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Supplementary Information

Monophenolase and catecholase activity of *Aspergillus oryzae* catechol oxidase: Insights from hybrid QM/MM calculations

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Part I. MD Simulation

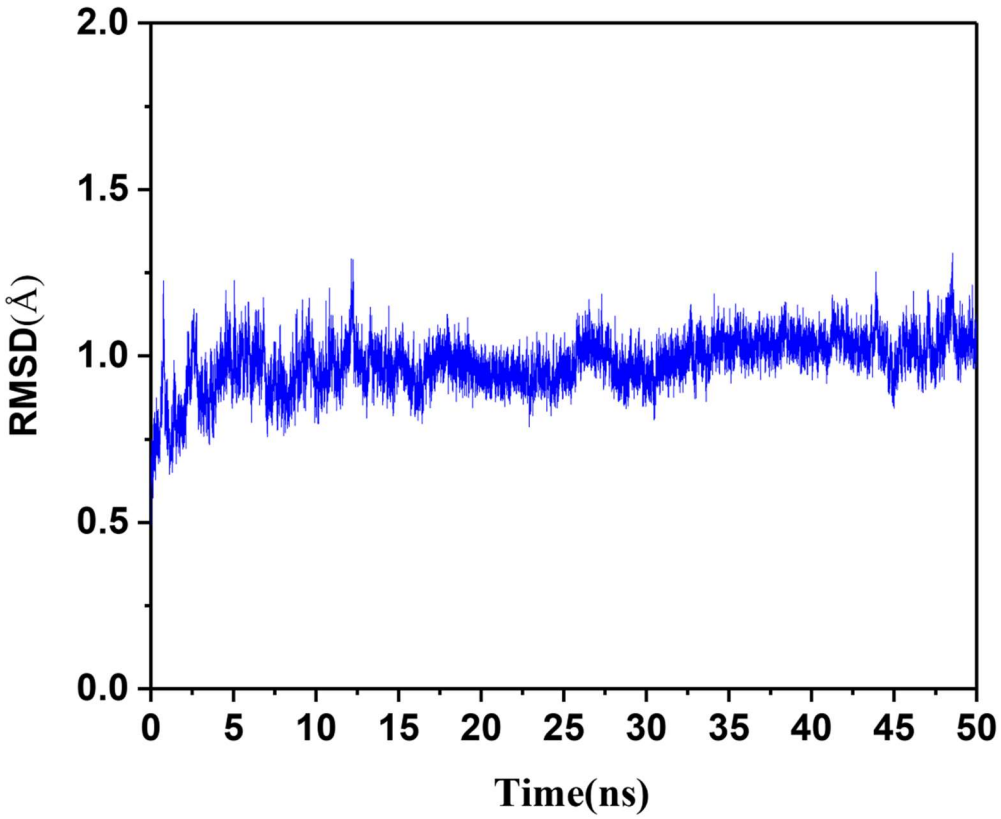

Fig. S1. The RMSD plot of backbone during MD simulations.

Part II. Computational Details

Region for the QM/MM optimization. QM/MM optimized region included the following set of residues: substrate RCO, CuA, CuB, dioxygen, Asp97, Phe98, Val99, Ala100, Thr101, His102, Ile103, Asn104, Gln105, Thr106, Gln107, Ile108, Ile109, His110, Tyr111, Thr112, Thr114, Phe115, Leu116, Ala117, Trp118, His119, Arg120,Tyr121, Phe122, Ile123, Tyr124, Tyr140, Tyr142, Trp143, Trp145, Met152, Leu230, Ile245, Leu246, Tyr249, Asn250, Leu258, Thr271, Met272, Gln273, Gly274, Ile281, Gly282, Val283, His284, Gly285, Gly286, Gly287, His288, Tyr289, Ser290, Met291, Gly292, Pro295, Gly296, Arg297, Asp298, Val299, Tyr300, Val301, Ser302, Pro303, Asp305, Ala307, Phe308, Trp309, Leu310, His311, His312, Gly313, Met314, Ile315, Asp316, Arg317, Trp319, Thr339, Phe340, Met341, Asn342, Ile355, Leu357, Ala360, Leu370, Tyr382; some crystal water: Wat494, Wat500, Wat514, Wat178, Wat551, Wat200, Wat575, Wat578, Wat586, Wat595, Wat596, Wat616, Wat622, Wat702, and solvent water: Solv2780.

Part III. QM/MM-optimized structure for the key species

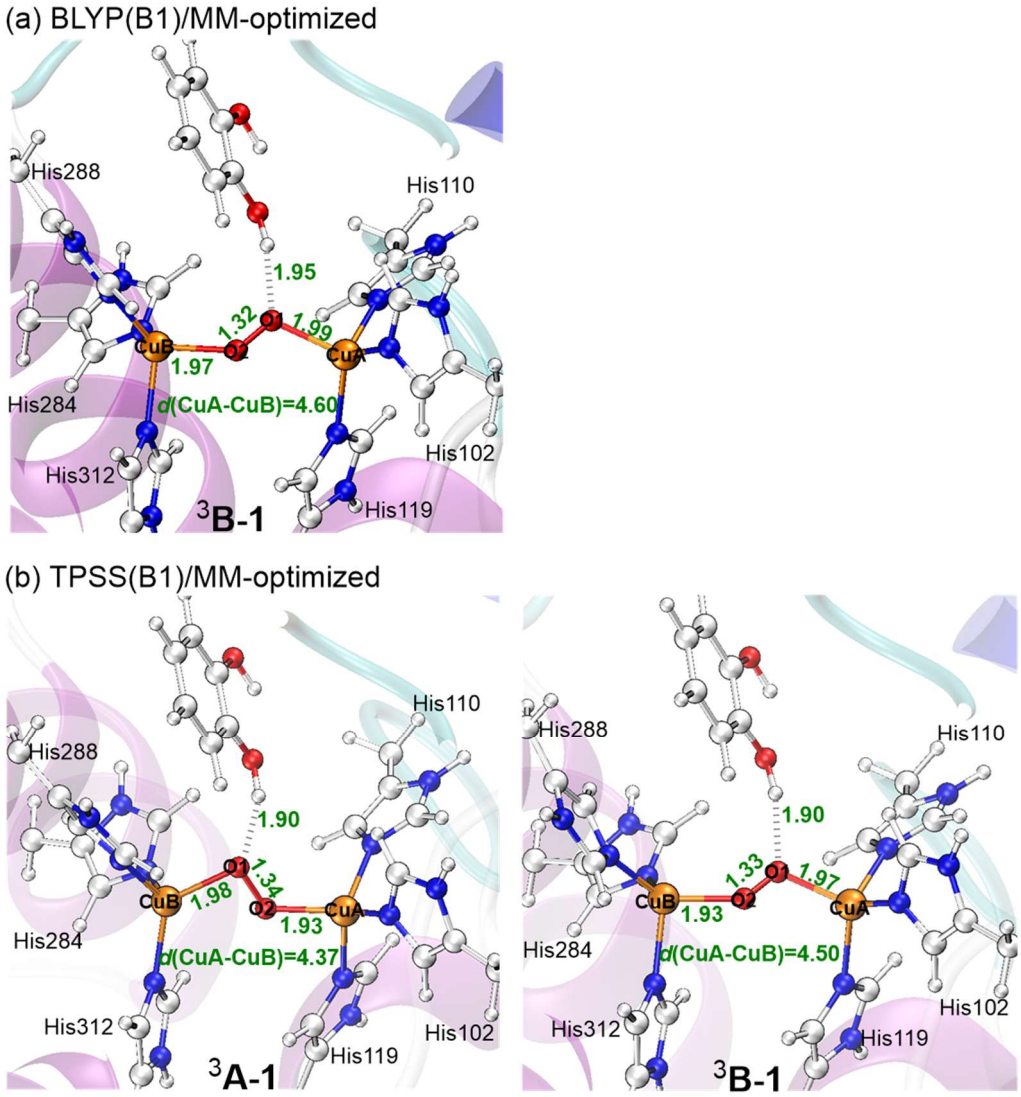

Fig. S2 QM/MM-optimized structures for the oxy-form of AoCO4: (a) at the BLYP(B1)/MM level (b) at the TPSS(B1)/MM level.

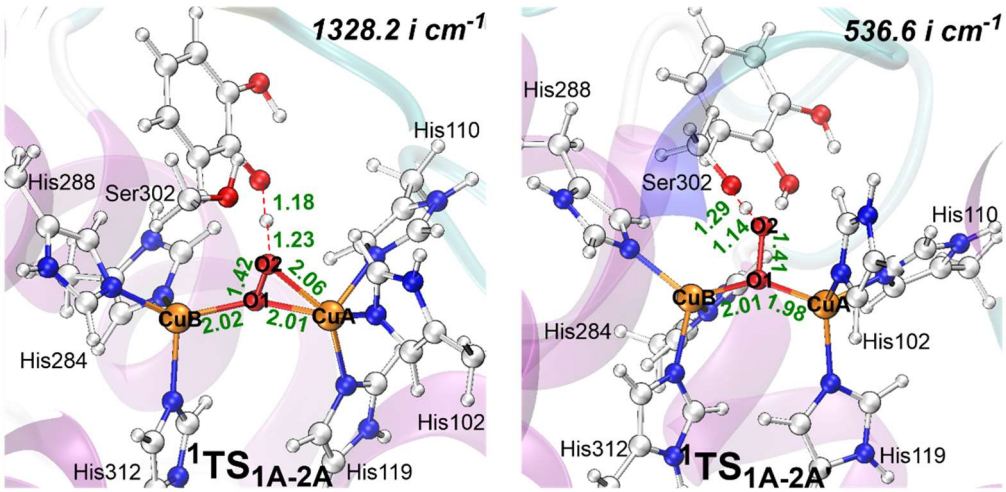

Fig. S3 QM/MM-optimized structures for the transition state of the initial proton coupled electron transfer from either catechol and Ser302 starting from ^{1}**A-1** using QM region QR2.

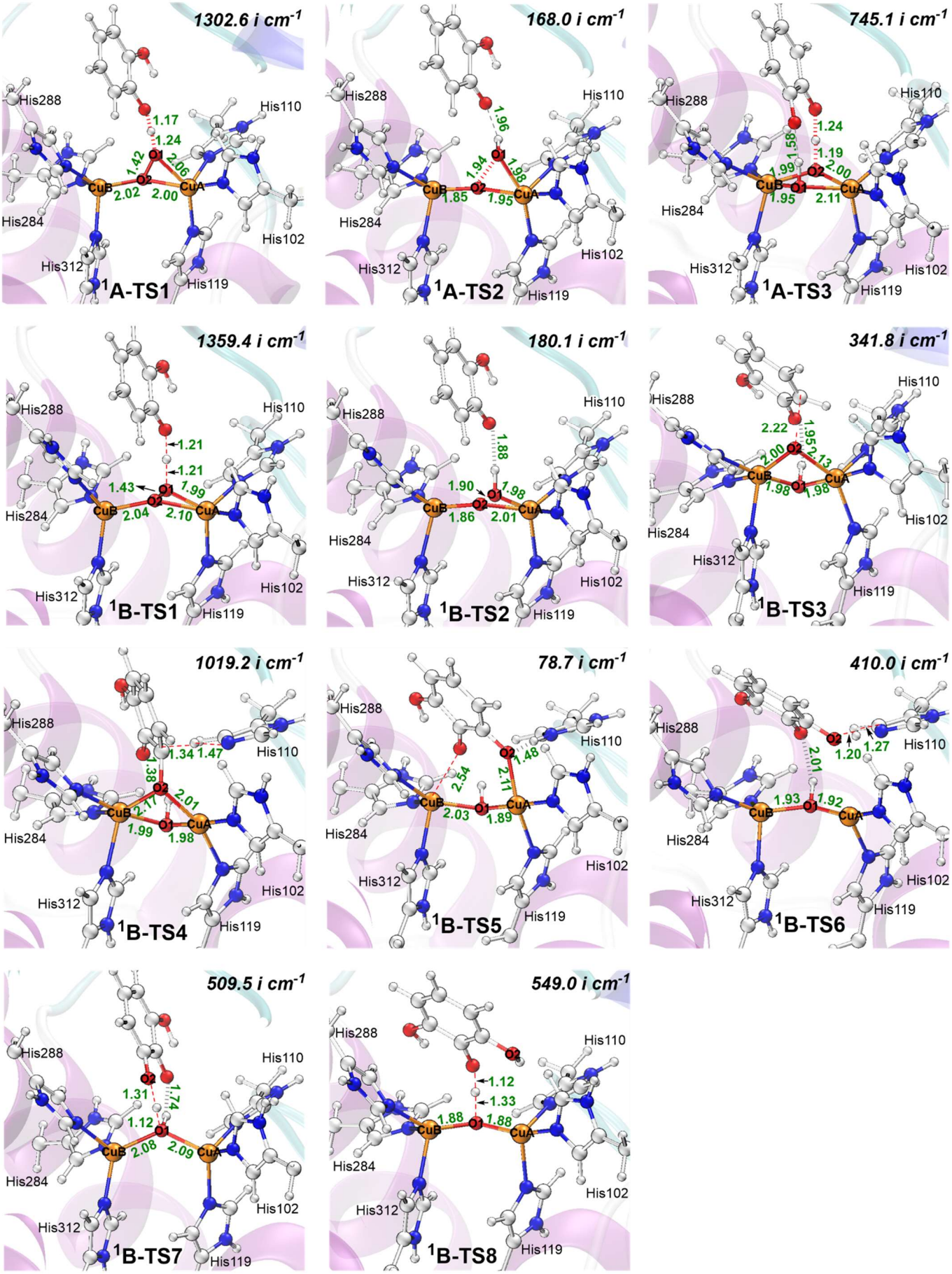

Fig. S4 QM/MM-optimized structures for the transition states involved in the singlet PES.

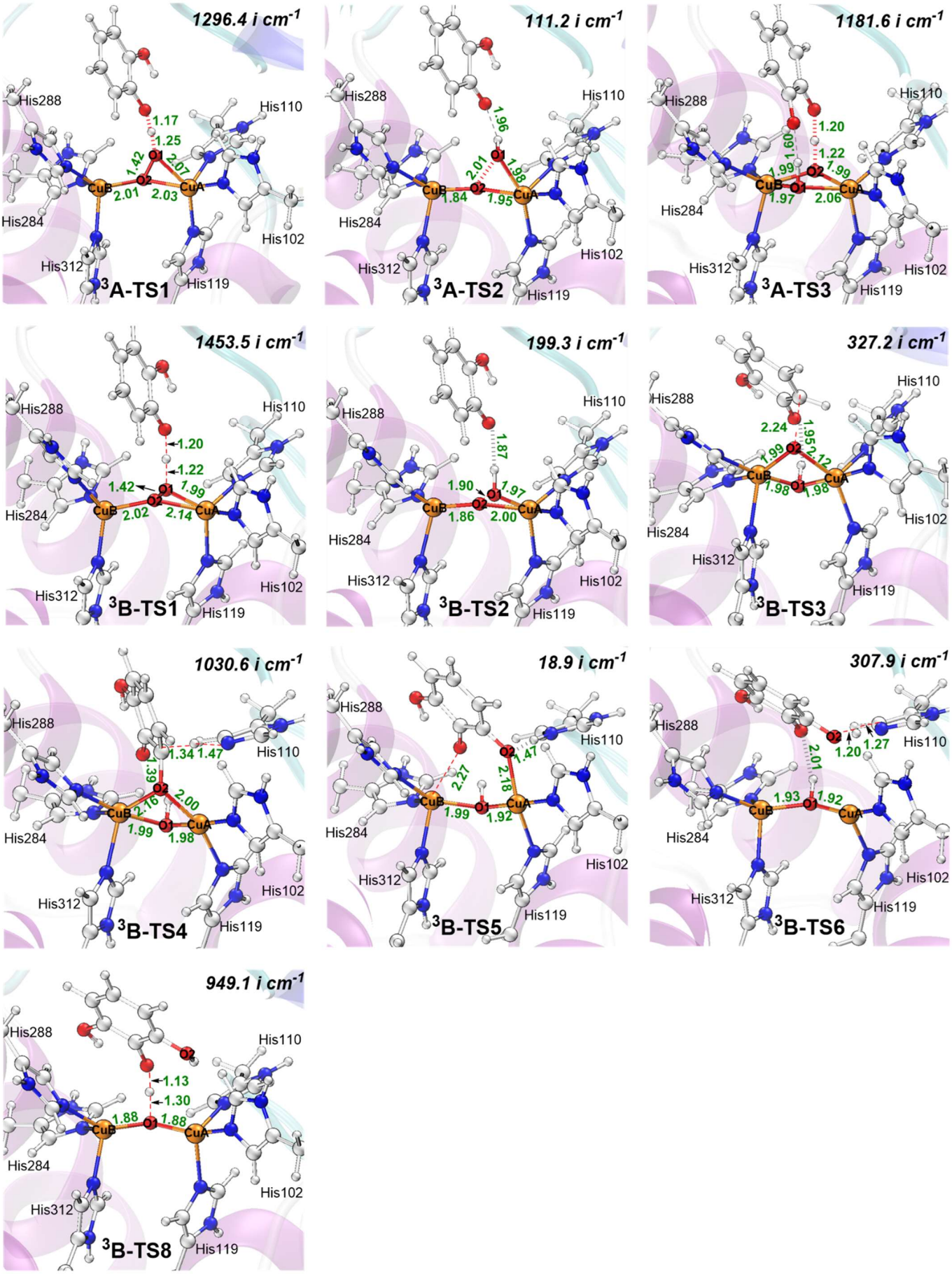

Fig. S5 QM/MM-optimized structures for the transition states involved in the triplet PES.

Part IV. Energy Profiles at the TPSSh/MM Level

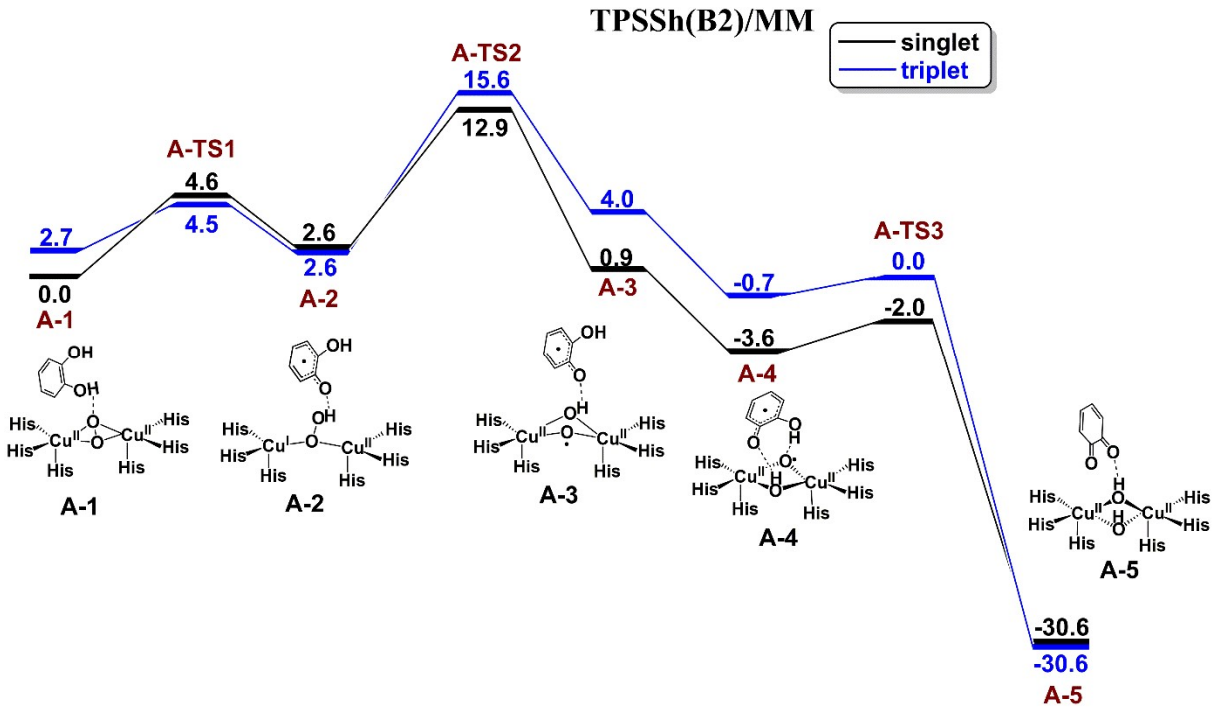

Fig. S6 Energy profile for the catechol oxidation starting from μ-η^2:η^2 peroxo dicopper(II,II) **A-1** in AoCO4. Relative energies (kcal mol^{-1}) were given at the UTPSSh(B2)/MM level with the inclusion of ZPE.

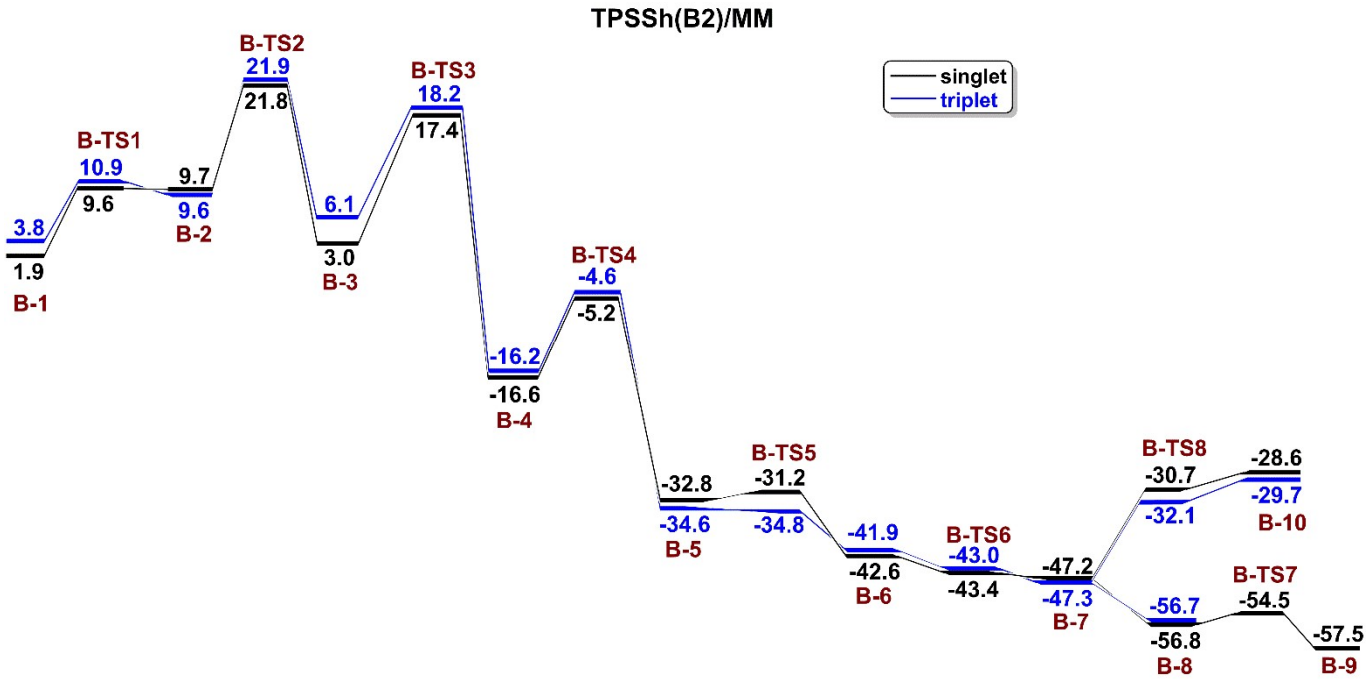

Fig. S7 Energy profile for the catechol oxidation starting from μ-η^2:η^2 peroxo dicopper(II,II) **B-1** in AoCO4. Relative energies (kcal mol^{-1}) were given at the TPSSh(B2)/MM level with the inclusion of ZPE.

Part V. Energies and Spin Densities for all Species

Table S1. Absolute energies (in Hartree) for the species involved in the proton coupled electron transfer from ^{1}**A-1** (using the larger QM region QR2).

species	B3LYP/B1		B3LYP/B2		TPSSh/B2	ZPE
	QM	QM/MM	QM	QM/MM	QM/MM	
^{1}**A-1**	-5521.207177	-5570.779352	-5524.158287	-5573.730462	-5573.759421	0.730131
^{1}**A-TS1**	-5521.182647	-5570.761121	-5524.134613	-5573.715000	-5573.744566	0.721720
^{1}**A-2**	-5521.188719	-5570.775419	-5524.142187	-5573.728887	-5573.753283	0.727482
^{1}**A-TS1'**	-5521.139833	-5570.723182	-5524.088926	-5573.672274	-5573.700791	0.720374
^{1}**A-2'**	-5521.146748	-5570.729644	-5524.096285	-5573.679181	-5573.704196	0.726359

Table S2. Relative energies (in kcal/mol) for the species involved in the proton coupled electron transfer from ^{1}**A-1** (using the larger QM region QR2).

species	**B3LYP/B1**		**B3LYP/B2**		**TPSSh/B2**		**B3LYP(B2) +ZPE**	**TPSSh(B2) +ZPE**
	QM	**QM/MM**	**QM**	**QM/MM**	**QM**	**QM/MM**		
^{1}**A-1**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
^{1}**A-TS1**	15.4	11.4	14.9	9.7	14.5	9.3	4.4	4.0
^{1}**A-2**	11.6	2.5	10.1	1.0	13.0	3.9	-0.7	2.2
^{1}**A-TS1'**	42.3	35.2	43.5	36.5	43.8	36.8	30.4	30.7
^{1}**A-2'**	37.9	31.2	38.9	32.2	41.4	34.7	29.8	32.3

Table S3. Spin density distribution at the B3LYP(B1)/MM level for the species in Table S1.

species	CuA	CuB	O1	O2	Sub	Ser302
^{1}**A-1**	-0.51	0.48	0.04	0.01	0.00	0.00
^{1}**A-TS1**	-0.49	0.23	-0.16	-0.13	0.60	0.00
^{1}**A-2**	-0.43	-0.16	-0.12	-0.23	1.00	0.00
^{1}**A-TS1'**	-0.38	-0.21	-0.26	-0.11	0.48	0.51
^{1}**A-2'**	-0.42	-0.23	-0.23	-0.07	0.02	0.98

Table S4. Absolute energies (in Hartree) for all the species involved in the pathway nascent from **A-1** (using the smaller QM region QR1).

species	B3LYP/B1		B3LYP/B2		TPSSh/B2	ZPE
	QM	QM/MM	QM	QM/MM	QM/MM	
^{1}**A-1**	-5405.547107	-5455.153534	-5408.359540	-5457.965968	-5457.997558	0.684424
^{1}**A-TS1**	-5405.524656	-5455.139213	-5408.335605	-5457.950163	-5457.982752	0.676940
^{1}**A-2**	-5405.536400	-5455.152315	-5408.349526	-5457.965441	-5457.992012	0.683031
^{1}**A-TS2**	-5405.508720	-5455.125190	-5408.325590	-5457.942059	-5457.973437	0.680806
^{1}**A-3**	-5405.539299	-5455.149763	-5408.352227	-5457.962690	-5457.994396	0.682618
^{1}**A-4**	-5405.560238	-5455.160585	-5408.370084	-5457.970431	-5458.001442	0.682581
^{1}**A-TS3**	-5405.556086	-5455.155381	-5408.364231	-5457.963526	-5457.994888	0.678632
^{1}**A-5**	-5405.611494	-5455.209487	-5408.424881	-5458.022874	-5458.044228	0.682327
^{3}**A-1**	-5405.543815	-5455.150175	-5408.355732	-5457.962093	-5457.991816	0.683031
^{3}**A-TS1**	-5405.525495	-5455.140223	-5408.330777	-5457.945504	-5457.982929	0.676890
^{3}**A-2**	-5405.536413	-5455.152328	-5408.349538	-5457.965454	-5457.992024	0.682987
^{3}**A-TS2**	-5405.504811	-5455.121385	-5408.321757	-5457.938331	-5457.969186	0.680871
^{3}**A-3**	-5405.536037	-5455.145857	-5408.348660	-5457.958481	-5457.989247	0.682547
^{3}**A-4**	-5405.557047	-5455.157392	-5408.366549	-5457.966894	-5457.996913	0.682713
^{3}**A-TS3**	-5405.553385	-5455.152742	-5408.361384	-5457.960740	-5457.991577	0.678456
^{3}**A-5**	-5405.611988	-5455.210003	-5408.425007	-5458.023022	-5458.044266	0.682300

Table S5. Absolute energies (in Hartree) for all the species involved in the pathway nascent from **B-1** (using the smaller QM region QR1).

species	B3LYP/B1		B3LYP/B2		TPSSh/B2	ZPE
	QM	QM/MM	QM	QM/MM	QM/MM	
^{1}**B-1**	-5405.545594	-5455.150814	-5408.357503	-5457.962723	-5457.994149	0.684108
^{1}**B-TS1**	-5405.527177	-5455.132539	-5408.337887	-5457.943248	-5457.975762	0.677873
^{1}**B-2**	-5405.535748	-5455.142160	-5408.348529	-5457.954941	-5457.981721	0.683989
^{1}**B-TS2**	-5405.507348	-5455.113893	-5408.321476	-5457.928021	-5457.959649	0.681205
^{1}**B-3**	-5405.544930	-5455.147597	-5408.357723	-5457.960390	-5457.991245	0.682841
^{1}**B-TS3**	-5405.525083	-5455.124874	-5408.335151	-5457.934942	-5457.966926	0.681444
^{1}**B-4**	-5405.594914	-5455.190452	-5408.400888	-5457.996426	-5458.024610	0.684974
^{1}**B-TS4**	-5405.572247	-5455.164945	-5408.376987	-5457.969686	-5458.001817	0.680384
^{1}**B-5**	-5405.622725	-5455.216940	-5408.426543	-5458.020757	-5458.050406	0.685041
^{1}**B-TS5**	-5405.618391	-5455.214664	-5408.423509	-5458.019783	-5458.047963	0.685041
^{1}**B-6**	-5405.629631	-5455.233354	-5408.439987	-5458.043709	-5458.065791	0.684732
^{1}**B-TS6**	-5405.626298	-5455.231366	-5408.436252	-5458.041321	-5458.063168	0.680939
^{1}**B-7**	-5405.629638	-5455.240900	-5408.439270	-5458.050532	-5458.073610	0.685204
^{1}**B-TS7**	-5405.639735	-5455.247460	-5408.447702	-5458.055427	-5458.079126	0.679133
^{1}**B-8**	-5405.648144	-5455.256380	-5408.457327	-5458.065564	-5458.088301	0.684641
^{1}**B-TS8**	-5405.597588	-5455.209967	-5408.406069	-5458.018448	-5458.043536	0.681538
^{1}**B-9**	-5405.644792	-5455.255369	-5408.465422	-5458.075999	-5458.086530	0.681739
^{1}**B-10**	-5405.598647	-5455.210387	-5408.408212	-5458.019952	-5458.043878	0.685191

Continued Table S5

species	B3LYP/B1		B3LYP/B2		TPSSh/B2	ZPE
	QM	QM/MM	QM	QM/MM	QM/MM	
^{3}**B-1**	-5405.543692	-5455.148733	-5408.354931	-5457.959971	-5457.989711	0.682684
^{3}**B-TS1**	-5405.526790	-5455.132032	-5408.337055	-5457.942297	-5457.973451	0.677718
^{3}**B-2**	-5405.535726	-5455.142138	-5408.348506	-5457.954918	-5457.981695	0.683900
^{3}**B-TS2**	-5405.507563	-5455.113557	-5408.321771	-5457.927764	-5457.959363	0.681176
^{3}**B-3**	-5405.541602	-5455.144606	-5408.353486	-5457.956490	-5457.986613	0.683163
^{3}**B-TS3**	-5405.524148	-5455.123774	-5408.334253	-5457.933879	-5457.965583	0.681441
^{3}**B-4**	-5405.594825	-5455.190295	-5408.400472	-5457.995941	-5458.023845	0.684852
^{3}**B-TS4**	-5405.571970	-5455.164713	-5408.376366	-5457.969108	-5458.000901	0.680358
^{3}**B-5**	-5405.624353	-5455.219416	-5408.428155	-5458.023218	-5458.052889	0.684661
^{3}**B-TS5**	-5405.622772	-5455.219339	-5408.426885	-5458.023453	-5458.052600	0.683948
^{3}**B-6**	-5405.628825	-5455.232651	-5408.439098	-5458.042924	-5458.064934	0.684960
^{3}**B-TS6**	-5405.625890	-5455.230960	-5408.435850	-5458.040920	-5458.062684	0.681060
^{3}**B-7**	-5405.629643	-5455.240904	-5408.439277	-5458.050539	-5458.073617	0.685085
^{3}**B-TS8**	-5405.599472	-5455.211642	-5408.407561	-5458.019732	-5458.045349	0.681069
^{3}**B-8**	-5405.648101	-5455.256338	-5408.457290	-5458.065527	-5458.088260	0.684733
^{3}**B-10**	-5405.601065	-5455.212986	-5408.410426	-5458.022347	-5458.046329	0.685904

Table S6. Relative energies (in kcal/mol) for all species (using the smaller QM region QR1).

species	B3LYP/B1		B3LYP/B2		TPSSh/B2		B3LYP(B2) +ZPE	TPSSh(B2) +ZPE
	QM	QM/MM	QM	QM/MM	QM	QM/MM		
^{1}**A-1**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
^{1}**A-TS1**	14.1	9.0	15.0	9.9	14.4	9.3	5.2	4.6
^{1}**A-2**	6.7	0.8	6.3	0.3	9.4	3.5	-0.5	2.6
^{1}**A-TS2**	24.1	17.8	21.3	15.0	21.4	15.1	12.7	12.9
^{1}**A-3**	4.9	2.4	4.6	2.1	4.5	2.0	0.9	0.9
^{1}**A-4**	-8.2	-4.4	-6.6	-2.8	-6.3	-2.4	-4.0	-3.6
^{1}**A-TS3**	-5.6	-1.2	-2.9	1.5	-2.8	1.7	-2.1	-2.0
^{1}**A-5**	-40.4	-35.1	-41.0	-35.7	-34.6	-29.3	-37.0	-30.6
^{3}**A-1**	2.1	2.1	2.4	2.4	3.6	3.6	1.6	2.7
^{3}**A-TS1**	13.6	8.4	18.0	12.8	14.4	9.2	8.1	4.5
^{3}**A-2**	6.7	0.8	6.3	0.3	9.4	3.5	-0.6	2.6
^{3}**A-TS2**	26.5	20.2	23.7	17.3	24.2	17.8	15.1	15.6
^{3}**A-3**	6.9	4.8	6.8	4.7	4.5	5.2	3.5	4.0
^{3}**A-4**	-6.2	-2.4	-4.4	-0.6	-3.4	0.4	-1.7	-0.7
^{3}**A-TS3**	-3.9	0.5	-1.2	3.3	-0.7	3.8	-0.5	0.0
^{3}**A-5**	-40.7	-35.4	-41.1	-35.8	-34.6	-29.3	-37.1	-30.6
^{1}**B-1**	0.9	1.7	1.3	2.0	1.4	2.1	1.8	1.9
^{1}**B-TS1**	12.5	13.2	13.6	14.3	13.0	13.7	10.1	9.6
^{1}**B-2**	7.1	7.1	6.9	6.9	9.9	9.9	6.6	9.7
^{1}**B-TS2**	24.9	24.9	23.9	23.8	23.9	23.8	21.8	21.8
^{1}**B-3**	1.4	3.7	1.1	3.5	1.6	4.0	2.5	3.0
^{1}**B-TS3**	13.8	18.0	15.3	19.5	15.1	19.2	17.6	17.4
^{1}**B-4**	-30.0	-23.2	-25.9	-19.1	-23.8	-17.0	-18.8	-16.6
^{1}**B-TS4**	-15.8	-7.2	-10.9	-2.3	-11.3	-2.7	-4.9	-5.2
^{1}**B-5**	-47.5	-39.8	-42.0	-34.4	-40.8	-33.2	-34.0	-32.8

Continued Table S6

species	B3LYP/B1		B3LYP/B2		TPSSh/B2		B3LYP(B2) +ZPE	TPSSh(B2) +ZPE
	QM	QM/MM	QM	QM/MM	QM	QM/MM		
^{1}**B-TS5**	-44.7	-38.4	-40.1	-33.8	-38.0	-31.6	-33.4	-31.2
^{1}**B-6**	-51.8	-50.1	-50.5	-48.8	-44.5	-42.8	-48.6	-42.6
^{1}**B-TS6**	-49.7	-48.8	-48.1	-47.3	-42.0	-41.2	-49.5	-43.4
^{1}**B-7**	-51.8	-54.8	-50.0	-53.1	-44.7	-47.7	-52.6	-47.2
^{1}**B-TS7**	-58.1	-58.9	-55.3	-56.1	-50.4	-51.2	-59.5	-54.5
^{1}**B-8**	-63.4	-64.5	-61.4	-62.5	-55.8	-56.9	-62.4	-56.8
^{1}**B-TS8**	-31.7	-35.4	-29.2	-32.9	-25.1	-28.9	-34.7	-30.7
^{1}**B-9**	-61.3	-63.9	-66.4	-69.0	-53.2	-55.8	-70.7	-57.5
^{1}**B-10**	-32.3	-35.7	-30.5	-33.9	-25.7	-29.1	-33.4	-28.6
^{3}**B-1**	2.1	3.0	2.9	3.8	4.1	4.9	2.7	3.8
^{3}**B-TS1**	12.7	13.5	14.1	14.9	14.4	15.1	10.6	10.9
^{3}**B-2**	7.1	7.2	6.9	6.9	9.9	10.0	6.6	9.6
^{3}**B-TS2**	24.8	25.1	23.7	24.0	23.7	24.0	21.9	21.9
^{3}**B-3**	3.5	5.6	3.8	5.9	4.7	6.9	5.2	6.1
^{3}**B-TS3**	14.4	18.7	15.9	20.1	15.8	20.1	18.3	18.2
^{3}**B-4**	-29.9	-23.1	-25.7	-18.8	-23.4	-16.5	-18.5	-16.2
^{3}**B-TS4**	-15.6	-7.0	-10.6	-2.0	-10.7	-2.1	-4.5	-4.6
^{3}**B-5**	-48.5	-41.3	-43.1	-35.9	-41.9	-34.7	-35.8	-34.6
^{3}**B-TS5**	-47.5	-41.3	-42.3	-36.1	-40.7	-34.5	-36.4	-34.8
^{3}**B-6**	-51.3	-49.6	-49.9	-48.3	-43.9	-42.3	-48.0	-41.9
^{3}**B-TS6**	-49.4	-48.6	-47.9	-47.0	-41.7	-40.9	-49.1	-43.0
^{3}**B-7**	-51.8	-54.8	-50.0	-53.1	-44.7	-47.7	-52.7	-47.3
^{3}**B-TS8**	-32.9	-36.5	-30.1	-33.7	-26.4	-30.0	-35.8	-32.1
^{3}**B-8**	-63.4	-64.5	-61.3	-62.5	-55.8	-56.9	-62.3	-56.7
^{3}**B-10**	-33.9	-37.3	-31.9	-35.4	-27.2	-30.6	-34.4	-29.7

