
O	4.7506218	-1.2672678	7.0980735	C	4.4392139	-10.5160141	-4.3923719
O	4.8457880	1.5112412	6.8452743	C	3.3761139	-9.8811689	-5.0518880
C	5.3005733	1.8506426	7.9899018	C	2.9388349	-8.6099716	-4.6248493
C	4.5890981	2.9659550	8.6957046	C	3.5709622	-7.9817923	-3.5368719
C	5.0082684	3.3873799	9.9747726	C	1.8233873	-7.9087003	-5.3430193
C	4.3595388	4.4578769	10.6083598	O	1.4067873	-6.8149707	-4.8348164
C	3.3052152	5.1234290	9.9650372	O	1.3865085	-8.4519215	-6.4137006
C	2.8813195	4.7037402	8.6870017	O	-1.4317274	-8.4304676	-6.4323763
C	3.5173288	3.6177134	8.0603894	O	-1.4014845	6.4666922	-8.4551177
O	6.3121239	1.3354803	8.5752988	O	1.4033200	8.4598251	-6.4531389
O	8.3277162	1.5290187	6.6154727	O	4.8488193	6.8477074	-1.3763352
O	8.4219353	6.4672735	1.4542265	O	4.8593276	6.8477039	1.4532114
O	8.4470342	6.4696392	-1.3662957	O	1.3750597	6.8879636	4.8960774
O	8.4603572	1.4005610	-6.4287224	O	-1.4433197	4.9365818	6.9031300
Cu	7.5284055	-0.0041059	-7.4889998	O	-1.4088600	8.5283299	6.4587899
O	6.4836749	1.4129449	-8.4198104	O	-1.4251458	-4.8578056	-6.8099646
C	5.4027399	1.8442805	-7.8926390	O	-6.4866512	1.4232101	-8.4448145
C	4.7053553	2.9753000	-8.5898460	O	-6.8422056	-1.3463178	4.9252512
C	5.1639502	3.4327826	-9.8428587	H	2.9129979	10.3481762	-5.9758501
C	4.5267273	4.5125393	-10.4722296	H	6.0265070	2.9309942	-10.3072648
C	3.4442825	5.1519561	-9.8497319	H	10.3302595	6.0078298	-2.8826514
C	2.9818904	4.6985359	-8.5965972	H	2.9442215	6.0124471	-10.3197342
C	3.6079774	3.6036761	-7.9743123	H	7.0063217	3.2499820	-3.2158995
C	1.8484025	5.3992025	-7.9066087	H	3.2507337	3.2500140	-6.9968909
O	1.4199572	6.4781981	-8.4403156	H	5.9860463	10.3474145	-2.8852737
Cu	0.0014081	7.5272740	-7.5187368	H	3.2383773	7.0158022	-3.2270923
O	-1.4152672	8.4564985	-6.4738192	H	10.3412079	2.9227744	-5.9612944
C	-1.8456373	7.9281886	-5.3929980	H	-2.9373194	-5.9307510	10.4210564
C	-2.9691130	8.6305598	-4.6887242	H	-2.9088271	-10.1940538	6.0990246
C	-3.6032236	8.0115746	-3.5966914	H	-3.2323538	-6.8864913	3.3191487
C	-4.6912003	8.6394369	-2.9641736	H	-6.0435358	-2.8745143	10.4060140
C	-5.1309861	9.9020054	-3.4135669	H	-3.1930212	-3.0773957	7.1568250
C	-4.4849982	10.5282199	-4.4899593	H	-5.9838379	-10.2183905	3.0116826
C	-3.4130186	9.8930399	-5.1345536	H	-10.3343270	-5.9482907	2.9773499
O	6.4729295	-1.4082546	-8.4272201	H	-10.3179394	-2.8910192	6.0834321
C	5.3979663	-1.8446642	-7.8920628	H	-7.0126245	-3.1855987	3.2994477
C	4.6970815	-2.9748987	-8.5869976	H	-2.9417461	10.3977918	5.9929204
C	5.1496496	-3.4328072	-9.8420453	H	-6.0728485	3.0414295	10.3795172
C	4.5091524	-4.5126662	-10.4680661	H	-10.3830047	5.9769323	2.8731552
C	3.4293820	-5.1517268	-9.8404153	H	-3.0000663	6.1330341	10.3649769
C	2.9727238	-4.6972961	-8.5856070	H	-7.0081199	3.2902260	3.2752834
C	3.6020794	-3.6024807	-7.9666698	H	-3.2813979	3.3226946	7.0800754
O	8.4442978	-1.4214210	-6.4317287	H	-6.0282229	10.3754145	2.9156510
O	4.8734294	-1.4173414	-6.8102515	H	-3.2713559	7.0519339	3.2613294
O	4.8694425	1.4111266	-6.8174523	H	-10.3730019	2.9176754	5.9773969
O	1.4103880	4.8710196	-6.8309426	H	-2.9401842	-10.3187247	-5.9437909
O	-1.4167441	6.8487378	-4.8649590	H	-6.0053153	-2.9121453	-10.3275331
O	-6.5003703	8.4758186	1.4185207	H	-10.3363827	-6.0005476	-2.9016171
O	8.4026330	-6.4846445	-1.3701140	H	-2.9178791	-5.9887394	-10.3208203
O	8.4330470	-6.4047667	1.4476784	H	-7.0343348	-3.2155489	-3.2242857
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418

