Hybrid Local Molecular Orbital: Molecular Orbital Calculations for Open Shell Systems

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Supporting Information Available

T_1 diagnostic in small benchmark system.

Table S1: T_1 diagnostic for systems in this study calculated with different methods. (a) $[MX_2]^+$ stands for the $[M^{II}(CH_3S)(H_2O)]^+$ complex. (b) $[MX_4]$ stands for the $[M^{II}(CH_3S)(NH_3)(H_2O)(CH_3COO)]$ complex. (c) $[MY_4]^{2+}$ stands for the $[M^{II}(H_2O)_2(H_2S)(NH_3)]^{2+}$ complex. (d) $[MX_6]^+$ stands for the $[M^{II}(H_2O)_2(SH)(CH_3COO)(Im)]\cdot H_2O$ complex.

coord	complex	UCCSD	LUCCSD	LMOMO	LMOMO-calc
LI	$[CuX_2]^{+(a)}$	0.028	0.018	0.015	0.019
	$[Cu(H_2O)_2]^{2+}$	0.018	0.012	0.010	0.012
	$[FeX_2]^+$	0.037	0.021	0.019	0.026
	$[Fe(H_2O)_2]^{2+}$	0.015	0.013	0.009	0.011
	$[MnX_2]^+$	0.025	0.018	0.016	0.021
	$[Mn(H_2O)_2]^{2+}$	0.013	0.012	0.009	0.011
TH	$[CuX_4]^{2+(b)}$	0.031	0.017	0.016	0.021
	$[Cu(H_2O)_4]^{2+}$	0.016	0.011	0.008	0.010
	$[FeX_4]^{2+}$	0.015	0.015	0.010	0.014
	$[Fe(H_2O)_4]^{2+}$	0.013	0.012	0.008	0.011
	$[MnX_4]^{2+}$	0.013	0.017	0.010	0.014
	$[Mn(H_2O)_4]^{2+}$	0.011	0.013	0.009	0.012
SQ	$[CuY_4]^{(c)}$	0.030	0.019	0.014	0.022
	$[Cu(H_2O)_4]^{2+}$	0.017	0.011	0.008	0.011
	$[FeY_4]$	0.042	0.018	0.016	0.026
	$[Fe(H_2O)_4]^{2+}$	0.013	0.012	0.007	0.009
	$[MnY_4]$	0.016	0.017	0.008	0.014
	$[Mn(H_2O)_4]^{2+}$	0.011	0.013	0.007	0.009
SP	$[CuX_6]^{(d)}$	-	0.018	0.012	0.019
	$[Cu(H_2O)_6]^{2+}$	-	0.010	0.007	0.009
	$[FeX_6]$	-	0.017	0.008	0.013
	$[Fe(H_2O)_6]^{2+}$	-	0.011	0.006	0.008
	$[MnX_6]$	-	0.018	0.008	0.014
	$[Mn(H_2O)_6]^{2+}$	-	0.013	0.006	0.009

Free Enthalpies of CuNiR

Table S2: Proton affinities calculated with LUCCSD(T0):LRMP2 in comparison with the LUCCSD(T0) and LRMP2 methods without entropy correction. All values are in kcal/mol.

	LRMP2	LUCCSD(T0):LRMP2			LUCCSD(T0)
		R1	R2	R3	
OS	247.8	246.9	247.8	248.4	249.8
SS	271.1	270.4	270.9	271.4	273.2
OES	278.6	277.8	278.9	279.6	280.2
P1ES	302.9	302.2	302.5	302.6	305.5

Table S3: Electron affinities calculated with LUCCSD(T0):LRMP2 in comparison with LUCCSD(T0) and LRMP2 methods without entropy correction. All values are in kcal/mol.

	LRMP2	LUCCSD(T0):LRMP2			LUCCSD(T0)
		R1	R2	R3	
OS	125.4	102.1	101.3	100.9	100.7
SS	100.6	76.5	75.9	76.0	73.8
P1WS	156.2	133.0	132.4	132.1	131.0
P1S	132.8	108.3	107.5	107.1	106.1

Table S4: pKa values and redox potentials with and without entropy correction calculated using LMOMO scheme with the R3 region selection.

state	OS	SS	OES	P1ES
pKa (without entropy)	–13.97	2.84	8.76	25.52
pKa (with entropy)	–14.88	3.91	8.13	24.43
state	OS	SS	P1WS	P1S
redox potential (without entropy)	0.10	–0.99	1.45	0.36
redox potential (with entropy)	0.10	–0.88	1.47	0.34

Table S5: Separate contributions to the free energy. All values are in a.u.

	cosmo	thermal	ZPE	entropy	enthalpy
NO2	-0.076588223	0.00291967	0.00825659	-0.02648957	0.00094421
H2O	-0.007256414	0.00283530	0.02121492	-0.02106050	0.00094421
OS	-0.055176370	0.03148263	0.54523461	-0.09362712	0.00094421
SS	-0.036469578	0.03273939	0.52884588	-0.09707765	0.00094421
P1WS	-0.147730512	0.03102256	0.55768895	-0.09163064	0.00094421
P1S	-0.053022911	0.03349553	0.54129462	-0.09940606	0.00094421
OES	-0.029251604	0.03166460	0.54156728	-0.09378550	0.00094421
P1ES	-0.073538453	0.03445415	0.52688361	-0.10109358	0.00094421
P1EWS	-0.053152278	0.03117970	0.55525580	-0.09240374	0.00094421
RS	-0.030750959	0.03371162	0.53852978	-0.09871860	0.00094421

T_1 diagnostic in CuNiR.

Table S6: T_1 diagnostic in CuNiR calculated using LUCCSD(T0) method and LMOMO scheme with R3 regions. LMOMO-R3-cor are corrected results for the number of electrons in high level region.

	LUCCSD(T0)	LMOMO-R3	LMOMO-R3-cor
OES	0.014	0.008	0.014
OS	0.014	0.008	0.016
P1ES	0.016	0.011	0.018
P1EWS	0.013	0.008	0.014
P1S	0.015	0.011	0.020
P1WS	0.013	0.008	0.016
RS	0.015	0.011	0.019
SS	0.016	0.012	0.020

Example of the Input File

Here are shown two examples of input files, one with the orbital selection for regions and one with the atom selection for regions.