Table S7. Spin density distribution for all species at the B3LYP(B1)/MM level (using the smaller QM region QR1).

species	CuA	CuB	O1	O2	Sub
^{1}**A-1**	-0.51	0.48	0.04	0.02	0.00
^{1}**A-TS1**	-0.49	0.25	-0.15	-0.12	0.56
^{1}**A-2**	-0.42	-0.17	-0.11	-0.23	1.00
^{1}**A-TS2**	-0.57	0.45	-0.52	-0.32	1.00
^{1}**A-3**	-0.59	0.59	-0.21	-0.78	1.00
^{1}**A-4**	-0.60	0.61	-0.22	-0.75	1.01
^{1}**A-TS3**	-0.62	0.63	-0.39	-0.60	1.01
^{1}**A-5**	-0.65	0.63	0.04	0.01	0.00
^{3}**A-1**	0.49	0.44	0.41	0.48	0.00
^{3}**A-TS1**	0.47	0.28	0.26	0.31	0.57
^{3}**A-2**	0.42	0.17	0.11	0.23	0.99
^{3}**A-TS2**	0.64	0.48	-0.33	0.02	1.00
^{3}**A-3**	0.65	0.63	-0.04	-0.49	1.00
^{3}**A-4**	0.67	0.65	-0.09	-0.52	1.00
^{3}**A-TS3**	0.68	0.67	-0.23	-0.41	0.98
^{3}**A-5**	0.64	0.63	0.24	0.27	-0.01
^{1}**B-1**	-0.51	0.47	0.01	0.06	0.00
^{1}**B-TS1**	-0.51	0.29	-0.15	-0.09	0.53
^{1}**B-2**	-0.44	-0.13	-0.13	-0.22	1.00
^{1}**B-TS2**	-0.60	0.38	-0.48	-0.22	1.01
^{1}**B-3**	-0.61	0.61	-0.16	-0.82	1.00
^{1}**B-TS3**	-0.62	0.60	0.03	-0.67	0.69
^{1}**B-4**	-0.63	0.62	0.02	0.00	0.00
^{1}**B-TS4**	-0.54	0.63	0.01	-0.07	-0.07
^{1}**B-5**	-0.54	0.50	-0.05	-0.10	0.24
^{1}**B-TS5**	-0.55	0.28	-0.11	-0.06	0.54
^{1}**B-6**	-0.27	-0.43	-0.14	0.14	0.80

Continued Table S7

species	CuA	CuB	O1	O2	Sub
^{1}**B-TS6**	-0.28	-0.44	-0.14	0.11	0.86
^{1}**B-7**	-0.44	-0.30	-0.15	0.07	0.93
^{1}**B-TS7**	-0.38	-0.25	-0.08	0.11	0.68
^{1}**B-8**	-0.47	-0.29	-0.14	0.07	0.93
^{1}**B-TS8**	-0.66	0.53	0.07	0.01	0.10
^{1}**B-9**	0.00	0.00	0.00	0.00	0.00
^{1}**B-10**	-0.65	0.54	0.12	0.01	0.02
^{3}**B-1**	0.48	0.44	0.43	0.47	0.00
^{3}**B-TS1**	0.50	0.32	0.23	0.28	0.54
^{3}**B-2**	0.44	0.13	0.13	0.22	0.99
^{3}**B-TS2**	0.62	0.40	-0.20	0.00	1.00
^{3}**B-3**	0.65	0.64	0.05	-0.60	1.00
^{3}**B-TS3**	0.62	0.60	0.29	-0.44	0.69
^{3}**B-4**	0.63	0.62	0.29	0.18	0.02
^{3}**B-TS4**	0.55	0.63	0.27	0.23	0.05
^{3}**B-5**	0.49	0.49	0.20	0.14	0.47
^{3}**B-TS5**	0.46	0.46	0.19	0.14	0.56
^{3}**B-6**	0.28	0.45	0.15	0.17	0.83
^{3}**B-TS6**	0.29	0.45	0.15	0.12	0.87
^{3}**B-7**	0.44	0.30	0.16	0.07	0.93
^{3}**B-TS8**	0.64	0.54	0.42	0.02	0.13
^{3}**B-8**	0.47	0.29	0.14	0.07	0.92
^{3}**B-10**	0.63	0.56	0.55	0.01	0.02

Part VI. Yamaguchi Spin Projection

For the dinuclear complex, the exchange coupling constant *J* is often used to describe the difference in energy between the high spin and broken symmetry (BS) state energies. This approach has been initiated by Noodleman. Positive value of *J* corresponds to ferromagnetic, while negative value corresponds to anti-ferromagnetic coupling. Since the broken symmetry approach to calculate the open-shell singlet species can results in spin contamination from higher spin states, the expression for J must account for spin contamination. Here, we used a formalism by Yamaguchi and coworkers to the calculate the *J* values for the diradical species. The formalism is given as $J = (E^{singlet} - E^{triplet})/[\langle S^2\rangle^{triplet} - \langle S^2\rangle^{singlet}]$. $E^{singlet}$ and $E^{triplet}$ are the energies of broken-symmetry singlet state and triplet state (B3LYP(B2)/MM values), while $\langle S^2\rangle^{singlet}$ and $\langle S^2\rangle^{triplet}$ are the calculated spin expectation values for the singlet and triplet spin states, respectively. Furthermore, the Yamaguchi's spin projected method was applied to calculate the ground state energy for the diradical species as shown below: $E_0 = E^{singlet} + a(E^{singlet} - E^{triplet})$, $a = \langle S^2\rangle^{singlet}/[\langle S^2\rangle^{triplet} - \langle S^2\rangle^{singlet}]$. The results are listed in Table S8. For some species having the tetraradical character, the Yamaguchi spin projection is not suitable to correct its energy. Although the difference in the absolute energies of the ground state caused by spin projection is about 0-3 kcal/mol, the differences in the calculated reaction barriers are within 1 kcal/mol.

Reference

1. L. Noodleman, *J. Chem. Phys.*, 1981, **74**, 5737-5743.
2. K. Yamaguchi, F. Jensen, A. Dorigo and K. N. Houk, *Chem. Phys. Lett.*, 1988, **149**, 537-542.

Table S8. Spin contamination for the biradical species, exchange coupling constant *J*, spin-corrected ground state energies (E_0), and the energy difference caused by spin projection.

species	$<S^2>^{singlet}$	$<S^2>^{triplet}$	*J* (kcal/mol)	E_0(Hartree)	ΔE(kcal/mol)
A-1	0.823327	2.010424	-2.0	-5457.968656	-1.7
A-TS1	0.957935	2.011384	-2.8	-5457.954300	-2.6
A-2	1.018952	2.019070	0.0	-5457.965428	0.0
A-TS2	1.589619	2.670530	-	-	-
A-3	1.790179	2.836299	-	-	-
A-4	1.795918	2.825602	-	-	-
A-TS3	1.816715	2.804243	-	-	-
A-5	0.994142	2.005313	0.1	-5458.022728	0.1
B-1	0.852736	2.010678	-1.5	-5457.964750	-1.3
B-TS1	0.919703	2.011177	-0.5	-5457.944049	-0.5
B-2	1.018443	2.019896	0.0	-5457.954964	0.0
B-TS2	1.581258	2.571498	-	-	-
B-3	1.855060	2.875878	-	-	-
B-TS3	1.716666	2.717915	-	-	-
B-4	0.981858	2.005274	-0.3	-5457.996891	-0.3
B-TS4	0.972919	2.006100	-0.4	-5457.970230	-0.3
B-5	1.006264	2.008910	1.5	-5458.018287	1.5
B-TS5	1.007694	2.010853	2.3	-5458.016096	2.3
B-6	0.959133	2.014824	-0.5	-5458.044422	-0.4
B-TS6	0.996229	2.018100	-0.2	-5458.041712	-0.2
B-7	1.021868	2.022422	0.0	-5458.050525	0.0
B-8	1.019629	2.021815	0.0	-5458.065602	0.0
B-TS8	0.999584	2.007156	0.8	-5458.017174	0.8
B-10	1.001459	2.008342	1.5	-5458.017570	1.5

Part VII. Cartesian Coordinates of the QM Region of all Species

^{1}**A-1** (QR2)

C	-8.7027739	-2.2120036	-7.7718161
H	-8.4715558	-2.8805537	-6.9291917
H	-8.5103856	-2.7873417	-8.6932395
C	-7.7999647	-1.0130691	-7.6982454
N	-7.4261579	-0.2659897	-8.7977771
H	-7.6835547	-0.4464272	-9.7751589
C	-6.5807197	0.7065982	-8.4116773
H	-6.1461865	1.4375632	-9.0946122
N	-6.3811993	0.6327047	-7.0976797
C	-7.1340391	-0.4303670	-6.6434897
H	-7.1596956	-0.7086004	-5.5979975
C	-7.5818441	7.2492806	-6.0009297
H	-8.3110566	7.6275086	-6.7298528
H	-6.6553830	7.8281494	-6.1497620
C	-7.3285420	5.8068839	-6.2849798
N	-8.1914752	5.0462180	-7.0483269
H	-9.1014643	5.3595362	-7.3970757
C	-7.6744803	3.8023900	-7.1687234
H	-8.1532125	3.0102378	-7.7417952
N	-6.5261687	3.7168847	-6.5146591
C	-6.2936721	4.9598134	-5.9712778
H	-5.3908929	5.1748518	-5.4061737
C	-4.4056741	1.0948926	-0.5218790
H	-4.2447751	1.9566015	0.1455553
H	-3.4293030	0.6183803	-0.7005305
C	-4.9680178	1.5023018	-1.8554395
N	-5.9235038	2.4835978	-2.0240253
H	-6.2681848	3.0858002	-1.2709211
C	-6.2463334	2.5572157	-3.3314442
H	-6.9691449	3.2615393	-3.7349280
N	-5.5445827	1.6753058	-4.0305736
C	-4.7455312	1.0099989	-3.1244764
H	-4.0600830	0.2206124	-3.4241246
C	1.2548864	7.1780094	-4.2937446
H	1.3349116	7.0960329	-3.1993180
H	1.0788174	8.2368901	-4.5229217
C	0.1354291	6.3407482	-4.8347320
N	-0.8783148	6.8499578	-5.6248510
H	-1.0037222	7.8240988	-5.8859854
C	-1.6511781	5.8237590	-6.0540575
H	-2.5071221	5.9345476	-6.7229273
N	-1.1892518	4.6771197	-5.5815055
C	-0.0840127	4.9812940	-4.8207600
H	0.5094297	4.2089309	-4.3349053
C	2.0670364	4.1212736	-10.2084539
H	2.1121803	5.1605903	-9.8554816
H	1.6266682	4.1613966	-11.2203416
C	1.1142025	3.3439182	-9.3556373
N	0.3935691	2.2833139	-9.8698950
H	0.4733697	1.9276115	-10.8197969
C	-0.5184189	1.8867344	-8.9613357
H	-1.2946576	1.1635754	-9.1907166
N	-0.4101795	2.6135807	-7.8577603
C	0.6007486	3.5293003	-8.0927873
H	0.8464185	4.2957036	-7.3661282
C	-1.9355898	0.2572511	-11.7562305
H	-0.9777155	0.0701703	-11.2349728
H	-1.6956597	0.7740098	-12.6972765
O	-2.7736302	1.0504591	-10.9334846
H	-3.2326154	1.6674669	-11.5345039
C	0.0862381	-0.9407821	-2.1997657
H	0.1262346	-1.8992042	-2.7344204
H	-0.5654383	-1.0788580	-1.3216179
C	-0.4888628	0.1496901	-3.0563704
N	-1.1034550	1.2523897	-2.4791377
H	-1.2377565	1.4019376	-1.4849229
C	-1.4790059	2.1011199	-3.4628173
H	-2.0022484	3.0380064	-3.2860117
N	-1.1384144	1.6165858	-4.6432220
C	-0.5168595	0.4051619	-4.4092072
H	-0.1461933	-0.2212741	-5.2167126
Cu	-5.3181960	1.9818343	-6.0778183
Cu	-1.7458633	2.7379649	-6.3496868
O	-3.6118098	2.6757906	-7.2125356
O	-3.6730603	3.0251270	-5.8412576
C	-2.7293494	4.2117240	-10.1304751
C	-3.2616171	5.2901120	-9.4267956
C	-3.1344291	6.6008078	-9.9280775
C	-2.4734891	6.8162233	-11.1377799
C	-1.9312674	5.7307631	-11.8385943

C	-2.0536261	4.4349449	-11.3361611
O	-3.6716492	7.6336153	-9.2190802
H	-4.2124901	7.2325493	-8.5205080
H	-2.4147347	7.8340285	-11.5296974
H	-1.4410020	5.8898707	-12.7970882
H	-1.6619643	3.5882388	-11.9019419
H	-2.8693772	3.1989276	-9.7537541
O	-3.9203136	5.1823946	-8.2330307
H	-3.9569403	4.2386811	-7.9443053
H	-9.7722301	-2.0066390	-7.7253904
H	-7.9712339	7.4814361	-5.0096951
H	-5.0403182	0.3740235	-0.0064752
H	2.2245954	6.9095480	-4.7128620
H	3.0823954	3.7302270	-10.2732228
H	-2.3553054	-0.7090173	-12.0359278
H	1.0883521	-0.6731109	-1.8648236

^{1}**TS$_{1A\text{-}2A}$** (QR2)

C	-8.7179634	-2.1692964	-7.7715254
H	-8.4785098	-2.8325318	-6.9267834
H	-8.5276907	-2.7505954	-8.6896992
C	-7.8156340	-0.9683457	-7.7147562
N	-7.3975395	-0.2750326	-8.8326172
H	-7.6407937	-0.4793227	-9.8081751
C	-6.5448533	0.6986492	-8.4596553
H	-6.0620671	1.3809291	-9.1598866
N	-6.3875498	0.6816059	-7.1401466
C	-7.1732472	-0.3469786	-6.6664683
H	-7.2387840	-0.5750367	-5.6105103
C	-7.5720471	7.3315341	-6.0046691
H	-8.3088540	7.7055595	-6.7278414
H	-6.6534941	7.9236038	-6.1513112
C	-7.3015402	5.8943733	-6.2940967
N	-8.1636308	5.1191913	-7.0428985
H	-9.0799519	5.4184932	-7.3870158
C	-7.6342789	3.8774565	-7.1520190
H	-8.1074118	3.0743439	-7.7154602
N	-6.4827905	3.8085847	-6.5053308
C	-6.2566016	5.0581746	-5.9797003
H	-5.3593301	5.2869235	-5.4092787
C	-4.3905149	1.1079677	-0.5887186
H	-4.2217443	1.9679161	0.0798222
H	-3.4169935	0.6291296	-0.7737971
C	-4.9451246	1.5323930	-1.9217909
N	-5.8996640	2.5168190	-2.0813897
H	-6.2604851	3.0976708	-1.3195968
C	-6.1825221	2.6397891	-3.3958165
H	-6.8992913	3.3533880	-3.7934285
N	-5.4555534	1.7902410	-4.1083326
C	-4.6850592	1.0895654	-3.2033041
H	-3.9888078	0.3161177	-3.5191448
C	1.2220477	7.1416213	-4.2182027
H	1.3469422	7.1002929	-3.1260249
H	1.0045951	8.1858428	-4.4771533
C	0.1200180	6.2409105	-4.6914091
N	-0.9472994	6.6715782	-5.4559572
H	-1.1470537	7.6335551	-5.7131112
C	-1.6634598	5.5853149	-5.8474716
H	-2.5493403	5.6283436	-6.4817358
N	-1.1115475	4.4804948	-5.3780802
C	-0.0113934	4.8701790	-4.6559079
H	0.6423541	4.1462207	-4.1718132
C	2.2425906	3.6870745	-10.2771820
H	2.1141539	4.7704866	-10.1403048
H	1.7324153	3.4223824	-11.2225693
C	1.5691018	2.9627618	-9.1576614
N	1.6608681	1.6002175	-8.9428268
H	2.2776438	0.9608634	-9.4398449
C	0.7942062	1.2615832	-7.9619741
H	0.7037822	0.2519922	-7.5722501
N	0.1336566	2.3265206	-7.5312982
C	0.6168267	3.3930201	-8.2637236
H	0.2468578	4.4046296	-8.1262362
C	-2.0491352	0.2917535	-11.6989772
H	-1.1557131	0.1526043	-11.0626931
H	-1.7039101	0.7864452	-12.6215318
O	-3.0009315	1.0877657	-11.0175409
H	-3.3325097	1.7265032	-11.6766022
C	0.1471627	-1.1098193	-1.9780822
H	0.1921237	-2.0812738	-2.4887452
H	-0.4735767	-1.2259677	-1.0754510
C	-0.4613168	-0.0523554	-2.8439267
N	-1.0432414	1.0794445	-2.2922465
H	-1.1588022	1.2632603	-1.3013368
C	-1.4100998	1.9063798	-3.3018685
H	-1.9027169	2.8644292	-3.1523242

N	-1.0982781	1.3741999	-4.4670802
C	-0.5063359	0.1583317	-4.2014236
H	-0.1608664	-0.5057987	-4.9894826
Cu	-5.2348615	2.0474809	-6.1671401
Cu	-1.4206989	2.4985412	-6.2096480
O	-3.8235623	2.5914092	-7.5635772
O	-3.4035645	2.8614140	-6.2294789
C	-2.3484192	3.8689662	-10.1693249
C	-3.1388862	4.9017454	-9.6138606
C	-3.2332518	6.1631874	-10.3115661
C	-2.5353936	6.3721600	-11.5035033
C	-1.7727892	5.3288033	-12.0295573
C	-1.6852191	4.0840645	-11.3658795
O	-4.0248139	7.1000146	-9.7750529
H	-4.4552724	6.6690710	-9.0103509
H	-2.6297704	7.3268887	-12.0239539
H	-1.2583212	5.4578598	-12.9811712
H	-1.1101333	3.2771818	-11.8240667
H	-2.3292639	2.8941525	-9.6843048
O	-3.8118112	4.8157179	-8.4933551
H	-3.8837436	3.7181472	-8.0576306
H	-9.7887474	-1.9720567	-7.7206856
H	-7.9612437	7.5496665	-5.0101789
H	-5.0188153	0.3885217	-0.0636447
H	2.1802018	6.8820182	-4.6683289
H	3.3056553	3.4742906	-10.3898008
H	-2.4165259	-0.6857853	-12.0112407
H	1.1535397	-0.8094551	-1.6864436

^{1}**A-2** (QR2)

C	-8.7458209	-2.2415153	-7.7729952
H	-8.5119533	-2.9052892	-6.9271301
H	-8.5557054	-2.8228668	-8.6911040
C	-7.8465090	-1.0416670	-7.7070061
N	-7.4739794	-0.2968495	-8.8074587
H	-7.7131372	-0.4710266	-9.7897962
C	-6.6337738	0.6797410	-8.4144754
H	-6.1857233	1.4004798	-9.0975484
N	-6.4406321	0.6163759	-7.1020917
C	-7.1877993	-0.4494574	-6.6525553
H	-7.2138149	-0.7278289	-5.6073760
C	-7.5281192	7.2916457	-5.9892876
H	-8.2453433	7.6811165	-6.7246512
H	-6.5985526	7.8708775	-6.1153009
C	-7.2716859	5.8530791	-6.2888463
N	-8.1494311	5.0903563	-7.0329394
H	-9.0693447	5.3967423	-7.3623948
C	-7.6281639	3.8479213	-7.1656539
H	-8.1181350	3.0518556	-7.7246768
N	-6.4644116	3.7660294	-6.5415903
C	-6.2248932	5.0084731	-6.0024871
H	-5.3166693	5.2248817	-5.4447903
C	-4.3701746	1.1059017	-0.5121002
H	-4.2139252	1.9602126	0.1665604
H	-3.3931775	0.6289549	-0.6837442
C	-4.9061247	1.5350137	-1.8493643
N	-5.8554090	2.5216512	-2.0177938
H	-6.2207421	3.1045049	-1.2599583
C	-6.1327467	2.6357652	-3.3344034
H	-6.8485637	3.3473893	-3.7376813
N	-5.4076909	1.7782613	-4.0377836
C	-4.6432126	1.0822057	-3.1265442
H	-3.9485020	0.3036526	-3.4330302
C	1.2112852	7.1401584	-4.2189207
H	1.3414049	7.0900423	-3.1277128
H	1.0052752	8.1889210	-4.4685902
C	0.0909278	6.2607439	-4.6872931
N	-0.9579477	6.7115762	-5.4654017
H	-1.1249072	7.6746954	-5.7403342
C	-1.7074528	5.6406158	-5.8390980
H	-2.5812235	5.7060719	-6.4877507
N	-1.1967969	4.5277533	-5.3449168
C	-0.0863911	4.8963194	-4.6253502
H	0.5415531	4.1605439	-4.1255475
C	2.1962038	3.7119835	-10.2952342
H	2.0820933	4.7976901	-10.1626477
H	1.7004444	3.4521516	-11.2497678
C	1.4940893	2.9986985	-9.1853379
N	1.5568890	1.6336519	-8.9805965
H	2.1592966	0.9844000	-9.4814192
C	0.6840513	1.3087451	-7.9985087
H	0.5772589	0.2994216	-7.6133920
N	0.0475143	2.3820146	-7.5578886
C	0.5506041	3.4416874	-8.2862997
H	0.2067342	4.4611756	-8.1351883
C	-1.9797289	0.3231141	-11.6246412

H	-0.9822472	0.1726867	-11.1762326
H	-1.8359153	0.9286883	-12.5356482
O	-2.8079231	0.9754739	-10.6772627
H	-3.3970573	1.5660185	-11.1684227
C	0.1476053	-1.0976372	-1.9683061
H	0.1859627	-2.0603421	-2.4957778
H	-0.4664268	-1.2276249	-1.0629202
C	-0.4669805	-0.0240946	-2.8096837
N	-1.0313645	1.1037852	-2.2321934
H	-1.1298596	1.2739522	-1.2371643
C	-1.4071669	1.9477465	-3.2257132
H	-1.8922790	2.9060453	-3.0541105
N	-1.1181529	1.4311769	-4.4031223
C	-0.5323146	0.2068048	-4.1631475
H	-0.2067489	-0.4502497	-4.9660297
Cu	-5.3045538	1.9923555	-6.1190521
Cu	-1.4492958	2.5453558	-6.1472465
O	-3.7747264	2.6540307	-7.6987790
O	-3.4750809	2.7186128	-6.2995831
C	-2.4135960	4.0663997	-10.2832263
C	-3.1043869	5.1868877	-9.7087889
C	-3.1703906	6.4312794	-10.4856797
C	-2.5723028	6.5308916	-11.7429209
C	-1.9189123	5.4110528	-12.2549414
C	-1.8387113	4.1901861	-11.5245197
O	-3.8401456	7.4273327	-9.9185668
H	-4.1712758	7.0492467	-9.0729005
H	-2.6471079	7.4583522	-12.3131915
H	-1.4747794	5.4527146	-13.2492436
H	-1.3343382	3.3381995	-11.9834379
H	-2.3808859	3.1231508	-9.7366281
O	-3.6714596	5.1983705	-8.5725429
H	-3.8652999	3.6153877	-7.9560486
H	-9.8146810	-2.0340909	-7.7222042
H	-7.9318789	7.5137663	-5.0015088
H	-5.0115164	0.3826215	-0.0085002
H	2.1655918	6.8750014	-4.6739561
H	3.2579555	3.4844941	-10.3900940
H	-2.3534067	-0.6431183	-11.9635015
H	1.1567509	-0.8041028	-1.6792919

^{1}**TS$_{1A\text{-}2A'}$** (QR2)

C	-8.6741853	-2.2749919	-7.8035168
H	-8.4433013	-2.9414938	-6.9590250
H	-8.5159653	-2.8634739	-8.7235319
C	-7.7388879	-1.1009737	-7.7574163
N	-7.4193742	-0.3276404	-8.8543092
H	-7.7293106	-0.4614390	-9.8227548
C	-6.5315825	0.6164538	-8.4864817
H	-6.1001870	1.3380805	-9.1781420
N	-6.2524007	0.5068869	-7.1947173
C	-6.9947609	-0.5601739	-6.7315078
H	-6.9528333	-0.8845741	-5.6984815
C	-7.5187139	7.2472115	-6.0153225
H	-8.2565026	7.6074255	-6.7454451
H	-6.6061164	7.8479400	-6.1638918
C	-7.2300009	5.8098168	-6.3013813
N	-8.0771330	5.0285084	-7.0610223
H	-8.9947985	5.3205376	-7.4088711
C	-7.5306123	3.7960370	-7.1833867
H	-7.9951046	2.9928894	-7.7540832
N	-6.3768634	3.7342884	-6.5359238
C	-6.1728982	4.9842479	-5.9945903
H	-5.2827320	5.2227327	-5.4166676
C	-4.3200283	1.1252038	-0.4708143
H	-4.1745747	1.9657479	0.2273389
H	-3.3416233	0.6424145	-0.6202472
C	-4.8082424	1.5875111	-1.8150900
N	-5.7339851	2.5937397	-1.9930528
H	-6.1225854	3.1611364	-1.2348692
C	-5.9540711	2.7521283	-3.3151063
H	-6.6503723	3.4805391	-3.7226039
N	-5.2128813	1.9055976	-4.0165377
C	-4.5017735	1.1673273	-3.0938920
H	-3.8106158	0.3846772	-3.3955076
C	1.1136807	6.9706176	-4.3101075
H	1.2148307	6.8767008	-3.2190712
H	0.8823750	8.0253065	-4.5152160
C	0.0310595	6.0754557	-4.8490756
N	-0.9851924	6.5245528	-5.6705835
H	-1.1571306	7.4908592	-5.9316515
C	-1.6923143	5.4507450	-6.1102770
H	-2.5271024	5.5222561	-6.8082139
N	-1.1898421	4.3320246	-5.6179789

C	-0.1230116	4.7051963	-4.8315377
H	0.4969891	3.9699620	-4.3209486
C	2.2493470	3.6417988	-10.3396998
H	2.1148242	4.7106680	-10.1196888
H	1.7685540	3.4553595	-11.3183489
C	1.5361815	2.8294143	-9.3106397
N	1.5330458	1.4480838	-9.2718344
H	2.1045870	0.8327051	-9.8485672
C	0.6397881	1.0487246	-8.3351474
H	0.4701895	0.0028324	-8.0942966
N	0.0565567	2.0937541	-7.7662871
C	0.6154132	3.2069747	-8.3614499
H	0.3153469	4.2176189	-8.0988251
C	-2.6561960	0.4685963	-10.7576932
H	-1.5729394	0.5867683	-10.5068124
H	-2.8467143	1.3234419	-11.4560912
O	-3.4427460	0.5376000	-9.6351228
H	-3.4379244	1.5444818	-8.8357257
C	0.1532399	-1.1198999	-2.0019054
H	0.2011049	-2.0994082	-2.4964482
H	-0.4734015	-1.2214723	-1.1011041
C	-0.4556794	-0.0833940	-2.8918036
N	-0.9709120	1.0952617	-2.3712142
H	-1.0352389	1.3316442	-1.3870271
C	-1.3702631	1.8778323	-3.4023458
H	-1.8277394	2.8557002	-3.2763311
N	-1.1433083	1.2751675	-4.5532512
C	-0.5749114	0.0536800	-4.2539053
H	-0.2993730	-0.6668486	-5.0195571
Cu	-5.2547095	1.9480301	-6.1164771
Cu	-1.4532967	2.2673047	-6.3531680
O	-3.4061178	2.1311195	-6.8059250
O	-3.5551736	2.4619576	-8.1663206
C	-2.0986192	3.9370337	-10.5025987
C	-2.9076167	4.9614047	-9.9991104
C	-3.0842389	6.1613787	-10.7590790
C	-2.4702571	6.3006859	-12.0119191
C	-1.7135082	5.2487406	-12.5151157
C	-1.5184180	4.0707466	-11.7589339
O	-3.8723643	7.1218604	-10.2588674
H	-4.2800658	6.7592843	-9.4510915
H	-2.6358637	7.2138859	-12.5851803
H	-1.2760422	5.3163577	-13.5101326
H	-0.9246402	3.2574900	-12.1805771
H	-1.9572119	3.0415471	-9.9027362
O	-3.5647654	4.9184928	-8.8317697
H	-3.6317696	3.9523679	-8.5016796
H	-9.7388156	-2.0505666	-7.7382323
H	-7.9151413	7.4756507	-5.0260160
H	-4.9810069	0.4002001	0.0040998
H	2.0869357	6.7496495	-4.7483018
H	3.3158660	3.4359176	-10.4303458
H	-2.7713934	-0.4414155	-11.3464839
H	1.1571577	-0.8149922	-1.7065296

^{1}**A-2′** (QR2)

C	-8.6699975	-2.2680275	-7.8055452
H	-8.4313935	-2.9311519	-6.9608038
H	-8.5067407	-2.8548896	-8.7257039
C	-7.7489013	-1.0818850	-7.7581663
N	-7.4645264	-0.2805393	-8.8442728
H	-7.7788313	-0.4160241	-9.8112578
C	-6.5853176	0.6721266	-8.4763903
H	-6.2056058	1.4345987	-9.1572255
N	-6.2761462	0.5375952	-7.1927233
C	-6.9910166	-0.5518614	-6.7366366
H	-6.9224843	-0.8985848	-5.7118191
C	-7.5603298	7.2393092	-6.0071546
H	-8.2952139	7.6039750	-6.7375249
H	-6.6393453	7.8248834	-6.1636308
C	-7.2950726	5.7952972	-6.2770374
N	-8.1424604	5.0228846	-7.0450814
H	-9.0488368	5.3278328	-7.4112902
C	-7.6241767	3.7770049	-7.1369631
H	-8.0944332	2.9757673	-7.7048585
N	-6.4884261	3.6985802	-6.4591646
C	-6.2655903	4.9519776	-5.9325777
H	-5.3810553	5.1812673	-5.3430926
C	-4.3226967	1.1362247	-0.4484349
H	-4.1760887	1.9730079	0.2538889
H	-3.3443526	0.6566682	-0.6071587
C	-4.8227011	1.6021272	-1.7864228
N	-5.7663522	2.5937023	-1.9512032
H	-6.1550933	3.1528165	-1.1868665

C	-6.0053551	2.7531453	-3.2681167
H	-6.7178713	3.4701814	-3.6671096
N	-5.2577178	1.9204138	-3.9795367
C	-4.5229923	1.1903767	-3.0688877
H	-3.8247448	0.4181982	-3.3809163
C	1.1191925	7.0125676	-4.3002764
H	1.2186475	6.9141966	-3.2096664
H	0.9035482	8.0702742	-4.5047257
C	0.0229253	6.1369361	-4.8403049
N	-0.9396852	6.5877283	-5.7230436
H	-1.0606019	7.5465566	-6.0364726
C	-1.6672361	5.5260557	-6.1541187
H	-2.4617296	5.6007996	-6.9011149
N	-1.2285394	4.4099055	-5.5940440
C	-0.1821710	4.7758512	-4.7751305
H	0.3901404	4.0418911	-4.2104709
C	2.2019574	3.6661668	-10.3431005
H	2.0694431	4.7407835	-10.1529057
H	1.7225157	3.4575103	-11.3179403
C	1.4841901	2.8836226	-9.2927421
N	1.5069018	1.5046556	-9.1965309
H	2.1043698	0.8805117	-9.7361159
C	0.6129403	1.1261524	-8.2518369
H	0.4716537	0.0899649	-7.9565652
N	0.0028946	2.1823032	-7.7322438
C	0.5449807	3.2811864	-8.3693396
H	0.2188405	4.2950065	-8.1561385
C	-2.4326805	0.4275222	-10.9906884
H	-1.3479720	0.5556686	-10.7695006
H	-2.6238589	1.2856496	-11.6909568
O	-3.1880948	0.6333068	-9.8840160
H	-3.4571298	1.8249523	-8.6136202
C	0.1543696	-1.1127267	-2.0101339
H	0.2012989	-2.0839643	-2.5207455
H	-0.4690550	-1.2293996	-1.1090935
C	-0.4595096	-0.0613973	-2.8795403
N	-0.9746298	1.1065103	-2.3353203
H	-1.0294105	1.3264348	-1.3465099
C	-1.3799369	1.9074995	-3.3498158
H	-1.8389580	2.8820786	-3.2032833
N	-1.1582318	1.3260585	-4.5128827
C	-0.5860938	0.1001257	-4.2385254
H	-0.3126912	-0.6062293	-5.0183854
Cu	-5.3292232	1.9617989	-6.0540570
Cu	-1.4849363	2.3709124	-6.2861371
O	-3.4516177	2.1202942	-6.6909692
O	-3.7249290	2.5661409	-8.0149393
C	-2.2332656	4.1373316	-10.4145160
C	-2.9524187	5.2181547	-9.9039109
C	-3.0508552	6.4160755	-10.6393769
C	-2.4448734	6.5040644	-11.8948416
C	-1.7525873	5.4046386	-12.4151201
C	-1.6381576	4.2263316	-11.6772209
O	-3.7545231	7.4582179	-10.1243128
H	-4.1882616	7.1237115	-9.3229194
H	-2.5500058	7.4277568	-12.4666716
H	-1.3165260	5.4564823	-13.4117453
H	-1.1067161	3.3706788	-12.0988518
H	-2.1578051	3.2247753	-9.8250843
O	-3.6008527	5.2110801	-8.6908442
H	-3.7842247	4.2827087	-8.4271538
H	-9.7365745	-2.0532459	-7.7395996
H	-7.9498421	7.4764171	-5.0171412
H	-4.9816057	0.4069923	0.0228669
H	2.0894066	6.7789434	-4.7386495
H	3.2679979	3.4541634	-10.4248241
H	-2.6194409	-0.4961006	-11.5385094
H	1.1589241	-0.8117152	-1.7129323

^{1}A-1

C	-8.6902805	-2.2072567	-7.7698392
H	-8.4605553	-2.8752068	-6.9263554
H	-8.4980532	-2.7836592	-8.6906587
C	-7.7863626	-1.0088730	-7.6957453
N	-7.4168491	-0.2569108	-8.7936421
H	-7.6755222	-0.4342608	-9.7714217
C	-6.5717444	0.7152826	-8.4058377
H	-6.1451672	1.4537683	-9.0854550
N	-6.3675598	0.6364294	-7.0927880
C	-7.1172916	-0.4298811	-6.6406853
H	-7.1393160	-0.7131474	-5.5964009
C	-7.5775673	7.2499550	-6.0043670
H	-8.3077998	7.6269496	-6.7329565
H	-6.6524120	7.8309277	-6.1525608
C	-7.3199484	5.8086286	-6.2899366
N	-8.1891772	5.0417586	-7.0397260

H	-9.1039383	5.3511212	-7.3798117
C	-7.6685130	3.7996473	-7.1623557
H	-8.1516400	3.0032474	-7.7256459
N	-6.5111417	3.7212460	-6.5234461
C	-6.2766694	4.9673530	-5.9876114
H	-5.3685678	5.1876684	-5.4330199
C	-4.4084676	1.1038526	-0.5148173
H	-4.2515773	1.9651119	0.1541336
H	-3.4303793	0.6300179	-0.6909948
C	-4.9667940	1.5114321	-1.8501165
N	-5.9258385	2.4885288	-2.0223781
H	-6.2767356	3.0881895	-1.2701036
C	-6.2410370	2.5636259	-3.3316038
H	-6.9651926	3.2649901	-3.7377123
N	-5.5308989	1.6867728	-4.0286978
C	-4.7343650	1.0232684	-3.1189141
H	-4.0428597	0.2380565	-3.4150342
C	1.2651839	7.1930731	-4.2699518
H	1.3501230	7.1157082	-3.1757247
H	1.0929277	8.2513264	-4.5040253
C	0.1396982	6.3599574	-4.8030940
N	-0.8767809	6.8732299	-5.5873907
H	-1.0009282	7.8487886	-5.8439274
C	-1.6530142	5.8501240	-6.0173964
H	-2.5049505	5.9602826	-6.6918541
N	-1.1894596	4.7017152	-5.5494744
C	-0.0810411	5.0011200	-4.7920043
H	0.5144991	4.2259926	-4.3134424
C	2.0771063	4.0911758	-10.2273288
H	2.1014780	5.1478440	-9.9296641
H	1.6189584	4.0620762	-11.2323136
C	1.1714199	3.3327289	-9.3115801
N	0.6180129	2.1209972	-9.6783189
H	0.8186116	1.6234869	-10.5420062
C	-0.2875148	1.7551237	-8.7497351
H	-0.9291219	0.8902700	-8.8548527
N	-0.3406911	2.6519359	-7.7780257
C	0.5616434	3.6449676	-8.1182455
H	0.6735192	4.5426703	-7.5203234
C	0.0899292	-0.9425799	-2.1861322
H	0.1285545	-1.8983112	-2.7256140
H	-0.5575428	-1.0856018	-1.3056701
C	-0.4912822	0.1508948	-3.0343502
N	-1.0956489	1.2547975	-2.4492079
H	-1.2189057	1.4032257	-1.4532739
C	-1.4780769	2.1065002	-3.4279206
H	-1.9947141	3.0456063	-3.2431878
N	-1.1520487	1.6227813	-4.6126452
C	-0.5332365	0.4086147	-4.3863680
H	-0.1741070	-0.2198004	-5.1976497
Cu	-5.3032747	1.9891761	-6.0781958
Cu	-1.7298523	2.7802666	-6.3136720
O	-3.5858095	2.6509960	-7.2103221
O	-3.6625008	3.0465449	-5.8523880
C	-2.5840995	4.1229461	-10.1101872
C	-3.1548673	5.2258874	-9.4787679
C	-3.0772064	6.5022042	-10.0693356
C	-2.4294200	6.6537772	-11.2963525
C	-1.8599231	5.5413651	-11.9300839
C	-1.9345694	4.2783876	-11.3405625
O	-3.6477346	7.5638887	-9.4340977
H	-4.1745088	7.1975031	-8.7064973
H	-2.4075397	7.6426119	-11.7595576
H	-1.3830550	5.6551769	-12.9027600
H	-1.5193434	3.4100837	-11.8558682
H	-2.6704519	3.1486395	-9.6302943
O	-3.8060127	5.1675330	-8.2754857
H	-3.8792858	4.2310450	-7.9724405
H	-9.7596831	-2.0012081	-7.7252471
H	-7.9677537	7.4804769	-5.0130645
H	-5.0429541	0.3809394	-0.0020893
H	2.2309879	6.9178257	-4.6936591
H	3.1001019	3.7198439	-10.2878194
H	1.0931770	-0.6747854	-1.8547012

