

Supporting information (SI)

A QM/MM study of the nitrogenase MoFe protein resting state: broken-symmetry states, protonation states and QM region convergence in the FeMoco active site

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Contents:

1. QM region definitions
2. Unconstrained model data
3. Localized orbital analysis
4. Scripts for QM/MM setup
5. Example QM inputfile
6. Cartesian coordinates of QM regions

1. QM region definitions

Included residues are mostly the sidechains of the residues, e.g. the inclusion of His442A refers to the methyleneimidazole group of His442A, except when mentioned otherwise.

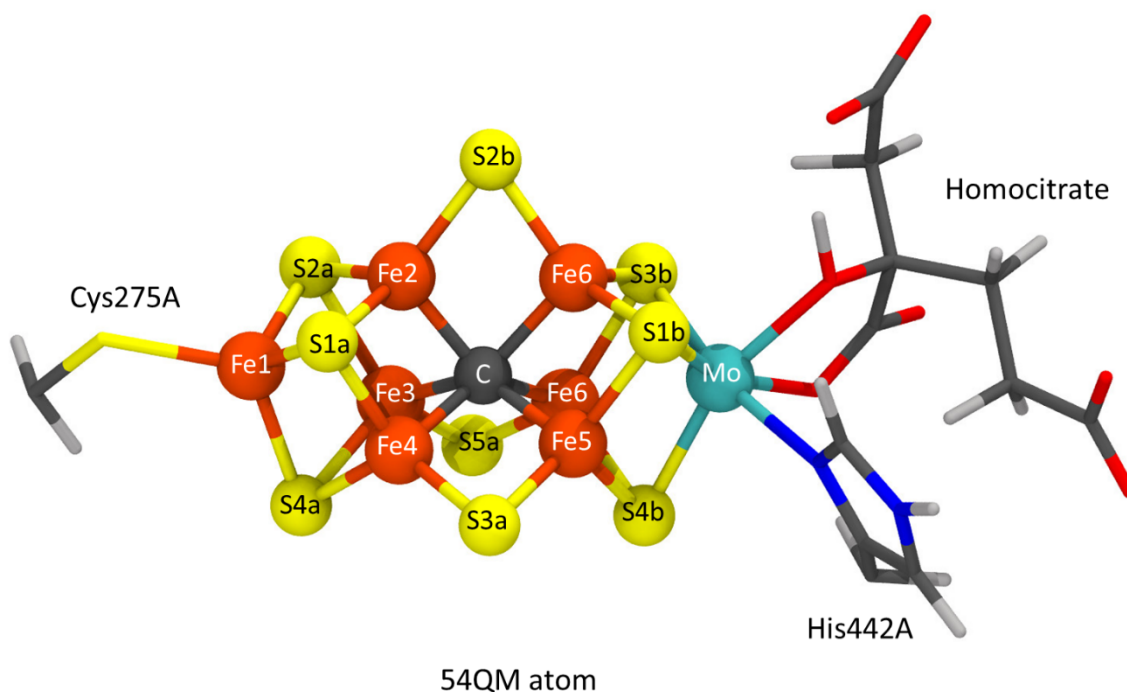


Figure S1: Minimal QM region, 54QM atoms. Contains Cys275A, His442A, homocitrate and FeMoco.

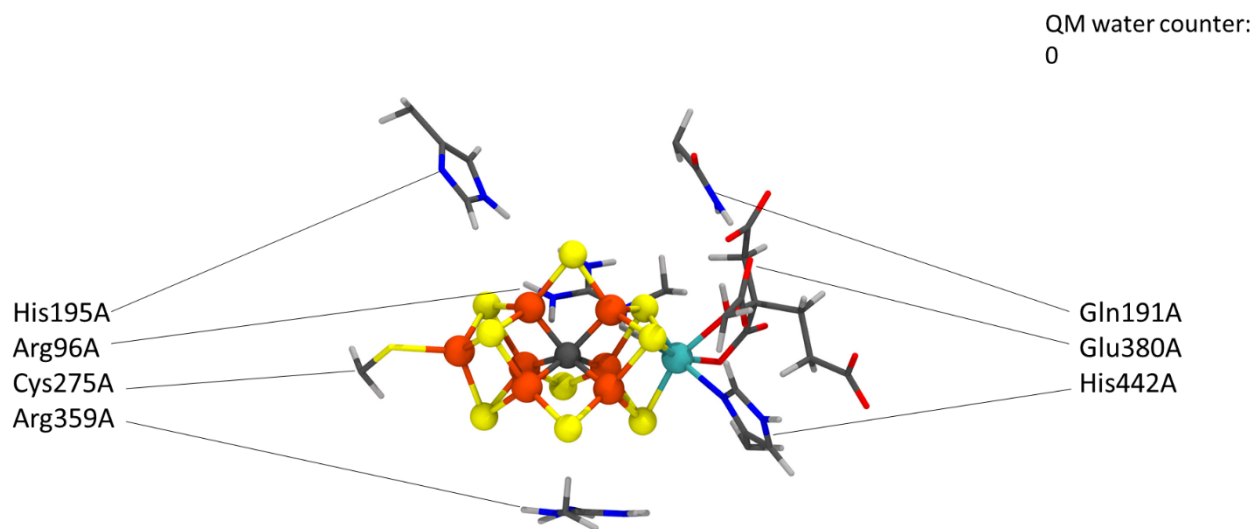


Figure S2: 103 QM atom model. contains FeMoco, Arg96A, Gln191A, His195A, Cys275A, Arg359A, Glu380A and His442A.

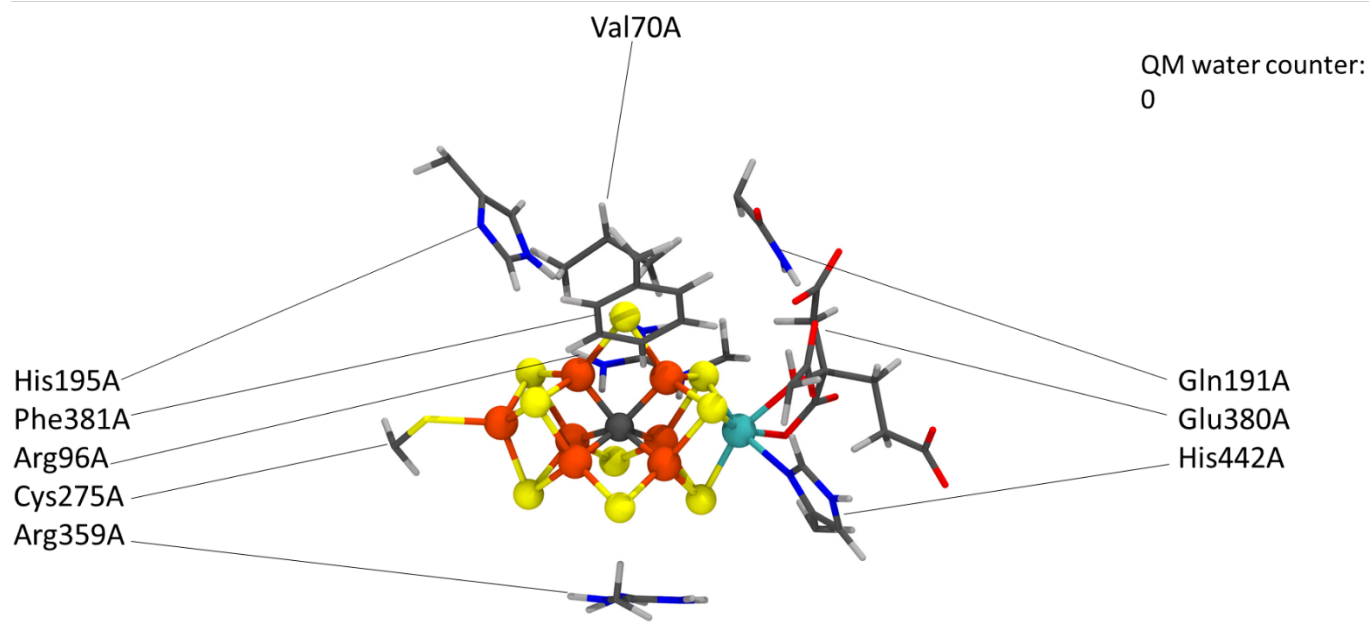


Figure S3: 127QM atom model. contains FeMoco, Val70A, Arg96A, Gln191A, His195A, Cys275A, Arg359A, Glu380A, Phe381A and His442A.

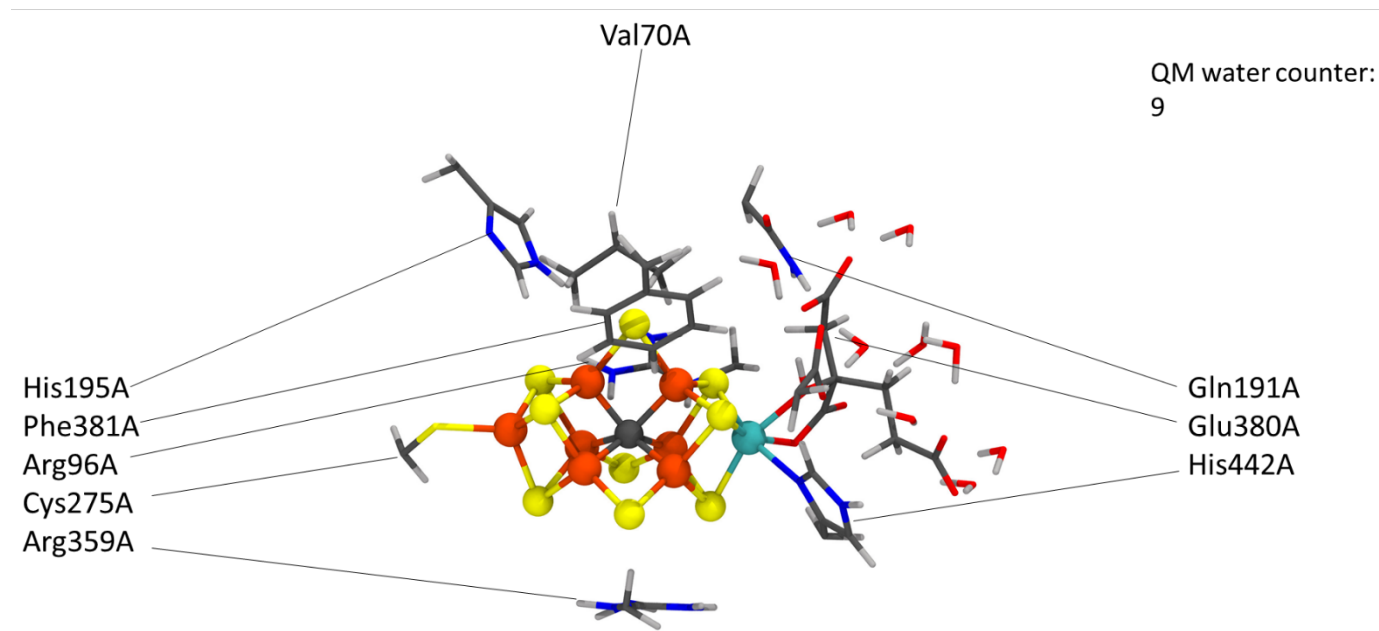


Figure S4: 154QM atom model: contains FeMoco, Val70A, Arg96A, Gln191A, His195A, Cys275A, Arg359A, Glu380A, Phe381A, His442A and 9 water molecules.

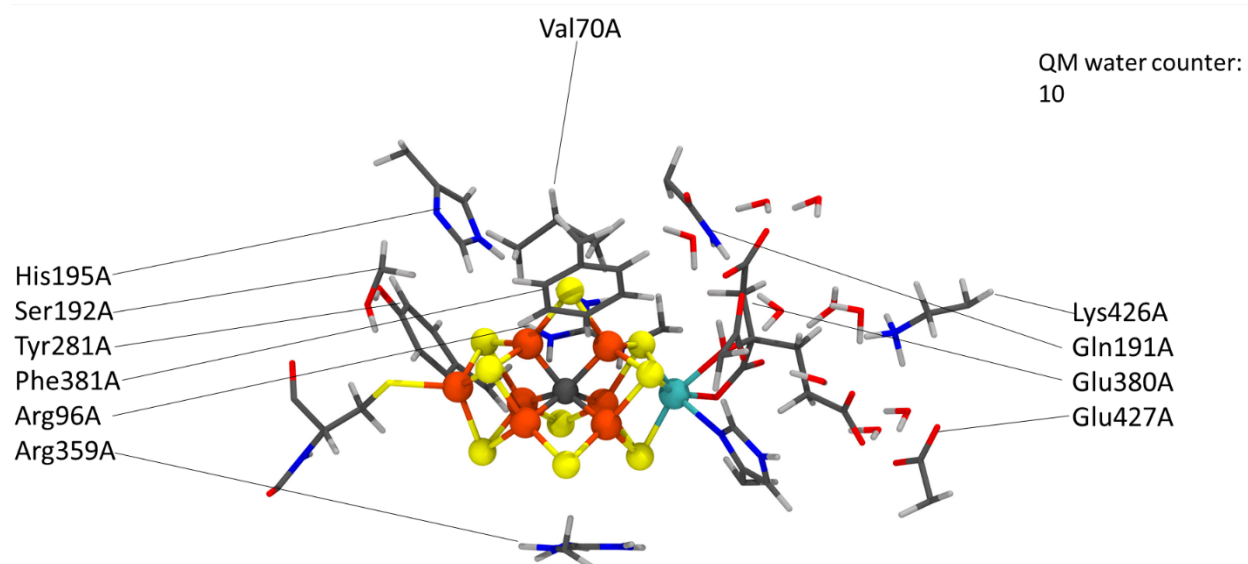


Figure S5: 198QM atom model: contains FeMoco, Val70A, Arg96A, Gln191A, His195A, increased Cys275A, Arg359A, Glu380A, Phe381A, Lys426A, Glu427A, His442A and 10 water molecules.

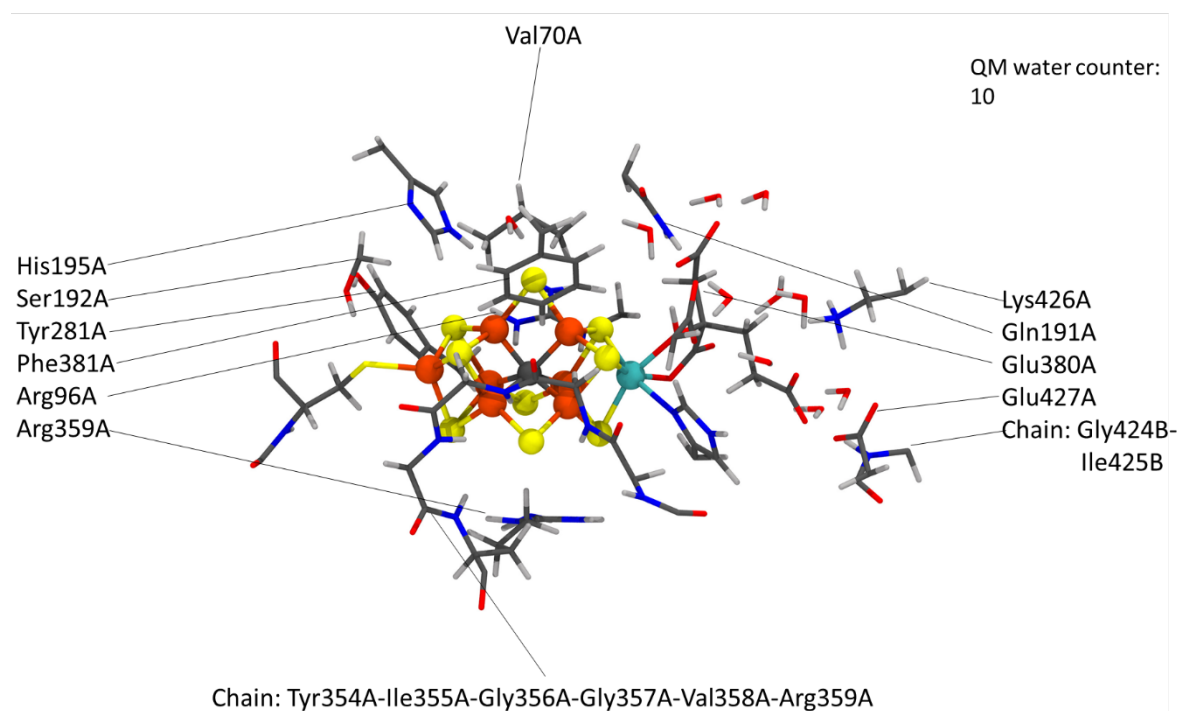


Figure S6: 247QM atom model: contains FeMoco, Val70A, Arg96A, Gln191A, His195A,

increased Cys275A, increased Arg359A, Glu380A, Phe381A, Lys426A, Glu427A, His442A, the chain part of Tyr354A-Ile355A-Gly356A-Gly357A-Val358A-Arg359A, the peptide chain part of Gly424B-425IleB and 10 water molecules.

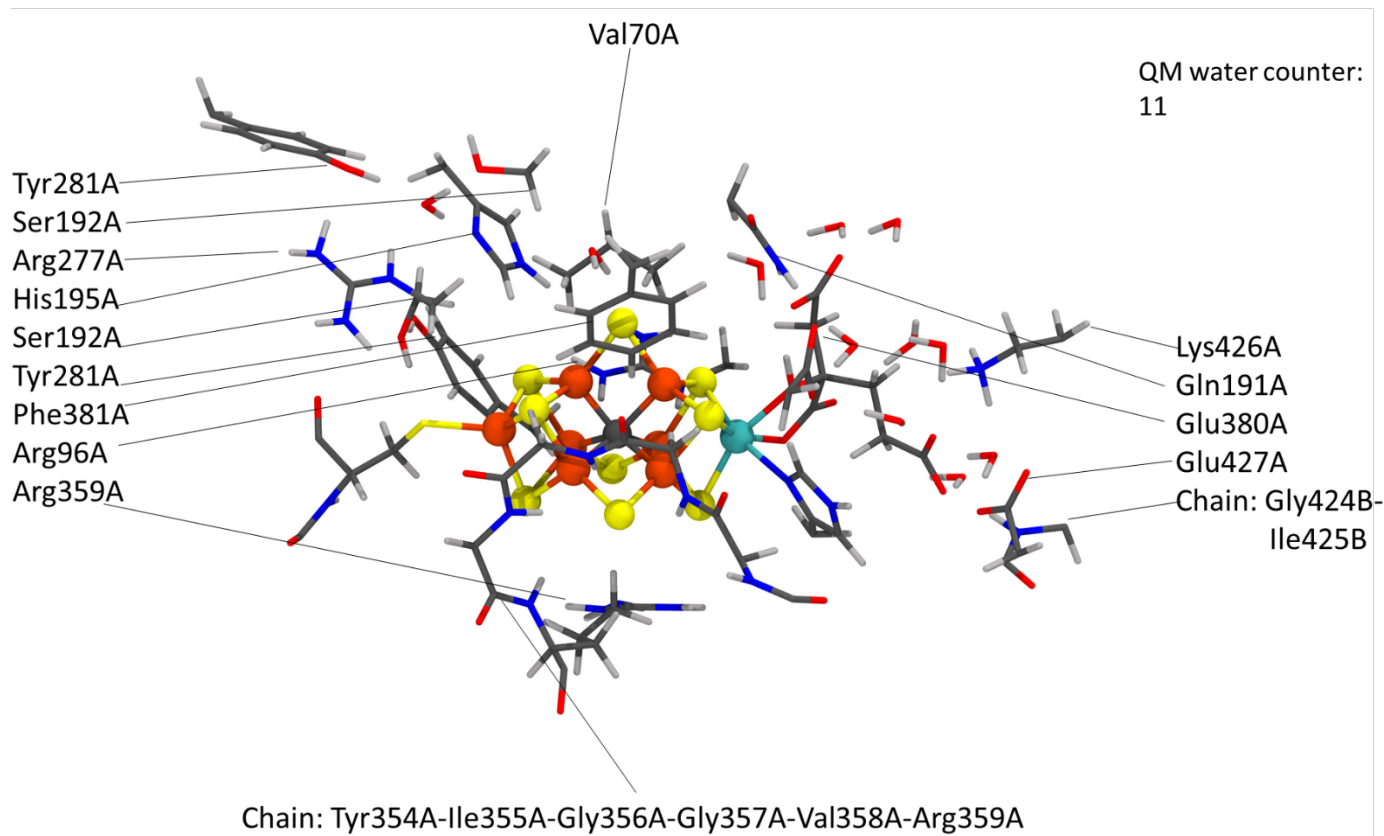


Figure S7: 282QM atom model: contains FeMoco, Val70A, Arg96A, Gln191A, Ser192A, His195A, increased Cys275A, Arg277A, Tyr281A, Arg359A, Glu380A, Phe381A, Lys426A, Glu427A, His442A, the peptide chain part of Tyr354A-Ile355A-Gly356A-Gly357A-Val358A-Arg359A, the chain part of Gly424B-425IleB and 10 water molecules.

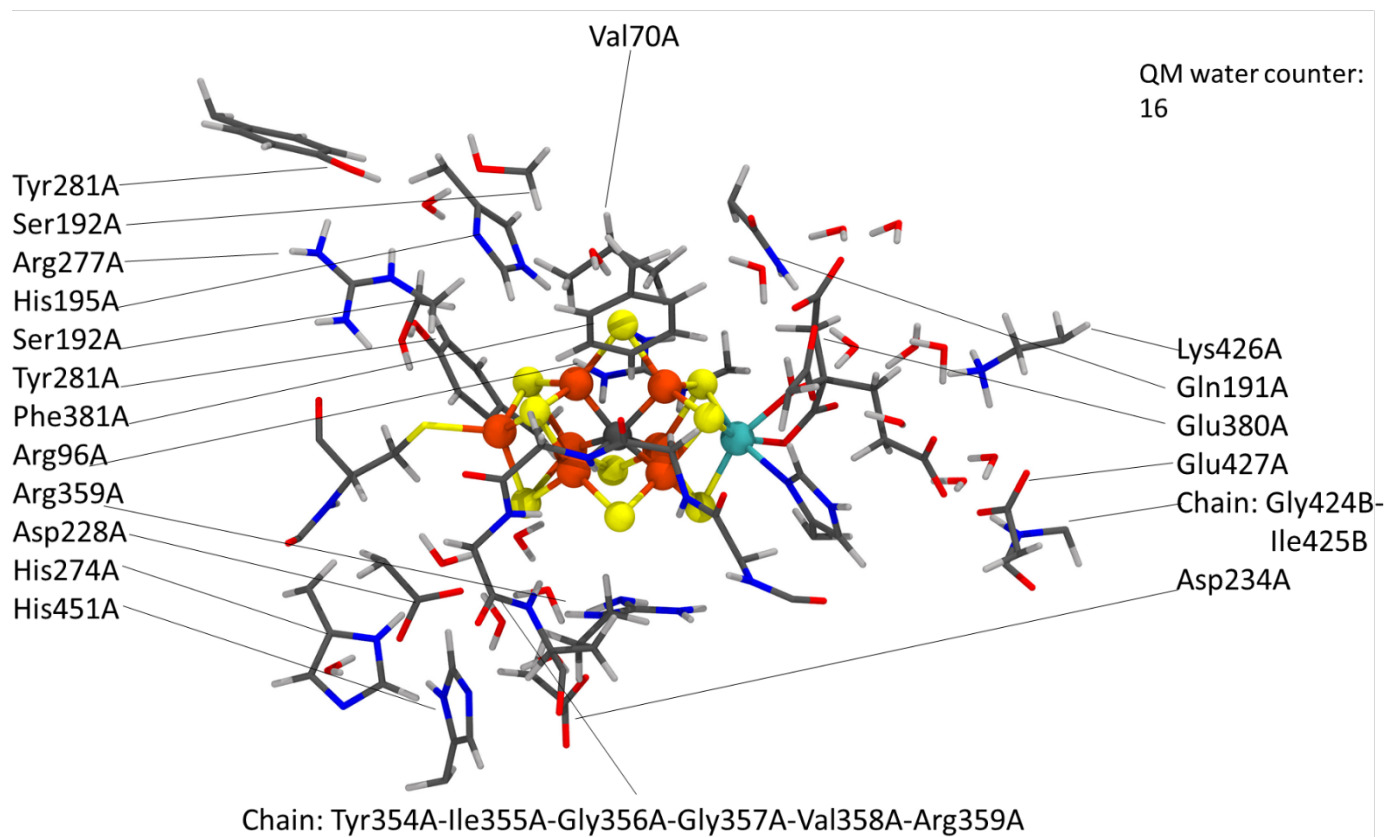


Figure S8: 335QM atom model: contains FeMoco, Val70A, Arg96A, Gln191A, Ser192A, His195A, Asp228A, Asp234A, His274A, increased Cys275A, Arg277A, Tyr281A, Arg359A, Glu380A, Phe381A, Lys426A, Glu427A, His442A, His451A, the peptide chain part of Tyr354A-Ile355A-Gly356A-Gly357A-Val358A-Arg359A, the peptide chain part of Gly424B-425IleB and 16 water molecules.