Orbital selection:

memory,2000,m

set,geomtype=xyz

geometry=oes.xyz

set,charge=0

set,spin=0

basis={default,cc-pVTZ,Cu=aug-cc-pVTZ-PP

set,jkfit

default,cc-pVTZ/JKFIT,Cu=def2-QZVPP/JKFIT

set,mp2fit

default,cc-pVTZ/MP2FIT,Cu=aug-cc-pVTZ-PP/MP2FIT

}

{df-rhf,basis=jkfit}

{df-luccsd(t),basis=mp2fit,loc_method=pipek,rclose=3,rweak=5,npasel=0.03

region,ccsd(t),default=mp2,type=inclusive,orbitals=[54,61,63,64,65,66,67,69,81,89,85,91,

93,60,62,71,57,59,68,48,50,51,88,90,92]}

Atom selection:

memory,2000,m

set,geomtype=xyz

geometry=os.xyz

set,charge=1

set,spin=1

basis={default,cc-pVTZ,Cu=aug-cc-pVTZ-PP

set,jkfit

default,cc-pVTZ/JKFIT,Cu=def2-QZVPP/JKFIT

set,mp2fit

default,cc-pVTZ/MP2FIT,Cu=aug-cc-pVTZ-PP/MP2FIT

}

{df-rhf,basis=jkfit}

{df-luccsd(t),basis=mp2fit,loc_ method=pipek,rclose=3,rweak=5,npasel=0.03

region,ccsd(t),default=mp2,type=inclusive,centers=[1,2,30,33,62,63]}

Cartesian Coordinates of the Small Benchmark Molecules

B3LYP/def2-TZVP structure of $[Cu^{II}(CH_3S)(H_2O)]^+$ in linear coordination geometry

9

C	-1.035070	-0.000903	-2.373454
S	0.547829	0.001098	-1.496665
Cu	0.082948	-0.000295	0.599499
O	-0.337705	-0.001556	2.496245
H	-1.616982	0.873890	-2.078764
H	-0.832776	0.016353	-3.441315
H	-1.594190	-0.899317	-2.105300
H	-1.223999	0.034449	2.878777
H	0.308185	-0.006229	3.215190

B3LYP/def2-TZVP structure of $[Cu^{II}(H_2O)_2]^+$ in linear coordination geometry

7

O	0.000076	0.000002	-1.862541
Cu	0.000017	0.000004	-0.000004
O	-0.000041	0.000006	1.862558
H	-0.000339	-0.796745	-2.439337
H	-0.001206	0.796596	-2.439548
H	-0.000493	-0.796802	2.439261
H	0.000374	0.796539	2.439649

B3LYP/def2-TZVP structure of $[Cu^{II}(H_2O)_2(H_2S)(NH_3)]^{2+}$ in tetrahedral coordination geometry

14

O	-0.879973	-1.688218	-1.071373
Cu	0.036393	-0.000542	-0.295436
N	1.960593	-0.003293	-0.793393

O	-0.873940	1.695392	-1.064654
S	-0.170473	-0.005277	2.087185
H	-0.740878	-2.600298	-0.774069
H	-1.544024	-1.729233	-1.777244
H	-1.618599	1.739011	-1.684730
H	-0.645731	2.612100	-0.847655
H	0.575050	1.050413	2.482966
H	0.727494	-0.923820	2.507828
H	2.538340	0.645673	-0.257416
H	2.045454	0.267605	-1.776276
H	2.386161	-0.927454	-0.704250

B3LYP/def2-TZVP structure of $[Cu^{II}(H_2O)_4]^{2+}$ in tetrahedral coordination geometry

13

O	1.166696	0.082614	-1.665518
Cu	-0.011138	-0.000009	0.000011
O	-1.138282	1.591705	0.079451
O	-1.137952	-1.591956	-0.078253
O	1.168417	-0.082328	1.664265
H	2.087224	-0.212144	-1.757771
H	0.913407	0.483229	-2.512709
H	-1.206015	-2.148017	-0.873625
H	-1.912753	-1.769239	0.481600
H	2.088974	0.212652	1.755582
H	0.916115	-0.482969	2.511741
H	-1.205595	2.147691	0.874925
H	-1.913713	1.768839	-0.479582

B3LYP/def2-TZVP structure of $[Cu^{II}(CH_3S)(NH_3)(H_2O)(CH_3COO)]$ in square planar coordination geometry

20

Cu	0.093677	-0.250413	-0.304871
O	2.114625	-0.110192	-0.808203
O	0.567760	-0.241918	1.601001
N	-1.888340	-0.387934	0.188765
S	-0.461223	-0.260357	-2.535644
H	2.672118	-0.520827	-0.133334
H	2.178594	-0.618953	-1.630933
H	-2.196086	-1.350290	0.282859
H	-2.453601	0.059322	-0.523379
H	-1.941208	0.083845	1.108901
C	-0.056986	0.216671	2.635161
C	0.771585	0.235243	3.908143
O	-1.225467	0.617365	2.652180
H	1.643712	0.876814	3.766951
H	0.178287	0.603084	4.742168
H	1.139246	-0.768958	4.126061
C	0.121149	1.374669	-3.131969
H	1.160747	1.562019	-2.866502
H	0.035194	1.375653	-4.219092
H	-0.496869	2.181152	-2.737915

B3LYP/def2-TZVP structure of $[Cu^{II}(H_2O)_4]$ in square planar coordination geometry

13

O	-0.452310	-0.000041	1.917616
Cu	0.000255	-0.000299	0.000138
O	1.917263	-0.000741	0.452593
O	-1.918446	0.000143	-0.452716
O	0.452807	-0.000558	-1.917279
H	-1.122916	0.559995	2.340729
H	-0.033002	-0.555421	2.594445
H	-2.341815	0.561108	-1.122347
H	-2.594918	-0.555476	-0.033080
H	1.123041	0.559803	-2.340582

H	0.026884	-0.549090	-2.595593
H	2.341552	0.566874	1.116171
H	2.595993	-0.549897	0.028108

B3LYP/def2-TZVP structure of $[Cu^{II}(H_2O)_2(SH)(CH_3COO)(Im)]\cdot H_2O$ in square pyramidal coordination geometry with one water in the second coordination shell

28

Cu	-0.415161	-0.926211	-0.950115
O	1.184673	0.746931	2.627077
O	1.736649	-1.103515	-0.778197
N	-0.090250	0.063550	-2.692746
S	-2.694210	-0.698117	-1.137698
O	-0.593231	-2.264494	0.527761
O	-0.196021	1.199207	0.239653
H	1.327350	-0.204472	2.444472
H	0.931576	0.814447	3.552421
C	-0.774516	0.009593	-3.886078
C	0.831527	0.996412	-2.815703
N	0.773131	1.541540	-4.047989
C	-0.244852	0.924747	-4.745173
H	-1.602862	-0.662793	-4.024227
H	1.520204	1.293227	-2.044438
H	-0.491543	1.186804	-5.758199
H	1.361751	2.283767	-4.386746
H	2.082596	-1.868627	-1.252012
H	1.738477	-1.354288	0.197818
H	-2.983309	-1.632439	-0.217635
C	0.174567	-2.417328	1.521919
C	-0.300317	-3.345859	2.620623
O	1.294722	-1.853398	1.667163
H	-1.157791	-3.932460	2.299299
H	0.516092	-3.996844	2.932154