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C	-8.6896774	-2.1948685	-7.7648220
H	-8.4490934	-2.8597961	-6.9219519
H	-8.5006412	-2.7732831	-8.6852208
C	-7.7921168	-0.9910069	-7.7019341
N	-7.4255027	-0.2488068	-8.8061013
H	-7.6789007	-0.4235513	-9.7850437
C	-6.5786887	0.7255464	-8.4238551
H	-6.1440244	1.4503377	-9.1115557
N	-6.3739578	0.6636756	-7.1128358
C	-7.1226833	-0.3983802	-6.6534782

H	-7.1425988	-0.6740860	-5.6073543
C	-7.5565630	7.3229675	-6.0062869
H	-8.2916539	7.6972503	-6.7312453
H	-6.6374166	7.9144386	-6.1512881
C	-7.2860331	5.8853228	-6.2955227
N	-8.1508650	5.1088453	-7.0398555
H	-9.0685612	5.4068262	-7.3824720
C	-7.6224132	3.8668802	-7.1478266
H	-8.1013898	3.0625807	-7.7044226
N	-6.4676816	3.7980940	-6.5061083
C	-6.2394622	5.0494607	-5.9843627
H	-5.3398633	5.2798841	-5.4183248
C	-4.3888421	1.1162296	-0.5669252
H	-4.2263188	1.9748160	0.1047543
H	-3.4130641	0.6395041	-0.7460004
C	-4.9350888	1.5411203	-1.9028914
N	-5.8907485	2.5227912	-2.0702864
H	-6.2564566	3.1049146	-1.3116834
C	-6.1660114	2.6426922	-3.3862981
H	-6.8823736	3.3533896	-3.7894384
N	-5.4330550	1.7929953	-4.0927414
C	-4.6660259	1.0962922	-3.1814796
H	-3.9646950	0.3241666	-3.4885260
C	1.2263262	7.1332769	-4.2196529
H	1.3484434	7.0893788	-3.1272623
H	1.0057957	8.1773659	-4.4767077
C	0.1294832	6.2287851	-4.6984706
N	-0.9405438	6.6571975	-5.4606188
H	-1.1468312	7.6196058	-5.7109248
C	-1.6486255	5.5691301	-5.8609919
H	-2.5338407	5.6100893	-6.4964406
N	-1.0886487	4.4648087	-5.3992717
C	0.0081127	4.8569206	-4.6729350
H	0.6667825	4.1343098	-4.1935554
C	2.2643547	3.6788370	-10.2614429
H	2.1359508	4.7600750	-10.1089361
H	1.7525456	3.4271603	-11.2093904
C	1.5896207	2.9399469	-9.1528572
N	1.6493044	1.5695777	-8.9783934
H	2.2499214	0.9302724	-9.4952977
C	0.7800461	1.2232698	-8.0028064
H	0.6669152	0.2049315	-7.6435644
N	0.1480505	2.2911827	-7.5368140
C	0.6548908	3.3669665	-8.2396935
H	0.3082684	4.3824264	-8.0729866
C	0.1590534	-1.1161246	-1.9774803
H	0.2044511	-2.0877732	-2.4876308
H	-0.4619813	-1.2314356	-1.0749746
C	-0.4498875	-0.0602075	-2.8443322
N	-1.0285872	1.0738900	-2.2939297
H	-1.1397426	1.2609106	-1.3030744
C	-1.3970065	1.8987758	-3.3040967
H	-1.8872830	2.8581250	-3.1555923
N	-1.0895962	1.3622378	-4.4688277
C	-0.4988139	0.1460619	-4.2021717
H	-0.1584834	-0.5216612	-4.9894201
Cu	-5.2156324	2.0340828	-6.1488728
Cu	-1.4018882	2.4793355	-6.2092920
O	-3.8043678	2.5752627	-7.5533075
O	-3.3853074	2.8478715	-6.2226580
C	-2.2166551	3.8478315	-10.0808390
C	-3.1014754	4.8486178	-9.6183968
C	-3.2836912	6.0389872	-10.4113261
C	-2.6032445	6.1977433	-11.6220578
C	-1.7768468	5.1696618	-12.0743069
C	-1.5794096	4.0025770	-11.3022270
O	-4.1306724	6.9636294	-9.9452263
H	-4.5334528	6.5722120	-9.1451757
H	-2.7668834	7.0981189	-12.2170377
H	-1.2860233	5.2549906	-13.0435087
H	-0.9261973	3.2177965	-11.6888474
H	-2.0658521	2.9645278	-9.4606125
O	-3.7799701	4.7949399	-8.4958382
H	-3.8556434	3.7152417	-8.0480022
H	-9.7601626	-1.9963718	-7.7126022
H	-7.9476044	7.5423180	-5.0127889
H	-5.0204412	0.3943621	-0.0491835
H	2.1860790	6.8769944	-4.6682734
H	3.3273033	3.4672363	-10.3773387
H	1.1650274	-0.8145591	-1.6856910

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C	-8.7368419	-2.2562526	-7.7766824
H	-8.5029893	-2.9213719	-6.9319496
H	-8.5508148	-2.8368504	-8.6961576
C	-7.8353365	-1.0579693	-7.7100029

N	-7.4843495	-0.2954013	-8.8052740
H	-7.7373448	-0.4577500	-9.7861900
C	-6.6428539	0.6796638	-8.4112592
H	-6.2171251	1.4182117	-9.0895735
N	-6.4261440	0.5977477	-7.1035244
C	-7.1598566	-0.4795017	-6.6582705
H	-7.1644705	-0.7771730	-5.6179663
C	-7.5163867	7.2739011	-5.9930022
H	-8.2329717	7.6625829	-6.7296218
H	-6.5873670	7.8542463	-6.1175532
C	-7.2567897	5.8358871	-6.2948123
N	-8.1376669	5.0708406	-7.0328907
H	-9.0603046	5.3753857	-7.3567897
C	-7.6129337	3.8308967	-7.1728614
H	-8.1058320	3.0341604	-7.7282265
N	-6.4428449	3.7519709	-6.5597594
C	-6.2035779	4.9948823	-6.0201504
H	-5.2911428	5.2135985	-5.4702459
C	-4.3655344	1.1101872	-0.4996807
H	-4.2134649	1.9636111	0.1810133
H	-3.3873912	0.6332124	-0.6653495
C	-4.8915708	1.5408681	-1.8403140
N	-5.8361428	2.5303386	-2.0164336
H	-6.2041434	3.1157639	-1.2618079
C	-6.1047358	2.6429053	-3.3349851
H	-6.8157726	3.3564416	-3.7433407
N	-5.3785954	1.7816246	-4.0329019
C	-4.6226357	1.0847641	-3.1150028
H	-3.9292249	0.3020208	-3.4132774
C	1.2114492	7.1315392	-4.2199626
H	1.3378621	7.0765446	-3.1286855
H	1.0040095	8.1811084	-4.4651182
C	0.0944781	6.2517999	-4.6968387
N	-0.9438749	6.7017486	-5.4894715
H	-1.1068102	7.6646145	-5.7679647
C	-1.6889367	5.6310489	-5.8718307
H	-2.5527281	5.6963663	-6.5337442
N	-1.1854578	4.5184050	-5.3693859
C	-0.0844477	4.8874511	-4.6351470
H	0.5362123	4.1521605	-4.1256557
C	2.2142275	3.7053799	-10.2725944
H	2.1005255	4.7891964	-10.1250984
H	1.7136872	3.4590303	-11.2280896
C	1.5147222	2.9785301	-9.1702815
N	1.5573955	1.6085365	-8.9945139
H	2.1507526	0.9609109	-9.5083776
C	0.6822875	1.2761088	-8.0170900
H	0.5598447	0.2602379	-7.6548421
N	0.0631248	2.3495712	-7.5520082
C	0.5821676	3.4166970	-8.2580399
H	0.2537756	4.4378222	-8.0855268
C	0.1478648	-1.0984756	-1.9641712
H	0.1862286	-2.0616397	-2.4907806
H	-0.4660332	-1.2274463	-1.0585489
C	-0.4671670	-0.0264435	-2.8067462
N	-1.0249609	1.1056704	-2.2310904
H	-1.1189892	1.2799669	-1.2362774
C	-1.4040896	1.9461797	-3.2258326
H	-1.8859038	2.9063360	-3.0555011
N	-1.1231188	1.4233506	-4.4026177
C	-0.5392476	0.1983056	-4.1607826
H	-0.2203439	-0.4633637	-4.9625408
Cu	-5.2922583	1.9826228	-6.1228951
Cu	-1.4469325	2.5280090	-6.1490609
O	-3.7241391	2.6474979	-7.7411210
O	-3.4670758	2.6988712	-6.3339425
C	-2.2076753	4.0364248	-10.2646950
C	-2.9868845	5.1383571	-9.7726035
C	-3.1392912	6.3148797	-10.6366631
C	-2.5524188	6.3627471	-11.9027423
C	-1.8342680	5.2530094	-12.3422933
C	-1.6549336	4.1013435	-11.5205611
O	-3.8773447	7.2990265	-10.1406221
H	-4.1852934	6.9598760	-9.2698574
H	-2.6916242	7.2390769	-12.5375443
H	-1.4070140	5.2492899	-13.3452837
H	-1.0814764	3.2632190	-11.9210060
H	-2.0831673	3.1684183	-9.6166237
O	-3.5621828	5.1860243	-8.6416245
H	-3.7930239	3.6099595	-7.9942788
H	-9.8050506	-2.0461165	-7.7233949
H	-7.9220807	7.4961767	-5.0060511
H	-5.0105642	0.3863871	-0.0015678
H	2.1675730	6.8697653	-4.6731383
H	3.2757205	3.4796492	-10.3743037
H	1.1569466	-0.8043458	-1.6755400

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C	-8.7329654	-2.2198748	-7.7481917
H	-8.5005237	-2.8884617	-6.9058078
H	-8.5365189	-2.7956675	-8.6686838
C	-7.8341980	-1.0190796	-7.6710491
N	-7.4530300	-0.2711894	-8.7668919
H	-7.6946530	-0.4308788	-9.7510610
C	-6.6047224	0.6949189	-8.3674428
H	-6.1436444	1.4187119	-9.0371641
N	-6.4151005	0.6242186	-7.0551579
C	-7.1740781	-0.4356096	-6.6114077
H	-7.2062073	-0.7198262	-5.5685203
C	-7.5774562	7.2905836	-5.9852106
H	-8.3095829	7.6627986	-6.7143444
H	-6.6547536	7.8762309	-6.1317216
C	-7.3144926	5.8494320	-6.2604952
N	-8.1809114	5.0726358	-7.0018911
H	-9.0929594	5.3754368	-7.3543864
C	-7.6624952	3.8240393	-7.0894434
H	-8.1440517	3.0167681	-7.6395256
N	-6.5155747	3.7525332	-6.4356489
C	-6.2789208	5.0076875	-5.9303703
H	-5.3788198	5.2362805	-5.3644912
C	-4.4061635	1.1157326	-0.5727201
H	-4.2478173	1.9786994	0.0942432
H	-3.4278287	0.6431415	-0.7496963
C	-4.9543376	1.5276492	-1.9123130
N	-5.9326675	2.4853128	-2.0908890
H	-6.3135490	3.0658166	-1.3390094
C	-6.2049997	2.5887083	-3.4097234
H	-6.9344523	3.2808077	-3.8216897
N	-5.4474110	1.7525212	-4.1064600
C	-4.6679058	1.0821636	-3.1862803
H	-3.9458220	0.3251776	-3.4815919
C	1.1887835	7.1366501	-4.2358130
H	1.3009093	7.0897233	-3.1423314
H	0.9762584	8.1826612	-4.4916743
C	0.0903943	6.2394689	-4.7275374
N	-0.9928840	6.6775917	-5.4669353
H	-1.2118807	7.6443433	-5.6883041
C	-1.6994766	5.5961902	-5.8865613
H	-2.5916630	5.6417354	-6.5139233
N	-1.1221331	4.4876878	-5.4584355
C	-0.0202752	4.8669374	-4.7333397
H	0.6472501	4.1364739	-4.2789527
C	2.2029900	3.7028830	-10.2464862
H	2.0878246	4.7872845	-10.1060547
H	1.6974488	3.4476808	-11.1971573
C	1.5085327	2.9828671	-9.1349323
N	1.5568303	1.6140401	-8.9455079
H	2.1463806	0.9636764	-9.4609173
C	0.6910781	1.2837262	-7.9633091
H	0.5704394	0.2701808	-7.5945028
N	0.0725103	2.3613617	-7.5024572
C	0.5798113	3.4269312	-8.2222829
H	0.2447335	4.4469501	-8.0599124
C	0.1594417	-1.1007838	-2.0044043
H	0.2044177	-2.0715640	-2.5162621
H	-0.4693525	-1.2162707	-1.1073686
C	-0.4375178	-0.0382815	-2.8728253
N	-1.0301630	1.0875116	-2.3204527
H	-1.1660862	1.2597631	-1.3299353
C	-1.3823226	1.9234015	-3.3259404
H	-1.8894177	2.8737066	-3.1770246
N	-1.0461065	1.4040678	-4.4910863
C	-0.4593797	0.1847369	-4.2291592
H	-0.1083924	-0.4773488	-5.0167466
Cu	-5.1606803	1.9860220	-6.1580576
Cu	-1.5145221	2.5304205	-6.2060583
O	-4.1882667	2.4271307	-7.8288609
O	-3.3497603	2.7074941	-6.0996926
C	-2.4494554	4.0444386	-10.1234874
C	-3.2045168	5.1722138	-9.6473481
C	-3.2681376	6.3633391	-10.5059283
C	-2.6178323	6.4025288	-11.7403272
C	-1.9185249	5.2715964	-12.1594203
C	-1.8300624	4.1032455	-11.3480985
O	-3.9856803	7.3756783	-10.0327897
H	-4.3474978	7.0383698	-9.1820640
H	-2.6955735	7.2895901	-12.3713298
H	-1.4404417	5.2653563	-13.1394582
H	-1.2761114	3.2455534	-11.7330795
H	-2.4091607	3.1615738	-9.4849035
O	-3.8138707	5.2265461	-8.5400299
H	-4.2354874	3.4026744	-7.9451964
H	-9.8031979	-2.0185327	-7.7020383
H	-7.9696171	7.5163244	-4.9935870

H	-5.0333944	0.3929423	-0.0509711
H	2.1514667	6.8779711	-4.6767128
H	3.2642620	3.4787096	-10.3537918
H	1.1642834	-0.8036708	-1.7042654

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C	-8.5629923	-2.1038617	-7.7109775
H	-8.3305895	-2.7664180	-6.8642588
H	-8.3638744	-2.6851058	-8.6278041
C	-7.6549285	-0.9032973	-7.6393513
N	-7.2821505	-0.1553307	-8.7389916
H	-7.5548501	-0.3087529	-9.7164409
C	-6.4060794	0.7930557	-8.3546332
H	-5.9694771	1.5224907	-9.0353782
N	-6.1852927	0.7109306	-7.0477636
C	-6.9570227	-0.3382716	-6.5913203
H	-6.9729578	-0.6228750	-5.5470631
C	-7.5330341	7.2802457	-6.0029310
H	-8.2673922	7.6506054	-6.7312041
H	-6.6155231	7.8744507	-6.1472093
C	-7.2557894	5.8426950	-6.2925385
N	-8.1224512	5.0637973	-7.0340494
H	-9.0433947	5.3598499	-7.3680999
C	-7.5824768	3.8273354	-7.1571397
H	-8.0624425	3.0239703	-7.7137447
N	-6.4189486	3.7656118	-6.5311681
C	-6.1976147	5.0144879	-5.9996091
H	-5.2890097	5.2300081	-5.4432288
C	-4.4185698	1.1151387	-0.5032546
H	-4.2697158	1.9765359	0.1673406
H	-3.4363296	0.6470202	-0.6725989
C	-4.9659236	1.5200789	-1.8438988
N	-5.9204711	2.4993823	-2.0346547
H	-6.2809477	3.1034052	-1.2912013
C	-6.2113234	2.5704065	-3.3513085
H	-6.9192448	3.2786592	-3.7734111
N	-5.4951262	1.6873405	-4.0327574
C	-4.7155128	1.0277108	-3.1065886
H	-4.0123805	0.2474608	-3.3867054
C	1.2500360	7.1670132	-4.2181056
H	1.3584962	7.0933156	-3.1254290
H	1.0732970	8.2252395	-4.4492390
C	0.1100390	6.3403974	-4.7299382
N	-1.0027654	6.8895421	-5.3411531
H	-1.1886350	7.8800702	-5.4653066
C	-1.7891403	5.8826179	-5.7921923
H	-2.7195160	6.0233806	-6.3402060
N	-1.2372374	4.7168644	-5.5076617
C	-0.0647663	4.9788585	-4.8431258
H	0.5960958	4.1798134	-4.5125293
C	2.0327687	3.9830586	-10.1456376
H	2.0425444	5.0592085	-9.9232936
H	1.5580756	3.8739970	-11.1384836
C	1.1535001	3.2828525	-9.1560579
N	0.7328828	1.9751565	-9.3251959
H	1.0598954	1.3359704	-10.0450513
C	-0.2223863	1.7037392	-8.4099187
H	-0.7717581	0.7732785	-8.3715549
N	-0.4394173	2.7541855	-7.6387908
C	0.4113439	3.7476649	-8.0917743
H	0.4107688	4.7452105	-7.6652356
C	0.1031222	-0.9357774	-2.2039332
H	0.1474714	-1.8886569	-2.7484708
H	-0.5463468	-1.0876017	-1.3262731
C	-0.4833602	0.1586258	-3.0475683
N	-1.0917134	1.2570430	-2.4568949
H	-1.2153499	1.4009588	-1.4606095
C	-1.4891977	2.1048633	-3.4351902
H	-2.0319400	3.0291337	-3.2516008
N	-1.1678884	1.6287118	-4.6222635
C	-0.5380099	0.4202812	-4.3992160
H	-0.1849842	-0.2110827	-5.2113461
Cu	-5.0331128	2.0795435	-6.0587539
Cu	-1.9969975	2.9009851	-6.2906929
O	-3.5112305	2.3987636	-7.4836630
O	-3.6328994	3.1967727	-5.3603403
C	-2.3535695	4.0111995	-10.3086153
C	-3.0743258	5.0993259	-9.7082597
C	-3.1998510	6.3430245	-10.4786554
C	-2.6205255	6.4709842	-11.7423937
C	-1.9442926	5.3752915	-12.2781926
C	-1.8072766	4.1528361	-11.5596856
O	-3.8990927	7.3094567	-9.8957979
H	-4.2096448	6.9096178	-9.0521083
H	-2.7346642	7.3982331	-12.3066845
H	-1.5272728	5.4366316	-13.2830394

H	-1.2812009	3.3253531	-12.0392020
H	-2.2722107	3.0948529	-9.7261358
O	-3.6055601	5.0725710	-8.5610064
H	-3.7337474	3.2753996	-7.8722196
H	-9.6367890	-1.9199620	-7.6762211
H	-7.9276089	7.5046498	-5.0119617
H	-5.0529320	0.3883604	0.0041351
H	2.2072899	6.8945658	-4.6625196
H	3.0641923	3.6376257	-10.2156936
H	1.1039046	-0.6658064	-1.8668623

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C	-8.5846472	-2.0382593	-7.7050164
H	-8.3410223	-2.6811155	-6.8468526
H	-8.3876439	-2.6372773	-8.6103442
C	-7.6855851	-0.8275675	-7.6810096
N	-7.2769722	-0.1796910	-8.8290054
H	-7.5349141	-0.4078751	-9.7959271
C	-6.4307203	0.8151408	-8.5062850
H	-5.9713931	1.4785550	-9.2398513
N	-6.2613262	0.8567942	-7.1889834
C	-7.0380480	-0.1564632	-6.6618317
H	-7.0959730	-0.3292507	-5.5937284
C	-7.7560668	7.2638979	-6.0664465
H	-8.5621555	7.5885347	-6.7365171
H	-6.8682542	7.8691191	-6.3155023
C	-7.4703368	5.8232967	-6.3236288
N	-8.2642121	5.0422260	-7.1383867
H	-9.1630652	5.3350664	-7.5304465
C	-7.7121062	3.8129321	-7.2339782
H	-8.1314187	3.0096015	-7.8356658
N	-6.6028731	3.7624941	-6.5101449
C	-6.4369646	5.0066334	-5.9443266
H	-5.5837373	5.2394274	-5.3149949
C	-4.3601086	1.1279733	-0.5526512
H	-4.1987407	1.9749531	0.1346517
H	-3.3843030	0.6504135	-0.7305809
C	-4.8966807	1.5755835	-1.8856290
N	-5.8929335	2.5184122	-2.0356046
H	-6.2878497	3.0665292	-1.2675845
C	-6.1568059	2.6594121	-3.3547708
H	-6.9104340	3.3429769	-3.7377953
N	-5.3805154	1.8694025	-4.0792988
C	-4.5953064	1.1844891	-3.1762376
H	-3.8523885	0.4575777	-3.4983291
C	1.2763930	7.1898545	-4.1833747
H	1.3923270	7.1214683	-3.0913311
H	1.1040351	8.2471033	-4.4212960
C	0.1250405	6.3741908	-4.6824857
N	-0.9979331	6.9440206	-5.2542761
H	-1.1743392	7.9380594	-5.3645066
C	-1.8099250	5.9608960	-5.6986899
H	-2.7546875	6.1254087	-6.2138198
N	-1.2618601	4.7825017	-5.4436886
C	-0.0639526	5.0169815	-4.8109756
H	0.5964622	4.2043568	-4.5167711
C	1.9929496	3.8489522	-10.1939616
H	1.9598743	4.9388648	-10.0519981
H	1.5305076	3.6475580	-11.1780509
C	1.1415684	3.1990567	-9.1443135
N	0.7504561	1.8708862	-9.1869733
H	1.0838608	1.1769150	-9.8514330
C	-0.1731168	1.6565908	-8.2191728
H	-0.6818654	0.7090737	-8.0634028
N	-0.3974033	2.7672281	-7.5381367
C	0.4128715	3.7344008	-8.1031564
H	0.4037935	4.7658954	-7.7630716
C	0.0710382	-0.8868316	-2.2328958
H	0.1084295	-1.7842762	-2.8651262
H	-0.5613090	-1.1247559	-1.3614557
C	-0.5420515	0.2726010	-2.9652393
N	-1.0066230	1.3834965	-2.2743379
H	-1.0181126	1.4905411	-1.2653733
C	-1.4391566	2.2982307	-3.1751154
H	-1.8717810	3.2557221	-2.8922711
N	-1.2828903	1.8497502	-4.4051229
C	-0.7308543	0.5885063	-4.2929262
H	-0.5139806	-0.0294171	-5.1613471
Cu	-5.1529203	2.3261229	-6.3107998
Cu	-2.0103882	3.0486402	-6.1436203
O	-3.2326215	1.7723346	-6.9202929
O	-3.8281746	3.7705031	-6.1666277
C	-2.3667465	4.2837188	-11.1959639
C	-3.0251186	4.2195346	-9.9146948
C	-3.5006463	5.4875140	-9.3374305
C	-3.3940884	6.6756526	-10.0775402

C	-2.7873613	6.6679690	-11.3280347
C	-2.2507721	5.4672394	-11.8781220
O	-4.0250954	5.5209715	-8.1234508
H	-3.9714012	4.6620748	-7.5955216
H	-3.7925103	7.5949164	-9.6430311
H	-2.7241612	7.5929784	-11.9067246
H	-1.7824078	5.4836731	-12.8625109
H	-2.0002897	3.3506644	-11.6224352
O	-3.1914011	3.1388480	-9.2886851
H	-3.2560044	2.0693634	-7.8563649
H	-9.6603335	-1.8652191	-7.6730390
H	-8.0697345	7.5059421	-5.0510187
H	-5.0005496	0.4032127	-0.0500341
H	2.2275641	6.9090243	-4.6355632
H	3.0391572	3.5470295	-10.2425291
H	1.0762174	-0.6382846	-1.8924467

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C	-8.5833840	-2.0431086	-7.7095823
H	-8.3405738	-2.6858520	-6.8509962
H	-8.3833081	-2.6407450	-8.6150780
C	-7.6880735	-0.8302634	-7.6806913
N	-7.2652682	-0.1841438	-8.8247784
H	-7.5145903	-0.4120314	-9.7944342
C	-6.4272322	0.8145605	-8.4955372
H	-5.9572060	1.4774145	-9.2233673
N	-6.2784203	0.8594043	-7.1748488
C	-7.0581127	-0.1549838	-6.6541609
H	-7.1314587	-0.3237608	-5.5864916
C	-7.7746236	7.2613178	-6.0771569
H	-8.5888823	7.5811881	-6.7394255
H	-6.8900175	7.8658439	-6.3392868
C	-7.4896193	5.8198916	-6.3310412
N	-8.2647131	5.0436124	-7.1678758
H	-9.1560623	5.3377205	-7.5756265
C	-7.7114176	3.8158840	-7.2607538
H	-8.1175330	3.0180669	-7.8783921
N	-6.6175293	3.7615758	-6.5124405
C	-6.4652826	5.0018698	-5.9332044
H	-5.6243937	5.2351516	-5.2887575
C	-4.3632796	1.1312749	-0.5494499
H	-4.2003315	1.9783792	0.1372121
H	-3.3880621	0.6528550	-0.7283149
C	-4.9015526	1.5776241	-1.8818274
N	-5.8968021	2.5212667	-2.0317980
H	-6.2888005	3.0719326	-1.2636949
C	-6.1650409	2.6597563	-3.3493153
H	-6.9180036	3.3438063	-3.7326624
N	-5.3911336	1.8663252	-4.0742996
C	-4.6036696	1.1823997	-3.1717555
H	-3.8612327	0.4549727	-3.4930505
C	1.3105522	7.1973073	-4.1593187
H	1.4351073	7.1293529	-3.0683229
H	1.1326297	8.2536703	-4.3961532
C	0.1591613	6.3791469	-4.6518785
N	-0.9623273	6.9496533	-5.2248969
H	-1.1376678	7.9438913	-5.3360336
C	-1.7726751	5.9710190	-5.6776340
H	-2.7113351	6.1361325	-6.2085517
N	-1.2235114	4.7908834	-5.4239928
C	-0.0273646	5.0223678	-4.7853557
H	0.6330220	4.2088087	-4.4935320
C	1.9921458	3.8735577	-10.1866045
H	1.9624966	4.9634482	-10.0448219
H	1.5309006	3.6739046	-11.1714579
C	1.1370160	3.2269006	-9.1382623
N	0.7325559	1.9029506	-9.1914132
H	1.0479184	1.2147418	-9.8705133
C	-0.1860831	1.6864239	-8.2221873
H	-0.7051808	0.7433199	-8.0771083
N	-0.3937324	2.7927864	-7.5275297
C	0.4215085	3.7597925	-8.0874773
H	0.4203509	4.7882424	-7.7393682
C	0.0670173	-0.8877351	-2.2288340
H	0.1034146	-1.7840734	-2.8627130
H	-0.5636593	-1.1273687	-1.3567254
C	-0.5477677	0.2726109	-2.9578350
N	-1.0159630	1.3806508	-2.2650282
H	-1.0289901	1.4847431	-1.2556416
C	-1.4482289	2.2975994	-3.1629074
H	-1.8812887	3.2544344	-2.8785123
N	-1.2893607	1.8522452	-4.3943001
C	-0.7336148	0.5918659	-4.2847861
H	-0.5086312	-0.0219462	-5.1539807
Cu	-5.1994699	2.3134417	-6.2816607
Cu	-1.9583562	3.0611751	-6.1298342

O	-3.2517933	1.8467991	-6.9413814
O	-3.8257765	3.7459195	-6.0830754
C	-2.5113379	4.3468567	-11.0593328
C	-3.0883173	4.2025378	-9.7501056
C	-3.4966994	5.4359650	-9.0388311
C	-3.3826435	6.6798990	-9.7210396
C	-2.8497092	6.7504254	-10.9926855
C	-2.3908968	5.5739957	-11.6601023
O	-3.9401745	5.4050113	-7.8217459
H	-3.8968550	4.4408819	-7.0416383
H	-3.7293292	7.5743368	-9.1973997
H	-2.7816287	7.7150287	-11.5027143
H	-1.9840564	5.6444983	-12.6703706
H	-2.2065736	3.4356298	-11.5732671
O	-3.2299019	3.0599139	-9.2173924
H	-3.2923183	2.2414559	-7.8671381
H	-9.6592460	-1.8710239	-7.6783700
H	-8.0776180	7.5067991	-5.0593161
H	-5.0036203	0.4066346	-0.0465317
H	2.2587279	6.9190931	-4.6193470
H	3.0371529	3.5667020	-10.2298035
H	1.0727333	-0.6394230	-1.8898016

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C	-8.5708452	-2.0208111	-7.6875080
H	-8.3290727	-2.6577165	-6.8246806
H	-8.3740209	-2.6280088	-8.5876537
C	-7.6663396	-0.8134230	-7.6749081
N	-7.2739841	-0.1713584	-8.8310893
H	-7.5470004	-0.3969366	-9.7936790
C	-6.4136639	0.8174914	-8.5228499
H	-5.9650738	1.4761713	-9.2662577
N	-6.2194349	0.8627578	-7.2114500
C	-6.9942966	-0.1433558	-6.6691437
H	-7.0322351	-0.3130001	-5.5993580
C	-7.8146186	7.2191226	-6.0871801
H	-8.6470699	7.5184205	-6.7366718
H	-6.9464573	7.8383952	-6.3699206
C	-7.5072679	5.7801035	-6.3341146
N	-8.2880130	4.9797644	-7.1436347
H	-9.1925507	5.2557593	-7.5324722
C	-7.7056033	3.7629461	-7.2385895
H	-8.1133240	2.9488997	-7.8335311
N	-6.5884110	3.7399421	-6.5256078
C	-6.4534030	4.9887792	-5.9595175
H	-5.5935351	5.2335270	-5.3463942
C	-4.3470080	1.1200481	-0.5558101
H	-4.1852670	1.9640564	0.1353000
H	-3.3715934	0.6399924	-0.7304367
C	-4.8739228	1.5748863	-1.8901326
N	-5.8620754	2.5261126	-2.0426172
H	-6.2581573	3.0750547	-1.2761967
C	-6.1126205	2.6752613	-3.3648339
H	-6.8565646	3.3683348	-3.7499236
N	-5.3382128	1.8830623	-4.0868738
C	-4.5665363	1.1878609	-3.1809500
H	-3.8259361	0.4588680	-3.5040137
C	1.2914866	7.1443563	-4.1907808
H	1.4154416	7.0722929	-3.0995065
H	1.1112412	8.2029820	-4.4202693
C	0.1406103	6.3275555	-4.6891951
N	-1.0265849	6.9046225	-5.1535109
H	-1.2370390	7.8971091	-5.1740165
C	-1.8421723	5.9292416	-5.6106935
H	-2.8338913	6.1004516	-6.0196521
N	-1.2560851	4.7507567	-5.4756307
C	-0.0279407	4.9770474	-4.9005339
H	0.6628994	4.1628089	-4.6920009
C	2.0116691	3.8206245	-10.2162166
H	1.9751148	4.9089378	-10.0611969
H	1.5539686	3.6282029	-11.2047489
C	1.1565943	3.1568402	-9.1787688
N	0.8047712	1.8177643	-9.2074620
H	1.1853830	1.1179988	-9.8398939
C	-0.1422392	1.5985755	-8.2593920
H	-0.6169422	0.6348319	-8.0895151
N	-0.4220343	2.7149441	-7.6112264
C	0.3800740	3.6906744	-8.1707323
H	0.3440448	4.7257074	-7.8409880
C	0.0599810	-0.8727215	-2.2368095
H	0.0939389	-1.7752597	-2.8624059
H	-0.5750781	-1.1021314	-1.3647827
C	-0.5464721	0.2827530	-2.9817026
N	-0.9984617	1.4084606	-2.3062385
H	-1.0108542	1.5300206	-1.2991422
C	-1.4269937	2.3123914	-3.2212404

H	-1.8522100	3.2773534	-2.9532355
N	-1.2801437	1.8438829	-4.4439468
C	-0.7398893	0.5803641	-4.3130684
H	-0.5356734	-0.0544931	-5.1719791
Cu	-5.0471857	2.3455464	-6.3608834
Cu	-2.0886912	3.0038534	-6.1976729
O	-3.2446083	1.5845489	-6.8581322
O	-3.8493874	3.9233011	-6.0672196
C	-2.2586521	4.2975749	-11.3095391
C	-3.0187361	4.2895639	-10.0603654
C	-3.5455753	5.6595619	-9.5350623
C	-3.4535151	6.8081811	-10.4428806
C	-2.7880091	6.6892848	-11.6163738
C	-2.1652285	5.4318506	-12.0404188
O	-3.9702601	5.7416992	-8.3948457
H	-3.9497015	4.3841901	-6.9222018
H	-3.9030892	7.7465977	-10.1108322
H	-2.7043116	7.5455393	-12.2913304
H	-1.6440158	5.4129965	-12.9987322
H	-1.8347449	3.3581722	-11.6644917
O	-3.2495031	3.2845007	-9.4082464
H	-3.2036403	1.5263293	-7.8246880
H	-9.6466958	-1.8480273	-7.6599829
H	-8.1032417	7.4703512	-5.0665689
H	-4.9917485	0.3959659	-0.0577327
H	2.2411293	6.8724396	-4.6515481
H	3.0594383	3.5247275	-10.2680926
H	1.0658138	-0.6271728	-1.8961152

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C	-8.6822863	-2.2144115	-7.7748534
H	-8.4526778	-2.8836324	-6.9323152
H	-8.4950260	-2.7911552	-8.6965958
C	-7.7718564	-1.0208201	-7.7022674
N	-7.4176513	-0.2562429	-8.7965692
H	-7.6896966	-0.4232847	-9.7725151
C	-6.5610660	0.7067252	-8.4104611
H	-6.1437480	1.4524870	-9.0882297
N	-6.3329155	0.6097527	-7.1023959
C	-7.0798616	-0.4597147	-6.6522935
H	-7.0818135	-0.7610074	-5.6126473
C	-7.5903270	7.2280639	-6.0227690
H	-8.3270414	7.6039272	-6.7454315
H	-6.6666133	7.8089993	-6.1797224
C	-7.3336556	5.7865456	-6.3104307
N	-8.2063567	5.0177145	-7.0537488
H	-9.1228726	5.3269644	-7.3892582
C	-7.6835270	3.7765517	-7.1808965
H	-8.1688586	2.9793514	-7.7412039
N	-6.5211641	3.7003922	-6.5511546
C	-6.2861107	4.9474701	-6.0168125
H	-5.3746220	5.1703646	-5.4687450
C	-4.3869429	1.0993102	-0.4922108
H	-4.2381226	1.9599363	0.1793993
H	-3.4069164	0.6242739	-0.6542797
C	-4.9255075	1.5089136	-1.8343593
N	-5.8687547	2.4981248	-2.0185398
H	-6.2242204	3.1003029	-1.2702196
C	-6.1661324	2.5775730	-3.3315313
H	-6.8794822	3.2864906	-3.7446795
N	-5.4580651	1.6919290	-4.0204116
C	-4.6837105	1.0169115	-3.1002685
H	-4.0004397	0.2210338	-3.3874901
C	1.2719696	7.1886624	-4.2662916
H	1.3592587	7.1113544	-3.1723629
H	1.0957568	8.2464294	-4.4998230
C	0.1494100	6.3507555	-4.7973065
N	-0.8526464	6.8536592	-5.6058784
H	-0.9705042	7.8257091	-5.8780295
C	-1.6246237	5.8243365	-6.0307752
H	-2.4643138	5.9325443	-6.7211196
N	-1.1732176	4.6824552	-5.5366120
C	-0.0760284	4.9927392	-4.7678606
H	0.5112027	4.2251366	-4.2671307
C	2.0774298	4.0943875	-10.2165566
H	2.1038809	5.1463049	-9.9024717
H	1.6206781	4.0825780	-11.2224247
C	1.1678839	3.3231004	-9.3149189
N	0.5988712	2.1285362	-9.7116560
H	0.7867886	1.6550994	-10.5915824
C	-0.3032067	1.7460566	-8.7856451
H	-0.9551046	0.8915792	-8.9113395
N	-0.3398780	2.6142810	-7.7880590
C	0.5706085	3.6067604	-8.1079586
H	0.6975908	4.4849676	-7.4844744
C	0.0815660	-0.9464576	-2.1725217

H	0.1192334	-1.9021499	-2.7120893
H	-0.5614256	-1.0900256	-1.2887936
C	-0.5065884	0.1445042	-3.0185316
N	-1.0889818	1.2605685	-2.4335057
H	-1.1899443	1.4218174	-1.4370005
C	-1.4889398	2.1024085	-3.4133275
H	-1.9903545	3.0498709	-3.2292149
N	-1.1958414	1.5998863	-4.5992888
C	-0.5786610	0.3845491	-4.3720550
H	-0.2397814	-0.2547048	-5.1835090
Cu	-5.2924091	1.9843914	-6.0808200
Cu	-1.7228435	2.7346092	-6.3008579
O	-3.5642964	2.8158220	-7.2555768
O	-3.7120998	3.1801362	-5.9243770
C	-2.5386840	4.1736434	-10.1868583
C	-3.1101878	5.3103689	-9.6185986
C	-3.0395103	6.5503573	-10.2822432
C	-2.3982477	6.6307686	-11.5195198
C	-1.8272155	5.4859127	-12.0897833
C	-1.8943786	4.2597304	-11.4268420
O	-3.6111270	7.6471817	-9.7139272
H	-4.1110249	7.3324127	-8.9448044
H	-2.3845833	7.5901632	-12.0405195
H	-1.3522839	5.5450667	-13.0686986
H	-1.4775198	3.3647974	-11.8924960
H	-2.6205507	3.2253364	-9.6556522
O	-3.7630759	5.3191872	-8.4116311
H	-3.8671331	4.3994180	-8.0830993
H	-9.7509819	-2.0053986	-7.7272119
H	-7.9723420	7.4596020	-5.0285250
H	-5.0303649	0.3775083	0.0108564
H	2.2376960	6.9158500	-4.6917472
H	3.0993985	3.7207673	-10.2802304
H	1.0859949	-0.6774781	-1.8456594

