

Mechanisms of the S/CO/Se interchange reactions at FeMo-co, the active site cluster of nitrogenase

Ian Dance

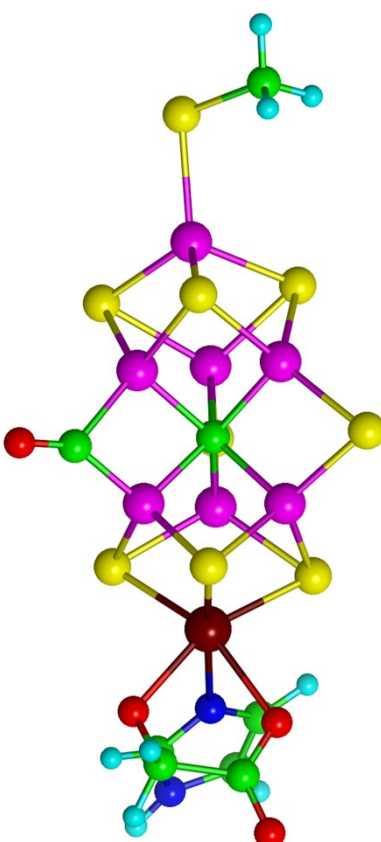
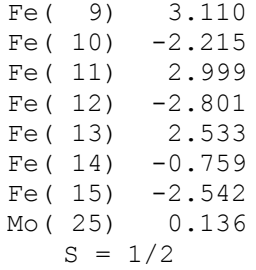
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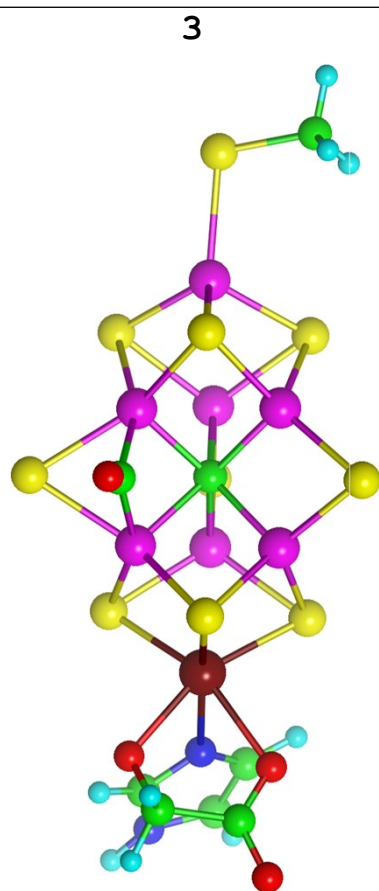
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Supplementary Information

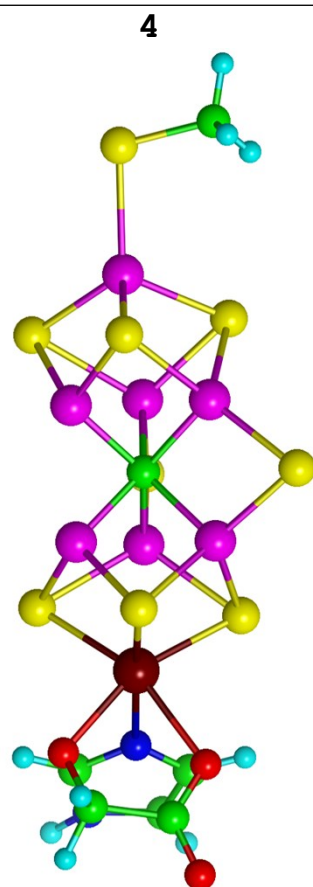
1. Details of calculated intermediates and transition states: pictorial representation, metal spin densities (Mulliken calculation), total spin S , and cartesian coordinates. The standard view direction is towards Fe2-Fe3-Fe6-Fe7 face, with S3A obscured behind C^c: in some instances a top view is included.