H	-0.587641	-2.743152	3.485752
H	-1.157522	1.195046	0.343234
H	0.190692	1.163139	1.138560

B3LYP/def2-TZVP structure of $[Cu^{II}(H_2O)_5]\cdot H_2O$ in square pyramidal coordination geometry with one water in the second coordination shell

19

Cu	-0.000697	-0.004239	-0.000003
O	-0.098389	1.536524	3.684800
O	1.967535	0.075195	-0.120530
O	0.108927	-1.541671	-3.685462
O	-1.967572	-0.085101	0.120407
O	-0.043022	-1.569793	-1.162431
O	0.040794	1.561784	1.161564
H	0.660197	1.720808	4.255558
H	-0.892088	1.735997	4.199674
H	-0.646279	-1.735201	-4.257683
H	0.905718	-1.734796	-4.197982
H	2.533575	-0.607499	-0.507726
H	2.505751	0.683147	0.406645
H	-2.505611	-0.692028	-0.408205
H	-2.534538	0.596906	0.507510
H	0.005255	-2.473126	-0.820899
H	0.031781	-1.579441	-2.192024
H	-0.006706	2.465422	0.820836
H	-0.026929	1.571672	2.191921

B3LYP/def2-TZVP structure of $[Fe^{II}(CH_3S)(H_2O)]^+$ in linear coordination geometry

9

C	-1.043140	0.000968	-2.396247
S	0.550752	-0.000485	-1.471692

Fe	0.093705	-0.000088	0.633454
O	-0.338809	0.000287	2.625610
H	-1.621995	0.889257	-2.156029
H	-0.775007	0.015398	-3.450107
H	-1.610106	-0.900443	-2.177227
H	-0.429868	0.782220	3.190537
H	-0.464488	-0.782171	3.183095

B3LYP/def2-TZVP structure of $[Fe^{II}(H_2O)_2]^+$ in linear coordination geometry

7

O	0.000002	-0.000002	-1.937229
Fe	0.000001	-0.000000	-0.000017
O	-0.000000	0.000001	1.937283
H	0.555795	-0.560282	-2.517861
H	-0.555884	0.560371	-2.517675
H	0.557750	0.558400	2.517836
H	-0.557760	-0.558404	2.517821

B3LYP/def2-TZVP structure of $[Fe^{II}(H_2O)_2(H_2S)(NH_3)]^{2+}$ in tetrahedral coordination geometry

14

O	0.079622	-1.926174	-1.041612
Fe	0.007307	0.002117	-0.331740
N	1.669875	1.090697	-1.071998
O	-1.737632	0.900880	-0.960878
S	0.075519	-0.026528	2.154474
H	0.481443	-2.689918	-0.597089
H	-0.223298	-2.234139	-1.911175
H	-2.610202	0.482298	-1.040526
H	-1.847159	1.826307	-1.231718
H	-1.077916	-0.648345	2.480808

H	-0.382500	1.204949	2.465164
H	1.696943	2.054625	-0.733160
H	1.697690	1.160864	-2.091601
H	2.571016	0.687981	-0.805110

B3LYP/def2-TZVP structure of $[Fe^{II}(H_2O)_4]^{2+}$ in tetrahedral coordination geometry

13

O	1.196396	1.177695	-1.162527
Fe	0.000000	-0.000000	-0.000001
O	-1.196006	1.180217	1.160366
O	-1.161657	-1.179860	-1.195127
O	1.161262	-1.178059	1.197300
H	2.056854	1.552221	-0.911692
H	0.975835	1.541175	-2.035885
H	-0.915698	-1.544822	-2.061061
H	-2.028939	-1.554115	-0.968666
H	2.028595	-1.552728	0.971732
H	0.915031	-1.541496	2.063797
H	-0.975491	1.545088	2.033156
H	-2.056143	1.554783	0.908537

B3LYP/def2-TZVP structure of $[Fe^{II}(CH_3S)(NH_3)(H_2O)(CH_3COO)]$ in square planar coordination geometry

20

Fe	-0.015768	0.029037	-0.302147
O	2.184205	0.023516	-1.022560
O	0.588769	0.021993	1.544023
N	-2.138695	0.034365	0.393035
S	-0.734000	0.037406	-2.495525
H	2.819295	0.334932	-0.365687
H	2.323743	0.531228	-1.830171

H	-2.666486	-0.765765	0.061099
H	-2.663029	0.865030	0.140220
H	-2.046458	-0.014352	1.416969
C	0.104242	-0.031300	2.751455
C	1.154878	-0.029368	3.844471
O	-1.091376	-0.079647	3.027040
H	0.688111	-0.084799	4.824993
H	1.829446	-0.876291	3.706130
H	1.756525	0.878982	3.772111
C	0.630356	-0.184022	-3.699987
H	1.215882	0.731907	-3.815075
H	1.285605	-1.008188	-3.420866
H	0.189434	-0.411252	-4.669948

B3LYP/def2-TZVP structure of $[Fe^{II}(H_2O)_4]$ in square planar coordination geometry

13

Fe	-0.000141	-0.006876	0.000121
O	-1.387033	-0.008029	1.541975
O	1.541421	0.011111	1.386758
O	1.386753	-0.005723	-1.541743
O	-1.541653	0.007104	-1.386453
H	-1.255230	-0.344041	2.443311
H	-2.297852	0.326189	1.505922
H	2.446731	-0.314619	1.256639
H	1.502018	0.351876	2.295052
H	1.255732	-0.342039	-2.443078
H	2.296901	0.330311	-1.505602
H	-2.446157	-0.320866	-1.256344
H	-1.503041	0.347792	-2.294810

B3LYP/def2-TZVP structure of $[Fe^{II}(H_2O)_2(SH)(CH_3COO)(Im)]\cdot H_2O$ in square pyramidal coordination geometry with one water in the second coordination shell

