Electronic Supplementary Material (ESI) for Dalton Transactions

A re-investigation of $[Fe(L\text{-cysteinate})_2(CO)_2]^{2-}$: an example of non-heme CO coordination of possible relevance to CO binding to ion channel receptors. Supplementary Material

Lindsay Hewison,[a] Tony R. Johnson,[a] Brian E. Mann,*[a] Anthony J. H. M. Meijer,[a] Philip Sawle[b] and Roberto Motterlini[c]

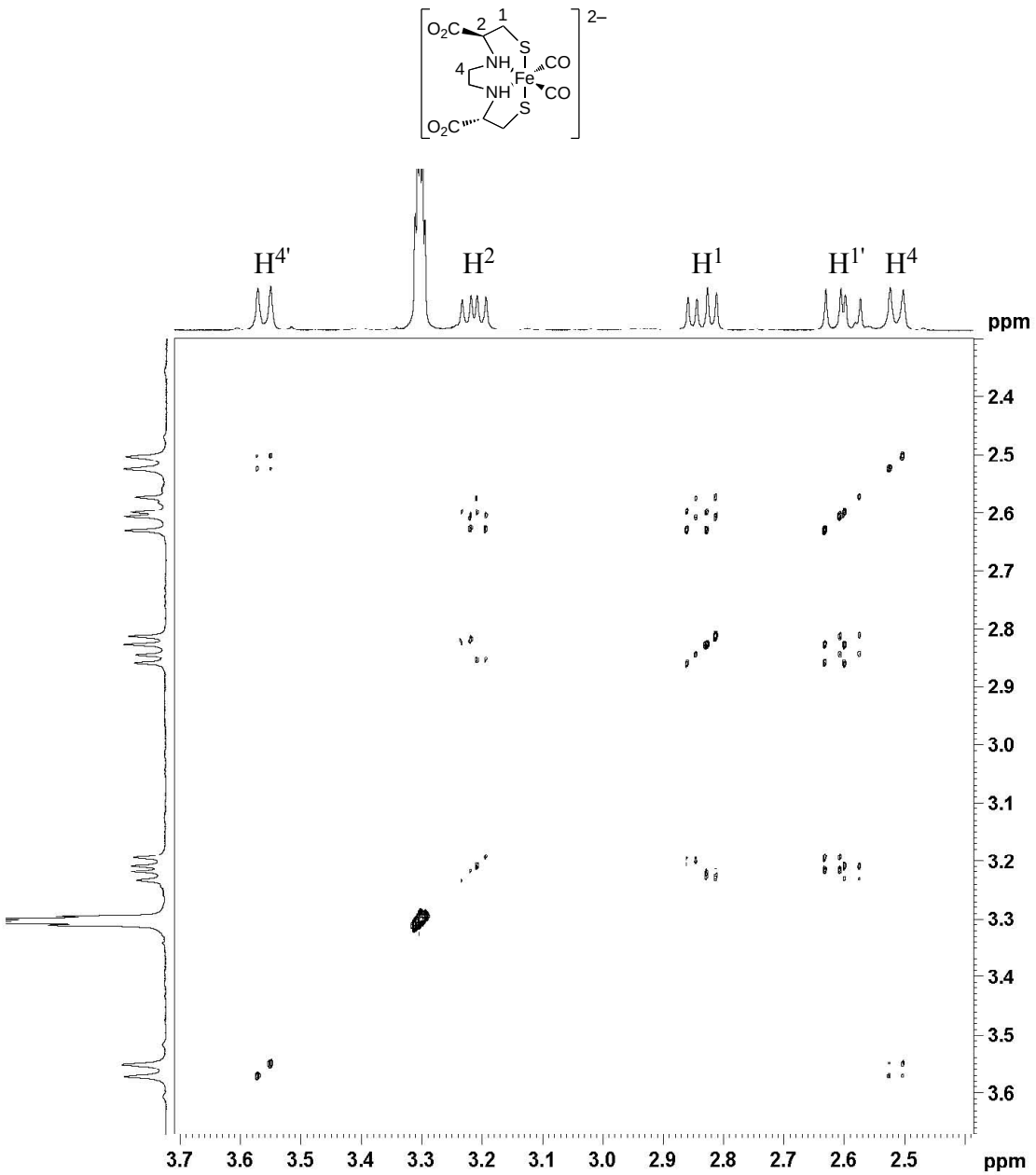

Fig. S1 400 MHz COSY-45 NMR spectrum of $K_2[Fe\{SCH_2CH(CO_2)NHCH_2\}_2(CO)_2]$ in CD_3OD.

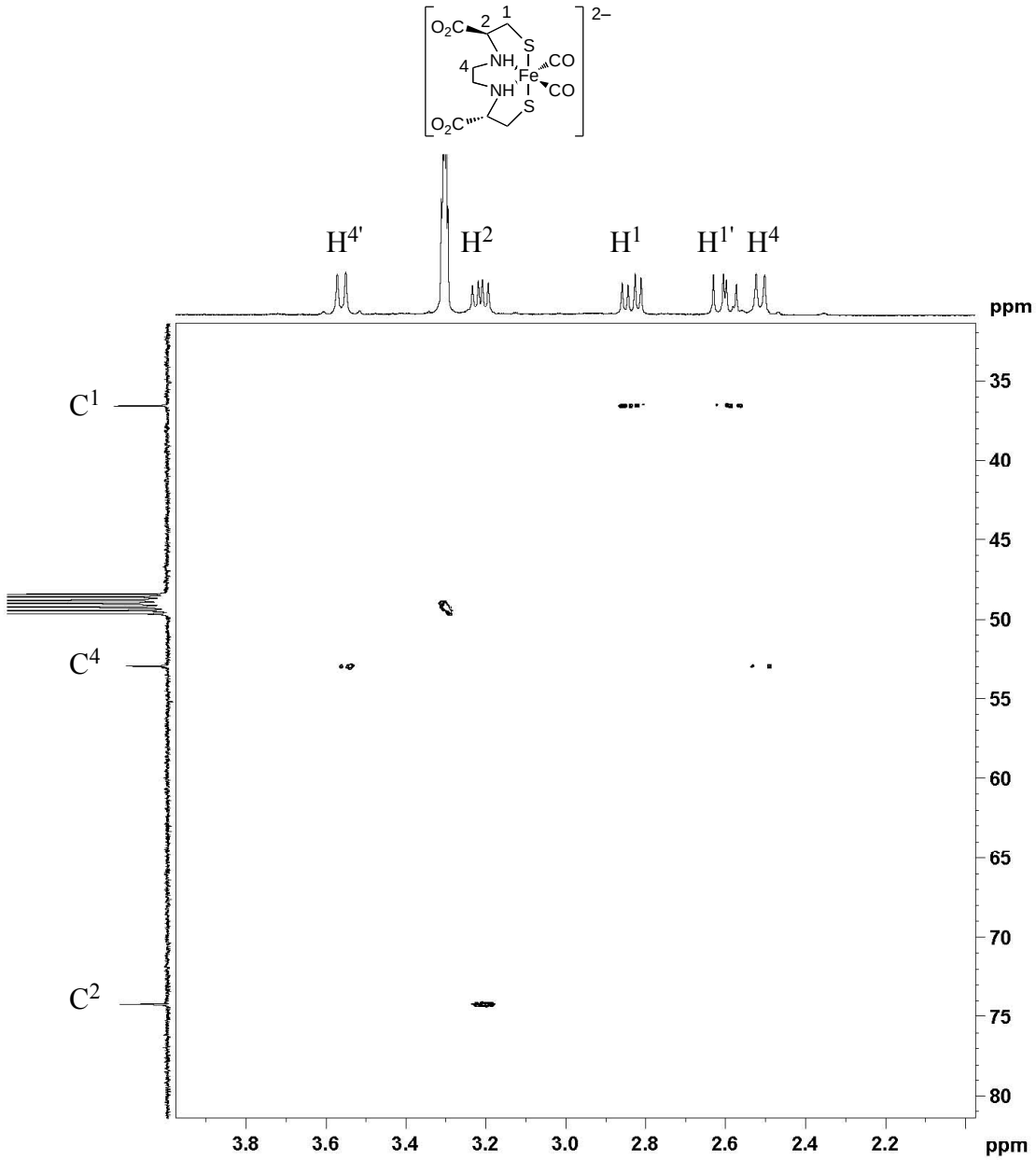

Fig. S2 100.62 MHz ^{13}C-^{1}H correlation NMR spectrum of $K_2[Fe\{SCH_2CH(CO_2)NHCH_2\}_2(CO)_2]$ in CD_3OD.

Electronic Supplementary Material (ESI) for Dalton Transactions

A re-investigation of $[Fe(L\text{-cysteinate})_2(CO)_2]^{2-}$: a mechanistic model for the possible binding of CO to ion channel receptors. Supplementary information

Lindsay Hewison,[1] Tony R. Johnson,[1] Brian E. Mann,[1] Anthony J. H. M. Meijer,[1] Philip Sawle,[2] and Roberto Motterlini[2,3]

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(Dated: May 13, 2011)

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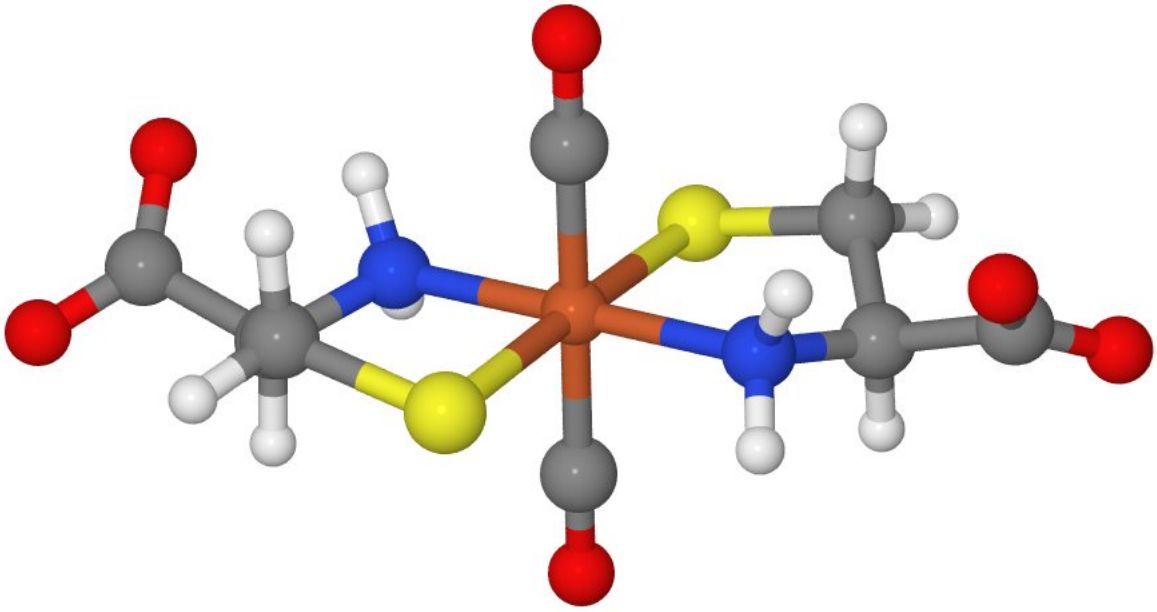
1. STRUCTURE 1 (*IN VACUO*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.28537934 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

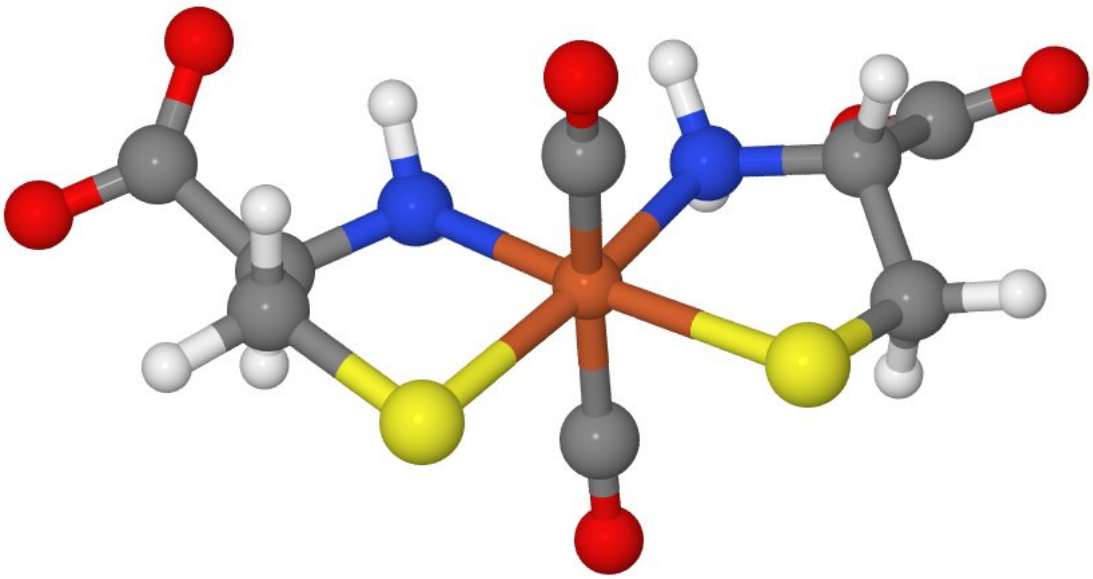
29

N	1.15206325	-1.53092420	0.74678236
H	1.26189315	-1.53346968	1.76882589
C	2.56987405	-1.59469283	0.27456447
H	2.58932066	-2.07376051	-0.70725477
C	3.10526252	-0.17256454	0.14177553
C	3.44373775	-2.42521715	1.28891444
H	3.18757153	0.26755732	1.14167917
H	4.10378361	-0.21102031	-0.29360700
S	2.01938438	0.89720964	-0.90189272
O	2.94185328	-2.54277277	2.43691921
H	0.72521061	-2.43794131	0.57582957
O	4.53209877	-2.83508992	0.84402442
Fe	-0.00665004	-0.04067471	-0.06488239
S	-2.03889942	-1.01830351	0.70895082
C	-3.05525589	0.48302883	0.35432583
C	-2.63721299	1.17940676	-0.93680573
H	-2.95236373	1.18995106	1.18497157
H	-4.10546350	0.20119150	0.27874821
N	-1.16622758	1.44510651	-0.88347536
H	-2.84129643	0.51500684	-1.77987957
C	-3.42721701	2.53009939	-1.12080956