species	cartesian coordinates				
	C1	1.074946112	8.252491045	1.006289005	
	C2	0.930587521	-3.693153008	-2.612125856	
	C3	0.472327428	-4.664383231	-3.477150743	
	C4	-0.979347102	-4.352577286	-1.797261434	
	C5	-0.841942880	-4.539694778	1.832853601	
	C6	0.690344462	-4.755018603	1.705084267	
	C7	-2.450570821	1.437862879	1.806882970	
	C8	0.113757462	1.594706668	0.219063312	
	Fe9	-0.300855954	5.258321294	0.177649745	
	Fe10	-1.289681390	2.847287487	0.967740620	
	Fe11	1.391875882	3.011413922	1.012614225	
	Fe12	0.035220741	2.917310026	-1.347180998	
	Fe13	0.126237164	0.269178823	-1.315582479	
	Fe14	-1.166812127	0.342945506	1.027249980	
	Fe15	1.476229817	0.352295560	1.047091267	
	H16	1.972371440	8.004384768	0.417578636	
	H17	1.026780352	9.350692679	1.138601433	
	H18	1.176632521	7.778775247	1.993807048	
	H19	1.826695162	-3.082328651	-2.635754665	
	H20	0.881385745	-5.097351710	-4.383255598	
	H21	-1.828768918	-4.445043794	-1.125244928	
	H22	-1.401935419	-5.744625441	-3.364406947	
	H23	-1.335033188	-5.526979981	1.668554760	
	H24	-1.019010415	-4.281858519	2.906901972	
	Mo25	0.016479015	-2.011096119	0.376749759	
	N26	0.023527140	-3.519816534	-1.583873956	
	N27	-0.751527607	-5.089833653	-2.940575494	
	O28	-3.468876394	1.504395992	2.475286320	
	O29	1.210044426	-5.831965325	2.124579376	
	O30	1.319416865	-3.759257367	1.173995919	
Fe (9)	3.110	O31	-1.361783853	-3.564401143	0.971655688
Fe (10)	-2.215	S32	-0.474172047	7.653395995	0.148614730
Fe (11)	2.999	S33	-1.997006686	4.100562265	-0.837302413
Fe (12)	-2.801	S34	-0.125251196	4.285090858	2.332941133
Fe (13)	2.533	S35	0.077205560	1.551534293	-3.167880643
Fe (14)	-0.759	S36	1.678194344	4.436029984	-0.876918045
Fe (15)	-2.542	S37	-1.799249264	-0.857333763	-0.754865840
Mo (25)	0.136	S38	0.076606810	-0.823656858	2.487376304
$S = 1/2$		S39	1.966791023	-1.027363659	-0.729834095
		S40	3.028156810	1.719059903	1.930039404



Fe (9) 3.187
 Fe (10) -2.256
 Fe (11) 2.899
 Fe (12) -2.753
 Fe (13) 2.516
 Fe (14) 1.792
 Fe (15) -2.566
 Mo (25) -0.279
 S=3/2

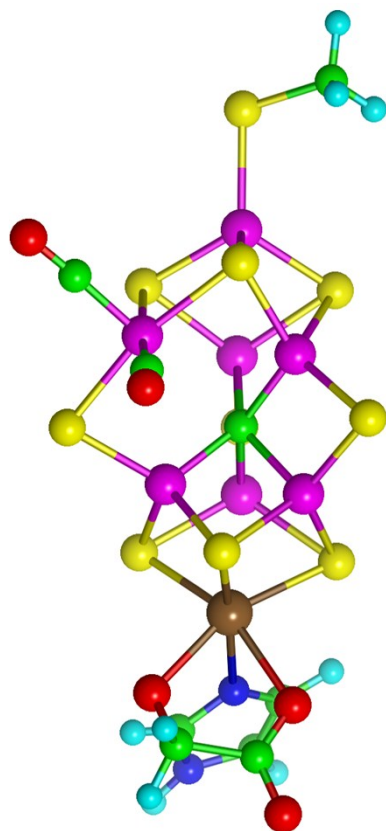
C1	2.002962277	8.061294159	0.490691452
C2	0.703342316	-3.788333495	-2.770965415
C3	0.124592915	-4.688405142	-3.643083780
C4	-1.226702609	-4.288796471	-1.899931379
C5	-0.946918838	-4.631114429	1.727792875
C6	0.577188571	-4.846754942	1.547272243
C7	-1.680703846	1.594050221	2.673714377
C8	0.036888833	1.612606101	0.302298626
Fe9	0.018519722	5.309063959	0.218329468
Fe10	-1.349207217	2.888547393	1.137045157
Fe11	1.360468739	2.905267314	1.122110674
Fe12	0.097803377	2.933559396	-1.252158808
Fe13	0.037300203	0.285233836	-1.213066905
Fe14	-1.366809918	0.321708800	1.143292485
Fe15	1.327829017	0.276413746	1.119280776
H16	2.645450880	7.497572655	-0.198252734
H17	2.216297414	9.140962605	0.384412542
H18	2.248153681	7.753757087	1.517097478
H19	1.657682750	-3.276627238	-2.825273304
H20	0.453008529	-5.122566748	-4.581157646
H21	-2.052372555	-4.318703659	-1.195039592
H22	-1.830055647	-5.600563815	-3.478238022
H23	-1.447003558	-5.614098589	1.565938567
H24	-1.092020988	-4.385558511	2.808200187
Mo25	-0.109012334	-2.064691682	0.340158750
N26	-0.143251991	-3.559542719	-1.705160596
N27	-1.114441798	-5.008506419	-3.070320914
O28	-1.881452827	1.612306928	3.860821127
O29	1.116342871	-5.920544260	1.939069306
O30	1.193438705	-3.848163770	0.998902715
O31	-1.487028239	-3.638768200	0.895760908
S32	0.201290924	7.717480682	0.110038700
S33	-1.723708385	4.320054026	-0.839452422
S34	-0.030748775	4.331015681	2.393640576
S35	0.084403724	1.571835695	-3.054730578
S36	1.917999392	4.253106010	-0.731815581
S37	-1.874854647	-0.910950970	-0.781791794
S38	-3.356477510	1.638268219	1.074505069
S39	-0.063781619	-1.014224514	2.477941526
S40	1.858887185	-1.045047522	-0.691846464
S41	2.896687270	1.547869067	2.083954858