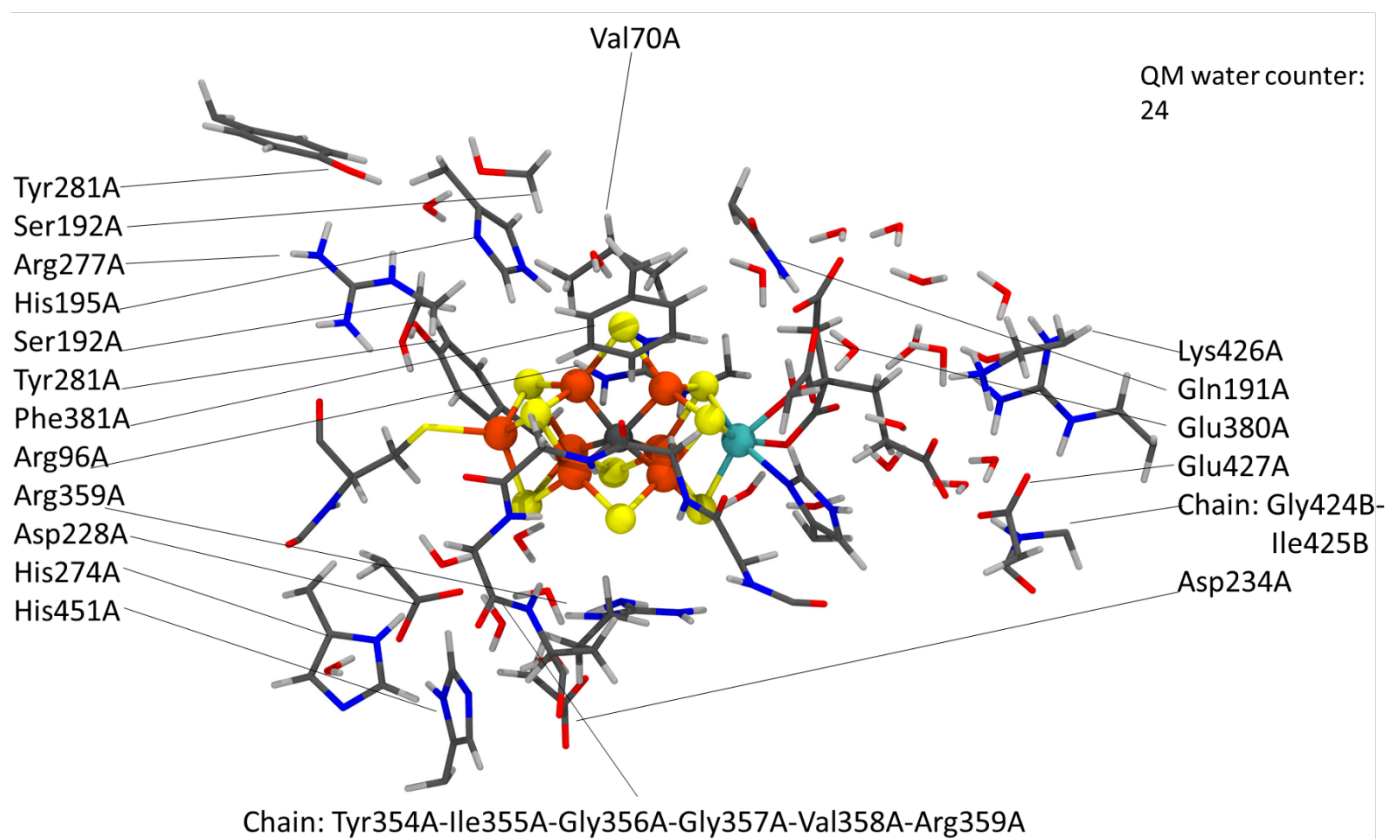


Figure S9: 367QM atom model: contains FeMoco, Val70A, Arg96A, Gln191A, Ser192A, His195A, Asp228A, Asp234A, His274A, increased Cys275A, Arg277A, Tyr281A, Arg359A, Glu380A, Phe381A, Lys426A, Glu427A, His442A, His451A, the peptide chain part of Tyr354A-Ile355A-Gly356A-Gly357A-Val358A-Arg359A, the peptide chain part of Gly424B-425IleB and 24 water molecules.

2. Unconstrained model data

Root-mean square deviations of the QM/MM calculations of the unconstrained model showing that the unconstrained model results in similar cofactor structures as the constrained model.

Table S1. RMSD values

QM region size (atoms)	[MoFe ₇ S ₉ C]	MoFe ₇ S ₉ C-HCA-His-Cys
54 constrained	0.040	0.105
103 constrained	0.039	0.099

127 constrained	0.043	0.102
154 constrained	0.044	0.104
198 constrained	0.050	0.103
247 constrained	0.044	0.100
282 constrained	0.045	0.101
334 constrained	0.046	0.106
367 constrained	0.046	0.100
54 (COSMO)	0.081	0.698
54 unconstrained	0.072	0.185
89 unconstrained	0.061	0.183
127 unconstrained	0.046	0.184
163 unconstrained	0.052	0.198
211 unconstrained	0.051	0.195

3. Localized orbitals

Localized orbitals were calculated using the Pipek-Mezey approach on the $M_S=3/2$ BS7-235 broken-symmetry solution of the QM/MM optimized geometries. The MM pointcharges were included in all calculations. The TPSSH functional was used as before.

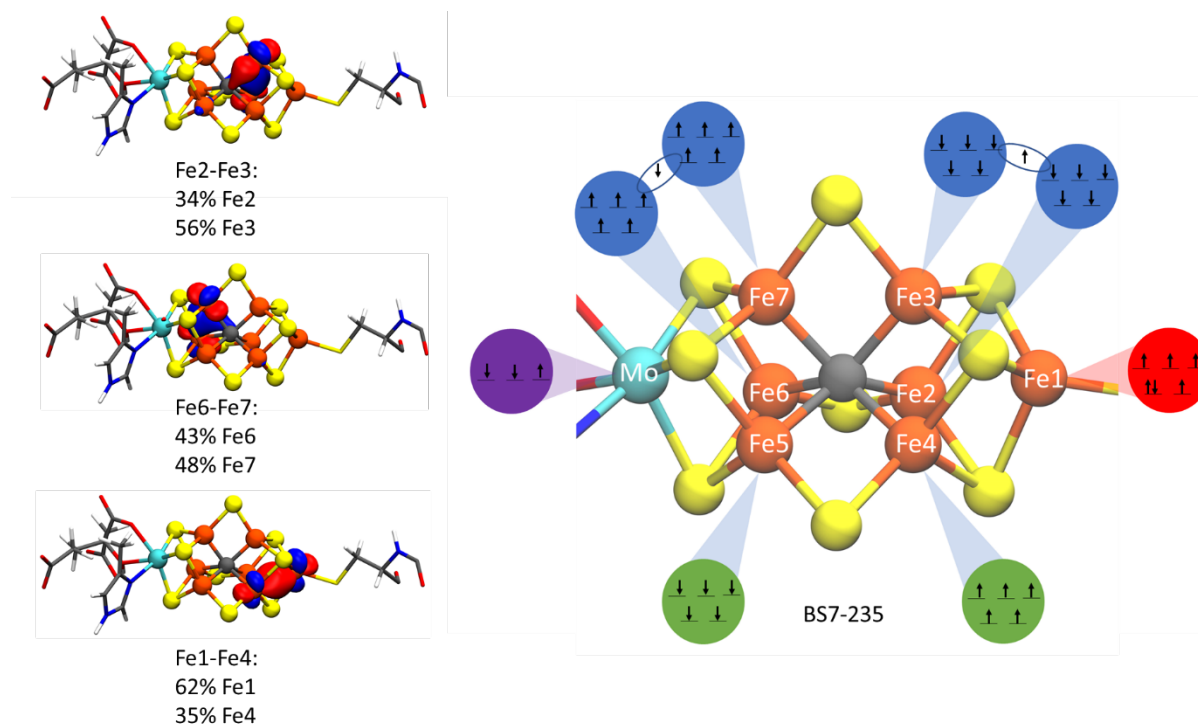


Figure S10: Localized orbitals of the electrons involved in the mixed-valence ferromagnetic pairs in FeMoco using 54 atom QM region.

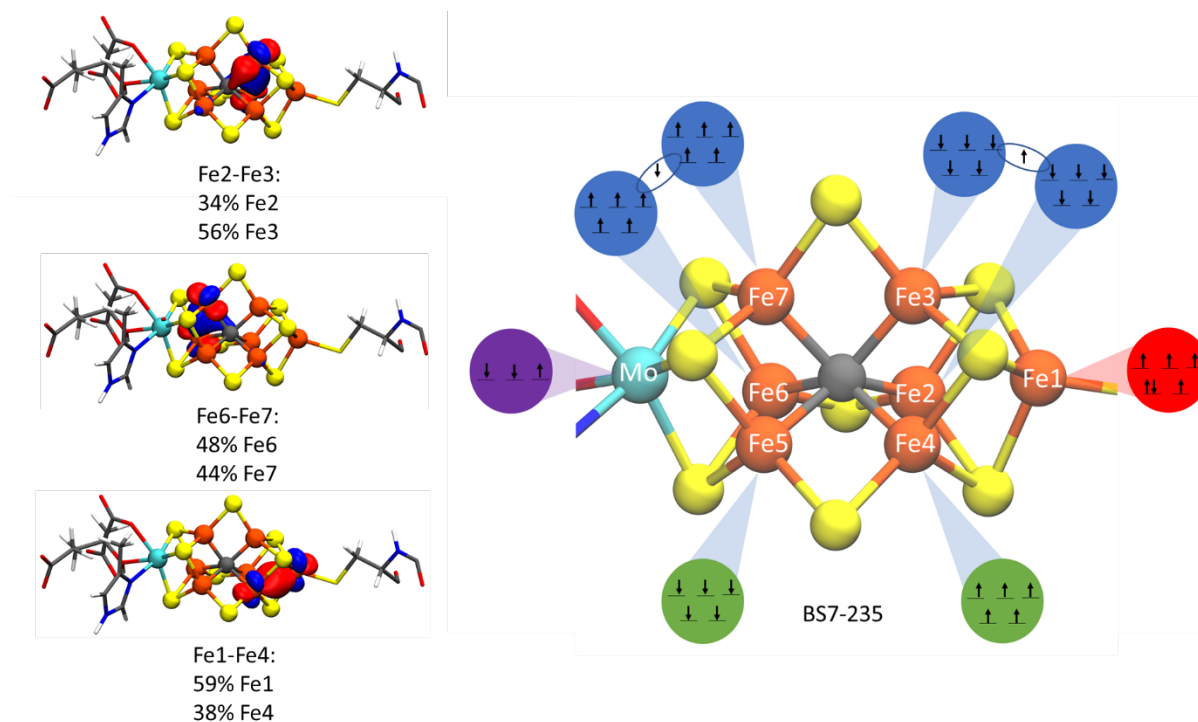


Figure S11: Localized orbitals of the electrons involved in the mixed-valence ferromagnetic pairs in FeMoco using 367 atom QM region.

Pipek, J.; Mezey, P. G. A fast intrinsic localization procedure applicable for ab initio and semiempirical linear combination of atomic orbital wave functions. *J. Chem. Phys.* **1989**, *90*, 4916.

4. Scripts for QM/MM setup involving GROMACS and Chemshell

Will be made available at:

<https://sites.google.com/site/ragnarbjoernsson/mm-and-qm-mm-setup>

5. Example ORCA Inputfile showing how the electronic structure was described in the QM/MM calculations

```

! TPSSh RIJCOSX D3BJ def2-SVP def2-TZVP/J ZORA Grid5 FinalGrid6 tightscf slowconv
%pointcharges "pointcharges.xyz"
%basis
newgto Fe "ZORA-def2-TZVP" end
newgto Mo "ZORA-def2-TZVP" end
newgto V "ZORA-def2-TZVP" end
newgto S "ZORA-def2-TZVP" end
end
%scf
directresetfreq 1
diismaxeq 20
MaxIter 1500
Flipspin X,X,X
FinalMs 1.5
end

*xyz CHARGE 36

```

6. QM/MM-optimized Cartesian coordinates (Å) of all QM regions (including link atoms).

54QM – [MoFe7S9C] – (56 atoms total with link atoms, marked with lowercase h)

C	49.8983182	64.9248471	104.8440244
H	50.3807384	64.5715409	103.9274703
H	49.2302666	65.7514754	104.5876694
S	51.2126319	65.4378481	106.0399219
C	61.1601568	66.3119473	99.5119699
H	62.0124726	66.6587762	98.9299222
H	60.3885569	67.0817005	99.4420086
N	61.0056323	66.9062308	101.9768937
C	61.6155725	66.2158975	100.9342834
C	61.8275395	66.8235189	103.0319191
H	61.6971149	67.2760679	104.0104038
N	62.9152000	66.0935435	102.7128729
H	63.7444037	65.9302273	103.3103937
C	62.8048579	65.7042692	101.3996452
H	63.5652890	65.1277655	100.8967025
Mo	59.0193656	68.0298049	101.9738854
Fe	52.9044338	66.1794930	104.7176283
Fe	54.8966709	67.9368709	104.8433900
Fe	54.1873066	66.8378200	102.5190731
Fe	55.4068798	65.4105679	104.3649077
Fe	57.7062424	66.1043552	103.3758401
Fe	57.1448975	68.6490909	103.7703841
Fe	56.4801974	67.5528045	101.5389222
S	54.5753941	66.2774580	106.3179863
S	52.8961540	68.2336297	103.8159636
S	53.6247827	64.7409342	103.0811625
S	59.0884672	67.6803411	104.2621807
S	57.3040642	69.6657974	101.7829515
S	58.0834274	66.0723283	101.1283195
S	56.0374563	69.7408693	105.3190329
S	57.2746591	64.1721579	104.4399961
S	54.6400170	67.2102860	100.3627880
C	55.9760369	67.0602000	103.4129859
O	60.4452206	69.6275785	102.2751968
O	59.5461650	68.8596492	100.0020322
O	60.1941825	70.7134756	98.8963721
O	60.4913317	71.5225705	103.9031018
O	60.9474307	73.5674732	103.0820864
O	64.6744970	68.2927328	99.3669693
O	64.7903706	69.1365913	101.4502008
C	60.7291293	70.5418061	101.2080537
C	60.0910018	70.0185023	99.9211340
C	60.0896971	71.8847234	101.5964589

C	60.5555167	72.3830928	102.9689817
C	62.2559551	70.5663137	100.9896833
C	62.7192485	69.3073363	100.2578227
C	64.1914489	68.8991919	100.3631064
H	60.3775951	70.2160502	103.1163858
H	62.1722932	68.4653812	100.6933145
H	62.4442482	69.3525666	99.1996035
H	62.5371499	71.4691642	100.4366478
H	62.7170377	70.6058936	101.9770587
H	59.0114692	71.6622205	101.6826273
H	60.2704167	72.6289006	100.8157268
h	60.7664621	65.3862086	99.0923516
h	49.2906940	64.0975661	105.2107206

103QM – [MoFe7S9C] – (110 atoms total with link atoms, marked with lowercase h)

C	56.4397277	71.4299747	98.8328029
H	57.3656423	71.2538732	99.3915797
H	56.0798328	72.4415154	99.0587797
N	55.4609054	70.4616533	99.2998878
H	55.8090432	69.6349869	99.7896900
C	54.1909252	70.7869295	99.5514216
N	53.6291726	71.8564003	98.9611147
H	54.0813312	72.3938153	98.2300362
H	52.7009832	72.1218361	99.2850918
N	53.4705143	70.0667901	100.4056953
H	53.8292364	69.1735978	100.7645317
H	52.4942007	70.3261717	100.5470487
C	59.4067212	73.1582531	107.4004873
H	59.2060735	73.0459790	106.3287632
H	59.6722445	74.2023447	107.6006160
C	60.5622245	72.2532161	107.8191974
O	60.9459536	72.1822121	109.0065340
N	61.1437014	71.5623279	106.8297707
H	60.8130863	71.6535092	105.8697743
H	61.8952271	70.8713427	107.0234571
C	51.0861190	72.2755268	109.4168143
H	51.2666192	72.1088764	110.4845158
H	50.1129893	71.8207725	109.1715841
N	52.6983787	70.4143576	109.3163331
C	52.1518111	71.5220565	108.6919776
C	53.4441106	69.8249937	108.3957999
H	54.0544216	68.9394451	108.5239705
N	53.4064432	70.4972876	107.2186853
H	53.9790208	70.2666193	106.4017226
C	52.5945878	71.5951831	107.3874256
H	52.4142713	72.3160233	106.6010964
C	49.9072939	64.9290668	104.8326759
H	50.3815290	64.5738968	103.9125668
H	49.2385228	65.7565143	104.5808764
S	51.2311024	65.4452153	106.0167437
C	56.5912963	62.4909552	101.3818172
H	56.6921044	63.3248707	102.0857455
H	57.5865111	62.2477388	101.0082102
N	55.7148562	62.8483619	100.2703050
H	54.7023419	62.7444215	100.4415870
C	56.1116289	63.4492749	99.1504942
N	57.4067641	63.6734480	98.9147690
H	58.1065804	63.4792171	99.6187778
H	57.7409944	64.1337814	98.0691111
N	55.2023616	63.8316406	98.2327378
H	54.3153728	63.3047609	98.2140657
H	55.5494084	64.0815506	97.3160008
C	63.1676258	67.3218414	107.9884765
H	64.1648934	67.4577279	108.4315186
H	63.1052909	66.3197390	107.5554327
C	62.9915900	68.4026290	106.8953918
O	63.0680956	69.6096338	107.2539998
O	62.8072869	68.0286533	105.6984659
C	61.1701139	66.2875065	99.5037950
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H	60.3958467	67.0545874	99.4407769
N	61.0409903	66.8908590	101.9657175
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C	61.8663173	66.8026741	103.0169430
H	61.7558696	67.2645934	103.9949122
N	62.9442820	66.0603239	102.6934831
H	63.7734880	65.8959078	103.2912199
C	62.8235639	65.6684009	101.3815567
H	63.5727009	65.0797784	100.8760980
Mo	59.0575496	68.0040562	101.9698271
Fe	52.9297158	66.1522064	104.6817649
Fe	54.9227248	67.9107314	104.7955089
Fe	54.2486722	66.7635823	102.4902466
Fe	55.4452038	65.3825600	104.3686822
Fe	57.7576869	66.0786450	103.3963026
Fe	57.1795572	68.6172697	103.7411949
Fe	56.5347158	67.4850387	101.5289394
S	54.5888427	66.2782519	106.2945577
S	52.9366167	68.1885615	103.7347029
S	53.6779029	64.6800677	103.0808204
S	59.1287667	67.6773271	104.2623965
S	57.3231138	69.6120675	101.7466494
S	58.1517475	66.0216946	101.1574247
S	56.0502137	69.7319979	105.2543693
S	57.3040207	64.1469832	104.4430467
S	54.7066502	67.1399027	100.3491851
C	56.0199903	67.0176326	103.4008722
O	60.4610901	69.6184393	102.2666557
O	59.5797865	68.8345510	99.9959846
O	60.1944700	70.6984283	98.8887908
O	60.4897799	71.5176970	103.8900747
O	60.9541722	73.5616216	103.0727259
O	64.6844719	68.2884108	99.3620459
O	64.7971797	69.1200330	101.4503135
C	60.7400399	70.5345524	101.1994115
C	60.1047445	70.0032534	99.9147903
C	60.1009343	71.8779808	101.5824334
C	60.5614776	72.3808488	102.9534648
C	62.2667318	70.5588389	100.9810102
C	62.7289650	69.2968572	100.2544957
C	64.1998067	68.8887284	100.3604024
H	60.3854445	70.2041414	103.1062998
H	62.1815141	68.4574210	100.6942394
H	62.4539692	69.3375525	99.1960796
H	62.5491896	71.4598116	100.4257197
H	62.7255643	70.6005621	101.9695312
H	59.0208521	71.6777657	101.6629404
H	60.2844172	72.6223329	100.8041276
h	60.7763070	65.3600823	99.0880213
h	49.3012377	64.1024299	105.2033974
h	51.0317172	73.3442077	109.2093802
h	56.6749390	71.3607597	97.7707520
h	56.2096072	61.6220481	101.9178966
h	58.4941380	72.9355893	107.9533706
h	62.4495933	67.4320814	108.8010918

127QM – [MoFe7S9C] – (136 atoms total with link atoms, marked with lowercase h)

C	53.7929055	72.8708018	103.3157950
H	53.7382335	73.5114220	104.1975841
C	52.8112701	71.7032115	103.4805951
H	53.1312048	71.0816950	104.3223154
H	51.7773774	72.0154662	103.6747549
H	52.8140509	71.0501552	102.6047316
C	55.2342204	72.3467613	103.1760942
H	55.9875267	73.1395574	103.2800709
H	55.4475662	71.6120348	103.9575732
H	55.3874353	71.8195254	102.2247695
C	56.4348182	71.4572158	98.8399542
H	57.3598388	71.2932494	99.4042247
H	56.0659733	72.4689690	99.0505590

N	55.4608805	70.4878595	99.3146130
H	55.8113052	69.6668116	99.8123939
C	54.1829115	70.7979287	99.5381188
N	53.6153090	71.8539922	98.9315037
H	54.0711786	72.3966514	98.2061060
H	52.6822198	72.1125173	99.2507046
N	53.4570482	70.0756586	100.3891669
H	53.8144648	69.1781930	100.7417663
H	52.4699644	70.3100058	100.4890688
C	59.3830054	73.1754385	107.3850339
H	59.1781927	73.0625576	106.3142452
H	59.6378786	74.2221761	107.5854443
C	60.5504259	72.2842630	107.7924353
O	60.9301729	72.1918043	108.9810206
N	61.1528979	71.6273292	106.7924947
H	60.8173092	71.7218536	105.8340345
H	61.8902560	70.9190230	106.9836220
C	51.0777287	72.2789657	109.4222985
H	51.2577647	72.1137305	110.4903674
H	50.1036961	71.8255941	109.1775360
N	52.6721352	70.4070424	109.3294976
C	52.1413487	71.5202981	108.7016989
C	53.4149074	69.8085531	108.4129174
H	54.0150689	68.9169097	108.5457866
N	53.3911425	70.4815290	107.2357210
H	53.9817976	70.2549933	106.4311218
C	52.5923548	71.5895846	107.3996377
H	52.4203878	72.3068493	106.6078682
C	49.9245770	64.9260309	104.8320401
H	50.4058729	64.5655955	103.9176745
H	49.2592652	65.7532419	104.5707007
S	51.2388051	65.4475862	106.0252460
C	56.5901728	62.5106972	101.3828332
H	56.7156610	63.3456667	102.0819329
H	57.5738498	62.2485922	100.9911319
N	55.7002867	62.8754286	100.2846355
H	54.6894978	62.7631878	100.4603964
C	56.0879093	63.4760220	99.1614795
N	57.3803974	63.7180139	98.9287626
H	58.0754335	63.5508361	99.6438403
H	57.7160128	64.1633148	98.0757622
N	55.1725850	63.8399598	98.2425218
H	54.2978545	63.2927233	98.2191264
H	55.5145498	64.1077485	97.3291101
C	63.1636365	67.3306594	107.9966522
H	64.1657294	67.4744020	108.4268719
H	63.1084504	66.3308948	107.5573637
C	62.9628162	68.4153474	106.9125792
O	62.9795986	69.6210996	107.2856241
O	62.8195269	68.0479492	105.7080737
C	58.9274093	69.1768927	111.5832870
H	58.1859811	69.7120293	112.1830615
H	59.8403909	69.7807980	111.5598798
C	58.4954306	68.9231498	110.1534150
C	57.3041494	68.2369068	109.8473933
H	56.6107714	67.9572399	110.6376039
C	57.0175680	67.8754597	108.5305825
H	56.1022448	67.3436813	108.2844309
C	57.9035005	68.2104234	107.5020550
H	57.6694313	67.9178094	106.4856157
C	59.3491358	69.2999771	109.1032574
H	60.2505111	69.8751616	109.3126883
C	59.0611026	68.9374493	107.7824917
H	59.7409552	69.2206424	106.9835085
C	61.1667291	66.2961935	99.5134419
H	62.0130131	66.6464496	98.9246935
H	60.3926410	67.0634232	99.4477189
N	61.0408580	66.9100307	101.9749175
C	61.6335934	66.2043153	100.9320698
C	61.8667940	66.8223356	103.0256431

H	61.7572239	67.2866169	104.0025648
N	62.9418797	66.0754771	102.7036341
H	63.7715236	65.9103144	103.3005463
C	62.8187184	65.6799134	101.3930959
H	63.5665362	65.0884140	100.8888581
Mo	59.0630869	68.0332378	101.9853240
Fe	52.9480398	66.1663059	104.7115511
Fe	54.9256857	67.9473830	104.8171549
Fe	54.2555783	66.7890413	102.5149540
Fe	55.4612741	65.4217425	104.4000451
Fe	57.7651003	66.1186191	103.4176264
Fe	57.1800472	68.6585015	103.7557154
Fe	56.5389660	67.5182523	101.5497363
S	54.6054759	66.3245154	106.3258221
S	52.9339063	68.1966220	103.7606623
S	53.7031112	64.7022866	103.1087956
S	59.1353806	67.7222984	104.2783694
S	57.3331840	69.6433093	101.7579043
S	58.1540311	66.0513371	101.1791901
S	56.0617639	69.7551874	105.3046190
S	57.3153012	64.1799730	104.4482615
S	54.7114218	67.1624651	100.3715430
C	56.0261490	67.0556726	103.4237230
O	60.4697301	69.6405269	102.2678480
O	59.5789821	68.8474726	100.0046220
O	60.1992498	70.7010481	98.8834622
O	60.4965094	71.5382740	103.8826872
O	60.9633635	73.5802029	103.0662241
O	64.6839722	68.2888057	99.3637358
O	64.7968923	69.1205922	101.4519860
C	60.7466056	70.5521034	101.1949852
C	60.1082746	70.0145575	99.9145227
C	60.1096454	71.8975254	101.5738614
C	60.5694253	72.4005438	102.9438046
C	62.2728684	70.5716887	100.9750984
C	62.7313268	69.3058158	100.2528204
C	64.2003843	68.8917281	100.3611089
H	60.3942830	70.2330060	103.1051567
H	62.1804922	68.4694291	100.6941264
H	62.4573406	69.3448270	99.1941047
H	62.5569509	71.4697894	100.4162565
H	62.7315172	70.6160308	101.9636612
H	59.0292389	71.7049841	101.6519187
H	60.2901930	72.6407115	100.7945996
h	60.7738276	65.3680725	99.0983672
h	49.3136797	64.1029274	105.2026778
h	51.0271863	73.3470117	109.2106612
h	56.6763142	71.3755529	97.7802004
h	56.2033632	61.6502251	101.9287573
h	58.4752698	72.9434179	107.9420345
h	62.4540502	67.4299921	108.8180458
h	53.6171727	73.5161099	102.4551193
h	59.2355425	68.2608984	112.0873460

154QM – [MoFe7S9C] – BS7-235 (163 atoms total with link atoms, marked with lowercase h)