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C	-5.3598248	7.9382127	-1.8313416	C	4.7172431	8.6386644	2.9997850
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C	-8.5836849	4.7110100	2.9841874	C	3.5719492	8.0742238	3.5849341
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C	-8.5930377	2.9828618	4.7024933	O	1.4760633	8.4330604	6.5411349
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Cu	-5.7720090	-0.0006313	5.7928859	C	-9.8528482	3.4523860	-5.1285667
O	-4.8533688	1.4114462	6.8482751	C	-7.8874246	5.4152054	-1.8281375
C	-1.8417765	-7.9260997	5.4053731	O	-8.4177630	6.4927296	-1.3923037
O	-1.4063474	-8.4619701	6.4803611	O	-6.8409997	-1.4034142	-4.8602716
Cu	0.0048441	-7.5314750	7.5329985	O	-4.8720341	-1.4090361	-6.8307568
O	1.4145805	-8.4615681	6.4785096	C	-5.4006407	-1.8409519	-7.9088295
C	1.8474934	-7.9263099	5.4021452	O	-6.4787199	-1.4082180	-8.4406305
O	1.4150106	-6.8473310	4.8761323	O	-6.4732567	-8.4576453	1.4173923
Cu	0.0033349	-5.7887253	5.7910323	O	-6.4696868	-8.4547993	-1.4032783
O	-1.4070773	-4.8747896	6.8519366	C	-5.3927304	-7.9205379	-1.8358849
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O	-1.4046761	-6.4783221	8.4650223	C	-5.1366090	-9.8752797	-3.4159766
C	-8.6176051	-4.6857071	-2.9587435	C	-4.4932179	-10.5041689	-4.4923482
C	-7.9962348	-3.5925688	-3.5887583	C	-3.4154986	-9.8754977	-5.1336859
C	-8.6201475	-2.9585516	-4.6780928	C	-2.9639991	-8.6165816	-4.6854071
C	-9.8806485	-3.4081319	-5.1238745	C	-3.5960185	-7.9946921	-3.5937479
C	-10.5088548	-4.4860740	-4.4825044	C	-1.8357441	-7.9202775	-5.3881987
C	-9.8779473	-5.1315555	-3.4085912	O	-1.4078062	-6.8382781	-4.8646686
C	-7.9245495	-1.8302307	-5.3813842	Cu	0.0043938	-5.7792059	-5.7790836
O	-8.4620196	-1.3947864	-6.4556905	O	1.4165275	-4.8649548	-6.8380529
Cu	-7.5292923	0.0088939	-7.5139948	C	1.8453032	-5.3894715	-7.9192464
O	-8.4478131	1.4263916	-6.4568690	O	1.4117314	-6.4661250	-8.4533865
C	-7.9086188	1.8591858	-5.3824540	Cu	0.0050765	-7.5222922	-7.5203203
O	-6.8282113	1.4257579	-4.8599885	O	-1.4099779	-6.4703214	-8.4467686
Cu	-5.7817718	0.0079462	-5.7771335	C	-1.8439011	-5.3940168	-7.9122446
O	-4.8719898	1.4191798	-6.8426384	C	-2.9758895	-4.6940070	-8.6054625
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C	-4.6993633	2.9755669	-8.6212598	C	-4.7003531	-2.9716346	-8.6037948
C	-5.1534556	3.4293733	-9.8772616	C	-5.1537261	-3.4282499	-9.8590202
C	-4.5142796	4.5075529	-10.5073907	C	-4.5136576	-4.5072813	-10.4867657
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C	-3.6043582	3.6058793	-8.0036803	O	-6.8375336	-4.8713436	1.4225951
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Cu	0.0073920	5.7839436	-5.8043130	O	-8.4399946	1.4169161	6.4788458
O	1.4280451	6.8358907	-4.8962628	O	-6.4666243	-1.4106472	8.4640568
C	1.8590410	7.9152903	-5.4225809	C	-5.3901493	-1.8455167	7.9306758
C	2.9911993	8.6078092	-4.7224051	O	-4.8636526	-1.4165638	6.8504499
C	3.4492215	9.8630340	-5.1741996	C	-4.6896755	-2.9754538	8.6264007
C	4.5285562	10.4890582	-4.5329406	C	-3.5957556	-3.6051978	8.0062275
C	5.1665221	9.8613203	-3.4527253	C	-2.9666487	-4.6990165	8.6271837
C	4.7123550	8.6058982	-2.9971940	C	-3.4222551	-5.1500483	9.8836102
C	3.6185657	7.9864348	-3.6277991	C	-4.5012523	-4.5092289	10.5106776
C	5.4089704	7.9135030	-1.8630397	C	-5.1416402	-3.4305108	9.8826963
O	6.4834766	8.4483727	-1.4257728	O	1.4169555	-6.4749080	8.4574241
Cu	7.5200089	7.5391864	0.0101055	C	1.8530704	-5.4005890	7.9205253
O	6.4518615	8.4852474	1.3949848	O	1.4219141	-4.8748622	6.8409122
C	5.3739696	7.9619967	1.8333971	C	2.9880228	-4.7035571	8.6115907