28

C	-0.208259	0.817467	-4.761379
C	-0.794017	-0.011469	-3.851402
N	-0.120860	0.078781	-2.653129
C	0.851091	0.949972	-2.824585
N	0.837054	1.420166	-4.091670
Fe	-0.661848	-0.754323	-0.727415
O	-0.220268	1.239454	0.174785
O	1.703218	-0.923274	-0.642623
S	-2.956620	-0.440288	-1.072377
O	-0.525433	-2.210389	0.672313
C	0.273306	-2.488339	1.617982
O	1.386890	-1.930347	1.801023
C	-0.181259	-3.558655	2.585844
O	1.187958	0.741224	2.442464
H	1.361188	-0.216293	2.309062
H	0.835316	0.827198	3.333400
H	-1.660256	-0.642246	-3.951960
H	1.549229	1.248599	-2.062266
H	-0.434714	1.034147	-5.789909
H	1.471134	2.102485	-4.471498
H	2.029385	-1.607075	-1.236883
H	1.788450	-1.292216	0.276501
H	-3.329934	-1.262607	-0.076728
H	-0.567147	-4.416644	2.035266
H	0.629557	-3.858322	3.245799
H	-1.007002	-3.161105	3.181228
H	-1.114292	1.556188	0.359880
H	0.252911	1.172330	1.039230

B3LYP/def2-TZVP structure of $[Fe^{II}(H_2O)_5]\cdot H_2O$ in square pyramidal coordination geometry with one water in the second coordination shell

19

O	-1.696640	1.486803	2.194593
O	0.938122	1.192805	1.676429
Fe	0.903852	0.044728	0.012774
O	0.869763	-1.113603	-1.661402
O	3.012848	0.050844	0.168727
O	-1.113597	-0.057734	-0.068524
O	-1.714027	-1.548765	-2.294085
H	-2.084534	1.078726	2.984124
H	-2.121845	2.354921	2.118740
H	-2.084107	-2.443474	-2.239981
H	-2.121177	-1.143532	-3.075478
H	3.624434	0.626161	-0.316786
H	3.549515	-0.607183	0.637366
H	-1.636171	-0.534680	-0.750102
H	-1.679197	0.387264	0.596194
H	1.608571	-1.487637	-2.160925
H	0.013399	-1.378148	-2.085962
H	1.688032	1.549246	2.171293
H	0.080458	1.467816	2.088978

B3LYP/def2-TZVP structure of $[Mn^{II}(CH_3S)(H_2O)]^+$ in linear coordination geometry

9

C	-1.038355	0.001022	-2.445141
S	0.547922	-0.000509	-1.498515
Mn	0.094728	-0.000101	0.649852
O	-0.337144	0.000287	2.697152
H	-1.621761	0.890164	-2.221389
H	-0.749279	0.014817	-3.493606
H	-1.609770	-0.900618	-2.241203
H	-0.424195	0.780470	3.265529
H	-0.461152	-0.779825	3.258653

B3LYP/def2-TZVP structure of $[Mn^{II}(H_2O)_2]^+$ in linear coordination geometry

7

O	0.000003	-0.000004	-1.994493
Mn	0.000001	-0.000001	0.000010
O	-0.000000	0.000001	1.994469
H	0.558463	-0.550766	-2.578753
H	-0.558583	0.550884	-2.578507
H	0.548288	0.561099	2.578543
H	-0.548301	-0.561104	2.578525

B3LYP/def2-TZVP structure of $[Mn^{II}(H_2O)_2(H_2S)(NH_3)]^{2+}$ in tetrahedral coordination geometry

14

O	-0.173910	-1.985338	-1.066119
Mn	0.008448	0.001702	-0.349579
N	1.847743	0.887239	-1.121036
O	-1.657356	1.146237	-1.004188
S	0.079081	-0.017193	2.237529
H	0.056548	-2.800670	-0.592631
H	-0.480128	-2.257790	-1.946217
H	-2.587908	0.871513	-0.973718
H	-1.647365	2.029546	-1.405765
H	-1.042619	-0.706397	2.537360
H	-0.477699	1.184936	2.497621
H	2.029620	1.842282	-0.806624
H	1.890177	0.926103	-2.141563
H	2.674993	0.354527	-0.843553

B3LYP/def2-TZVP structure of $[Mn^{II}(H_2O)_4]^{2+}$ in tetrahedral coordination geometry

13

O	1.232396	1.214791	-1.201315
Mn	0.000000	-0.000000	-0.000001
O	-1.231632	1.217677	1.199162
O	-1.200633	-1.216945	-1.230943
O	1.199862	-1.215523	1.233101
H	2.093439	1.590841	-0.955706
H	1.014568	1.580220	-2.074321
H	-0.960247	-1.583767	-2.097427
H	-2.067625	-1.592825	-1.006987
H	2.066795	-1.592058	1.010019
H	0.959113	-1.580822	2.100128
H	-1.013696	1.584346	2.071620
H	-2.092260	1.594120	0.952699

B3LYP/def2-TZVP structure of $[Mn^{II}(CH_3S)(NH_3)(H_2O)(CH_3COO)]$ in square planar coordination geometry

20

Mn	-0.003880	0.012019	-0.302934
O	2.186269	-0.017885	-1.028619
O	0.624017	0.034749	1.591152
N	-2.177035	0.041693	0.417119
S	-0.747338	-0.014892	-2.545617
H	2.373996	0.175299	-1.954183
H	2.965481	0.193139	-0.501265
H	-2.725506	-0.750276	0.098210
H	-2.690470	0.879644	0.165628
H	-2.066733	-0.001327	1.441056
C	0.110219	-0.010897	2.782438
C	1.128064	-0.008962	3.908541
O	-1.094361	-0.054784	3.030928
H	1.754893	0.882034	3.837560

H	0.630218	-0.033989	4.874955
H	1.785002	-0.875374	3.809219
C	0.630123	-0.026198	-3.756867
H	1.257702	-0.912814	-3.648766
H	0.205651	-0.042764	-4.760240
H	1.242915	0.876375	-3.681885

B3LYP/def2-TZVP structure of $[Mn^{II}(H_2O)_4]$ in square planar coordination geometry

13

O	0.000163	1.696173	-1.285775
Mn	0.000105	0.000000	0.000038
O	0.000178	1.285736	1.696108
O	0.000033	-1.285789	-1.696103
O	0.000047	-1.696077	1.285779
H	0.502490	1.800642	-2.110117
H	-0.505873	2.516088	-1.165503
H	0.506145	-2.107619	-1.802302
H	-0.508296	-1.167406	-2.514891
H	0.503632	-1.802057	2.109167
H	-0.506283	-2.515725	1.164830
H	0.500890	2.111083	1.800356
H	-0.505203	1.164321	2.516230