C	53.807963	72.867022	103.298791
H	53.773438	73.502656	104.184900
C	52.825393	71.703067	103.476245
H	53.156947	71.079224	104.311734
H	51.796044	72.018941	103.687520
H	52.811701	71.051852	102.599285
C	55.244929	72.340595	103.123948
H	56.002505	73.130197	103.229685
H	55.473709	71.593325	103.889514
H	55.380958	71.829217	102.161922
C	56.440520	71.432280	98.823646
H	57.367827	71.237789	99.371902
H	56.108118	72.448679	99.064555
N	55.452071	70.477892	99.298717
H	55.789003	69.646348	99.787561

C	54.180172	70.805757	99.529104
N	53.625690	71.873414	98.931312
H	54.090652	72.417901	98.213017
H	52.695738	72.141495	99.249229
N	53.446606	70.087933	100.377723
H	53.796794	69.188803	100.731277
H	52.463463	70.338426	100.484510
C	59.350498	73.220457	107.365046
H	59.133379	73.115356	106.295817
H	59.596661	74.267567	107.571381
C	60.533953	72.343163	107.750106
O	60.920003	72.232018	108.934212
N	61.143413	71.719115	106.732478
H	60.789719	71.812517	105.782938
H	61.887183	71.020524	106.914200
C	51.079762	72.278410	109.421013
H	51.259202	72.113034	110.489147
H	50.106268	71.824458	109.175395
N	52.675566	70.407320	109.327656
C	52.144814	71.521154	108.700636
C	53.421666	69.811553	108.412063
H	54.022883	68.920499	108.544916
N	53.400219	70.486901	107.236023
H	53.991740	70.262815	106.431745
C	52.599131	71.593482	107.399836
H	52.428263	72.311490	106.608431
C	49.934244	64.929169	104.828856
H	50.413977	64.566888	103.914453
H	49.269336	65.756560	104.567165
S	51.250801	65.453372	106.018752
C	56.608524	62.492314	101.366269
H	56.770501	63.328090	102.057408
H	57.575309	62.198737	100.954850
N	55.707941	62.871878	100.282852
H	54.698013	62.760897	100.464245
C	56.091970	63.474492	99.159548
N	57.384350	63.714796	98.924891
H	58.081924	63.535248	99.634600
H	57.719942	64.155338	98.069202
N	55.173889	63.843767	98.245622
H	54.299917	63.295251	98.221674
H	55.512949	64.117299	97.332786
C	63.092499	67.363563	107.933892
H	64.112828	67.453917	108.333547
H	62.996791	66.388120	107.450403
C	62.904670	68.511704	106.915936
O	62.899409	69.686377	107.341649
O	62.801961	68.205857	105.673086
C	58.942343	69.177169	111.590063
H	58.197949	69.708392	112.189662
H	59.856131	69.780501	111.577747
C	58.520336	68.937889	110.154377
C	57.343629	68.233693	109.831996
H	56.652076	67.927190	110.613807
C	57.068501	67.890255	108.507887
H	56.163989	67.346617	108.248530
C	57.951825	68.258331	107.488401
H	57.727296	67.978351	106.466366
C	59.368412	69.351632	109.113287
H	60.256596	69.943281	109.333279
C	59.092201	69.005534	107.785161
H	59.766468	69.318169	106.992325
C	61.165114	66.301540	99.486114
H	62.001568	66.656594	98.886159
H	60.385670	67.063266	99.424540
N	61.055044	66.929591	101.942745
C	61.645620	66.222568	100.899998
C	61.888237	66.851599	102.987820
H	61.770597	67.315662	103.962209
N	62.966264	66.110568	102.663972

H	63.807923	65.964694	103.252410
C	62.836641	65.707324	101.356525
H	63.581050	65.111929	100.852333
Mo	59.077755	68.049815	101.962190
Fe	52.963358	66.180159	104.710150
Fe	54.944584	67.965353	104.810614
Fe	54.269074	66.806767	102.510795
Fe	55.478475	65.437740	104.391195
Fe	57.780876	66.134691	103.402865
Fe	57.198976	68.678134	103.743863
Fe	56.550353	67.538868	101.540997
S	54.625926	66.340970	106.319352
S	52.948082	68.210936	103.760103
S	53.719063	64.718373	103.104707
S	59.157715	67.738531	104.256877
S	57.351627	69.662196	101.745279
S	58.160954	66.069407	101.163804
S	56.080298	69.775297	105.294291
S	57.330702	64.195950	104.435315
S	54.721471	67.180320	100.367488
C	56.042582	67.074187	103.414561
O	60.500113	69.663423	102.213440
O	59.589598	68.853043	99.978061
O	60.168330	70.693524	98.826576
O	60.471176	71.581847	103.821374
O	60.982856	73.601104	103.002787
O	64.680173	68.292338	99.289334
O	64.837139	69.123151	101.360311
C	60.768819	70.575042	101.136346
C	60.111784	70.019641	99.870770
C	60.120662	71.923395	101.501220
C	60.560541	72.427023	102.874598
C	62.292428	70.619860	100.901338
C	62.747291	69.341865	100.193333
C	64.205138	68.911155	100.278896
H	60.410858	70.243025	103.046485
H	62.199803	68.505459	100.641157
H	62.472642	69.382148	99.135668
H	62.535421	71.493571	100.290375
H	62.777666	70.723568	101.874253
H	59.041130	71.723302	101.572049
H	60.318764	72.665215	100.724461
O	63.974147	69.561104	96.865719
H	63.000378	69.533254	96.811222
H	64.214794	69.034687	97.657931
O	67.288223	68.637657	102.392620
H	67.473896	67.765891	102.806194
H	66.411903	68.572987	101.962400
O	61.863290	73.068354	98.444072
H	61.296724	72.289189	98.611903
H	62.189660	73.341140	99.331728
O	65.035589	68.491388	104.172251
H	64.236951	68.378945	104.733484
H	64.697869	68.737618	103.294954
O	63.255323	74.317970	104.405172
H	63.646426	73.603372	104.953635
H	62.383028	73.986283	104.120244
O	59.843605	75.603964	101.496191
H	58.961076	75.203528	101.398503
H	60.293607	74.962873	102.085690
O	57.668690	73.906689	100.906841
H	58.055646	73.038850	100.734448
H	56.951056	73.728637	101.534735
O	64.934286	71.552956	102.543174
H	64.986921	70.669869	102.104665
H	64.251458	71.369480	103.223233
O	62.935928	70.488659	104.252696
H	62.051288	70.890049	104.212942
H	62.832345	69.651805	104.793253
h	60.771289	65.369124	99.081679

h	49.322601	64.107424	105.201275
h	51.028255	73.346561	109.210141
h	56.666055	71.364388	97.759413
h	56.210543	61.646026	101.926158
h	58.452816	72.972620	107.931448
h	62.411558	67.446719	108.780929
h	53.619591	73.519286	102.446069
h	59.248291	68.257472	112.088682

154QM – [MoFe7S9C] – BS7-247 (162 atoms total with link atoms, marked with lowercase h)

C	53.80961972	72.86639759	103.3093803
H	53.78205869	73.50678521	104.1920901
C	52.81601797	71.71336345	103.4935928
H	53.14210999	71.09025924	104.3314308
H	51.78972154	72.03878094	103.7047358
H	52.795104	71.05729107	102.6204203
C	55.24092608	72.32321638	103.1386223
H	56.0064793	73.10663587	103.2333201
H	55.46399439	71.58087461	103.9113673
H	55.36918946	71.80141362	102.1810545
C	56.43092673	71.42089929	98.80899954
H	57.35401694	71.22342128	99.3630788
H	56.0993044	72.43670112	99.05163976
N	55.43359377	70.46913173	99.27183292
H	55.76309296	69.61996982	99.73119544
C	54.1688394	70.80908524	99.52501014
N	53.61994957	71.88849094	98.94450677
H	54.07110099	72.41577176	98.20419299
H	52.69385708	72.16109522	99.26941886
N	53.44060673	70.09450321	100.3806807
H	53.78983612	69.1989125	100.7409124
H	52.45946832	70.34990785	100.4980888
C	59.34579444	73.22520932	107.3624441
H	59.12779239	73.11815021	106.2936184
H	59.58846494	74.27325313	107.5680961
C	60.53283026	72.35194474	107.7466056
O	60.9201291	72.24343954	108.9304303
N	61.14573255	71.73112752	106.72882
H	60.78512924	71.8150145	105.781146
H	61.88584731	71.02860095	106.9113924
C	51.08117394	72.27833391	109.4181314
H	51.25703079	72.11143029	110.4866769
H	50.10873066	71.82438602	109.168561
N	52.67869853	70.40856575	109.3277686
C	52.15055693	71.52379358	108.700921
C	53.4328495	69.81741108	108.4159532
H	54.03612337	68.92803772	108.5506656
N	53.41956437	70.49737612	107.2424155
H	54.01722541	70.27630984	106.4424376
C	52.6145388	71.60168349	107.4039034
H	52.44761609	72.32206797	106.6138403
C	49.88850273	64.93307352	104.7971393
H	50.3666704	64.5719509	103.8818682
H	49.21544455	65.75534912	104.5404228
S	51.20121801	65.4707913	105.9726904
C	56.61351298	62.5115937	101.3762306
H	56.78609148	63.34938792	102.0627335
H	57.57570512	62.20604576	100.9626422
N	55.71231223	62.89268975	100.2934256
H	54.70200967	62.79005629	100.4781021
C	56.0983951	63.47647592	99.16169408
N	57.39268483	63.69821921	98.91836722
H	58.09188947	63.51819674	99.62662855
H	57.7282032	64.13093157	98.05888236
N	55.18133875	63.84707784	98.24629556
H	54.30343908	63.30478577	98.22923789
H	55.52212382	64.10060159	97.32821088
C	63.08845391	67.36390448	107.9374598
H	64.11051199	67.44870316	108.3341344
H	62.98603747	66.38940349	107.4534182

C	62.90347257	68.51270373	106.9196856
O	62.88442305	69.6870005	107.3466564
O	62.81673644	68.20719475	105.6758576
C	58.94825724	69.17616411	111.6023323
H	58.20111475	69.70423201	112.2014058
H	59.86144359	69.78050161	111.5959401
C	58.53305126	68.94049865	110.1641368
C	57.36385033	68.22689551	109.8338866
H	56.67008154	67.9131138	110.6109085
C	57.10018262	67.88224073	108.5076773
H	56.20122521	67.3318313	108.2441176
C	57.98781608	68.25684189	107.494218
H	57.77762434	67.9717655	106.4705322
C	59.38375064	69.36244761	109.1285722
H	60.26674631	69.95967597	109.3541406
C	59.11980704	69.01334955	107.7987647
H	59.79805755	69.32752993	107.010088
C	61.16116388	66.30637693	99.48438098
H	61.99663405	66.66206769	98.88326894
H	60.38007641	67.06659088	99.4229595
N	61.05368393	66.93653835	101.9408171
C	61.64311331	66.22893373	100.8976434
C	61.88807985	66.85859708	102.9853168
H	61.76867078	67.32324094	103.959328
N	62.96487942	66.11684058	102.6603661
H	63.80659014	65.97075638	103.2485078
C	62.83411142	65.7130447	101.3530982
H	63.57801949	65.11795949	100.8477255
Mo	59.07757652	68.05167274	101.9591774
Fe	53.01349844	66.18397957	104.8304501
Fe	54.95733685	67.97335695	104.8106853
Fe	54.2427917	66.80578723	102.544388
Fe	55.51379152	65.44276168	104.3925974
Fe	57.80776721	66.19830025	103.3661236
Fe	57.20336493	68.67355401	103.7388161
Fe	56.48179315	67.52917562	101.5082711
S	54.63356936	66.3176095	106.3528163
S	52.99137042	68.24865059	103.808126
S	53.74684546	64.69152421	103.2244716
S	59.1912411	67.77309564	104.2518323
S	57.31633279	69.62971889	101.7355177
S	58.13959034	66.08885556	101.132845
S	56.13712361	69.74891872	105.3354345
S	57.37416727	64.25079553	104.4211587
S	54.65168229	67.13108694	100.36977
C	56.02705759	67.09594179	103.3847693
O	60.49737006	69.66253072	102.2021611
O	59.5733325	68.8658019	99.96040172
O	60.16904586	70.70595638	98.81701657
O	60.47288489	71.5801903	103.8137435
O	60.97631775	73.60159944	102.9945995
O	64.67863124	68.29198027	99.28762886
O	64.83444825	69.12759597	101.3566054
C	60.766002	70.57534828	101.1263964
C	60.10784563	70.02591345	99.85789434
C	60.11433181	71.92139837	101.4947528
C	60.55697579	72.4261456	102.868383
C	62.28924607	70.62313261	100.8925121
C	62.74509982	69.34374735	100.1873807
C	64.2031125	68.91322422	100.2755721
H	60.42138336	70.2350453	103.0403987
H	62.19649797	68.50812629	100.635226
H	62.47263184	69.38259024	99.12907342
H	62.52993724	71.49464236	100.2775445
H	62.77584567	70.73156054	101.8643622
H	59.03506176	71.71941931	101.5666319
H	60.31092103	72.66375921	100.7176752
O	63.97366551	69.56161447	96.8651142
H	63.00005933	69.5327398	96.80929977
H	64.21418078	69.03345135	97.65625437

O	67.28669246	68.63888083	102.388348
H	67.4704101	67.76697609	102.8022723
H	66.40924584	68.57620044	101.9601361
O	61.86455137	73.07539244	98.4374575
H	61.29798606	72.29556068	98.60318133
H	62.19131877	73.34572744	99.32563357
O	65.04164746	68.49714977	104.1722115
H	64.24741541	68.38211702	104.7396104
H	64.69586084	68.74073957	103.2973476
O	63.25296632	74.31662287	104.4062273
H	63.64213333	73.60102741	104.9550151
H	62.38010317	73.98707221	104.1214135
O	59.84587065	75.61445055	101.4945429
H	58.95715986	75.22691599	101.4038423
H	60.2919163	74.96858208	102.0819919
O	57.68398374	73.91488529	100.8999441
H	58.1241602	73.06929984	100.7466383
H	56.95959855	73.70555702	101.5097264
O	64.93262988	71.55188346	102.5443137
H	64.98719259	70.6704235	102.1026262
H	64.25155764	71.3636776	103.2250742
O	62.9334214	70.48592308	104.2518861
H	62.04737282	70.88426849	104.2134841
H	62.83459071	69.64931965	104.794506
h	60.76864921	65.37282317	99.08129692
h	49.28924229	64.10724654	105.1804979
h	51.02893279	73.34676908	109.2088845
h	56.66218887	71.35528017	97.74585369
h	56.20918717	61.67176719	101.9412786
h	58.44955763	72.97520924	107.9301823
h	62.41041889	67.4483708	108.7866954
h	53.62559255	73.51718778	102.454586
h	59.25369417	68.25474591	112.0980781

154QM – [MoFe7S9C] – BS7-346 (162 atoms total with link atoms, marked with lowercase h)

C	53.7961674	72.8689822	103.3084040
H	53.7495684	73.5067964	104.1925062
C	52.8140524	71.7027034	103.4771172
H	53.1350900	71.0830357	104.3197961
H	51.7808750	72.0163069	103.6726097
H	52.8147520	71.0481512	102.6024567
C	55.2352773	72.3438949	103.1529053
H	55.9916152	73.1333622	103.2659688
H	55.4542719	71.5986191	103.9231587
H	55.3844187	71.8307794	102.1938564
C	56.4415324	71.4373147	98.8324722
H	57.3685198	71.2478297	99.3834082
H	56.1025762	72.4520841	99.0715177
N	55.4566259	70.4774345	99.3046276
H	55.7977580	69.6491642	99.7961716
C	54.1833147	70.8001155	99.5340496
N	53.6249139	71.8649419	98.9347791
H	54.0885271	72.4108685	98.2168033
H	52.6940558	72.1297627	99.2534552
N	53.4519390	70.0801680	100.3828496
H	53.8040651	69.1807425	100.7346144
H	52.4674779	70.3247908	100.4871378
C	59.3702938	73.1933691	107.3826668
H	59.1633700	73.0789160	106.3124689
H	59.6189391	74.2415835	107.5816121
C	60.5455192	72.3125125	107.7864858
O	60.9242704	72.2100590	108.9733760
N	61.1581952	71.6736298	106.7797334
H	60.8168701	71.7723141	105.8260320
H	61.8971913	70.9738999	106.9737540
C	51.0787021	72.2786624	109.4227544
H	51.2588898	72.1137457	110.4908223
H	50.1049110	71.8247631	109.1781300
N	52.6724370	70.4060923	109.3288065
C	52.1425069	71.5203187	108.7019751

C	53.4163495	69.8087643	108.4124408
H	54.0156468	68.9164329	108.5446595
N	53.3942811	70.4835747	107.2361532
H	53.9853369	70.2583871	106.4317492
C	52.5952646	71.5915038	107.4006549
H	52.4244125	72.3096964	106.6094424
C	49.9274895	64.9266421	104.8318656
H	50.4084495	64.5656757	103.9176070
H	49.2625687	65.7541386	104.5705283
S	51.2424363	65.4489268	106.0242410
C	56.5892909	62.5113925	101.3830000
H	56.7127931	63.3470959	102.0815643
H	57.5740018	62.2497923	100.9934046
N	55.7007872	62.8743008	100.2831661
H	54.6898499	62.7621920	100.4582839
C	56.0890987	63.4742231	99.1598134
N	57.3816402	63.7153628	98.9267909
H	58.0786816	63.5388255	99.6377919
H	57.7174795	64.1590053	98.0729457
N	55.1736426	63.8397343	98.2414159
H	54.2983575	63.2932741	98.2193254
H	55.5154834	64.1037998	97.3268155
C	63.1561536	67.3354169	108.0668039
H	64.1573542	67.4753705	108.4983950
H	63.1009920	66.3453280	107.6075434
C	62.9422264	68.4440981	107.0212531
O	62.9297901	69.6365967	107.4063246
O	62.8092220	68.0983310	105.7978631
C	58.9254471	69.1756654	111.5840133
H	58.1808341	69.7151989	112.1758057
H	59.8392054	69.7786647	111.5638099
C	58.5024279	68.9175648	110.1525132
C	57.3150056	68.2270554	109.8412014
H	56.6208715	67.9407287	110.6283907
C	57.0311328	67.8731343	108.5218480
H	56.1178966	67.3401227	108.2711375
C	57.9163406	68.2177552	107.4958741
H	57.6824521	67.9319124	106.4773385
C	59.3560717	69.3036070	109.1054439
H	60.2538732	69.8831369	109.3184346
C	59.0712432	68.9469269	107.7822358
H	59.7492747	69.2385304	106.9846609
C	61.1708753	66.3028468	99.4987367
H	62.0119025	66.6546687	98.9034973
H	60.3938697	67.0668435	99.4329298
N	61.0466224	66.9285223	101.9555944
C	61.6435541	66.2225436	100.9154447
C	61.8755958	66.8522544	103.0044532
H	61.7519699	67.3176248	103.9769093
N	62.9552519	66.1114842	102.6863114
H	63.7949550	65.9671524	103.2774612
C	62.8329996	65.7086688	101.3780049
H	63.5817456	65.1153049	100.8776781
Mo	59.0625978	68.0407412	101.9689139
Fe	52.9550299	66.1700631	104.7152402
Fe	54.9311183	67.9564147	104.8183149
Fe	54.2575054	66.7942000	102.5163104
Fe	55.4691334	65.4249857	104.4025520
Fe	57.7736054	66.1235924	103.4104329
Fe	57.1861982	68.6697871	103.7501997
Fe	56.5381764	67.5258834	101.5447267
S	54.6143863	66.3317777	106.3264274
S	52.9378355	68.2001006	103.7638894
S	53.7112849	64.7069370	103.1121430
S	59.1431781	67.7308626	104.2645069
S	57.3357459	69.6506097	101.7499395
S	58.1513230	66.0576486	101.1707954
S	56.0686879	69.7656635	105.3004917
S	57.3254098	64.1879968	104.4455057
S	54.7093867	67.1655262	100.3722261

C	56.0315648	67.0633075	103.4228647
O	60.4723996	69.6534285	102.2376202
O	59.5829788	68.8506242	99.9903347
O	60.1808822	70.6916671	98.8489241
O	60.4079023	71.5557486	103.8578170
O	60.9925444	73.5633296	103.0488883
O	64.6813610	68.3008623	99.3201389
O	64.8330841	69.1394680	101.3896061
C	60.7561029	70.5654620	101.1649218
C	60.1111611	70.0155894	99.8908094
C	60.1111072	71.9129097	101.5322813
C	60.5426529	72.3993574	102.9159148
C	62.2827215	70.6058605	100.9529936
C	62.7440569	69.3431454	100.2232946
C	64.2034320	68.9200360	100.3079624
H	60.3547178	70.2352261	103.0679315
H	62.1996675	68.4952049	100.6526652
H	62.4740061	69.4017429	99.1653162
H	62.5449714	71.4917838	100.3683091
H	62.7487515	70.6828764	101.9376303
H	59.0306370	71.7175089	101.5937094
H	60.3174148	72.6602632	100.7635297
O	63.9750341	69.5615708	96.8775675
H	63.0011752	69.5356362	96.8236896
H	64.2130293	69.0410925	97.6740014
O	67.2853506	68.6391382	102.4050622
H	67.4748983	67.7647288	102.8114070
H	66.4026906	68.5807290	101.9864089
O	61.9111141	73.0358226	98.4624292
H	61.3306343	72.2669453	98.6301977
H	62.2289522	73.3084874	99.3528767
O	64.9878678	68.4760403	104.2001755
H	64.1976766	68.3594912	104.7720854
H	64.6348898	68.7396962	103.3348011
O	63.2599428	74.3115340	104.4109811
H	63.6469341	73.5927672	104.9569814
H	62.3863658	73.9779088	104.1292674
O	59.8778673	75.5767835	101.5219729
H	59.0057159	75.1597310	101.4033485
H	60.3252021	74.9420396	102.1200562
O	57.6714920	73.9060698	100.9401516
H	57.9780886	73.0034634	100.7842406
H	56.9666243	73.8072426	101.5991483
O	64.9003070	71.5563848	102.5839085
H	64.9266467	70.6602985	102.1658053
H	64.2300020	71.4225580	103.2813720
O	62.8444351	70.3731174	104.4001396
H	61.9132775	70.6564815	104.3513280
H	62.7838705	69.6414559	105.0658856
h	60.7774581	65.3718388	99.0906752
h	49.3158950	64.1041298	105.2026658
h	51.0277346	73.3466508	109.2109286
h	56.6702609	71.3685351	97.7689781
h	56.2027493	61.6505797	101.9285769
h	58.4658638	72.9545008	107.9421446
h	62.4414775	67.4233864	108.8850745
h	53.6153462	73.5177755	102.4514104
h	59.2285318	68.2633424	112.0976996

153QM – neg2 – HCA-deprot(162 atoms total with link atoms, marked with lowercase h)

C	53.7845103	72.86153598	103.3131822
H	53.71473705	73.50043755	104.1966595
C	52.81703236	71.68040607	103.4658202
H	53.13413388	71.06263094	104.3113927
H	51.7755852	71.9790921	103.6444416
H	52.84364833	71.02551784	102.5911937
C	55.23384787	72.35708874	103.1765569
H	55.97707236	73.15650451	103.3046849
H	55.45300463	71.60806111	103.9439102
H	55.40486753	71.85188315	102.2170221

C	56.52984624	71.41376215	98.867927
H	57.48265929	71.19645238	99.35768514
H	56.23493503	72.42759548	99.1649517
N	55.56058308	70.4510038	99.36543478
H	55.921337	69.65786912	99.90146136
C	54.27802242	70.74228386	99.56215066
N	53.70762985	71.79962554	98.94953639
H	54.25529417	72.48587647	98.4475869
H	52.78472309	72.06262165	99.29718269
N	53.53234171	69.98356294	100.3641505
H	53.88171834	69.06611976	100.6788504
H	52.55109905	70.22931238	100.4733753
C	59.35683911	73.18117078	107.3358262
H	59.13697309	73.06188835	106.2687817
H	59.60412153	74.23110397	107.5307297
C	60.54976526	72.31148564	107.715127
O	60.93304632	72.20290719	108.9063922
N	61.15964092	71.69780439	106.6965179
H	60.84288343	71.82494355	105.7265424
H	61.91571587	71.0192899	106.8759787
C	51.07970786	72.27925489	109.4201138
H	51.25746371	72.11460728	110.489007
H	50.10564776	71.82620822	109.1740957
N	52.6679622	70.40402866	109.340656
C	52.14614635	71.51727003	108.7052442
C	53.41392234	69.79919192	108.4290152
H	54.01177573	68.90645264	108.5665313
N	53.39934122	70.4668697	107.2501603
H	53.99995922	70.23334209	106.4505135
C	52.60473622	71.57847777	107.4049577
H	52.44215237	72.29343857	106.6090566
C	49.92764999	64.93443924	104.8276378
H	50.41033171	64.57778586	103.9121693
H	49.25639738	65.75705481	104.565183
S	51.24342716	65.46422064	106.0162685
C	56.56977859	62.56464284	101.3903485
H	56.75846726	63.39029373	102.0878755
H	57.52115371	62.27971446	100.936037
N	55.6468503	62.9646278	100.3308944
H	54.6393414	62.81716528	100.4936511
C	56.03474862	63.58708507	99.22001083
N	57.32080296	63.92200701	99.05923279
H	57.87391481	64.1376698	99.8832124
H	57.66175772	64.34289639	98.19556812
N	55.15419063	63.84541237	98.24275587
H	54.28597425	63.2980917	98.16571306
H	55.47577714	64.30829545	97.4055481
C	63.18361803	67.35787309	108.0305684
H	64.18767549	67.48947798	108.4606499
H	63.12104024	66.36367288	107.5801803
C	62.9912283	68.45744183	106.9588054
O	63.0034231	69.65348212	107.3230546
O	62.864766	68.07058071	105.7464927
C	58.94711308	69.18463425	111.6175831
H	58.19911617	69.71362237	112.2155871
H	59.86202814	69.78655929	111.6130043
C	58.53632755	68.94864833	110.178625
C	57.36382649	68.24161015	109.8475026
H	56.6692443	67.92923994	110.6249965
C	57.09622452	67.90635942	108.5196443
H	56.1944051	67.36341591	108.2479811
C	57.98423325	68.28577377	107.5085259
H	57.76687707	68.01466449	106.482925
C	59.39296731	69.36718593	109.1467254
H	60.27588719	69.96529352	109.3724492
C	59.12405443	69.03002334	107.8149032
H	59.79825718	69.35124238	107.0255354
C	61.19263507	66.30963054	99.53658056
H	62.02171358	66.67292238	98.92984307
H	60.41150559	67.07273959	99.49225748