Fe (8)	3.168
Fe (9)	-2.642
Fe (10)	2.935
Fe (11)	-2.874
Fe (12)	2.676
Fe (13)	2.412
Fe (14)	-2.711
Mo (24)	-0.215
$S=3/2$	

C1	1.261576770	8.329699769	0.544129125
C2	0.812283060	-3.996749794	-2.123729345
C3	0.294035805	-4.820001875	-3.101684993
C4	-1.343978042	-3.954841113	-1.838170228
C5	-1.049291142	-4.499279021	2.089539009
C6	0.485719618	-4.708043864	1.982580433
C7	-0.059428530	1.734860045	0.375931712
Fe8	-0.453735159	5.439125608	0.260772847
Fe9	-1.424244927	3.005353469	0.986927467
Fe10	1.190058265	3.128339576	1.183418673
Fe11	-0.081218290	3.020634944	-1.239944473
Fe12	-0.053678562	0.303940188	-1.082889129
Fe13	-1.327869743	0.436048977	1.140870758
Fe14	1.286535328	0.476283145	1.284789573
H15	1.938849645	7.732216412	-0.081171616
H16	1.427312075	9.404092285	0.337338095
H17	1.507988796	8.131200477	1.598111244
H18	1.839744901	-3.725799609	-1.909168155
H19	0.753063679	-5.414547148	-3.885043683
H20	-2.325385499	-3.706638277	-1.456838613
H21	-1.796181475	-5.206715891	-3.512245115
H22	-1.534205358	-5.487965154	1.910446514
H23	-1.242186570	-4.255363314	3.166308449
Mo24	-0.199783644	-2.000479394	0.600576747
N25	-0.210266517	-3.474318910	-1.355322816
N26	-1.095323379	-4.798120718	-2.903011438
O27	1.008135925	-5.769111360	2.438136414
O28	1.116557963	-3.726140388	1.429352304
O29	-1.562766790	-3.518740777	1.233790223
S30	-0.515360971	7.863475679	0.173093627
S31	-2.149923530	4.253431580	-0.810831631
S32	-0.421486331	4.404386468	2.443786673
S33	-0.014065248	1.555442118	-2.978390500
S34	1.548434429	4.569743745	-0.695318159
S35	-2.055812247	-0.859577247	-0.574736622
S36	-0.150784526	-0.739386618	2.690967655
S37	1.771259516	-1.002254017	-0.467387678
S38	2.825420985	1.875800189	2.145016566

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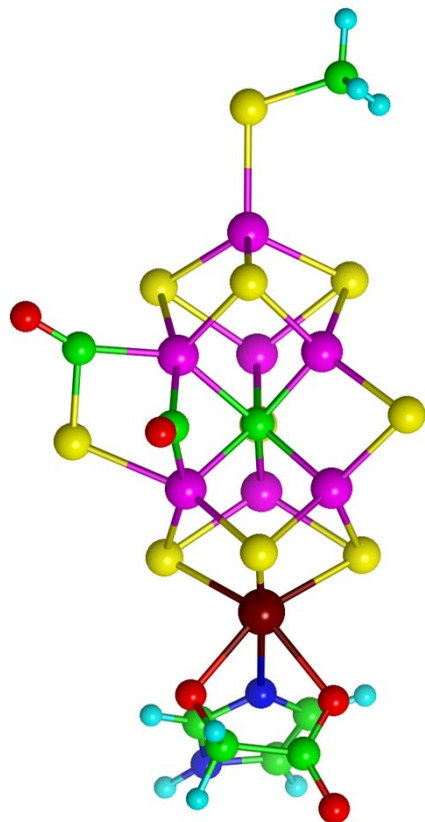