H	-1.12727189	2.36910343	-0.43476650
O	-2.77793455	3.56206298	-0.80916601
O	-4.60075331	2.41141319	-1.51977050
H	-0.85242087	1.65337837	-1.82807446
C	0.14979780	0.92416352	1.47443569
O	0.24860173	1.52935469	2.44025421
C	-0.16202313	-1.00340366	-1.60209525
O	-0.25967199	-1.60861218	-2.56994128

2. STRUCTURE 2 (*IN VACUO*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]	
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$	
Charge	:	-2	
Multiplicity	:	1	
Energy	:	-2932.28456247	a.u.
Number of imaginary frequencies	:	0	

Cartesian Co-ordinates (XYZ format)

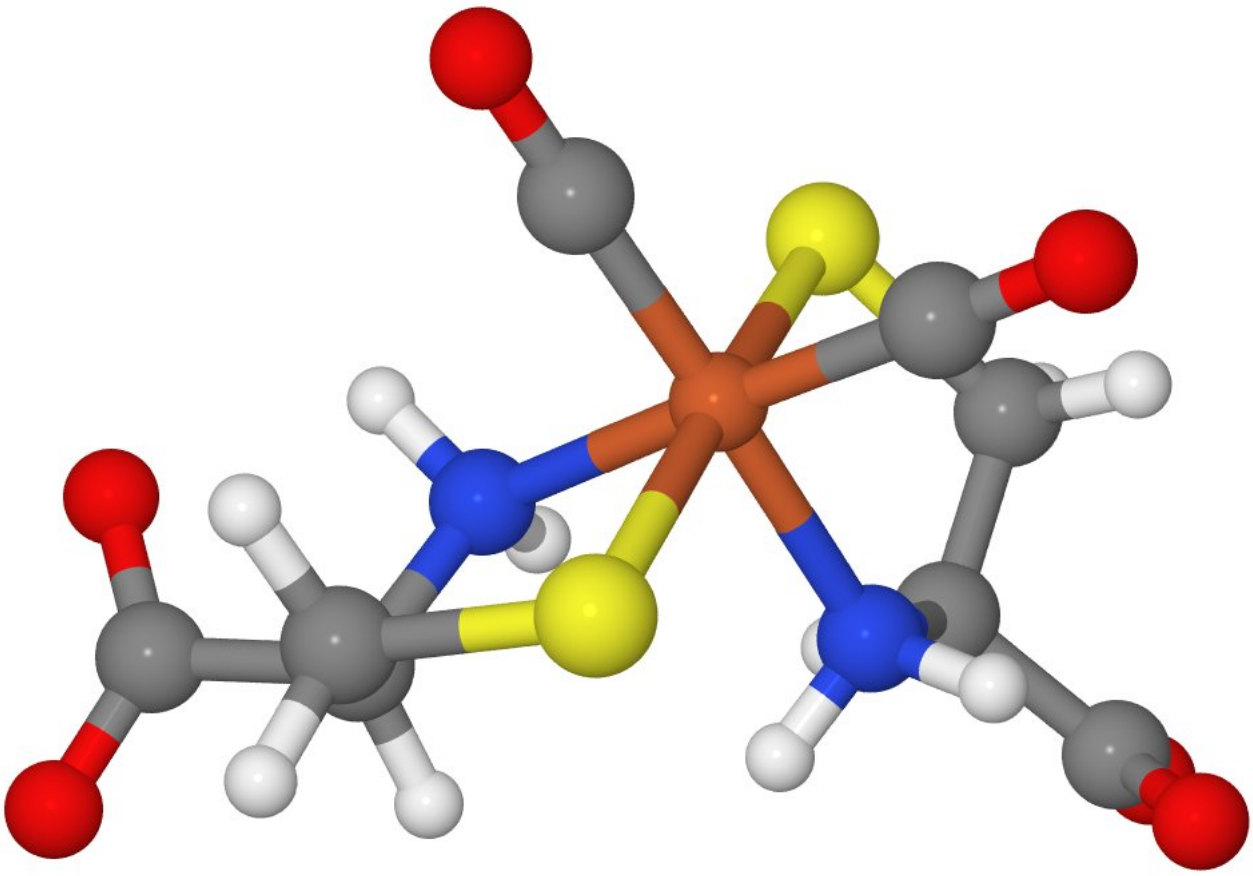
29

N	1.24031305	-1.10264802	0.55627751
H	1.25715625	-1.19145787	1.58366549
C	2.70614862	-1.08083737	0.25207576
H	2.87149382	-1.55624676	-0.71760410
C	3.16732955	0.37008405	0.17645805
C	3.49036193	-1.86478102	1.37142515
H	3.11504388	0.80996621	1.17876768
H	4.20814085	0.39516538	-0.14764574
S	2.13709664	1.36938429	-0.98180103
O	2.84352994	-2.03557086	2.43966794
H	0.88790345	-2.00876927	0.25729766
O	4.65507364	-2.19242311	1.08199286
Fe	0.08076427	0.39060587	-0.24019514
S	-1.43349922	2.03063703	-1.10834074
C	-2.90025163	0.92110449	-0.97003555
C	-2.90302348	0.12969889	0.33275363
H	-2.90258741	0.21781756	-1.81041622
H	-3.81292653	1.51508784	-1.02637708
N	-1.58651066	-0.56975418	0.47130027
H	-3.02292442	0.82311779	1.16847086
C	-4.06892729	-0.92996854	0.34693617
H	-1.81233752	-1.48982155	0.06366280

O	-3.70215583	-2.11256790	0.11101732
O	-5.20705414	-0.47361007	0.55685472
H	-1.46577930	-0.78384244	1.45833421
C	0.23173973	1.51680768	1.18438613
O	0.34665430	2.28997397	2.02289629
C	0.01241160	-0.33884579	-1.90859962
O	-0.02004349	-0.71578568	-2.99071097

3. STRUCTURE 3A (*IN VACUO*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.29962596 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

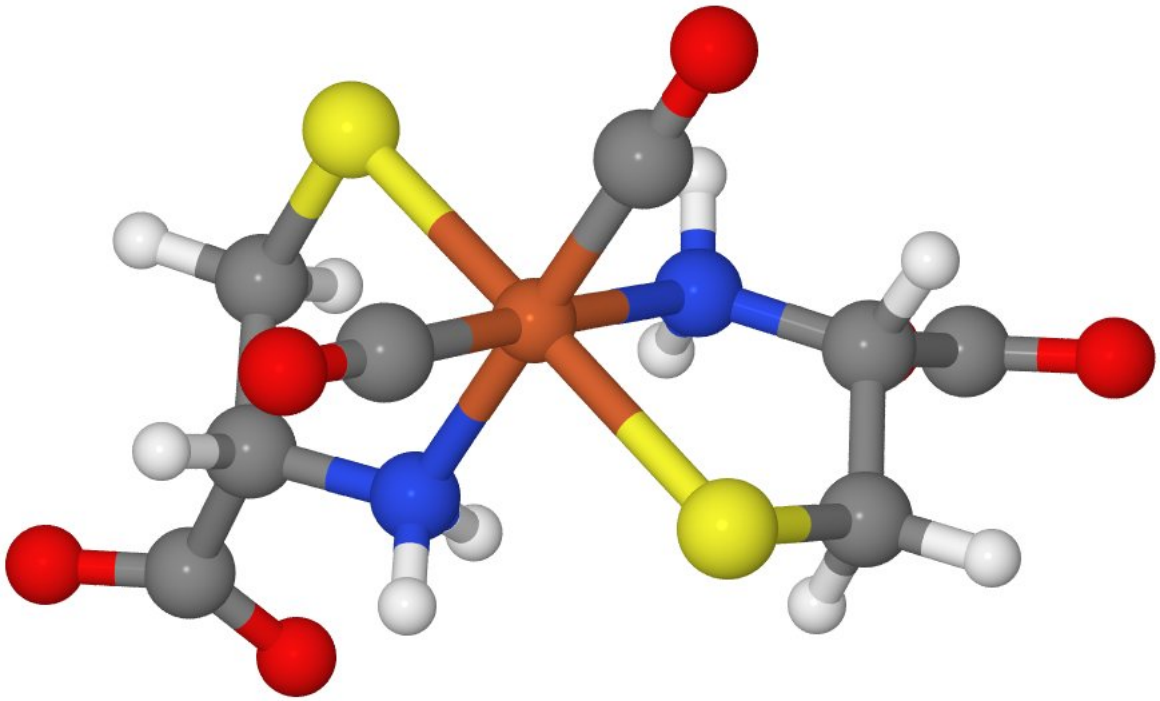
29

N	0.88826460	-0.62092507	1.09170771
H	0.93432862	-0.62696910	2.12019277
C	2.33244896	-0.62252235	0.71225119
H	2.45995736	-1.17480028	-0.22229035
C	2.77955437	0.82016408	0.50747794
C	3.19618082	-1.30571938	1.84409308
H	2.80086470	1.32731354	1.47760487
H	3.79064965	0.83103043	0.09984917
S	1.65264475	1.74131048	-0.63180023
O	2.63023639	-1.36881590	2.96524954
H	0.47160619	-1.52578247	0.88441020

O	4.33885622	-1.65850496	1.49907100
Fe	-0.33639625	0.80421615	0.24119887
S	-2.21722507	-0.39234489	1.03747582
C	-2.64725542	-1.12960410	-0.60187501
C	-1.40882671	-1.56748700	-1.37480533
H	-3.19416666	-0.38955882	-1.19517267
H	-3.30112290	-1.98859119	-0.44959670
N	-0.44562522	-0.42710212	-1.41018605
H	-0.94648737	-2.41546559	-0.86313599
C	-1.80510080	-1.99648476	-2.84206247
H	-0.68159473	0.02840957	-2.30280590
O	-1.57945991	-1.12413847	-3.71914721
O	-2.32629871	-3.12228918	-2.94282198
H	0.49665725	-0.77116126	-1.58084273
C	-0.19910431	1.81323171	1.68922782
O	-0.10822655	2.47836804	2.62128878
C	-1.40390384	1.98125958	-0.53938752
O	-2.10679960	2.74433899	-1.03243542

4. STRUCTURE 3B (*IN VACUO*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.29471357 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

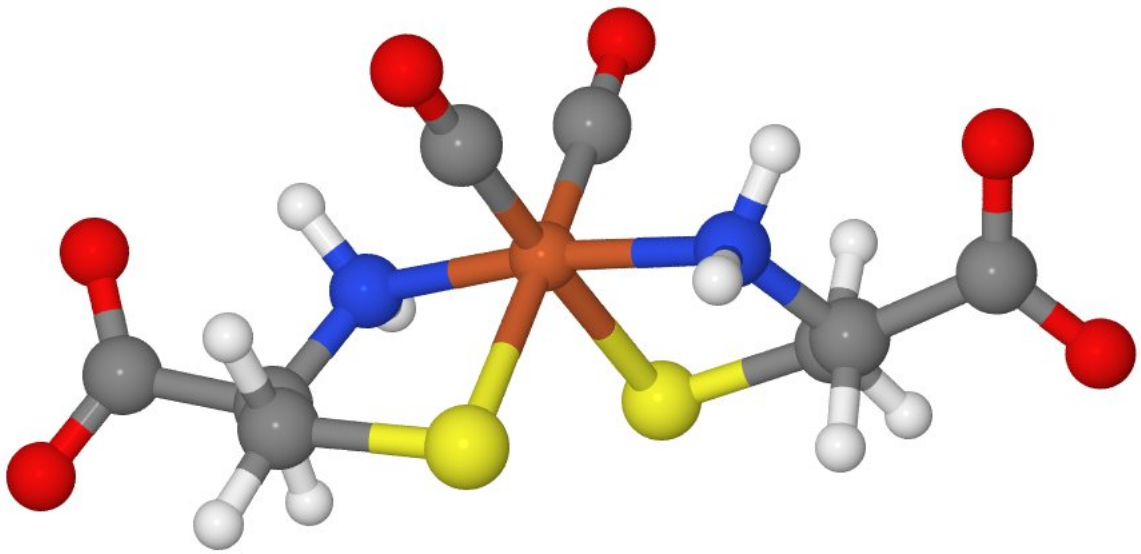
29

N	1.21736336	-0.51731163	0.75866812
H	1.30143523	-0.43027744	1.76907754
C	2.58267999	-0.54626358	0.15663163
C	2.43007970	-0.43863922	-1.35459435
H	3.41683793	-0.34015319	-1.80609214
H	1.97163367	-1.35687447	-1.73581719
S	1.38748527	1.01332593	-1.84568369
H	0.88419610	-1.48180306	0.65694225
Fe	-0.02776810	0.95645678	0.05547335
S	-1.43824232	0.71447212	1.94517982
C	-2.39785194	-0.72871017	1.28726518
C	-2.54793572	-0.67136866	-0.22705109
H	-3.38737822	-0.73885411	1.74332726
H	-1.88672471	-1.65686977	1.56273854
N	-1.18797088	-0.49608314	-0.81616509
H	-1.27893436	-0.29911262	-1.81040967
H	-0.80005527	-1.44534099	-0.82355362
C	0.98979247	2.17994595	0.83660376