B3LYP/def2-TZVP structure of $[Mn^{II}(H_2O)_2(SH)(CH_3COO)(Im)]\cdot H_2O$ in square pyramidal coordination geometry with one water in the second coordination shell

28

N	0.957012	1.149728	-4.413995
C	-0.274901	0.763065	-4.897554
C	-0.881885	0.105997	-3.869788
N	-0.038085	0.084861	-2.778867
C	1.058123	0.724424	-3.136694

Mn	-0.591067	-0.554715	-0.716631
O	-0.441342	-2.254370	0.496356
C	0.291301	-2.467959	1.506621
C	-0.090387	-3.623026	2.409179
O	-0.413387	1.231167	0.567101
O	1.835251	-0.667541	-0.545131
S	-2.981647	-0.181279	-0.963577
O	1.300835	-1.775204	1.814674
O	0.968324	0.741250	2.846190
H	1.169897	-0.198065	2.641240
H	0.666147	0.769683	3.758977
H	-1.864156	-0.331915	-3.817377
H	1.913028	0.897002	-2.504654
H	-0.597591	0.989638	-5.897888
H	1.653731	1.676023	-4.913974
H	2.196228	-1.395704	-1.063750
H	1.801573	-1.018577	0.388324
H	-3.342888	-1.174488	-0.133752
H	-0.657324	-4.373154	1.861472
H	0.795089	-4.061525	2.866015
H	-0.725641	-3.236349	3.210985
H	-1.355144	1.419854	0.695666
H	0.023683	1.175607	1.451787

B3LYP/def2-TZVP structure of $[Mn^{II}(H_2O)_5]\cdot H_2O$ in square pyramidal coordination geometry with one water in the second coordination shell

19

O	-0.084228	1.585499	3.795585
O	-0.018688	1.677674	1.237354
Mn	0.010626	-0.003269	-0.000417
O	-2.126445	-0.057419	0.021493
O	0.037887	-1.685664	-1.236614

O	2.148237	0.050677	-0.023023
O	0.052313	-1.597056	-3.795475
H	0.682649	1.758918	4.358109
H	-0.865596	1.793090	4.325598
H	-0.718960	-1.793376	-4.344250
H	0.830154	-1.773105	-4.341824
H	2.732795	-0.573834	-0.476926
H	2.710210	0.690819	0.437634
H	-2.687341	-0.703878	-0.431546
H	-2.711557	0.572043	0.467733
H	0.053986	-2.607021	-0.942883
H	0.048054	-1.689542	-2.258193
H	-0.008475	2.599583	0.945061
H	-0.047921	1.680421	2.258555

Cartesian Coordinates of the Copper Nitrite Reductase

B3LYP-D3/def2-SVP structure of OS state

65

Cu	4.616966	70.064627	-2.480324
O	4.189094	71.259202	-4.079149
H	5.118252	71.206606	-4.469660
H	4.168856	72.233175	-3.851579
O	4.839547	73.775404	-3.631508
H	4.809769	74.341741	-4.415175
H	5.783275	73.441264	-3.588975
O	7.279275	72.693423	-3.420701
O	6.713917	70.820316	-4.500779
C	7.544884	71.556677	-3.854246
C	8.922394	70.949049	-3.584443
H	8.754057	70.152588	-2.834127
H	9.236108	70.419667	-4.499367

H	9.642344	72.476528	-2.212068
H	10.228374	72.672509	-3.870506
C	9.993606	71.925960	-3.097400
H	10.921864	71.393298	-2.838718
H	6.142066	75.535730	-1.937187
H	4.553611	76.194429	-1.514040
H	6.020658	76.885687	-0.765618
C	5.454865	74.946897	0.047706
H	4.874122	75.378783	0.880975
H	6.460056	74.746519	0.449633
C	5.549315	75.952863	-1.111580
C	4.847611	73.643656	-0.361772
N	3.485003	73.401568	-0.354326
H	2.778913	74.040489	-0.005427
C	3.244779	72.187600	-0.900799
H	2.258649	71.745500	-1.026498
N	4.395029	71.632657	-1.253295
C	5.401874	72.520456	-0.929309
H	6.439534	72.341529	-1.195358
N	2.735197	69.031571	-1.903019
C	1.414749	69.288477	-2.225924
H	1.148320	69.957388	-3.042277
C	0.574389	68.580880	-1.385992
N	1.431120	67.883667	-0.551562
C	2.712576	68.180924	-0.892430
H	3.584027	67.766303	-0.390046
H	1.145047	67.245660	0.183046
C	-0.921733	68.547369	-1.247016
H	-1.349731	68.896412	-2.199394
H	-1.224432	69.299289	-0.495322
C	-1.528702	67.187530	-0.862138
H	-2.625738	67.254067	-0.825185
H	-1.259905	66.407862	-1.592073
H	-1.191441	66.852579	0.133387

H	10.217516	68.461300	0.824660
H	10.252312	69.123939	2.466012
H	9.796575	70.168523	1.089634
C	9.706307	69.155637	1.511591
C	8.234391	68.767888	1.719675
H	7.754160	69.461016	2.426815
H	8.173960	67.767752	2.185588
C	7.434311	68.779377	0.457617
N	7.742940	67.989195	-0.638438
H	8.514085	67.332041	-0.698135
C	6.862242	68.247996	-1.631631
H	6.868752	67.769899	-2.607219
C	6.335615	69.508733	0.063539
H	5.782035	70.254481	0.626040
N	5.994315	69.168349	-1.233382
O	5.323554	68.796494	-3.952589
H	4.671202	68.727676	-4.665761
H	6.041616	69.432154	-4.296627

B3LYP-D3/def2-SVP structure of SS state

65

Cu	-2.012734	70.864692	2.173497
O	-1.879038	69.958552	0.418191
H	-2.752830	69.529700	0.195480
H	-1.713261	70.594577	-0.368340
O	-4.322254	69.355669	-0.382050
H	-4.750692	69.824670	0.347868
H	-4.169305	70.030317	-1.092902
O	-3.533076	71.222758	-2.234690
C	-2.334364	71.550922	-2.436859
O	-1.395084	71.476092	-1.594507
C	-2.003643	72.126503	-3.824145
H	-2.379923	73.166683	-3.827465