Fe (10) 1.105
 Fe (11) -0.142
 Fe (12) 1.752
 Fe (13) -2.756
 Fe (14) 2.073
 Fe (15) 1.329
 Fe (16) -2.331
 Mo (26) -0.093

S=1/2

C1	1.974653296	7.705706512	0.305083931
C2	0.987413159	-3.877975598	-2.882847631
C3	0.461719035	-4.781027731	-3.781740810
C4	-0.944459189	-4.456141913	-2.078394257
C5	-0.882391177	-4.802368410	1.466219979
C6	0.636440516	-5.042230719	1.365764463
C7	-1.413961887	2.185787827	3.303654510
C8	0.279855269	1.208664376	0.105554580
C9	-2.797663989	3.989900789	2.142337457
Fe10	0.285389157	4.922928206	-0.062227610
Fe11	-1.543254983	2.872865886	1.686026143
Fe12	1.321174348	2.548521074	1.013127704
Fe13	0.172598153	2.572780489	-1.334077556
Fe14	0.258958993	-0.036504113	-1.392440389
Fe15	-1.118479394	0.105584989	0.735082259
Fe16	1.485382217	-0.074120451	0.969014777
H17	2.765572865	7.194526148	-0.267287144
H18	2.094075538	8.801692482	0.190501108
H19	2.106184565	7.443447339	1.366986346
H20	1.919904516	-3.318379862	-2.902979066
H21	0.824749677	-5.182698992	-4.723733559
H22	-1.773648647	-4.516813151	-1.371448784
H23	-1.453418538	-5.765266670	-3.676839153
H24	-1.387912463	-5.784315961	1.292969085
H25	-1.071956515	-4.548631223	2.541749918
Mo26	0.079850326	-2.294390688	0.118020974
N27	0.111023131	-3.700486712	-1.842318872
N28	-0.776315135	-5.141781638	-3.252331374
O29	-1.399264155	1.828643440	4.424722283
O30	1.137265686	-6.124439663	1.771319764
O31	1.294588671	-4.050315531	0.863447246
O32	-1.363610545	-3.820060754	0.610754108
O33	-3.672560650	4.696207151	2.513106501
S34	0.296583049	7.188279610	-0.282008336
S35	-1.581462130	3.861139962	-0.622901457
S36	0.309852052	4.253341830	2.048068561
S37	0.173041158	1.292970467	-3.160763214
S38	2.032423856	3.802724469	-0.783757513
S39	-1.655994296	-1.134577826	-1.019719813
S40	-2.969797624	1.158294053	1.073668149
S41	-0.014166821	-1.194916208	2.220763244
S42	2.066488577	-1.304641156	-0.833563917
S43	2.745141264	1.318094369	2.143436392

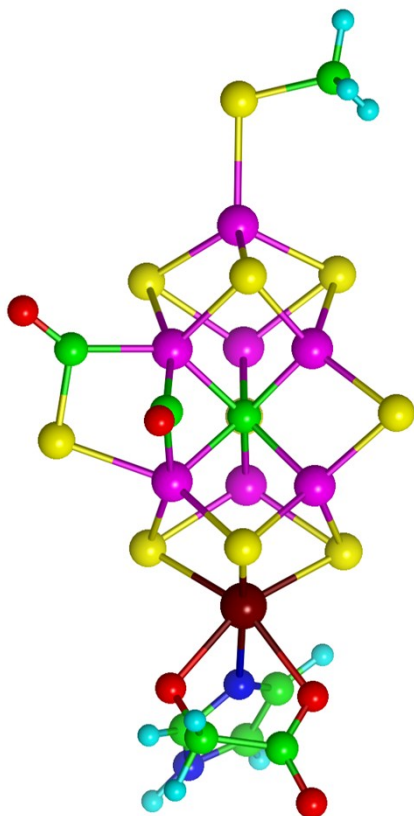
TS 6-7



Fe (10) 2.955
Fe (11) -1.319
Fe (12) 2.262
Fe (13) -2.742
Fe (14) 2.295
Fe (15) -0.254
Fe (16) -2.358
Mo (26) -0.012
S=1/2