O	1.63884521	2.98510981	1.33746004
C	-1.11461306	2.20189357	-0.58482736
O	-1.80854702	3.02179098	-0.99305439
C	3.36322927	-1.85590148	0.55605906
O	2.64367652	-2.78226995	1.00146556
O	4.59314060	-1.81232202	0.35630375
H	3.13468480	0.32384485	0.52078563
H	-3.14966416	0.20169361	-0.49174622
C	-3.25320411	-1.96940327	-0.77630091
O	-2.48255515	-2.79696965	-1.31993949
O	-4.48340416	-2.01839590	-0.57970226

5. STRUCTURE 4A (*IN VACUO*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.28997292 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

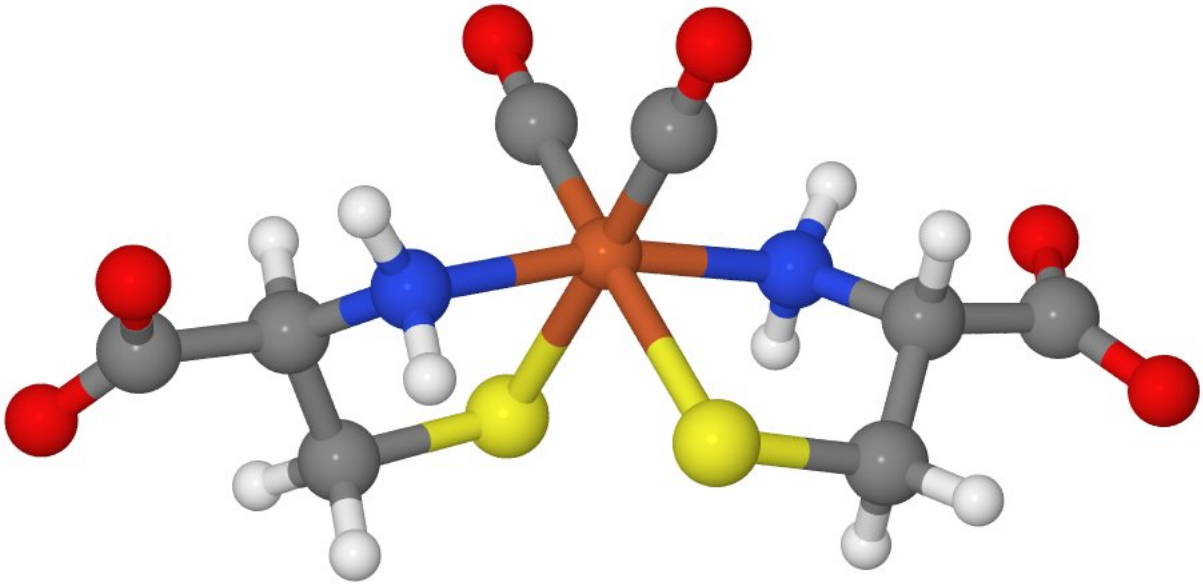
29

N	1.04339039	-1.37864006	1.09757996
H	1.03726017	-1.49597120	2.12314725
C	2.51872230	-1.32939005	0.82722050
H	2.72387934	-1.89980149	-0.08044112
C	2.94947028	0.11449991	0.59875679
C	3.29089069	-1.97204006	2.04296970
H	2.89940548	0.66637403	1.54364336
H	3.98581314	0.12680888	0.26148650
S	1.87492669	0.92421710	-0.66184062
O	2.59589958	-2.14006615	3.08149362
H	0.69522846	-2.26309586	0.73614991
O	4.49532652	-2.21062922	1.84403098
Fe	-0.16201524	0.07058121	0.29710275
S	-0.69708616	-1.43937254	-1.50016320
C	-2.15975022	-0.45967001	-2.04809165
C	-1.82468033	1.02610064	-2.10055614
H	-2.99807930	-0.62288642	-1.36219764
H	-2.47254539	-0.78839564	-3.03905582
N	-1.20487237	1.44921052	-0.80097198
H	-1.09958911	1.18966889	-2.89979434
C	-3.11344552	1.89489233	-2.36802292
H	-2.00462580	1.91882110	-0.34770602
O	-3.52671909	2.54824829	-1.37197781

O	-3.58391404	1.81204462	-3.51648498
H	-0.54874831	2.19903374	-1.00440001
C	0.19591138	1.26361763	1.56095922
O	0.39196634	2.05704331	2.37074614
C	-1.60923660	-0.64605701	1.03242862
O	-2.52355504	-1.12525249	1.54048169

6. STRUCTURE 4B (*IN VACUO*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.28682698 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

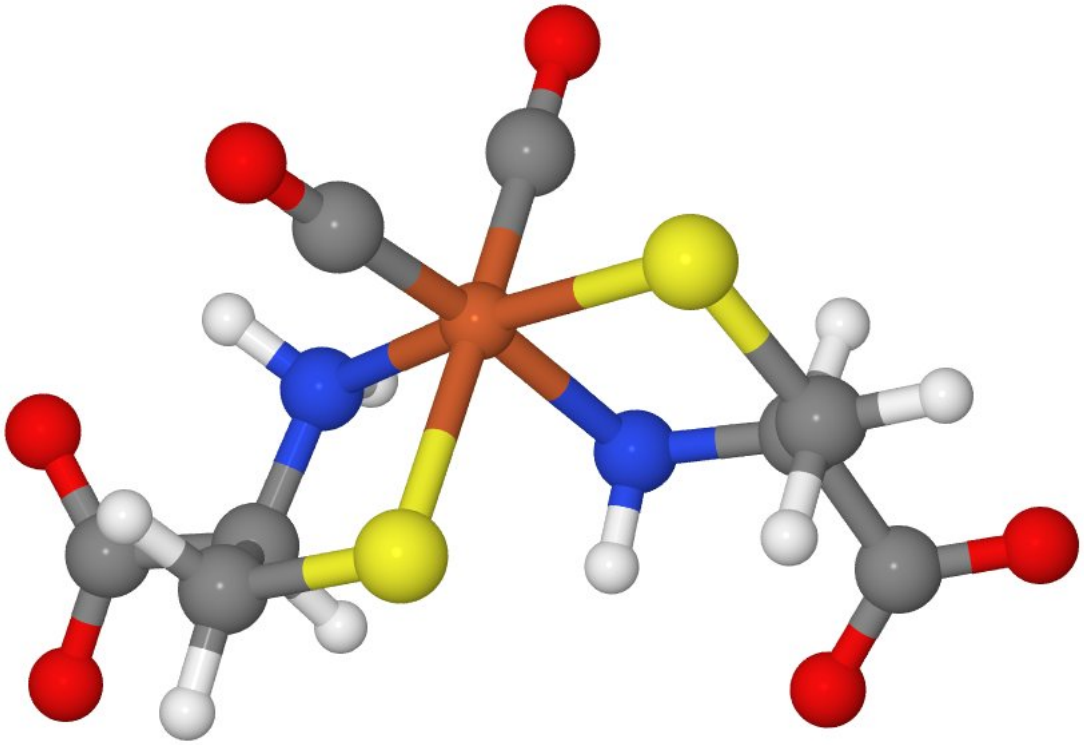
29

N	0.83500898	-1.71228564	0.71702290
H	1.02590322	-1.33115482	1.64381504
C	2.16731572	-1.97419190	0.09514874
H	1.97200406	-2.34766245	-0.91662210
C	2.89480519	-0.64863181	-0.02429143
C	2.91402602	-3.13243413	0.85997963
H	3.11580157	-0.25403625	0.97301096
H	3.83761120	-0.79976976	-0.54562235
S	1.85223770	0.57089508	-0.94408733
O	2.15227079	-3.87758970	1.52958322
H	0.47183657	-2.64575982	0.92149967
O	4.14304876	-3.20500088	0.67489433
Fe	-0.30331644	-0.29779899	-0.20230567
S	-0.37275556	0.88179171	1.93193150
C	-1.03402960	2.47554946	1.26645207
C	-1.92435741	2.21271133	0.06692453
H	-0.19735679	3.11921287	0.97518456
H	-1.60631192	2.99054861	2.03507710
N	-1.13989234	1.41273725	-0.92051029
H	-2.75625849	1.57795835	0.39303076
C	-2.57111382	3.46889138	-0.63148308
H	-0.34816128	1.99625254	-1.19131947

O	-2.67714834	3.36157799	-1.88093579
O	-2.94214702	4.38410950	0.12662283
H	-1.72539055	1.41454566	-1.75851536
C	-0.27783448	-1.08410871	-1.78971887
O	-0.31186330	-1.57659066	-2.82919312
C	-1.82811940	-0.98330992	0.38417920
O	-2.79980278	-1.47780168	0.75229967

7. STRUCTURE 5A (*IN VACUO*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.29194657 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

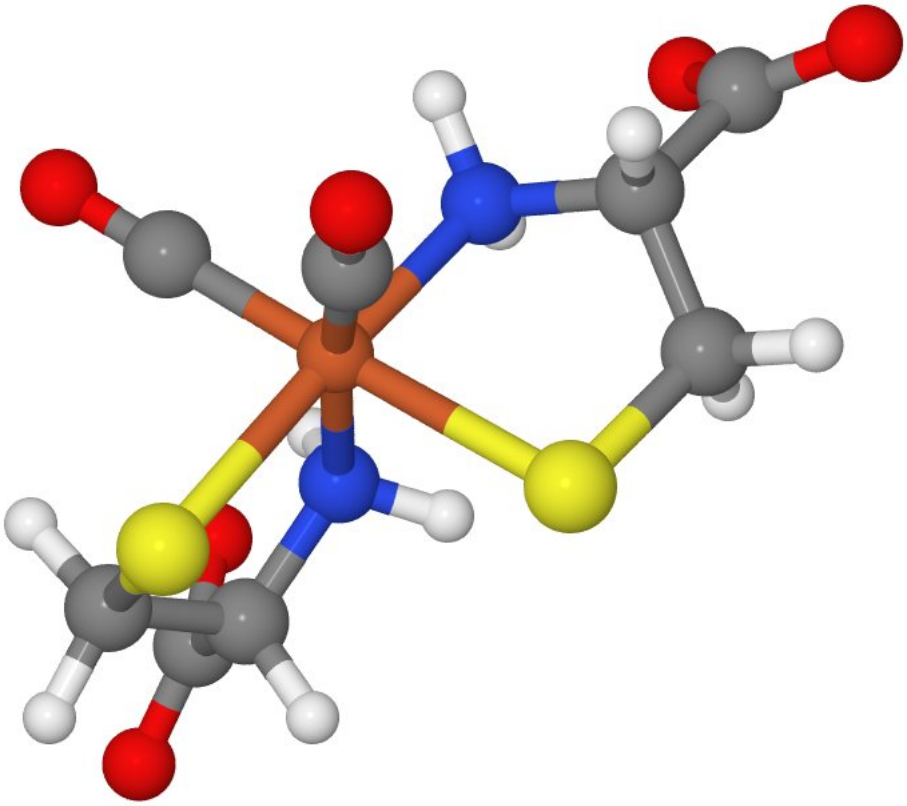
29

N	1.14446068	-0.94744319	0.16923824
H	1.27722275	-0.64690477	1.13728559
C	2.48522711	-1.01719260	-0.47778749
H	2.30931807	-1.26953244	-1.53058660
C	3.09777975	0.36752197	-0.42850977
C	3.33914280	-2.20092130	0.11631901
H	3.31627536	0.64318979	0.60817313
H	4.03434515	0.37152979	-0.98269719
S	1.93865812	1.61487401	-1.16545093
O	2.64830279	-3.11871576	0.62821901
H	0.86178499	-1.92748845	0.25751042
O	4.57294083	-2.11848187	-0.03686812
Fe	-0.10112783	0.50421405	-0.56431192
S	-0.18381517	1.45596576	1.63633788
C	-1.90437448	0.88927764	1.99188936
C	-2.16111207	-0.51965725	1.47519362

H	-2.60998011	1.58093429	1.51882422
H	-2.08592534	0.91475588	3.06652164
N	-1.71056080	-0.60768259	0.04776403
H	-1.58312821	-1.22909582	2.07157898
C	-3.69437361	-0.88366306	1.55760729
H	-2.60458636	-0.45903444	-0.44616479
O	-4.29861259	-0.85637546	0.45124426
O	-4.12769938	-1.12097573	2.69810915
H	-1.50537026	-1.58620560	-0.13864154
C	-1.02050138	1.97207344	-0.96532530
O	-1.58323634	2.93755460	-1.23287559
C	-0.08970996	-0.14797679	-2.21098614
O	-0.11268157	-0.53626090	-3.29449177

8. STRUCTURE 5B (*IN VACUO*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.29098763 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