C	3.6174607	-3.6088198	7.9920891	C	4.5607157	4.5318053	10.5553265
C	4.7165074	-2.9857977	8.6100873	C	3.4677771	5.1590421	9.9369216
C	5.1733843	-3.4487943	9.8618427	C	2.9838979	4.6783150	8.7032535
C	4.5327329	-4.5280405	10.4882702	C	3.5925258	3.5641227	8.1020423
C	3.4482927	-5.1618026	9.8637260	O	6.4716050	1.3775660	8.5329453
C	5.4178522	-1.8521818	7.9210801	O	8.4423172	1.4609764	6.5353395
O	6.5043506	-1.4360264	8.4491959	O	8.4281608	6.5178867	1.4532048
Cu	7.5380170	0.0085865	7.5533762	O	8.4629793	6.4597560	-1.3710343
O	8.4812356	-1.3617605	6.4602102	O	8.4571453	1.4141678	-6.4507258
C	7.9377081	-1.7963936	5.3887168	Cu	7.5340395	0.0077334	-7.5200533
O	6.8482508	-1.3731109	4.8772390	O	6.4892238	1.4185014	-8.4556029
Cu	5.7917957	0.0288919	5.8115380	C	5.4095954	1.8505166	-7.9261546
O	6.8410887	1.4637697	4.9197170	C	4.7059097	2.9745840	-8.6281303
C	7.9098089	1.9050979	5.4627936	C	5.1562633	3.4242231	-9.8869524
C	8.5780444	3.0702241	4.7963052	C	4.5118667	4.4969785	-10.5210747
C	9.7514498	3.6308914	5.3430386	C	3.4305599	5.1374876	-9.8976452
C	10.3335608	4.7574636	4.7442145	C	2.9764852	4.6915981	-8.6388635
C	9.7393058	5.3409625	3.6150757	C	3.6094963	3.6035423	-8.0117988
C	8.5664927	4.7848780	3.0645728	C	1.8451120	5.3928918	-7.9464958
C	8.0005028	3.6385594	3.6478732	O	1.4106792	6.4683605	-8.4822276
C	7.8935317	5.4503343	1.9029327	Cu	0.0061107	7.5261774	-7.5468758
O	6.8260978	4.9083336	1.4516175	O	-1.3961728	8.4600785	-6.4846932
Cu	5.7729537	5.8037262	0.0136447	C	-1.8261615	7.9270010	-5.4061194
O	6.8421451	4.8646541	-1.3738654	C	-2.9477615	8.6269979	-4.6966117
C	7.9270709	5.3829985	-1.8016174	C	-3.5743013	8.0070952	-3.6006502
C	8.6241382	4.6752884	-2.9261299	C	-4.6604470	8.6325680	-2.9628620
C	7.9973997	3.5908759	-3.5660330	C	-5.1066874	9.8931677	-3.4117253
C	8.6201424	2.9619600	-4.6592255	C	-4.4687560	10.5199107	-4.4925882
C	9.8844914	3.4071143	-5.0982428	C	-3.3979423	9.8874462	-5.1417376
C	10.5183514	4.4753323	-4.4462898	O	6.4768407	-1.4014691	-8.4528564
C	9.8887488	5.1163301	-3.3690850	C	5.3992705	-1.8343435	-7.9202825
C	7.9204454	1.8428824	-5.3735167	C	4.6968233	-2.9630899	-8.6161619
O	6.8349003	1.4161093	-4.8564885	C	5.1460859	-3.4165031	-9.8739979
Cu	5.7866228	0.0063630	-5.7827597	C	4.5043786	-4.4944236	-10.5020036
O	6.8448405	-1.4106967	-4.8729337	C	3.4268657	-5.1362219	-9.8733998
C	7.9268154	-1.8390254	-5.3960062	C	2.9736620	-4.6867132	-8.6155373
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C	10.5084963	-4.4986066	-4.5009011	O	4.8728126	-1.4044461	-6.8403365
C	9.8808959	-5.1387882	-3.4218811	O	4.8822515	1.4230081	-6.8459265
C	8.6233522	-4.6887290	-2.9683677	O	1.4154238	4.8683635	-6.8656342
C	8.0015979	-3.5966151	-3.5995348	O	-1.3988237	6.8439772	-4.8842189
C	7.9285303	-5.3893974	-1.8380858	O	-6.4150206	8.4650814	1.4260690
O	6.8479835	-4.8643119	-1.4086167	O	8.4638274	-6.4651039	-1.4034706
Cu	5.7896092	-5.7725198	0.0091439	O	8.4617202	-6.4425274	1.4150477
O	4.8756386	-6.8310506	-1.4018639	C	7.9257724	-5.3652276	1.8447809
C	5.4010178	-7.9122259	-1.8298652	O	6.8402305	-4.8476025	1.4186542
O	6.4772940	-8.4459353	-1.3951566	C	8.6265406	-4.6524135	2.9639688
Cu	7.5354580	-7.5113119	0.0114904	C	9.8909159	-5.0930367	3.4075950
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C	5.4105054	-7.9110537	1.8567549	C	9.8979441	-3.3656042	5.1184272