C1	1.720160161	7.899143210	0.353676943
C2	1.128716871	-4.082153997	-2.623783976
C3	0.516366353	-4.911860501	-3.538298954
C4	-0.935333697	-4.237784965	-1.983467341
C5	-0.513425289	-4.661156914	1.708203558
C6	1.005768777	-4.825240412	1.520857849
C7	-1.443590205	1.328040805	2.556700566
C8	0.156765795	1.386333588	0.192859887
C9	-3.184953567	2.806358043	1.481798808
Fe10	-0.027851181	4.988932396	0.090876362
Fe11	-1.334408123	2.674483667	1.151247119
Fe12	1.355070326	2.743918875	0.941601265
Fe13	0.147958857	2.694990794	-1.346728771
Fe14	0.234853664	0.109098236	-1.312675538
Fe15	-1.190727353	0.156272137	0.978355713
Fe16	1.534051696	0.167017610	0.942426473
H17	2.421954516	7.382348024	-0.317336331
H18	1.798513588	8.990633437	0.185954660
H19	2.018410481	7.682277878	1.391027689
H20	2.157095406	-3.734376667	-2.573331181
H21	0.877041733	-5.437092017	-4.418827267
H22	-1.840515378	-4.104148517	-1.398510954
H23	-1.565536406	-5.460041456	-3.605369334
H24	-0.973768244	-5.670938888	1.574621184
H25	-0.652440986	-4.405177578	2.793023946
Mo26	0.235171346	-2.152766079	0.259402705
N27	0.218751242	-3.678000908	-1.678315708
N28	-0.805961259	-5.008767427	-3.109189913
O29	-1.652570811	1.225614352	3.731847876
O30	1.591421452	-5.859718334	1.931840681
O31	1.577975930	-3.821679024	0.935435080
O32	-1.096557514	-3.721638187	0.871357977
O33	-4.178426095	3.404962035	1.839603575
S34	-0.012359288	7.340819631	0.019904600
S35	-1.685214905	3.950405130	-0.940670960
S36	-0.006861063	4.051208619	2.215017250
S37	0.175024886	1.367059919	-3.132835094
S38	1.872734766	4.081312167	-0.833244402
S39	-1.582825545	-1.130797761	-0.846257882
S40	-3.296137147	1.054171777	0.588174088
S41	0.187054679	-1.044214763	2.316263627
S42	2.102506685	-1.092123772	-0.837392529
S43	2.946094847	1.554275838	1.924156650

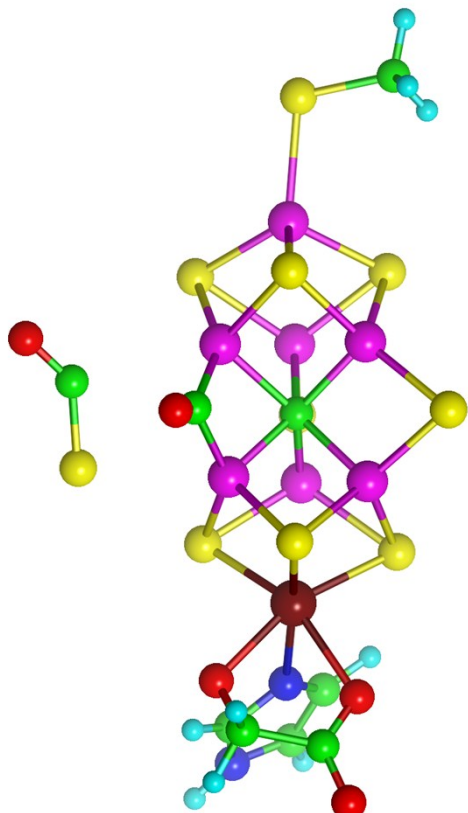
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Fe (10) 3.123
 Fe (11) -0.928
 Fe (12) 1.086
 Fe (13) -2.675
 Fe (14) 2.406
 Fe (15) 0.225
 Fe (16) -2.309
 Mo (26) -0.113
 S=1/2