N	61.12117081	66.92707514	101.9988656
C	61.68945259	66.21930399	100.9466047
C	61.95600979	66.82853754	103.0349848
H	61.8463695	67.28430253	104.0132336
N	63.02162469	66.07151044	102.7007289
H	63.86270538	65.92328112	103.2862488
C	62.8769331	65.68226265	101.3896763
H	63.6046292	65.07518078	100.8754305
Mo	59.18642612	68.15476923	102.054131
Fe	52.98999636	66.15431348	104.6981652
Fe	54.96718542	67.95522088	104.8273084
Fe	54.34933188	66.76057516	102.5151972
Fe	55.52499158	65.43223596	104.4319898
Fe	57.85574297	66.14765997	103.4869087
Fe	57.25507537	68.69514272	103.8150543
Fe	56.63975735	67.54898422	101.6065442
S	54.61925433	66.33234894	106.347944
S	52.98387319	68.17156073	103.726859
S	53.77908818	64.67342847	103.1213816
S	59.22145158	67.77814039	104.3434823
S	57.38173376	69.68947666	101.8258411
S	58.29487259	66.12109478	101.2545339
S	56.05578672	69.78135353	105.3454302
S	57.37245677	64.18218229	104.5010361
S	54.83800251	67.10223724	100.372492
C	56.09893836	67.06462512	103.4658343
O	60.5405687	69.60680864	102.202601
O	59.56364442	68.87362927	99.98556043
O	60.14992605	70.71804809	98.84825798
O	60.25027346	71.86569921	103.9798434
O	61.10709806	73.62409796	102.8806844
O	64.6728693	68.32072223	99.29563567
O	64.8625197	69.19407084	101.3442686
C	60.74676631	70.54508152	101.2015829
C	60.09654123	70.04121056	99.89665147
C	60.07273568	71.88762684	101.5920972
C	60.51079523	72.48830959	102.9389135
C	62.26765802	70.64990022	100.9087462
C	62.73843597	69.35909399	100.2311902
C	64.20212119	68.95289249	100.2839318
H	62.2155323	68.53899605	100.7368694
H	62.42578425	69.34733921	99.1827786
H	62.45969736	71.50843934	100.2572011
H	62.77820049	70.80001748	101.8606135
H	59.00522714	71.63695141	101.6868363
H	60.23278519	72.61181766	100.7831248
O	63.97076083	69.56037566	96.86711146
H	62.99499593	69.55814419	96.83998471
H	64.2110486	69.06233661	97.67975484
O	67.28495206	68.66538064	102.3774614
H	67.43301168	67.79176185	102.7964748
H	66.39960554	68.64087519	101.9541154
O	61.78550936	73.07028439	98.41066817
H	61.21956167	72.29474695	98.61272853
H	62.13077212	73.35424427	99.28928257
O	65.02290686	68.50677861	104.1652163
H	64.24219134	68.39868165	104.7537562
H	64.65059454	68.79466713	103.3149284
O	63.24310971	74.32108224	104.3886018
H	63.54543829	73.54801847	104.9094712
H	62.39322635	74.03201858	103.9797707
O	59.86365923	75.61577549	101.5144688
H	58.97307352	75.22708734	101.4595383
H	60.35268334	74.94636675	102.054543
O	57.70580034	73.88824009	100.9473681
H	58.30782883	73.12754986	100.9512225
H	57.02116753	73.65087527	101.5908481
O	64.93525723	71.59074849	102.5725027
H	64.92763492	70.70477046	102.1330887
H	64.24215341	71.47759782	103.2505192

O	62.66390664	70.27657846	104.1660741
H	61.75226744	70.34646278	103.8283193
H	62.65914454	69.48508862	104.7631501
h	60.79729486	65.37987724	99.12751816
h	49.32101521	64.10707589	105.1957835
h	51.02831167	73.34735035	109.2089322
h	56.69407545	71.37389839	97.79112302
h	56.17555039	61.72000088	101.955354
h	58.46561134	72.93830451	107.9144419
h	62.472069	67.45267101	108.8507992
h	53.60334148	73.50445364	102.451845
h	59.25140044	68.26341655	112.1144073

154QM – [MoFe7S9C]³⁻ – (163 atoms total with link atoms, marked with lowercase h)

C	53.7864813	72.8472102	103.2940850
H	53.7179543	73.4791959	104.1843191
C	52.8249730	71.6608554	103.4405244
H	53.1558888	71.0263251	104.2683640
H	51.7840840	71.9545054	103.6357937
H	52.8462368	71.0163007	102.5580580
C	55.2358506	72.3425622	103.1501338
H	55.9816316	73.1419310	103.2817681
H	55.4572151	71.5865275	103.9137079
H	55.4051934	71.8392740	102.1895210
C	56.5412084	71.4440172	98.8837783
H	57.5054374	71.2494540	99.3650408
H	56.2253872	72.4585775	99.1652209
N	55.6179542	70.4586817	99.4104707
H	56.0321429	69.7671918	100.0563772
C	54.3195024	70.6981170	99.5729673
N	53.7181021	71.7141221	98.9029040
H	54.2777234	72.4627860	98.5160424
H	52.7957929	71.9614511	99.2750537
N	53.5944836	69.9302141	100.3775695
H	53.9545119	68.9921822	100.6626727
H	52.6027569	70.1289516	100.4586857
C	59.3398975	73.1551502	107.3548545
H	59.1125774	73.0027017	106.2939016
H	59.5735666	74.2136818	107.5185961
C	60.5451123	72.3159969	107.7579650
O	60.9406380	72.2506483	108.9454926
N	61.1687454	71.6861043	106.7553265
H	60.8168872	71.7502903	105.8008980
H	61.9219683	71.0015139	106.9485165
C	51.0809130	72.2802414	109.4297554
H	51.2645092	72.1215485	110.4990386
H	50.1038658	71.8273492	109.1937353
N	52.6443127	70.3891806	109.3565529
C	52.1397629	71.5061260	108.7147767
C	53.3658093	69.7585390	108.4381887
H	53.9360627	68.8463000	108.5686833
N	53.3505181	70.4124514	107.2549947
H	53.9532685	70.1591457	106.4513291
C	52.5836070	71.5409814	107.4071730
H	52.4253118	72.2471577	106.6024495
C	49.8424221	64.9287929	104.8361709
H	50.3555742	64.5922063	103.9290109
H	49.1532209	65.7347749	104.5633179
S	51.1366011	65.4881339	106.0336615
C	56.5714250	62.5387895	101.3822784
H	56.7658952	63.3715772	102.0732801
H	57.5321184	62.2638990	100.9334133
N	55.6583974	62.9241838	100.3091541
H	54.6467878	62.8561836	100.5043452
C	56.0558073	63.5767004	99.2171983
N	57.3500367	63.8872506	99.0659561
H	57.8715057	64.1624566	99.8968215
H	57.6827813	64.3178805	98.2045735
N	55.1898935	63.8683569	98.2433782
H	54.2784785	63.3912034	98.1682283

H	55.4942361	64.4306225	97.4641592
C	63.1575095	67.3728212	107.9891072
H	64.1660948	67.4645185	108.4211749
H	63.0733334	66.3951501	107.5077677
C	63.0078047	68.5143778	106.9543679
O	62.9780861	69.6928618	107.3738208
O	62.9631725	68.1932661	105.7183139
C	58.9280654	69.1936642	111.5879871
H	58.1871541	69.7287235	112.1909351
H	59.8439288	69.7955340	111.5666372
C	58.5031674	68.9452378	110.1544650
C	57.3220605	68.2459136	109.8367021
H	56.6328128	67.9448995	110.6246870
C	57.0381085	67.9044930	108.5134570
H	56.1297511	67.3680780	108.2431606
C	57.9212784	68.2668217	107.4903815
H	57.6943518	67.9898382	106.4669119
C	59.3586381	69.3399101	109.1122489
H	60.2555219	69.9190710	109.3332362
C	59.0751831	68.9939343	107.7856441
H	59.7476724	69.2885104	106.9846055
C	61.1887727	66.2713725	99.5357764
H	62.0148499	66.6334207	98.9238793
H	60.4031394	67.0320238	99.5056584
N	61.0893996	66.8862757	101.9822700
C	61.6866154	66.1835424	100.9436806
C	61.9060296	66.7996008	103.0337314
H	61.7516717	67.2500472	104.0080367
N	62.9926415	66.0577731	102.7192490
H	63.8204774	65.9059858	103.3160907
C	62.8731927	65.6606934	101.4054099
H	63.6135566	65.0531907	100.9095688
Mo	59.1385785	68.0148202	101.9508466
Fe	52.9369354	66.1379542	104.8488763
Fe	54.9033120	67.9210577	104.9166123
Fe	54.2861991	66.7426631	102.6312151
Fe	55.5649061	65.3962088	104.5014112
Fe	57.8462853	66.1450505	103.5339861
Fe	57.1407175	68.6943384	103.8479680
Fe	56.5837339	67.5389470	101.6490122
S	54.5968720	66.2969395	106.4616174
S	52.9023916	68.1686296	103.8310362
S	53.7103257	64.6400730	103.2560785
S	59.2031807	67.8185363	104.3080475
S	57.4084336	69.7046169	101.8195145
S	58.1814629	66.0280240	101.2757351
S	55.9599727	69.8241928	105.4197603
S	57.4289506	64.1264101	104.5058083
S	54.7527946	67.0553558	100.4374246
C	56.0706579	67.0504889	103.5347105
O	60.5956418	69.6518555	102.1644396
O	59.5800299	68.9090474	99.9354165
O	60.2047596	70.7517441	98.7961206
O	60.5957611	71.6122382	103.8235559
O	61.0367327	73.6305666	102.9618798
O	64.6982144	68.3084895	99.2456317
O	64.8989161	69.1838574	101.2913938
C	60.8056466	70.5888060	101.1050548
C	60.1186107	70.0526979	99.8393230
C	60.1490070	71.9205246	101.5134396
C	60.6311515	72.4370379	102.8643732
C	62.3196397	70.6466913	100.8156796
C	62.7604540	69.3110252	100.2097679
C	64.2284759	68.9279356	100.2402399
H	60.4889681	70.1799212	103.0070261
H	62.2583093	68.5184126	100.7782176
H	62.4115374	69.2405157	99.1759045
H	62.5172922	71.4608752	100.1112117
H	62.8481435	70.8467199	101.7504623
H	59.0791104	71.6740716	101.6288366

H	60.2929066	72.6678238	100.7285584
O	63.9786640	69.5655151	96.8510130
H	63.0023266	69.5655559	96.8201618
H	64.2175654	69.0489753	97.6526426
O	67.2961677	68.6785448	102.3565329
H	67.4222309	67.8091972	102.7904622
H	66.4196587	68.6560819	101.9135796
O	61.8139717	73.0841868	98.4086349
H	61.2463610	72.2972754	98.5802479
H	62.1431385	73.3506311	99.2964706
O	65.0891795	68.4547045	104.1207371
H	64.3150336	68.3586717	104.7229516
H	64.7091244	68.7136890	103.2649013
O	63.2572082	74.3460250	104.3983099
H	63.6206736	73.6167605	104.9454470
H	62.3948226	74.0210284	104.0639488
O	59.8361682	75.6036352	101.4970838
H	58.9606979	75.1808616	101.4103703
H	60.3106692	74.9543472	102.0646912
O	57.6683973	73.8897076	100.9618270
H	58.0746303	73.0215627	100.8242660
H	56.9644321	73.7072194	101.6060445
O	64.9646576	71.5639573	102.5608054
H	65.0159150	70.7059107	102.0736577
H	64.2837360	71.3302912	103.2322743
O	63.0143124	70.4613024	104.2433593
H	62.1175100	70.8335601	104.1573531
H	62.9214009	69.6334781	104.7956051
h	60.7855630	65.3442673	99.1283885
h	49.2518729	64.0847215	105.1923481
h	51.0290464	73.3470732	109.2123920
h	56.6976517	71.3954397	97.8061732
h	56.1618786	61.7192057	101.9727201
h	58.4497360	72.9166204	107.9369053
h	62.4496152	67.4590785	108.8134327
h	53.6021294	73.4957690	102.4376663
h	59.2394507	68.2786036	112.0917434

154QM – [MoFe7S9C]* – (163 atoms total with link atoms, marked with lowercase h)

C	53.6663819	72.8085222	103.3653581
H	53.6585423	73.4435441	104.2499079
C	52.5935735	71.7162465	103.5203092
H	52.8415356	71.0989551	104.3905369
H	51.5771533	72.0925630	103.6797710
H	52.5739376	71.0521807	102.6521829
C	55.0462337	72.1510863	103.2483523
H	55.8755939	72.8622102	103.2868556
H	55.2000146	71.4542342	104.0756885
H	55.1369800	71.5555649	102.3309500
C	56.3831535	71.5105941	98.7948369
H	57.2775753	71.4039930	99.4178306
H	55.9824403	72.5193176	98.9377070
N	55.3883303	70.5554507	99.2650651
H	55.7191689	69.6912398	99.6855182
C	54.1156264	70.8814466	99.5004399
N	53.5585185	71.9474935	98.9142721
H	53.9609774	72.4087761	98.0986493
H	52.6168447	72.1976754	99.2109926
N	53.3853113	70.1668194	100.3613994
H	53.7545048	69.3180552	100.7834101
H	52.3979031	70.4150342	100.4699950
C	59.3029806	73.3297117	107.3185465
H	59.0775572	73.2549993	106.2477819
H	59.5353084	74.3718454	107.5545402
C	60.5019396	72.4600743	107.6674441
O	60.8881847	72.3059094	108.8427113
N	61.1241621	71.8814634	106.6260490
H	60.7472807	71.9755606	105.6871901
H	61.8480407	71.1607848	106.8006095
C	51.0614625	72.2867957	109.3982887

H	51.2124926	72.1003447	110.4672939
H	50.0991348	71.8342788	109.1123863
N	52.7101770	70.4543231	109.2878473
C	52.1646541	71.5788191	108.6925680
C	53.5485660	69.9559364	108.3997888
H	54.2085410	69.1088826	108.5399078
N	53.5735271	70.7057684	107.2643662
H	54.2455082	70.5864450	106.5125078
C	52.7017745	71.7589270	107.4361928
H	52.5461354	72.5203556	106.6832201
C	49.9402761	64.9594952	104.7775417
H	50.3799778	64.5853964	103.8491817
H	49.2903955	65.8078224	104.5528484
S	51.2946218	65.4614720	105.9238657
C	56.6029243	62.3999278	101.3240254
H	56.7053027	63.2323410	102.0297641
H	57.5980253	62.1601395	100.9522563
N	55.7226578	62.7697689	100.2214579
H	54.7113582	62.6429081	100.3848985
C	56.1052528	63.3990931	99.1098944
N	57.3971881	63.6506092	98.8694088
H	58.1357818	63.2264338	99.4216112
H	57.6970887	64.0795798	97.9967760
N	55.1748780	63.8297979	98.2345023
H	54.2881370	63.2965707	98.2320839
H	55.4943668	64.0483346	97.2976367
C	63.0139910	67.4107311	107.9052413
H	64.0467543	67.5234300	108.2628564
H	62.9240045	66.4356630	107.4200047
C	62.7541443	68.5566300	106.9028933
O	62.7116802	69.7297575	107.3274294
O	62.6282862	68.2513589	105.6564207
C	58.9744443	69.1159624	111.6645695
H	58.1928616	69.6132072	112.2444024
H	59.8739296	69.7360420	111.7285231
C	58.6358906	68.9337632	110.1990249
C	57.5604321	68.1292265	109.7646493
H	56.8734988	67.6821806	110.4789879
C	57.3850839	67.8636554	108.4051386
H	56.5581144	67.2410289	108.0736897
C	58.2717120	68.3977412	107.4658901
H	58.1457255	68.1651836	106.4166888
C	59.4802527	69.5113520	109.2347473
H	60.2976130	70.1662050	109.5320588
C	59.3100088	69.2358645	107.8740529
H	59.9988473	69.6613913	107.1507388
C	61.1930467	66.3221559	99.4715205
H	62.0395685	66.6480228	98.8704293
H	60.4335612	67.1033449	99.3889430
N	61.0605002	67.0261358	101.9036080
C	61.6549656	66.2787658	100.8885928
C	61.8947857	66.9795632	102.9570165
H	61.7889018	67.4732849	103.9197359
N	62.9619915	66.2187541	102.6607914
H	63.8093200	66.0872061	103.2526322
C	62.8382753	65.7727370	101.3694852
H	63.5854097	65.1631132	100.8868085
Mo	59.0666816	68.0879401	101.8981000
Fe	52.9795356	66.2230510	104.7060562
Fe	55.0669139	67.8893981	104.8881758
Fe	54.3017559	66.6811487	102.4537242
Fe	55.6240805	65.3741527	104.3213563
Fe	57.8574337	66.1242558	103.2951531
Fe	57.2075546	68.6346357	103.6912653
Fe	56.5272589	67.5507865	101.5122316
S	54.6884046	66.2028551	106.2738454
S	53.1156979	68.1989441	103.7315409
S	53.7557077	64.6577333	103.1729233
S	59.1632896	67.7264741	104.1832446
S	57.2780220	69.6513414	101.7330042

S	58.1438619	66.1157856	101.0627522
S	56.1975325	69.6433893	105.3339655
S	57.4411657	64.1916049	104.3186490
S	54.6847177	67.1622947	100.3877684
C	56.0519747	67.0243119	103.3793439
O	60.3486027	69.7165774	102.1964277
O	59.5363972	68.8471773	99.9612260
O	60.1850463	70.6358885	98.7719026
O	60.2721634	71.5776761	103.7373762
O	60.9166249	73.5852494	102.9994709
O	64.6627412	68.2606142	99.3364927
O	64.7170103	69.0500032	101.4318422
C	60.7161978	70.5862152	101.1040999
C	60.1000369	70.0139456	99.8316661
C	60.0961227	71.9675401	101.4015193
C	60.4579426	72.4441091	102.8046022
C	62.2587258	70.5810448	100.9925981
C	62.7730447	69.4838568	100.0626608
C	64.1687909	68.9056408	100.2979554
H	60.2302582	70.3806585	103.0292009
H	62.1164309	68.6105369	100.1456046
H	62.7375393	69.8177784	99.0215653
H	62.6055729	71.5568835	100.6450177
H	62.6352212	70.4311220	102.0091290
H	59.0033521	71.8840599	101.3776274
H	60.3960289	72.6960256	100.6472936
O	64.0142748	69.5529529	96.8876560
H	63.0474359	69.4726879	96.7904159
H	64.2553738	69.0056498	97.6642703
O	67.2523002	68.6028579	102.4161329
H	67.4976274	67.7325346	102.8070450
H	66.3731079	68.4946248	102.0071704
O	61.9471896	73.0399208	98.4642820
H	61.3902969	72.2564400	98.6184801
H	62.2810600	73.3021167	99.3511400
O	64.9687750	68.5664659	104.2551696
H	64.1541881	68.4359802	104.7832859
H	64.6620138	68.7745550	103.3572336
O	63.2365259	74.2931329	104.4017963
H	63.6441124	73.5865625	104.9492728
H	62.3574191	73.9592601	104.1555132
O	59.8398661	75.6209038	101.4727166
H	58.9499452	75.2290731	101.4596992
H	60.3121215	74.9849540	102.0471857
O	57.7107113	73.9351268	101.9886910
H	56.9191095	73.5342978	101.6063127
H	57.3826254	74.3727933	102.8041878
O	64.8832923	71.5346649	102.5169974
H	64.9193951	70.6307059	102.1241629
H	64.1854311	71.4158981	103.1903261
O	62.7907136	70.5144487	104.2495787
H	61.9110288	70.9213031	104.2168350
H	62.6815484	69.6773036	104.7927357
h	60.7906692	65.3882413	99.0791391
h	49.3334549	64.1497277	105.1826487
h	51.0156662	73.3578302	109.2011720
h	56.6724825	71.3838091	97.7516296
h	56.2289448	61.5238385	101.8538122
h	58.4166099	73.0544078	107.8900549
h	62.3665980	67.4715977	108.7800240
h	53.5560374	73.4780379	102.5123399
h	59.2710942	68.1789710	112.1358582

198QM – [MoFe7S9C] – (212 atoms total with link atoms, marked with lowercase h)

C	53.8794629	72.9237593	103.1898968
H	53.8553184	73.5586080	104.0772277
C	52.9323495	71.7347146	103.3908471
H	53.3135414	71.1093572	104.2036438
H	51.9041869	72.0229731	103.6436693
H	52.8973774	71.0929404	102.5071284

C	55.3230946	72.4309121	102.9773823
H	56.0627682	73.2363359	103.0880855
H	55.5809146	71.6744567	103.7256171
H	55.4505994	71.9403545	102.0032663
C	56.4692322	71.3930223	98.7796799
H	57.3680308	71.2127808	99.3806747
H	56.1049115	72.4047205	98.9910390
N	55.4673480	70.4297391	99.2054042
H	55.7939150	69.5834359	99.6747422
C	54.1970654	70.7649054	99.4509802
N	53.6580660	71.8627816	98.8948902
H	54.0923437	72.3798518	98.1364495
H	52.7182544	72.1087484	99.2076234
N	53.4514369	70.0285905	100.2689022
H	53.7998785	69.1362799	100.6392373
H	52.4777996	70.3079282	100.4055470
C	59.2779526	73.1927274	107.4129972
H	59.0607556	73.0998322	106.3423506
H	59.5187514	74.2392230	107.6296311
C	60.4765678	72.3281337	107.7809309
O	60.8619638	72.1973070	108.9616396
N	61.0995266	71.7383951	106.7488661
H	60.7573287	71.8513578	105.7977595
H	61.8646424	71.0630184	106.9091778
C	51.0354850	72.2518934	109.3928368
H	51.2793831	72.1137406	110.4517223
H	50.0564929	71.7745179	109.2213626
N	52.6033863	70.3653168	109.2154991
C	52.0685965	71.4949416	108.6214566
C	53.3306629	69.7833942	108.2768126
H	53.9282743	68.8863531	108.3817984
N	53.2951130	70.4847632	107.1160840
H	53.8705324	70.2723845	106.2973134
C	52.5052646	71.5926126	107.3155781
H	52.3351929	72.3278640	106.5405639
C	51.0290059	68.6361017	98.6519751
H	51.8942167	67.9680334	98.7122063
H	51.3621997	69.6094339	98.2751321
C	50.3433384	68.7826112	100.0004154
C	49.3262026	69.7435109	100.1810344
H	49.0406655	70.3719439	99.3331745
C	48.7860498	70.0173437	101.4373796
H	48.0615707	70.8164263	101.5788518
C	49.2099704	69.2695312	102.5504218
O	48.7490099	69.6148371	103.7608812
H	49.0861496	68.9953073	104.4622429
C	50.6764642	67.9836547	101.1002325
H	51.4272551	67.2030364	100.9999586
C	50.0920418	68.1979526	102.3498506
H	50.3862565	67.5861621	103.1962934
C	47.7458913	62.0044377	104.6756280
O	48.0331359	61.3793032	105.7101087
N	48.1806891	63.2545919	104.4432323
H	47.9783279	63.7320320	103.5651894
C	49.1153817	63.8989959	105.3830541
H	49.8596300	63.1397616	105.6541473
C	49.8612330	65.0649370	104.7574627
H	50.3530976	64.7603960	103.8288488
H	49.1707602	65.8890584	104.5480163
S	51.1286201	65.6038026	105.9691992
C	48.3891674	64.3403311	106.6950794
O	48.0389956	65.4993677	106.8375135
C	50.1000135	69.1372794	106.7287510
H	49.7854955	70.1455477	106.4382358
H	51.1947973	69.1023714	106.6819264
O	49.5282259	68.2173031	105.8179231
H	50.0650117	67.3838093	105.8538378
C	56.5839162	62.4823089	101.3322760
H	56.7913533	63.3187272	102.0107312
H	57.5256648	62.1595384	100.8856879