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C	5.1622679	-9.8655912	3.4383704	C	8.0051796	-3.5593581	3.5945824
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C	3.6110253	-7.9933763	3.6111960	C	5.1479500	-9.8675132	-3.4099285
O	4.8827559	-1.4000992	6.8546380	C	4.5071879	-10.4964020	-4.4878804
O	4.8905170	1.4325681	6.8990493	C	3.4310903	-9.8677191	-5.1319321
C	5.4043893	1.8309702	7.9988765	C	2.9784640	-8.6088253	-4.6847479
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C	2.9388001	-4.7111510	-8.6452133	H	-6.9814156	3.2416309	3.2379731
C	3.5688713	-3.6153579	-8.0287175	H	-3.2474302	3.2448456	6.9894688
O	8.4269349	-1.4169042	-6.5209713	H	-5.8967850	10.3695810	2.8536776
O	4.8366500	-1.4203372	-6.8842250	H	-3.1870127	7.0080151	3.2159639
O	4.8458057	1.4071636	-6.9017272	H	-10.3198035	2.9116139	5.9789160
O	1.3714698	4.8438148	-6.9332108	H	-2.9350256	-10.3728523	-6.0096457
O	-1.4371304	6.8215302	-4.9496562	H	-6.0583774	-2.9690366	-10.3370043
O	-6.4113730	8.4595472	1.3827491	H	-10.3832048	-6.0143946	-2.9136033
O	8.4470815	-6.4580838	-1.4340110	H	-2.9685378	-6.0430996	-10.3419424
O	8.4539732	-6.4187489	1.3824263	H	-7.0477051	-3.2716973	-3.2573471
C	7.9156995	-5.3401913	1.8052172	H	-3.2853777	-3.2767926	-7.0233014
O	6.8240866	-4.8323594	1.3827125	H	-6.0256378	-10.3694804	-2.9364398
C	8.6212478	-4.6103688	2.9108200	H	-3.2751652	-7.0389758	-3.2645198
C	9.8978392	-5.0279437	3.3413456	H	-10.3926129	-2.9254283	-5.9882291
C	10.5365697	-4.3593972	4.3965013	H	-2.9871112	5.9619478	-10.4144657
C	9.8999628	-3.2875818	5.0399667	H	-6.0001602	10.3357120	-2.9600341
C	8.6229454	-2.8664953	4.6139442	H	-10.3608488	2.9151943	-5.9866551
C	7.9916690	-3.5224262	3.5416981	H	-3.2548069	7.0035572	-3.3091765
O	4.8750799	-6.8303781	1.4068304	H	-6.0660628	2.8772951	-10.3806027
O	-1.4417239	-6.8898829	4.8559745	H	-3.2940347	3.2253824	-7.0702109
C	4.6821775	-8.6111106	-2.9758953	H	-2.9553192	10.3215775	-6.0786027
C	5.1351197	-9.8684939	-3.4269843	H	-10.3324731	5.9984123	-2.9061532
C	4.4953534	-10.5003522	-4.5037706	H	-7.0111207	3.2402284	-3.2586539
C	3.4160480	-9.8760901	-5.1467762	H	2.9127788	-10.3884662	5.9509562
C	2.9591567	-8.6186286	-4.6998786	H	6.0831703	-3.0749943	10.2541659
C	3.5876222	-7.9937789	-3.6077352	H	10.3733035	-5.8838472	2.8384888
C	1.8282923	-7.9278240	-5.4043750	H	2.9825089	-6.1382522	10.2769881
O	1.3945224	-6.8477480	-4.8815183	H	6.9954959	-3.1973878	3.2099385
O	1.3974845	-8.4653637	-6.4803894	H	3.2470805	-3.3308450	6.9892537
O	-1.4236017	-8.4847768	-6.4798154	H	6.0265333	-10.3328254	2.9016906
O	-1.4622781	6.4413711	-8.5385325	H	3.2386678	-7.0334141	3.2302253
O	1.3754199	8.4345561	-6.5906527	H	10.3767204	-2.7656633	5.8836720
O	4.8458852	6.8392834	-1.5336444	H	2.8412336	5.9067988	10.4216143
O	4.7936357	6.9041765	1.2958631	H	6.0858133	10.2850836	2.9526793
O	1.4749535	6.7964279	4.8811461	H	9.9917593	3.2354452	6.2603747
O	-1.4113347	4.8695859	6.8128211	H	3.1736675	10.1397712	6.1924346
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O	-1.4425818	-4.8934071	-6.8521452	H	5.8330204	2.7368487	10.4820870
O	-6.5232915	1.3743151	-8.4822061	H	3.1541560	3.1550489	7.0994419
O	-6.8375241	-1.4373956	4.8637095	H	10.0223110	6.2809246	3.1407008
H	2.9151389	10.3121081	-6.1522597	H	6.9033557	3.2719461	3.2241254