C1	2.319764314	7.645609731	0.429406250
C2	0.792574111	-3.781372493	-2.797543988
C3	0.225166002	-4.700849647	-3.653911493
C4	-1.042357102	-4.428973514	-1.836783095
C5	-1.040510874	-4.562172492	1.698019482
C6	0.468435571	-4.863792516	1.616418478
C7	-1.377795410	1.593939851	2.496843107
C8	0.260041345	1.393575473	0.200902679
C9	-2.996897233	2.868821070	1.253844556
Fe10	0.366426721	4.983320129	0.092615468
Fe11	-1.083067467	2.750315109	1.066734813
Fe12	1.566332232	2.594776205	1.001347938
Fe13	0.443423517	2.685654851	-1.317144291
Fe14	0.334549729	0.096020360	-1.317087551
Fe15	-1.231053366	0.261263521	0.872569981
Fe16	1.446108088	0.020457907	1.043253682
H17	2.981964546	6.997170045	-0.163651674
H18	2.586313429	8.704991554	0.244837700
H19	2.488663827	7.421244708	1.494984833
H20	1.700580411	-3.192347033	-2.895824208
H21	0.521224227	-5.084414391	-4.626553958
H22	-1.819735669	-4.489863629	-1.070774726
H23	-1.641481478	-5.745077218	-3.397185839
H24	-1.579459730	-5.533918325	1.570673844
H25	-1.224480766	-4.245534544	2.758042517
Mo26	0.016682778	-2.156234545	0.244545802
N27	-0.000625787	-3.633600942	-1.688191903
N28	-0.947021890	-5.109845598	-3.021925427
O29	-1.611804770	1.441157024	3.659537408
O30	0.929632011	-5.932375358	2.097053329
O31	1.159259408	-3.934301364	1.040797341
O32	-1.483121425	-3.613609686	0.785551461
O33	-3.890070607	3.647426083	1.555480423
S34	0.559139308	7.341599556	-0.040647426
S35	-1.323897170	4.037670748	-1.004146904
S36	0.340268226	4.040370219	2.197456588
S37	0.514355703	1.374631071	-3.110489870
S38	2.249736246	3.940842165	-0.668454336
S39	-1.614205843	-0.977421314	-0.978377149
S40	-3.323680569	1.162806171	0.548630142
S41	-0.083395696	-1.038597863	2.313330975
S42	2.046571679	-1.267068055	-0.702777359
S43	2.997449425	1.287706979	2.008592398

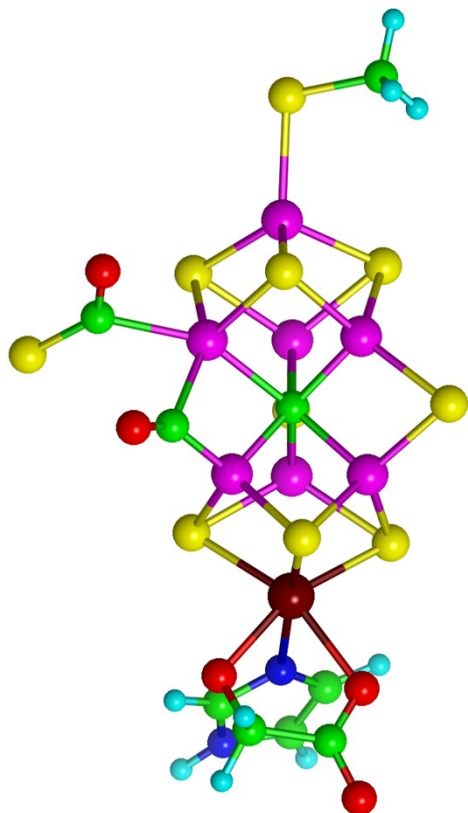
TS 7-2



Fe (10) 3.075
Fe (11) -2.045
Fe (12) 2.916
Fe (13) -2.583
Fe (14) 2.456
Fe (15) -1.396
Fe (16) -2.391
Mo (26) 0.217
S=1/2