H	-2.630411	71.588276	-4.552214
C	-0.528632	72.096419	-4.218038
H	-0.360082	72.615281	-5.176110
H	-0.160322	71.062910	-4.320770
H	0.083334	72.584830	-3.444700
C	-6.139390	73.516871	-1.685681
H	-6.834974	72.774290	-1.262919
H	-6.666161	74.072030	-2.477441
H	-5.306144	72.957144	-2.140024
C	-5.648568	74.476437	-0.595253
H	-6.508175	75.001283	-0.139168
H	-5.027980	75.267327	-1.058162
C	-4.858053	73.802479	0.485720
C	-4.055132	72.681575	0.479020
H	-3.846122	72.020123	-0.360234
N	-4.763972	74.295897	1.778319
H	-5.248244	75.110627	2.136040
C	-3.933479	73.480287	2.488862
H	-3.680240	73.637116	3.536731
N	-3.493532	72.499718	1.726590
N	-1.785195	71.289312	4.188953
C	-2.721137	70.943311	5.142384
H	-3.766631	70.811827	4.877883
C	-2.095646	70.718781	6.347564
N	-0.752069	70.955245	6.092574
C	-0.608548	71.287679	4.785744
H	0.343681	71.497761	4.303638
H	0.000755	70.861683	6.764399
C	-2.602512	70.208055	7.660617
H	-3.657731	70.508129	7.756813
C	-2.480307	68.681496	7.812836
H	-3.041796	68.169226	7.017834
H	-1.431100	68.354863	7.732378
H	-2.872765	68.350811	8.787007

H	-2.068236	70.713236	8.484122
C	1.609469	75.020871	0.776188
H	2.511517	75.095067	1.411725
H	0.926093	75.808156	1.131562
H	2.462922	76.267567	-0.799223
C	2.001089	75.274954	-0.682865
H	1.126134	75.216197	-1.348724
H	2.743113	74.540339	-1.038842
C	0.937285	73.700119	0.990360
C	-0.084808	73.299001	1.821307
H	-0.668939	73.893749	2.519834
N	1.301730	72.551251	0.305439
H	1.964556	72.499223	-0.458680
H	0.530032	70.531934	0.284095
C	0.512100	71.531272	0.710800
N	-0.329484	71.953868	1.636965
O	-3.477874	69.521536	2.675287
N	-2.905215	68.429924	3.174633
O	-1.648124	68.486097	3.239187

B3LYP-D3/def2-SVP structure of P1WS state

66

N	5.901291	69.487922	-1.047097
C	6.488927	68.310090	-1.234488
N	7.362258	68.075499	-0.230388
C	7.338785	69.141733	0.653799
C	6.418003	70.016240	0.123083
C	8.214389	69.217444	1.861247
C	9.706308	69.155637	1.511592
Cu	4.395136	70.232126	-2.222829
O	5.070739	68.921044	-3.664901
O	4.048947	71.474247	-3.899309
N	4.095812	71.808906	-1.039136

C	3.122522	72.048714	-0.172131
N	3.271911	73.296929	0.331203
C	4.387293	73.891504	-0.234525
C	4.893568	72.937358	-1.089080
C	4.859087	75.278607	0.081074
C	5.549314	75.952862	-1.111581
N	2.627343	69.203930	-1.697030
C	1.312645	69.485858	-2.023766
C	0.467684	68.700827	-1.266006
N	1.312801	67.939700	-0.477226
C	2.595816	68.264572	-0.762214
C	-1.024961	68.596424	-1.192258
C	-1.528701	67.187532	-0.862138
O	6.617966	71.032369	-4.330284
C	7.538830	71.653115	-3.788759
C	8.803307	70.993936	-3.314738
C	9.993605	71.925959	-3.097400
O	7.460712	72.943128	-3.545499
O	5.139780	74.162891	-4.130038
H	4.940900	71.463465	-4.322879
H	3.888413	72.422066	-3.747421
H	5.029392	74.531031	-5.022791
H	5.077556	74.927605	-3.533474
H	8.520789	70.486087	-2.371779
H	9.026837	70.185547	-4.027921
H	9.753344	72.717531	-2.374135
H	10.302842	72.408814	-4.036166
H	10.850651	71.355640	-2.711789
H	6.391420	75.350591	-1.488160
H	4.824562	76.131987	-1.925047
H	5.957292	76.930887	-0.819990
H	4.003695	75.887716	0.417026
H	5.555285	75.242845	0.937459
H	2.651142	73.734517	1.007101

H	2.313323	71.369091	0.087358
H	5.781160	72.987436	-1.710506
H	1.053106	70.219739	-2.784017
H	3.458820	67.809530	-0.280909
H	1.011829	67.226080	0.179776
H	-1.434437	68.938879	-2.154864
H	-1.402049	69.309878	-0.437995
H	-2.625833	67.143831	-0.920641
H	-1.128208	66.443389	-1.568312
H	-1.253072	66.877832	0.160191
H	9.980505	68.198571	1.037649
H	10.320227	69.261049	2.417322
H	9.983442	69.964231	0.817429
H	7.980859	70.154499	2.389422
H	7.952796	68.402228	2.558815
H	7.938473	67.243651	-0.135160
H	6.299622	67.634471	-2.065102
H	6.102384	70.977256	0.516369
H	4.414779	68.699586	-4.344937
H	5.795909	69.416932	-4.115067
H	6.611972	73.346221	-3.880196

B3LYP-D3/def2-SVP structure of P1S state

66

C	0.361720	72.069673	2.517527
N	0.792199	73.115333	3.199396
C	1.953292	73.541825	2.581922
C	2.222632	72.748714	1.487394
N	1.196512	71.816162	1.474545
Cu	-0.034301	74.055401	4.940718
N	-0.458645	75.964484	3.909344
C	-0.936815	77.212748	4.275789
C	-1.040716	78.021367	3.159391

N	-0.611621	77.223320	2.114964
C	-0.272518	76.004908	2.601621
C	-1.484940	79.431501	2.907576
C	-2.009233	80.165945	4.137267
C	3.281322	72.852974	0.428767
C	3.897476	71.532339	-0.053581
N	-1.974877	73.407784	4.718981
C	-2.989692	73.878809	3.906566
C	-4.145776	73.164152	4.144088
N	-3.791655	72.250821	5.126110
C	-2.489475	72.430005	5.449997
C	-5.501587	73.213158	3.503678
C	-6.708893	73.225273	4.460003
O	1.773269	74.763978	5.443213
N	2.702193	73.887605	5.763830
O	2.377633	72.731451	5.727471
O	-0.224615	73.386411	6.902006
O	-1.900423	75.084507	7.842139
C	-1.884181	76.260626	8.189279
O	-0.790842	76.965369	8.367288
C	-3.159032	77.017269	8.444909
C	-4.374484	76.109019	8.363150
O	1.338209	75.464440	8.046570
H	0.606298	73.459633	7.396031
H	-0.837791	74.034521	7.356433
H	1.617227	75.477826	7.100629
H	2.132367	75.667473	8.561246
H	-3.208581	77.845590	7.715594
H	-3.064187	77.507811	9.428228
H	-5.292297	76.670311	8.596307
H	-4.288976	75.274797	9.074090
H	-4.477254	75.671546	7.359057
H	-1.226776	80.275269	4.904258
H	-2.360780	81.171017	3.863236