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C	-8.6969614	-2.2048031	-7.7669741
H	-8.4583205	-2.8691270	-6.9230442
H	-8.5092106	-2.7850601	-8.6864126
C	-7.7961479	-1.0037799	-7.7041412
N	-7.4298130	-0.2594269	-8.8069524
H	-7.6839509	-0.4317641	-9.7860275
C	-6.5793462	0.7114181	-8.4226685
H	-6.1439202	1.4368189	-9.1092037
N	-6.3722238	0.6451892	-7.1124805
C	-7.1226786	-0.4164181	-6.6553717
H	-7.1421305	-0.6952412	-5.6100387
C	-7.5588177	7.3208437	-6.0047643
H	-8.2934524	7.6948299	-6.7303382
H	-6.6391787	7.9115523	-6.1498643
C	-7.2891885	5.8826044	-6.2923069
N	-8.1528927	5.1061858	-7.0380322
H	-9.0692515	5.4047375	-7.3836420
C	-7.6251510	3.8635174	-7.1430874
H	-8.1032115	3.0589691	-7.7001403
N	-6.4723868	3.7941806	-6.4981729
C	-6.2444120	5.0458960	-5.9771267
H	-5.3464855	5.2761616	-5.4083648
C	-4.3873679	1.1151952	-0.5589945
H	-4.2242082	1.9725981	0.1139977
H	-3.4120809	0.6381920	-0.7395368
C	-4.9340938	1.5407232	-1.8943365
N	-5.8886590	2.5232816	-2.0611153
H	-6.2538645	3.1052922	-1.3022294
C	-6.1671464	2.6408305	-3.3767490
H	-6.8841222	3.3515229	-3.7789829
N	-5.4363259	1.7895260	-4.0831875
C	-4.6687399	1.0932834	-3.1725399
H	-3.9710088	0.3180156	-3.4800559
C	1.2313141	7.1343562	-4.2150583
H	1.3569553	7.0935258	-3.1229689
H	1.0094495	8.1778086	-4.4737185
C	0.1329645	6.2293021	-4.6886579
N	-0.9366678	6.6575486	-5.4512193
H	-1.1414149	7.6197577	-5.7035398
C	-1.6459579	5.5695891	-5.8494314
H	-2.5313466	5.6097522	-6.4847156
N	-1.0878092	4.4653329	-5.3856576
C	0.0097220	4.8575626	-4.6604846
H	0.6681873	4.1347966	-4.1810450
C	2.2644120	3.6807979	-10.2608592
H	2.1379160	4.7621741	-10.1072818
H	1.7539889	3.4329633	-11.2108586
C	1.5877239	2.9417369	-9.1535557
N	1.6472036	1.5714109	-8.9786729
H	2.2472797	0.9317209	-9.4956870

C	0.7770202	1.2254238	-8.0037540
H	0.6641073	0.2071981	-7.6441143
N	0.1449354	2.2934189	-7.5381761
C	0.6521714	3.3688137	-8.2411264
H	0.3075130	4.3846226	-8.0727072
C	0.1579548	-1.1140929	-1.9805108
H	0.2032000	-2.0868115	-2.4886228
H	-0.4637622	-1.2278594	-1.0782217
C	-0.4512679	-0.0592713	-2.8488395
N	-1.0318997	1.0740993	-2.2987624
H	-1.1422025	1.2616139	-1.3079116
C	-1.4052038	1.8965069	-3.3090108
H	-1.8967024	2.8551989	-3.1606308
N	-1.0991882	1.3594987	-4.4739978
C	-0.5034971	0.1454073	-4.2069131
H	-0.1633784	-0.5224497	-4.9941061
Cu	-5.2292021	2.0263855	-6.1399029
Cu	-1.4093708	2.4795960	-6.2105263
O	-3.8239813	2.5831088	-7.5533998
O	-3.3838175	2.8716508	-6.2399202
C	-2.1981958	3.8638382	-10.0752136
C	-3.0830116	4.8605952	-9.6057196
C	-3.2890606	6.0443790	-10.4012777
C	-2.6182488	6.2079565	-11.6174141
C	-1.7884527	5.1852423	-12.0747191
C	-1.5761197	4.0196879	-11.3036577
O	-4.1397533	6.9607682	-9.9277052
H	-4.5289811	6.5647965	-9.1226809
H	-2.7932270	7.1051035	-12.2140031
H	-1.3086932	5.2699715	-13.0494685
H	-0.9291317	3.2336043	-11.6976749
H	-2.0417718	2.9791491	-9.4585304
O	-3.7429677	4.8077322	-8.4708155
H	-3.8485847	3.7262364	-8.0483337
H	-9.7669150	-2.0035645	-7.7143544
H	-7.9497822	7.5411854	-5.0114553
H	-5.0198342	0.3925947	-0.0433382
H	2.1898959	6.8778609	-4.6660545
H	3.3272764	3.4684640	-10.3761853
H	1.1638431	-0.8132638	-1.6876681

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C	-8.7368419	-2.2562526	-7.7766824
H	-8.5029893	-2.9213719	-6.9319496
H	-8.5508148	-2.8368504	-8.6961576
C	-7.8353365	-1.0579693	-7.7100029
N	-7.4843495	-0.2954013	-8.8052740
H	-7.7373448	-0.4577500	-9.7861900
C	-6.6428539	0.6796638	-8.4112592
H	-6.2171251	1.4182117	-9.0895735
N	-6.4261440	0.5977477	-7.1035244
C	-7.1598566	-0.4795017	-6.6582705
H	-7.1644705	-0.7771730	-5.6179663
C	-7.5163867	7.2739011	-5.9930022
H	-8.2329717	7.6625829	-6.7296218
H	-6.5873670	7.8542463	-6.1175532
C	-7.2567897	5.8358871	-6.2948123
N	-8.1376669	5.0708406	-7.0328907
H	-9.0603046	5.3753857	-7.3567897
C	-7.6129337	3.8308967	-7.1728614
H	-8.1058320	3.0341604	-7.7282265
N	-6.4428449	3.7519709	-6.5597594
C	-6.2035779	4.9948823	-6.0201504
H	-5.2911428	5.2135985	-5.4702459
C	-4.3655344	1.1101872	-0.4996807
H	-4.2134649	1.9636111	0.1810133
H	-3.3873912	0.6332124	-0.6653495
C	-4.8915708	1.5408681	-1.8403140
N	-5.8361428	2.5303386	-2.0164336
H	-6.2041434	3.1157639	-1.2618079
C	-6.1047358	2.6429053	-3.3349851
H	-6.8157726	3.3564416	-3.7433407
N	-5.3785954	1.7816246	-4.0329019
C	-4.6226357	1.0847641	-3.1150028
H	-3.9292249	0.3020208	-3.4132774
C	1.2114492	7.1315392	-4.2199626
H	1.3378621	7.0765446	-3.1286855
H	1.0040095	8.1811084	-4.4651182
C	0.0944781	6.2517999	-4.6968387
N	-0.9438749	6.7017486	-5.4894715
H	-1.1068102	7.6646145	-5.7679647
C	-1.6889367	5.6310489	-5.8718307
H	-2.5527281	5.6963663	-6.5337442
N	-1.1854578	4.5184050	-5.3693859
C	-0.0844477	4.8874511	-4.6351470
H	0.5362123	4.1521605	-4.1256557

C	2.2142275	3.7053799	-10.2725944
H	2.1005255	4.7891964	-10.1250984
H	1.7136872	3.4590303	-11.2280896
C	1.5147222	2.9785301	-9.1702815
N	1.5573955	1.6085365	-8.9945139
H	2.1507526	0.9609109	-9.5083776
C	0.6822875	1.2761088	-8.0170900
H	0.5598447	0.2602379	-7.6548421
N	0.0631248	2.3495712	-7.5520082
C	0.5821676	3.4166970	-8.2580399
H	0.2537756	4.4378222	-8.0855268
C	0.1478648	-1.0984756	-1.9641712
H	0.1862286	-2.0616397	-2.4907806
H	-0.4660332	-1.2274463	-1.0585489
C	-0.4671670	-0.0264435	-2.8067462
N	-1.0249609	1.1056704	-2.2310904
H	-1.1189892	1.2799669	-1.2362774
C	-1.4040896	1.9461797	-3.2258326
H	-1.8859038	2.9063360	-3.0555011
N	-1.1231188	1.4233506	-4.4026177
C	-0.5392476	0.1983056	-4.1607826
H	-0.2203439	-0.4633637	-4.9625408
Cu	-5.2922583	1.9826228	-6.1228951
Cu	-1.4469325	2.5280090	-6.1490609
O	-3.7241391	2.6474979	-7.7411210
O	-3.4670758	2.6988712	-6.3339425
C	-2.2076753	4.0364248	-10.2646950
C	-2.9868845	5.1383571	-9.7726035
C	-3.1392912	6.3148797	-10.6366631
C	-2.5524188	6.3627471	-11.9027423
C	-1.8342680	5.2530094	-12.3422933
C	-1.6549336	4.1013435	-11.5205611
O	-3.8773447	7.2990265	-10.1406221
H	-4.1852934	6.9598760	-9.2698574
H	-2.6916242	7.2390769	-12.5375443
H	-1.4070140	5.2492899	-13.3452837
H	-1.0814764	3.2632190	-11.9210060
H	-2.0831673	3.1684183	-9.6166237
O	-3.5621828	5.1860243	-8.6416245
H	-3.7930239	3.6099595	-7.9942788
H	-9.8050506	-2.0461165	-7.7233949
H	-7.9220807	7.4961767	-5.0060511
H	-5.0105642	0.3863871	-0.0015678
H	2.1675730	6.8697653	-4.6731383
H	3.2757205	3.4796492	-10.3743037
H	1.1569466	-0.8043458	-1.6755400

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C	-8.7257995	-2.2153060	-7.7381007
H	-8.4949135	-2.8812189	-6.8933037
H	-8.5283241	-2.7949160	-8.6561074
C	-7.8245500	-1.0157374	-7.6650600
N	-7.4548488	-0.2651166	-8.7630157
H	-7.7055249	-0.4224974	-9.7452917
C	-6.5970530	0.6957079	-8.3718685
H	-6.1421937	1.4204013	-9.0449051
N	-6.3889369	0.6196660	-7.0624925
C	-7.1467975	-0.4389118	-6.6123053
H	-7.1652222	-0.7286172	-5.5705554
C	-7.5739845	7.2856023	-5.9874470
H	-8.3096436	7.6541379	-6.7148934
H	-6.6539251	7.8745349	-6.1371092
C	-7.3057795	5.8454032	-6.2624034
N	-8.1723052	5.0628431	-6.9975409
H	-9.0870049	5.3614124	-7.3467889
C	-7.6474668	3.8170032	-7.0868683
H	-8.1277974	3.0068346	-7.6337965
N	-6.4961840	3.7526042	-6.4396569
C	-6.2633100	5.0101538	-5.9379290
H	-5.3610942	5.2456543	-5.3782771
C	-4.4004614	1.1130760	-0.5891867
H	-4.2446341	1.9793967	0.0740064
H	-3.4211768	0.6399047	-0.7597303
C	-4.9384436	1.5227124	-1.9343123
N	-5.9094991	2.4853758	-2.1233358
H	-6.2979186	3.0662089	-1.3753765
C	-6.1625496	2.5952082	-3.4458161
H	-6.8842525	3.2916783	-3.8643635
N	-5.3987788	1.7584804	-4.1365207
C	-4.6366522	1.0804955	-3.2063936
H	-3.9158424	0.3186039	-3.4922391
C	1.2069788	7.1253931	-4.2197743
H	1.3331539	7.0908738	-3.1274424
H	0.9765098	8.1662305	-4.4817100
C	0.1181599	6.2054759	-4.6895390
N	-0.9683047	6.6129713	-5.4411635

H	-1.1996823	7.5716370	-5.6836807
C	-1.6605060	5.5114919	-5.8346464
H	-2.5537626	5.5314190	-6.4621581
N	-1.0719907	4.4200154	-5.3800379
C	0.0238757	4.8314478	-4.6650365
H	0.7012349	4.1219342	-4.1921129
C	2.1971327	3.6943196	-10.2139414
H	2.0811379	4.7757380	-10.0523577
H	1.6864768	3.4589966	-11.1665783
C	1.5095066	2.9513788	-9.1123329
N	1.5798792	1.5815279	-8.9364907
H	2.1790094	0.9454865	-9.4588185
C	0.7194846	1.2268384	-7.9586618
H	0.6149814	0.2069104	-7.6029098
N	0.0817917	2.2892569	-7.4885017
C	0.5724202	3.3710985	-8.1964354
H	0.2204953	4.3835288	-8.0232925
C	0.1696248	-1.1216392	-1.9930773
H	0.2183893	-2.0977218	-2.4943282
H	-0.4600998	-1.2285717	-1.0957271
C	-0.4283278	-0.0716592	-2.8748622
N	-1.0151994	1.0642798	-2.3370310
H	-1.1479806	1.2516623	-1.3488152
C	-1.3707614	1.8862038	-3.3508178
H	-1.8687549	2.8431388	-3.2172684
N	-1.0424500	1.3457403	-4.5097273
C	-0.4560655	0.1291005	-4.2341246
H	-0.1096382	-0.5439692	-5.0137834
Cu	-5.1102253	2.0000795	-6.2029237
Cu	-1.5112697	2.4169660	-6.2044920
O	-4.2326959	2.4229018	-7.9267214
O	-3.3148434	2.7663131	-6.1760956
C	-2.4335859	4.0536843	-10.1174746
C	-3.1856941	5.1820826	-9.6390106
C	-3.2573762	6.3724664	-10.4974799
C	-2.6168546	6.4103831	-11.7372436
C	-1.9210315	5.2779608	-12.1598744
C	-1.8252616	4.1104968	-11.3477270
O	-3.9750668	7.3787887	-10.0128533
H	-4.3203740	7.0326300	-9.1574099
H	-2.6995009	7.2953447	-12.3704365
H	-1.4514070	5.2697679	-13.1441327
H	-1.2762535	3.2508807	-11.7358737
H	-2.3903245	3.1710503	-9.4789062
O	-3.7934287	5.2398660	-8.5310777
H	-4.2506274	3.4027596	-8.0151963
H	-9.7964146	-2.0152903	-7.6951650
H	-7.9645258	7.5107910	-4.9950590
H	-5.0285332	0.3929670	-0.0647486
H	2.1669908	6.8731550	-4.6701292
H	3.2583361	3.4736267	-10.3288694
H	1.1731696	-0.8185175	-1.6946118

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C	-8.5574904	-2.0956448	-7.7053444
H	-8.3267845	-2.7594991	-6.8591483
H	-8.3561119	-2.6754696	-8.6225466
C	-7.6476980	-0.8961481	-7.6298889
N	-7.2633170	-0.1535461	-8.7296427
H	-7.5337907	-0.3059221	-9.7080009
C	-6.3833656	0.7899884	-8.3432875
H	-5.9364342	1.5149277	-9.0222025
N	-6.1711732	0.7097424	-7.0348324
C	-6.9528881	-0.3322675	-6.5790425
H	-6.9766736	-0.6122910	-5.5339015
C	-7.5381510	7.2748627	-6.0031594
H	-8.2740047	7.6443002	-6.7303310
H	-6.6205654	7.8682425	-6.1504745
C	-7.2618931	5.8367530	-6.2912508
N	-8.1260907	5.0577531	-7.0356080
H	-9.0463270	5.3536890	-7.3715103
C	-7.5854394	3.8213327	-7.1569479
H	-8.0634031	3.0178733	-7.7151136
N	-6.4239305	3.7600559	-6.5271675
C	-6.2046507	5.0089089	-5.9948640
H	-5.2976662	5.2243449	-5.4360224
C	-4.4256230	1.1101586	-0.5120060
H	-4.2767587	1.9752424	0.1537268
H	-3.4428515	0.6432392	-0.6816046
C	-4.9771879	1.5077212	-1.8532607
N	-5.9266003	2.4910349	-2.0479330
H	-6.2817767	3.1020834	-1.3076379
C	-6.2232077	2.5517486	-3.3644265
H	-6.9275170	3.2623167	-3.7886953
N	-5.5148272	1.6598365	-4.0421073
C	-4.7367426	1.0023535	-3.1130243

H	-4.0407363	0.2137722	-3.3880286
C	1.2567203	7.1728745	-4.2172805
H	1.3663413	7.1023352	-3.1244961
H	1.0786018	8.2301600	-4.4517212
C	0.1185888	6.3427859	-4.7273138
N	-0.9966086	6.8883273	-5.3370966
H	-1.1865379	7.8781958	-5.4595905
C	-1.7783393	5.8779540	-5.7896640
H	-2.7111032	6.0155018	-6.3344291
N	-1.2213996	4.7140658	-5.5084460
C	-0.0505231	4.9806223	-4.8437383
H	0.6143618	4.1843371	-4.5140283
C	2.0307882	3.9832443	-10.1414685
H	2.0404016	5.0583812	-9.9141767
H	1.5564727	3.8787272	-11.1349731
C	1.1506986	3.2782805	-9.1557543
N	0.7319847	1.9708073	-9.3305441
H	1.0618794	1.3342825	-10.0514031
C	-0.2233319	1.6949482	-8.4163638
H	-0.7710325	0.7634509	-8.3826507
N	-0.4434079	2.7417647	-7.6411615
C	0.4075910	3.7375659	-8.0896454
H	0.4067286	4.7332531	-7.6587435
C	0.0968683	-0.9334054	-2.2066687
H	0.1435203	-1.8852816	-2.7527379
H	-0.5508756	-1.0891940	-1.3283707
C	-0.4962532	0.1585696	-3.0488603
N	-1.0998039	1.2599089	-2.4584558
H	-1.2113271	1.4111612	-1.4617848
C	-1.5109700	2.1000590	-3.4376084
H	-2.0497000	3.0265318	-3.2528315
N	-1.2036598	1.6157761	-4.6253274
C	-0.5680192	0.4103760	-4.4014605
H	-0.2224177	-0.2250246	-5.2135644
Cu	-5.0077470	2.0819702	-6.0670363
Cu	-2.0131627	2.8865422	-6.2897978
O	-3.5600385	2.3959386	-7.4922057
O	-3.6489811	3.2483181	-5.3656668
C	-2.3606830	4.0032828	-10.3061565
C	-3.0870849	5.0866743	-9.7047128
C	-3.2107992	6.3339628	-10.4695152
C	-2.6263810	6.4684549	-11.7303683
C	-1.9466314	5.3761113	-12.2684651
C	-1.8098497	4.1509809	-11.5544465
O	-3.9138340	7.2966347	-9.8852399
H	-4.2283959	6.8927194	-9.0449838
H	-2.7402439	7.3977821	-12.2913160
H	-1.5260523	5.4422916	-13.2715007
H	-1.2800525	3.3264188	-12.0349173
H	-2.2775768	3.0854212	-9.7264693
O	-3.6247232	5.0532444	-8.5605363
H	-3.7661827	3.2828050	-7.8682667
H	-9.6316501	-1.9133489	-7.6734754
H	-7.9299853	7.5010429	-5.0115068
H	-5.0575837	0.3848727	0.0004903
H	2.2133595	6.8998627	-4.6626707
H	3.0621175	3.6377868	-10.2127807
H	1.0974861	-0.6614910	-1.8706730

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C	-8.5821601	-2.0294189	-7.7019922
H	-8.3375454	-2.6721453	-6.8440471
H	-8.3822604	-2.6269145	-8.6076451
C	-7.6870556	-0.8153075	-7.6764596
N	-7.2733004	-0.1706062	-8.8245625
H	-7.5272836	-0.4018414	-9.7918573
C	-6.4310229	0.8272335	-8.5011086
H	-5.9702813	1.4901381	-9.2343741
N	-6.2693259	0.8737801	-7.1829673
C	-7.0466237	-0.1390250	-6.6559520
H	-7.1100944	-0.3071182	-5.5874271
C	-7.7506097	7.2545345	-6.0674718
H	-8.5525344	7.5845289	-6.7400533
H	-6.8580635	7.8539318	-6.3135154
C	-7.4725346	5.8119697	-6.3247772
N	-8.2750681	5.0324536	-7.1330300
H	-9.1728427	5.3299004	-7.5242426
C	-7.7293806	3.8002929	-7.2285819
H	-8.1544214	2.9972301	-7.8264745
N	-6.6161351	3.7476052	-6.5111239
C	-6.4402318	4.9913908	-5.9503555
H	-5.5796422	5.2204293	-5.3291991
C	-4.3598921	1.1278715	-0.5527753
H	-4.1992425	1.9751754	0.1342798
H	-3.3838574	0.6502955	-0.7293705
C	-4.8942133	1.5754044	-1.8865945

N	-5.8891044	2.5192721	-2.0388141
H	-6.2861367	3.0669849	-1.2715336
C	-6.1469541	2.6636932	-3.3586811
H	-6.8985494	3.3485799	-3.7432661
N	-5.3678145	1.8750008	-4.0819619
C	-4.5878693	1.1866166	-3.1766421
H	-3.8445739	0.4592818	-3.4967442
C	1.2813422	7.1938387	-4.1804067
H	1.4001372	7.1307771	-3.0883871
H	1.1070426	8.2496758	-4.4231771
C	0.1302559	6.3744438	-4.6730601
N	-0.9901218	6.9401406	-5.2536037
H	-1.1654488	7.9332907	-5.3729966
C	-1.8002635	5.9529446	-5.6930000
H	-2.7424331	6.1143533	-6.2142288
N	-1.2548481	4.7764130	-5.4250967
C	-0.0593286	5.0161698	-4.7909532
H	0.6003162	4.2059548	-4.4882312
C	1.9901808	3.8504814	-10.1893502
H	1.9577947	4.9402222	-10.0459398
H	1.5273950	3.6508589	-11.1736477
C	1.1376228	3.1996433	-9.1406914
N	0.7464742	1.8715294	-9.1857373
H	1.0810281	1.1781484	-9.8502200
C	-0.1795588	1.6566803	-8.2201183
H	-0.6879375	0.7084918	-8.0672091
N	-0.4063840	2.7662897	-7.5384679
C	0.4060647	3.7335253	-8.1004357
H	0.3964552	4.7645607	-7.7588684
C	0.0710570	-0.8882174	-2.2323587
H	0.1092163	-1.7856243	-2.8645693
H	-0.5600333	-1.1272019	-1.3602742
C	-0.5459340	0.2692766	-2.9643180
N	-1.0071027	1.3821975	-2.2743579
H	-1.0106902	1.4936203	-1.2657923
C	-1.4502344	2.2916320	-3.1751380
H	-1.8821099	3.2495121	-2.8925727
N	-1.3050029	1.8374882	-4.4045267
C	-0.7474469	0.5785170	-4.2916597
H	-0.5357905	-0.0428337	-5.1589666
Cu	-5.1348294	2.3371133	-6.3181373
Cu	-2.0276209	3.0402381	-6.1349838
O	-3.2731685	1.7784345	-6.9516249
O	-3.8354475	3.8071098	-6.1854063
C	-2.3677891	4.2861820	-11.1993107
C	-3.0301707	4.2260739	-9.9201298
C	-3.5044430	5.4966319	-9.3466125
C	-3.3927266	6.6830497	-10.0897048
C	-2.7825572	6.6712918	-11.3380574
C	-2.2469458	5.4678211	-11.8835668
O	-4.0333679	5.5358374	-8.1355088
H	-3.9770558	4.6805634	-7.5985108
H	-3.7903753	7.6039541	-9.6578119
H	-2.7157444	7.5946351	-11.9190075
H	-1.7754081	5.4801645	-12.8664516
H	-2.0023253	3.3514458	-11.6230113
O	-3.2014581	3.1451556	-9.2952655
H	-3.2830532	2.1088529	-7.8777430
H	-9.6584210	-1.8597595	-7.6712585
H	-8.0654068	7.4989613	-5.0529646
H	-5.0007110	0.4032736	-0.0504054
H	2.2314595	6.9119676	-4.6341603
H	3.0362438	3.5482191	-10.2389102
H	1.0761867	-0.6386438	-1.8925150

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C	-8.5830586	-2.0328717	-7.7041868
H	-8.3403861	-2.6779419	-6.8472845
H	-8.3806797	-2.6268986	-8.6114002
C	-7.6881595	-0.8191509	-7.6699600
N	-7.2525625	-0.1771109	-8.8118788
H	-7.4946320	-0.4057489	-9.7832289
C	-6.4142837	0.8195724	-8.4765141
H	-5.9356747	1.4796244	-9.2011202
N	-6.2771608	0.8666920	-7.1548820
C	-7.0663084	-0.1425077	-6.6390974
H	-7.1495505	-0.3092361	-5.5719153
C	-7.7682343	7.2414684	-6.0693157
H	-8.5773894	7.5641325	-6.7366846
H	-6.8798210	7.8416344	-6.3284467
C	-7.4888048	5.7980124	-6.3191096
N	-8.2734822	5.0201410	-7.1462325
H	-9.1635929	5.3181187	-7.5537832
C	-7.7266216	3.7890278	-7.2343068
H	-8.1390798	2.9881917	-7.8436443
N	-6.6288271	3.7350867	-6.4919667

C	-6.4658131	4.9772979	-5.9228752
H	-5.6177410	5.2071483	-5.2861857
C	-4.3588251	1.1295921	-0.5369237
H	-4.2001477	1.9764268	0.1510442
H	-3.3823460	0.6530899	-0.7137699
C	-4.8948465	1.5759288	-1.8698971
N	-5.8891129	2.5202732	-2.0217471
H	-6.2835284	3.0706641	-1.2547042
C	-6.1542297	2.6593315	-3.3396098
H	-6.9064380	3.3439230	-3.7235297
N	-5.3792446	1.8654862	-4.0628320
C	-4.5949729	1.1801749	-3.1588137
H	-3.8543708	0.4499718	-3.4782206
C	1.3105443	7.1970566	-4.1598846
H	1.4362520	7.1303736	-3.0690306
H	1.1313373	8.2529127	-4.3980633
C	0.1590480	6.3772086	-4.6493272
N	-0.9584067	6.9455009	-5.2326084
H	-1.1296937	7.9390065	-5.3553461
C	-1.7707715	5.9631385	-5.6749289
H	-2.7099384	6.1284873	-6.2033229
N	-1.2279956	4.7838328	-5.4058434
C	-0.0331440	5.0195794	-4.7672007
H	0.6247934	4.2082207	-4.4639307
C	1.9846899	3.8727475	-10.1769783
H	1.9565629	4.9624755	-10.0332805
H	1.5240831	3.6756740	-11.1626923
C	1.1260974	3.2248584	-9.1313178
N	0.7190012	1.9020106	-9.1891644
H	1.0367372	1.2145913	-9.8679082
C	-0.2033079	1.6854032	-8.2225803
H	-0.7237356	0.7423456	-8.0808913
N	-0.4122906	2.7900814	-7.5261168
C	0.4077250	3.7559236	-8.0809984
H	0.4095080	4.7831987	-7.7291014
C	0.0693896	-0.8928088	-2.2266152
H	0.1075078	-1.7887154	-2.8608868
H	-0.5604480	-1.1338395	-1.3542860
C	-0.5493350	0.2661750	-2.9543789
N	-1.0125932	1.3761141	-2.2608204
H	-1.0149346	1.4847579	-1.2518752
C	-1.4560714	2.2885582	-3.1577465
H	-1.8871958	3.2460887	-2.8727406
N	-1.3089234	1.8385850	-4.3888245
C	-0.7494850	0.5796877	-4.2806284
H	-0.5339322	-0.0370479	-5.1502730
Cu	-5.1731902	2.3171917	-6.2671715
Cu	-1.9876074	3.0468297	-6.1118693
O	-3.2871494	1.8294763	-6.9461661
O	-3.8383159	3.7813796	-6.0829164
C	-2.5094322	4.3531763	-11.0620375
C	-3.1008655	4.2038465	-9.7590007
C	-3.5242753	5.4345675	-9.0499044
C	-3.3974382	6.6810538	-9.7222475
C	-2.8493818	6.7561653	-10.9874669
C	-2.3844562	5.5818356	-11.6558698
O	-4.0016137	5.3984282	-7.8442839
H	-3.9278621	4.4675972	-7.0861996
H	-3.7498606	7.5727871	-9.1984483
H	-2.7737224	7.7229537	-11.4922377
H	-1.9678802	5.6578731	-12.6612660
H	-2.1954553	3.4454708	-11.5767346
O	-3.2457812	3.0626829	-9.2315338
H	-3.3166298	2.2303046	-7.8639791
H	-9.6592194	-1.8624833	-7.6739838
H	-8.0750758	7.4902705	-5.0534357
H	-5.0005360	0.4037978	-0.0374277
H	2.2584422	6.9189627	-4.6205579
H	3.0292721	3.5646221	-10.2213999
H	1.0747275	-0.6425802	-1.8878708

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C	-8.5714079	-2.0214846	-7.6877928
H	-8.3296143	-2.6589434	-6.8253693
H	-8.3745015	-2.6280026	-8.5883716
C	-7.6670081	-0.8140278	-7.6746399
N	-7.2746067	-0.1714964	-8.8305030
H	-7.5476308	-0.3968851	-9.7930964
C	-6.4136787	0.8167738	-8.5216422
H	-5.9651416	1.4757434	-9.2649054
N	-6.2192122	0.8614441	-7.2103366
C	-6.9941909	-0.1448473	-6.6687515
H	-7.0311988	-0.3159392	-5.5991676
C	-7.8145342	7.2187012	-6.0873022
H	-8.6471020	7.5184930	-6.7364208
H	-6.9461730	7.8376612	-6.3700555

C	-7.5076120	5.7796517	-6.3347160
N	-8.2891647	4.9791880	-7.1432753
H	-9.1932764	5.2557058	-7.5327542
C	-7.7071970	3.7619942	-7.2376016
H	-8.1148784	2.9476425	-7.8321652
N	-6.5898480	3.7388683	-6.5251452
C	-6.4539295	4.9879036	-5.9602805
H	-5.5937509	5.2332813	-5.3476446
C	-4.3469635	1.1199817	-0.5554886
H	-4.1862749	1.9643440	0.1354463
H	-3.3711351	0.6404191	-0.7291467
C	-4.8729724	1.5744345	-1.8903444
N	-5.8614906	2.5251450	-2.0436929
H	-6.2587655	3.0735978	-1.2775564
C	-6.1089888	2.6764506	-3.3661986
H	-6.8530260	3.3691736	-3.7518327
N	-5.3324001	1.8857517	-4.0877459
C	-4.5624684	1.1894668	-3.1810177
H	-3.8210327	0.4609608	-3.5033198
C	1.2924742	7.1446481	-4.1912018
H	1.4172454	7.0747580	-3.0998559
H	1.1122745	8.2029200	-4.4224449
C	0.1409723	6.3271798	-4.6867862
N	-1.0260954	6.9036627	-5.1523781
H	-1.2370276	7.8960467	-5.1733686
C	-1.8424320	5.9272580	-5.6063234
H	-2.8350269	6.0967685	-6.0144563
N	-1.2568724	4.7490046	-5.4683019
C	-0.0282919	4.9762707	-4.8950020
H	0.6629057	4.1624504	-4.6858366
C	2.0123520	3.8203096	-10.2165154
H	1.9760701	4.9087003	-10.0618638
H	1.5549765	3.6277732	-11.2051963
C	1.1565032	3.1572246	-9.1791925
N	0.8044313	1.8181971	-9.2071088
H	1.1865572	1.1176106	-9.8377063
C	-0.1437850	1.6002149	-8.2596672
H	-0.6189903	0.6365985	-8.0895434
N	-0.4239696	2.7170762	-7.6126687
C	0.3786483	3.6919622	-8.1725394
H	0.3423254	4.7274361	-7.8440876
C	0.0602247	-0.8739908	-2.2362078
H	0.0941229	-1.7776067	-2.8601752
H	-0.5744793	-1.1018306	-1.3634991
C	-0.5466715	0.2807909	-2.9816892
N	-0.9966767	1.4069132	-2.3057090
H	-1.0074292	1.5283589	-1.2985830
C	-1.4275909	2.3103232	-3.2198284
H	-1.8508683	3.2758247	-2.9508163
N	-1.2839109	1.8412341	-4.4427372
C	-0.7437189	0.5773938	-4.3127772
H	-0.5422351	-0.0580050	-5.1719923
Cu	-5.0411804	2.3469263	-6.3605620
Cu	-2.0968956	3.0013885	-6.1905528
O	-3.2420398	1.5784158	-6.8597661
O	-3.8504898	3.9323997	-6.0824490
C	-2.2584411	4.2957540	-11.3067992
C	-3.0208813	4.2899018	-10.0594234
C	-3.5483756	5.6608183	-9.5375037
C	-3.4547553	6.8079954	-10.4467142
C	-2.7868616	6.6871350	-11.6186320
C	-2.1636905	5.4288083	-12.0393715
O	-3.9743434	5.7447781	-8.3979234
H	-3.9473570	4.3821778	-6.9442403
H	-3.9039897	7.7471267	-10.1163118
H	-2.7006109	7.5424992	-12.2943236
H	-1.6405179	5.4081665	-12.9965770
H	-1.8333484	3.3560510	-11.6593817
O	-3.2530364	3.2858042	-9.4058745
H	-3.2061430	1.5545109	-7.8281823
H	-9.6472649	-1.8487405	-7.6602665
H	-8.1028365	7.4697334	-5.0665520
H	-4.9916977	0.3958079	-0.0575362
H	2.2419028	6.8717890	-4.6518531
H	3.0600906	3.5242551	-10.2681094
H	1.0660239	-0.6278751	-1.8958234

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C	-8.7149861	-2.1817987	-7.7545230
H	-8.4812504	-2.8349892	-6.9008698
H	-8.5227129	-2.7737800	-8.6653359
C	-7.8150337	-0.9786494	-7.7108967
N	-7.4289920	-0.2813166	-8.8378097
H	-7.6816519	-0.4969085	-9.8092956
C	-6.5951719	0.7134462	-8.4852907
H	-6.1586170	1.4181613	-9.1936099

N	-6.4152580	0.7023559	-7.1673460
C	-7.1689224	-0.3423185	-6.6735403
H	-7.2124975	-0.5647381	-5.6150692
C	-7.6906257	7.2472081	-6.0365444
H	-8.4537669	7.6121310	-6.7358716
H	-6.7733248	7.8256558	-6.2362250
C	-7.4465849	5.8016094	-6.3092728
N	-8.2785276	5.0507508	-7.1145910
H	-9.1740583	5.3722268	-7.4931181
C	-7.7715387	3.8034993	-7.2203592
H	-8.2258803	3.0159159	-7.8182047
N	-6.6558310	3.7098638	-6.5114414
C	-6.4365921	4.9468348	-5.9484019
H	-5.5673739	5.1550136	-5.3314023
C	-4.3736895	1.1214577	-0.5397709
H	-4.2111862	1.9729435	0.1411618
H	-3.3987431	0.6426791	-0.7186444
C	-4.9191290	1.5577261	-1.8723001
N	-5.9001463	2.5156095	-2.0231652
H	-6.2769061	3.0794751	-1.2566381
C	-6.1874667	2.6376654	-3.3369270
H	-6.9361844	3.3257009	-3.7209398
N	-5.4376940	1.8182160	-4.0597647
C	-4.6469103	1.1354739	-3.1588308
H	-3.9262552	0.3850678	-3.4767063
C	1.3135171	7.2214127	-4.2301837
H	1.4074167	7.1458596	-3.1368418
H	1.1482120	8.2797086	-4.4674640
C	0.1754427	6.4033995	-4.7541648
N	-0.8482763	6.9422994	-5.5109926
H	-0.9658069	7.9240841	-5.7464547
C	-1.6397439	5.9404124	-5.9533907
H	-2.5081975	6.0793214	-6.6013348
N	-1.1763736	4.7777447	-5.5153423
C	-0.0530108	5.0468450	-4.7680141
H	0.5425641	4.2541506	-4.3205303
C	2.0679526	4.0206348	-10.2608157
H	2.0733211	5.0956676	-10.0348314
H	1.6075009	3.9141314	-11.2599076
C	1.1843753	3.3133199	-9.2838781
N	0.6795849	2.0487408	-9.5249626
H	0.9187461	1.4623792	-10.3199515
C	-0.2278562	1.7525693	-8.5695578
H	-0.8270333	0.8504887	-8.5724369
N	-0.3290723	2.7458733	-7.7031667
C	0.5433537	3.7269884	-8.1383197
H	0.6177652	4.6893524	-7.6427262
C	0.0660719	-0.9030477	-2.1993768
H	0.1008233	-1.8263979	-2.7928847
H	-0.5681084	-1.1002328	-1.3193177
C	-0.5368712	0.2299649	-2.9785754
N	-1.0598037	1.3400782	-2.3294116
H	-1.1145178	1.4661483	-1.3241392
C	-1.4742078	2.2283678	-3.2636846
H	-1.9404801	3.1805982	-3.0192903
N	-1.2497299	1.7624608	-4.4775949
C	-0.6661067	0.5202696	-4.3186268
H	-0.3844503	-0.1000732	-5.1664665
Cu	-5.3739804	2.1272188	-6.2308846
Cu	-1.7595493	2.9596091	-6.2190609
O	-3.7785979	3.3302856	-6.3229441
O	-3.4148421	2.1448333	-7.0040528
C	-2.8145997	4.2135930	-9.7823196
C	-3.3284038	5.3926316	-9.2444389
C	-3.1919980	6.6130828	-9.9347119
C	-2.5336950	6.6391514	-11.1649221
C	-2.0047980	5.4581248	-11.7003861
C	-2.1447494	4.2500424	-11.0130594
O	-3.7097414	7.7496439	-9.3929681
H	-4.2197154	7.4789865	-8.6141419
H	-2.4674542	7.5878224	-11.7018660
H	-1.5120052	5.4783493	-12.6732725
H	-1.7603616	3.3291937	-11.4545846
H	-2.9534058	3.2757673	-9.2391875
O	-3.9794100	5.4824055	-8.0370217
H	-4.0223436	4.6165484	-7.5713570
H	-9.7853339	-1.9799431	-7.7135796
H	-8.0369995	7.4881942	-5.0315482
H	-5.0125565	0.3986927	-0.0323004
H	2.2719561	6.9363484	-4.6640032
H	3.0992035	3.6709250	-10.3086818
H	1.0726619	-0.6476045	-1.8683302

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C	-8.7057584	-2.1428810	-7.7576098
H	-8.4610801	-2.7908375	-6.9032050