N	55.6535475	62.8745222	100.2798158
H	54.6495857	62.7250063	100.4660065
C	56.0133255	63.4812265	99.1517104
N	57.2988026	63.7527569	98.9158677
H	57.9925072	63.6115732	99.6368760
H	57.6367007	64.1509069	98.0402168
N	55.0796060	63.8238133	98.2437503
H	54.2330029	63.2328268	98.2066208
H	55.4041334	64.1368308	97.3385834
C	63.0924067	67.3584070	107.7916053
H	64.1061213	67.4466147	108.2071962
H	62.9979167	66.3872568	107.2995518
C	62.9129038	68.5180708	106.7912932
O	62.9232919	69.6887041	107.2178938
O	62.7913384	68.2160832	105.5433644
C	58.9357908	69.1305101	111.5395455
H	58.1943021	69.6509364	112.1522981
H	59.8478397	69.7351740	111.5202833
C	58.4999153	68.9022839	110.1074941
C	57.3187130	68.2052693	109.7900015
H	56.6373295	67.8894166	110.5771501
C	57.0294640	67.8791057	108.4643298
H	56.1196682	67.3439573	108.2071968
C	57.9024738	68.2553422	107.4390835
H	57.6655261	67.9880590	106.4161844
C	59.3380567	69.3252835	109.0621686
H	60.2277727	69.9141630	109.2829771
C	59.0477240	68.9966058	107.7327718
H	59.7144362	69.3190639	106.9372634
C	69.0295376	71.7502962	103.6376778
H	69.9195461	72.1076482	104.1706080
H	68.4503110	72.6405985	103.3578775
C	68.2298330	70.9111949	104.6329529
H	68.8218373	70.0695559	105.0091562
H	67.9440348	71.5331125	105.4858337
N	66.9889192	70.3256176	104.0531086
H	67.2041079	69.5948647	103.3002568
H	66.4093628	69.8118443	104.7319740
H	66.3448476	71.0149427	103.6037423
C	69.8776556	64.8163080	103.9499709
H	69.2201793	64.0480581	104.3728261
H	70.7680952	64.9091105	104.5852639
C	69.1048346	66.1599496	103.9568169
O	68.0001728	66.1800106	103.3268212
O	69.6457380	67.1210493	104.5496729
C	61.0717071	66.3022804	99.4016610
H	61.8652410	66.7054180	98.7742917
H	60.2540070	67.0232207	99.3710723
N	61.0186877	66.9179987	101.8644500
C	61.5956183	66.2288528	100.8008645
C	61.8650817	66.8211798	102.8964874
H	61.7592815	67.2699470	103.8800817
N	62.9415061	66.0887524	102.5432568
H	63.7820070	65.9150475	103.1225617
C	62.7961576	65.7099191	101.2295725
H	63.5428930	65.1361292	100.7016895
Mo	59.0414114	68.0519563	101.9237423
Fe	52.9080359	66.2502240	104.6984421
Fe	54.9066015	68.0032726	104.7762282
Fe	54.2171088	66.8357752	102.4926336
Fe	55.4191516	65.4664703	104.3729345
Fe	57.7333763	66.1424813	103.3784924
Fe	57.1654728	68.6934867	103.7046042
Fe	56.5124606	67.5315942	101.5120981
S	54.5755568	66.3856130	106.2982960
S	52.9098308	68.2668540	103.7362262
S	53.6374179	64.7615137	103.1061377
S	59.1256259	67.7432733	104.2168008
S	57.3157885	69.6572705	101.6975905
S	58.1240800	66.0649878	101.1396644

S	56.0324893	69.8313779	105.2188488
S	57.2618643	64.2067386	104.4042107
S	54.6949635	67.1264605	100.3418781
C	55.9992122	67.0935459	103.3897924
O	60.4568493	69.6675353	102.1990473
O	59.5688579	68.8741030	99.9497608
O	60.2047917	70.7028049	98.8094308
O	60.5111718	71.5966429	103.7973184
O	61.0559481	73.6049195	102.9677965
O	64.6718951	68.2608374	99.2525110
O	64.8373070	69.0892829	101.3246608
C	60.7662342	70.5703337	101.1246966
C	60.1170409	70.0290359	99.8526518
C	60.1580890	71.9411101	101.4752119
C	60.6141817	72.4377826	102.8466641
C	62.2980997	70.5769284	100.9249503
C	62.7494254	69.3374964	100.1510017
C	64.2000939	68.8837875	100.2398686
H	60.3893927	70.2514787	103.0325604
H	62.1812014	68.4813892	100.5313955
H	62.5021852	69.4457739	99.0918232
H	62.5943372	71.4832809	100.3905825
H	62.7383388	70.5919361	101.9244023
H	59.0707443	71.7952183	101.5384600
H	60.3821799	72.6734794	100.6969306
O	63.9603743	69.6675270	96.8936718
H	62.9961483	69.5466809	96.8017020
H	64.2309385	69.1047577	97.6502912
O	67.3179843	68.4514521	102.1552016
H	67.4614446	67.6003322	102.6705095
H	66.4066568	68.4806774	101.7828981
O	61.9418718	73.0334545	98.4584842
H	61.3843017	72.2452870	98.6194148
H	62.2580536	73.3103035	99.3464622
O	65.0045187	68.3391379	104.0802436
H	64.2007150	68.2677273	104.6512781
H	64.6812817	68.6328195	103.2096914
O	63.2687245	74.3615523	104.5222819
H	63.6354119	73.6102609	105.0441420
H	62.3982947	74.0616296	104.2012464
O	59.8972489	75.2946720	101.1573306
H	58.9965966	74.9213254	101.1492414
H	60.3618734	74.7489386	101.8299616
O	57.5353931	73.8875283	100.7441190
H	57.7775705	72.9758990	100.5336881
H	56.8590083	73.7982326	101.4347327
O	64.9235096	71.4666330	102.6035282
H	64.9251595	70.6354466	102.0642035
H	64.2141301	71.2623699	103.2628944
O	62.9561494	70.4898014	104.2042418
H	62.0789260	70.9128833	104.1859417
H	62.8419713	69.6343220	104.7219537
h	60.7082751	65.3535206	99.0068962
h	47.0294966	61.5892676	103.9667701
h	48.2859884	63.5457383	107.4340269
h	69.3580883	71.2511460	102.7261019
h	70.1776145	64.4828859	102.9565317
h	49.8306665	68.9393918	107.7662286
h	50.3028156	68.2054861	97.9625660
h	50.9608802	73.3173699	109.1754410
h	56.7593581	71.3249786	97.7312219
h	56.1808315	61.6532526	101.9138733
h	58.3814972	72.9286286	107.9739666
h	62.3976653	67.4396284	108.6275506
h	53.6428194	73.5698734	102.3445544
h	59.2572530	68.2101105	112.0269813

247QM – [MoFe7S9C] – BS7-235 (267 atoms total with link atoms, marked with lowercase h)

C	53.9039525	72.8935945	103.1863625
H	53.8791750	73.5220897	104.0778966

C	52.9613981	71.6994624	103.3828616
H	53.3445666	71.0722334	104.1937912
H	51.9329234	71.9854790	103.6370183
H	52.9274743	71.0615774	102.4961298M
C	55.3505611	72.4102237	102.9687273
H	56.0851989	73.2196012	103.0843224
H	55.6132049	71.6493594	103.7108439
H	55.4799336	71.9271910	101.9909423
C	56.4867658	71.3718170	98.7790241
H	57.3882861	71.1873192	99.3743949
H	56.1240439	72.3824774	98.9979913
N	55.4854368	70.4070266	99.2029216
H	55.8125637	69.5602261	99.6701671
C	54.2144594	70.7410818	99.4472804
N	53.6771203	71.8420928	98.8962710
H	54.1097313	72.3611145	98.1380833
H	52.7352730	72.0842444	99.2069247
N	53.4670242	70.0008391	100.2604083
H	53.8121936	69.1052465	100.6252941
H	52.4930752	70.2796511	100.3955452
C	59.2956191	73.1554969	107.4351614
H	59.0855925	73.0756309	106.3619481
H	59.5565907	74.1958170	107.6602619
C	60.4714342	72.2598273	107.8060535
O	60.8519150	72.1196411	108.9872641
N	61.0768667	71.6506259	106.7751908
H	60.7451904	71.7818733	105.8228900
H	61.8493320	70.9815509	106.9310214
C	51.0562872	72.2375757	109.4043907
H	51.2935975	72.1059537	110.4654975
H	50.0790264	71.7573282	109.2311230
N	52.6236841	70.3463199	109.2495386
C	52.0944036	71.4746541	108.6437457
C	53.3516324	69.7533474	108.3191879
H	53.9342560	68.8491416	108.4340037
N	53.3118130	70.4358205	107.1490760
H	53.8913057	70.2192968	106.3361187
C	52.5309721	71.5531771	107.3371059
H	52.3606345	72.2778441	106.5519352
C	51.0267221	68.6281587	98.6481070
H	51.8915416	67.9592770	98.7060324
H	51.3600293	69.6021619	98.2730928
C	50.3430312	68.7714785	99.9976373
C	49.3304747	69.7359126	100.1855077
H	49.0445038	70.3691155	99.3414287
C	48.7949112	70.0060487	101.4447158
H	48.0740649	70.8074144	101.5913401
C	49.2182050	69.2499771	102.5524026
O	48.7636557	69.5891949	103.7673018
H	49.1004978	68.9611764	104.4604627
C	50.6739651	67.9641721	101.0918539
H	51.4194432	67.1795300	100.9848523
C	50.0929093	68.1741607	102.3435146
H	50.3828899	67.5543365	103.1854463
C	47.7394275	61.9888241	104.6785649
O	48.0246150	61.3644110	105.7137068
N	48.1759210	63.2381672	104.4466007
H	47.9765469	63.7150614	103.5676950
C	49.1099168	63.8758837	105.3895490
H	49.8423972	63.1085062	105.6670519
C	49.8737478	65.0301504	104.7656838
H	50.3552722	64.7214416	103.8332200
H	49.1999170	65.8699671	104.5649157
S	51.1556066	65.5349234	105.9781954
C	48.3870738	64.3278985	106.6996780
O	48.0525969	65.4920581	106.8393228
C	50.1248542	69.1012972	106.7178350
H	49.8071781	70.1055724	106.4174063
H	51.2197438	69.0713563	106.6740714
O	49.5593834	68.1722993	105.8113023

H	50.0966970	67.3415271	105.8536417
C	64.1346711	61.7808919	105.6434196
O	64.6031527	62.2653850	104.6148419
N	62.8756559	61.9969480	106.0650934
H	62.6178419	61.7139508	107.0107749
C	61.9892447	62.8895367	105.3190951
H	62.6605969	63.5476467	104.7475800
C	61.3017659	63.7809656	106.3735803
O	61.8953609	64.0151911	107.4243874
N	60.0857547	64.3163637	106.1052981
H	59.5925645	64.1061337	105.2390629
C	59.5637971	65.4115859	106.9016656
H	60.4098340	65.9083348	107.3697058
H	59.0704724	66.1085387	106.2186003
C	58.5819234	65.0533150	108.0203210
O	58.8675233	65.2279501	109.2035574
N	57.3774288	64.5809634	107.5857240
H	57.1936849	64.6695882	106.5807405
C	56.2707395	64.4101297	108.4988619
H	56.6939266	64.2733644	109.4954169
H	55.6585978	65.3200008	108.5552923
C	55.2712980	63.2912452	108.2349651
O	54.5139436	62.9278586	109.1474070
N	55.1976818	62.7419417	107.0056719
H	55.7367751	63.1616262	106.2487004
C	54.2562116	61.6523937	106.7195387
H	53.8464661	61.3357218	107.6797348
C	55.0338501	60.4723203	106.1373586
O	55.0924766	59.3524553	106.6581674
N	55.6787978	60.7604922	104.9840104
H	55.6283059	61.7026826	104.6050662
C	56.4458994	59.7871746	104.2350194
H	55.7611005	59.0524851	103.7817111
C	57.1447013	60.5328546	103.0885417
H	57.7228483	61.3688091	103.5078925
H	57.8436848	59.8509143	102.6017258
C	56.1252858	61.0563890	102.0539650
H	55.9688045	60.2889223	101.2868353
H	55.1450326	61.2361532	102.5171166
C	56.5789444	62.3606558	101.3968522
H	56.5950132	63.1663663	102.1413659
H	57.6011463	62.2496575	101.0267524
N	55.6992581	62.7211666	100.2914375
H	54.6864167	62.6009905	100.4677419
C	56.0760064	63.3567948	99.1802992
N	57.3620891	63.6201847	98.9405063
H	58.0789972	63.4124357	99.6219650
H	57.6843727	64.0542914	98.0758053
N	55.1477572	63.7431596	98.2860408
H	54.2777014	63.1850034	98.2485507
H	55.4760587	64.0501318	97.3796715
C	57.3895947	58.8720941	105.0506648
O	57.4591096	57.7248899	104.6236304
C	63.1179694	67.3542501	107.8230464
H	64.1313615	67.4507477	108.2371442
H	63.0178234	66.3660687	107.3672194
C	62.9387715	68.4891104	106.7968456
O	62.9791453	69.6699011	107.1946390
O	62.7824910	68.1634540	105.5584985
C	58.8528281	69.1376235	111.4392840
H	58.1225782	69.6780648	112.0480818
H	59.7518796	69.7560451	111.3584762
C	58.3738763	68.8361139	110.0352513
C	57.1755251	68.1427654	109.7878952
H	56.5144639	67.8772057	110.6098618
C	56.8395273	67.7630300	108.4893259
H	55.9062726	67.2448145	108.2891535
C	57.6882607	68.0581495	107.4228041
H	57.4165590	67.7374729	106.4229780
C	59.1820859	69.1998482	108.9432619

H	60.0835411	69.7886482	109.1121198
C	58.8478189	68.8054599	107.6436448
H	59.4904965	69.0838042	106.8117370
C	67.5183416	66.0606346	99.8317082
O	68.5841681	65.4430944	99.8665822
N	67.3566471	67.2705125	99.2465192
H	66.4078696	67.6772521	99.2851101
C	68.3328643	67.9584063	98.4076385
H	68.6852739	67.2656210	97.6338396
C	69.0372299	71.7430701	103.6436141
H	69.9249025	72.1063412	104.1763673
H	68.4520272	72.6300312	103.3645616
C	68.2438408	70.8986506	104.6390180
H	68.8400924	70.0592192	105.0131610
H	67.9557670	71.5182477	105.4927898
N	67.0051922	70.3064261	104.0601134
H	67.2225941	69.5688045	103.3103229
H	66.4264808	69.7963108	104.7423651
H	66.3612845	70.9924186	103.6099401
C	69.8804456	64.8016355	103.9443982
H	69.2176747	64.0315430	104.3559099
H	70.7668265	64.8880274	104.5863961
C	69.1086115	66.1428395	103.9600946
O	67.9931810	66.1616622	103.3472531
O	69.6506969	67.1055775	104.5494013
C	61.0889786	66.2763529	99.4147142
H	61.8841692	66.6820978	98.7922603
H	60.2719612	66.9978494	99.3860481
N	61.0199223	66.8670462	101.8820184
C	61.6044853	66.1873741	100.8160162
C	61.8560950	66.7537596	102.9216634
H	61.7468730	67.1948777	103.9082929
N	62.9314141	66.0192182	102.5702796
H	63.7718394	65.8413374	103.1536171
C	62.7978983	65.6565651	101.2506339
H	63.5465198	65.0820095	100.7260366
Mo	59.0408096	67.9966411	101.9252302
Fe	52.9318655	66.1468589	104.6907937
Fe	54.9071983	67.9146842	104.7482685
Fe	54.2145501	66.7456136	102.4682165
Fe	55.4417173	65.3781508	104.3295827
Fe	57.7311013	66.0696214	103.3144705
Fe	57.1640863	68.6077967	103.6916194
Fe	56.5065130	67.4817540	101.4856945
S	54.6176538	66.2852739	106.2621295
S	52.9063881	68.1625527	103.7253997
S	53.6513675	64.6611795	103.0880640
S	59.1029828	67.6280980	104.2205295
S	57.3144054	69.6014861	101.7053139
S	58.1247886	66.0290921	101.0841819
S	56.0104046	69.7595974	105.1618548
S	57.3147478	64.1467570	104.3573867
S	54.6822530	67.0854078	100.3233458
C	55.9982713	67.0130633	103.3534651
O	60.4428414	69.6219240	102.2130606
O	59.5648409	68.8330854	99.9552675
O	60.1881933	70.6729318	98.8268971
O	60.4995056	71.5493388	103.8141991
O	61.0447695	73.5600192	102.9875918
O	64.6367121	68.2200908	99.2445157
O	64.8244746	69.0478944	101.3162254
C	60.7510517	70.5291356	101.1408903
C	60.1040265	69.9926708	99.8661095
C	60.1442755	71.8994950	101.4940965
C	60.6020278	72.3935045	102.8659701
C	62.2827002	70.5354925	100.9375205
C	62.7263328	69.2941161	100.1624687
C	64.1761325	68.8448390	100.2465930
H	60.3762740	70.2051249	103.0480524
H	62.1619851	68.4394029	100.5513983

H	62.4708929	69.3976642	99.1047476
H	62.5794379	71.4406342	100.4013208
H	62.7270384	70.5490726	101.9352565
H	59.0564879	71.7557742	101.5560745
H	60.3709555	72.6322988	100.7168693
O	63.9481750	69.6529880	96.8914545
H	62.9813628	69.5519418	96.7949456
H	64.2019081	69.0819583	97.6463024
O	67.3281406	68.4134052	102.1920700
H	67.4932894	67.5594016	102.7067110
H	66.4181303	68.4126048	101.8289547
O	61.9383148	72.9991515	98.4745674
H	61.3761737	72.2147796	98.6362164
H	62.2526608	73.2766417	99.3632797
O	65.0054396	68.3263883	104.0984415
H	64.2040658	68.2315571	104.6688150
H	64.6697665	68.6163619	103.2328137
O	63.2611722	74.3388837	104.5292850
H	63.6314583	73.5852177	105.0457433
H	62.3906208	74.0363117	104.2113028
O	59.9097899	75.2673609	101.1712033
H	59.0056181	74.9030527	101.1572907
H	60.3650577	74.7172665	101.8462549
O	57.5467987	73.8759061	100.7309941
H	57.8022778	72.9688153	100.5176470
H	56.8647281	73.7753882	101.4144161
O	64.9164370	71.4320136	102.6068579
H	64.9226314	70.6010541	102.0711433
H	64.2128917	71.2242309	103.2710988
O	55.9282388	70.6820977	108.2895815
H	56.1450024	70.4455578	107.3698356
H	56.3982861	70.0088732	108.7992657
O	62.9475875	70.4373528	104.2019452
H	62.0724142	70.8645460	104.1967523
H	62.8372451	69.5859729	104.7264155
h	60.7264563	65.3293662	99.0148881
h	47.0246478	61.5751948	103.9671804
h	48.2747865	63.5359189	107.4401015
h	69.3688696	71.2444811	102.7328500
h	70.1859124	64.4755120	102.9502148
h	49.8524250	68.9102196	107.7557843
h	50.3001267	68.1993180	97.9580185
h	50.9779087	73.3017380	109.1819438
h	56.7714870	71.3105425	97.7286687
h	58.3889112	72.9057377	107.9861318
h	62.4248820	67.4654335	108.6569141
h	53.6628296	73.5445865	102.3460433
h	59.1975961	68.2465188	111.9638166
h	64.7134284	61.0658902	106.2281243
h	61.3788051	62.3790874	104.5741977
h	53.4320562	61.9683818	106.0800182
h	57.9905828	59.1349474	105.9211754
h	67.8355633	68.8026574	97.9301461
h	69.2469868	68.2439485	98.9281314
h	66.5862442	65.6989940	100.2658484

247QM – [MoFe7S9C] – BS7-247 (267 atoms total with link atoms, marked with lowercase h)

C	53.9096834	72.8906523	103.1969564
H	53.8889960	73.5227905	104.0857777
C	52.9590504	71.7039570	103.3972664
H	53.3384744	71.0748176	104.2082091
H	51.9329569	71.9966768	103.6530865
H	52.9186090	71.0642893	102.5120565
C	55.3526143	72.3942373	102.9840499
H	56.0934742	73.1992359	103.0907150
H	55.6098190	71.6375146	103.7330681
H	55.4772785	71.9020578	102.0100651
C	56.4790538	71.3602620	98.7631735
H	57.3760694	71.1740764	99.3649252
H	56.1138806	72.3692530	98.9835421

N	55.4715613	70.3948122	99.1717826
H	55.7945225	69.5306073	99.6053111
C	54.2067011	70.7352967	99.4408805
N	53.6724808	71.8476364	98.9109983
H	54.0898494	72.3561475	98.1365831
H	52.7337670	72.0902236	99.2313614
N	53.4657353	69.9921031	100.2567574
H	53.8134532	69.1010567	100.6278442
H	52.4940302	70.2728722	100.4051854
C	59.2959551	73.1490047	107.4351063
H	59.0855503	73.0676438	106.3620850
H	59.5564268	74.1898324	107.6587788
C	60.4725476	72.2543562	107.8069711
O	60.8532265	72.1162234	108.9883337
N	61.0783370	71.6444255	106.7768962
H	60.7451288	71.7729998	105.8249346
H	61.8504533	70.9749069	106.9334074
C	51.0560355	72.2406427	109.3991921
H	51.2875973	72.1061152	110.4612715
H	50.0798322	71.7606599	109.2193286
N	52.6215186	70.3483920	109.2468183
C	52.0995948	71.4810498	108.6427615
C	53.3590301	69.7606783	108.3207885
H	53.9405245	68.8559487	108.4363916
N	53.3328700	70.4512812	107.1549894
H	53.9198383	70.2379124	106.3471107
C	52.5503866	71.5679705	107.3415611
H	52.3880107	72.2975043	106.5591649
C	51.0338289	68.6201714	98.6557323
H	51.8953054	67.9471248	98.7153759
H	51.3725903	69.5920936	98.2799723
C	50.3498089	68.7706529	100.0045655
C	49.3281210	69.7276975	100.1822809
H	49.0366363	70.3490716	99.3314066
C	48.7905103	70.0071741	101.4380831
H	48.0606759	70.8019203	101.5758586
C	49.2245874	69.2725005	102.5564818
O	48.7622281	69.6232744	103.7639857
H	49.0979977	69.0055387	104.4683661
C	50.6952519	67.9863372	101.1110067
H	51.4500195	67.2091013	101.0123482
C	50.1182729	68.2090690	102.3626834
H	50.4235926	67.6083970	103.2136995
C	47.7243188	61.9793414	104.6701090
O	48.0154707	61.3593731	105.7058291
N	48.1489969	63.2316338	104.4341999
H	47.9432975	63.7023208	103.5536008
C	49.0818511	63.8823500	105.3677797
H	49.8302664	63.1275617	105.6381724
C	49.8184840	65.0462984	104.7306119
H	50.3016459	64.7427267	103.7980470
H	49.1291982	65.8739710	104.5321278
S	51.0945822	65.5807276	105.9258407
C	48.3684280	64.3266173	106.6865068
O	48.0259299	65.4877533	106.8312358
C	50.1230578	69.1287702	106.7313918
H	49.8177122	70.1414103	106.4464102
H	51.2179337	69.0868998	106.6894451
O	49.5471869	68.2204188	105.8112712
H	50.0753647	67.3809774	105.8381314
C	64.1389842	61.7787714	105.6444854
O	64.6078466	62.2611318	104.6148641
N	62.8807118	61.9967053	106.0661745
H	62.6231328	61.7170683	107.0129466
C	61.9959766	62.8904926	105.3197718
H	62.6684138	63.5482581	104.7492289
C	61.3075297	63.7812192	106.3744963
O	61.8978955	64.0110907	107.4284752
N	60.0947568	64.3186938	106.1018079
H	59.6061251	64.1162073	105.2306894

C	59.5666454	65.4115140	106.8968186
H	60.4089303	65.9174576	107.3618768
H	59.0664137	66.1001680	106.2101084
C	58.5900759	65.0479460	108.0194241
O	58.8769117	65.2300405	109.2016232
N	57.3887176	64.5631923	107.5901703
H	57.2067537	64.6349016	106.5826513
C	56.2852193	64.3894529	108.5071712
H	56.7106149	64.2480138	109.5020281
H	55.6741680	65.2996285	108.5714408
C	55.2838651	63.2715576	108.2455701
O	54.5627632	62.8755335	109.1743904
N	55.1670871	62.7587609	107.0036313
H	55.6597639	63.2161029	106.2358848
C	54.2350552	61.6591879	106.7266666
H	53.8324746	61.3421434	107.6895243
C	55.0204791	60.4831740	106.1440292
O	55.0775392	59.3603783	106.6588504
N	55.6719602	60.7783750	104.9962337
H	55.6274604	61.7241382	104.6252112
C	56.4380281	59.8077600	104.2427065
H	55.7523551	59.0764651	103.7850747
C	57.1376120	60.5588476	103.1001923
H	57.7134087	61.3948753	103.5226845
H	57.8383430	59.8802609	102.6111405
C	56.1180711	61.0846296	102.0674778
H	55.9581327	60.3174575	101.3006101
H	55.1395241	61.2683489	102.5325922
C	56.5755178	62.3870661	101.4099604
H	56.5949588	63.1935316	102.1538958
H	57.5969329	62.2722149	101.0387473
N	55.6958048	62.7488161	100.3045343
H	54.6825985	62.6319560	100.4813313
C	56.0752478	63.3633494	99.1833348
N	57.3630565	63.6142281	98.9378245
H	58.0779100	63.4220065	99.6259653
H	57.6861304	64.0397309	98.0694674
N	55.1490716	63.7420396	98.2829315
H	54.2774996	63.1861792	98.2508095
H	55.4801146	64.0322700	97.3720136
C	57.3801285	58.8866044	105.0530063
O	57.4462729	57.7404745	104.6217923
C	63.1281585	67.3540447	107.8303452
H	64.1398021	67.4537116	108.2481111
H	63.0317111	66.3648664	107.3758892
C	62.9498999	68.4862468	106.8011977
O	62.9828291	69.6682580	107.1967647
O	62.8020546	68.1574565	105.5629387
C	58.8510862	69.1374372	111.4364595
H	58.1205600	69.6790837	112.0439094
H	59.7488647	69.7571685	111.3517212
C	58.3717462	68.8278116	110.0344302
C	57.1751213	68.1301271	109.7914312
H	56.5138012	67.8691644	110.6147579
C	56.8416268	67.7394043	108.4954178
H	55.9086383	67.2188612	108.3008320
C	57.6925847	68.0239592	107.4281825
H	57.4287173	67.6887042	106.4310139
C	59.1798281	69.1854155	108.9400848
H	60.0796378	69.7776796	109.1056130
C	58.8493048	68.7775297	107.6440606
H	59.4918597	69.0484139	106.8095687
C	67.5171885	66.0612868	99.8310920
O	68.5830762	65.4438301	99.8659038
N	67.3554389	67.2708684	99.2453628
H	66.4069101	67.6778601	99.2837286
C	68.3320943	67.9584348	98.4066982
H	68.6842491	67.2654707	97.6329366
C	69.0404054	71.7434482	103.6433676
H	69.9281661	72.1050190	104.1771141