C1	2.146531324	7.756687085	0.198488198
C2	0.827927350	-3.739829445	-2.754382607
C3	0.218018680	-4.676676942	-3.557941718
C4	-0.908011290	-4.427429408	-1.648327438
C5	-0.688501855	-4.488946130	1.883395481
C6	0.820247656	-4.785789720	1.718698703
C7	-1.590037210	1.545753509	2.372045054
C8	0.326180732	1.441779424	0.170162908
C9	-3.903027847	2.037112085	1.040967787
Fe10	0.173248769	5.024146832	0.080937705
Fe11	-1.106765675	2.732542106	0.943432604
Fe12	1.618946635	2.787297731	0.932292327
Fe13	0.286970316	2.732595004	-1.347095380
Fe14	0.410072035	0.140799229	-1.332508603
Fe15	-0.960574359	0.253266626	0.978443823
Fe16	1.664258545	0.166098693	0.976371041
H17	2.788323114	7.119326216	-0.428387721
H18	2.350817124	8.817668148	-0.033798639
H19	2.411620000	7.572238447	1.252487056
H20	1.708805521	-3.121427628	-2.926763230
H21	0.452644939	-5.063780653	-4.545252474
H22	-1.629361286	-4.495454213	-0.830492962
H23	-1.588057709	-5.772231448	-3.147947728
H24	-1.229885601	-5.463216567	1.813220631
H25	-0.813906395	-4.142192074	2.943323389
Mo26	0.269790191	-2.108307925	0.320300051
N27	0.124266177	-3.608363953	-1.585153661
N28	-0.888285226	-5.108449880	-2.835374463
O29	-1.946868735	1.502779206	3.516033400
O30	1.310791777	-5.847597064	2.188409305
O31	1.468277123	-3.861929651	1.092726683
O32	-1.178140198	-3.564699510	0.972569905
O33	-4.780420998	2.846622076	1.292822724
S34	0.363040480	7.375426859	-0.116049824
S35	-1.578591093	3.995930388	-0.923428891
S36	0.198650756	4.115231435	2.211972372
S37	0.344070657	1.417510095	-3.139436252
S38	2.032122371	4.089650238	-0.944104065
S39	-1.430274191	-1.005393804	-0.871280704
S40	-3.792984978	0.420746148	0.607103070
S41	0.286146695	-0.963712950	2.389806624
S42	2.211678307	-1.156279346	-0.768773096
S43	3.200247373	1.510500732	1.840488619

8

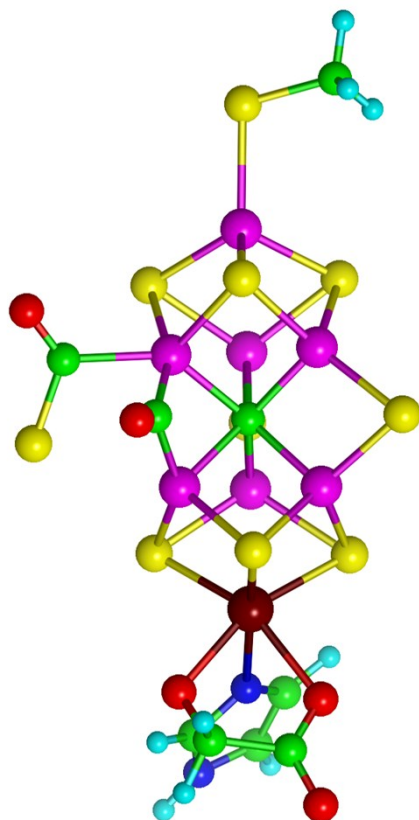


Fe (10)	3.049
Fe (11)	-2.258
Fe (12)	2.926
Fe (13)	-2.629
Fe (14)	2.267
Fe (15)	-0.689
Fe (16)	-2.398
Mo (26)	0.151