H	-2.854824	79.625337	4.592026
H	-0.641241	79.996200	2.469447
H	-2.268158	79.417632	2.126934
H	-1.166147	77.458348	5.310227
H	-0.546435	77.513927	1.145499
H	0.097813	75.192984	1.982578
H	2.517367	74.387711	2.966513
H	-0.526402	71.482130	2.742081
H	1.098226	71.055184	0.810976
H	4.070239	73.510012	0.826239
H	4.345171	70.966970	0.779138
H	3.152771	70.884144	-0.546535
H	4.686316	71.728979	-0.793948
H	2.856383	73.388271	-0.440869
H	-5.598828	72.352417	2.815675
H	-5.523727	74.108147	2.862308
H	-7.643659	73.274956	3.882420
H	-6.675198	74.090516	5.140801
H	-6.755522	72.312728	5.078097
H	-2.826547	74.699120	3.213343
H	-4.413710	71.576901	5.559354
H	-1.957339	71.877466	6.220795
H	0.032048	76.398857	8.249731

B3LYP-D3/def2-SVP structure of OES state

65

Cu	4.479061	70.000517	-2.328615
O	4.222022	71.028786	-4.133275
H	5.169290	70.997328	-4.453169
H	4.184344	71.974591	-3.853220
O	4.793614	73.635817	-3.478539
H	4.889195	74.032952	-4.354983
H	5.714851	73.263265	-3.303176

O	7.198082	72.623948	-3.093838
O	6.803206	70.939902	-4.524172
C	7.514055	71.560216	-3.678139
C	8.863592	70.924431	-3.314657
H	8.685925	70.367676	-2.377313
H	9.118990	70.177364	-4.081551
H	9.666533	72.703398	-2.390865
H	10.271492	72.431099	-4.037144
C	9.993606	71.925960	-3.097400
H	10.896928	71.437873	-2.694761
H	6.231124	75.404834	-1.778067
H	4.678194	76.245254	-1.718423
H	6.049792	76.866431	-0.751063
C	5.137925	75.061389	0.071392
H	4.451852	75.613661	0.740025
H	6.027171	74.828034	0.678447
C	5.549314	75.952862	-1.111580
C	4.511762	73.766246	-0.336709
N	3.181523	73.645687	-0.694064
H	2.511839	74.404433	-0.727755
C	2.962352	72.366734	-1.105621
H	2.001661	72.002126	-1.465495
N	4.069469	71.655955	-1.014525
C	5.042679	72.512711	-0.544259
H	6.079035	72.200325	-0.444132
N	2.757115	68.783374	-2.061853
C	1.443173	69.114185	-2.320765
H	1.182981	69.787239	-3.136151
C	0.606264	68.477510	-1.424800
N	1.458332	67.739892	-0.618509
C	2.738076	67.956226	-1.037043
H	3.611808	67.506155	-0.569299
H	1.176362	67.146482	0.152101
C	-0.875773	68.533979	-1.203986

H	-1.334562	68.956829	-2.111268
H	-1.099360	69.254608	-0.394667
C	-1.528702	67.187531	-0.862138
H	-2.612139	67.304326	-0.706525
H	-1.371796	66.450526	-1.665845
H	-1.116339	66.759881	0.067763
H	10.322614	68.601346	0.784625
H	10.195030	69.055659	2.493757
H	9.722371	70.215910	1.214983
C	9.706307	69.155637	1.511591
C	8.269659	68.610991	1.559167
H	7.685936	69.169468	2.307106
H	8.288669	67.563099	1.913636
C	7.522018	68.692244	0.264640
N	7.938909	68.088374	-0.913696
H	8.796103	67.565379	-1.045653
C	7.035940	68.370698	-1.895186
H	7.107636	68.060944	-2.944044
C	6.340463	69.315632	-0.068753
H	5.681252	69.905532	0.564777
N	6.055339	69.109777	-1.405543
O	6.385921	68.300227	-4.830415
H	5.464273	68.373019	-4.540571
H	6.673834	69.246748	-4.829103

B3LYP-D3/def2-SVP structure of P1ES state

65

N	4.290564	70.040631	-2.665296
C	4.231372	71.145374	-3.386282
N	5.420049	71.340000	-4.035135
C	6.288410	70.314091	-3.690388
C	5.553229	69.519792	-2.838186
C	7.682760	70.157287	-4.212186

C	8.595798	71.379466	-4.038094
Cu	2.878394	69.462744	-1.260980
N	2.742443	67.392293	-1.300204
C	1.920011	66.768471	-0.386238
C	2.317720	65.459944	-0.220409
N	3.401751	65.301870	-1.073709
C	3.617451	66.496302	-1.702352
C	1.786360	64.346765	0.621079
C	1.312190	63.137983	-0.196157
O	1.058278	70.427347	-1.605043
N	3.672454	70.064290	0.577535
C	2.893089	70.840047	1.317590
N	3.622600	71.691056	2.078793
C	4.957290	71.473081	1.796632
C	4.966195	70.444984	0.873371
C	6.057311	72.327883	2.345799
C	6.039301	72.525432	3.868546
O	2.657168	73.862655	0.003363
C	3.882075	74.164650	0.056343
C	4.762149	73.798117	-1.150299
C	5.285481	75.037307	-1.878920
O	4.461779	74.739649	1.020355
O	2.522574	74.114906	2.736276
O	1.849587	72.916138	-2.534965
N	0.036262	70.273933	-0.854455
H	2.074090	74.017054	1.865889
H	3.334067	74.550076	2.355820
H	5.608516	73.200558	-0.770986
H	4.175838	73.167480	-1.827325
H	5.817839	75.696903	-1.173810
H	4.453727	75.611760	-2.320961
H	5.981264	74.770716	-2.695393
H	5.091591	72.985473	4.191255
H	6.155499	71.571258	4.409344