H	68.4565300	72.6314493	103.3648288
C	68.2452943	70.8987432	104.6371566
H	68.8405199	70.0584768	105.0110616
H	67.9567153	71.5175809	105.4912973
N	67.0070720	70.3079312	104.0560792
H	67.2247184	69.5717678	103.3052062
H	66.4276249	69.7951470	104.7359397
H	66.3630513	70.9945236	103.6073433
C	69.8800163	64.8031190	103.9441809
H	69.2171938	64.0333504	104.3562013
H	70.7663904	64.8896973	104.5861789
C	69.1084371	66.1445923	103.9591233
O	67.9935420	66.1638095	103.3453804
O	69.6504909	67.1071218	104.5488676
C	61.0881539	66.2846606	99.4164004
H	61.8829718	66.6903221	98.7933617
H	60.2706552	67.0059026	99.3882576
N	61.0161491	66.8754396	101.8829094
C	61.6027441	66.1959414	100.8177161
C	61.8505790	66.7614729	102.9242471
H	61.7361562	67.2018849	103.9104953
N	62.9259586	66.0269802	102.5743108
H	63.7653292	65.8480272	103.1586950
C	62.7950003	65.6644350	101.2542712
H	63.5444112	65.0891361	100.7315091
Mo	59.0348545	67.9961673	101.9222523
Fe	52.9771894	66.1402832	104.8009739
Fe	54.9158010	67.9195508	104.7493309
Fe	54.1906064	66.7378791	102.5044463
Fe	55.4714930	65.3768603	104.3294572
Fe	57.7553120	66.1259774	103.2853537
Fe	57.1650868	68.5977920	103.6853162
Fe	56.4361901	67.4649535	101.4553759
S	54.6230524	66.2550466	106.2903921
S	52.9497688	68.1931760	103.7638676
S	53.6806146	64.6262807	103.1976276
S	59.1308086	67.6632606	104.2159025
S	57.2691960	69.5628804	101.6939904
S	58.1034362	66.0418817	101.0604724
S	56.0707125	69.7265720	105.2120418
S	57.3497320	64.1968534	104.3605458
S	54.6156159	67.0261588	100.3265213
C	55.9807765	67.0278042	103.3289725
O	60.4302364	69.6222877	102.2054242
O	59.5440255	68.8481299	99.9402034
O	60.1858446	70.6874296	98.8214925
O	60.5041387	71.5470746	103.8110035
O	61.0419452	73.5601242	102.9847454
O	64.6312400	68.2225405	99.2414662
O	64.8202462	69.0500027	101.3130387
C	60.7433338	70.5303911	101.1354274
C	60.0961012	70.0011384	99.8572253
C	60.1380089	71.9006651	101.4923078
C	60.6011631	72.3926261	102.8644843
C	62.2757733	70.5367590	100.9371346
C	62.7212328	69.2975843	100.1596721
C	64.1714222	68.8475905	100.2438485
H	60.3783661	70.1980408	103.0457812
H	62.1570628	68.4418304	100.5463405
H	62.4666791	69.4034657	99.1019409
H	62.5740854	71.4434850	100.4043748
H	62.7178506	70.5475213	101.9360756
H	59.0498128	71.7617949	101.5573522
H	60.3643673	72.6344315	100.7157216
O	63.9480750	69.6553066	96.8899255
H	62.9811175	69.5554024	96.7936372
H	64.2008415	69.0841301	97.6451640
O	67.3277006	68.4144529	102.1876994
H	67.4928874	67.5613877	102.7040104
H	66.4168955	68.4134949	101.8269184

O	61.9379082	73.0061657	98.4729459
H	61.3756039	72.2216066	98.6338353
H	62.2527052	73.2825660	99.3618646
O	65.0141900	68.3289077	104.0960527
H	64.2165124	68.2314463	104.6719087
H	64.6715400	68.6185439	103.2331962
O	63.2594515	74.3367624	104.5293220
H	63.6291388	73.5820416	105.0447541
H	62.3888749	74.0348186	104.2109944
O	59.9091951	75.2721896	101.1721581
H	59.0034765	74.9127103	101.1584705
H	60.3627963	74.7196912	101.8466727
O	57.5460239	73.8787922	100.7143100
H	57.8194295	72.9787104	100.4950832
H	56.8618850	73.7631871	101.3930461
O	64.9128524	71.4312674	102.6059806
H	64.9192060	70.6004057	102.0700828
H	64.2114568	71.2214645	103.2718431
O	55.9361110	70.6644307	108.3320948
H	56.1652377	70.4258158	107.4158368
H	56.4090451	69.9988712	108.8494937
O	62.9483354	70.4260565	104.2000276
H	62.0730636	70.8526609	104.1982540
H	62.8424467	69.5760059	104.7286417
h	60.7264862	65.3368527	99.0177480
h	47.0106308	61.5636028	103.9588580
h	48.2693854	63.5336585	107.4277720
h	69.3721171	71.2453953	102.7323364
h	70.1855041	64.4763352	102.9502207
h	49.8476701	68.9272521	107.7665822
h	50.3065884	68.1944944	97.9643659
h	50.9777605	73.3052632	109.1789120
h	56.7710401	71.3023588	97.7146229
h	58.3897995	72.8994249	107.9870657
h	62.4316788	67.4648007	108.6614386
h	53.6720610	73.5405965	102.3548310
h	59.1977208	68.2485694	111.9635512
h	64.7175123	61.0641252	106.2298513
h	61.3855150	62.3808082	104.5743688
h	53.4069767	61.9657913	106.0876459
h	57.9835882	59.1458576	105.9228864
h	67.8350377	68.8027501	97.9290649
h	69.2464505	68.2436131	98.9269802
h	66.5852662	65.6998722	100.2657958

247QM – [MoFe7S9C] – BS7-346 (395 atoms total with link atoms, marked with lowercase h)

C	53.8992479	72.8853555	103.1884585
H	53.8736990	73.5146229	104.0795017
C	52.9560113	71.6917145	103.3843920
H	53.3349591	71.0666594	104.1989471
H	51.9264111	71.9781670	103.6334060
H	52.9258520	71.0502076	102.4998654
C	55.3457144	72.4005744	102.9732919
H	56.0804522	73.2112739	103.0784001
H	55.6091338	71.6472240	103.7227073
H	55.4719746	71.9085395	101.9994861
C	56.5175020	71.3082161	98.7689789
H	57.4241295	71.1163966	99.3537771
H	56.1486962	72.3106388	99.0123003
N	55.5202519	70.3303989	99.1717040
H	55.8449299	69.4548787	99.5807991
C	54.2539384	70.6607076	99.4438620
N	53.7197582	71.7833261	98.9346061
H	54.1268553	72.2971315	98.1585458
H	52.7759491	72.0108354	99.2560263
N	53.5141043	69.8978242	100.2431993
H	53.8729030	69.0074580	100.6074042
H	52.5430066	70.1696665	100.4006030
C	59.2912200	73.1450352	107.4367732
H	59.0806047	73.0635645	106.3637627

H	59.5528646	74.1857633	107.6597095
C	60.4672468	72.2490392	107.8082614
O	60.8459547	72.1065367	108.9896690
N	61.0744025	71.6423101	106.7770486
H	60.7457982	71.7782565	105.8244003
H	61.8489560	70.9752465	106.9325163
C	51.0479147	72.2452417	109.4139683
H	51.2814783	72.1127189	110.4758031
H	50.0719830	71.7640946	109.2360063
N	52.6140750	70.3532807	109.2524333
C	52.0910126	71.4889795	108.6554499
C	53.3528679	69.7731319	108.3229970
H	53.9363194	68.8690650	108.4333807
N	53.3265070	70.4723560	107.1619569
H	53.9147018	70.2685828	106.3530185
C	52.5426307	71.5866112	107.3557127
H	52.3802383	72.3220006	106.5787874
C	51.0142401	68.6123568	98.6529875
H	51.8740344	67.9375980	98.7173616
H	51.3551895	69.5830298	98.2761559
C	50.3267631	68.7671566	99.9993992
C	49.3251838	69.7451066	100.1811584
H	49.0460558	70.3769035	99.3339001
C	48.7952800	70.0307557	101.4392328
H	48.0836819	70.8411924	101.5803464
C	49.2150645	69.2820986	102.5539312
O	48.7678821	69.6404862	103.7658054
H	49.0995540	69.0174483	104.4662718
C	50.6535393	67.9682940	101.1007239
H	51.3922883	67.1764000	100.9990359
C	50.0816755	68.1982277	102.3535331
H	50.3757430	67.5885914	103.2021990
C	47.7404409	62.0004415	104.6837034
O	48.0229108	61.3783923	105.7208618
N	48.1759300	63.2501825	104.4501584
H	47.9802625	63.7226914	103.5680459
C	49.1069336	63.8958603	105.3916180
H	49.8509407	63.1379785	105.6655208
C	49.8510501	65.0604303	104.7629174
H	50.3361437	64.7550710	103.8314791
H	49.1616668	65.8868786	104.5594684
S	51.1285299	65.6014750	105.9634370
C	48.3837220	64.3399906	106.7038452
O	48.0456380	65.5025666	106.8478773
C	50.1214019	69.1387344	106.7385846
H	49.8119936	70.1500240	106.4531729
H	51.2166220	69.1017370	106.6991837
O	49.5517268	68.2284673	105.8168406
H	50.0777746	67.3885572	105.8551438
C	64.1403796	61.7786462	105.6427775
O	64.6110285	62.2643336	104.6156707
N	62.8800355	61.9922051	106.0607486
H	62.6195622	61.7092588	107.0056810
C	61.9948466	62.8830152	105.3116258
H	62.6673037	63.5406134	104.7408805
C	61.3036041	63.7743769	106.3633525
O	61.8912040	64.0076910	107.4180471
N	60.0900194	64.3105378	106.0885268
H	59.5999375	64.1038543	105.2190411
C	59.5630911	65.4021273	106.8854882
H	60.4060931	65.9087096	107.3486867
H	59.0593892	66.0912534	106.2019979
C	58.5881408	65.0383008	108.0084463
O	58.8727053	65.2261740	109.1901089
N	57.3892002	64.5480349	107.5786207
H	57.2071976	64.6206444	106.5710207
C	56.2851502	64.3786290	108.4958629
H	56.7097586	64.2410569	109.4916127
H	55.6751114	65.2895349	108.5543857
C	55.2825727	63.2625430	108.2365787

O	54.5502208	62.8790028	109.1617808
N	55.1769046	62.7395560	106.9985280
H	55.6875312	63.1817323	106.2342603
C	54.2384243	61.6469949	106.7170956
H	53.8345245	61.3280448	107.6788685
C	55.0209641	60.4713449	106.1307287
O	55.0819337	59.3492026	106.6467364
N	55.6683986	60.7684317	104.9815510
H	55.6200517	61.7140782	104.6106428
C	56.4404664	59.8034180	104.2266161
H	55.7589401	59.0700220	103.7662594
C	57.1378415	60.5615919	103.0866777
H	57.7119310	61.3972808	103.5119212
H	57.8398148	59.8863056	102.5950721
C	56.1156716	61.0898438	102.0570323
H	55.9477441	60.3207681	101.2937367
H	55.1402034	61.2784536	102.5268481
C	56.5732267	62.3889087	101.3920202
H	56.6127241	63.1935658	102.1369779
H	57.5853466	62.2663190	100.9982523
N	55.6792125	62.7583869	100.3010651
H	54.6683141	62.6242446	100.4767320
C	56.0518070	63.3896929	99.1861051
N	57.3351320	63.6847368	98.9654028
H	58.0154538	63.6236636	99.7098748
H	57.6643603	64.1076120	98.0982580
N	55.1276985	63.7275581	98.2705558
H	54.2756254	63.1432360	98.2192880
H	55.4533586	64.0738130	97.3781816
C	57.3829789	58.8844368	105.0397898
O	57.4497461	57.7372290	104.6119830
C	63.1139021	67.3550731	107.8207626
H	64.1254667	67.4504271	108.2394945
H	63.0149564	66.3675742	107.3631760
C	62.9399836	68.4919085	106.7963166
O	62.9846346	69.6720419	107.1959210
O	62.7828678	68.1693687	105.5572601
C	58.8329057	69.1329874	111.4284469
H	58.1033212	69.6744705	112.0370617
H	59.7276020	69.7561975	111.3371910
C	58.3479815	68.8168298	110.0297852
C	57.1504616	68.1180765	109.7930533
H	56.4926108	67.8591307	110.6197093
C	56.8104082	67.7263215	108.4987871
H	55.8770459	67.2051083	108.3069614
C	57.6571138	68.0097129	107.4279636
H	57.3870180	67.6706513	106.4338199
C	59.1512973	69.1728544	108.9316072
H	60.0514550	69.7659476	109.0925099
C	58.8149336	68.7633278	107.6377962
H	59.4549968	69.0333913	106.8011711
C	67.5198274	66.0615272	99.8361988
O	68.5855161	65.4437059	99.8692462
N	67.3578805	67.2710026	99.2500342
H	66.4093581	67.6782007	99.2882981
C	68.3337676	67.9575491	98.4095417
H	68.6854648	67.2637843	97.6363141
C	69.0411904	71.7435639	103.6445123
H	69.9293388	72.1068943	104.1763929
H	68.4556685	72.6304956	103.3659770
C	68.2486194	70.8992028	104.6405626
H	68.8445909	70.0591824	105.0138406
H	67.9619469	71.5187250	105.4948575
N	67.0090015	70.3079685	104.0627635
H	67.2254393	69.5694581	103.3133310
H	66.4303019	69.7992809	104.7459332
H	66.3658911	70.9943825	103.6122598
C	69.8834539	64.8036005	103.9460671
H	69.2220147	64.0333189	104.3592994
H	70.7705528	64.8915590	104.5868495

C	69.1104147	66.1439643	103.9617170
O	67.9947891	66.1620178	103.3491508
O	69.6513973	67.1073233	104.5509379
C	61.1162100	66.2798825	99.4223045
H	61.9160923	66.6817326	98.8034437
H	60.3009898	67.0031813	99.3904248
N	61.0392154	66.8785616	101.8896195
C	61.6234771	66.1920862	100.8269077
C	61.8689895	66.7610912	102.9338693
H	61.7574699	67.2041804	103.9194075
N	62.9394168	66.0166313	102.5893994
H	63.7768075	65.8356830	103.1759780
C	62.8099147	65.6531242	101.2694195
H	63.5552521	65.0696231	100.7501255
Mo	59.0611578	67.9918551	101.9399334
Fe	52.9261688	66.0971447	104.6627877
Fe	54.8888459	67.9112820	104.7444264
Fe	54.2595212	66.7161951	102.4721931
Fe	55.4703005	65.3848058	104.3301977
Fe	57.7792816	66.1232730	103.3031396
Fe	57.1430122	68.6376813	103.7448007
Fe	56.5394158	67.4612738	101.5002761
S	54.6194142	66.2178037	106.2392587
S	52.9607583	68.1540996	103.6111847
S	53.6399425	64.6175827	103.1391962
S	59.1116442	67.6774313	104.2446287
S	57.3032894	69.5753238	101.7333331
S	58.1875511	66.0273615	101.0799459
S	56.0022797	69.7564875	105.2269152
S	57.3365619	64.1741643	104.3302291
S	54.7585899	66.9446661	100.3188847
C	56.0192541	67.0471090	103.3678819
O	60.4493151	69.6322047	102.2218802
O	59.5696819	68.8335793	99.9608740
O	60.1914303	70.6737885	98.8324689
O	60.5018955	71.5664470	103.8169232
O	61.0440096	73.5737349	102.9807542
O	64.6387822	68.2251972	99.2435904
O	64.8300874	69.0522014	101.3153845
C	60.7567108	70.5337210	101.1454996
C	60.1101726	69.9922986	99.8718431
C	60.1475622	71.9048972	101.4934936
C	60.6032045	72.4058461	102.8650305
C	62.2882033	70.5424471	100.9405691
C	62.7312731	69.3020182	100.1634977
C	64.1803840	68.8504334	100.2462238
H	60.3857111	70.2152993	103.0552284
H	62.1665091	68.4472752	100.5516081
H	62.4758956	69.4078029	99.1060497
H	62.5831323	71.4485586	100.4049773
H	62.7333996	70.5558393	101.9378546
H	59.0594634	71.7635644	101.5551871
H	60.3744430	72.6356842	100.7143552
O	63.9446484	69.6534766	96.8910933
H	62.9782574	69.5493296	96.7948285
H	64.2004634	69.0831934	97.6459534
O	67.3318699	68.4147375	102.1956810
H	67.4963531	67.5600373	102.7096691
H	66.4227450	68.4140318	101.8305798
O	61.9360721	73.0043825	98.4725145
H	61.3779180	72.2177451	98.6365467
H	62.2525012	73.2836234	99.3599463
O	65.0074119	68.3283945	104.0971649
H	64.2051280	68.2354753	104.6662653
H	64.6738918	68.6154646	103.2297432
O	63.2627229	74.3424586	104.5274542
H	63.6319691	73.5882996	105.0439600
H	62.3917862	74.0420864	104.2087429
O	59.9028928	75.2738255	101.1646755
H	58.9980437	74.9121969	101.1517482

H	60.3582845	74.7242481	101.8403171
O	57.5437916	73.8685434	100.7013068
H	57.8276169	72.9707891	100.4854446
H	56.8557044	73.7466051	101.3748193
O	64.9218530	71.4349554	102.6075464
H	64.9282231	70.6036082	102.0722167
H	64.2182597	71.2277610	103.2717397
O	55.9276138	70.6617480	108.3626300
H	56.1524941	70.4448321	107.4404183
H	56.4011092	69.9841813	108.8636474
O	62.9494354	70.4428700	104.2021556
H	62.0759856	70.8729858	104.1991942
H	62.8383568	69.5911077	104.7263300
h	60.7523645	65.3336756	99.0218347
h	47.0271361	61.5840573	103.9724456
h	48.2756108	63.5457087	107.4424217
h	69.3720579	71.2448761	102.7335215
h	70.1878803	64.4766929	102.9518221
h	49.8458557	68.9360854	107.7735121
h	50.2898069	68.1841948	97.9602098
h	50.9709491	73.3090998	109.1895815
h	56.7929329	71.2717198	97.7149994
h	58.3849894	72.8968577	107.9892415
h	62.4173617	67.4651501	108.6518954
h	53.6576318	73.5356885	102.3477709
h	59.1843850	68.2468451	111.9569176
h	64.7185456	61.0643998	106.2289885
h	61.3864941	62.3713328	104.5658674
h	53.4116761	61.9613226	106.0801084
h	57.9852028	59.1449224	105.9101580
h	67.8368071	68.8017113	97.9315379
h	69.2481981	68.2434328	98.9293055
h	66.5888491	65.7011741	100.2737971

282QM – [MoFe7S9C] – (305 atoms total with link atoms, marked with lowercase h)

C	53.9049260	72.8981490	103.1922517
H	53.8823167	73.5310145	104.0809549
C	52.9618842	71.7055358	103.3960868
H	53.3467988	71.0823007	104.2097087
H	51.9337437	71.9933978	103.6497238
H	52.9260911	71.0632199	102.5125054
C	55.3505037	72.4117781	102.9740303
H	56.0866988	73.2202407	103.0856403
H	55.6129338	71.6526375	103.7179658
H	55.4772723	71.9257328	101.9974161
C	56.4879013	71.3719458	98.7798133
H	57.3893368	71.1862227	99.3749246
H	56.1268738	72.3832978	98.9984118
N	55.4849040	70.4092178	99.2047563
H	55.8105000	69.5628947	99.6737668
C	54.2145793	70.7460648	99.4494199
N	53.6787770	71.8468485	98.8965960
H	54.1106303	72.3621355	98.1352744
H	52.7369920	72.0903757	99.2057506
N	53.4665563	70.0094086	100.2652527
H	53.8098539	69.1134104	100.6308078
H	52.4926848	70.2900787	100.3990672
C	59.2924056	73.1439181	107.4342633
H	59.0804325	73.0612923	106.3616154
H	59.5516871	74.1853782	107.6564476
C	60.4705551	72.2506991	107.8046025
O	60.8512676	72.1095246	108.9856144
N	61.0770361	71.6437773	106.7731446
H	60.7464204	71.7771676	105.8207548
H	61.8516655	70.9768892	106.9285935
C	55.4484541	71.0290290	112.9586759
H	55.9099407	70.1203393	112.5632913
H	56.1657814	71.5069098	113.6339489
O	54.2659724	70.6476970	113.6575447
H	54.0157205	71.3311076	114.3148278

C	51.0545383	72.2288740	109.4444405
H	51.2826546	72.1103929	110.5086078
H	50.0779176	71.7486850	109.2698007
N	52.6181578	70.3301959	109.3241085
C	52.0933388	71.4527754	108.7006873
C	53.3548188	69.7177022	108.4099819
H	53.9360178	68.8161253	108.5475993
N	53.3205095	70.3822192	107.2333318
H	53.9061142	70.1534887	106.4261326
C	52.5415018	71.5049241	107.3979882
H	52.3769807	72.2167812	106.5998181
C	51.0280564	68.6266686	98.6472924
H	51.8921639	67.9569820	98.7063590
H	51.3623734	69.5999899	98.2714656
C	50.3436556	68.7718241	99.9960079
C	49.3313085	69.7368453	100.1816749
H	49.0468269	70.3696001	99.3367515
C	48.7931122	70.0071484	101.4396534
H	48.0717322	70.8082537	101.5850799
C	49.2132949	69.2499957	102.5475246
O	48.7548920	69.5870709	103.7615916
H	49.0868107	68.9533693	104.4515256
C	50.6724923	67.9643791	101.0907000
H	51.4175859	67.1792351	100.9849332
C	50.0886013	68.1742806	102.3408882
H	50.3756238	67.5541600	103.1836318
C	47.7371661	61.9876997	104.6798337
O	48.0208299	61.3653518	105.7163442
N	48.1754649	63.2363038	104.4464778
H	47.9787740	63.7124999	103.5666365
C	49.1119945	63.8708187	105.3880424
H	49.8424247	63.1012900	105.6647489
C	49.8786765	65.0217653	104.7625860
H	50.3646821	64.7098612	103.8335260
H	49.2056168	65.8606011	104.5555232
S	51.1549961	65.5282711	105.9798700
C	48.3921987	64.3284525	106.6981529
O	48.0580799	65.4930171	106.8332409
C	53.3766800	66.8227602	112.2101436
H	53.7502096	65.8714533	112.5772088
H	54.1380970	67.5776708	112.4478475
N	52.1521127	67.1848853	112.9071983
H	51.8016936	68.1120405	112.6499036
C	51.4588782	66.4753202	113.8018157
N	51.7550803	65.2161997	114.1245373
H	52.5188884	64.6657175	113.6797256
H	51.3193037	64.7128534	114.9068468
N	50.3702810	67.0788025	114.3459260
H	50.3405650	68.0989971	114.2828345
H	49.9929119	66.6808532	115.2163461
C	50.1262471	69.0909255	106.6915257
H	49.8104012	70.0947793	106.3873799
H	51.2208507	69.0554106	106.6427623
O	49.5535832	68.1592874	105.7941106
H	50.0859434	67.3257628	105.8429403
C	44.9700631	71.5913022	112.6518144
H	44.9976016	72.0491739	111.6596082
H	44.5687752	72.3345874	113.3525262
C	46.3875991	71.2020227	113.0350374
C	46.7115781	70.5700562	114.2497168
H	45.9215514	70.3572579	114.9693137
C	48.0196373	70.1878003	114.5444791
H	48.2575642	69.6778663	115.4769242
C	49.0570279	70.4342265	113.6294819
O	50.3096761	70.0055966	113.9271158
H	50.9166962	70.1059022	113.1318097
C	47.4408476	71.4667503	112.1468841
H	47.2276038	71.9267486	111.1818573
C	48.7608666	71.1028096	112.4330604
H	49.5510106	71.2754574	111.7072865

C	64.1332373	61.7808920	105.6446408
O	64.6012175	62.2660831	104.6161674
N	62.8743675	61.9963142	106.0666886
H	62.6166014	61.7123565	107.0121761
C	61.9874570	62.8886343	105.3208277
H	62.6587011	63.5473748	104.7498770
C	61.2988147	63.7794568	106.3751243
O	61.8924196	64.0149909	107.4256610
N	60.0817683	64.3128680	106.1076574
H	59.5893842	64.1034731	105.2407501
C	59.5596085	65.4080409	106.9041824
H	60.4056606	65.9032471	107.3738369
H	59.0678994	66.1062800	106.2210889
C	58.5763696	65.0509641	108.0221878
O	58.8603958	65.2285562	109.2052556
N	57.3719708	64.5772695	107.5872279
H	57.1895975	64.6643610	106.5818483
C	56.2644369	64.4065658	108.4993089
H	56.6862504	64.2690423	109.4962687
H	55.6524456	65.3165869	108.5545179
C	55.2628918	63.2901781	108.2326783
O	54.5001170	62.9306985	109.1419480
N	55.1930286	62.7392453	107.0040629
H	55.7379040	63.1546073	106.2489370
C	54.2522074	61.6492653	106.7169115
H	53.8414925	61.3323145	107.6765772
C	55.0316362	60.4698491	106.1359267
O	55.0910539	59.3502536	106.6569668
N	55.6775260	60.7589523	104.9834989
H	55.6245579	61.7006149	104.6036793
C	56.4458407	59.7866881	104.2344055
H	55.7619749	59.0514918	103.7805393
C	57.1437106	60.5339236	103.0884557
H	57.7211418	61.3701808	103.5082368
H	57.8432891	59.8530788	102.6010574
C	56.1233008	61.0570167	102.0545984
H	55.9674619	60.2898841	101.2870533
H	55.1429442	61.2353212	102.5181003
C	56.5753639	62.3620145	101.3979500
H	56.5913071	63.1675786	102.1427167
H	57.5974232	62.2515137	101.0272625
N	55.6950495	62.7222256	100.2928909
H	54.6822926	62.5995409	100.4681221
C	56.0714966	63.3585874	99.1820487
N	57.3572843	63.6251826	98.9440138
H	58.0741082	63.4153749	99.6248904
H	57.6803291	64.0565316	98.0781716
N	55.1432588	63.7435421	98.2871628
H	54.2747338	63.1827927	98.2483108
H	55.4718266	64.0510127	97.3810183
C	57.3898749	58.8721077	105.0503317
O	57.4603606	57.7251383	104.6230153
C	63.1155962	67.3538244	107.8228000
H	64.1287035	67.4494024	108.2377295
H	63.0147651	66.3656629	107.3671139
C	62.9383754	68.4887088	106.7965469
O	62.9830042	69.6694683	107.1940846
O	62.7790493	68.1634351	105.5585062
C	58.8525305	69.1434011	111.4393977
H	58.1228461	69.6861707	112.0466536
H	59.7502253	69.7622789	111.3503833
C	58.3677855	68.8331393	110.0395746
C	57.1686370	68.1374918	109.8012173
H	56.5120975	67.8736086	110.6279697
C	56.8269743	67.7541393	108.5049392
H	55.8932246	67.2349183	108.3094141
C	57.6698372	68.0463667	107.4331339
H	57.3934645	67.7219130	106.4357463
C	59.1707112	69.1934028	108.9422893
H	60.0725191	69.7832631	109.1054778