H	-8.5177684	-2.7397518	-8.6663865
C	-7.8074313	-0.9369364	-7.7317136
N	-7.4427634	-0.2481180	-8.8702221
H	-7.7139832	-0.4709264	-9.8344056
C	-6.6016529	0.7491838	-8.5392559
H	-6.1829725	1.4516617	-9.2608283
N	-6.3947233	0.7482157	-7.2264200
C	-7.1399521	-0.2926014	-6.7116275
H	-7.1628138	-0.5064904	-5.6500986
C	-7.7868250	7.2809075	-6.0661688
H	-8.5718194	7.6468820	-6.7398959
H	-6.8766398	7.8612356	-6.2923995
C	-7.5508302	5.8349602	-6.3433572
N	-8.3790756	5.0900824	-7.1581362
H	-9.2721624	5.4151560	-7.5387562
C	-7.8771884	3.8395855	-7.2608898
H	-8.3287162	3.0545862	-7.8646083
N	-6.7698203	3.7406077	-6.5417060
C	-6.5494428	4.9748400	-5.9740384
H	-5.6851812	5.1733955	-5.3472208
C	-4.3829860	1.1370985	-0.5870878
H	-4.2084357	1.9850597	0.0956076
H	-3.4119320	0.6580577	-0.7841348
C	-4.9439046	1.5842139	-1.9106164
N	-5.9354354	2.5341410	-2.0429784
H	-6.3111970	3.0858174	-1.2678141
C	-6.2262257	2.6740590	-3.3557104
H	-6.9839741	3.3597908	-3.7259434
N	-5.4713254	1.8760987	-4.0944803
C	-4.6721131	1.1876171	-3.2061455
H	-3.9454934	0.4494781	-3.5382648
C	1.3467196	7.1321960	-4.2190828
H	1.4697591	7.0858277	-3.1265701
H	1.1241287	8.1779221	-4.4698886
C	0.2417625	6.2432889	-4.6982971
N	-0.8518368	6.7188933	-5.3944772
H	-1.0493062	7.6926973	-5.6036732
C	-1.6003485	5.6632075	-5.7971348
H	-2.5084005	5.7612420	-6.3904301
N	-1.0483153	4.5299176	-5.3986502
C	0.0933703	4.8736258	-4.7121711
H	0.7610070	4.1207827	-4.2963630
C	2.1574790	4.0973587	-10.2905438
H	2.1797804	5.1466810	-9.9675893
H	1.7154476	4.0862486	-11.3035031
C	1.2500069	3.3171608	-9.4018137
N	0.7352048	2.0926496	-9.7792282
H	0.9634516	1.6007961	-10.6393961
C	-0.1557502	1.6946591	-8.8443704
H	-0.7616793	0.8033466	-8.9420321
N	-0.2388188	2.5846715	-7.8717330
C	0.6291450	3.6052327	-8.2092155
H	0.7173091	4.5029963	-7.6051197
C	0.1193504	-1.0429897	-2.0406006
H	0.1535807	-2.0055086	-2.5685713
H	-0.5043909	-1.1726515	-1.1414737
C	-0.4827405	0.0352288	-2.8881297
N	-1.0484364	1.1638530	-2.3105353
H	-1.1534966	1.3299004	-1.3154005
C	-1.4206096	2.0113595	-3.2981198
H	-1.9046716	2.9699123	-3.1269830
N	-1.1277013	1.4955740	-4.4769219
C	-0.5420775	0.2678904	-4.2417103
H	-0.2087952	-0.3804517	-5.0482984
Cu	-5.3988949	2.2403975	-6.3084441
Cu	-1.4393180	2.5599633	-6.2086850
O	-3.9159763	3.5615517	-6.3601107
O	-3.3678829	2.3295136	-6.8240644
C	-2.7830004	4.0528267	-9.7360723
C	-3.3931432	5.2113682	-9.2051247
C	-3.3852611	6.4240247	-9.9864684
C	-2.7584142	6.4645548	-11.2344123
C	-2.1544591	5.3079891	-11.7279603
C	-2.1709016	4.1093812	-10.9796727
O	-3.9941051	7.5008029	-9.4697107
H	-4.3718501	7.2057254	-8.6190566
H	-2.7724261	7.3917869	-11.8105108
H	-1.6933393	5.3156153	-12.7162585
H	-1.7045780	3.2213160	-11.4075084
H	-2.8098660	3.1387990	-9.1401805
O	-3.9637945	5.2966127	-8.0255923
H	-3.9635468	4.3425698	-7.2818439
H	-9.7770894	-1.9479865	-7.7093144
H	-8.1025820	7.5184569	-5.0503272
H	-5.0113977	0.4116134	-0.0705255
H	2.3076359	6.8816148	-4.6684328
H	3.1796578	3.7218964	-10.3379255
H	1.1285186	-0.7597365	-1.7415793

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C	-8.7101051	-2.1764169	-7.7737714
H	-8.4675209	-2.8304128	-6.9231556
H	-8.5305721	-2.7704131	-8.6862633
C	-7.8025755	-0.9786649	-7.7415042
N	-7.4618951	-0.2581908	-8.8673075
H	-7.7479591	-0.4566565	-9.8321548
C	-6.6048762	0.7233633	-8.5249061
H	-6.1991032	1.4438552	-9.2356012
N	-6.3649765	0.6817052	-7.2197062
C	-7.1041363	-0.3704597	-6.7203066
H	-7.0994788	-0.6230051	-5.6669136
C	-7.7863442	7.2732453	-6.0659491
H	-8.5709464	7.6392177	-6.7401496
H	-6.8751656	7.8518884	-6.2937060
C	-7.5553994	5.8251072	-6.3378571
N	-8.3694057	5.0881362	-7.1733687
H	-9.2533752	5.4186160	-7.5694979
C	-7.8770977	3.8309181	-7.2573795
H	-8.3229368	3.0486954	-7.8692962
N	-6.7914279	3.7191917	-6.5094420
C	-6.5753939	4.9528253	-5.9387474
H	-5.7305645	5.1431320	-5.2833086
C	-4.3752575	1.1402302	-0.5437512
H	-4.2029766	1.9837700	0.1449134
H	-3.4035137	0.6636280	-0.7434637
C	-4.9410736	1.5910372	-1.8629930
N	-5.9446769	2.5294787	-1.9864057
H	-6.3205897	3.0754758	-1.2075425
C	-6.2512017	2.6640593	-3.2955624
H	-7.0201540	3.3400830	-3.6602787
N	-5.4941330	1.8734260	-4.0390601
C	-4.6767342	1.1959226	-3.1597839
H	-3.9444892	0.4671601	-3.4997995
C	1.3348303	7.1101049	-4.2291812
H	1.4571396	7.0601090	-3.1364206
H	1.1152433	8.1579617	-4.4752554
C	0.2248407	6.2270916	-4.7093128
N	-0.8894423	6.7166639	-5.3609296
H	-1.0940562	7.6944128	-5.5410499
C	-1.6510582	5.6646140	-5.7560344
H	-2.5817272	5.7775968	-6.3066969
N	-1.0899815	4.5237258	-5.3997193
C	0.0732167	4.8573366	-4.7455344
H	0.7499069	4.0960518	-4.3602236
C	2.1774245	4.1062525	-10.2923352
H	2.2025290	5.1491635	-9.9494457
H	1.7381692	4.1147058	-11.3066170
C	1.2679889	3.3100943	-9.4208683
N	0.7716900	2.0832795	-9.8135679
H	1.0234445	1.5940665	-10.6685748
C	-0.1199598	1.6664709	-8.8846161
H	-0.7082293	0.7649806	-8.9914901
N	-0.2259190	2.5484081	-7.9079587
C	0.6319449	3.5816743	-8.2321621
H	0.7085273	4.4740315	-7.6178007
C	0.1463913	-1.0707969	-2.0132744
H	0.1820490	-2.0429590	-2.5235477
H	-0.4817086	-1.1811063	-1.1147675
C	-0.4420902	-0.0048504	-2.8842156
N	-1.0322683	1.1226539	-2.3312051
H	-1.1693278	1.2946082	-1.3412866
C	-1.3707727	1.9644665	-3.3381453
H	-1.8670547	2.9204220	-3.1889451
N	-1.0323239	1.4468860	-4.5031331
C	-0.4521298	0.2239318	-4.2398723
H	-0.0890835	-0.4279921	-5.0304885
Cu	-5.4374689	2.1665369	-6.2146684
Cu	-1.3848003	2.5020793	-6.2361237
O	-3.9154103	3.6148429	-6.2182122
O	-3.4104690	2.3495508	-6.6759509
C	-2.7419527	4.0628892	-9.8179094
C	-3.4081968	5.2425456	-9.3466274
C	-3.4018111	6.4329362	-10.2068197
C	-2.7467025	6.4303252	-11.4408902
C	-2.1153729	5.2590241	-11.8514100
C	-2.1116268	4.0866059	-11.0384259
O	-4.0478826	7.4897531	-9.7338383
H	-4.4109469	7.1938437	-8.8692798
H	-2.7588022	7.3218675	-12.0703084
H	-1.6283936	5.2223562	-12.8268194
H	-1.6021145	3.2006854	-11.4178894
H	-2.7484385	3.1824083	-9.1724637
O	-3.9949703	5.3589936	-8.2271193
H	-4.0043302	4.1650972	-7.0528786
H	-9.7792945	-1.9717748	-7.7187973
H	-8.1009748	7.5147276	-5.0506854

H	-5.0060226	0.4107370	-0.0357732
H	2.2967712	6.8610663	-4.6771945
H	3.1983845	3.7280614	-10.3440907
H	1.1549008	-0.7835232	-1.7158707

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C	-8.6652888	-2.0830278	-7.7342632
H	-8.4218932	-2.7305896	-6.8792627
H	-8.4680054	-2.6782579	-8.6422813
C	-7.7702004	-0.8727250	-7.7023696
N	-7.3819092	-0.2002844	-8.8432003
H	-7.6430652	-0.4303651	-9.8083583
C	-6.5452694	0.8004076	-8.5090775
H	-6.1132023	1.4933480	-9.2315002
N	-6.3644310	0.8178861	-7.1933666
C	-7.1217447	-0.2137335	-6.6778253
H	-7.1665005	-0.4074613	-5.6128068
C	-7.8863738	7.2671057	-6.1065498
H	-8.7119359	7.6039984	-6.7451851
H	-6.9990021	7.8586790	-6.3894069
C	-7.6361523	5.8195851	-6.3620842
N	-8.4096549	5.0653204	-7.2205070
H	-9.2880943	5.3807044	-7.6390952
C	-7.8896621	3.8195056	-7.2920854
H	-8.3009644	3.0288886	-7.9163624
N	-6.8218716	3.7346992	-6.5129441
C	-6.6511511	4.9715759	-5.9319875
H	-5.8250374	5.1768122	-5.2595237
C	-4.3828019	1.1323825	-0.5608610
H	-4.2045467	1.9780896	0.1235495
H	-3.4131655	0.6522586	-0.7641420
C	-4.9580328	1.5774162	-1.8784750
N	-5.9565546	2.5215856	-2.0003439
H	-6.3206301	3.0779794	-1.2233074
C	-6.2789731	2.6401390	-3.3082960
H	-7.0452958	3.3208756	-3.6702859
N	-5.5398320	1.8338377	-4.0518573
C	-4.7151749	1.1640251	-3.1740912
H	-3.9927427	0.4241422	-3.5118848
C	1.3007480	7.0495982	-4.2505307
H	1.4053802	6.9757484	-3.1573932
H	1.0777871	8.1022619	-4.4743917
C	0.2021150	6.1745372	-4.7749947
N	-0.9318147	6.6902268	-5.3722557
H	-1.1596106	7.6742320	-5.4725662
C	-1.6819555	5.6635435	-5.8377629
H	-2.6225332	5.8018447	-6.3646050
N	-1.0921986	4.5086364	-5.5788109
C	0.0755123	4.8086191	-4.9137341
H	0.7664088	4.0296555	-4.5958401
C	2.1957018	4.0421982	-10.2938389
H	2.2017325	5.0971566	-9.9886554
H	1.7421449	4.0025415	-11.3012825
C	1.3187563	3.2589798	-9.3779115
N	0.8820987	1.9855060	-9.6883120
H	1.1679983	1.4455118	-10.5010375
C	-0.0065455	1.5962862	-8.7485635
H	-0.5537653	0.6649787	-8.7946163
N	-0.1640557	2.5399634	-7.8375475
C	0.6528656	3.5862044	-8.2201330
H	0.6808787	4.5221383	-7.6713378
C	0.1380555	-1.0132937	-2.0973357
H	0.1749118	-1.9872800	-2.6043005
H	-0.5077504	-1.1207692	-1.2109382
C	-0.4299161	0.0547842	-2.9829654
N	-1.0537132	1.1702086	-2.4432887
H	-1.2285919	1.3329349	-1.4578244
C	-1.3811196	2.0083946	-3.4568114
H	-1.9093525	2.9487929	-3.3157241
N	-1.0010868	1.5046996	-4.6142793
C	-0.4074390	0.2915197	-4.3386585
H	-0.0173135	-0.3551929	-5.1209297
Cu	-5.3586627	2.3109933	-6.2647818
Cu	-1.6212941	2.5897906	-6.4083077
O	-4.0775943	3.7930155	-5.9584292
O	-3.4105593	2.2046937	-6.7540187
C	-2.8653638	4.1835210	-9.7079213
C	-3.4393035	5.4240222	-9.2631987
C	-3.3503951	6.5839626	-10.1622990
C	-2.7123507	6.4954248	-11.4015904
C	-2.1575016	5.2731704	-11.7753912
C	-2.2347475	4.1283841	-10.9279118
O	-3.9077311	7.7018813	-9.7158125
H	-4.2725289	7.4603936	-8.8347806
H	-2.6729065	7.3658067	-12.0597789
H	-1.6755923	5.1738931	-12.7496762

H	-1.7905493	3.1987124	-11.2838388
H	-2.9486722	3.3188860	-9.0447430
O	-4.0015309	5.6145352	-8.1442971
H	-4.1219641	4.3106021	-6.7979893
H	-9.7388123	-1.8985152	-7.6946526
H	-8.1562433	7.5153274	-5.0800884
H	-5.0114947	0.4057083	-0.0463160
H	2.2707408	6.8180466	-4.6904903
H	3.2246488	3.6868908	-10.3494384
H	1.1431621	-0.7356286	-1.7799569

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C	-8.5900755	-2.0128772	-7.7068659
H	-8.3428679	-2.6502220	-6.8457833
H	-8.3923472	-2.6168345	-8.6090243
C	-7.6947983	-0.7993873	-7.6910248
N	-7.3137257	-0.1414649	-8.8425970
H	-7.5849319	-0.3778156	-9.8033647
C	-6.4631980	0.8545862	-8.5273286
H	-6.0358222	1.5355625	-9.2635670
N	-6.2663945	0.8878882	-7.2150902
C	-7.0281900	-0.1323868	-6.6809261
H	-7.0632187	-0.3143950	-5.6130173
C	-7.8249633	7.2685438	-6.0809460
H	-8.6542620	7.5779166	-6.7294780
H	-6.9537841	7.8863660	-6.3571410
C	-7.5248482	5.8293954	-6.3318299
N	-8.3068920	5.0351167	-7.1459792
H	-9.2085527	5.3160537	-7.5392387
C	-7.7374805	3.8127781	-7.2348881
H	-8.1461196	3.0016960	-7.8333963
N	-6.6274436	3.7804080	-6.5107746
C	-6.4813586	5.0291549	-5.9471386
H	-5.6258609	5.2708839	-5.3263716
C	-4.3563142	1.1487186	-0.5559772
H	-4.1893699	1.9898352	0.1373770
H	-3.3825329	0.6710199	-0.7440839
C	-4.9010855	1.6085678	-1.8816407
N	-5.9016345	2.5495464	-2.0145660
H	-6.2923267	3.0887819	-1.2385101
C	-6.1733771	2.7046481	-3.3310692
H	-6.9313267	3.3895072	-3.7024893
N	-5.3997442	1.9266898	-4.0688314
C	-4.6063108	1.2348124	-3.1793400
H	-3.8645340	0.5135619	-3.5173232
C	1.3355463	7.2116656	-4.1877810
H	1.4585072	7.1569149	-3.0954967
H	1.1643779	8.2667190	-4.4368110
C	0.1755086	6.3970543	-4.6627101
N	-0.9501232	6.9723877	-5.2226217
H	-1.1130616	7.9665668	-5.3498374
C	-1.7894051	5.9912543	-5.6189364
H	-2.7468110	6.1601931	-6.1049330
N	-1.2574421	4.8098349	-5.3484475
C	-0.0394036	5.0406225	-4.7535634
H	0.6144335	4.2245991	-4.4538336
C	1.9975836	3.9684985	-10.1470130
H	2.0157594	5.0517827	-9.9600300
H	1.5292750	3.8313642	-11.1392822
C	1.1068304	3.3119013	-9.1343966
N	0.6067438	2.0309330	-9.2943501
H	0.8712608	1.3819835	-10.0301680
C	-0.3295558	1.8077831	-8.3397648
H	-0.9250025	0.9029663	-8.2801852
N	-0.4585580	2.8607685	-7.5547450
C	0.4280179	3.8049993	-8.0388686
H	0.4964209	4.8005408	-7.6098183
C	0.0754935	-0.8697322	-2.2369013
H	0.1092566	-1.7613264	-2.8771890
H	-0.5560689	-1.1146689	-1.3668191
C	-0.5347707	0.3000688	-2.9553381
N	-1.0047949	1.3970189	-2.2460947
H	-1.0231916	1.4841046	-1.2352866
C	-1.4296292	2.3302696	-3.1299658
H	-1.8653089	3.2820421	-2.8330032
N	-1.2620275	1.9049933	-4.3674213
C	-0.7105720	0.6419884	-4.2785118
H	-0.4867216	0.0455369	-5.1602046
Cu	-5.1414229	2.3825894	-6.3302687
Cu	-2.0742031	3.0668597	-6.0220466
O	-3.8402514	3.9446057	-6.1386440
O	-3.3179412	1.8164631	-6.7447688
C	-2.7613662	4.2268701	-9.8742048
C	-3.3465253	5.4650629	-9.4375292
C	-3.3305977	6.5994642	-10.3710269
C	-2.7298774	6.4975737	-11.6264807

C	-2.1488691	5.2834277	-11.9873150
C	-2.1721277	4.1558980	-11.1136202
O	-3.9152195	7.7079683	-9.9359274
H	-4.2404614	7.4754967	-9.0369638
H	-2.7399367	7.3503150	-12.3076445
H	-1.6921678	5.1766579	-12.9724579
H	-1.7228336	3.2261656	-11.4636404
H	-2.8018634	3.3721050	-9.1952753
O	-3.8689003	5.6756410	-8.3038479
H	-3.9022337	4.4564511	-6.9793507
H	-9.6660915	-1.8420629	-7.6740244
H	-8.1140687	7.5133028	-5.0589003
H	-4.9932627	0.4205761	-0.0538103
H	2.2841864	6.9238398	-4.6408866
H	3.0283808	3.6192012	-10.2063013
H	1.0820090	-0.6270606	-1.8961617

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C	-8.5401061	-2.0872560	-7.6548958
H	-8.3275311	-2.7368024	-6.7934973
H	-8.3397296	-2.6916234	-8.5560822
C	-7.5986265	-0.9098480	-7.6116812
N	-7.1306151	-0.2867861	-8.7512964
H	-7.4034353	-0.4657945	-9.7247684
C	-6.2121435	0.6338087	-8.4103193
H	-5.6694949	1.2319471	-9.1366775
N	-6.0553102	0.6632547	-7.0926844
C	-6.9173755	-0.2898830	-6.5817949
H	-7.0026636	-0.4624235	-5.5165311
C	-7.8808138	7.1162853	-6.0708077
H	-8.7545840	7.3774771	-6.6819530
H	-7.0420680	7.7440010	-6.4199377
C	-7.5598342	5.6743401	-6.2900489
N	-8.2118943	4.9097668	-7.2352296
H	-9.0600508	5.1965620	-7.7257926
C	-7.6188156	3.6941245	-7.2880883
H	-7.9449650	2.9053676	-7.9630466
N	-6.6153202	3.6325702	-6.4237612
C	-6.5774802	4.8553000	-5.7949895
H	-5.8421190	5.0881798	-5.0307348
C	-4.4149151	1.1024074	-0.5339360
H	-4.2772907	1.9717912	0.1292603
H	-3.4283034	0.6387954	-0.6892786
C	-4.9528000	1.4898597	-1.8844044
N	-5.9582860	2.4140976	-2.0862862
H	-6.3623438	2.9980277	-1.3495908
C	-6.2345346	2.4685455	-3.4086049
H	-6.9902850	3.1258593	-3.8297806
N	-5.4548001	1.6377848	-4.0865335
C	-4.6552698	1.0209631	-3.1473722
H	-3.9015357	0.2859913	-3.4178350
C	1.3674050	7.1212127	-4.1711015
H	1.5244174	7.0637191	-3.0829864
H	1.1692482	8.1764957	-4.4057118
C	0.2042960	6.3011341	-4.6287715
N	-1.0153454	6.8864175	-4.9021794
H	-1.2418720	7.8694640	-4.7982859
C	-1.8494354	5.9430205	-5.3866496
H	-2.8743526	6.1405747	-5.6857229
N	-1.2321972	4.7753659	-5.4537267
C	0.0405310	4.9758717	-4.9702209
H	0.7612031	4.1635750	-4.9064549
C	2.0679055	3.8633148	-10.1654319
H	2.0565034	4.9512404	-10.0074182
H	1.6182968	3.6805979	-11.1601030
C	1.1789654	3.2261919	-9.1431190
N	0.8616087	1.8790960	-9.1273644
H	1.2872931	1.1638248	-9.7126312
C	-0.1261992	1.6778626	-8.2237502
H	-0.5676857	0.7105923	-8.0104009
N	-0.4675251	2.8172053	-7.6471018
C	0.3389460	3.7898839	-8.2058027
H	0.2598724	4.8373843	-7.9294602
C	0.0445025	-0.8671251	-2.2707448
H	0.0903839	-1.8135587	-2.8266832
H	-0.6081752	-1.0340271	-1.3976715
C	-0.5525769	0.2280574	-3.1093784
N	-1.1390128	1.3403386	-2.5218428
H	-1.2307927	1.5047446	-1.5252286
C	-1.5862438	2.1599172	-3.5039450
H	-2.1327364	3.0815932	-3.3227967
N	-1.3182930	1.6566965	-4.6932701
C	-0.6716072	0.4559337	-4.4633114
H	-0.3481960	-0.1980556	-5.2696024
Cu	-4.9632967	2.1228718	-6.1724994
Cu	-2.1002859	3.0619432	-6.3817795

O	-3.7510195	3.4665388	-5.3763513
O	-3.4585093	2.3354475	-7.6601347
C	-4.1444027	3.9360388	-9.0384810
C	-3.7797689	5.2006114	-8.3889729
C	-2.8641687	6.1093664	-9.0975468
C	-2.3281106	5.7601282	-10.3139162
C	-2.6964460	4.5274479	-10.9095384
C	-3.6056276	3.6564169	-10.3002843
O	-2.5917808	7.2651861	-8.4866604
H	-3.1911388	7.3032656	-7.7155917
H	-1.6694691	6.4747067	-10.8055664
H	-2.3182142	4.2813127	-11.9041907
H	-3.9768570	2.8035319	-10.8684463
H	-5.0728302	3.4775310	-8.7090113
O	-4.2056040	5.5834023	-7.2788289
H	-4.0649350	4.2495782	-5.8671883
H	-9.6130257	-1.8955090	-7.6429315
H	-8.1211458	7.3925607	-5.0441729
H	-5.0490183	0.3779509	-0.0229150
H	2.3061960	6.8591971	-4.6590418
H	3.1077920	3.5384228	-10.1993087
H	1.0440201	-0.6056338	-1.9233929

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C	-8.5231893	-2.0719607	-7.6402944
H	-8.3057566	-2.7128246	-6.7740889
H	-8.2990748	-2.6747595	-8.5370894
C	-7.6225154	-0.8638810	-7.5859645
N	-7.2252680	-0.1697884	-8.7106406
H	-7.4839654	-0.3458944	-9.6886391
C	-6.3582201	0.7941492	-8.3540559
H	-5.9144437	1.4772120	-9.0731434
N	-6.1625248	0.7799313	-7.0404594
C	-6.9479331	-0.2462836	-6.5501390
H	-6.9911022	-0.4698024	-5.4920184
C	-7.7587246	7.3304323	-5.9817412
H	-8.5964293	7.6396089	-6.6188048
H	-6.8968197	7.9639853	-6.2524807
C	-7.4448906	5.8961724	-6.2542952
N	-8.1785278	5.1277841	-7.1339954
H	-9.0631987	5.4124341	-7.5616748
C	-7.6028446	3.9049164	-7.2165063
H	-7.9880761	3.1111472	-7.8542408
N	-6.5363375	3.8414583	-6.4321744
C	-6.4312600	5.0740992	-5.8297546
H	-5.6473754	5.3053999	-5.1138081
C	-4.4445580	1.1141670	-0.5249292
H	-4.2954048	1.9785370	0.1420429
H	-3.4615236	0.6500822	-0.6996217
C	-5.0025908	1.5147004	-1.8630175
N	-5.9786691	2.4741023	-2.0450712
H	-6.3531580	3.0635033	-1.2965794
C	-6.2747052	2.5452963	-3.3607550
H	-7.0027660	3.2381156	-3.7735986
N	-5.5390812	1.6860081	-4.0520826
C	-4.7450568	1.0366808	-3.1302829
H	-4.0257116	0.2725958	-3.4134735
C	1.3950528	7.1626839	-4.0957256
H	1.5677759	7.1051556	-3.0101820
H	1.2014526	8.2179627	-4.3298219
C	0.2185508	6.3553346	-4.5367416
N	-0.9934024	6.9565827	-4.8093647
H	-1.2071203	7.9428756	-4.7101860
C	-1.8434279	6.0224707	-5.2846587
H	-2.8562546	6.2421233	-5.6052393
N	-1.2440197	4.8454755	-5.3428614
C	0.0337340	5.0309116	-4.8676432
H	0.7478388	4.2116181	-4.8140726
C	1.9917459	3.9684514	-10.1401119
H	1.9896051	5.0591180	-10.0049905
H	1.5234303	3.7706165	-11.1229299
C	1.1242977	3.3465162	-9.0884682
N	0.8457056	1.9921752	-9.0376727
H	1.2315836	1.2780782	-9.6508952
C	-0.1148145	1.7814183	-8.1143835
H	-0.5279548	0.8067993	-7.8938659
N	-0.4838978	2.9201153	-7.5534110
C	0.2871762	3.9067567	-8.1457151
H	0.1879251	4.9556119	-7.8819371
C	0.0664271	-0.8712100	-2.2590885
H	0.1123458	-1.8107718	-2.8262682
H	-0.5841431	-1.0491665	-1.3867949
C	-0.5334174	0.2358140	-3.0793623
N	-1.1482115	1.3200427	-2.4685688
H	-1.2481554	1.4579948	-1.4687900
C	-1.5931361	2.1617756	-3.4311481

H	-2.1577101	3.0687707	-3.2345453
N	-1.2981860	1.6973981	-4.6304978
C	-0.6315979	0.5024125	-4.4275334
H	-0.2842860	-0.1196850	-5.2489132
Cu	-5.0350172	2.1976639	-6.0635240
Cu	-2.0845175	3.0776879	-6.2573209
O	-3.7194479	3.4227219	-5.2121628
O	-3.6304995	2.5279274	-7.5807819
C	-3.9037110	3.3589634	-8.6748650
C	-3.5794082	4.8322407	-8.4456388
C	-3.0304156	5.6335755	-9.5460990
C	-2.6017375	5.0232737	-10.6853289
C	-2.7959017	3.6054571	-10.9005682
C	-3.4011619	2.8230309	-9.9815743
O	-2.8554999	6.9427395	-9.2944280
H	-3.2349274	7.0969552	-8.4097351
H	-2.1285905	5.6197348	-11.4674875
H	-2.4624088	3.2036568	-11.8547094
H	-3.6931816	1.7903171	-10.1982054
H	-5.0098929	3.4464791	-8.8369235
O	-3.7752399	5.3878329	-7.3580907
H	-3.9622029	4.2251274	-5.7114432
H	-9.5984899	-1.8936707	-7.6375330
H	-8.0452565	7.5524697	-4.9537989
H	-5.0717902	0.3865921	-0.0098747
H	2.3257712	6.8949653	-4.5958821
H	3.0272021	3.6311662	-10.1863264
H	1.0664312	-0.6118206	-1.9115610

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C	-8.4663910	-1.9737243	-7.6685783
H	-8.2470258	-2.6268618	-6.8115637
H	-8.2360954	-2.5591271	-8.5753640
C	-7.5702073	-0.7621617	-7.5813821
N	-7.1873851	-0.0100909	-8.6753842
H	-7.4444313	-0.1591112	-9.6592220
C	-6.3233346	0.9409002	-8.2795287
H	-5.8764721	1.6572124	-8.9633312
N	-6.1153698	0.8648303	-6.9684705
C	-6.8884539	-0.1932477	-6.5235645
H	-6.9182779	-0.4741833	-5.4787844
C	-7.7840218	7.6139811	-6.3026427
H	-8.6834026	7.9462573	-6.8382612
H	-6.9913704	8.3409793	-6.5438631
C	-7.3593552	6.2764523	-6.8197513
N	-8.1940025	5.4129316	-7.5055321
H	-9.2011704	5.5488372	-7.6364907
C	-7.4605064	4.3854573	-7.9902737
H	-7.8674567	3.5964839	-8.6209727
N	-6.1920184	4.5305200	-7.6287295
C	-6.1143205	5.7065373	-6.9066890
H	-5.1653696	6.0846589	-6.5419331
C	-4.4677575	1.1061110	-0.4686554
H	-4.3312708	1.9733662	0.1968356
H	-3.4801662	0.6504555	-0.6376378
C	-5.0207408	1.4938566	-1.8104304
N	-5.9688594	2.4764834	-2.0124660
H	-6.3391940	3.0756689	-1.2688716
C	-6.2591437	2.5335842	-3.3292146
H	-6.9585597	3.2478766	-3.7562769
N	-5.5511414	1.6344585	-3.9989785
C	-4.7769902	0.9805099	-3.0644792
H	-4.0795709	0.1908592	-3.3317791
C	1.5627411	7.1543898	-3.9798604
H	1.8348608	7.1868818	-2.9124901
H	1.2784525	8.1771241	-4.2659743
C	0.4123137	6.2452288	-4.2406630
N	-0.8824036	6.7155648	-4.1595856
H	-1.1615960	7.6512404	-3.8895399
C	-1.7233354	5.7254840	-4.5220565
H	-2.7984426	5.8548212	-4.5664261
N	-1.0468883	4.6351867	-4.8290244
C	0.2830017	4.9356153	-4.6448524
H	1.0643847	4.2018856	-4.8269978
C	1.9731987	3.9763772	-10.0101308
H	1.9842148	5.0654085	-9.8639139
H	1.4939599	3.7949017	-10.9905118
C	1.1053397	3.3559989	-8.9558965
N	0.7618374	2.0142569	-8.9577233
H	1.1047148	1.3125579	-9.6089212
C	-0.1699340	1.8024224	-8.0052249
H	-0.6239770	0.8399081	-7.8132462
N	-0.4565039	2.9281785	-7.3737775
C	0.3312752	3.9084207	-7.9553573
H	0.2739150	4.9491266	-7.6493796
C	0.1495670	-1.0530976	-2.1456597

H	0.2128714	-2.0004093	-2.6972197
H	-0.4807929	-1.2272477	-1.2589188
C	-0.4930033	0.0293120	-2.9600026
N	-1.1278820	1.0887549	-2.3279493
H	-1.2119543	1.2135601	-1.3250639
C	-1.5867175	1.9389395	-3.2749578
H	-2.1549528	2.8384366	-3.0628449
N	-1.2881562	1.5007427	-4.4823224
C	-0.5999669	0.3147791	-4.3029194
H	-0.2411651	-0.2854198	-5.1356783
Cu	-4.8516333	2.0826442	-5.9158740
Cu	-1.9778214	3.0715235	-5.9953906
O	-3.6549576	3.3432005	-4.9630254
O	-3.5582569	2.5351407	-7.3847110
C	-3.7176753	3.4958482	-8.3652124
C	-3.1938670	4.8303772	-8.0665631
C	-2.8977134	5.7337717	-9.1601779
C	-2.9287405	5.2872293	-10.4566023
C	-3.3258922	3.9489336	-10.7468079
C	-3.6892400	3.0765069	-9.7601011
O	-2.4824959	6.9656431	-8.8077009
H	-2.5345383	6.9779255	-7.8324604
H	-2.6554645	5.9670654	-11.2666466
H	-3.3438033	3.6345794	-11.7828302
H	-4.0600380	2.0769170	-10.0039405
H	-4.9515506	3.9888562	-8.1999291
O	-3.0456577	5.2509112	-6.8805954
H	-3.8291259	4.1736239	-5.4482717
H	-9.5437202	-1.8081099	-7.6687504
H	-8.0089260	7.6971280	-5.2393595
H	-5.0957417	0.3734278	0.0381758
H	2.4648184	6.9063539	-4.5391467
H	3.0048241	3.6292253	-10.0675857
H	1.1457576	-0.7533602	-1.8203473

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C	-8.6522979	-2.1709242	-7.7071951
H	-8.4463838	-2.8229856	-6.8460122
H	-8.4483532	-2.7739667	-8.6089172
C	-7.7228785	-0.9913705	-7.6506253
N	-7.3587145	-0.2636710	-8.7658746
H	-7.6460770	-0.4157833	-9.7401386
C	-6.4611830	0.6695864	-8.4149622
H	-6.0007928	1.3720104	-9.1027992
N	-6.2142401	0.6023746	-7.1086139
C	-6.9953388	-0.4299609	-6.6222516
H	-6.9911912	-0.7042486	-5.5756365
C	-7.7316308	7.7076031	-6.2700743
H	-8.5634463	8.1561377	-6.8301458
H	-6.8568583	8.3544997	-6.4438300
C	-7.4365768	6.3553408	-6.8281645
N	-8.3785493	5.5872792	-7.4954593
H	-9.3779316	5.8030674	-7.5870753
C	-7.7916344	4.4898553	-8.0001201
H	-8.2741380	3.7273014	-8.6095344
N	-6.5096643	4.5203130	-7.6684759
C	-6.2582214	5.6629223	-6.9476366
H	-5.2569974	5.9043960	-6.6008234
C	-4.4715528	1.0781021	-0.5687176
H	-4.3418452	1.9656639	0.0705171
H	-3.4810911	0.6198753	-0.7132919
C	-5.0104037	1.4251605	-1.9296316
N	-5.9333894	2.4213117	-2.1748656
H	-6.2901705	3.0582741	-1.4573570
C	-6.2255423	2.4203035	-3.4958068
H	-6.9170824	3.1274362	-3.9481679
N	-5.5418406	1.4757884	-4.1271707
C	-4.7801519	0.8526726	-3.1621210
H	-4.1002766	0.0345682	-3.3854410
C	1.6054594	7.3104126	-4.0130199
H	1.8480651	7.3493514	-2.9392146
H	1.3818600	8.3363679	-4.3319675
C	0.4227763	6.4508204	-4.2795843
N	-0.8123189	6.9930398	-4.5697505
H	-1.0294680	7.9815859	-4.6315745
C	-1.6777370	5.9799178	-4.8015532
H	-2.7169981	6.1341687	-5.0746550
N	-1.0706796	4.8159228	-4.6776678
C	0.2337341	5.0900610	-4.3475125
H	0.9690659	4.2989364	-4.2098618
C	2.0960246	3.9116520	-10.0439496
H	2.0808637	5.0001053	-9.8914706
H	1.5928749	3.7229823	-11.0101778
C	1.2840877	3.2590708	-8.9708056
N	0.8586586	1.9456227	-9.0446405
H	1.1130647	1.2767897	-9.7663407

C	-0.0167353	1.7193333	-8.0416783
H	-0.5250526	0.7764882	-7.8969812
N	-0.1789850	2.8063651	-7.3064116
C	0.6320805	3.7725576	-7.8715302
H	0.6421873	4.7955593	-7.5155502
C	0.1351360	-1.0026148	-2.1710171
H	0.1878854	-1.9401910	-2.7398860
H	-0.5045272	-1.1845472	-1.2925194
C	-0.4763004	0.1111806	-2.9691050
N	-1.1194949	1.1547388	-2.3191758
H	-1.2515348	1.2332565	-1.3166527
C	-1.5075561	2.0638197	-3.2400442
H	-2.0507005	2.9743279	-3.0092231
N	-1.1477236	1.6767628	-4.4492159
C	-0.5047796	0.4624727	-4.3006902
H	-0.1175982	-0.1014038	-5.1457756
Cu	-4.9187866	1.8386807	-6.1801251
Cu	-1.7110933	3.0903999	-5.9278093
O	-3.6571469	2.9846726	-5.3179592
O	-4.6487448	2.8132034	-8.0002700
C	-3.7186571	3.3671466	-8.8047700
C	-2.8039974	4.3373563	-8.2988822
C	-1.9717769	5.0708251	-9.1913585
C	-1.9432799	4.7762704	-10.5460048
C	-2.7943267	3.7764456	-11.0275667
C	-3.6868952	3.0954442	-10.1907342
O	-1.2034903	6.0458290	-8.6500399
H	-1.4374183	6.0267367	-7.7019040
H	-1.2701592	5.3132930	-11.2135361
H	-2.7626678	3.5554657	-12.0893565
H	-4.4095649	2.3966696	-10.6193548
H	-5.7440688	3.7591104	-7.8942953
O	-2.6594511	4.5978064	-7.0110506
H	-3.7572672	3.7929169	-5.8601111
H	-9.7209804	-1.9568850	-7.6941072
H	-7.9955370	7.7693226	-5.2143231
H	-5.0984877	0.3594419	-0.0409424
H	2.5095590	7.0028669	-4.5384588
H	3.1337435	3.5880492	-10.1244936
H	1.1331188	-0.7207531	-1.8353823

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C	-8.6805874	-2.1760982	-7.7020178
H	-8.4743140	-2.8223799	-6.8367837
H	-8.4740608	-2.7841263	-8.5997667
C	-7.7551893	-0.9935024	-7.6534698
N	-7.4020736	-0.2699321	-8.7744800
H	-7.6909541	-0.4312923	-9.7465273
C	-6.5082692	0.6704629	-8.4346761
H	-6.0569839	1.3716080	-9.1300563
N	-6.2528989	0.6122756	-7.1294483
C	-7.0249743	-0.4220905	-6.6324836
H	-7.0126441	-0.6903670	-5.5843423
C	-7.7601989	7.7176852	-6.2597686
H	-8.5950674	8.1670906	-6.8147775
H	-6.8847227	8.3610935	-6.4421887
C	-7.4749751	6.3626566	-6.8141693
N	-8.4265413	5.5939906	-7.4670546
H	-9.4260426	5.8118939	-7.5517124
C	-7.8500874	4.4910005	-7.9694536
H	-8.3393328	3.7235561	-8.5668939
N	-6.5647040	4.5205591	-7.6502523
C	-6.2998451	5.6667496	-6.9396246
H	-5.2916214	5.8995225	-6.6075834
C	-4.4694994	1.0758105	-0.5977275
H	-4.3301707	1.9619243	0.0416879
H	-3.4831096	0.6120119	-0.7512993
C	-5.0101157	1.4311325	-1.9562775
N	-5.9397994	2.4228921	-2.1953314
H	-6.3033831	3.0508132	-1.4736758
C	-6.2235640	2.4360052	-3.5184952
H	-6.9192440	3.1417119	-3.9666474
N	-5.5270537	1.5060983	-4.1572290
C	-4.7660928	0.8772122	-3.1947874
H	-4.0735694	0.0717000	-3.4237313
C	1.5626547	7.2767667	-4.0175180
H	1.8057817	7.3018903	-2.9433984
H	1.3339330	8.3065120	-4.3207124
C	0.3854396	6.4135510	-4.3022462
N	-0.8553944	6.9518580	-4.5740809
H	-1.0848894	7.9390810	-4.5985605
C	-1.7105136	5.9378562	-4.8414372
H	-2.7534236	6.0891336	-5.0990053
N	-1.0906739	4.7769966	-4.7586920
C	0.2106117	5.0538932	-4.4162940
H	0.9523550	4.2652041	-4.2997815