H	2.8866491	-6.0245575	-10.3683030
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H	10.3269713	-5.9930130	-2.9534849
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H	-4.8722441	11.4710604	-4.9095725
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H	-4.9244883	4.8041779	-11.5407496
H	-11.5356378	-4.8555213	-4.8349034
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H	-4.9019448	4.9056255	11.4214515
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H	4.7090515	4.6941406	11.6095923
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H	4.8479045	-11.4847763	-4.8518773
H	11.4831711	4.7989593	-4.8428877
H	5.0991618	11.2973929	5.0421630
H	-4.7160861	11.5265442	4.7584511
O	4.5378219	6.3693822	6.6476404
C	5.6627790	6.0226046	6.2798358
N	6.3518674	6.6580186	5.2588356
N	6.3496630	4.9639040	6.8622814
H	7.0962152	6.1657644	4.7557900
H	5.7927572	7.3143895	4.7072636
H	7.3661796	4.8916743	6.7673499
H	5.9481901	4.6123282	7.7350926

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Energy = -54158.24884898 , Urea @ LCW

C	-5.1472760	-9.8673508	3.4233861
C	-4.7033197	-8.6055267	2.9758284
C	-3.6103530	-7.9839869	3.6060578
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C	-5.4112418	-7.9069621	1.8524659
O	-4.8919743	-6.8219048	1.4271272
Cu	-5.8075916	-5.7686459	0.0119973
O	-6.8658071	-4.8628623	-1.4055873
C	-7.9448823	-5.3905981	-1.8357830
O	-8.4782330	-6.4670752	-1.4009277
Cu	-7.5440859	-7.5167299	0.0096107
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C	-7.9472826	-5.3893676	1.8550314
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C	-9.8966950	-3.4285092	5.1659107