C	58.8305202	68.7946100	107.6458055
H	59.4689532	69.0705141	106.8098090
C	67.5169749	66.0609105	99.8322786
O	68.5826599	65.4432306	99.8672550
N	67.3555152	67.2706922	99.2471593
H	66.4068265	67.6774784	99.2854866
C	68.3320031	67.9581227	98.4081178
H	68.6842188	67.2650036	97.6345402
C	69.0385169	71.7431710	103.6438285
H	69.9265030	72.1062069	104.1762050
H	68.4533719	72.6302836	103.3651445
C	68.2454879	70.8987827	104.6395032
H	68.8416219	70.0590509	105.0131583
H	67.9581086	71.5182893	105.4935723
N	67.0062544	70.3069482	104.0612359
H	67.2229599	69.5687955	103.3116736
H	66.4276237	69.7978115	104.7442218
H	66.3627438	70.9930706	103.6108899
C	69.8794918	64.8015706	103.9440694
H	69.2167071	64.0314034	104.3554354
H	70.7657050	64.8880327	104.5862681
C	69.1076330	66.1427500	103.9597414
O	67.9918055	66.1615057	103.3474713
O	69.6500447	67.1055689	104.5486148
C	61.0819064	66.2795755	99.4194224
H	61.8775546	66.6854744	98.7975247
H	60.2642517	67.0003671	99.3897964
N	61.0108930	66.8704202	101.8873225
C	61.5962508	66.1912512	100.8212355
C	61.8471872	66.7573564	102.9270144
H	61.7381282	67.1983483	103.9137040
N	62.9231633	66.0238289	102.5755796
H	63.7639696	65.8461971	103.1583842
C	62.7901223	65.6613866	101.2559085
H	63.5398539	65.0880789	100.7313711
Mo	59.0326410	68.0048741	101.9333130
Fe	52.9275352	66.1523166	104.6978739
Fe	54.8992517	67.9218841	104.7616858
Fe	54.2082921	66.7552052	102.4784829
Fe	55.4356986	65.3861657	104.3383666
Fe	57.7239198	66.0790766	103.3230091
Fe	57.1569038	68.6192189	103.7073069
Fe	56.4987845	67.4936931	101.4984488
S	54.6093273	66.2909395	106.2731767
S	52.8980548	68.1697280	103.7379473
S	53.6475495	64.6693291	103.0942286
S	59.0971861	67.6361768	104.2289333
S	57.3079714	69.6124790	101.7190086
S	58.1141391	66.0391836	101.0920029
S	55.9992338	69.7675735	105.1856695
S	57.3079714	64.1532715	104.3596619
S	54.6769906	67.0946388	100.3341608
C	55.9913239	67.0236172	103.3656202
O	60.4402083	69.6250921	102.2173783
O	59.5545620	68.8365446	99.9625450
O	60.1844633	70.6715529	98.8297990
O	60.4989989	71.5526031	103.8160899
O	61.0448185	73.5626334	102.9885584
O	64.6334582	68.2195493	99.2460392
O	64.8229248	69.0480223	101.3172519
C	60.7488911	70.5304804	101.1435840
C	60.0991164	69.9936902	99.8704026
C	60.1436225	71.9018368	101.4958057
C	60.6018225	72.3964044	102.8673195
C	62.2804143	70.5352740	100.9391839
C	62.7230483	69.2923204	100.1660718
C	64.1735379	68.8441768	100.2483753
H	60.3753649	70.2100463	103.0517529
H	62.1601213	68.4383067	100.5585210
H	62.4652885	69.3929053	99.1086031

H	62.5772831	71.4394616	100.4014254
H	62.7254974	70.5502275	101.9365799
H	59.0556806	71.7595049	101.5582573
H	60.3709842	72.6337704	100.7179646
O	52.1049834	69.9476123	112.0501194
H	52.9098906	70.2732108	112.5031036
H	52.2468946	70.0432404	111.0601112
O	63.9475924	69.6542198	96.8921837
H	62.9807165	69.5534670	96.7959667
H	64.2010889	69.0830040	97.6468723
O	67.3278749	68.4136958	102.1933017
H	67.4930691	67.5593096	102.7075815
H	66.4180323	68.4127121	101.8299422
O	61.9372306	72.9985119	98.4748086
H	61.3754380	72.2141614	98.6369711
H	62.2519801	73.2764029	99.3632807
O	65.0043028	68.3276153	104.0991579
H	64.2025100	68.2327469	104.6686552
H	64.6694029	68.6174654	103.2331601
O	63.2627221	74.3392286	104.5291673
H	63.6329055	73.5851473	105.0451063
H	62.3917448	74.0374594	104.2117399
O	59.9103448	75.2688284	101.1700585
H	59.0063656	74.9041245	101.1561191
H	60.3656226	74.7196481	101.8457458
O	57.5480746	73.8762220	100.7295376
H	57.8029093	72.9692823	100.5148283
H	56.8654613	73.7752259	101.4122777
O	64.9169128	71.4320532	102.6067891
H	64.9228488	70.6007741	102.0715385
H	64.2136988	71.2247133	103.2713126
O	55.9164701	70.6685340	108.3387030
H	56.1379013	70.4428161	107.4169864
H	56.4169950	70.0146192	108.8450565
O	62.9467194	70.4370540	104.2015245
H	62.0723352	70.8656306	104.1968192
H	62.8354334	69.5859152	104.7261583
h	60.7209807	65.3320861	99.0193428
h	47.0228268	61.5746526	103.9676689
h	48.2819335	63.5399391	107.4425690
h	69.3697310	71.2445817	102.7329097
h	70.1853397	64.4754199	102.9500120
h	49.8569444	68.9055685	107.7313267
h	50.3010716	68.1974608	97.9578428
h	50.9796297	73.2896157	109.2051020
h	56.7723620	71.3101240	97.7294194
h	58.3873734	72.8937616	107.9878025
h	62.4221003	67.4657565	108.6562278
h	53.6639881	73.5464608	102.3498101
h	59.2007807	68.2555500	111.9671376
h	64.7124678	61.0658657	106.2288468
h	61.3776748	62.3782300	104.5753612
h	53.4285250	61.9641345	106.0762307
h	57.9899830	59.1351516	105.9213916
h	67.8349554	68.8023420	97.9303057
h	69.2462274	68.2435223	98.9285100
h	66.5848371	65.6994370	100.2664709
h	55.2546589	71.6945090	112.1174583
h	44.2837298	70.7456342	112.6086927
h	53.2535107	66.7697221	111.1284397

334QM – [MoFe7S9C] – (361 atoms total with link atoms, marked with lowercase h)

C	53.910798	72.911820	103.205912
H	53.888860	73.547166	104.092791
C	52.965829	71.720964	103.411676
H	53.348610	71.099997	104.228000
H	51.937200	72.010053	103.661935
H	52.932093	71.075891	102.530173
C	55.354925	72.420002	102.990552
H	56.094444	73.226178	103.096224

H	55.615001	71.664397	103.738991
H	55.478988	71.926774	102.017261
C	56.490331	71.375764	98.776726
H	57.392292	71.181114	99.368092
H	56.140142	72.390457	98.997646
N	55.479235	70.423590	99.206013
H	55.797301	69.574931	99.676448
C	54.214194	70.775270	99.456433
N	53.685949	71.876832	98.897350
H	54.118828	72.381284	98.129461
H	52.749921	72.134441	99.210979
N	53.464329	70.055487	100.285089
H	53.797954	69.154477	100.649222
H	52.492164	70.343878	100.415091
C	59.292970	73.139428	107.436167
H	59.080899	73.055429	106.363671
H	59.552295	74.181264	107.656853
C	60.471290	72.246623	107.807478
O	60.852034	72.106396	108.988687
N	61.077926	71.639269	106.776470
H	60.748617	71.774032	105.823749
H	61.853865	70.973873	106.931832
C	55.455407	71.037213	112.969011
H	55.920793	70.129324	112.576375
H	56.170317	71.518515	113.644332
O	54.273055	70.653970	113.666738
H	54.022129	71.335235	114.326400
C	51.062417	72.229599	109.450977
H	51.292913	72.115475	110.515054
H	50.085791	71.748018	109.280224
N	52.625486	70.329670	109.333862
C	52.099107	71.450110	108.707837
C	53.357660	69.712698	108.418913
H	53.938780	68.811183	108.557499
N	53.318053	70.371670	107.239396
H	53.899721	70.138974	106.430022
C	52.540877	71.495715	107.402777
H	52.373468	72.204380	106.602450
C	47.420727	64.135316	98.414101
H	47.162714	63.320532	99.099496
H	46.472693	64.484150	97.985847
C	48.295273	63.541398	97.282227
O	49.330242	64.134477	96.891771
O	47.861015	62.444852	96.811981
C	51.054310	68.674349	98.646775
H	51.913757	67.998145	98.693277
H	51.383693	69.649261	98.271957
C	50.375592	68.803904	100.000635
C	49.367201	69.768686	100.204542
H	49.086624	70.420471	99.372899
C	48.821140	70.006365	101.465107
H	48.101945	70.806258	101.627764
C	49.228900	69.216006	102.554328
O	48.764585	69.528377	103.772235
H	49.102206	68.893870	104.459751
C	50.682335	67.954319	101.070341
H	51.401647	67.150553	100.930062
C	50.091840	68.134112	102.322428
H	50.362648	67.483349	103.147630
C	51.181063	62.784296	94.499829
H	51.335628	63.848620	94.691789
H	50.580884	62.419824	95.341988
C	52.509096	62.024404	94.611320
O	52.664329	60.944678	94.010629
O	53.333349	62.553590	95.432720
C	47.080614	61.585073	101.893852
H	46.146721	61.535075	101.329432
H	47.528504	62.564508	101.722528
N	49.322550	60.590636	101.169084
H	49.838906	61.474652	101.087225

C	47.981532	60.468806	101.475547
C	49.795442	59.342948	100.881568
H	50.813028	59.172479	100.556034
N	48.846187	58.429458	100.987223
C	47.717854	59.116473	101.365661
H	46.777098	58.616476	101.556067
C	47.737592	61.969696	104.760783
O	47.980247	61.356609	105.812377
N	48.205055	63.205779	104.508363
H	48.010765	63.664391	103.620281
C	49.134366	63.855368	105.443965
H	49.862303	63.089160	105.737949
C	49.908388	64.989249	104.800081
H	50.398374	64.653631	103.880680
H	49.239951	65.826067	104.569842
S	51.180541	65.510047	106.013641
C	48.407276	64.333211	106.741378
O	48.083560	65.501797	106.864955
C	53.401499	66.821186	112.216710
H	53.775889	65.870247	112.584405
H	54.164244	67.576546	112.448744
N	52.179775	67.188476	112.917251
H	51.834448	68.118265	112.661564
C	51.482021	66.480498	113.809675
N	51.770372	65.217940	114.126731
H	52.533866	64.666965	113.682072
H	51.331182	64.714589	114.906961
N	50.396514	67.086522	114.356516
H	50.362762	68.106146	114.290186
H	50.016142	66.688197	115.225180
C	50.130488	69.071451	106.697716
H	49.807406	70.070004	106.384068
H	51.224989	69.041662	106.644591
O	49.560280	68.126355	105.812261
H	50.099004	67.297274	105.867749
C	44.975724	71.592057	112.639287
H	45.005035	72.036958	111.641269
H	44.574954	72.344723	113.330281
C	46.393094	71.204373	113.026289
C	46.717973	70.586668	114.248139
H	45.928616	70.382562	114.970884
C	48.026402	70.208618	114.546941
H	48.266109	69.712914	115.486597
C	49.063546	70.442502	113.628285
O	50.315113	70.015335	113.930381
H	50.924694	70.110283	113.135866
C	47.446401	71.458807	112.134703
H	47.233977	71.909661	111.165206
C	48.766738	71.097753	112.424265
H	49.555894	71.263066	111.695760
C	64.125730	61.780494	105.644413
O	64.594803	62.264778	104.615943
N	62.866179	61.995997	106.064538
H	62.606057	61.712181	107.009343
C	61.979474	62.885450	105.314959
H	62.650871	63.544114	104.744179
C	61.285682	63.776719	106.365127
O	61.872303	64.011572	107.419989
N	60.071268	64.311969	106.088872
H	59.582775	64.101942	105.219943
C	59.542048	65.402440	106.886475
H	60.383774	65.901924	107.359762
H	59.047378	66.098796	106.203794
C	58.558513	65.035320	108.000167
O	58.838600	65.210425	109.184554
N	57.358203	64.555701	107.559576
H	57.177355	64.645175	106.553831
C	56.249374	64.384501	108.469923
H	56.671206	64.249616	109.466956
H	55.636717	65.294335	108.522812

C	55.247590	63.267405	108.208868
O	54.494529	62.907570	109.126395
N	55.164662	62.718092	106.979416
H	55.703747	63.132256	106.219516
C	54.226075	61.622873	106.703878
H	53.825999	61.310557	107.669634
C	55.004984	60.440860	106.126228
O	55.081956	59.331021	106.666257
N	55.633489	60.713836	104.960243
H	55.554170	61.642282	104.554138
C	56.407348	59.734084	104.225764
H	55.729055	58.984089	103.788507
C	57.095179	60.463717	103.063556
H	57.646047	61.326126	103.466765
H	57.821904	59.789754	102.607091
C	56.079739	60.930224	101.994786
H	56.032648	60.177433	101.199894
H	55.063151	61.007964	102.403961
C	56.466487	62.285889	101.402028
H	56.373165	63.065165	102.169725
H	57.522057	62.266757	101.116247
N	55.649750	62.634308	100.246386
H	54.633248	62.484708	100.351343
C	56.074185	63.377314	99.217231
N	57.378585	63.587613	98.996970
H	58.101610	63.149653	99.552706
H	57.703111	64.096627	98.175594
N	55.171176	63.938148	98.402124
H	54.265688	63.426235	98.356614
H	55.509204	64.279082	97.511263
C	57.365647	58.842472	105.049834
O	57.449690	57.692238	104.632829
C	63.111797	67.350978	107.818941
H	64.123614	67.444701	108.237400
H	63.010886	66.363720	107.361290
C	62.939192	68.488193	106.794634
O	62.988938	69.668096	107.194198
O	62.777720	68.165537	105.556336
C	58.848475	69.144195	111.436120
H	58.120544	69.688492	112.044117
H	59.745908	69.762965	111.343094
C	58.359537	68.830121	110.038519
C	57.159295	68.134414	109.806178
H	56.504924	67.874613	110.635888
C	56.813540	67.745894	108.512525
H	55.879671	67.224738	108.322534
C	57.652767	68.034652	107.436895
H	57.372938	67.707381	106.441379
C	59.159539	69.185642	108.937521
H	60.062485	69.775031	109.096217
C	58.814452	68.783171	107.643512
H	59.449755	69.056313	106.804198
C	67.513443	66.061906	99.832067
O	68.579337	65.444119	99.866608
N	67.352292	67.271879	99.246664
H	66.403816	67.679073	99.285280
C	68.329372	67.958531	98.407790
H	68.681202	67.264963	97.634403
C	69.037532	71.743257	103.643321
H	69.925561	72.105988	104.175856
H	68.452699	72.630536	103.364509
C	68.243924	70.899094	104.638755
H	68.839746	70.059232	105.012632
H	67.956457	71.518729	105.492683
N	67.004857	70.307710	104.059970
H	67.221734	69.569848	103.310264
H	66.425664	69.798059	104.742193
H	66.361454	70.994124	103.609735
C	69.876151	64.800412	103.942734
H	69.212390	64.030351	104.352745

H	70.761950	64.885477	104.585728
C	69.105394	66.142415	103.959179
O	67.988950	66.162026	103.348301
O	69.649679	67.104642	104.547488
C	61.072708	66.285188	99.427373
H	61.871081	66.686212	98.805697
H	60.257429	67.008791	99.395514
N	60.992296	66.875354	101.893960
C	61.583157	66.198094	100.830053
C	61.825691	66.763421	102.936208
H	61.713630	67.204353	103.922370
N	62.904940	66.032885	102.588060
H	63.744843	65.856450	103.171896
C	62.777084	65.670765	101.267794
H	63.530553	65.100097	100.745467
C	49.971876	58.761466	95.466809
H	49.700253	59.461564	94.672828
H	49.039398	58.263178	95.757835
N	49.874012	60.733210	96.991017
H	49.080689	61.259054	96.569610
C	50.467896	59.534298	96.646489
C	50.455690	61.181595	98.123042
H	50.199991	62.127003	98.584537
N	51.399725	60.350268	98.541957
C	51.406515	59.309513	97.629871
H	52.056274	58.454111	97.732129
Mo	59.012208	68.018740	101.933562
Fe	52.924208	66.148675	104.703324
Fe	54.885431	67.922402	104.762592
Fe	54.181924	66.773448	102.477834
Fe	55.421157	65.385565	104.316646
Fe	57.702061	66.083847	103.297915
Fe	57.139862	68.623784	103.710261
Fe	56.473304	67.523772	101.497664
S	54.616965	66.281344	106.265588
S	52.872472	68.173516	103.760713
S	53.620308	64.676512	103.079576
S	59.074661	67.629986	104.225068
S	57.296750	69.636996	101.730804
S	58.083950	66.070652	101.067015
S	55.985932	69.764916	105.197713
S	57.291883	64.152210	104.321676
S	54.643237	67.145389	100.342778
C	55.969433	67.032144	103.357343
O	60.434176	69.630598	102.220382
O	59.541551	68.851416	99.964366
O	60.184773	70.682673	98.833813
O	60.500610	71.560223	103.820993
O	61.047210	73.569425	102.991369
O	64.627128	68.220870	99.248332
O	64.821953	69.051124	101.318103
C	60.745899	70.536434	101.147940
C	60.094274	70.004151	99.873830
C	60.143547	71.908679	101.500970
C	60.603340	72.403112	102.871703
C	62.277120	70.538210	100.942232
C	62.717253	69.290660	100.174844
C	64.168969	68.845218	100.251655
H	60.371756	70.213875	103.054897
H	62.157349	68.438912	100.576483
H	62.453270	69.383770	99.118191
H	62.573406	71.439342	100.398964
H	62.724177	70.558178	101.938591
H	59.055535	71.767343	101.564851
H	60.371003	72.640030	100.722610
O	51.995872	64.577736	96.794427
H	52.518711	63.831564	96.403516
H	51.055264	64.286192	96.770352
O	46.677912	60.540126	98.326965
H	47.044086	61.259855	97.765761

H	47.387134	60.291635	98.931105
O	51.815007	65.070907	99.384249
H	52.030363	64.834461	98.437201
H	52.643491	65.399192	99.772080
O	52.116093	69.950109	112.060259
H	52.919759	70.281677	112.511307
H	52.255364	70.044063	111.069382
O	63.943247	69.655358	96.894399
H	62.975754	69.558047	96.800161
H	64.195768	69.085102	97.650143
O	52.952476	61.741631	100.922764
H	52.535629	61.198618	100.226678
H	52.260731	62.376953	101.182205
O	67.326193	68.414105	102.192264
H	67.490239	67.560019	102.707226
H	66.416189	68.414353	101.829142
O	50.532595	63.294233	100.960907
H	51.017950	63.910867	100.344321
H	49.892482	63.865976	101.423133
O	61.937019	73.000839	98.475808
H	61.374156	72.217143	98.639117
H	62.252164	73.279059	99.363996
O	65.003222	68.331267	104.098072
H	64.200822	68.236017	104.666715
H	64.668854	68.620783	103.231667
O	63.265356	74.341838	104.529735
H	63.634800	73.587210	105.045391
H	62.394071	74.041093	104.211836
O	59.908130	75.270539	101.171099
H	59.004703	74.904396	101.157310
H	60.364489	74.722480	101.847170
O	57.548041	73.873494	100.728956
H	57.807789	72.966998	100.517793
H	56.863685	73.770732	101.409740
O	64.916196	71.434565	102.607164
H	64.921561	70.603329	102.071726
H	64.213180	71.227191	103.272018
O	53.415719	62.094943	98.000138
H	53.435422	62.063828	97.012717
H	52.732405	61.462410	98.289914
O	55.914040	70.670148	108.349499
H	56.126868	70.449618	107.424444
H	56.414943	70.010008	108.847292
O	62.946602	70.440649	104.202283
H	62.072283	70.869445	104.197391
H	62.835078	69.588877	104.725841
h	60.709562	65.337099	99.030738
h	47.083573	61.598633	103.971708
h	48.281964	63.547738	107.486627
h	69.368655	71.244555	102.732431
h	70.182716	64.474911	102.948684
h	49.866075	68.894070	107.740160
h	50.318181	68.244164	97.967715
h	50.986631	73.289418	109.207856
h	56.770417	71.313305	97.725195
h	58.387939	72.890282	107.990165
h	62.415693	67.462296	108.650274
h	53.673055	73.558826	102.361562
h	59.197406	68.257214	111.964873
h	64.705009	61.066015	106.229241
h	61.371518	62.372864	104.569498
h	53.392831	61.927815	106.070804
h	57.967096	59.118653	105.915889
h	67.832820	68.802805	97.929560
h	69.243857	68.243344	98.928045
h	66.581346	65.700699	100.266569
h	55.260302	71.700169	112.126105
h	44.287176	70.747809	112.604454
h	53.274096	66.765666	111.135621
h	47.842720	64.941589	99.014027

h	50.657251 62.695016 93.548137
h	50.666294 58.020590 95.070636
h	46.868771 61.472436 102.957103

367QM – [MoFe7S9C] – (395 atoms total with link atoms, marked with lowercase h)

C	53.9146196	72.9151833	103.2049631
H	53.8942357	73.5492218	104.0928508
C	52.9705684	71.7235882	103.4107054
H	53.3544768	71.1023034	104.2262794
H	51.9419758	72.0119849	103.6619097
H	52.9362621	71.0789710	102.5287741
C	55.3581983	72.4239534	102.9847370
H	56.0975713	73.2308283	103.0866212
H	55.6214478	71.6693141	103.7328560
H	55.4780450	71.9298538	102.0112984
C	56.5044617	71.3271111	98.7359324
H	57.4111400	71.1038741	99.3098832
H	56.1707171	72.3409497	98.9851734
N	55.4811765	70.3870507	99.1560931
H	55.7823568	69.4913707	99.5409429
C	54.2300229	70.7589934	99.4398921
N	53.7189829	71.8876326	98.9181796
H	54.1320055	72.3771090	98.1295073
H	52.7895342	72.1521301	99.2451354
N	53.4775655	70.0386772	100.2655545
H	53.8107360	69.1388418	100.6310572
H	52.5102706	70.3375861	100.4080157
C	59.2944215	73.1411970	107.4432529
H	59.0849565	73.0565953	106.3702981
H	59.5534300	74.1831242	107.6637524
C	60.4711728	72.2476334	107.8175790
O	60.8502485	72.1063496	108.9988923
N	61.0790863	71.6397155	106.7871422
H	60.7510268	71.7784441	105.8351473
H	61.8540454	70.9731786	106.9422913
C	55.4534585	71.0371049	112.9719561
H	55.9197278	70.1294441	112.5797903
H	56.1677055	71.5191231	113.6474830
O	54.2709758	70.6533270	113.6688759
H	54.0197799	71.3341689	114.3290245
C	51.0635775	72.2290500	109.4508299
H	51.2946507	72.1150287	110.5147714
H	50.0869481	71.7473344	109.2807084
N	52.6269512	70.3292450	109.3327770
C	52.0997613	71.4494610	108.7069495
C	53.3580347	69.7119212	108.4173433
H	53.9392154	68.8104107	108.5558723
N	53.3171170	70.3703801	107.2374852
H	53.8985457	70.1384642	106.4280931
C	52.5401060	71.4945270	107.4013689
H	52.3718448	72.2029744	106.6010233
C	47.4210873	64.1407817	98.4149378
H	47.1625589	63.3263223	99.1005271
H	46.4733995	64.4906932	97.9867909
C	48.2953114	63.5456253	97.2832753
O	49.3317070	64.1368500	96.8940251
O	47.8595333	62.4505535	96.8113547
C	51.0565805	68.6768739	98.6420602
H	51.9158806	68.0005096	98.6880651
H	51.3853999	69.6515471	98.2663322
C	50.3788750	68.8076836	99.9962742
C	49.3722265	69.7742976	100.2008915
H	49.0919857	70.4269267	99.3698768
C	48.8256277	70.0108978	101.4615364
H	48.1070608	70.8112992	101.6242954
C	49.2317218	69.2189053	102.5502391
O	48.7650509	69.5289714	103.7680159
H	49.1026032	68.8942146	104.4550966
C	50.6851048	67.9576310	101.0657677
H	51.4025115	67.1523244	100.9245234