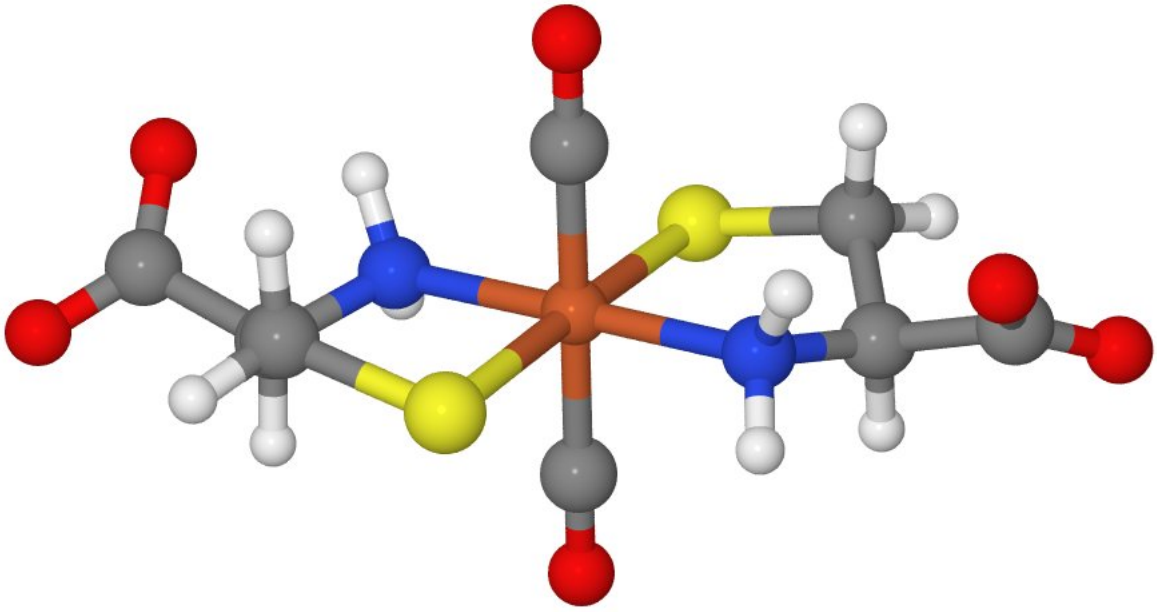
29

N	1.17547548	-0.70035768	0.57291216
H	1.17809522	-0.84513962	1.59534550
C	2.64184618	-0.59419769	0.28464523
H	2.86097312	-1.18387794	-0.60707074
C	3.00702310	0.85726970	0.00355599
C	3.46943140	-1.15534735	1.50439215
H	2.95041299	1.43733525	0.93056548
H	4.03428793	0.90595359	-0.35788420
S	1.88077962	1.59986818	-1.25522459
O	2.80129194	-1.34753025	2.55435824
H	0.84949309	-1.56921768	0.15633895
O	4.68627262	-1.31172895	1.29298341
Fe	-0.07832737	0.71569633	-0.24753669
S	-0.52844906	-0.84740520	-2.02376819

C	-1.95607078	-1.71324563	-1.21759105
C	-2.69224215	-0.81827521	-0.23096679
H	-1.59098375	-2.59970665	-0.68610716
H	-2.65959096	-2.05206132	-1.97764671
N	-1.67890668	-0.17892019	0.66394198
H	-3.20213270	-0.02254023	-0.77994043
C	-3.74845958	-1.62785673	0.61073327
H	-1.44517577	-0.92160118	1.33062863
O	-3.40002918	-1.87576699	1.79290307
O	-4.78592157	-1.93824601	-0.00461508
H	-2.19178391	0.46896502	1.25687587
C	0.20536813	1.89229286	1.04429102
O	0.35974184	2.68551278	1.86387789
C	-1.06682336	1.80795574	-1.23915744
O	-1.66395473	2.53747797	-1.89683974

9. STRUCTURE 1 (*IN METHANOL*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.51914101 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

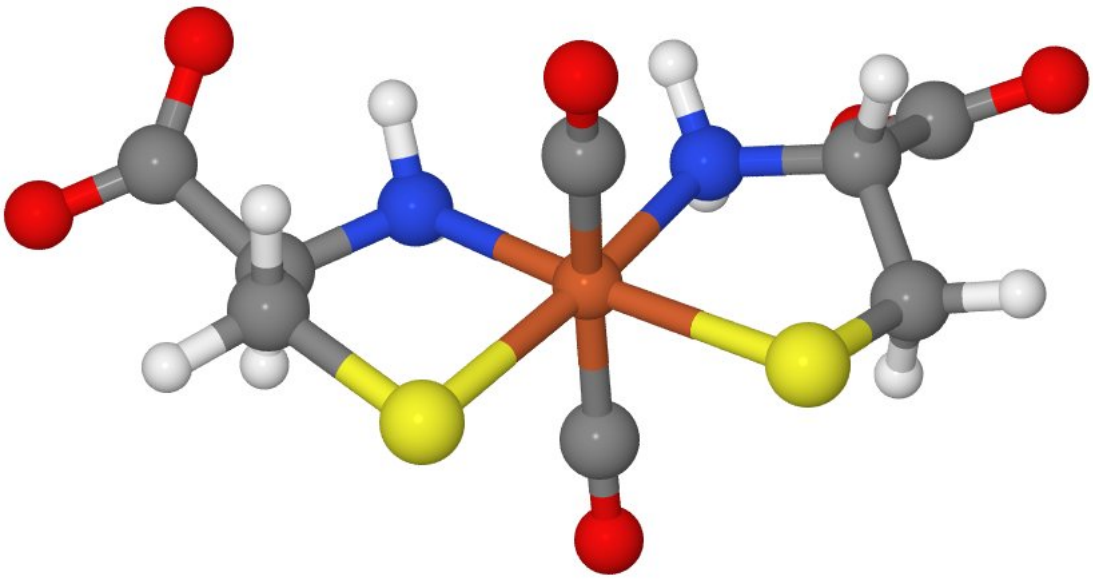
29

N	-1.88084340	-0.82297200	0.14723130
H	-2.13875747	-1.31500888	-0.71399510
C	-3.01262307	0.12778310	0.35782155
H	-3.11090803	0.31369826	1.42900813
C	-2.70429850	1.44584811	-0.34946659
C	-4.34487247	-0.47381511	-0.19227830
H	-2.70814991	1.28259110	-1.43200767
H	-3.48234439	2.17163634	-0.11431257
S	-1.06473255	2.12328696	0.15419793
O	-4.21817732	-1.40606177	-1.02818453
H	-1.95002878	-1.55113971	0.85429418
O	-5.39456415	0.05981139	0.22498482
Fe	-0.00000853	-0.00017874	0.14711419
S	1.06481242	-2.12359285	0.14953159
C	2.70428610	-1.44508803	-0.35300103
C	3.01265049	-0.12844364	0.35690749
H	2.70796776	-1.27964413	-1.43521166
H	3.48239660	-2.17131877	-0.11942922
N	1.88078976	0.82268012	0.14841138
H	3.11109900	-0.31652722	1.42770147
C	4.34478903	0.47434101	-0.19215626

H	2.13850665	1.31642222	-0.71189541
O	4.21792936	1.40820909	-1.02622437
O	5.39456320	-0.05999792	0.22398047
H	1.95010543	1.54947436	0.85687339
C	-0.00025682	0.00171221	-1.68072402
O	-0.00038070	0.00291482	-2.82221675
C	0.00023153	-0.00211429	1.97588611
O	0.00038172	-0.00336087	3.11734676

10. STRUCTURE 2 (*IN METHANOL*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.52041738 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

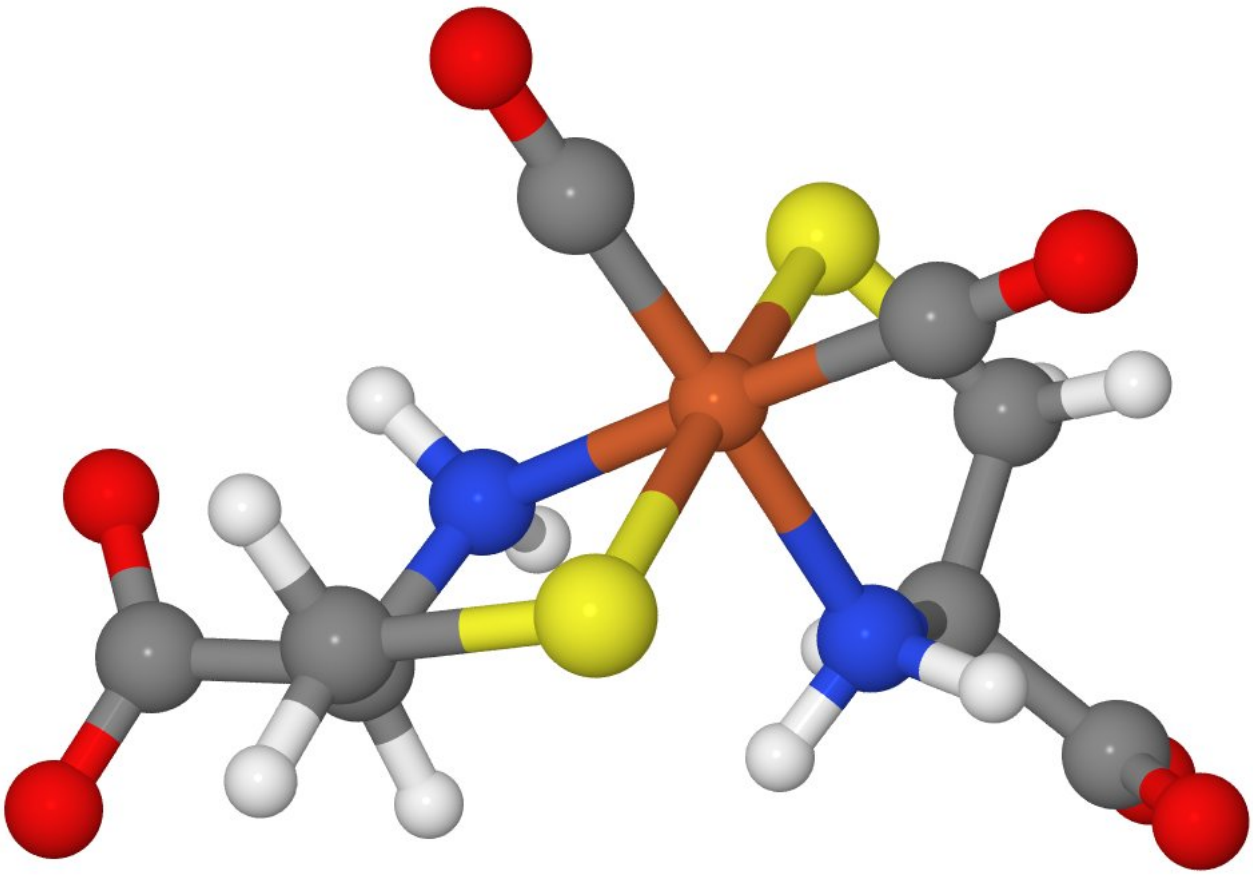
29

N	1.43810380	1.01033092	0.15472607
H	1.57638931	1.57919705	-0.68775606
C	2.82189178	0.55195498	0.47882590
H	2.89701796	0.41943270	1.55972898
C	3.08374763	-0.78625989	-0.20777735
C	3.87029719	1.60953534	0.00610623
H	3.11576247	-0.63414305	-1.29147947
H	4.05218077	-1.17376363	0.10794675
S	1.77449727	-2.02037263	0.19007699
O	3.46811676	2.42018867	-0.86919028
H	1.17149138	1.69420540	0.85953861
O	5.00702572	1.51557076	0.51484770
Fe	-0.00001447	-0.43582454	0.00024147
S	-1.77460289	-2.02055764	-0.18734233
C	-3.08375001	-0.78585911	0.20902744
C	-2.82195592	0.55139810	-0.47945827
H	-3.11558795	-0.63225949	1.29252505
H	-4.05224752	-1.17375851	-0.10601223
N	-1.43808377	1.01017368	-0.15627310
H	-2.89730763	0.41738957	-1.56016254
C	-3.87021852	1.60968781	-0.00801239
H	-1.57620597	1.58038080	0.68533212

O	-3.46779442	2.42163324	0.86597514
O	-5.00707817	1.51499927	-0.51632589
H	-1.17152393	1.69290328	-0.86221164
C	0.18233886	-0.63925189	-1.80638313
O	0.29749912	-0.86383468	-2.92125058
C	-0.18236278	-0.63676143	1.80714083
O	-0.29750943	-0.85981387	2.92231798

11. STRUCTURE 3A (*IN METHANOL*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.53285350 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