C	2.0737424	3.9217874	-10.0893723
H	2.0585602	5.0114949	-9.9462204
H	1.5806394	3.7233982	-11.0592378
C	1.2557410	3.2793842	-9.0152006
N	0.9022113	1.9431726	-9.0335916
H	1.2202530	1.2518372	-9.7070605
C	0.0115237	1.7217909	-8.0417382
H	-0.4350178	0.7568424	-7.8458369
N	-0.2349380	2.8342604	-7.3714476
C	0.5406071	3.8134099	-7.9654094
H	0.4936863	4.8526090	-7.6579181
C	0.1622178	-1.0637709	-2.0822157
H	0.2134527	-2.0070136	-2.6422347
H	-0.4642936	-1.2337617	-1.1922787
C	-0.4567858	0.0388220	-2.8860582
N	-1.0764471	1.1040353	-2.2488851
H	-1.1941158	1.2053410	-1.2465935
C	-1.4537889	2.0029644	-3.1884069
H	-1.9779144	2.9293580	-2.9716103
N	-1.1120177	1.5856723	-4.3910884
C	-0.4913129	0.3652221	-4.2229747
H	-0.1195907	-0.2231257	-5.0587448
Cu	-4.9383800	1.8507087	-6.2259393
Cu	-1.6691836	3.0143407	-5.8960750
O	-3.6416062	2.9678969	-5.4240636
O	-4.7030120	2.8119297	-8.0880016
C	-3.7908538	3.4051662	-8.8624456
C	-2.9888311	4.4831905	-8.3378425
C	-2.1004645	5.2075496	-9.2055945
C	-1.9460574	4.8460954	-10.5316620
C	-2.7150128	3.7833862	-11.0245203
C	-3.6365044	3.0882583	-10.2262069
O	-1.4117880	6.2188670	-8.6408394
H	-1.7233812	6.2282003	-7.7142514
H	-1.2387818	5.3731822	-11.1704506
H	-2.5897550	3.5113521	-12.0691872
H	-4.2849744	2.3333467	-10.6783824
H	-5.8112434	3.7713198	-7.9029632
O	-2.9878508	4.8262652	-7.0901543
H	-3.7186661	3.7805777	-5.9704531
H	-9.7495500	-1.9633597	-7.6907157
H	-8.0171491	7.7822839	-5.2024748
H	-5.0945833	0.3600283	-0.0638807
H	2.4676849	6.9816095	-4.5484314
H	3.1121170	3.5976542	-10.1585275
H	1.1636212	-0.7709823	-1.7667280

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C	-8.6647327	-2.1748913	-7.7703452
H	-8.4571224	-2.8391931	-6.9182226
H	-8.4742843	-2.7678295	-8.6819232
C	-7.7235277	-1.0066155	-7.6971659
N	-7.3830907	-0.2217501	-8.7805043
H	-7.6823373	-0.3345172	-9.7555386
C	-6.4583294	0.6795705	-8.4045762
H	-6.0009401	1.4184577	-9.0635871
N	-6.1768695	0.5329430	-7.1121912
C	-6.9564988	-0.5151458	-6.6633344
H	-6.9159095	-0.8651608	-5.6395551
C	-7.8834563	7.7851651	-6.3284185
H	-8.7761117	8.1815329	-6.8313801
H	-7.0610328	8.4810422	-6.5590087
C	-7.5342353	6.4521071	-6.8982763
N	-8.4566166	5.5878201	-7.4658265
H	-9.4718233	5.7297577	-7.4947086
C	-7.8147397	4.5410758	-8.0114087
H	-8.2753185	3.7277626	-8.5702242
N	-6.5165335	4.6966775	-7.7971766
C	-6.3115648	5.8729131	-7.1174997
H	-5.3061398	6.2107969	-6.8896154
C	-4.3863780	1.1251492	-0.4582573
H	-4.2662077	1.9879195	0.2160122
H	-3.3961432	0.6607618	-0.5872643
C	-4.8799886	1.5230868	-1.8206134
N	-5.7781566	2.5405739	-2.0593538
H	-6.1418930	3.1615187	-1.3315727
C	-6.0301198	2.5888853	-3.3899502
H	-6.7086048	3.3117108	-3.8390590
N	-5.3416449	1.6572329	-4.0293875
C	-4.6232425	0.9870994	-3.0651193
H	-3.9598155	0.1586087	-3.3021299
C	1.3909436	7.1034720	-4.1030290
H	1.5810932	7.1029910	-3.0184903
H	1.1290380	8.1346702	-4.3778446
C	0.2800569	6.1807625	-4.4921163
N	-0.9920342	6.6301743	-4.7866980

H	-1.3192206	7.5874964	-4.7156384
C	-1.7335773	5.5809010	-5.2130911
H	-2.7664062	5.6607404	-5.5340803
N	-1.0059056	4.4791477	-5.2199002
C	0.2390023	4.8303276	-4.7567946
H	1.0362102	4.0984870	-4.6473236
C	2.2241337	3.7469347	-10.2089289
H	2.1312318	4.8303139	-10.0469169
H	1.7199105	3.5213152	-11.1678854
C	1.5005710	3.0246124	-9.1217059
N	1.4376496	1.6469813	-9.0187195
H	1.9579396	0.9831937	-9.5883142
C	0.5614826	1.3284595	-8.0428448
H	0.3582202	0.3089862	-7.7352038
N	0.0455269	2.4240308	-7.5037573
C	0.6291132	3.4893016	-8.1649120
H	0.3703891	4.5224977	-7.9485490
C	0.1848792	-1.1228848	-2.0132011
H	0.2396945	-2.0997439	-2.5125076
H	-0.4441823	-1.2334306	-1.1157669
C	-0.4277219	-0.0787966	-2.8921149
N	-1.0552393	1.0307592	-2.3450687
H	-1.1965867	1.2037619	-1.3558220
C	-1.4347200	1.8476967	-3.3557552
H	-1.9712798	2.7819571	-3.2144941
N	-1.0845005	1.3350128	-4.5185342
C	-0.4560951	0.1377698	-4.2495581
H	-0.0837874	-0.5176060	-5.0330169
Cu	-4.8878679	1.6910037	-6.1528370
Cu	-1.4866985	2.6310133	-6.1799953
O	-3.3895533	2.8675384	-5.9367601
O	-4.7394175	3.1339783	-8.7557797
C	-3.7627079	3.6860370	-9.3738208
C	-3.0542600	4.8103282	-8.7307753
C	-1.9106448	5.4002278	-9.4041602
C	-1.4981402	4.9453752	-10.6337597
C	-2.2292505	3.9022394	-11.2649402
C	-3.3222162	3.2912791	-10.6674741
O	-1.2700497	6.3781256	-8.7272532
H	-1.8215735	6.5251674	-7.9341188
H	-0.6232035	5.3806757	-11.1167415
H	-1.9214601	3.5877098	-12.2638944
H	-3.9143107	2.5463164	-11.2020885
H	-5.7225598	4.0327827	-8.1736518
O	-3.3956622	5.2627582	-7.5919491
H	-3.5879759	3.6453320	-6.4974597
H	-9.7315212	-1.9532085	-7.7405885
H	-8.0831258	7.8316455	-5.2578868
H	-5.0370962	0.3959015	0.0242674
H	2.3278760	6.8618054	-4.6048470
H	3.2809223	3.4991769	-10.3083288
H	1.1860000	-0.8140391	-1.7124722

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C	-8.6764621	-2.1827140	-7.7733183
H	-8.4634619	-2.8488978	-6.9240510
H	-8.4872687	-2.7717326	-8.6876517
C	-7.7376495	-1.0126688	-7.6995403
N	-7.4142413	-0.2125102	-8.7768818
H	-7.7208554	-0.3132587	-9.7510133
C	-6.4886919	0.6872940	-8.4009634
H	-6.0491767	1.4353934	-9.0603410
N	-6.1885407	0.5252497	-7.1147171
C	-6.9583918	-0.5319334	-6.6697717
H	-6.9005477	-0.8964913	-5.6518724
C	-7.9121287	7.7044292	-6.2943084
H	-8.8108917	8.0828323	-6.8006535
H	-7.1008193	8.4097418	-6.5361358
C	-7.5454856	6.3693421	-6.8496535
N	-8.4504620	5.5019173	-7.4347252
H	-9.4642415	5.6404618	-7.4837232
C	-7.7778555	4.4668155	-7.9783180
H	-8.2354358	3.6587388	-8.5485358
N	-6.4825899	4.6217592	-7.7512431
C	-6.3158784	5.7971479	-7.0582782
H	-5.3266351	6.1650658	-6.8070267
C	-4.3938532	1.1343538	-0.4656707
H	-4.2732305	1.9954971	0.2105685
H	-3.4038344	0.6695358	-0.5948629
C	-4.8860224	1.5363022	-1.8275715
N	-5.7682304	2.5673794	-2.0674428
H	-6.1235693	3.1950039	-1.3407334
C	-6.0201505	2.6200545	-3.3969261
H	-6.6876148	3.3528959	-3.8466813
N	-5.3458112	1.6766081	-4.0352962
C	-4.6375951	0.9949805	-3.0713689

H	-3.9895683	0.1542953	-3.3083275
C	1.3889731	7.1051683	-4.0907482
H	1.5752956	7.0888717	-3.0057951
H	1.1395168	8.1425523	-4.3530291
C	0.2671917	6.2016432	-4.4960049
N	-0.9861913	6.6758644	-4.8297619
H	-1.2920073	7.6421129	-4.7826527
C	-1.7403617	5.6390494	-5.2633254
H	-2.7628564	5.7435980	-5.6093258
N	-1.0381707	4.5202775	-5.2389750
C	0.2024229	4.8492974	-4.7467203
H	0.9801680	4.1011335	-4.6095593
C	2.2056453	3.7380704	-10.2156301
H	2.1078779	4.8230335	-10.0675841
H	1.7015065	3.4966373	-11.1707151
C	1.4886091	3.0269052	-9.1160358
N	1.4521460	1.6515156	-8.9779513
H	1.9909961	0.9848415	-9.5266902
C	0.5784375	1.3403284	-7.9974093
H	0.3971503	0.3247351	-7.6627643
N	0.0379363	2.4388081	-7.4882038
C	0.6034421	3.4977922	-8.1747595
H	0.3264131	4.5308214	-7.9831825
C	0.1749889	-1.1111922	-2.0167853
H	0.2260196	-2.0836052	-2.5251576
H	-0.4531237	-1.2286542	-1.1195277
C	-0.4371101	-0.0581532	-2.8860445
N	-1.0606133	1.0495087	-2.3306096
H	-1.1982955	1.2171868	-1.3397964
C	-1.4441255	1.8721745	-3.3352244
H	-1.9779257	2.8068898	-3.1850149
N	-1.0998697	1.3652007	-4.5026924
C	-0.4718295	0.1652831	-4.2422359
H	-0.1052530	-0.4882529	-5.0301371
Cu	-4.9176117	1.6913684	-6.1361930
Cu	-1.5056928	2.6565706	-6.1683107
O	-3.4141538	2.8752455	-5.9577195
O	-4.7838871	3.1885394	-8.8160155
C	-3.7900100	3.7355090	-9.4478007
C	-3.0607224	4.8397762	-8.8110160
C	-1.9182944	5.4170748	-9.5051597
C	-1.5151673	4.9394288	-10.7312138
C	-2.2557437	3.8945561	-11.3345550
C	-3.3616825	3.3067969	-10.7203530
O	-1.2632372	6.3927137	-8.8465146
H	-1.7959184	6.5506147	-8.0424353
H	-0.6380347	5.3549147	-11.2270425
H	-1.9493511	3.5516322	-12.3241884
H	-3.9591323	2.5522548	-11.2351511
H	-5.5608063	3.9140243	-8.2532504
O	-3.3632831	5.2812159	-7.6609590
H	-3.6143891	3.6577607	-6.5090468
H	-9.7435991	-1.9634643	-7.7384665
H	-8.1125820	7.7654197	-5.2246519
H	-5.0447152	0.4042825	0.0154124
H	2.3259796	6.8595234	-4.5904920
H	3.2634242	3.4942336	-10.3141888
H	1.1775509	-0.8085714	-1.7145328

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C	-8.6595113	-2.2156589	-7.7308538
H	-8.4355500	-2.8707250	-6.8760423
H	-8.4592871	-2.8071510	-8.6405002
C	-7.7573039	-1.0149261	-7.6683772
N	-7.3824531	-0.2775836	-8.7736866
H	-7.6275266	-0.4284998	-9.7586050
C	-6.5404921	0.6982749	-8.3890462
H	-6.0990630	1.4179336	-9.0766040
N	-6.3409156	0.6445354	-7.0754898
C	-7.0922357	-0.4187424	-6.6179577
H	-7.1182479	-0.6899598	-5.5705013
C	-7.5781436	7.2683321	-5.9088828
H	-8.3324203	7.6367963	-6.6161625
H	-6.6663348	7.8660874	-6.0715493
C	-7.2972227	5.8356513	-6.2282678
N	-8.1406482	5.0807202	-7.0215163
H	-9.0625112	5.3786886	-7.3567535
C	-7.5827039	3.8677368	-7.2172464
H	-8.0374079	3.0885780	-7.8275558
N	-6.4150467	3.7933087	-6.5864204
C	-6.2288972	5.0129987	-5.9669846
H	-5.3399540	5.2221238	-5.3790423
C	-4.3814316	1.1175976	-0.4487215
H	-4.2390182	1.9705168	0.2343547
H	-3.3986686	0.6502763	-0.6147636
C	-4.9178017	1.5363073	-1.7880432

N	-5.8935613	2.4939353	-1.9664258
H	-6.2742464	3.0741673	-1.2144005
C	-6.1827800	2.5718497	-3.2845004
H	-6.9225733	3.2553286	-3.6926467
N	-5.4421586	1.7213854	-3.9778531
C	-4.6525359	1.0679938	-3.0584463
H	-3.9376991	0.3010135	-3.3463671
C	1.3461683	7.1481843	-4.0876348
H	1.5306177	7.1210743	-3.0030672
H	1.1194410	8.1907368	-4.3455259
C	0.2045191	6.2725074	-4.4955723
N	-1.0037489	6.7817491	-4.9274806
H	-1.2630891	7.7623481	-4.9538497
C	-1.7839742	5.7514092	-5.3365284
H	-2.7779154	5.8826213	-5.7547603
N	-1.1411341	4.6063541	-5.2011399
C	0.0875483	4.9108376	-4.6669355
H	0.8239016	4.1386440	-4.4511983
C	2.1425695	3.7810125	-10.2021811
H	2.0589923	4.8677489	-10.0580366
H	1.6448186	3.5454794	-11.1621684
C	1.4018012	3.0820680	-9.1076210
N	1.3569332	1.7084385	-8.9609104
H	1.9042545	1.0355509	-9.4927162
C	0.4643092	1.4100667	-7.9899676
H	0.2771620	0.3982590	-7.6483045
N	-0.0832789	2.5104028	-7.4975381
C	0.5002891	3.5603124	-8.1824921
H	0.2360627	4.5968230	-7.9914035
C	0.1458144	-1.0776335	-2.0042184
H	0.1879337	-2.0370703	-2.5372376
H	-0.4733872	-1.2161425	-1.1036033
C	-0.4719650	-0.0015229	-2.8411160
N	-1.0488314	1.1154302	-2.2542491
H	-1.1456942	1.2778449	-1.2577022
C	-1.4449233	1.9575797	-3.2392513
H	-1.9484035	2.9043219	-3.0603889
N	-1.1568779	1.4531185	-4.4223508
C	-0.5491648	0.2363525	-4.1932095
H	-0.2229071	-0.4162404	-4.9996683
Cu	-5.2501556	2.0620918	-6.0977290
Cu	-1.6044630	2.7059644	-6.0922355
O	-3.5570924	3.0128440	-5.9980551
O	-4.7852886	3.3155554	-9.0628022
C	-3.7449568	3.8980611	-9.6512544
C	-3.0955713	5.0047331	-8.9681603
C	-1.9371615	5.6140507	-9.6086336
C	-1.4690947	5.1480319	-10.8230898
C	-2.1455528	4.0852759	-11.4514395
C	-3.2706587	3.4642873	-10.8788512
O	-1.3402584	6.6043983	-8.9308832
H	-1.8963167	6.7590979	-8.1429832
H	-0.5867199	5.5944887	-11.2802817
H	-1.7905150	3.7360461	-12.4229028
H	-3.8218707	2.6849920	-11.4040132
H	-5.0603084	3.8185029	-8.2711959
O	-3.4936632	5.4149880	-7.8406790
H	-3.6602276	3.8113823	-6.5427195
H	-9.7299907	-2.0131257	-7.6973783
H	-7.9508933	7.4804919	-4.9068287
H	-5.0231767	0.3858512	0.0419688
H	2.2787872	6.8884616	-4.5884668
H	3.1979567	3.5252580	-10.2960640
H	1.1525746	-0.7850089	-1.7061057

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C	-8.6555093	-2.2342473	-7.7661504
H	-8.4223753	-2.8870469	-6.9120722
H	-8.4733621	-2.8298513	-8.6768439
C	-7.7447215	-1.0396029	-7.7247645
N	-7.3934474	-0.3062874	-8.8392868
H	-7.6688982	-0.4740039	-9.8137230
C	-6.5371061	0.6667038	-8.4787352
H	-6.1073170	1.3791079	-9.1833940
N	-6.3045427	0.6130735	-7.1707278
C	-7.0506401	-0.4457241	-6.6930063
H	-7.0505404	-0.7187372	-5.6452781
C	-7.6246932	7.2860004	-5.9496691
H	-8.4027779	7.6336946	-6.6404691
H	-6.7279713	7.8989129	-6.1403643
C	-7.3337079	5.8518371	-6.2527974
N	-8.1388658	5.0952787	-7.0808550
H	-9.0425472	5.3940355	-7.4599869
C	-7.5916712	3.8678505	-7.2155211
H	-8.0224349	3.0819590	-7.8340846
N	-6.4738584	3.7884784	-6.5060683

C	-6.2976982	5.0178463	-5.9099819
H	-5.4431432	5.2404652	-5.2764756
C	-4.3451124	1.1608608	-0.4814442
H	-4.2054450	2.0035266	0.2153352
H	-3.3623885	0.6901391	-0.6388950
C	-4.8500911	1.6127260	-1.8240526
N	-5.8352352	2.5608626	-1.9992616
H	-6.2492489	3.1083127	-1.2397625
C	-6.0669396	2.7049029	-3.3218395
H	-6.8104037	3.3878984	-3.7239251
N	-5.2760139	1.9091176	-4.0284473
C	-4.5181803	1.2180599	-3.1048357
H	-3.7747852	0.4818002	-3.3996059
C	1.2945212	7.1791995	-4.1376625
H	1.4407820	7.1117328	-3.0498517
H	1.1144588	8.2355453	-4.3709440
C	0.1304513	6.3597450	-4.5978297
N	-0.9211324	6.8982980	-5.3121509
H	-1.0411131	7.8777220	-5.5537603
C	-1.7444005	5.8931094	-5.6937271
H	-2.6281380	6.0405591	-6.3153973
N	-1.2829177	4.7302514	-5.2617979
C	-0.1198351	5.0066643	-4.5768386
H	0.4926501	4.2187002	-4.1430671
C	2.0964650	3.8620745	-10.2603596
H	2.0384684	4.9466709	-10.0925704
H	1.6290747	3.6669352	-11.2437997
C	1.2951419	3.1553475	-9.2147618
N	1.1124146	1.7858241	-9.1963682
H	1.5689725	1.1171489	-9.8123632
C	0.2222608	1.4844132	-8.2236859
H	-0.0801085	0.4711465	-7.9911828
N	-0.1890822	2.5778312	-7.6054944
C	0.4737980	3.6275488	-8.2140487
H	0.3148182	4.6611950	-7.9183673
C	0.1271521	-1.0046976	-2.0877675
H	0.1574698	-1.9443086	-2.6551612
H	-0.5019918	-1.1686872	-1.1979464
C	-0.4683897	0.1118317	-2.8911830
N	-0.9737038	1.2425026	-2.2647238
H	-1.0305784	1.3881805	-1.2621200
C	-1.3605423	2.1240609	-3.2147614
H	-1.8068120	3.0908152	-2.9945707
N	-1.1363614	1.6312223	-4.4197946
C	-0.5803245	0.3793046	-4.2359698
H	-0.3083797	-0.2672814	-5.0668281
Cu	-5.3290973	2.1148089	-6.1865933
Cu	-1.6011857	2.7765091	-6.0785459
O	-3.5317588	2.9673901	-6.8377282
O	-3.1266853	2.9809108	-9.2231990
C	-2.9986967	4.1234214	-9.7921423
C	-3.4421174	5.3571792	-9.0935842
C	-3.3812169	6.6276559	-9.8098937
C	-2.8463390	6.6982225	-11.0727903
C	-2.3610066	5.5045724	-11.6893034
C	-2.4294820	4.2666465	-11.0830421
O	-3.8570798	7.6934305	-9.1416905
H	-4.1839344	7.3329074	-8.2931491
H	-2.8056994	7.6537632	-11.5983284
H	-1.9544349	5.5695572	-12.7004556
H	-2.0932031	3.3737351	-11.6065464
H	-3.3875740	2.8711746	-7.9395883
O	-3.8513105	5.3736885	-7.8922450
H	-3.7430313	3.9342721	-6.9249196
H	-9.7243895	-2.0263199	-7.7179042
H	-7.9761791	7.5002848	-4.9404088
H	-4.9934936	0.4277041	-0.0017052
H	2.2352518	6.9001875	-4.6122621
H	3.1465497	3.5748525	-10.3141383
H	1.1353920	-0.7368775	-1.7718700

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C	-8.6668184	-2.2223384	-7.7453689
H	-8.4348756	-2.8717558	-6.8884833
H	-8.4756247	-2.8187494	-8.6536737
C	-7.7656981	-1.0198342	-7.7020624
N	-7.4133202	-0.2909553	-8.8192483
H	-7.6767073	-0.4691463	-9.7952394
C	-6.5760313	0.6975367	-8.4579212
H	-6.1535253	1.4113140	-9.1655548
N	-6.3563186	0.6578776	-7.1467989
C	-7.0909543	-0.4073156	-6.6677393
H	-7.0994531	-0.6678391	-5.6173044
C	-7.6109808	7.2882038	-5.9478126
H	-8.3810292	7.6483988	-6.6413865
H	-6.7085858	7.8964302	-6.1255309

C	-7.3259192	5.8559046	-6.2644799
N	-8.1516700	5.1012644	-7.0741988
H	-9.0647698	5.3996794	-7.4306221
C	-7.6039562	3.8763105	-7.2303800
H	-8.0508153	3.0926795	-7.8400595
N	-6.4660140	3.7971555	-6.5547805
C	-6.2773464	5.0236710	-5.9569525
H	-5.4050719	5.2423685	-5.3468134
C	-4.3513618	1.1564315	-0.4995214
H	-4.2134838	2.0046456	0.1907473
H	-3.3672480	0.6877547	-0.6544073
C	-4.8570878	1.5964927	-1.8461767
N	-5.8413548	2.5439481	-2.0320970
H	-6.2548704	3.0999918	-1.2788214
C	-6.0714206	2.6729191	-3.3575038
H	-6.8117802	3.3546131	-3.7679694
N	-5.2816991	1.8678689	-4.0545176
C	-4.5245431	1.1881496	-3.1227786
H	-3.7796312	0.4491993	-3.4072826
C	1.2888166	7.1881618	-4.1498694
H	1.4336401	7.1237274	-3.0615643
H	1.1112687	8.2442094	-4.3865911
C	0.1248858	6.3673406	-4.6072034
N	-0.9310686	6.9003722	-5.3197786
H	-1.0532689	7.8782180	-5.5658577
C	-1.7556939	5.8894486	-5.6881290
H	-2.6449315	6.0318349	-6.3020498
N	-1.2901043	4.7314229	-5.2504666
C	-0.1243285	5.0141194	-4.5764880
H	0.4900391	4.2300434	-4.1385127
C	2.0788596	3.8677344	-10.2156005
H	2.0274614	4.9526733	-10.0473309
H	1.6056092	3.6757457	-11.1969255
C	1.2768777	3.1637900	-9.1665804
N	1.1025631	1.7930635	-9.1397233
H	1.5690687	1.1228299	-9.7463854
C	0.2066628	1.4932011	-8.1714169
H	-0.0891039	0.4797072	-7.9316530
N	-0.2172983	2.5876679	-7.5644650
C	0.4438832	3.6371405	-8.1749900
H	0.2774892	4.6714530	-7.8857166
C	0.1318023	-1.0077390	-2.0837454
H	0.1619929	-1.9477354	-2.6505135
H	-0.4971168	-1.1711241	-1.1937003
C	-0.4634038	0.1081309	-2.8878337
N	-0.9689340	1.2393207	-2.2628105
H	-1.0262107	1.3860433	-1.2604216
C	-1.3550394	2.1198292	-3.2144867
H	-1.8029637	3.0865805	-2.9972275
N	-1.1299041	1.6255353	-4.4184589
C	-0.5743998	0.3741192	-4.2329771
H	-0.3034464	-0.2744035	-5.0627235
Cu	-5.2687621	2.1369853	-6.2372195
Cu	-1.6854685	2.7515091	-6.0709439
O	-3.5577643	2.9914190	-6.7116684
O	-2.9519831	3.0233796	-9.2755135
C	-2.9000546	4.2080065	-9.8797762
C	-3.4091086	5.4000617	-9.2156662
C	-3.4060813	6.6557202	-9.9666064
C	-2.8701013	6.7303073	-11.2391180
C	-2.3385510	5.5564354	-11.8104731
C	-2.3511422	4.3201952	-11.1505741
O	-3.9388807	7.7035173	-9.3299079
H	-4.2501896	7.3458157	-8.4734941
H	-2.8794160	7.6738790	-11.7867137
H	-1.9346239	5.5947934	-12.8230430
H	-1.9699240	3.4309767	-11.6503149
H	-3.2641710	3.0248141	-8.3202228
O	-3.8417212	5.4226816	-8.0219480
H	-3.7519165	3.9336184	-6.8975766
H	-9.7371625	-2.0205041	-7.7042259
H	-7.9682739	7.4975387	-4.9395533
H	-4.9971179	0.4247164	-0.0140746
H	2.2298912	6.9056101	-4.6216845
H	3.1274084	3.5766143	-10.2777379
H	1.1401971	-0.7394502	-1.7687413

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C	-8.6442097	-2.1832264	-7.6807542
H	-8.4238781	-2.8328041	-6.8211999
H	-8.4281944	-2.7768776	-8.5852925
C	-7.7508786	-0.9735883	-7.6188759
N	-7.3571677	-0.2597181	-8.7345353
H	-7.5933782	-0.4245042	-9.7204155
C	-6.5263111	0.7262677	-8.3641154
H	-6.0747298	1.4368962	-9.0553650

N	-6.3485158	0.7034001	-7.0426542
C	-7.1073315	-0.3512756	-6.5699757
H	-7.1539015	-0.5936560	-5.5169604
C	-7.6088258	7.2415599	-5.9067107
H	-8.3697588	7.6041355	-6.6096490
H	-6.6965808	7.8339283	-6.0852307
C	-7.3360253	5.8043754	-6.2087146
N	-8.1861390	5.0403498	-6.9855297
H	-9.1022765	5.3427524	-7.3321473
C	-7.6422611	3.8180599	-7.1531396
H	-8.1028869	3.0305852	-7.7470876
N	-6.4761760	3.7492936	-6.5173505
C	-6.2744750	4.9808660	-5.9293654
H	-5.3760853	5.1994098	-5.3616391
C	-4.3788769	1.1162077	-0.4895587
H	-4.2414344	1.9772369	0.1843525
H	-3.3939310	0.6488530	-0.6429741
C	-4.9010094	1.5266806	-1.8383615
N	-5.8784504	2.4802046	-2.0321971
H	-6.2763095	3.0571048	-1.2854468
C	-6.1369894	2.5721316	-3.3542259
H	-6.8713610	3.2560098	-3.7719223
N	-5.3713306	1.7332761	-4.0396741
C	-4.6002017	1.0729391	-3.1063684
H	-3.8752433	0.3119001	-3.3841119
C	1.3453172	7.1454960	-4.0953376
H	1.5223083	7.1225984	-3.0095006
H	1.1212611	8.1878766	-4.3570127
C	0.2014302	6.2747454	-4.5068699
N	-1.0104217	6.7948232	-4.9151307
H	-1.2589587	7.7784232	-4.9401753
C	-1.8023378	5.7779739	-5.3262097
H	-2.7971900	5.9115064	-5.7435113
N	-1.1660084	4.6257438	-5.2098608
C	0.0738528	4.9157961	-4.6900270
H	0.8080973	4.1375331	-4.4905252
C	2.1494087	3.7742656	-10.0698676
H	2.0771760	4.8620731	-9.9287900
H	1.6360114	3.5435558	-11.0223971
C	1.4051819	3.0900396	-8.9669442
N	1.3286895	1.7163710	-8.8237525
H	1.8563487	1.0333045	-9.3622757
C	0.4256004	1.4301107	-7.8641889
H	0.2113205	0.4221316	-7.5289125
N	-0.0980895	2.5446712	-7.3703196
C	0.5109075	3.5881824	-8.0464369
H	0.2467406	4.6278358	-7.8720446
C	0.1104863	-1.0132164	-2.0853757
H	0.1499744	-1.9676552	-2.6268878
H	-0.5203860	-1.1593112	-1.1936414
C	-0.4973057	0.0727073	-2.9208239
N	-1.0429474	1.2049274	-2.3322752
H	-1.1061534	1.3819666	-1.3351525
C	-1.4651268	2.0380846	-3.3103123
H	-1.9443721	2.9960040	-3.1273306
N	-1.2238608	1.5136039	-4.4973317
C	-0.6186725	0.2916264	-4.2734479
H	-0.3258605	-0.3754833	-5.0804024
Cu	-5.1816944	2.1047785	-6.1565882
Cu	-1.7274538	2.7378089	-6.1515464
O	-3.5721075	3.0735058	-6.1685312
O	-4.9219154	3.1804120	-9.0519099
C	-3.8085826	3.7637210	-9.5592511
C	-3.1561036	4.7402225	-8.7804938
C	-2.0010376	5.3556420	-9.3015121
C	-1.4946679	4.9819724	-10.5483912
C	-2.1572662	4.0058106	-11.2992998
C	-3.3219954	3.3985868	-10.8122827
O	-1.3602346	6.3013316	-8.5529216
H	-1.9610906	6.5124682	-7.8216455
H	-0.5875184	5.4621427	-10.9165274
H	-1.7863387	3.7358442	-12.2895876
H	-3.9020106	2.6942788	-11.4070804
H	-5.2834861	3.7657791	-8.3641383
O	-3.6485504	5.0765475	-7.5681918
H	-3.6537224	4.1761607	-6.9070567
H	-9.7173970	-1.9934758	-7.6625792
H	-7.9703570	7.4599925	-4.9018978
H	-5.0204662	0.3898723	0.0093067
H	2.2814072	6.8860005	-4.5897707
H	3.2012872	3.5084553	-10.1745726
H	1.1160053	-0.7336661	-1.7709723

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C	-8.7550232	-2.3647081	-7.8485067
H	-8.5287599	-3.0452368	-7.0139434

H	-8.5925952	-2.9351045	-8.7782533
C	-7.8330746	-1.1874593	-7.7637092
N	-7.4893473	-0.3817837	-8.8281907
H	-7.7360612	-0.5009634	-9.8163342
C	-6.6499590	0.5809944	-8.3953610
H	-6.2266292	1.3412710	-9.0499518
N	-6.4283969	0.4484089	-7.0945243
C	-7.1509865	-0.6545366	-6.6945991
H	-7.1376696	-1.0069606	-5.6711130
C	-7.5486198	7.2805499	-5.8997358
H	-8.2916120	7.6451617	-6.6211875
H	-6.6344661	7.8793305	-6.0488785
C	-7.2680242	5.8415353	-6.1967677
N	-8.0662884	5.0992466	-7.0431700
H	-8.9659484	5.4034565	-7.4269053
C	-7.5280129	3.8632361	-7.1674680
H	-7.9648260	3.0856153	-7.7936726
N	-6.4255936	3.7583411	-6.4380026
C	-6.2514572	4.9868287	-5.8362048
H	-5.4133659	5.1948562	-5.1738970
C	-4.3259173	1.1374680	-0.3864223
H	-4.1696440	1.9634233	0.3265865
H	-3.3519050	0.6565889	-0.5651655
C	-4.8525497	1.6163910	-1.7077670
N	-5.8012431	2.6064462	-1.8382506
H	-6.1685281	3.1604694	-1.0607996
C	-6.0949541	2.7555827	-3.1458407
H	-6.8238659	3.4669813	-3.5212455
N	-5.3810526	1.9163507	-3.8817397
C	-4.6072325	1.1943511	-2.9981930
H	-3.9216455	0.4196173	-3.3306825
C	1.2153710	7.1106410	-4.2010886
H	1.3529197	7.0533799	-3.1114089
H	1.0048515	8.1608928	-4.4403962
C	0.0922510	6.2332921	-4.6682028
N	-0.9569956	6.6919720	-5.4404009
H	-1.1268433	7.6585446	-5.7007809
C	-1.7051370	5.6225555	-5.8232409
H	-2.5861557	5.7031501	-6.4590917
N	-1.1971962	4.5031790	-5.3408288
C	-0.0866474	4.8682006	-4.6174040
H	0.5440589	4.1280656	-4.1280836
C	2.2114782	3.7046508	-10.3895282
H	2.0948754	4.7864444	-10.2297434
H	1.7364409	3.4691790	-11.3605417
C	1.4913630	2.9629404	-9.3135087
N	1.4880405	1.5872785	-9.1909208
H	2.0455784	0.9378797	-9.7418025
C	0.6291322	1.2507628	-8.1985543
H	0.4734162	0.2261442	-7.8758293
N	0.0665662	2.3281285	-7.6763197
C	0.6001365	3.4006994	-8.3611696
H	0.3213325	4.4268726	-8.1352588
C	0.1434728	-1.0946333	-1.9930163
H	0.1866228	-2.0594038	-2.5163366
H	-0.4761118	-1.2221144	-1.0909510
C	-0.4701378	-0.0279588	-2.8439596
N	-1.0142533	1.1141406	-2.2751411
H	-1.0977934	1.3000777	-1.2816987
C	-1.3957666	1.9470979	-3.2755667
H	-1.8653354	2.9135010	-3.1097860
N	-1.1304749	1.4105756	-4.4507189
C	-0.5550913	0.1814088	-4.1997373
H	-0.2537730	-0.4947077	-4.9960464
Cu	-5.7507819	1.8075893	-5.8409389
Cu	-1.2785526	2.4986174	-6.1738850
O	-3.3500199	2.6939687	-6.9117465
O	-2.8185407	3.1748158	-9.5371643
C	-2.7091828	4.1848698	-10.2260757
C	-3.3707459	5.4862865	-9.6978685
C	-3.3825409	6.6821749	-10.5783540
C	-2.7153001	6.6437443	-11.7618506
C	-2.0420133	5.4266699	-12.1928491
C	-2.0095262	4.2661351	-11.4821434
O	-4.0238815	7.7518951	-10.0982329
H	-4.3935531	7.4911903	-9.2339404
H	-2.6947963	7.5219391	-12.4097654
H	-1.5548383	5.4470895	-13.1683819
H	-1.5317109	3.3705851	-11.8780266
H	-3.3333271	2.8903969	-7.8740124
O	-3.8434833	5.5481597	-8.5764390
H	-3.9751198	3.3419431	-6.5548096
H	-9.8158789	-2.1251520	-7.7759498
H	-7.9372473	7.5018077	-4.9057136
H	-4.9852599	0.4035453	0.0769255
H	2.1675113	6.8520698	-4.6643770
H	3.2752884	3.4789581	-10.4632640
H	1.1498287	-0.7979479	-1.6975644

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C	-8.6383385	-2.1769540	-7.6900518
H	-8.4154579	-2.8278043	-6.8320766
H	-8.4238866	-2.7688562	-8.5961183
C	-7.7462917	-0.9664981	-7.6277450
N	-7.3524891	-0.2514655	-8.7424398
H	-7.5887613	-0.4169666	-9.7282346
C	-6.5222757	0.7349981	-8.3707795
H	-6.0697822	1.4456799	-9.0619921
N	-6.3454104	0.7106431	-7.0492662
C	-7.1039294	-0.3446465	-6.5779563
H	-7.1517005	-0.5884696	-5.5252540
C	-7.5940096	7.2460010	-5.9079045
H	-8.3518065	7.6103923	-6.6134791
H	-6.6817528	7.8403170	-6.0795766
C	-7.3181670	5.8101542	-6.2150278
N	-8.1729786	5.0450415	-6.9852660
H	-9.0924530	5.3455720	-7.3248297
C	-7.6269014	3.8242716	-7.1595288
H	-8.0911509	3.0363207	-7.7500899
N	-6.4551447	3.7570883	-6.5345525
C	-6.2516612	4.9883670	-5.9466467
H	-5.3494792	5.2066718	-5.3843509
C	-4.3783804	1.1196402	-0.4934972
H	-4.2415751	1.9801245	0.1812434
H	-3.3932161	0.6528513	-0.6471766
C	-4.8994640	1.5308288	-1.8426372
N	-5.8786276	2.4824562	-2.0376083
H	-6.2786420	3.0582687	-1.2912539
C	-6.1343721	2.5753710	-3.3602682
H	-6.8686500	3.2585047	-3.7792377
N	-5.3653378	1.7391298	-4.0449713
C	-4.5947410	1.0794699	-3.1107236
H	-3.8668215	0.3211337	-3.3881105
C	1.3484022	7.1524993	-4.0905241
H	1.5253112	7.1261795	-3.0048000
H	1.1280699	8.1960776	-4.3499059
C	0.2011345	6.2870987	-4.5038990
N	-1.0029526	6.8135085	-4.9263922
H	-1.2456697	7.7984596	-4.9581464
C	-1.7989545	5.8001810	-5.3378562
H	-2.7903827	5.9446503	-5.7580245
N	-1.1726678	4.6436539	-5.2089664
C	0.0649073	4.9279298	-4.6797596
H	0.7927352	4.1459071	-4.4711590
C	2.1389559	3.7770712	-10.0703457
H	2.0651590	4.8653419	-9.9341372
H	1.6255002	3.5413885	-11.0215188
C	1.3957082	3.0958272	-8.9648264
N	1.3179721	1.7223816	-8.8200616
H	1.8420499	1.0383079	-9.3607921
C	0.4187467	1.4379748	-7.8564859
H	0.2046815	0.4303383	-7.5202980
N	-0.1014935	2.5535041	-7.3607611
C	0.5054861	3.5957627	-8.0412386
H	0.2413142	4.6359676	-7.8707830
C	0.1100330	-1.0066752	-2.0855842
H	0.1477069	-1.9572463	-2.6339701
H	-0.5197681	-1.1588549	-1.1941290
C	-0.4968854	0.0861209	-2.9125730
N	-1.0338548	1.2185256	-2.3164971
H	-1.0941074	1.3904762	-1.3182378
C	-1.4524671	2.0600849	-3.2889091
H	-1.9251954	3.0199914	-3.0991532
N	-1.2165339	1.5407767	-4.4792222
C	-0.6194387	0.3134519	-4.2637015
H	-0.3331898	-0.3511879	-5.0750687
Cu	-5.1672306	2.1002587	-6.1621703
Cu	-1.7320546	2.7474531	-6.1407579
O	-3.5577913	3.0516227	-6.1870397
O	-4.8799430	3.1818116	-9.0701770
C	-3.7754009	3.7717058	-9.5959056
C	-3.1148992	4.7627404	-8.8535227
C	-1.9670296	5.3688154	-9.3883466
C	-1.4718695	4.9745186	-10.6347313
C	-2.1413337	3.9852269	-11.3595381
C	-3.2991577	3.3860624	-10.8481631
O	-1.3128162	6.3211323	-8.6583068
H	-1.8962079	6.5410207	-7.9159969
H	-0.5670669	5.4457240	-11.0193065
H	-1.7796320	3.6955145	-12.3476476
H	-3.8834292	2.6664164	-11.4199273
H	-5.2657145	3.7779999	-8.4067505
O	-3.5913714	5.1367299	-7.6292603
H	-3.6203963	4.2975473	-7.0111718
H	-9.7115709	-1.9877065	-7.6694560
H	-7.9614741	7.4610311	-4.9045111