C	-8.6405840	-2.9722576	4.7147061
C	-8.0209997	-3.5990445	3.6187548
C	-7.9443162	-1.8441321	5.4178083
O	-8.4784346	-1.4100779	6.4942252
Cu	-7.5466228	-0.0000108	7.5481825
O	-6.4904191	1.4104684	8.4762303
C	-5.4153620	1.8445499	7.9392224
C	-4.7126095	2.9752942	8.6314692
C	-5.1624025	3.4338106	9.8872878
C	-4.5203549	4.5136471	10.5116503
C	-3.4415684	5.1519614	9.8816369
C	-2.9876354	4.6970627	8.6260150
C	-3.6186876	3.6023659	8.0085070
C	-1.8565949	5.3944217	7.9287006
O	-1.4214990	6.4726702	8.4579191
Cu	-0.0026470	7.5167341	7.5251571
O	1.3977991	6.4725489	8.4744355
C	1.8294485	5.3893890	7.9514557
O	1.4014523	4.8565964	6.8740136
Cu	-0.0046606	5.7610783	5.7960331
O	-1.4114527	6.8245613	4.8730110
C	-1.8386596	7.9088016	5.3919885
C	-2.9664829	8.6041016	4.6874255
C	-3.4139463	9.8662078	5.1308451
C	-4.4916635	10.4945671	4.4893055
C	-5.1392006	9.8620915	3.4176127
C	-4.6957056	8.5999915	2.9703690
C	-3.6026860	7.9784099	3.6004700
C	-5.4043114	7.9012025	1.8475727
O	-4.8852182	6.8162226	1.4218546
Cu	-5.8027830	5.7619594	0.0085839
O	-4.8792617	6.8115415	-1.4036372
C	-5.3962848	7.8964640	-1.8318970
O	-6.4730600	8.4342820	-1.4033517
Cu	-7.5375905	7.5117135	0.0050909
O	-8.4737492	6.4629747	1.4159721
C	-7.9429241	5.3855402	1.8515325
C	-8.6389199	4.6881695	2.9832550
C	-8.0185203	3.5961372	3.6160643
C	-8.6390091	2.9701554	4.7119596
C	-9.8952165	3.4271209	5.1621655
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C	-7.9435714	1.8421125	5.4160016
O	-6.8637563	1.4111459	4.8904595
Cu	-5.8058685	-0.0012762	5.8044589
O	-4.8922901	1.4142843	6.8578960
C	-1.8466090	-7.9143379	5.3978452
O	-1.4121382	-8.4540341	6.4714690
Cu	-0.0094171	-7.5231443	7.5299343
O	1.4081525	-8.4300121	6.4615322
C	1.8431995	-7.8846740	5.3912018
O	1.4109435	-6.8019436	4.8731192
Cu	-0.0098471	-5.7684157	5.7998587
O	-1.4293173	-4.8666418	6.8556596
C	-1.8603638	-5.3978771	7.9328383
O	-1.4271374	-6.4769018	8.4620137
C	-8.6390232	-4.6916831	-2.9677569
C	-8.0163398	-3.6005515	-3.5997411
C	-8.6350351	-2.9730338	-4.6957695
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C	-10.5216650	-4.5033538	-4.5035791