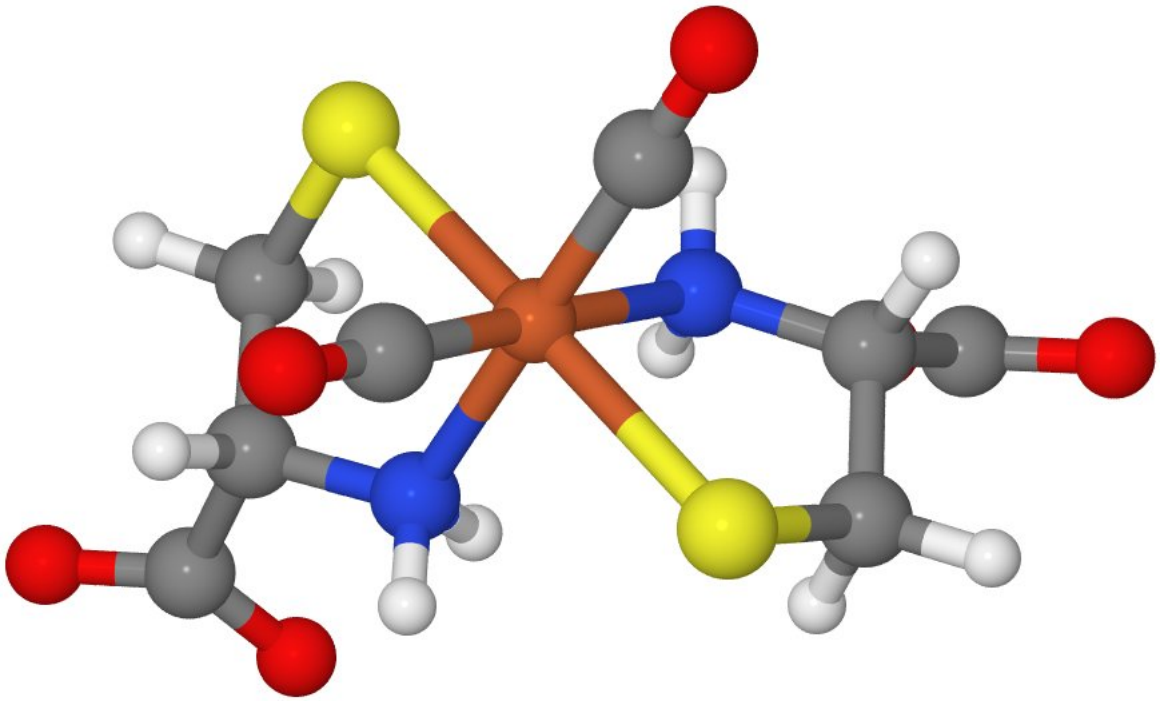
29

N	-1.24366176	-0.58583462	-0.67553109
H	-1.86995494	-0.31263834	-1.44050014
C	-2.16200471	-1.22170722	0.31219214
H	-1.61642694	-1.99629617	0.85496569
C	-2.63716602	-0.15824772	1.29755449
C	-3.38603497	-1.86953032	-0.41451910
H	-3.29950571	0.54449242	0.78304243
H	-3.20266128	-0.62610978	2.10345459
S	-1.21379709	0.77065897	2.01771450
O	-3.62058330	-1.43648648	-1.57248783
H	-0.65950716	-1.30009961	-1.10467780

O	-4.02337456	-2.71686220	0.24528080
Fe	0.00001664	0.91041255	0.00002392
S	1.21385109	0.77077591	-2.01765966
C	2.63717294	-0.15825081	-1.29756677
C	2.16194987	-1.22178531	-0.31231648
H	3.29953194	0.54441196	-0.78297395
H	3.20266342	-0.62605780	-2.10350275
N	1.24362075	-0.58596104	0.67544973
H	1.61635423	-1.99630249	-0.85517406
C	3.38593483	-1.86971962	0.41436449
H	1.86991251	-0.31286144	1.44045568
O	3.62037373	-1.43688762	1.57243478
O	4.02336216	-2.71689343	-0.24555355
H	0.65942132	-1.30023718	1.10451734
C	-1.11931133	2.14723849	-0.61688131
O	-1.85025668	2.93697190	-1.00663066
C	1.11939383	2.14712286	0.61707449
O	1.85036075	2.93677807	1.00694036

12. STRUCTURE 3B (*IN METHANOL*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.53159340 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

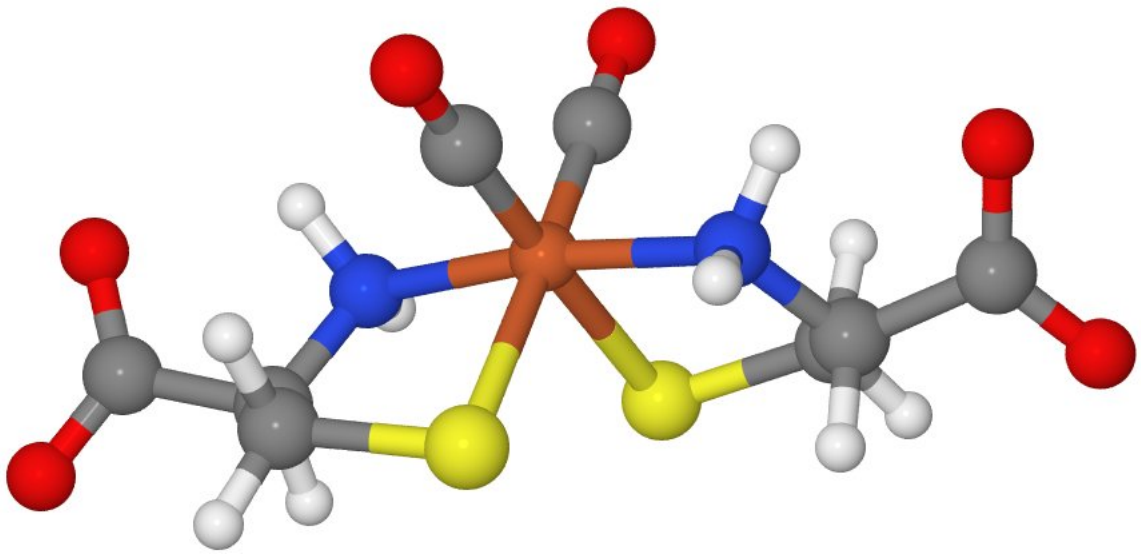
29

N	-1.17087030	0.40652975	0.81083065
H	-1.35158336	0.19531797	1.78968823
C	-2.46824002	0.68317229	0.13179594
C	-2.26220870	0.60616988	-1.37844396
H	-3.22711992	0.67133069	-1.88093555
H	-1.65570116	1.45508897	-1.70796108
S	-1.43171918	-0.96718013	-1.87289262
H	-0.71600103	1.32380414	0.85659891
Fe	-0.00006168	-1.07699275	-0.00010991
S	1.43159521	-0.96751183	1.87269533
C	2.26217794	0.60588378	1.37853169
C	2.46803904	0.68323332	-0.13171287
H	3.22715235	0.67083353	1.88092983
H	1.65578353	1.45478213	1.70831120
N	1.17053008	0.40693066	-0.81061339
H	1.35102367	0.19618419	-1.78961420
H	0.71565503	1.32422721	-0.85583270
C	-1.05036807	-2.31231570	0.73435980

O	-1.73336983	-3.10514092	1.19776046
C	1.05042708	-2.31195521	-0.73492444
O	1.73352671	-3.10456491	-1.19854999
C	-3.01263332	2.09514213	0.52088600
O	-2.15906310	2.90159678	0.97208500
O	-4.22800064	2.28677368	0.30368617
H	-3.18482232	-0.08203422	0.43636119
H	3.18448997	-0.08197836	-0.43657389
C	3.01252246	2.09523749	-0.52051413
O	2.15898132	2.90182471	-0.97152758
O	4.22788286	2.28678036	-0.30319831

13. STRUCTURE 4A (*IN METHANOL*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.52564930 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

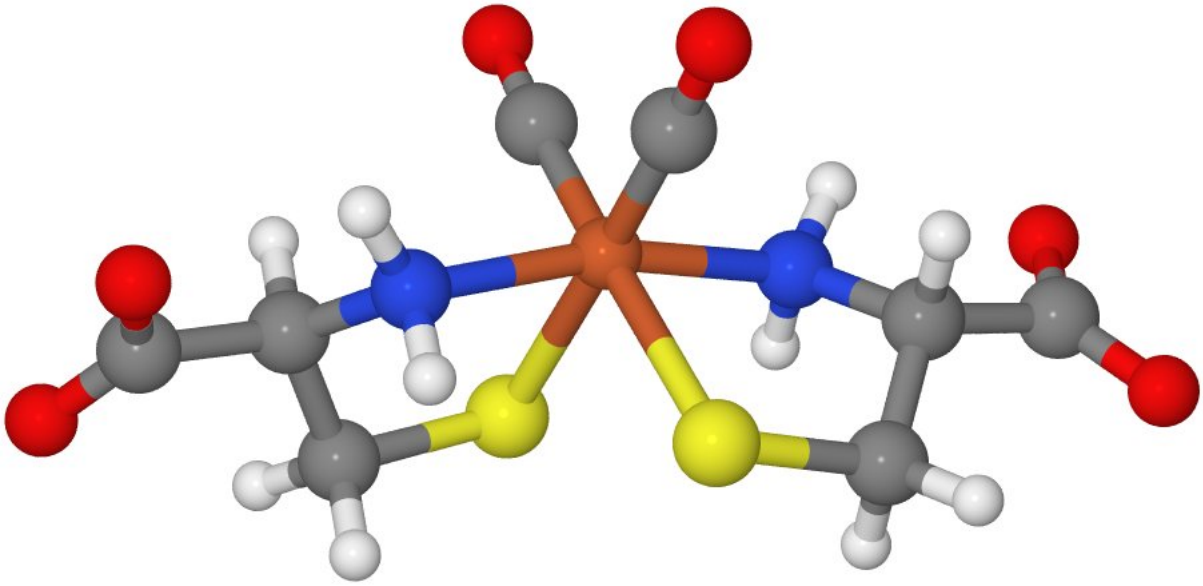
29

N	1.88258779	0.23194255	0.78922641
H	2.44117832	1.09321892	0.80740935
C	2.81520081	-0.75063068	0.15417261
H	2.64024711	-1.73010957	0.60178578
C	2.53568459	-0.83226162	-1.34313560
C	4.29610586	-0.31794351	0.40491450
H	2.83137274	0.10582951	-1.82365239
H	3.13046312	-1.63406920	-1.78008819
S	0.74900341	-1.15186775	-1.65709627
O	4.46417522	0.88334256	0.74355507
H	1.79089963	-0.02404881	1.76970792
O	5.15977955	-1.19706690	0.20557439
Fe	-0.00033983	0.40848747	0.01295489
S	-0.74457818	-1.27066875	1.56607366
C	-2.53150010	-0.92737114	1.28116608
C	-2.81598258	-0.74048948	-0.20572935
H	-2.82432842	-0.02467789	1.82678723
H	-3.12645602	-1.75671422	1.66267908
N	-1.88376343	0.28287885	-0.77370393
H	-2.64466619	-1.68638575	-0.72198677
C	-4.29731178	-0.28893656	-0.41866875
H	-2.44257021	1.14331353	-0.73346508
O	-4.46448708	0.93232614	-0.67653775

O	-5.16184425	-1.17746603	-0.27140385
H	-1.79203618	0.09367298	-1.76921594
C	0.48949662	1.63336897	-1.18637455
O	0.79257572	2.41826296	-1.96348882
C	-0.49253279	1.54514396	1.29519963
O	-0.79645038	2.27381325	2.12495661

14. STRUCTURE 4B (*IN METHANOL*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.52493796 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

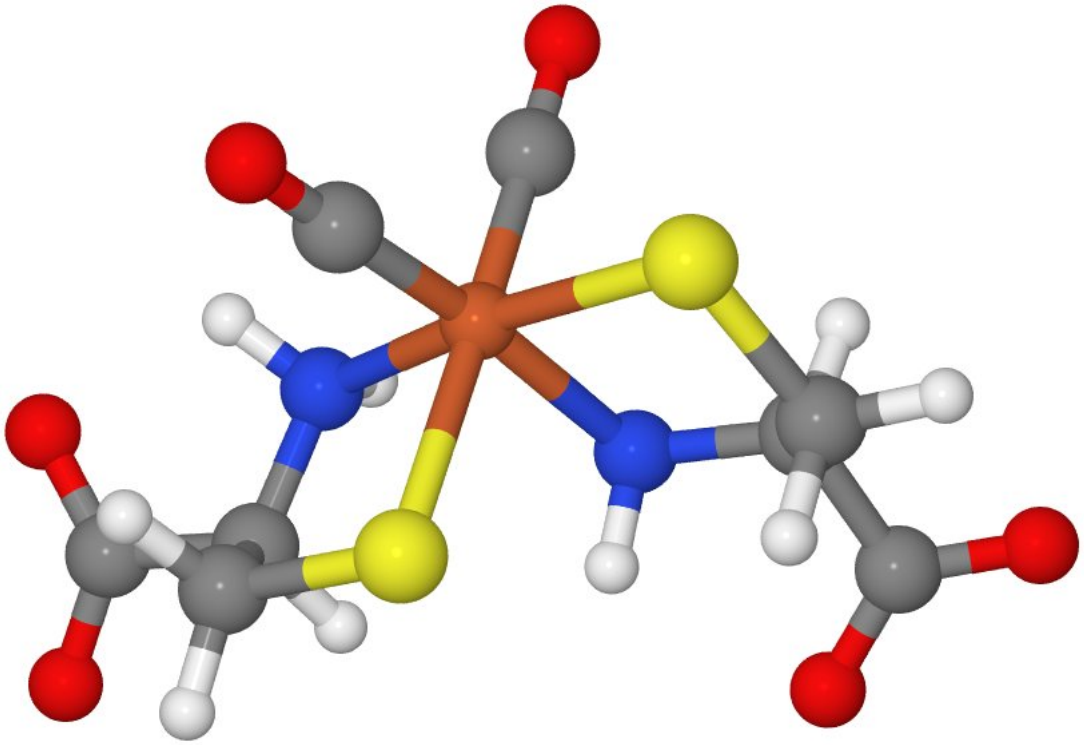
29

N	-1.97444856	0.53410542	0.51311827
H	-2.11526537	0.05906855	1.40936351
C	-2.86825848	-0.20830967	-0.42455360
H	-3.11270809	0.45260847	-1.25857520
C	-2.12721825	-1.43219328	-0.95006704
C	-4.18481731	-0.63912821	0.29813340
H	-1.95233917	-2.12723255	-0.12456372
H	-2.73829889	-1.93140984	-1.70179057
S	-0.50599688	-0.96775711	-1.68514538
O	-4.13872051	-0.65806371	1.55514181
H	-2.39124250	1.45033145	0.66258591
O	-5.13386536	-0.95500898	-0.45094422
Fe	0.00008165	0.67257255	0.00390112
S	0.50572675	-0.98737526	1.67401505
C	2.12706661	-1.44337380	0.93385845
C	2.86827922	-0.21358030	0.42252058
H	1.95231855	-2.12901020	0.10049049
H	2.73801684	-1.95115066	1.67994130
N	1.97467089	0.53988653	-0.50648016
H	3.11283851	0.43758246	1.26414812
C	4.18480110	-0.63608617	-0.30514768
H	2.11576366	0.07554954	-1.40830064