C	50.0950255	68.1373923	102.3181033
H	50.3652488	67.4859051	103.1430188
C	51.1842588	62.7870028	94.4977681
H	51.3403366	63.8515489	94.6868701
H	50.5829653	62.4264489	95.3408683
C	52.5110487	62.0255672	94.6127387
O	52.6662457	60.9445106	94.0147958
O	53.3344602	62.5554620	95.4349759
C	47.0810589	61.5850723	101.8963160
H	46.1468668	61.5348318	101.3322538
H	47.5274312	62.5651168	101.7244510
N	49.3229778	60.5920527	101.1686214
H	49.8393282	61.4760043	101.0868785
C	47.9823442	60.4698014	101.4766250
C	49.7957369	59.3444971	100.8802787
H	50.8130109	59.1751368	100.5531274
N	48.8471279	58.4305356	100.9879775
C	47.7191660	59.1173509	101.3678672
H	46.7780763	58.6181059	101.5587622
C	47.7398090	61.9708203	104.7629642
O	47.9819563	61.3576571	105.8147306
N	48.2082082	63.2059504	104.5101760
H	48.0133642	63.6653443	103.6224741
C	49.1391889	63.8563566	105.4441585
H	49.8676279	63.0905589	105.7380038
C	49.9128338	64.9890858	104.7966327
H	50.3987706	64.6506917	103.8761409
H	49.2445028	65.8260873	104.5668198
S	51.1911133	65.5136031	106.0025490
C	48.4131177	64.3347581	106.7416468
O	48.0930531	65.5040736	106.8661467
C	53.4024971	66.8200729	112.2162615
H	53.7775983	65.8694157	112.5840103
H	54.1647012	67.5759963	112.4483189
N	52.1804584	67.1864969	112.9167257
H	51.8346587	68.1160694	112.6610656
C	51.4830805	66.4785483	113.8096350
N	51.7722244	65.2164223	114.1274835
H	52.5348063	64.6651345	113.6816046
H	51.3331168	64.7128477	114.9077545
N	50.3973212	67.0843595	114.3560432
H	50.3630446	68.1039478	114.2895355
H	50.0165365	66.6861336	115.2245857
C	50.1320776	69.0706059	106.6944968
H	49.8086732	70.0691826	106.3812237
H	51.2266059	69.0414156	106.6413632
O	49.5626041	68.1256768	105.8084511
H	50.1025057	67.2973850	105.8629171
C	44.9758993	71.5918475	112.6388175
H	45.0051870	72.0366826	111.6407815
H	44.5753882	72.3446334	113.3298125
C	46.3932095	71.2038047	113.0256498
C	46.7180335	70.5867489	114.2478442
H	45.9286762	70.3833754	114.9707871
C	48.0263504	70.2084025	114.5467419
H	48.2659564	69.7131076	115.4866337
C	49.0634217	70.4412617	113.6277916
O	50.3148340	70.0135583	113.9298748
H	50.9242762	70.1083902	113.1354193
C	47.4464986	71.4573667	112.1337334
H	47.2342084	71.9082188	111.1642056
C	48.7667859	71.0960445	112.4234469
H	49.5560648	71.2611832	111.6950171
C	64.1265633	61.7795136	105.6446489
O	64.5954864	62.2653423	104.6169463
N	62.8663243	61.9935867	106.0645037
H	62.6057061	61.7078503	107.0085831
C	61.9799667	62.8831462	105.3150483
H	62.6520772	63.5410392	104.7441312
C	61.2873632	63.7756449	106.3649148

O	61.8749113	64.0117253	107.4189620
N	60.0730203	64.3107784	106.0888154
H	59.5836244	64.0997466	105.2205467
C	59.5432853	65.4013425	106.8858159
H	60.3847405	65.8999429	107.3604543
H	59.0496215	66.0982064	106.2027859
C	58.5583057	65.0345680	107.9986203
O	58.8369174	65.2108956	109.1830669
N	57.3588897	64.5536980	107.5569326
H	57.1794596	64.6435024	106.5509978
C	56.2487760	64.3829950	108.4658868
H	56.6693006	64.2482737	109.4634805
H	55.6361895	65.2929778	108.5173574
C	55.2472766	63.2656798	108.2042136
O	54.4966484	62.9030550	109.1227359
N	55.1612941	62.7200390	106.9735981
H	55.6988231	63.1357767	106.2136712
C	54.2231388	61.6245184	106.6973908
H	53.8227334	61.3119453	107.6629535
C	55.0028357	60.4424927	106.1204364
O	55.0802646	59.3335496	106.6616955
N	55.6313150	60.7150112	104.9549132
H	55.5478154	61.6416894	104.5456765
C	56.4053912	59.7348342	104.2208228
H	55.7272473	58.9851346	103.7827976
C	57.0955168	60.4636010	103.0594169
H	57.6502921	61.3230103	103.4636014
H	57.8195454	59.7869963	102.6024949
C	56.0822623	60.9350962	101.9904001
H	56.0411782	60.1889799	101.1889841
H	55.0635470	61.0053262	102.3956262
C	56.4651312	62.2969390	101.4087736
H	56.3645410	63.0711125	102.1806424
H	57.5219432	62.2851512	101.1272798
N	55.6513498	62.6488533	100.2522681
H	54.6349961	62.4940342	100.3520923
C	56.0791689	63.3813761	99.2177244
N	57.3845069	63.5908380	98.9994533
H	58.1068513	63.1588779	99.5607320
H	57.7100125	64.0996942	98.1784171
N	55.1790895	63.9335059	98.3935027
H	54.2725152	63.4222090	98.3514647
H	55.5198849	64.2600850	97.4982259
C	57.3626180	58.8428217	105.0460312
O	57.4458537	57.6922249	104.6293714
C	63.1104913	67.3493074	107.8202325
H	64.1219040	67.4414492	108.2399082
H	63.0086597	66.3625314	107.3617887
C	62.9393037	68.4876711	106.7978179
O	62.9907196	69.6674063	107.1981544
O	62.7761374	68.1676942	105.5587136
C	58.8444309	69.1435372	111.4349266
H	58.1165875	69.6876709	112.0431850
H	59.7414848	69.7628119	111.3413437
C	58.3546695	68.8289968	110.0376866
C	57.1537751	68.1342549	109.8059853
H	56.4996681	67.8752270	110.6361305
C	56.8073725	67.7450999	108.5126286
H	55.8731685	67.2242071	108.3236800
C	57.6461331	68.0327288	107.4361666
H	57.3652438	67.7054086	106.4409006
C	59.1542575	69.1833582	108.9360440
H	60.0578602	69.7717541	109.0943981
C	58.8081572	68.7808490	107.6423273
H	59.4428800	69.0537871	106.8025230
C	67.5188033	66.0627754	99.8323954
O	68.5829593	65.4426647	99.8676217
N	67.3607165	67.2735556	99.2460380
H	66.4143636	67.6852709	99.2838502
C	68.3388365	67.9551653	98.4039094

H	68.6900065	67.2574608	97.6340781
C	69.0488041	71.7411537	103.6438998
H	69.9392171	72.1149179	104.1646002
H	68.4521486	72.6218082	103.3685307
C	68.2757300	70.8924025	104.6513486
H	68.8810356	70.0563091	105.0185107
H	67.9949517	71.5112555	105.5081880
N	67.0329173	70.2934732	104.0887952
H	67.2405910	69.5603868	103.3297062
H	66.4671616	69.7812909	104.7792518
H	66.3792733	70.9778606	103.6537998
C	69.8753864	64.8039308	103.9425081
H	69.2113837	64.0344154	104.3531881
H	70.7609604	64.8891701	104.5857043
C	69.1053095	66.1460551	103.9579537
O	67.9898165	66.1668091	103.3451308
O	69.6485622	67.1077717	104.5481177
C	61.0758322	66.2973573	99.4188856
H	61.8666091	66.7029723	98.7902504
H	60.2526775	67.0105015	99.3838889
N	61.0103655	66.8885226	101.8879913
C	61.5950647	66.2144788	100.8184405
C	61.8449285	66.7653090	102.9278884
H	61.7340845	67.1970611	103.9183622
N	62.9193793	66.0310595	102.5729861
H	63.7589683	65.8472204	103.1555555
C	62.7872828	65.6784999	101.2505515
H	63.5357131	65.1052947	100.7237955
C	49.9718389	58.7630268	95.4676299
H	49.7009931	59.4626574	94.6729572
H	49.0386443	58.2653260	95.7573732
N	49.8731153	60.7370500	96.9896598
H	49.0799435	61.2625288	96.5677629
C	50.4668661	59.5374044	96.6468805
C	50.4551311	61.1872040	98.1208286
H	50.1998267	62.1335784	98.5805086
N	51.3987078	60.3561362	98.5413647
C	51.4054540	59.3140749	97.6306416
H	52.0544601	58.4583453	97.7347957
C	68.0963267	72.7525657	94.1452138
H	67.8941955	71.8010116	93.6357672
H	68.5375242	72.5346467	95.1238112
C	66.8014150	73.5519513	94.3495629
H	67.0168886	74.4418998	94.9514238
H	66.4021654	73.9024451	93.3874105
N	65.7781218	72.7841384	95.0619293
H	65.5798826	71.8204008	94.7539355
C	64.9802807	73.2681607	96.0363532
N	64.9451170	74.5824588	96.3094325
H	65.2869068	75.2747210	95.6509472
H	64.6441997	74.8677778	97.2617570
N	64.2224478	72.4411659	96.7572379
H	64.3190880	71.4127762	96.7503349
H	63.4976283	72.8090046	97.3830653
Mo	59.0346340	68.0272623	101.9358911
Fe	52.9348085	66.1500757	104.6870131
Fe	54.8964402	67.9263991	104.7477067
Fe	54.2023717	66.7698475	102.4628858
Fe	55.4371505	65.3923274	104.3080851
Fe	57.7194412	66.0925129	103.2948804
Fe	57.1518590	68.6326936	103.6975297
Fe	56.4967741	67.5288948	101.4814626
S	54.6252290	66.2879066	106.2526331
S	52.8875072	68.1719812	103.7371924
S	53.6411329	64.6750615	103.0697020
S	59.0865099	67.6420940	104.2255174
S	57.3170448	69.6402019	101.7123534
S	58.1129255	66.0755037	101.0694974
S	55.9950268	69.7707154	105.1832125
S	57.3089879	64.1625236	104.3192548

S	54.6675403	67.1332240	100.3287359
C	55.9861757	67.0375411	103.3440477
O	60.4571495	69.6543193	102.2177312
O	59.5941824	68.8668138	99.9673332
O	60.2110564	70.7015015	98.8329880
O	60.5067627	71.5883843	103.8217123
O	61.0032296	73.6145087	103.0116220
O	64.6536301	68.2583766	99.2423424
O	64.8353864	69.0683542	101.3221763
C	60.7710631	70.5648021	101.1499215
C	60.1263070	70.0251488	99.8789985
C	60.1679319	71.9373941	101.4979221
C	60.5988685	72.4315056	102.8763515
C	62.3006646	70.5712666	100.9335476
C	62.7436344	69.3280436	100.1609245
C	64.1934868	68.8787761	100.2460131
H	60.3861610	70.2314412	103.0512903
H	62.1812690	68.4709191	100.5487472
H	62.4914900	69.4323252	99.1027274
H	62.5862939	71.4773162	100.3940037
H	62.7533988	70.5918313	101.9270166
H	59.0787996	71.8003751	101.5471886
H	60.4016877	72.6703471	100.7232060
O	58.8250373	68.8505228	95.4669814
H	58.4333357	68.4554436	96.2717399
H	59.7198686	69.1161437	95.7504287
O	51.9953537	64.5785630	96.7946858
H	52.5189421	63.8335353	96.4025650
H	51.0547891	64.2870070	96.7699462
O	57.9055257	68.0274654	98.0114328
H	57.4056682	67.2988070	98.4021302
H	58.5066439	68.3390460	98.7199492
O	46.6764584	60.5513999	98.3255731
H	47.0390555	61.2712587	97.7619001
H	47.3871903	60.3089050	98.9302582
O	51.8175404	65.0730121	99.3844781
H	52.0323385	64.8363949	98.4371508
H	52.6461430	65.4012941	99.7717520
O	52.1164813	69.9482040	112.0600962
H	52.9193646	70.2803971	112.5120204
H	52.2561116	70.0427098	111.0695540
O	63.9832107	69.6272888	96.8432296
H	63.0084048	69.5717258	96.7559616
H	64.2343532	69.0870127	97.6226678
O	61.2377078	69.9650385	96.4538532
H	61.2895929	70.8285265	95.9956114
H	60.7922985	70.1693882	97.3131830
O	52.9575207	61.7458520	100.9232708
H	52.5400664	61.2014567	100.2286382
H	52.2642777	62.3785574	101.1850379
O	67.3350500	68.4249541	102.1976201
H	67.4953658	67.5654702	102.7051866
H	66.4263587	68.4324013	101.8307616
O	50.5348211	63.2969555	100.9635259
H	51.0197004	63.9128163	100.3459067
H	49.8913939	63.8681203	101.4218371
O	61.8900478	73.0608851	98.4946650
H	61.3659985	72.2505303	98.6488916
H	62.2765276	73.3122355	99.3643284
O	65.0063525	68.3243186	104.0971800
H	64.2021960	68.2321740	104.6627821
H	64.6770939	68.6049723	103.2260490
O	63.2628503	74.3558117	104.4983527
H	63.6248971	73.5996285	105.0184226
H	62.3777492	74.0734551	104.2024272
O	62.7264925	74.1201916	100.8970405
H	62.0714219	74.0629840	101.6227829
H	63.5897786	74.1582164	101.3740637
O	59.8931412	75.2693819	101.1677803
H	58.9985530	74.8878163	101.0941709

H	60.2988417	74.7476073	101.8943015
O	57.5493997	73.8487386	100.7000678
H	57.7539268	72.9347488	100.4611921
H	56.8773803	73.7663980	101.3959045
O	64.9157830	71.4024484	102.6793812
H	64.9270749	70.5975554	102.1018963
H	64.1978935	71.1742937	103.3272592
O	65.0101538	72.3526902	99.9668558
H	64.6215339	72.2282533	100.8524041
H	65.9340126	72.5925168	100.1990386
O	64.5209748	74.8996954	98.9767702
H	64.6734040	73.9840598	99.3173166
H	63.7361362	75.1729740	99.4760080
O	53.4184502	62.0957477	98.0012730
H	53.4379601	62.0652606	97.0136883
H	52.7302499	61.4679390	98.2900986
O	55.9146150	70.6718159	108.3359206
H	56.1315955	70.4482401	107.4126117
H	56.4108580	70.0117369	108.8384067
O	62.9376683	70.4396941	104.2227417
H	62.0649030	70.8693280	104.2105603
H	62.8280366	69.5830645	104.7429154
h	60.7144868	65.3468530	99.0264086
h	47.0853274	61.5996144	103.9743407
h	48.2854700	63.5490683	107.4862707
h	69.3744581	71.2424330	102.7310503
h	70.1821535	64.4771802	102.9489311
h	49.8679741	68.8928760	107.7369596
h	50.3202180	68.2461422	97.9636006
h	50.9875025	73.2889016	109.2079427
h	56.7686724	71.2907887	97.6790783
h	58.3875233	72.8926579	107.9944617
h	62.4137733	67.4610343	108.6509962
h	53.6752562	73.5633471	102.3619589
h	59.1937489	68.2568103	111.9638496
h	64.7059670	61.0652004	106.2295550
h	61.3721182	62.3707586	104.5693632
h	53.3900397	61.9295627	106.0641761
h	57.9643843	59.1185925	105.9119960
h	67.8431869	68.7974262	97.9212138
h	69.2529939	68.2405573	98.9244234
h	66.5862093	65.7030332	100.2670460
h	55.2580748	71.6997238	112.1288496
h	44.2872188	70.7477009	112.6041368
h	53.2753909	66.7643894	111.1351461
h	47.8440545	64.9465355	99.0148767
h	50.6604934	62.6967388	93.5461435
h	50.6659569	58.0216438	95.0718791
h	46.8697792	61.4729465	102.9597330
h	68.8152128	73.3168361	93.5511861

205QM – [MoFe7S9C] - BS7-235 (218 atoms total with link atoms, marked with lowercase h)

C	54.3073837	72.8414072	102.8678061
H	54.1221856	73.4649733	103.7468007
C	53.6078706	71.4925062	103.0394963
H	53.8303267	71.0991833	104.0339620
H	52.5197263	71.5265964	102.9184099
H	54.0005046	70.7583642	102.3347373
C	55.8216716	72.6145700	102.7013851
H	56.0053140	71.8937041	101.8952733
H	56.4063591	73.5123713	102.4792152
H	56.2471935	72.1843084	103.6120775
C	56.2236567	71.5269929	98.8194920
H	57.0495454	71.4425769	99.5335938
H	55.7857921	72.5228048	98.9290083
N	55.2283529	70.5221937	99.1770578
H	55.5881107	69.6240139	99.5020642
C	53.9407367	70.7687692	99.4260230
N	53.3093277	71.8213461	98.8542013
H	53.8172787	72.4195055	98.2099659

H	52.5526159	72.2684626	99.3802597
N	53.2661576	69.9663919	100.2383203
H	53.7084258	69.1029654	100.5790153
H	52.2584974	70.0344932	100.3382825
C	59.4357648	73.1239788	107.7432281
H	59.2369421	73.1683007	106.6713281
H	59.8204561	74.0915825	108.0811029
C	60.4555485	72.0461767	108.0623548
O	60.9025028	71.8650809	109.2172475
N	60.8649588	71.3097484	107.0192847
H	60.4687370	71.4532538	106.0991585
H	61.5950337	70.5869418	107.1232567
C	51.2198479	72.5611633	108.8714489
H	51.1501063	72.1767680	109.8974979
H	50.3720620	72.1431087	108.3081115
N	53.1839121	71.0763346	109.1176537
C	52.5130286	72.0168283	108.3550040
C	54.2181612	70.6908073	108.3849376
H	54.9687255	69.9578001	108.6553598
N	54.2398302	71.3404451	107.1954172
H	54.8564821	71.0876577	106.4161705
C	53.1546071	72.1781311	107.1450170
H	52.8973232	72.7386909	106.2578506
C	50.9455810	68.9152873	98.4936042
H	51.7872804	68.2128439	98.4583273
H	51.2794361	69.8778478	98.0911231
C	50.4232609	69.0683955	99.9196411
C	49.8838690	70.2912041	100.3600426
H	49.8344795	71.1392825	99.6816183
C	49.4188263	70.4579067	101.6663261
H	49.0267396	71.4170576	101.9935062
C	49.4742148	69.3917582	102.5763122
O	49.0956516	69.6272049	103.8577140
H	49.2608130	68.8664524	104.4705859
C	50.4450932	68.0033678	100.8404588
H	50.8739458	67.0454355	100.5552330
C	49.9525977	68.1477853	102.1370786
H	50.0033255	67.3106354	102.8295503
C	49.6737730	64.9612444	104.9536770
H	50.0902958	64.6812376	103.9814273
H	48.9661206	65.7835603	104.8111677
S	51.0578101	65.4662692	106.0695978
C	50.0268871	69.0363317	106.9112584
H	49.6511436	70.0241416	106.6271678
H	51.1213945	69.0715955	106.8395718
O	49.4886806	68.0840775	106.0053480
H	50.0909368	67.2927967	106.0099016
C	57.0103995	62.1626693	100.9441950
H	57.6065704	62.9508947	101.4206200
H	57.6823977	61.4935458	100.3893271
N	56.0109650	62.7432294	100.0551421
H	55.0221769	62.6166886	100.3180868
C	56.2948935	63.4839228	98.9847637
N	57.5620856	63.7114357	98.6445964
H	58.3338859	63.2588297	99.1357412
H	57.8187091	64.2716534	97.8330259
N	55.2929853	64.0133013	98.2574651
H	54.3945858	63.5051366	98.2791024
H	55.5282484	64.3996373	97.3529494
C	63.0185870	67.2288661	107.9864200
H	64.0110752	67.3863732	108.4316413
H	62.9505251	66.2011954	107.6219259
C	62.8698486	68.2241870	106.8311955
O	62.9031544	69.4552216	107.0912380
O	62.7624694	67.7484277	105.6552112
C	58.6400946	69.2979738	111.3784007
H	57.9456507	69.8752826	111.9943954
H	59.5280236	69.9115859	111.2031833
C	58.0890903	68.9449462	110.0148100
C	56.8186277	68.3754077	109.8327864

H	56.1620332	68.2277813	110.6891233
C	56.4137031	67.9529592	108.5662439
H	55.4358839	67.5006430	108.4147942
C	57.2634168	68.1006783	107.4672366
H	56.9460847	67.7418824	106.4946028
C	58.9103222	69.1430819	108.8921130
H	59.8788424	69.6240121	109.0219948
C	58.5037861	68.7214828	107.6245086
H	59.1528012	68.8736809	106.7654011
C	68.9070860	71.9169496	103.5712257
H	69.7877484	72.3249321	104.0859816
H	68.2788828	72.7667229	103.2775133
C	68.1641857	71.0425875	104.5862798
H	68.7865844	70.2148096	104.9452462
H	67.8742730	71.6461962	105.4526908
N	66.9280086	70.4304044	104.0299273
H	66.2412398	71.1138362	103.6329822
H	67.1562979	69.7342014	103.2484985
H	66.3859642	69.8607179	104.6986496
C	69.8849506	65.0538487	104.0915896
H	69.2061698	64.2743272	104.4628678
H	70.7506826	65.1443572	104.7574081
C	69.1311646	66.4088428	104.0793775
O	68.0048606	66.4083943	103.4914460
O	69.7238977	67.3778864	104.6019464
C	61.2680189	66.4237254	99.2809528
H	62.1668262	66.6453172	98.7018101
H	60.5665268	67.2492961	99.1636096
N	60.9552117	66.7844625	101.8115791
C	61.6604426	66.2783579	100.7192311
C	61.7352001	66.6101350	102.8851466
H	61.5185686	66.9054431	103.9049045
N	62.8924789	66.0111693	102.5352332
H	63.7153151	65.8619226	103.1418180
C	62.8628291	65.7928640	101.1788322
H	63.6680071	65.3236780	100.6380777
Mo	58.9425920	67.8963044	101.8679523
Fe	52.7165666	66.1174858	104.6241244
Fe	54.7169093	67.8545985	104.6326700
Fe	54.0484647	66.6998171	102.3791016
Fe	55.2370185	65.3059003	104.2753512
Fe	57.5919967	65.9719582	103.3182441
Fe	57.0142814	68.5162934	103.5778429
Fe	56.3993610	67.3373190	101.4049797
S	54.4171895	66.2626097	106.1844884
S	52.6981292	68.1217298	103.6174109
S	53.4277291	64.6282747	103.0222125
S	58.9609987	67.6025188	104.1719854
S	57.1921862	69.4533198	101.5727205
S	58.0514999	65.8846476	101.0931922
S	55.8352794	69.6870105	104.9852664
S	57.0912984	64.0509841	104.3935449
S	54.5423076	67.0499308	100.2438434
C	55.8434624	66.9156566	103.2799229
O	60.3317636	69.4990967	102.1257091
O	59.4558175	68.6902433	99.8983040
O	60.0504570	70.4986891	98.7382234
O	60.0294942	71.2011308	103.7725968
O	60.1250053	73.3444540	103.2759629
O	64.6702970	68.3654578	99.4058240
O	64.8131196	69.4502470	101.3518403
C	60.5591701	70.4392475	101.0890163
C	59.9637988	69.8610817	99.8057020
C	59.8577023	71.7763042	101.4482393
C	60.0368760	72.1699910	102.8996483
C	62.0835372	70.6338936	100.8559917
C	62.6740619	69.3608724	100.2479666
C	64.1658505	69.0708320	100.3455097
H	60.1106104	70.2834873	103.1850945
H	62.2197130	68.5144082	100.7766613

H	62.3742351	69.2627508	99.2000127
H	62.2409428	71.4984927	100.2005553
H	62.5478100	70.8694449	101.8176748
H	58.7719315	71.6552178	101.3174047
H	60.1875312	72.5872920	100.7958361
O	58.5708048	68.6393488	95.6410731
H	59.5062488	68.6906140	95.9126723
H	58.1091816	68.2737853	96.4191206
O	62.6139846	69.4984234	103.6202463
H	61.8474792	69.2690160	103.0658338
H	62.5228622	68.9672541	104.4515613
O	57.4161785	67.9860216	98.1564837
H	56.7780445	67.4264126	98.6241671
H	58.1177783	68.1872675	98.8067448
O	64.0160853	66.2138981	97.7908288
H	64.6070877	66.4028744	97.0337071
H	64.2257157	66.9169659	98.4454883
O	63.9335016	69.0501431	96.8990195
H	64.1776188	68.8630812	97.8439642
H	64.3255606	68.2986861	96.4156713
O	61.1156247	69.1930498	96.6003429
H	62.0798922	69.1412765	96.7622620
H	60.7063017	69.6098334	97.3829848
O	67.2761115	68.5867332	102.1429764
H	67.4025477	67.7724201	102.7115610
H	66.3460786	68.6687921	101.8315465
O	61.8337096	72.1829064	97.6939940
H	61.2382927	71.5893045	98.2161799
H	61.5275600	72.0274745	96.7817169
O	64.9775410	68.4143237	104.1866127
H	64.3150703	68.1478708	104.8625072
H	64.3838262	68.8380343	103.5314716
O	58.3449034	74.9501745	101.9020442
H	57.6687656	75.2493965	102.5366931
H	58.9522253	74.4147806	102.4459999
O	61.5376079	74.6091983	99.0336058
H	61.5516482	73.7250471	98.6130902
H	61.7003670	74.4989580	100.0045742
O	61.9408623	74.5274127	101.6438958
H	61.2322177	74.2273554	102.2453540
H	62.5940551	74.9563954	102.2323511
O	64.6965572	71.6706475	102.9342372
H	64.5757735	70.8712061	102.3672075
H	64.1695619	71.4882791	103.7429121
O	57.8453670	71.9968705	105.3560623
H	58.5442521	71.6279471	104.7959363
H	57.2460062	71.2393168	105.4747921
h	60.8233054	65.5169076	98.8711009
h	49.1212490	64.0901610	105.3058106
h	56.6199150	71.4019509	97.8118160
h	56.5004113	61.6018218	101.7274123
h	51.1230988	73.6468221	108.8642543
h	53.9513002	73.4225270	102.0171761
h	58.4792645	72.9525346	108.2369703
h	62.2907815	67.4061398	108.7782156
h	59.0080210	68.4373487	111.9369898
h	69.2491923	71.4280137	102.6591006
h	70.2494841	64.7489775	103.1106533
h	49.8022530	68.8459484	107.9607158
h	50.1497327	68.5230204	97.8605012