C	-9.8958629	-5.1422523	-3.4226642	O	-1.3982477	-6.8285700	-4.8373481
C	-7.9367774	-1.8461663	-5.3986273	Cu	0.0083698	-5.7625443	-5.7563524
O	-8.4672362	-1.4138975	-6.4775884	O	1.4172824	-4.8541966	-6.8287055
Cu	-7.5315133	-0.0048325	-7.5292249	C	1.8482392	-5.3870286	-7.9047988
O	-8.4654719	1.4064346	-6.4791682	O	1.4172193	-6.4684725	-8.4311806
C	-7.9344332	1.8392800	-5.4007113	Cu	0.0170491	-7.5181759	-7.4854755
O	-6.8550116	1.4097369	-4.8730606	O	-1.4024833	-6.4781851	-8.4211496
Cu	-5.7955373	-0.0050643	-5.7807029	C	-1.8400497	-5.4001286	-7.8935087
O	-4.8763292	1.4077410	-6.8330619	C	-2.9714706	-4.7052856	-8.5925763
C	-5.3976942	1.8390532	-7.9147521	C	-3.6032191	-3.6094347	-7.9777940
C	-4.6936621	2.9705631	-8.6046566	C	-4.6972437	-2.9842659	-8.6024699
C	-5.1432899	3.4326732	-9.8591938	C	-5.1469609	-3.4463845	-9.8569729
C	-4.5002335	4.5133377	-10.4811233	C	-4.5046240	-4.5277486	-10.4784347
C	-3.4203409	5.1487134	-9.8500546	C	-3.4253008	-5.1637264	-9.8469918
C	-2.9665545	4.6902485	-8.5956287	O	-4.8840814	-6.8210123	-1.3982827
C	-3.5989512	3.5949997	-7.9804328	O	-6.8694753	-4.8596750	1.4238767
C	-1.8346092	5.3846091	-7.8969323	O	-6.8629145	4.8554759	-1.4072787
O	-1.4049143	4.8499357	-6.8208051	O	-6.8645320	4.8556248	1.4220814
Cu	0.0136504	5.7470633	-5.7597600	O	-8.4768398	1.4108642	6.4939733
O	1.4373523	6.7748283	-4.8308030	O	-6.4923521	-1.4115729	8.4766427
C	1.8762588	7.8547831	-5.3492975	C	-5.4163202	-1.8451617	7.9411811
C	3.0129890	8.5363013	-4.6452226	O	-4.8916313	-1.4143488	6.8608638
C	3.4634527	9.7998541	-5.0812921	C	-4.7144874	-2.9760649	8.6341020
C	4.5450622	10.4202795	-4.4388637	C	-3.6208113	-3.6041209	8.0116960
C	5.1929741	9.7784990	-3.3731838	C	-2.9908446	-4.6991670	8.6297076
C	4.7484926	8.5135282	-2.9343593	C	-3.4455900	-5.1533990	9.8852753
C	3.6517938	7.8994045	-3.5658546	C	-4.5241137	-4.5141029	10.5147369
C	5.4601110	7.8103112	-1.8159049	C	-5.1651031	-3.4339342	9.8898652
O	6.5043796	8.3761937	-1.3452132	O	1.3923822	-6.4801642	8.4782596
Cu	7.5890611	7.4463269	0.0423444	C	1.8262918	-5.3985625	7.9539045
O	6.5444142	8.3511835	1.4685951	O	1.3991400	-4.8660832	6.8759695
C	5.4419522	7.8380997	1.8618823	C	2.9522633	-4.7013481	8.6586099
C	4.7261006	8.5404617	2.9775475	C	3.5866292	-3.6057527	8.0461727
C	5.1747276	9.8009729	3.4249959	C	4.6779612	-2.9807774	8.6755479
C	4.5244902	10.4404230	4.4905293	C	5.1215369	-3.4420169	9.9324271
C	3.4395635	9.8197152	5.1271221	C	4.4758457	-4.5224994	10.5519965
C	2.9872572	8.5591680	4.6844519	C	3.3997967	-5.1589552	9.9156809
C	3.6252348	7.9267007	3.6019685	C	5.3852828	-1.8495387	7.9880632
C	1.8512894	7.8746335	5.3869512	O	6.4619089	-1.4230668	8.5281035
O	1.4158107	8.4216517	6.4562528	Cu	7.5254470	-0.0065467	7.6175775
C	-8.6317036	2.9672984	-4.6987212	O	8.4798515	-1.4081376	6.5734108
C	-8.0129404	3.5944529	-3.6025223	C	7.9490884	-1.8431265	5.4954238
C	-8.6346705	4.6866035	-2.9713616	O	6.8631057	-1.4261474	4.9736647
C	-9.8905828	5.1386687	-3.4273496	Cu	5.7963839	-0.0065358	5.8576222
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C	-9.8877171	3.4230043	-5.1507636	C	7.9510332	1.8281766	5.4948026
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O	-6.8571388	-1.4169890	-4.8711222	C	10.5334934	4.4896500	4.6042685
O	-4.8787970	-1.4206833	-6.8314518	C	9.9196579	5.1094645	3.5058219
C	-5.4003405	-1.8518425	-7.9131223	C	8.6736556	4.6421609	3.0374109
O	-6.4739250	-1.4175468	-8.4528024	C	8.0505699	3.5519058	3.6704308
O	-6.4863457	-8.4439863	1.4184457	C	7.9873033	5.3273622	1.8946714
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C	-5.1325188	-9.8653577	-3.3967859	C	8.0306523	5.3152734	-1.7861505
C	-4.4806653	-10.4981516	-4.4657101	C	8.7443680	4.6078245	-2.8983568
C	-3.3998740	-9.8703681	-5.1025640	C	8.0741860	3.5954609	-3.6037908
C	-2.9537548	-8.6084375	-4.6571323	C	8.7203940	2.9060634	-4.6436316
C	-3.5942736	-7.9825374	-3.5727712	C	10.0445809	3.2462793	-4.9896527
C	-1.8232783	-7.9133533	-5.3572936	C	10.7131411	4.2616942	-4.2888045