H	-5.0195133	0.3926009	0.0049292
H	2.2834907	6.8908046	-4.5856926
H	3.1908737	3.5111545	-10.1743830
H	1.1163034	-0.7299025	-1.7711272

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C	-8.7192578	-2.1946810	-7.7606556
H	-8.4866839	-2.8505916	-6.9086589
H	-8.5304884	-2.7849173	-8.6733718
C	-7.8158101	-0.9947361	-7.7130228
N	-7.4408598	-0.2810004	-8.8333768
H	-7.6980782	-0.4860340	-9.8058821
C	-6.6023746	0.7077052	-8.4731899
H	-6.1728523	1.4221920	-9.1762755
N	-6.4076982	0.6772065	-7.1575495
C	-7.1571863	-0.3747952	-6.6738475
H	-7.1878649	-0.6176241	-5.6196673
C	-7.6734045	7.2499253	-6.0449181
H	-8.4307585	7.6216057	-6.7471307
H	-6.7529919	7.8264537	-6.2348495
C	-7.4313365	5.8053046	-6.3243029
N	-8.2815243	5.0498920	-7.1054440
H	-9.1833340	5.3703569	-7.4699198
C	-7.7764294	3.8012018	-7.2141404
H	-8.2445469	3.0100164	-7.7966373
N	-6.6450425	3.7106315	-6.5313854
C	-6.4123733	4.9521433	-5.9834098
H	-5.5293630	5.1648440	-5.3873147
C	-4.3632780	1.1193729	-0.5318308
H	-4.2049786	1.9702855	0.1508139
H	-3.3874127	0.6388520	-0.7011953
C	-4.8915746	1.5600752	-1.8695516
N	-5.8547298	2.5338268	-2.0307140
H	-6.2351000	3.0997955	-1.2672050
C	-6.1189050	2.6689687	-3.3473908
H	-6.8520980	3.3697349	-3.7388712
N	-5.3698517	1.8415362	-4.0634334
C	-4.6060028	1.1393783	-3.1537088
H	-3.8933972	0.3784851	-3.4643906
C	1.3053331	7.2137378	-4.2366964
H	1.3997665	7.1428664	-3.1431034
H	1.1338923	8.2704371	-4.4773076
C	0.1722931	6.3845146	-4.7547710
N	-0.8417741	6.9038091	-5.5375580
H	-0.9570292	7.8797532	-5.7972170
C	-1.6291079	5.8898903	-5.9623063
H	-2.4856755	6.0163997	-6.6287388
N	-1.1738281	4.7386159	-5.4878640
C	-0.0587813	5.0282699	-4.7357188
H	0.5325013	4.2483101	-4.2608419
C	2.0716317	4.0276781	-10.2719367
H	2.0783419	5.1005741	-10.0361581
H	1.6130119	3.9312997	-11.2727664
C	1.1864511	3.3110189	-9.3036536
N	0.6658485	2.0583052	-9.5697867
H	0.8894132	1.4904224	-10.3824231
C	-0.2335156	1.7482287	-8.6103812
H	-0.8443702	0.8536384	-8.6299706
N	-0.3141473	2.7205845	-7.7190154
C	0.5628662	3.7026076	-8.1406484
H	0.6517420	4.6515892	-7.6219256
C	0.0672037	-0.9219702	-2.1844104
H	0.1032433	-1.8476745	-2.7740208
H	-0.5634370	-1.1170418	-1.3013455
C	-0.5442120	0.2039952	-2.9662860
N	-1.0512579	1.3244954	-2.3219042
H	-1.0845904	1.4646697	-1.3174900
C	-1.4830003	2.2009525	-3.2586709
H	-1.9390623	3.1592408	-3.0191644
N	-1.2860320	1.7163178	-4.4705107
C	-0.7006471	0.4749879	-4.3070580
H	-0.4350222	-0.1559494	-5.1521573
Cu	-5.3661120	2.1140303	-6.2169024
Cu	-1.7266445	2.8955787	-6.1990618
O	-3.7918450	3.3379360	-6.4964133
O	-3.3664645	2.1946203	-7.1465899
C	-2.7522228	4.2635991	-9.8890804
C	-3.2770944	5.4508243	-9.3808714
C	-3.1562142	6.6543211	-10.1021530
C	-2.5007430	6.6538540	-11.3345454
C	-1.9628506	5.4645468	-11.8413704
C	-2.0883838	4.2733090	-11.1231754
O	-3.6882860	7.7991372	-9.5941150
H	-4.1849347	7.5485797	-8.8002007
H	-2.4464684	7.5874263	-11.8984222
H	-1.4715625	5.4649379	-12.8150401

H	-1.6977084	3.3441364	-11.5411196
H	-2.8767224	3.3381230	-9.3225046
O	-3.9286459	5.5611225	-8.1727750
H	-4.0310372	4.6891650	-7.7381074
H	-9.7888582	-1.9894566	-7.7170174
H	-8.0252145	7.4864621	-5.0407535
H	-5.0080220	0.3979567	-0.0299041
H	2.2656035	6.9318753	-4.6685537
H	3.1022234	3.6759882	-10.3194899
H	1.0738822	-0.6612239	-1.8577974

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C	-8.7153708	-2.1542900	-7.7632448
H	-8.4712100	-2.8049039	-6.9106316
H	-8.5288182	-2.7484913	-8.6740579
C	-7.8175967	-0.9489737	-7.7331481
N	-7.4545148	-0.2533497	-8.8679094
H	-7.7223510	-0.4734155	-9.8336525
C	-6.6180711	0.7457778	-8.5305135
H	-6.2000272	1.4526543	-9.2480841
N	-6.4125278	0.7389501	-7.2174444
C	-7.1538895	-0.3075479	-6.7093011
H	-7.1776453	-0.5277708	-5.6492127
C	-7.7792644	7.2846917	-6.0713933
H	-8.5625634	7.6532314	-6.7455474
H	-6.8686145	7.8655711	-6.2943963
C	-7.5441120	5.8394178	-6.3524927
N	-8.3761898	5.0959800	-7.1646353
H	-9.2701313	5.4218308	-7.5425803
C	-7.8770263	3.8442001	-7.2676415
H	-8.3315519	3.0598191	-7.8699172
N	-6.7680732	3.7431703	-6.5518652
C	-6.5434101	4.9770244	-5.9856586
H	-5.6763571	5.1749186	-5.3623753
C	-4.3818185	1.1330509	-0.5806644
H	-4.2099734	1.9816023	0.1019643
H	-3.4100478	0.6538085	-0.7739045
C	-4.9410128	1.5785048	-1.9052769
N	-5.9273857	2.5334151	-2.0391552
H	-6.3001031	3.0885189	-1.2648441
C	-6.2205757	2.6698995	-3.3514558
H	-6.9754359	3.3583843	-3.7224193
N	-5.4716623	1.8645338	-4.0885795
C	-4.6743353	1.1747874	-3.1995614
H	-3.9535968	0.4303258	-3.5302791
C	1.3488343	7.1363192	-4.2200998
H	1.4702292	7.0888765	-3.1274676
H	1.1285553	8.1825497	-4.4708079
C	0.2434425	6.2496461	-4.7014350
N	-0.8465122	6.7274621	-5.4014502
H	-1.0409920	7.7016257	-5.6119491
C	-1.5958921	5.6734925	-5.8066423
H	-2.4993254	5.7736426	-6.4070486
N	-1.0476953	4.5390816	-5.4059873
C	0.0920063	4.8803496	-4.7150460
H	0.7568523	4.1263260	-4.2970186
C	2.1627265	4.0914931	-10.2955047
H	2.1814890	5.1419982	-9.9759940
H	1.7189456	4.0749226	-11.3075891
C	1.2621304	3.3087467	-9.4024511
N	0.7460323	2.0849059	-9.7799938
H	0.9689146	1.5952229	-10.6428975
C	-0.1361534	1.6824776	-8.8385204
H	-0.7426398	0.7915642	-8.9353642
N	-0.2123655	2.5684594	-7.8617458
C	0.6508123	3.5914369	-8.2036901
H	0.7425112	4.4870356	-7.5970144
C	0.1159688	-1.0360627	-2.0483438
H	0.1503359	-1.9964043	-2.5802220
H	-0.5075741	-1.1695249	-1.1496058
C	-0.4871200	0.0451692	-2.8916252
N	-1.0528490	1.1720260	-2.3104944
H	-1.1546797	1.3361444	-1.3146700
C	-1.4294742	2.0206027	-3.2953693
H	-1.9139013	2.9783683	-3.1210826
N	-1.1390850	1.5069697	-4.4757661
C	-0.5509213	0.2796726	-4.2446094
H	-0.2194877	-0.3670072	-5.0532557
Cu	-5.4159016	2.2243086	-6.2899489
Cu	-1.4425347	2.5641924	-6.2038076
O	-3.9253081	3.5393216	-6.3580487
O	-3.3490568	2.3344244	-6.8444485
C	-2.7308873	4.0633615	-9.7088478
C	-3.3619421	5.2114300	-9.1820418
C	-3.4046615	6.4131442	-9.9782318
C	-2.7937266	6.4600427	-11.2337069

C	-2.1712537	5.3129247	-11.7261368
C	-2.1483335	4.1210112	-10.9670108
O	-4.0364827	7.4724530	-9.4555887
H	-4.3866531	7.1654522	-8.5963350
H	-2.8341515	7.3828204	-11.8153375
H	-1.7225388	5.3225089	-12.7199960
H	-1.6682330	3.2395459	-11.3938588
H	-2.7213000	3.1557539	-9.1041592
O	-3.9036503	5.3080596	-7.9882223
H	-3.9436688	4.3481078	-7.2638976
H	-9.7860941	-1.9564533	-7.7134588
H	-8.0964444	7.5201240	-5.0555021
H	-5.0119171	0.4079681	-0.0655943
H	2.3096327	6.8841297	-4.6688017
H	3.1860509	3.7192249	-10.3433588
H	1.1250959	-0.7536062	-1.7484317

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C	-8.7101051	-2.1764169	-7.7737714
H	-8.4675209	-2.8304128	-6.9231556
H	-8.5305721	-2.7704131	-8.6862633
C	-7.8025755	-0.9786649	-7.7415042
N	-7.4618951	-0.2581908	-8.8673075
H	-7.7479591	-0.4566565	-9.8321548
C	-6.6048762	0.7233633	-8.5249061
H	-6.1991032	1.4438552	-9.2356012
N	-6.3649765	0.6817052	-7.2197062
C	-7.1041363	-0.3704597	-6.7203066
H	-7.0994788	-0.6230051	-5.6669136
C	-7.7863442	7.2732453	-6.0659491
H	-8.5709464	7.6392177	-6.7401496
H	-6.8751656	7.8518884	-6.2937060
C	-7.5553994	5.8251072	-6.3378571
N	-8.3694057	5.0881362	-7.1733687
H	-9.2533752	5.4186160	-7.5694979
C	-7.8770977	3.8309181	-7.2573795
H	-8.3229368	3.0486954	-7.8692962
N	-6.7914279	3.7191917	-6.5094420
C	-6.5753939	4.9528253	-5.9387474
H	-5.7305645	5.1431320	-5.2833086
C	-4.3752575	1.1402302	-0.5437512
H	-4.2029766	1.9837700	0.1449134
H	-3.4035137	0.6636280	-0.7434637
C	-4.9410736	1.5910372	-1.8629930
N	-5.9446769	2.5294787	-1.9864057
H	-6.3205897	3.0754758	-1.2075425
C	-6.2512017	2.6640593	-3.2955624
H	-7.0201540	3.3400830	-3.6602787
N	-5.4941330	1.8734260	-4.0390601
C	-4.6767342	1.1959226	-3.1597839
H	-3.9444892	0.4671601	-3.4997995
C	1.3348303	7.1101049	-4.2291812
H	1.4571396	7.0601090	-3.1364206
H	1.1152433	8.1579617	-4.4752554
C	0.2248407	6.2270916	-4.7093128
N	-0.8894423	6.7166639	-5.3609296
H	-1.0940562	7.6944128	-5.5410499
C	-1.6510582	5.6646140	-5.7560344
H	-2.5817272	5.7775968	-6.3066969
N	-1.0899815	4.5237258	-5.3997193
C	0.0732167	4.8573366	-4.7455344
H	0.7499069	4.0960518	-4.3602236
C	2.1774245	4.1062525	-10.2923352
H	2.2025290	5.1491635	-9.9494457
H	1.7381692	4.1147058	-11.3066170
C	1.2679889	3.3100943	-9.4208683
N	0.7716900	2.0832795	-9.8135679
H	1.0234445	1.5940665	-10.6685748
C	-0.1199598	1.6664709	-8.8846161
H	-0.7082293	0.7649806	-8.9914901
N	-0.2259190	2.5484081	-7.9079587
C	0.6319449	3.5816743	-8.2321621
H	0.7085273	4.4740315	-7.6178007
C	0.1463913	-1.0707969	-2.0132744
H	0.1820490	-2.0429590	-2.5235477
H	-0.4817086	-1.1811063	-1.1147675
C	-0.4420902	-0.0048504	-2.8842156
N	-1.0322683	1.1226539	-2.3312051
H	-1.1693278	1.2946082	-1.3412866
C	-1.3707727	1.9644665	-3.3381453
H	-1.8670547	2.9204220	-3.1889451
N	-1.0323239	1.4468860	-4.5031331
C	-0.4521298	0.2239318	-4.2398723
H	-0.0890835	-0.4279921	-5.0304885
Cu	-5.4374689	2.1665369	-6.2146684
Cu	-1.3848003	2.5020793	-6.2361237

O	-3.9154103	3.6148429	-6.2182122
O	-3.4104690	2.3495508	-6.6759509
C	-2.7419527	4.0628892	-9.8179094
C	-3.4081968	5.2425456	-9.3466274
C	-3.4018111	6.4329362	-10.2068197
C	-2.7467025	6.4303252	-11.4408902
C	-2.1153729	5.2590241	-11.8514100
C	-2.1116268	4.0866059	-11.0384259
O	-4.0478826	7.4897531	-9.7338383
H	-4.4109469	7.1938437	-8.8692798
H	-2.7588022	7.3218675	-12.0703084
H	-1.6283936	5.2223562	-12.8268194
H	-1.6021145	3.2006854	-11.4178894
H	-2.7484385	3.1824083	-9.1724637
O	-3.9949703	5.3589936	-8.2271193
H	-4.0043302	4.1650972	-7.0528786
H	-9.7792945	-1.9717748	-7.7187973
H	-8.1009748	7.5147276	-5.0506854
H	-5.0060226	0.4107370	-0.0357732
H	2.2967712	6.8610663	-4.6771945
H	3.1983845	3.7280614	-10.3440907
H	1.1549008	-0.7835232	-1.7158707

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C	-8.6636158	-2.0805998	-7.7329035
H	-8.4202678	-2.7281762	-6.8778976
H	-8.4656786	-2.6753629	-8.6411600
C	-7.7680105	-0.8699800	-7.7008971
N	-7.3798076	-0.1983062	-8.8423018
H	-7.6415920	-0.4286490	-9.8072900
C	-6.5436591	0.8031345	-8.5085224
H	-6.1129560	1.4957044	-9.2319953
N	-6.3619498	0.8226200	-7.1929780
C	-7.1190772	-0.2099303	-6.6772533
H	-7.1635091	-0.4029774	-5.6120626
C	-7.8889698	7.2693262	-6.1063766
H	-8.7160226	7.6058685	-6.7432133
H	-7.0029390	7.8622196	-6.3906737
C	-7.6396053	5.8220857	-6.3632110
N	-8.4152704	5.0703124	-7.2214254
H	-9.2920376	5.3889214	-7.6411596
C	-7.9003631	3.8222596	-7.2911738
H	-8.3134325	3.0328688	-7.9157933
N	-6.8336907	3.7344827	-6.5113056
C	-6.6578762	4.9706531	-5.9320832
H	-5.8281933	5.1722867	-5.2623857
C	-4.3826645	1.1326699	-0.5602801
H	-4.2048730	1.9783957	0.1242120
H	-3.4128148	0.6530168	-0.7636873
C	-4.9584955	1.5779632	-1.8773890
N	-5.9573402	2.5221225	-1.9975727
H	-6.3205161	3.0784330	-1.2201803
C	-6.2814959	2.6409321	-3.3049280
H	-7.0469599	3.3223706	-3.6672782
N	-5.5435974	1.8347670	-4.0492308
C	-4.7171729	1.1650444	-3.1733399
H	-3.9942403	0.4264425	-3.5129181
C	1.3005413	7.0468910	-4.2514067
H	1.4053919	6.9717056	-3.1584044
H	1.0781530	8.0999542	-4.4741211
C	0.1991221	6.1745614	-4.7753064
N	-0.9334596	6.6956592	-5.3699937
H	-1.1547266	7.6808125	-5.4733708
C	-1.6901258	5.6729421	-5.8335971
H	-2.6310273	5.8158710	-6.3585943
N	-1.1066687	4.5150657	-5.5761945
C	0.0644986	4.8091339	-4.9132908
H	0.7517452	4.0265517	-4.5958616
C	2.1988836	4.0448207	-10.3019139
H	2.2040926	5.0995468	-9.9959343
H	1.7471617	4.0066223	-11.3102603
C	1.3244161	3.2592944	-9.3866822
N	0.8926741	1.9840110	-9.6954319
H	1.1753084	1.4475628	-10.5117927
C	0.0142546	1.5891448	-8.7483183
H	-0.5263001	0.6538895	-8.7923079
N	-0.1414428	2.5312517	-7.8350014
C	0.6655005	3.5816946	-8.2239044
H	0.6943551	4.5173730	-7.6746518
C	0.1383003	-1.0112717	-2.0992628
H	0.1750684	-1.9855481	-2.6056142
H	-0.5080494	-1.1173458	-1.2130942
C	-0.4312819	0.0547021	-2.9863750
N	-1.0556582	1.1709128	-2.4485762
H	-1.2230600	1.3390047	-1.4625828
C	-1.3924668	2.0031221	-3.4636582

H	-1.9216932	2.9431274	-3.3246653
N	-1.0175494	1.4946450	-4.6209523
C	-0.4176476	0.2848031	-4.3433255
H	-0.0303196	-0.3635244	-5.1255820
Cu	-5.3563204	2.3228762	-6.2544129
Cu	-1.6197191	2.5844369	-6.4032558
O	-4.0824444	3.7951264	-5.9484732
O	-3.4094333	2.1825063	-6.6889157
C	-2.8586671	4.1770573	-9.7099197
C	-3.4368964	5.4140299	-9.2622584
C	-3.3560976	6.5756227	-10.1595401
C	-2.7155117	6.4924761	-11.3978002
C	-2.1573859	5.2730806	-11.7751320
C	-2.2301236	4.1254428	-10.9312893
O	-3.9208692	7.6896809	-9.7128453
H	-4.2849889	7.4478057	-8.8319098
H	-2.6761237	7.3642986	-12.0537704
H	-1.6759927	5.1790761	-12.7499371
H	-1.7838858	3.1979636	-11.2902342
H	-2.9367894	3.3115933	-9.0472967
O	-3.9962091	5.5997203	-8.1414471
H	-4.0917485	4.2972737	-6.7979576
H	-9.7373227	-1.8970107	-7.6939777
H	-8.1577584	7.5164205	-5.0793598
H	-5.0113385	0.4057918	-0.0460003
H	2.2708379	6.8162164	-4.6911568
H	3.2276150	3.6883882	-10.3542021
H	1.1433897	-0.7342512	-1.7812666

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C	-8.5828322	-2.0141779	-7.6936484
H	-8.3408881	-2.6491158	-6.8293988
H	-8.3785384	-2.6205781	-8.5925742
C	-7.6881263	-0.7999738	-7.6747941
N	-7.2905231	-0.1520072	-8.8266372
H	-7.5537506	-0.3901374	-9.7892272
C	-6.4411849	0.8439267	-8.5091834
H	-6.0016532	1.5181442	-9.2443520
N	-6.2605615	0.8862466	-7.1949392
C	-7.0323854	-0.1267130	-6.6614601
H	-7.0801986	-0.2988481	-5.5925439
C	-7.8486833	7.2506224	-6.0921289
H	-8.6876264	7.5535341	-6.7310639
H	-6.9833705	7.8708979	-6.3814035
C	-7.5462270	5.8117961	-6.3414734
N	-8.3195413	5.0178519	-7.1640422
H	-9.2177700	5.2980235	-7.5654750
C	-7.7489723	3.7955087	-7.2462041
H	-8.1514626	2.9846907	-7.8488788
N	-6.6468382	3.7630824	-6.5102006
C	-6.5077352	5.0110440	-5.9450356
H	-5.6612032	5.2529250	-5.3115031
C	-4.3596297	1.1329134	-0.5547043
H	-4.1967699	1.9787997	0.1336365
H	-3.3844690	0.6542053	-0.7335637
C	-4.8967942	1.5829517	-1.8865114
N	-5.8842390	2.5352279	-2.0341041
H	-6.2728142	3.0866677	-1.2653998
C	-6.1493358	2.6783482	-3.3531505
H	-6.8968360	3.3698581	-3.7339339
N	-5.3838582	1.8804868	-4.0795248
C	-4.6036897	1.1883452	-3.1780638
H	-3.8699211	0.4522996	-3.5012030
C	1.3286581	7.1930919	-4.1944948
H	1.4424141	7.1260188	-3.1020722
H	1.1588346	8.2509295	-4.4329251
C	0.1740712	6.3842429	-4.6935548
N	-0.9409947	6.9680163	-5.2653105
H	-1.1021182	7.9640366	-5.3793190
C	-1.7688770	5.9926803	-5.6984452
H	-2.7129012	6.1740427	-6.2070877
N	-1.2406006	4.8069969	-5.4404138
C	-0.0370707	5.0290611	-4.8138773
H	0.6110342	4.2084888	-4.5138682
C	2.0266254	3.9531546	-10.1654167
H	2.0388277	5.0361848	-9.9764232
H	1.5626438	3.8144647	-11.1595648
C	1.1354349	3.2923133	-9.1575818
N	0.6450762	2.0070933	-9.3150455
H	0.9207988	1.3551599	-10.0442318
C	-0.2981739	1.7825607	-8.3691479
H	-0.8907254	0.8754903	-8.3117537
N	-0.4397079	2.8401513	-7.5918159
C	0.4454304	3.7879349	-8.0713687
H	0.5030105	4.7861899	-7.6479042
C	0.0550918	-0.8519040	-2.2479480

H	0.0911950	-1.7534238	-2.8743325
H	-0.5794701	-1.0840524	-1.3763167
C	-0.5549111	0.3045644	-2.9885711
N	-1.0351130	1.4126638	-2.3037432
H	-1.0573366	1.5215876	-1.2952399
C	-1.4728521	2.3199112	-3.2098773
H	-1.9189743	3.2730560	-2.9333505
N	-1.3037301	1.8701652	-4.4376067
C	-0.7360813	0.6166120	-4.3186228
H	-0.5034407	0.0025167	-5.1859361
Cu	-5.1237829	2.3757337	-6.3322161
Cu	-2.0666965	3.0704798	-6.1609490
O	-3.8751715	3.9042126	-6.0173952
O	-3.3301518	1.9200947	-7.0229841
C	-2.8665762	4.2073167	-9.7704001
C	-3.4266803	5.4522410	-9.3200015
C	-3.3880864	6.5979472	-10.2394488
C	-2.7805123	6.5025556	-11.4924244
C	-2.2206310	5.2824048	-11.8657934
C	-2.2706506	4.1441061	-11.0072973
O	-3.9551422	7.7114161	-9.7933058
H	-4.2900770	7.4744139	-8.8992717
H	-2.7710637	7.3637845	-12.1632038
H	-1.7616145	5.1788903	-12.8504042
H	-1.8368513	3.2120845	-11.3699358
H	-2.9324081	3.3431437	-9.1035869
O	-3.9421522	5.6614623	-8.1812842
H	-3.9707466	4.4482468	-6.8348038
H	-9.6593509	-1.8450511	-7.6697710
H	-8.1261783	7.4974244	-5.0673598
H	-5.0002879	0.4081731	-0.0523348
H	2.2804563	6.9105970	-4.6443207
H	3.0592485	3.6085308	-10.2201006
H	1.0608411	-0.6072450	-1.9063681

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C	-8.5399212	-2.0870912	-7.6548448
H	-8.3274724	-2.7366041	-6.7933972
H	-8.3396091	-2.6915113	-8.5560285
C	-7.5982455	-0.9097519	-7.6113950
N	-7.1298164	-0.2865665	-8.7508632
H	-7.4027661	-0.4655404	-9.7244046
C	-6.2120371	0.6346305	-8.4096447
H	-5.6688096	1.2323879	-9.1360012
N	-6.0562694	0.6642970	-7.0916793
C	-6.9178344	-0.2894611	-6.5811630
H	-7.0030681	-0.4621732	-5.5159723
C	-7.8808556	7.1158453	-6.0707032
H	-8.7546910	7.3771033	-6.6818136
H	-7.0423131	7.7437190	-6.4199933
C	-7.5595199	5.6737619	-6.2899420
N	-8.2115799	4.9091737	-7.2351052
H	-9.0599347	5.1961296	-7.7254729
C	-7.6182771	3.6937062	-7.2885277
H	-7.9450915	2.9052959	-7.9634756
N	-6.6140869	3.6321584	-6.4245990
C	-6.5767612	4.8548097	-5.7952497
H	-5.8420032	5.0879137	-5.0305454
C	-4.4146967	1.1024794	-0.5335643
H	-4.2771498	1.9718781	0.1295281
H	-3.4281420	0.6388500	-0.6892587
C	-4.9526595	1.4900498	-1.8837200
N	-5.9579990	2.4143420	-2.0857619
H	-6.3622275	2.9983349	-1.3492250
C	-6.2346121	2.4679047	-3.4080977
H	-6.9900577	3.1254768	-3.8295031
N	-5.4553096	1.6365719	-4.0855252
C	-4.6555121	1.0205004	-3.1465004
H	-3.9015011	0.2859697	-3.4174759
C	1.3675164	7.1212594	-4.1711507
H	1.5243184	7.0636047	-3.0830131
H	1.1696500	8.1766832	-4.4047558
C	0.2042134	6.3020063	-4.6294953
N	-1.0157981	6.8871432	-4.9010300
H	-1.2422526	7.8702883	-4.7970643
C	-1.8498886	5.9430821	-5.3851464
H	-2.8753306	6.1409325	-5.6825614
N	-1.2326691	4.7756689	-5.4538275
C	0.0404390	4.9769432	-4.9719260
H	0.7616848	4.1649136	-4.9094589
C	2.0682524	3.8634587	-10.1662427
H	2.0565916	4.9513092	-10.0077471
H	1.6186226	3.6807684	-11.1608883
C	1.1798709	3.2260366	-9.1439347
N	0.8626252	1.8789583	-9.1282429
H	1.2881079	1.1635024	-9.7133441

C	-0.1250931	1.6781757	-8.2241370
H	-0.5675799	0.7112863	-8.0110436
N	-0.4661996	2.8172035	-7.6475344
C	0.3400000	3.7895998	-8.2064048
H	0.2601959	4.8370455	-7.9299645
C	0.0443905	-0.8671037	-2.2707933
H	0.0902523	-1.8135558	-2.8267247
H	-0.6082912	-1.0339162	-1.3976895
C	-0.5527674	0.2280026	-3.1094678
N	-1.1389186	1.3404524	-2.5218571
H	-1.2305228	1.5050673	-1.5253031
C	-1.5862286	2.1598702	-3.5040346
H	-2.1321425	3.0818564	-3.3229355
N	-1.3190443	1.6563617	-4.6932559
C	-0.6722252	0.4556515	-4.4634215
H	-0.3488058	-0.1982507	-5.2697357
Cu	-4.9610363	2.1236158	-6.1735882
Cu	-2.1084000	3.0531071	-6.3829366
O	-3.7574760	3.4685270	-5.3704316
O	-3.4550307	2.3280635	-7.6568235
C	-4.1517395	3.9428659	-9.0453145
C	-3.7817968	5.2025830	-8.3902263
C	-2.8623403	6.1090379	-9.0964647
C	-2.3256079	5.7585589	-10.3136459
C	-2.6940578	4.5282773	-10.9101424
C	-3.6071104	3.6580274	-10.3014111
O	-2.5892836	7.2638641	-8.4859232
H	-3.1884850	7.3022035	-7.7144234
H	-1.6679821	6.4731739	-10.8055267
H	-2.3179406	4.2824212	-11.9057514
H	-3.9754666	2.8024568	-10.8676567
H	-5.0769157	3.4826417	-8.7139482
O	-4.2050950	5.5814514	-7.2779840
H	-4.0672977	4.2492421	-5.8680067
H	-9.6128509	-1.8954006	-7.6428825
H	-8.1211759	7.3923959	-5.0441398
H	-5.0489292	0.3779756	-0.0227710
H	2.3063091	6.8593120	-4.6591243
H	3.1081370	3.5385235	-10.1997652
H	1.0439014	-0.6055824	-1.9234450

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C	-8.5237322	-2.0721453	-7.6399341
H	-8.3066580	-2.7133584	-6.7738732
H	-8.2995510	-2.6748090	-8.5368137
C	-7.6228286	-0.8642329	-7.5855383
N	-7.2258058	-0.1704008	-8.7104449
H	-7.4848654	-0.3465903	-9.6882859
C	-6.3585561	0.7935221	-8.3540737
H	-5.9149844	1.4762827	-9.0736530
N	-6.1624453	0.7797507	-7.0405511
C	-6.9478491	-0.2463341	-6.5500494
H	-6.9896296	-0.4705210	-5.4920243
C	-7.7591803	7.3299574	-5.9818661
H	-8.5971067	7.6388397	-6.6188056
H	-6.8973936	7.9635783	-6.2528103
C	-7.4449600	5.8957909	-6.2545847
N	-8.1778839	5.1273226	-7.1347746
H	-9.0626350	5.4116807	-7.5624440
C	-7.6007626	3.9051861	-7.2184501
H	-7.9850541	3.1115842	-7.8568740
N	-6.5340040	3.8421582	-6.4344985
C	-6.4304111	5.0743954	-5.8309815
H	-5.6471286	5.3058134	-5.1145063
C	-4.4443231	1.1138708	-0.5242604
H	-4.2959083	1.9786782	0.1422960
H	-3.4610157	0.6499719	-0.6978916
C	-5.0009503	1.5133652	-1.8631486
N	-5.9768888	2.4723332	-2.0476649
H	-6.3527738	3.0622796	-1.3003574
C	-6.2703004	2.5426154	-3.3641631
H	-6.9975931	3.2354479	-3.7785828
N	-5.5329020	1.6833565	-4.0536172
C	-4.7409622	1.0345727	-3.1296952
H	-4.0217256	0.2696114	-3.4109215
C	1.3966224	7.1637417	-4.0960685
H	1.5694639	7.1061620	-3.0105481
H	1.2033020	8.2190923	-4.3300313
C	0.2202393	6.3563938	-4.5367988
N	-0.9919846	6.9572261	-4.8087771
H	-1.2057839	7.9435682	-4.7105576
C	-1.8413523	6.0224888	-5.2844425
H	-2.8548016	6.2420359	-5.6029273
N	-1.2416055	4.8459291	-5.3435944
C	0.0358986	5.0320846	-4.8686402
H	0.7504905	4.2131269	-4.8158963

C	1.9906453	3.9689928	-10.1375650
H	1.9887018	5.0596455	-10.0021958
H	1.5215390	3.7714443	-11.1200618
C	1.1235423	3.3463328	-9.0858189
N	0.8455078	1.9917822	-9.0365746
H	1.2313190	1.2785106	-9.6508071
C	-0.1146438	1.7796503	-8.1130946
H	-0.5273259	0.8045405	-7.8937697
N	-0.4840630	2.9172929	-7.5503551
C	0.2864227	3.9049041	-8.1418695
H	0.1870688	4.9532473	-7.8760172
C	0.0652566	-0.8676344	-2.2613365
H	0.1102386	-1.8073839	-2.8282878
H	-0.5850861	-1.0452161	-1.3887527
C	-0.5358475	0.2393007	-3.0811750
N	-1.1501146	1.3234304	-2.4694110
H	-1.2488028	1.4612462	-1.4694713
C	-1.6003826	2.1632123	-3.4309617
H	-2.1637063	3.0707968	-3.2333597
N	-1.3090107	1.6980331	-4.6308899
C	-0.6396615	0.5041512	-4.4293063
H	-0.2941294	-0.1178369	-5.2515155
Cu	-5.0256387	2.2000626	-6.0672377
Cu	-2.0937641	3.0698260	-6.2556866
O	-3.7257645	3.4410038	-5.2125850
O	-3.6264360	2.5179974	-7.5852983
C	-3.9045767	3.3569924	-8.6737407
C	-3.5789081	4.8294904	-8.4439154
C	-3.0310544	5.6313691	-9.5445570
C	-2.6020210	5.0212781	-10.6837774
C	-2.7972575	3.6036516	-10.8994100
C	-3.4029635	2.8211986	-9.9807878
O	-2.8580269	6.9406966	-9.2933031
H	-3.2362855	7.0946044	-8.4080491
H	-2.1284908	5.6177587	-11.4657320
H	-2.4640722	3.2018730	-11.8536799
H	-3.6946169	1.7883047	-10.1968421
H	-5.0108360	3.4449540	-8.8336663
O	-3.7746457	5.3851384	-7.3563452
H	-3.9631961	4.2384927	-5.7230840
H	-9.5990263	-1.8938122	-7.6374436
H	-8.0453524	7.5520498	-4.9538354
H	-5.0716737	0.3862864	-0.0093637
H	2.3272165	6.8954297	-4.5961382
H	3.0259408	3.6313661	-10.1848717
H	1.0655112	-0.6094712	-1.9136168

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C	-8.4668441	-1.9720578	-7.6666963
H	-8.2477222	-2.6258387	-6.8101057
H	-8.2365949	-2.5562620	-8.5742799
C	-7.5701474	-0.7606837	-7.5786120
N	-7.1869068	-0.0097321	-8.6732392
H	-7.4452485	-0.1582091	-9.6567710
C	-6.3230436	0.9416066	-8.2783770
H	-5.8781513	1.6568854	-8.9644562
N	-6.1149156	0.8673178	-6.9671526
C	-6.8880768	-0.1904519	-6.5212772
H	-6.9170179	-0.4706838	-5.4763657
C	-7.7817318	7.6158701	-6.3003822
H	-8.6828232	7.9468200	-6.8339306
H	-6.9926764	8.3472521	-6.5405142
C	-7.3536722	6.2817803	-6.8231567
N	-8.1878466	5.4164174	-7.5079343
H	-9.1960375	5.5493615	-7.6357164
C	-7.4521238	4.3919427	-7.9956541
H	-7.8569789	3.6013746	-8.6251709
N	-6.1830160	4.5412516	-7.6387156
C	-6.1067621	5.7170159	-6.9162110
H	-5.1577279	6.0989167	-6.5558694
C	-4.4669340	1.1037772	-0.4655796
H	-4.3323273	1.9712891	0.1999370
H	-3.4787331	0.6487297	-0.6329415
C	-5.0153933	1.4902831	-1.8093397
N	-5.9634074	2.4719670	-2.0160666
H	-6.3382581	3.0708652	-1.2745034
C	-6.2506039	2.5256104	-3.3337929
H	-6.9500104	3.2383814	-3.7636162
N	-5.5385079	1.6269120	-4.0000429
C	-4.7683393	0.9740256	-3.0618483
H	-4.0712886	0.1825255	-3.3248091
C	1.5610521	7.1551637	-3.9809499
H	1.8328147	7.1880531	-2.9135377
H	1.2761933	8.1776114	-4.2675802
C	0.4114901	6.2447362	-4.2415963
N	-0.8832058	6.7150117	-4.1623496

H	-1.1624754	7.6519519	-3.8967075
C	-1.7239478	5.7232885	-4.5209914
H	-2.7987707	5.8534674	-4.5680134
N	-1.0476617	4.6318887	-4.8238777
C	0.2822543	4.9333764	-4.6409738
H	1.0640714	4.1989785	-4.8188176
C	1.9693623	3.9789005	-10.0069068
H	1.9812928	5.0679578	-9.8613349
H	1.4895338	3.7970517	-10.9869841
C	1.1014022	3.3591088	-8.9523040
N	0.7589547	2.0170427	-8.9549371
H	1.1018660	1.3162464	-9.6071263
C	-0.1718717	1.8037083	-8.0019048
H	-0.6243981	0.8404627	-7.8104429
N	-0.4588779	2.9283105	-7.3689077
C	0.3283384	3.9096367	-7.9496222
H	0.2692944	4.9496235	-7.6412515
C	0.1463131	-1.0484131	-2.1513251
H	0.2085149	-1.9963099	-2.7019847
H	-0.4838249	-1.2225688	-1.2643208
C	-0.4986781	0.0343149	-2.9642227
N	-1.1327931	1.0928503	-2.3294158
H	-1.2126587	1.2172725	-1.3261164
C	-1.5984666	1.9416620	-3.2738759
H	-2.1644599	2.8418040	-3.0588807
N	-1.3055962	1.5036098	-4.4826859
C	-0.6127899	0.3194820	-4.3065872
H	-0.2564328	-0.2792544	-5.1414331
Cu	-4.8378731	2.0872912	-5.9195448
Cu	-1.9924640	3.0678326	-5.9951062
O	-3.6721581	3.3738012	-4.9674707
O	-3.5509898	2.5258726	-7.3913662
C	-3.7105930	3.4969109	-8.3666131
C	-3.1835972	4.8284413	-8.0701833
C	-2.8902813	5.7305910	-9.1649983
C	-2.9252772	5.2834830	-10.4615048
C	-3.3259370	3.9463824	-10.7492372
C	-3.6878298	3.0755786	-9.7601507
O	-2.4724993	6.9620784	-8.8143930
H	-2.5227378	6.9749899	-7.8389603
H	-2.6532455	5.9624284	-11.2726988
H	-3.3488980	3.6306521	-11.7846414
H	-4.0610728	2.0762315	-10.0009369
H	-4.9459517	3.9951288	-8.2012417
O	-3.0340981	5.2526665	-6.8841919
H	-3.8262050	4.1973565	-5.4728205
H	-9.5443803	-1.8077950	-7.6669052
H	-8.0070824	7.6962331	-5.2369795
H	-5.0956202	0.3712123	0.0405516
H	2.4636934	6.9076836	-4.5395720
H	3.0007792	3.6313578	-10.0657266
H	1.1425589	-0.7499428	-1.8250180