H	6.851911	73.200976	4.182224
H	7.016620	71.882138	2.030328
H	5.976217	73.319638	1.864966
H	3.220078	72.552100	2.522074
H	1.804991	70.808988	1.301790
H	5.823429	69.978838	0.389157
H	1.112681	67.334027	0.080531
H	4.409324	66.658296	-2.432780
H	3.938204	64.453423	-1.202710
H	0.950871	64.750927	1.213294
H	2.550009	64.020751	1.352986
H	0.883261	62.357780	0.453867
H	0.543384	63.440321	-0.924281
H	2.139209	62.676855	-0.762821
H	8.213603	72.251421	-4.594219
H	9.607182	71.163528	-4.419627
H	8.674632	71.672967	-2.979808
H	8.123853	69.294293	-3.688074
H	7.659842	69.875969	-5.283434
H	5.646156	72.152376	-4.595472
H	3.382428	71.847644	-3.391412
H	5.872353	68.613642	-2.326642
H	1.420677	72.066472	-2.290126
H	2.077833	73.289697	-1.650530
O	0.142366	69.425788	0.034986

B3LYP-D3/def2-SVP structure of P1EWS state

66

C	0.395566	72.241689	2.449632
N	1.106415	73.055353	3.205214
C	2.351119	73.153509	2.622085
C	2.400508	72.379352	1.485149
N	1.140154	71.809935	1.395582

Cu	0.460089	74.116716	4.828620
O	-1.609647	73.946026	4.564674
C	3.475406	72.177149	0.470558
C	3.043329	72.582420	-0.941098
N	1.375390	73.353223	6.500142
C	2.275229	72.388180	6.443596
N	2.890007	72.248500	7.649101
C	2.352512	73.175824	8.525597
C	1.406267	73.849833	7.787870
C	2.765643	73.275767	9.955328
C	2.636049	71.938762	10.684451
N	1.465609	75.968882	4.737565
C	1.192141	77.101854	3.992054
C	2.329450	77.867504	3.867337
N	3.304254	77.163436	4.553932
C	2.747787	76.033379	5.064299
C	2.566472	79.182095	3.193991
C	1.260009	79.874197	2.802382
O	-0.368449	76.474205	6.904809
O	-1.737588	74.892242	2.034406
C	-1.674920	76.068497	1.719743
C	-1.427870	76.543270	0.306980
C	-1.513641	75.445402	-0.747795
O	-1.800652	77.075428	2.580134
O	-2.331909	76.498611	5.152280
H	-2.080097	74.683206	4.996281
H	-1.729586	74.168279	3.613342
H	-1.646455	76.622048	5.866608
H	-3.160810	76.851985	5.506295
H	-0.429710	77.018873	0.310298
H	-2.133520	77.365862	0.107315
H	-1.259352	75.851985	-1.738287
H	-2.524948	75.014483	-0.797737
H	-0.817054	74.625882	-0.514803

H	0.634237	80.072533	3.685699
H	1.465886	80.833118	2.304984
H	0.668834	79.256315	2.109112
H	3.151108	79.834739	3.867417
H	3.196632	79.035319	2.297569
H	0.205448	77.298511	3.586672
H	4.268402	77.456093	4.671987
H	3.285711	75.304927	5.668349
H	0.741647	74.651805	8.101886
H	2.510197	71.786377	5.567338
H	3.602398	71.564251	7.877307
H	2.133847	74.036661	10.437167
H	1.600212	71.566609	10.653977
H	3.280984	71.166820	10.233315
H	2.939715	72.033012	11.738313
H	3.804838	73.646290	10.029799
H	3.809887	71.123872	0.469839
H	4.345833	72.771849	0.787103
H	3.867954	72.447106	-1.657961
H	2.717998	73.634107	-0.975022
H	2.203659	71.964774	-1.300821
H	3.134835	73.778158	3.046667
H	0.821044	71.183907	0.664537
H	-0.637777	71.948945	2.625582
H	-2.001525	76.774296	3.509994
H	0.256104	76.058420	6.267918
H	0.085821	77.276287	7.200078

B3LYP-D3/def2-SVP structure of RS state

66

C	-0.618602	72.092741	1.194558
N	0.163156	73.027554	1.697267
C	1.435367	72.783228	1.217595

C	1.420500	71.677031	0.399375
N	0.100431	71.254318	0.393539
Cu	-0.261869	74.501473	3.036270
N	-0.142184	76.502834	2.592265
C	-0.826475	77.475583	3.289807
C	-0.270421	78.711490	3.040346
N	0.775123	78.454355	2.165703
C	0.818116	77.112746	1.927372
C	-0.600469	80.081665	3.544652
C	-2.009232	80.165945	4.137268
C	2.503110	70.985755	-0.364985
C	3.897477	71.532339	-0.053581
N	-2.084503	74.059697	3.926211
C	-3.261180	73.870448	3.227482
C	-4.168166	73.177855	3.999739
N	-3.505785	72.969156	5.201592
C	-2.256118	73.507833	5.115299
C	-5.526830	72.636131	3.677527
C	-6.708893	73.225273	4.460003
O	1.297519	74.645095	4.553075
N	2.492263	75.031566	4.225223
O	2.773412	74.924509	3.042980
O	0.247612	73.522913	6.981263
O	-1.723568	75.602958	7.552272
C	-2.158516	76.708469	7.281074
O	-1.504997	77.612565	6.574107
C	-3.516857	77.201748	7.743917
C	-4.374483	76.109020	8.363149
O	0.841500	76.753781	6.090992
H	0.779766	73.800862	6.211958
H	-0.166882	74.347192	7.290654
H	0.914605	75.880808	5.614177
H	1.447702	77.317068	5.592050
H	-4.013831	77.685015	6.886161

H	-3.324273	78.017076	8.463673
H	-5.307721	76.522264	8.776207
H	-3.828633	75.598671	9.170422
H	-4.635188	75.343677	7.615009
H	-2.116223	79.465280	4.979779
H	-2.218184	81.178603	4.516409
H	-2.768292	79.912916	3.380780
H	0.137591	80.380720	4.312471
H	-0.484315	80.810260	2.720832
H	-1.651841	77.223762	3.950348
H	1.402452	79.146561	1.774447
H	1.572996	76.626260	1.313690
H	2.263754	73.412087	1.531252
H	-1.681398	71.971612	1.400448
H	-0.260953	70.444865	-0.096430
H	2.304198	71.078564	-1.450488
H	3.971117	72.602030	-0.305268
H	4.136124	71.421135	1.015707
H	4.661812	70.995039	-0.633710
H	2.472299	69.902708	-0.139791
H	-5.516729	71.538049	3.817508
H	-5.689718	72.805753	2.600415
H	-7.652863	72.764604	4.128136
H	-6.781518	74.313483	4.304051
H	-6.614683	73.044466	5.544216
H	-3.384142	74.235488	2.209361
H	-3.876391	72.490466	6.013958
H	-1.496881	73.450846	5.904456
H	-0.567345	77.265805	6.347190

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