C 10.0673373 4.9466964 -3.2477157
C 7.9917442 1.8175557 -5.3704240
O 6.9122092 1.3860805 -4.8275747
Cu 5.8226403 -0.0106594 -5.7703893
O 6.9172709 -1.4010518 -4.8231346
C 7.9888688 -1.8436412 -5.3726119
C 8.7159320 -2.9329098 -4.6454769
C 10.0382027 -3.2777597 -4.9942124
C 10.7056401 -4.2935243 -4.2928119
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C 8.7390964 -4.6314596 -2.8971148
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C 8.0257400 -5.3359066 -1.7827691
O 6.9818404 -4.7621275 -1.3186503
Cu 5.8563484 -5.7036990 0.0391147
O 4.9731316 -6.7083736 -1.4286727
C 5.4532206 -7.8276417 -1.8112244
O 6.4939206 -8.3966493 -1.3364379
Cu 7.5820826 -7.4649369 0.0474188
O 6.5388200 -8.3653762 1.4771509
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O 8.5411223 6.3795440 1.4252970
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O 8.4921960 1.3987907 -6.4623179
Cu 7.5528947 -0.0120512 -7.5301393
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C 5.4332672 1.8392483 -7.9115292
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C 5.1646464 3.4177510 -9.8657079
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O 1.4215434 6.4491801 -8.4357562
Cu 0.0237014 7.5017744 -7.4898073
O -1.3752032 8.4395676 -6.4329466
C -1.8164829 7.8996012 -5.3621603
C -2.9461092 8.5962712 -4.6621993
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O 1.4247338 4.8388466 -6.8293544
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C 9.8997042 -3.4317877 5.2512255
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C 8.0467795 -3.5690018 3.6730292
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H -11.5057007 -4.8540617 -4.8546468
H -11.5060468 4.8569515 4.8688831
H -11.4997942 4.8520267 -4.8603496
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H 4.8593036 4.8410811 -11.4800086
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H 4.8812141 -11.4292447 -4.7698732
H 11.7495555 4.5228598 -4.5574413
H 4.8733889 11.4273487 4.8351876
H -4.8369089 11.4825717 4.8346096
O 6.8827499 -0.0081089 0.1931215
C 6.7811001 -0.0084783 -1.0428159
N 6.6993557 1.1573858 -1.7724063
N 6.6961022 -1.1749573 -1.7714802
H 6.7872024 1.1758694 -2.7968008
H 6.8503870 2.0309377 -1.2626680
H 6.7919815 -1.1941499 -2.7952416
H 6.8483221 -2.0476591 -1.2605034

10

Energy = -283.8833977040 , Clycine

N	-0.5139553	3.7082060	4.6548661
H	0.4354609	3.5849207	4.2711994
H	-1.1039572	3.9173787	3.8350615
C	-0.9523954	2.4641799	5.2535336
C	-0.9525464	1.2540659	4.3173250
H	-0.3161254	2.2135756	6.1336594
H	-1.9814451	2.5755690	5.6666450
O	-1.3758175	0.1258655	4.9444872
O	-0.6170232	1.2790947	3.1484521
H	-1.3413814	-0.5943997	4.2672636

8

Energy = -224.8331549433 , urea

O	-2.2561332	2.0461025	5.0640541
C	-1.1375002	2.4743794	5.3223562
N	-0.5578741	3.5483071	4.6477490
N	-0.3259842	1.9320915	6.3184150
H	0.4622843	3.5940772	4.5708278
H	-1.0663535	3.8184388	3.8020037
H	0.3565498	2.5344084	6.7877464
H	-0.8190065	1.2787758	6.9321070

24

Energy = -679.1043093450 , Caffeine

N	3.7403140	1.5126902	0.4052535
C	2.9642678	2.6499505	0.4030990
C	1.5713799	2.5862463	0.4576023
C	0.8282289	1.3552975	0.5203621
N	1.7132099	0.2338209	0.5179317
C	3.1276340	0.2490705	0.4641471
N	3.4112125	3.9354013	0.3496050
N	1.1503144	3.9090117	0.4354131

O -0.3972641 1.2355376 0.5704181

O 3.7718172 -0.7939378 0.4690331

C 1.1166581 -1.0990643 0.5777689

H 1.4086166 -1.6915793 -0.3146990

H 1.4741411 -1.6403838 1.4789610

H 0.0187727 -0.9638435 0.6141955

C 5.1930022 1.6132192 0.3476046

H 5.5958699 0.5825218 0.3510961

H 5.5041007 2.1472609 -0.5757693

H 5.5744422 2.1796868 1.2241911

C 2.2905680 4.6605396 0.3711401

C -0.2270123 4.3725435 0.4762970

H -0.7213227 4.0329730 1.4101753

H -0.2301493 5.4805951 0.4318033

H -0.7979525 3.9602452 -0.3812645

H 2.2514586 5.7593310 0.3411287

14

Energy = -436.0324888780 , Niacine

N 3.5006495 -4.7942555 -0.3647869

C 3.9649977 -3.6147657 -0.8096320

C 3.3915441 -2.8986945 -1.8772176

C 2.2721283 -3.4428847 -2.5154773

C 1.7715648 -4.6786214 -2.0622477

C 2.4275028 -5.3093374 -0.9820331

H 4.8511409 -3.2114409 -0.2834965

H 3.8184131 -1.9344048 -2.1970090

H 1.7701623 -2.9397252 -3.3576014

C 0.5767935 -5.2591240 -2.7429157

H 2.0567626 -6.2793243 -0.6062744

O 0.1983484 -6.4524188 -2.2125735

O -0.0108573 -4.7368124 -3.6746868

H -0.5907222 -6.7390050 -2.7340571