O	4.13838911	-0.64133865	-1.56228292
O	5.13414574	-0.95979381	0.44019681
H	2.39148927	1.45783079	-0.64490497
C	-0.32978430	1.85154557	-1.29224348
O	-0.52944684	2.60462809	-2.13180423
C	0.32986635	1.83702552	1.31313848
O	0.52966321	2.58081818	2.16090536

15. STRUCTURE 5A (*IN METHANOL*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]	
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$	
Charge	:	-2	
Multiplicity	:	1	
Energy	:	-2932.52879001	a.u.
Number of imaginary frequencies	:	0	

Cartesian Co-ordinates (XYZ format)

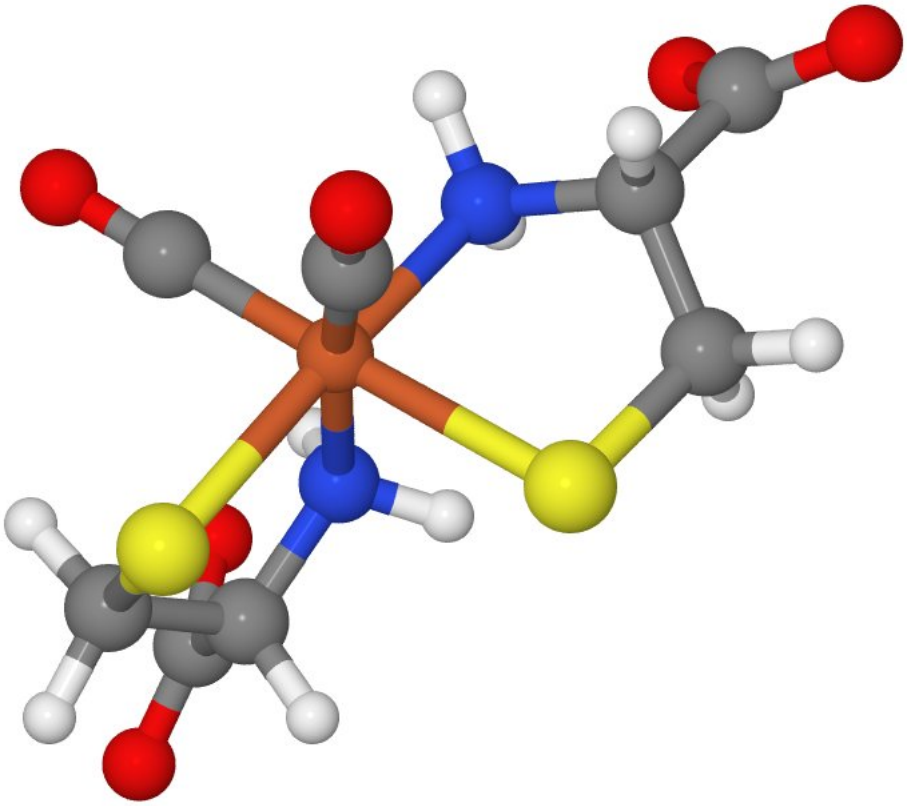
29

N	-1.14781570	-0.83533949	0.50096136
H	-0.91347802	-1.55457532	-0.18747449
C	-2.62130761	-0.64758927	0.39607263
H	-2.95989799	-0.13024937	1.29638171
C	-2.91556334	0.22549975	-0.81781089
C	-3.37298107	-2.01247239	0.28197441
H	-2.65891051	-0.31900617	-1.73070896
H	-3.97880197	0.46230856	-0.84691471
S	-1.95122302	1.79715431	-0.75806421
O	-2.67690682	-3.00260782	-0.05424792
H	-0.96224684	-1.27679873	1.39942968
O	-4.60254669	-1.96451771	0.50861865
Fe	0.01782593	0.81929559	0.13990150
S	0.63872045	-0.15501040	-1.95374453
C	2.32661629	-0.65986711	-1.41238499
C	2.31190753	-1.19102514	0.01641492

H	2.99714041	0.20330644	-1.47270465
H	2.70915365	-1.42862809	-2.08351827
N	1.61874330	-0.20587343	0.90227479
H	1.75993454	-2.13192821	0.04539411
C	3.77339077	-1.42812693	0.51739931
H	2.38938189	0.38651156	1.23127687
O	4.24456215	-0.53029299	1.26364851
O	4.33265495	-2.45980263	0.09157201
H	1.33780003	-0.70262676	1.74527848
C	0.97880149	2.20564151	-0.43237492
O	1.57148981	3.09993458	-0.83315194
C	-0.43039247	1.57056475	1.69320679
O	-0.72317058	2.08579779	2.67335272

16. STRUCTURE 5B (*IN METHANOL*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.52865957 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

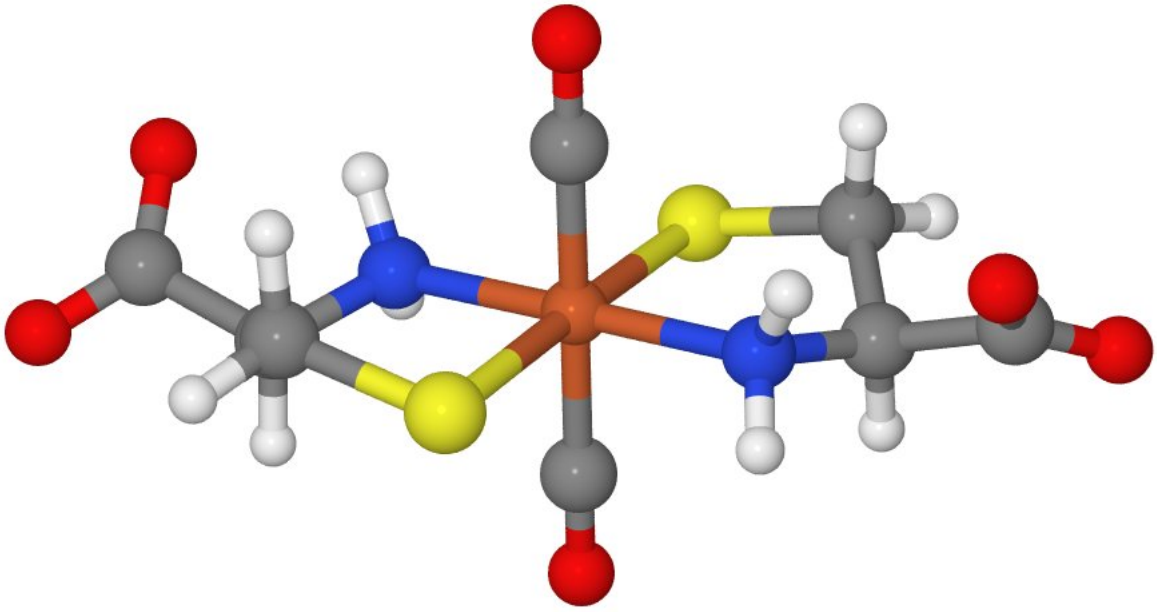
29

N	1.03037083	-0.96221876	-0.03399895
H	1.16439593	-1.54190707	0.80322272
C	2.40733266	-0.87656730	-0.60661119
H	2.32865167	-0.91432899	-1.69385946
C	3.05122781	0.44680986	-0.20667951
C	3.27909946	-2.07544947	-0.10967527
H	3.26229024	0.44537550	0.86707157
H	3.99663162	0.56989813	-0.73479331
S	1.94674671	1.86767209	-0.60609895
O	2.83585954	-2.69870067	0.89048338
H	0.47621515	-1.53134406	-0.66905141
O	4.34351683	-2.26673388	-0.73476660
Fe	-0.00563462	0.80352968	0.21180299
S	-0.90971869	0.48271486	-1.98182619

C	-2.25975132	-0.68011451	-1.49260747
C	-2.78032613	-0.38674319	-0.08956795
H	-1.88279986	-1.70733333	-1.52784693
H	-3.08037758	-0.60546941	-2.20575142
N	-1.62376070	-0.26965564	0.84644216
H	-3.31298661	0.56605506	-0.09036492
C	-3.74341393	-1.52851915	0.36796522
H	-1.40872395	-1.24072051	1.09383094
O	-3.22913098	-2.40811586	1.10618830
O	-4.90729284	-1.46983159	-0.08138123
H	-1.98178208	0.11214241	1.71897566
C	0.65543097	1.05512035	1.84698343
O	1.09000087	1.24086678	2.89027452
C	-0.87958544	2.35553885	0.16972694
O	-1.40750051	3.36979270	0.10767785

17. STRUCTURE 1 (*IN WATER*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.52378554 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

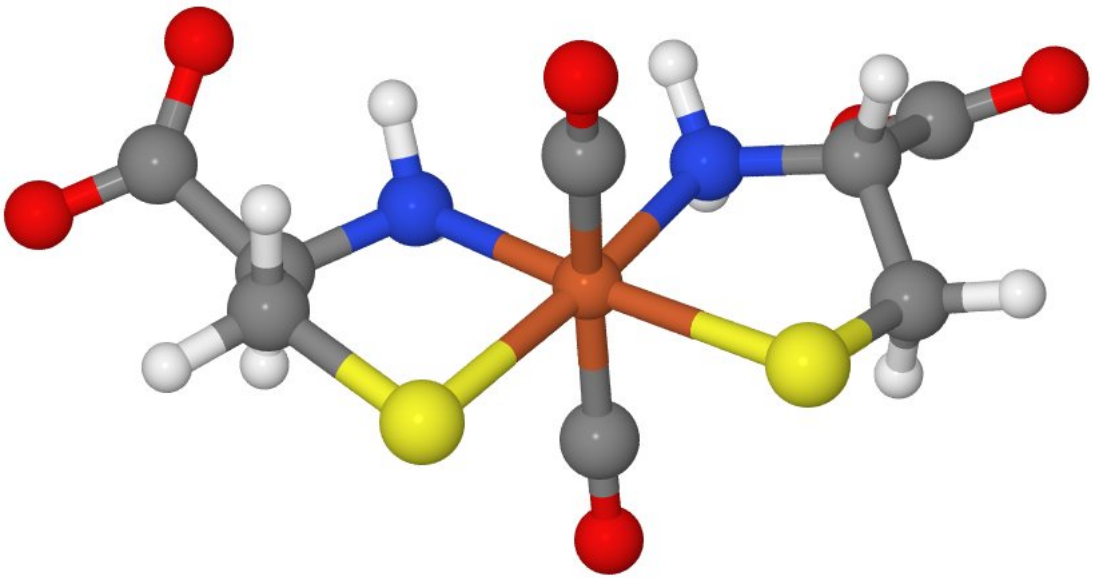
29

N	-1.88105285	-0.82249534	0.15454128
H	-2.13553739	-1.31895268	-0.70517117
C	-3.01402068	0.12876797	0.35601020
H	-3.11955476	0.31650227	1.42618001
C	-2.70147538	1.44578171	-0.35172969
C	-4.34201479	-0.47433877	-0.20204060
H	-2.69903445	1.28092301	-1.43400049
H	-3.48028302	2.17263293	-0.12229520
S	-1.06447506	2.12294841	0.16052753
O	-4.20943737	-1.40746236	-1.03617573
H	-1.95239496	-1.54672062	0.86543757
O	-5.39539766	0.05781438	0.20799775
Fe	-0.00003726	-0.00011142	0.15459377
S	1.06449902	-2.12339616	0.15466602
C	2.70159578	-1.44501698	-0.35569787
C	3.01397371	-0.12958118	0.35503352
H	2.69938588	-1.27774239	-1.43759906
H	3.48035789	-2.17237782	-0.12772132
N	1.88103545	0.82211417	0.15543838
H	3.11929607	-0.31966928	1.42480958
C	4.34206581	0.47478941	-0.20141584

H	2.13537550	1.32004130	-0.70346582
O	4.20958519	1.40930295	-1.03400207
O	5.39536428	-0.05863465	0.20719656
H	1.95260763	1.54514110	0.86753500
C	-0.00045026	0.00189377	-1.67301512
O	-0.00062638	0.00315035	-2.81450319
C	0.00009836	-0.00162961	1.98387253
O	0.00011379	-0.00252957	3.12518048

18. STRUCTURE 2 (*IN WATER*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]	
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$	
Charge	:	-2	
Multiplicity	:	1	
Energy	:	-2932.52522483	a.u.
Number of imaginary frequencies	:	0	