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C	-8.6589270	-2.1836019	-7.7132241
H	-8.4530134	-2.8349910	-6.8514808
H	-8.4588384	-2.7887823	-8.6144021
C	-7.7253617	-1.0078215	-7.6597023
N	-7.3668783	-0.2761200	-8.7738920
H	-7.6597901	-0.4239931	-9.7468943
C	-6.4632667	0.6524214	-8.4239665
H	-6.0060320	1.3576807	-9.1113699
N	-6.2073796	0.5775509	-7.1203577
C	-6.9884463	-0.4541286	-6.6339063
H	-6.9763059	-0.7354300	-5.5889494
C	-7.7355976	7.7123960	-6.2676426
H	-8.5670191	8.1615789	-6.8278276
H	-6.8597607	8.3576721	-6.4420354
C	-7.4432810	6.3589155	-6.8241913
N	-8.3871830	5.5903029	-7.4881093
H	-9.3864080	5.8071614	-7.5788910
C	-7.8026291	4.4914739	-7.9922203
H	-8.2865280	3.7276700	-8.5990550
N	-6.5199608	4.5218620	-7.6629821
C	-6.2657181	5.6654607	-6.9446841
H	-5.2634820	5.9058132	-6.6004537
C	-4.4683135	1.0814422	-0.5597996
H	-4.3371678	1.9658426	0.0835382
H	-3.4785430	0.6222537	-0.7062616
C	-5.0073374	1.4346415	-1.9189178
N	-5.9316489	2.4304052	-2.1596900
H	-6.2877680	3.0646173	-1.4395689
C	-6.2251025	2.4326460	-3.4811812
H	-6.9208982	3.1375950	-3.9302816
N	-5.5415571	1.4912705	-4.1158251
C	-4.7776883	0.8670586	-3.1537878

H	-4.0967030	0.0508944	-3.3809970
C	1.6023155	7.3037746	-4.0120943
H	1.8426489	7.3380368	-2.9376399
H	1.3797322	8.3312250	-4.3270291
C	0.4196451	6.4456855	-4.2859544
N	-0.8151213	6.9896132	-4.5745729
H	-1.0330058	7.9785075	-4.6276880
C	-1.6792154	5.9775783	-4.8180379
H	-2.7184764	6.1336952	-5.0902967
N	-1.0716719	4.8130247	-4.7031488
C	0.2315827	5.0853253	-4.3666027
H	0.9664952	4.2932364	-4.2314554
C	2.0984116	3.9145568	-10.0532537
H	2.0831485	5.0032385	-9.9025708
H	1.5974730	3.7233343	-11.0201795
C	1.2860173	3.2637665	-8.9800060
N	0.8682994	1.9475896	-9.0474719
H	1.1293263	1.2758415	-9.7641220
C	-0.0073322	1.7218431	-8.0446715
H	-0.5085371	0.7761674	-7.8929942
N	-0.1777243	2.8125735	-7.3164474
C	0.6286242	3.7803202	-7.8855229
H	0.6327594	4.8055665	-7.5354299
C	0.1414837	-1.0147596	-2.1548816
H	0.1933392	-1.9551091	-2.7193369
H	-0.4974795	-1.1910665	-1.2748004
C	-0.4680252	0.0964687	-2.9572880
N	-1.1074176	1.1450960	-2.3120677
H	-1.2426455	1.2264372	-1.3102099
C	-1.4895439	2.0524949	-3.2378628
H	-2.0284404	2.9666227	-3.0107171
N	-1.1298207	1.6590102	-4.4446490
C	-0.4931036	0.4427226	-4.2901296
H	-0.1078808	-0.1268754	-5.1323442
Cu	-4.9187706	1.8098035	-6.1844970
Cu	-1.7001579	3.0695841	-5.9364269
O	-3.6176308	2.9435574	-5.3537704
O	-4.6503508	2.8309112	-8.0390115
C	-3.7289024	3.3819462	-8.8372706
C	-2.8221933	4.3652889	-8.3208329
C	-1.9751651	5.0991009	-9.2078426
C	-1.9212243	4.7909340	-10.5551950
C	-2.7626646	3.7812969	-11.0438914
C	-3.6664714	3.1007785	-10.2222285
O	-1.2188134	6.0757223	-8.6568498
H	-1.4640203	6.0584967	-7.7113965
H	-1.2375963	5.3216856	-11.2167990
H	-2.7118602	3.5556495	-12.1044398
H	-4.3787398	2.3979334	-10.6613576
H	-5.7552374	3.7681569	-7.9000995
O	-2.6951810	4.6235302	-7.0408492
H	-3.7504341	3.7572284	-5.8799872
H	-9.7267866	-1.9656771	-7.6973798
H	-7.9988099	7.7749770	-5.2117689
H	-5.0962834	0.3613018	-0.0352826
H	2.5073387	6.9982715	-4.5371347
H	3.1361291	3.5902155	-10.1307875
H	1.1400496	-0.7318250	-1.8218940

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C	-8.6716031	-2.1842504	-7.7203473
H	-8.4641412	-2.8349013	-6.8584165
H	-8.4732870	-2.7902024	-8.6214325
C	-7.7378091	-1.0084944	-7.6704522
N	-7.3859529	-0.2760180	-8.7860734
H	-7.6829092	-0.4263546	-9.7573306
C	-6.4784461	0.6511864	-8.4410081
H	-6.0245637	1.3573120	-9.1302699
N	-6.2143874	0.5746186	-7.1392924
C	-6.9936605	-0.4564394	-6.6489759
H	-6.9746876	-0.7393823	-5.6044526
C	-7.7429602	7.7114272	-6.2709164
H	-8.5743477	8.1621107	-6.8299911
H	-6.8660575	8.3546033	-6.4476480
C	-7.4534945	6.3568932	-6.8271210
N	-8.4000109	5.5867779	-7.4858587
H	-9.3998620	5.8026756	-7.5724361
C	-7.8172711	4.4884437	-7.9926884
H	-8.3029783	3.7237037	-8.5969708
N	-6.5332398	4.5206105	-7.6695695
C	-6.2757577	5.6646446	-6.9529187
H	-5.2718550	5.9051075	-6.6138489
C	-4.4609948	1.0820313	-0.5656895
H	-4.3221369	1.9637916	0.0797111
H	-3.4747385	0.6170652	-0.7186330
C	-5.0029335	1.4414015	-1.9220297

N	-5.9227259	2.4422242	-2.1585296
H	-6.2755389	3.0753939	-1.4360489
C	-6.2188612	2.4482261	-3.4802801
H	-6.9144768	3.1555873	-3.9259190
N	-5.5409770	1.5058630	-4.1184281
C	-4.7790730	0.8758241	-3.1590528
H	-4.1033359	0.0560666	-3.3892031
C	1.5863163	7.2696195	-4.0006802
H	1.8316765	7.2978697	-2.9272075
H	1.3514779	8.2973317	-4.3060942
C	0.4120775	6.4006156	-4.2803750
N	-0.8324514	6.9342530	-4.5453866
H	-1.0661678	7.9206041	-4.5631574
C	-1.6828509	5.9174372	-4.8159979
H	-2.7264058	6.0662444	-5.0745085
N	-1.0573283	4.7592825	-4.7409572
C	0.2433038	5.0405357	-4.4013993
H	0.9895033	4.2551163	-4.2910634
C	2.1007659	3.8873457	-10.0902459
H	2.0725148	4.9771501	-9.9495931
H	1.6018049	3.6796988	-11.0550482
C	1.3001876	3.2377606	-9.0078823
N	0.9374983	1.9039068	-9.0321859
H	1.2416305	1.2163054	-9.7162461
C	0.0601208	1.6785307	-8.0309279
H	-0.3910897	0.7154954	-7.8371267
N	-0.1664344	2.7879784	-7.3467155
C	0.6073528	3.7670169	-7.9420006
H	0.5691797	4.8037866	-7.6289900
C	0.1590003	-1.0464248	-2.1238903
H	0.2124881	-1.9954899	-2.6736244
H	-0.4777888	-1.2090531	-1.2397558
C	-0.4525696	0.0508590	-2.9424591
N	-1.1011483	1.1046170	-2.3153445
H	-1.2438382	1.1993992	-1.3157249
C	-1.4798428	1.9981790	-3.2567276
H	-2.0265808	2.9117074	-3.0458913
N	-1.1089249	1.5910877	-4.4552608
C	-0.4691184	0.3799631	-4.2795065
H	-0.0754246	-0.2006829	-5.1102555
Cu	-4.9159645	1.7950568	-6.2074306
Cu	-1.6728217	3.0117471	-5.9587777
O	-3.5785367	2.9051727	-5.4030449
O	-4.6522969	2.8444322	-8.0973831
C	-3.7359076	3.4041829	-8.8817053
C	-2.8505427	4.4087690	-8.3488280
C	-1.9890384	5.1491771	-9.2245548
C	-1.8992527	4.8301257	-10.5654256
C	-2.7170134	3.8032567	-11.0655091
C	-3.6325533	3.1159413	-10.2631589
O	-1.2538744	6.1313399	-8.6580376
H	-1.5221211	6.1162784	-7.7184439
H	-1.2047474	5.3605416	-11.2158805
H	-2.6352453	3.5685314	-12.1229950
H	-4.3234399	2.4001271	-10.7154901
H	-5.7693478	3.7760937	-7.9217674
O	-2.7550039	4.6690210	-7.0763370
H	-3.7155862	3.7259046	-5.9188602
H	-9.7394230	-1.9663156	-7.7021399
H	-8.0042117	7.7762617	-5.2146917
H	-5.0896935	0.3633407	-0.0400582
H	2.4913342	6.9770239	-4.5330305
H	3.1424664	3.5756429	-10.1661911
H	1.1576786	-0.7565861	-1.797238

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C	-8.6615274	-2.1758816	-7.7736663
H	-8.4546801	-2.8442237	-6.9244715
H	-8.4722093	-2.7652224	-8.6877856
C	-7.7174894	-1.0102219	-7.6947054
N	-7.3740187	-0.2197292	-8.7732583
H	-7.6742772	-0.3248726	-9.7488962
C	-6.4445014	0.6745755	-8.3923355
H	-5.9837523	1.4160100	-9.0469322
N	-6.1625013	0.5176418	-7.1010112
C	-6.9467869	-0.5298078	-6.6585481
H	-6.9055065	-0.8886574	-5.6378068
C	-7.8700783	7.7762177	-6.3306306
H	-8.7600900	8.1735975	-6.8377523
H	-7.0461923	8.4713506	-6.5582656
C	-7.5207135	6.4425732	-6.9011712
N	-8.4448482	5.5820722	-7.4723416
H	-9.4598606	5.7256815	-7.5002681
C	-7.8043756	4.5371153	-8.0236910
H	-8.2666405	3.7275670	-8.5867088
N	-6.5056361	4.6887553	-7.8099741

C	-6.2988976	5.8616916	-7.1245994
H	-5.2924857	6.1963347	-6.8953018
C	-4.3857287	1.1271025	-0.4510936
H	-4.2657943	1.9884054	0.2250262
H	-3.3956002	0.6626018	-0.5804386
C	-4.8782955	1.5269707	-1.8128702
N	-5.7755330	2.5451057	-2.0520729
H	-6.1398114	3.1657695	-1.3241939
C	-6.0271419	2.5941866	-3.3822454
H	-6.7041663	3.3177227	-3.8323525
N	-5.3397261	1.6608363	-4.0205981
C	-4.6219512	0.9898283	-3.0566140
H	-3.9603707	0.1598535	-3.2934627
C	1.3939330	7.1024881	-4.0979201
H	1.5858451	7.1012576	-3.0137566
H	1.1316609	8.1337812	-4.3719483
C	0.2820969	6.1805355	-4.4856507
N	-0.9892321	6.6321478	-4.7807981
H	-1.3145633	7.5901934	-4.7101708
C	-1.7322425	5.5851042	-5.2086898
H	-2.7641789	5.6654925	-5.5323667
N	-1.0062415	4.4823129	-5.2147914
C	0.2392072	4.8301903	-4.7501404
H	1.0355069	4.0971194	-4.6418887
C	2.2160542	3.7478898	-10.2048838
H	2.1246372	4.8317763	-10.0456117
H	1.7118009	3.5209701	-11.1635006
C	1.4901490	3.0297793	-9.1156185
N	1.4260620	1.6524104	-9.0079368
H	1.9457422	0.9865705	-9.5756862
C	0.5485446	1.3374497	-8.0323622
H	0.3445136	0.3189608	-7.7219045
N	0.0321697	2.4349668	-7.4970930
C	0.6169117	3.4979624	-8.1617789
H	0.3559028	4.5317783	-7.9515026
C	0.1865139	-1.1269296	-2.0112060
H	0.2415552	-2.1029653	-2.5120420
H	-0.4416047	-1.2390373	-1.1133296
C	-0.4279123	-0.0816126	-2.8872484
N	-1.0539039	1.0268037	-2.3362253
H	-1.1925139	1.1973570	-1.3461435
C	-1.4353098	1.8462077	-3.3440245
H	-1.9713070	2.7802534	-3.1989712
N	-1.0880637	1.3360715	-4.5089389
C	-0.4591619	0.1380245	-4.2441204
H	-0.0884369	-0.5158608	-5.0296031
Cu	-4.8868821	1.6796181	-6.1243318
Cu	-1.4983771	2.6446000	-6.1629666
O	-3.4001684	2.8748083	-5.9199747
O	-4.7436430	3.1254273	-8.7875018
C	-3.7668716	3.6856693	-9.4035120
C	-3.0494437	4.7901045	-8.7453948
C	-1.9148949	5.3942933	-9.4170149
C	-1.5062682	4.9576118	-10.6556996
C	-2.2380539	3.9223221	-11.2956882
C	-3.3317291	3.3062195	-10.7015839
O	-1.2705375	6.3618818	-8.7272964
H	-1.8152726	6.4880946	-7.9258358
H	-0.6324412	5.3988801	-11.1351667
H	-1.9312357	3.6159011	-12.2974966
H	-3.9233227	2.5634210	-11.2393020
H	-5.7114555	4.0213058	-8.1951019
O	-3.3699503	5.2093254	-7.5841427
H	-3.5978878	3.6432379	-6.4975404
H	-9.7281140	-1.9534232	-7.7424929
H	-8.0748024	7.8248809	-5.2611511
H	-5.0374033	0.3968997	0.0286883
H	2.3300448	6.8614296	-4.6015588
H	3.2726582	3.4992522	-10.3040499
H	1.1875543	-0.8174721	-1.7108386

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C	-8.6764513	-2.1827090	-7.7733343
H	-8.4634517	-2.8488941	-6.9240681
H	-8.4872581	-2.7717260	-8.6876680
C	-7.7376402	-1.0126623	-7.6995527
N	-7.4142317	-0.2125014	-8.7768927
H	-7.7208461	-0.3132503	-9.7510241
C	-6.4886840	0.6873033	-8.4009744
H	-6.0491674	1.4354040	-9.0603512
N	-6.1885320	0.5252554	-7.1147277
C	-6.9583822	-0.5319301	-6.6697837
H	-6.9005390	-0.8964905	-5.6518852
C	-7.9121246	7.7044333	-6.2943036
H	-8.8108890	8.0828352	-6.8006482
H	-7.1008141	8.4097464	-6.5361286

C	-7.5454820	6.3693467	-6.8496544
N	-8.4504581	5.5019236	-7.4347276
H	-9.4642392	5.6404665	-7.4837194
C	-7.7778509	4.4668211	-7.9783141
H	-8.2354289	3.6587493	-8.5485385
N	-6.4825866	4.6217674	-7.7512381
C	-6.3158752	5.7971532	-7.0582786
H	-5.3266309	6.1650677	-6.8070282
C	-4.3938446	1.1343466	-0.4656794
H	-4.2732236	1.9954889	0.2105613
H	-3.4038256	0.6695290	-0.5948730
C	-4.8860145	1.5362965	-1.8275801
N	-5.7682246	2.5673733	-2.0674493
H	-6.1235638	3.1949957	-1.3407385
C	-6.0201445	2.6200544	-3.3969311
H	-6.6876087	3.3528937	-3.8466856
N	-5.3458024	1.6766080	-4.0353058
C	-4.6375863	0.9949780	-3.0713773
H	-3.9895587	0.1542958	-3.3083372
C	1.3889784	7.1051716	-4.0907438
H	1.5752976	7.0888736	-3.0057908
H	1.1395223	8.1425550	-4.3530240
C	0.2671977	6.2016459	-4.4959999
N	-0.9861841	6.6758665	-4.8297598
H	-1.2920052	7.6421151	-4.7826443
C	-1.7403574	5.6390564	-5.2633251
H	-2.7628528	5.7435970	-5.6093288
N	-1.0381643	4.5202849	-5.2389780
C	0.2024299	4.8493021	-4.7467211
H	0.9801746	4.1011383	-4.6095625
C	2.2056517	3.7380887	-10.2156331
H	2.1078831	4.8230513	-10.0675856
H	1.7015132	3.4966586	-11.1707189
C	1.4886145	3.0269216	-9.1160415
N	1.4521526	1.6515308	-8.9779577
H	1.9910029	0.9848572	-9.5266999
C	0.5784455	1.3403391	-7.9974190
H	0.3971573	0.3247469	-7.6627758
N	0.0379428	2.4388196	-7.4882089
C	0.6034483	3.4978089	-8.1747624
H	0.3264187	4.5308356	-7.9831843
C	0.1749996	-1.1111923	-2.0167990
H	0.2260306	-2.0836040	-2.5251728
H	-0.4531132	-1.2286567	-1.1195419
C	-0.4371008	-0.0581525	-2.8860558
N	-1.0606048	1.0495073	-2.3306202
H	-1.1982872	1.2171832	-1.3398054
C	-1.4441173	1.8721762	-3.3352313
H	-1.9779193	2.8068904	-3.1850203
N	-1.0998618	1.3652034	-4.5027011
C	-0.4718211	0.1652860	-4.2422475
H	-0.1052437	-0.4882465	-5.0301492
Cu	-4.9176044	1.6913721	-6.1361924
Cu	-1.5056874	2.6565866	-6.1683089
O	-3.4141474	2.8752542	-5.9577185
O	-4.7838643	3.1884988	-8.8160376
C	-3.7899959	3.7355368	-9.4478065
C	-3.0607165	4.8397679	-8.8110458
C	-1.9182965	5.4170880	-9.5051557
C	-1.5151619	4.9394329	-10.7312233
C	-2.2557291	3.8945858	-11.3345559
C	-3.3616822	3.3068187	-10.7203509
O	-1.2632316	6.3927298	-8.8465086
H	-1.7959173	6.5506251	-8.0424331
H	-0.6380306	5.3549425	-11.2270395
H	-1.9493449	3.5516501	-12.3241919
H	-3.9591265	2.5522811	-11.2351591
H	-5.5608140	3.9140607	-8.2532342
O	-3.3632752	5.2812265	-7.6609364
H	-3.6143855	3.6577662	-6.5090573
H	-9.7435884	-1.9634600	-7.7384821
H	-8.1125785	7.7654209	-5.2246470
H	-5.0447061	0.4042738	0.0154021
H	2.3259848	6.8595310	-4.5904899
H	3.2634307	3.4942524	-10.3141927
H	1.1775612	-0.8085711	-1.7145458

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C	-8.6595113	-2.2156589	-7.7308538
H	-8.4355500	-2.8707250	-6.8760423
H	-8.4592871	-2.8071510	-8.6405002
C	-7.7573039	-1.0149261	-7.6683772
N	-7.3824531	-0.2775836	-8.7736866
H	-7.6275266	-0.4284998	-9.7586050
C	-6.5404921	0.6982749	-8.3890462
H	-6.0990630	1.4179336	-9.0766040

N	-6.3409156	0.6445354	-7.0754898
C	-7.0922357	-0.4187424	-6.6179577
H	-7.1182479	-0.6899598	-5.5705013
C	-7.5781436	7.2683321	-5.9088828
H	-8.3324203	7.6367963	-6.6161625
H	-6.6663348	7.8660874	-6.0715493
C	-7.2972227	5.8356513	-6.2282678
N	-8.1406482	5.0807202	-7.0215163
H	-9.0625112	5.3786886	-7.3567535
C	-7.5827039	3.8677368	-7.2172464
H	-8.0374079	3.0885780	-7.8275558
N	-6.4150467	3.7933087	-6.5864204
C	-6.2288972	5.0129987	-5.9669846
H	-5.3399540	5.2221238	-5.3790423
C	-4.3814316	1.1175976	-0.4487215
H	-4.2390182	1.9705168	0.2343547
H	-3.3986686	0.6502763	-0.6147636
C	-4.9178017	1.5363073	-1.7880432
N	-5.8935613	2.4939353	-1.9664258
H	-6.2742464	3.0741673	-1.2144005
C	-6.1827800	2.5718497	-3.2845004
H	-6.9225733	3.2553286	-3.6926467
N	-5.4421586	1.7213854	-3.9778531
C	-4.6525359	1.0679938	-3.0584463
H	-3.9376991	0.3010135	-3.3463671
C	1.3461683	7.1481843	-4.0876348
H	1.5306177	7.1210743	-3.0030672
H	1.1194410	8.1907368	-4.3455259
C	0.2045191	6.2725074	-4.4955723
N	-1.0037489	6.7817491	-4.9274806
H	-1.2630891	7.7623481	-4.9538497
C	-1.7839742	5.7514092	-5.3365284
H	-2.7779154	5.8826213	-5.7547603
N	-1.1411341	4.6063541	-5.2011399
C	0.0875483	4.9108376	-4.6669355
H	0.8239016	4.1386440	-4.4511983
C	2.1425695	3.7810125	-10.2021811
H	2.0589923	4.8677489	-10.0580366
H	1.6448186	3.5454794	-11.1621684
C	1.4018012	3.0820680	-9.1076210
N	1.3569332	1.7084385	-8.9609104
H	1.9042545	1.0355509	-9.4927162
C	0.4643092	1.4100667	-7.9899676
H	0.2771620	0.3982590	-7.6483045
N	-0.0832789	2.5104028	-7.4975381
C	0.5002891	3.5603124	-8.1824921
H	0.2360627	4.5968230	-7.9914035
C	0.1458144	-1.0776335	-2.0042184
H	0.1879337	-2.0370703	-2.5372376
H	-0.4733872	-1.2161425	-1.1036033
C	-0.4719650	-0.0015229	-2.8411160
N	-1.0488314	1.1154302	-2.2542491
H	-1.1456942	1.2778449	-1.2577022
C	-1.4449233	1.9575797	-3.2392513
H	-1.9484035	2.9043219	-3.0603889
N	-1.1568779	1.4531185	-4.4223508
C	-0.5491648	0.2363525	-4.1932095
H	-0.2229071	-0.4162404	-4.9996683
Cu	-5.2501556	2.0620918	-6.0977290
Cu	-1.6044630	2.7059644	-6.0922355
O	-3.5570924	3.0128440	-5.9980551
O	-4.7852886	3.3155554	-9.0628022
C	-3.7449568	3.8980611	-9.6512544
C	-3.0955713	5.0047331	-8.9681603
C	-1.9371615	5.6140507	-9.6086336
C	-1.4690947	5.1480319	-10.8230898
C	-2.1455528	4.0852759	-11.4514395
C	-3.2706587	3.4642873	-10.8788512
O	-1.3402584	6.6043983	-8.9308832
H	-1.8963167	6.7590979	-8.1429832
H	-0.5867199	5.5944887	-11.2802817
H	-1.7905150	3.7360461	-12.4229028
H	-3.8218707	2.6849920	-11.4040132
H	-5.0603084	3.8185029	-8.2711959
O	-3.4936632	5.4149880	-7.8406790
H	-3.6602276	3.8113823	-6.5427195
H	-9.7299907	-2.0131257	-7.6973783
H	-7.9508933	7.4804919	-4.9068287
H	-5.0231767	0.3858512	0.0419688
H	2.2787872	6.8884616	-4.5884668
H	3.1979567	3.5252580	-10.2960640
H	1.1525746	-0.7850089	-1.7061057

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C	-8.6668184	-2.2223384	-7.7453689
H	-8.4348756	-2.8717558	-6.8884833

H	-8.4756247	-2.8187494	-8.6536737
C	-7.7656981	-1.0198342	-7.7020624
N	-7.4133202	-0.2909553	-8.8192483
H	-7.6767073	-0.4691463	-9.7952394
C	-6.5760313	0.6975367	-8.4579212
H	-6.1535253	1.4113140	-9.1655548
N	-6.3563186	0.6578776	-7.1467989
C	-7.0909543	-0.4073156	-6.6677393
H	-7.0994531	-0.6678391	-5.6173044
C	-7.6109808	7.2882038	-5.9478126
H	-8.3810292	7.6483988	-6.6413865
H	-6.7085858	7.8964302	-6.1255309
C	-7.3259192	5.8559046	-6.2644799
N	-8.1516700	5.1012644	-7.0741988
H	-9.0647698	5.3996794	-7.4306221
C	-7.6039562	3.8763105	-7.2303800
H	-8.0508153	3.0926795	-7.8400595
N	-6.4660140	3.7971555	-6.5547805
C	-6.2773464	5.0236710	-5.9569525
H	-5.4050719	5.2423685	-5.3468134
C	-4.3513618	1.1564315	-0.4995214
H	-4.2134838	2.0046456	0.1907473
H	-3.3672480	0.6877547	-0.6544073
C	-4.8570878	1.5964927	-1.8461767
N	-5.8413548	2.5439481	-2.0320970
H	-6.2548704	3.0999918	-1.2788214
C	-6.0714206	2.6729191	-3.3575038
H	-6.8117802	3.3546131	-3.7679694
N	-5.2816991	1.8678689	-4.0545176
C	-4.5245431	1.1881496	-3.1227786
H	-3.7796312	0.4491993	-3.4072826
C	1.2888166	7.1881618	-4.1498694
H	1.4336401	7.1237274	-3.0615643
H	1.1112687	8.2442094	-4.3865911
C	0.1248858	6.3673406	-4.6072034
N	-0.9310686	6.9003722	-5.3197786
H	-1.0532689	7.8782180	-5.5658577
C	-1.7556939	5.8894486	-5.6881290
H	-2.6449315	6.0318349	-6.3020498
N	-1.2901043	4.7314229	-5.2504666
C	-0.1243285	5.0141194	-4.5764880
H	0.4900391	4.2300434	-4.1385127
C	2.0788596	3.8677344	-10.2156005
H	2.0274614	4.9526733	-10.0473309
H	1.6056092	3.6757457	-11.1969255
C	1.2768777	3.1637900	-9.1665804
N	1.1025631	1.7930635	-9.1397233
H	1.5690687	1.1228299	-9.7463854
C	0.2066628	1.4932011	-8.1714169
H	-0.0891039	0.4797072	-7.9316530
N	-0.2172983	2.5876679	-7.5644650
C	0.4438832	3.6371405	-8.1749900
H	0.2774892	4.6714530	-7.8857166
C	0.1318023	-1.0077390	-2.0837454
H	0.1619929	-1.9477354	-2.6505135
H	-0.4971168	-1.1711241	-1.1937003
C	-0.4634038	0.1081309	-2.8878337
N	-0.9689340	1.2393207	-2.2628105
H	-1.0262107	1.3860433	-1.2604216
C	-1.3550394	2.1198292	-3.2144867
H	-1.8029637	3.0865805	-2.9972275
N	-1.1299041	1.6255353	-4.4184589
C	-0.5743998	0.3741192	-4.2329771
H	-0.3034464	-0.2744035	-5.0627235
Cu	-5.2687621	2.1369853	-6.2372195
Cu	-1.6854685	2.7515091	-6.0709439
O	-3.5577643	2.9914190	-6.7116684
O	-2.9519831	3.0233796	-9.2755135
C	-2.9000546	4.2080065	-9.8797762
C	-3.4091086	5.4000617	-9.2156662
C	-3.4060813	6.6557202	-9.9666064
C	-2.8701013	6.7303073	-11.2391180
C	-2.3385510	5.5564354	-11.8104731
C	-2.3511422	4.3201952	-11.1505741
O	-3.9388807	7.7035173	-9.3299079
H	-4.2501896	7.3458157	-8.4734941
H	-2.8794160	7.6738790	-11.7867137
H	-1.9346239	5.5947934	-12.8230430
H	-1.9699240	3.4309767	-11.6503149
H	-3.2641710	3.0248141	-8.3202228
O	-3.8417212	5.4226816	-8.0219480
H	-3.7519165	3.9336184	-6.8975766
H	-9.7371625	-2.0205041	-7.7042259
H	-7.9682739	7.4975387	-4.9395533
H	-4.9971179	0.4247164	-0.0140746
H	2.2298912	6.9056101	-4.6216845
H	3.1274084	3.5766143	-10.2777379
H	1.1401971	-0.7394502	-1.7687413

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C	-8.6443363	-2.1852748	-7.6849861
H	-8.4232573	-2.8362053	-6.8265538
H	-8.4305047	-2.7779748	-8.5906578
C	-7.7505062	-0.9764661	-7.6219333
N	-7.3566497	-0.2598171	-8.7356614
H	-7.5935644	-0.4220434	-9.7217052
C	-6.5251692	0.7250604	-8.3622554
H	-6.0736016	1.4378070	-9.0519142
N	-6.3470211	0.6980138	-7.0410568
C	-7.1061363	-0.3575898	-6.5717651
H	-7.1529705	-0.6044298	-5.5197609
C	-7.6095081	7.2479340	-5.9070000
H	-8.3720974	7.6098659	-6.6084445
H	-6.6989903	7.8428128	-6.0860963
C	-7.3354217	5.8113744	-6.2105815
N	-8.1864999	5.0464455	-6.9849607
H	-9.1035272	5.3478456	-7.3300489
C	-7.6425489	3.8235475	-7.1509004
H	-8.1048461	3.0351031	-7.7424149
N	-6.4763818	3.7548304	-6.5160793
C	-6.2734342	4.9878898	-5.9319498
H	-5.3745405	5.2085001	-5.3654745
C	-4.3789032	1.1174314	-0.4874989
H	-4.2414590	1.9777706	0.1873066
H	-3.3938766	0.6505209	-0.6414366
C	-4.8999808	1.5295931	-1.8361387
N	-5.8773343	2.4831556	-2.0302629
H	-6.2767407	3.0588607	-1.2833244
C	-6.1319889	2.5793262	-3.3524515
H	-6.8651157	3.2637563	-3.7714678
N	-5.3633671	1.7428683	-4.0381122
C	-4.5951915	1.0793073	-3.1044218
H	-3.8685884	0.3199484	-3.3821831
C	1.3482366	7.1519220	-4.0945738
H	1.5265789	7.1302923	-3.0088500
H	1.1248109	8.1940255	-4.3573776
C	0.2028295	6.2813974	-4.5018480
N	-1.0078405	6.8011755	-4.9134910
H	-1.2548738	7.7850424	-4.9450157
C	-1.8013670	5.7829904	-5.3192160
H	-2.7974925	5.9177950	-5.7332714
N	-1.1671508	4.6304007	-5.1958934
C	0.0729268	4.9215701	-4.6773549
H	0.8068382	4.1433439	-4.4757918
C	2.1483612	3.7773237	-10.0683841
H	2.0776240	4.8649803	-9.9255111
H	1.6356280	3.5482490	-11.0216552
C	1.4025938	3.0915850	-8.9675996
N	1.3219944	1.7174610	-8.8308889
H	1.8461971	1.0351535	-9.3736785
C	0.4198737	1.4298877	-7.8704996
H	0.2024044	0.4208381	-7.5407678
N	-0.0992937	2.5435109	-7.3702818
C	0.5117837	3.5880944	-8.0427276
H	0.2504258	4.6276487	-7.8636621
C	0.1130347	-1.0197284	-2.0788061
H	0.1521802	-1.9720614	-2.6240004
H	-0.5154974	-1.1696957	-1.1861036
C	-0.4971266	0.0695257	-2.9075482
N	-1.0350436	1.2017693	-2.3119795
H	-1.0937877	1.3744245	-1.3137603
C	-1.4551906	2.0419338	-3.2850228
H	-1.9271380	3.0024021	-3.0959785
N	-1.2207318	1.5212182	-4.4750066
C	-0.6209447	0.2955084	-4.2587019
H	-0.3338001	-0.3688484	-5.0699726
Cu	-5.1835895	2.0970783	-6.1445501
Cu	-1.7185423	2.7358534	-6.1355432
O	-3.5699038	3.0604758	-6.1930687
O	-4.9142442	3.1770341	-9.0609146
C	-3.8047285	3.7655870	-9.5689024
C	-3.1501974	4.7388662	-8.7861641
C	-1.9949978	5.3575495	-9.3071795
C	-1.4922049	4.9912701	-10.5571731
C	-2.1559767	4.0174864	-11.3104884
C	-3.3182062	3.4050972	-10.8229015
O	-1.3541417	6.2983465	-8.5543512
H	-1.9490725	6.5016404	-7.8159800
H	-0.5855616	5.4729897	-10.9243687
H	-1.7865299	3.7503283	-12.3020396
H	-3.8965411	2.6982708	-11.4163216
H	-5.2734415	3.7543634	-8.3650838
O	-3.6331042	5.0631282	-7.5702470
H	-3.6485768	4.1500931	-6.9045295
H	-9.7171713	-1.9937459	-7.6647829
H	-7.9706218	7.4646569	-4.9016670

H	-5.0205884	0.3905800	0.0104907
H	2.2835770	6.8901885	-4.5892458
H	3.1999696	3.5102323	-10.1725398
H	1.1187523	-0.7388946	-1.7661864

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C	-8.6443743	-2.1874605	-7.6992256
H	-8.4205160	-2.8400331	-6.8427005
H	-8.4322601	-2.7777056	-8.6069379
C	-7.7513775	-0.9782002	-7.6350245
N	-7.3588012	-0.2579698	-8.7465963
H	-7.5951458	-0.4193798	-9.7329623
C	-6.5268018	0.7258831	-8.3706451
H	-6.0728976	1.4382890	-9.0591942
N	-6.3487799	0.6947525	-7.0498782
C	-7.1068971	-0.3622717	-6.5833422
H	-7.1531430	-0.6124344	-5.5320748
C	-7.5947529	7.2485736	-5.9069514
H	-8.3526517	7.6123510	-6.6126922
H	-6.6826435	7.8429782	-6.0794180
C	-7.3190280	5.8121754	-6.2123042
N	-8.1708885	5.0471258	-6.9853695
H	-9.0889133	5.3476795	-7.3286380
C	-7.6244903	3.8253256	-7.1553366
H	-8.0871532	3.0372369	-7.7472073
N	-6.4558364	3.7566723	-6.5252047
C	-6.2547464	4.9888226	-5.9386362
H	-5.3568470	5.2101285	-5.3701560
C	-4.3785227	1.1260284	-0.4909366
H	-4.2413210	1.9848748	0.1858483
H	-3.3933130	0.6602139	-0.6469532
C	-4.9000804	1.5408644	-1.8387384
N	-5.8851439	2.4870139	-2.0312449
H	-6.2885688	3.0584849	-1.2833604
C	-6.1388627	2.5851688	-3.3537635
H	-6.8769340	3.2646890	-3.7716900
N	-5.3626987	1.7573979	-4.0406855
C	-4.5891711	1.0981734	-3.1082360
H	-3.8553911	0.3465584	-3.3882984
C	1.3478285	7.1485188	-4.0927055
H	1.5243433	7.1204850	-3.0069687
H	1.1268881	8.1923595	-4.3504306
C	0.2002917	6.2834335	-4.5062440
N	-1.0018629	6.8113465	-4.9318563
H	-1.2407506	7.7970605	-4.9700672
C	-1.8000751	5.7983064	-5.3398395
H	-2.7907753	5.9451779	-5.7609055
N	-1.1774924	4.6401728	-5.2057792
C	0.0605807	4.9239076	-4.6766734
H	0.7865000	4.1407448	-4.4658364
C	2.1434792	3.7787571	-10.0811799
H	2.0694504	4.8665938	-9.9415860
H	1.6313198	3.5456572	-11.0336783
C	1.4012616	3.0940986	-8.9774797
N	1.3277943	1.7202984	-8.8340650
H	1.8511700	1.0380459	-9.3777092
C	0.4328447	1.4326281	-7.8673897
H	0.2212923	0.4240358	-7.5322370
N	-0.0875984	2.5463065	-7.3679207
C	0.5135263	3.5907473	-8.0498799
H	0.2474653	4.6301228	-7.8772954
C	0.1156216	-1.0151955	-2.0731569
H	0.1512670	-1.9644231	-2.6239206
H	-0.5135208	-1.1673683	-1.1813027
C	-0.4881364	0.0811345	-2.8971697
N	-1.0170673	1.2154866	-2.2978166
H	-1.0763537	1.3848036	-1.2990033
C	-1.4269927	2.0637560	-3.2683024
H	-1.8909439	3.0273335	-3.0750330
N	-1.1938252	1.5463771	-4.4598761
C	-0.6075549	0.3135629	-4.2476161
H	-0.3248788	-0.3505044	-5.0608163
Cu	-5.1715956	2.0769151	-6.1513936
Cu	-1.7088587	2.7319970	-6.1373341
O	-3.5382485	2.9737079	-6.2471362
O	-4.8835604	3.1840132	-9.0813725
C	-3.7792864	3.7754350	-9.6041734
C	-3.1166542	4.7650695	-8.8631757
C	-1.9695665	5.3720978	-9.3957322
C	-1.4734846	4.9770402	-10.6416746
C	-2.1430397	3.9876964	-11.3661391
C	-3.3012775	3.3890986	-10.8557489
O	-1.3136132	6.3228590	-8.6648566
H	-1.8953086	6.5443845	-7.9219942
H	-0.5677280	5.4470205	-11.0254338
H	-1.7797467	3.6970685	-12.3533417

H	-3.8856269	2.6688579	-11.4265628
H	-5.2681064	3.7727681	-8.4111073
O	-3.5897744	5.1356913	-7.6321264
H	-3.6179607	4.2990534	-7.0348666
H	-9.7170695	-1.9955791	-7.6752890
H	-7.9617489	7.4645711	-4.9035943
H	-5.0190632	0.3974627	0.0060206
H	2.2834656	6.8876550	-4.5872758
H	3.1957849	3.5138020	-10.1837377
H	1.1226321	-0.7396373	-1.7600050