Cartesian Co-ordinates (XYZ format)

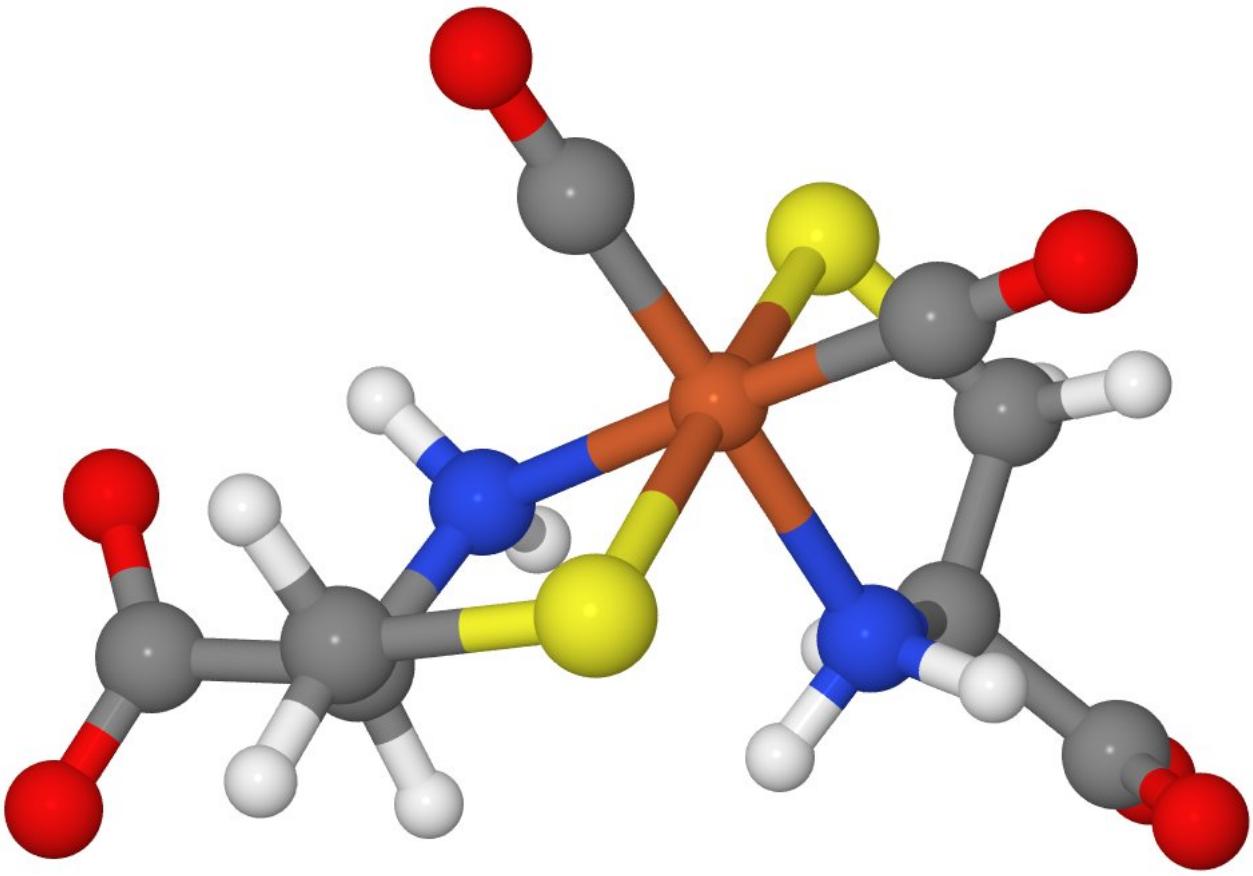
29

N	1.43863356	1.01074147	0.15354203
H	1.57625163	1.57848942	-0.68962973
C	2.82177162	0.55164421	0.47849447
H	2.89566994	0.41887465	1.55944705
C	3.08422542	-0.78643930	-0.20827727
C	3.87151766	1.60811257	0.00727880
H	3.11702180	-0.63432062	-1.29190850
H	4.05221224	-1.17434740	0.10824660
S	1.77404714	-2.02011633	0.18816502
O	3.47159624	2.42060304	-0.86722183
H	1.17200160	1.69525456	0.85774779
O	5.00824928	1.51194847	0.51613742
Fe	-0.00009068	-0.43472001	0.00047010
S	-1.77414620	-2.02034616	-0.18674156
C	-3.08405137	-0.78623164	0.20925038
C	-2.82190061	0.55110645	-0.47905362
H	-3.11624074	-0.63301176	1.29274344
H	-4.05222511	-1.17441916	-0.10635987
N	-1.43868148	1.01063037	-0.15503871
H	-2.89614677	0.41710386	-1.55983007
C	-3.87155151	1.60805309	-0.00870150
H	-1.57615006	1.57985091	0.68716770

O	-3.47100043	2.42240119	0.86378109
O	-5.00831175	1.51158595	-0.51744187
H	-1.17205656	1.69387925	-0.86047274
C	0.18078700	-0.63711864	-1.80670309
O	0.29513463	-0.86172366	-2.92154670
C	-0.18102115	-0.63408279	1.80798888
O	-0.29542816	-0.85688102	2.92318845

19. STRUCTURE 3A (*IN WATER*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.53745613 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

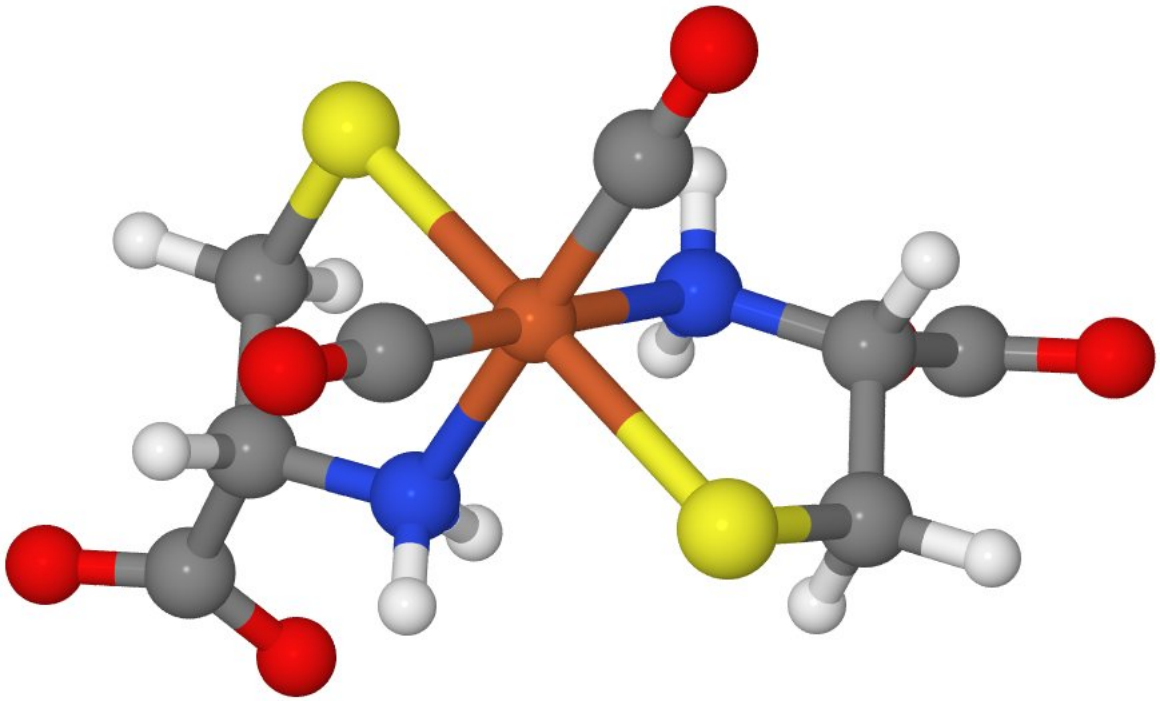
29

N	-1.24450815	-0.58797818	-0.67482924
H	-1.86879587	-0.31357950	-1.44086659
C	-2.16518307	-1.22152638	0.31219473
H	-1.62195849	-1.99803078	0.85456824
C	-2.63801575	-0.15768595	1.29842401
C	-3.39048529	-1.86557496	-0.41501880
H	-3.29945207	0.54669130	0.78500777
H	-3.20357180	-0.62495923	2.10458779
S	-1.21245849	0.76802009	2.01819921
O	-3.62134695	-1.43532503	-1.57476950
H	-0.66134065	-1.30396283	-1.10243368

O	-4.03340530	-2.70816445	0.24573138
Fe	0.00000296	0.90778995	0.00004477
S	1.21253252	0.76820856	-2.01809311
C	2.63802767	-0.15765831	-1.29840112
C	2.16511869	-1.22158849	-0.31230748
H	3.29949045	0.54662269	-0.78488636
H	3.20357656	-0.62486255	-2.10460925
N	1.24445713	-0.58810973	0.67477185
H	1.62185442	-1.99799502	-0.85478032
C	3.39038348	-1.86579156	0.41483968
H	1.86875367	-0.31382152	1.44083989
O	3.62135029	-1.43559647	1.57458985
O	4.03322601	-2.70836854	-0.24599987
H	0.66125792	-1.30411625	1.10229588
C	-1.11939132	2.14471102	-0.61718082
O	-1.85027897	2.93413830	-1.00738358
C	1.11944652	2.14462519	0.61735648
O	1.85038769	2.93398261	1.00759840

20. STRUCTURE 3B (*IN WATER*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.53637468 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

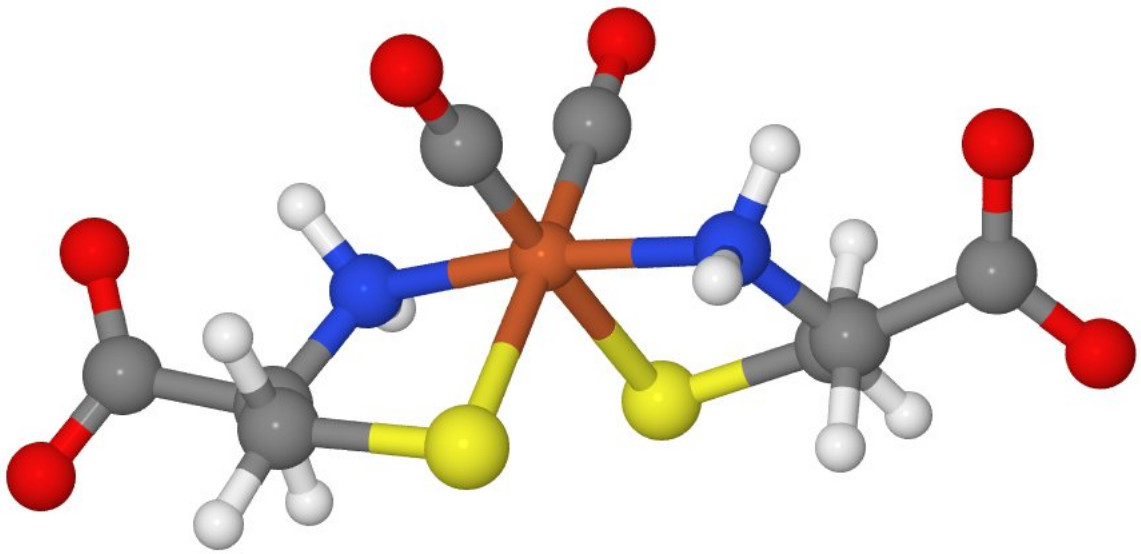
29

N	-1.16973376	0.40286461	0.81162703
H	-1.35309029	0.19029298	1.78967834
C	-2.46510959	0.68531495	0.13124268
C	-2.25881982	0.60654205	-1.37905025
H	-3.22315550	0.67402488	-1.88243210
H	-1.64966798	1.45324266	-1.70941615
S	-1.43320870	-0.96978724	-1.87168610
H	-0.71127939	1.31819963	0.85937309
Fe	-0.00008047	-1.08116579	-0.00003314
S	1.43304992	-0.96991438	1.87163699
C	2.25894713	0.60630596	1.37908578
C	2.46477246	0.68537015	-0.13125491
H	3.22345972	0.67340684	1.88218153
H	1.65013027	1.45310903	1.70981252
N	1.16903830	0.40353015	-0.81118435
H	1.35183012	0.19173655	-1.78951359
H	0.71058840	1.31891143	-0.85791487
C	-1.04963839	-2.31694174	0.73575586

O	-1.73226106	-3.10958171	1.19966781
C	1.04991233	-2.31632948	-0.73623323
O	1.73280704	-3.10859370	-1.20038545
C	-3.00226665	2.10000134	0.51917094
O	-2.14391828	2.90436578	0.96558523
O	-4.21749830	2.29710269	0.30602032
H	-3.18563080	-0.07601007	0.43591249
H	3.18490529	-0.07614900	-0.43636629
C	3.00227284	2.09996510	-0.51902586
O	2.14402056	2.90473390	-0.96488011
O	4.21764946	2.29662251	-0.30625787

21. STRUCTURE 4A (*IN WATER*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.53040800 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

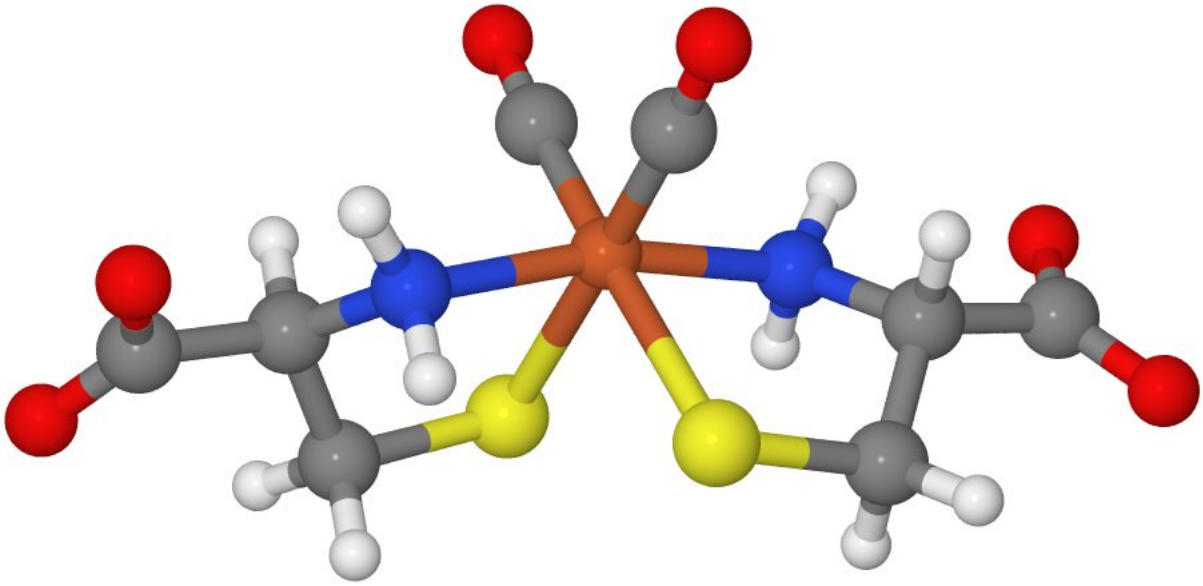
29

N	1.88427114	0.23848197	0.78633434
H	2.44362307	1.09911108	0.79675347
C	2.81182170	-0.75097704	0.15512864
H	2.62983346	-1.72832453	0.60451233
C	2.53429556	-0.83331114	-1.34246922
C	4.29510736	-0.32855827	0.40660104
H	2.83345509	0.10344147	-1.82334101
H	3.12709308	-1.63736522	-1.77796221
S	0.74720454	-1.14757705	-1.65901983
O	4.47287560	0.87376690	0.73578179
H	1.79557788	-0.01014174	1.76900172
O	5.15203953	-1.21681046	0.21716346
Fe	-0.00031975	0.41382471	0.01309061
S	-0.74226952	-1.26674616	1.56671941
C	-2.52987790	-0.92809182	1.28073180
C	-2.81292129	-0.74067295	-0.20630637
H	-2.82539701	-0.02658392	1.82675922
H	-3.12263441	-1.75936222	1.66150105
N	-1.88554537	0.28895867	-0.77041084
H	-2.63479185	-1.68450558	-0.72376126
C	-4.29653358	-0.29937774	-0.42152613
H	-2.44507909	1.14829385	-0.72296923
O	-4.47297573	0.92213941	-0.67100763

O	-5.15464115	-1.19614828	-0.28475934
H	-1.79689956	0.10679922	-1.76755571
C	0.48763752	1.63985491	-1.18643916
O	0.78998220	2.42476940	-1.96351826
C	-0.49092788	1.55094445	1.29617250
O	-0.79408020	2.27906227	2.12641072

22. STRUCTURE 4B (*IN WATER*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.52998186 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

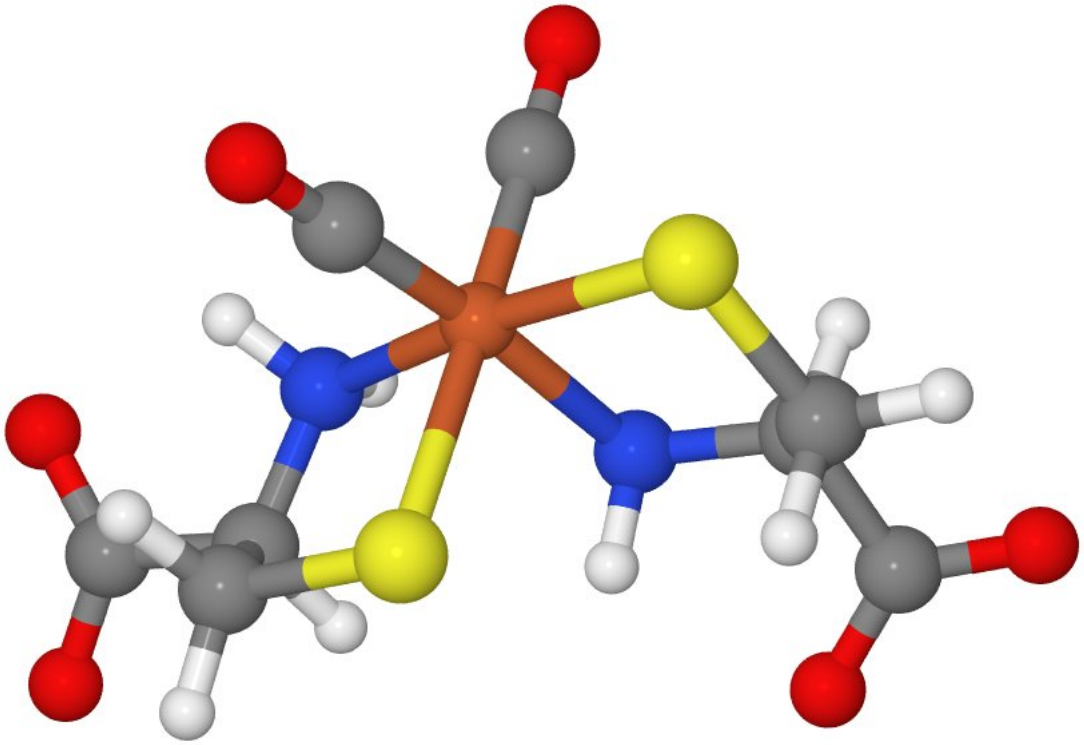
29

N	-1.97704625	0.54311216	0.50393689
H	-2.12116480	0.07724526	1.40468347
C	-2.86756039	-0.21117121	-0.42732784
H	-3.12529063	0.44487360	-1.26110578
C	-2.11959863	-1.43041229	-0.95486951
C	-4.17290401	-0.65667397	0.30623019
H	-1.94183338	-2.12599373	-0.13059431
H	-2.72838259	-1.93154335	-1.70728374
S	-0.50063539	-0.95811456	-1.68936455
O	-4.11349630	-0.68121856	1.56287813
H	-2.39496040	1.46074879	0.64119643
O	-5.12664747	-0.97998804	-0.43357632
Fe	0.00002658	0.68132859	0.00375006
S	0.50029105	-0.97655076	1.67806613
C	2.11914611	-1.44110990	0.93859273
C	2.86759710	-0.21618228	0.42516381
H	1.94129133	-2.12701511	0.10628771
H	2.72754669	-1.95117366	1.68529177
N	1.97737277	0.54889262	-0.49751675
H	3.12520862	0.43025047	1.26644015
C	4.17313051	-0.65355718	-0.31299260
H	2.12164283	0.09355722	-1.40358984

O	4.11416149	-0.66410166	-1.56982923
O	5.12659073	-0.98521101	0.42350146
H	2.39525819	1.46809638	-0.62398666
C	-0.32370391	1.86197078	-1.29280949
O	-0.52012157	2.61530709	-2.13261271
C	0.32416302	1.84694052	1.31379390
O	0.52062601	2.59043479	2.16230154

23. STRUCTURE 5A (*IN WATER*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.53375627 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

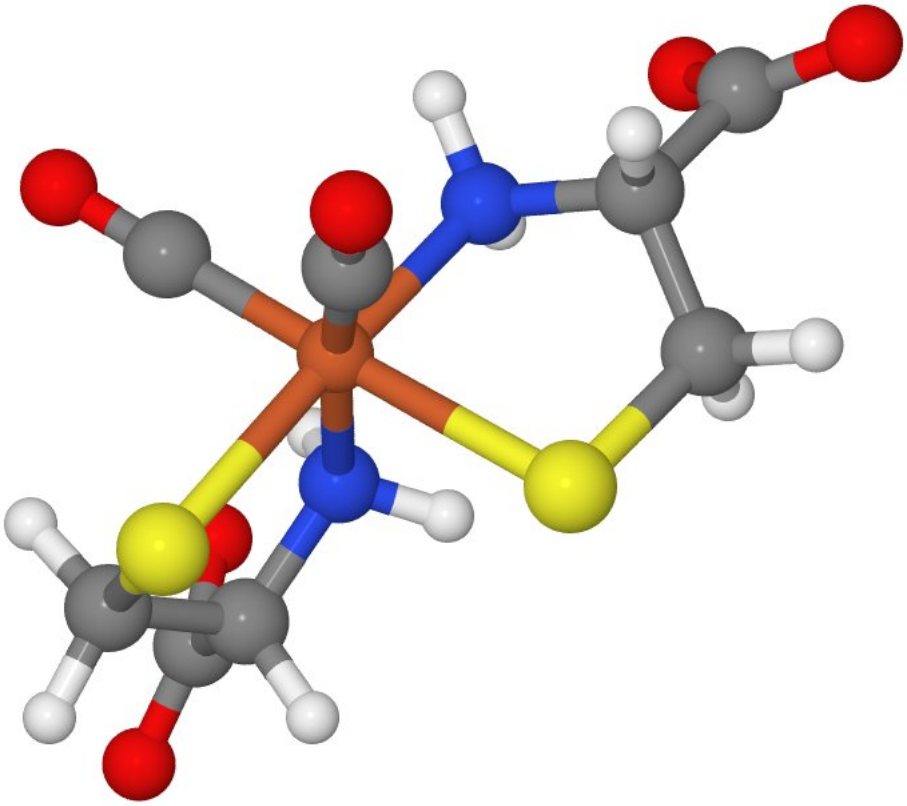
29

N	-1.14941490	-0.82814401	0.51922631
H	-0.90873671	-1.55778885	-0.15625811
C	-2.62278986	-0.64919460	0.39730427
H	-2.97739506	-0.14070573	1.29625797
C	-2.91034222	0.22670095	-0.81669682
C	-3.36026597	-2.01959467	0.26106977
H	-2.64274883	-0.31429881	-1.72841501
H	-3.97440529	0.45896816	-0.85515004
S	-1.95429289	1.80240893	-0.74470514
O	-2.65436387	-2.99483848	-0.09863265
H	-0.96984637	-1.25350392	1.42668498
O	-4.58955002	-1.99079430	0.49170074
Fe	0.01672471	0.82394898	0.14568593
S	0.62554067	-0.16109335	-1.94794893
C	2.31553841	-0.66496992	-1.41242290
C	2.30583930	-1.19141185	0.01826543

H	2.98613906	0.19770667	-1.47819781
H	2.69477367	-1.43611038	-2.08272576
N	1.61930370	-0.20190686	0.90401018
H	1.75152969	-2.13071275	0.05289171
C	3.76874542	-1.43213797	0.51227587
H	2.39151859	0.39130390	1.22716892
O	4.24782562	-0.53469247	1.25363827
O	4.32204723	-2.46711564	0.08590972
H	1.34134901	-0.69482219	1.75023413
C	0.97967154	2.20541787	-0.43548083
O	1.57410836	3.09545803	-0.84284735
C	-0.42254981	1.58142710	1.69896400
O	-0.71107239	2.10017300	2.67825127

24. STRUCTURE 5B (*IN WATER*)

General Information



SMILES	:	C1C([NH2][Fe]2(S1)([NH2]C(CS2)C(=O)[O])([C][O])[C][O])C(=O)[O]
Formula	:	$C_8H_{10}FeN_2O_6S_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-2932.53350358 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

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N	1.03139043	-0.96259046	-0.03273424
H	1.16514063	-1.54030991	0.80571514
C	2.40806866	-0.87654734	-0.60570604
H	2.32899308	-0.91437662	-1.69292247
C	3.05171037	0.44717556	-0.20643011
C	3.28065825	-2.07505441	-0.11022107
H	3.26234531	0.44690928	0.86737287
H	3.99713278	0.57048649	-0.73440880
S	1.94655037	1.86715102	-0.60719991
O	2.83942032	-2.69916296	0.89022762
H	0.47776634	-1.53356647	-0.66659039
O	4.34443188	-2.26608062	-0.73681027
Fe	-0.00551107	0.80286652	0.21141437
S	-0.90965617	0.48072675	-1.98218107

C	-2.26096153	-0.68070114	-1.49305248
C	-2.78006768	-0.38641596	-0.08959883
H	-1.88507783	-1.70824611	-1.52872241
H	-3.08167577	-0.60476786	-2.20599103
N	-1.62304425	-0.27079317	0.84584546
H	-3.31103849	0.56725603	-0.08992771
C	-3.74502039	-1.52625203	0.36787015
H	-1.40678442	-1.24176466	1.09208655
O	-3.23189259	-2.40935206	1.10265136
O	-4.91005611	-1.46365118	-0.07842326
H	-1.98027718	0.11037767	1.71900582
C	0.65429103	1.05494797	1.84742868
O	1.08875120	1.24098706	2.89051008
C	-0.88089067	2.35446095	0.16963917
O	-1.40971088	3.36805081	0.10691778