S=1/2

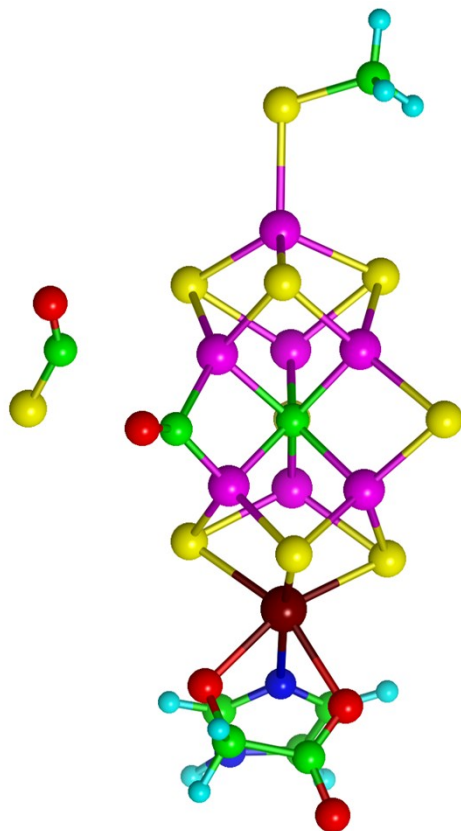
C1	1.931231526	7.598369682	0.493326814
C2	1.062436600	-3.937051908	-2.596344094
C3	0.457457505	-4.801349674	-3.482710111
C4	-0.954791483	-4.226107501	-1.854178307
C5	-0.595221029	-4.654282128	1.764201140
C6	0.920388538	-4.884186517	1.604864755
C7	-2.056502226	1.060465762	2.092568292
C8	0.290276528	1.374582680	0.211393979
C9	-3.386594386	3.080929595	0.946838748
Fe10	0.105496297	4.896289100	0.083144908
Fe11	-1.340084073	2.646232538	0.895194433
Fe12	1.535975936	2.722724788	1.018094008
Fe13	0.374221278	2.617619828	-1.340360648
Fe14	0.364921814	0.055102040	-1.263870516
Fe15	-0.885251013	0.133282265	1.041512612
Fe16	1.661306481	0.123008271	1.028510103
H17	2.638888033	6.988792273	-0.088242503
H18	2.164135591	8.670475547	0.343411040
H19	2.068169899	7.354493430	1.558594883
H20	2.063607078	-3.513777482	-2.597775348
H21	0.805454724	-5.297016385	-4.384472633
H22	-1.826452121	-4.161376484	-1.207009106
H23	-1.582532312	-5.494894283	-3.438756374
H24	-1.100112145	-5.635765263	1.596598075
H25	-0.748166313	-4.407724719	2.846725175
Mo26	0.269393242	-2.167513742	0.339518453
N27	0.178079323	-3.600180426	-1.602407728
N28	-0.833165335	-4.980886642	-2.990542558
O29	-2.824425947	1.033181605	3.013512542
O30	1.445613998	-5.950132962	2.021184647
O31	1.544214050	-3.901737502	1.044939056
O32	-1.115758736	-3.668664790	0.934477934
O33	-3.337920712	3.965438965	1.797594881
S34	0.205484448	7.237106144	-0.046801776
S35	-1.496189051	3.868901456	-1.079571154
S36	0.031658404	3.970422168	2.212740914
S37	0.446785305	1.272106379	-3.101658908
S38	2.047320097	4.022160870	-0.830700998
S39	-1.539888919	-1.003576786	-0.721802810
S40	-4.658576638	2.364098133	0.062437769
S41	0.350913984	-1.049855605	2.446323057
S42	2.189903094	-1.188954682	-0.736237077
S43	3.128265506	1.469251975	1.965725388

TS 7-8



C1	1.828050446	7.825603244	0.244971212
C2	0.873594502	-3.719957300	-2.796356715
C3	0.340603962	-4.707346562	-3.592722409
C4	-0.807012195	-4.531263607	-1.687407585
C5	-0.531862137	-4.604106109	1.850875720
C6	0.982437579	-4.804358322	1.645154887
C7	-1.547757743	1.473615605	2.472632533
C8	0.193195195	1.425909738	0.147602268
C9	-3.275605890	2.543127676	1.147201197
Fe10	0.063599024	4.993245190	0.054222667
Fe11	-1.266283726	2.628171630	0.976559754
Fe12	1.491515471	2.769932975	0.909451983
Fe13	0.165189229	2.683535994	-1.354569362
Fe14	0.237137996	0.112518158	-1.313182950
Fe15	-1.090776475	0.147061788	1.032708956
Fe16	1.571189421	0.156806783	0.940933760
H17	2.531691134	7.244450538	-0.372480740
H18	1.974702438	8.903409223	0.039952306
H19	2.067867538	7.635571578	1.303379339
H20	1.710460619	-3.049414245	-2.966260958
H21	0.604508986	-5.081478641	-4.577532047
H22	-1.515758386	-4.661973335	-0.865145297
H23	-1.390361517	-5.925788094	-3.185153362
H24	-1.014170622	-5.608883237	1.786110018
H25	-0.650743021	-4.272666771	2.912594411
Mo26	0.238811095	-2.153958704	0.307809664
N27	0.156884372	-3.633274920	-1.627203492
N28	-0.732998254	-5.221314634	-2.869532326
O29	-1.902128346	1.400886557	3.611512979
O30	1.553344679	-5.834256560	2.087587968
O31	1.559560889	-3.835728319	1.012094303
O32	-1.105189318	-3.704096860	0.961954928
O33	-3.974587038	3.451837445	1.585083806
S34	0.089574061	7.344736574	-0.144834355
S35	-1.665266446	3.939971144	-0.943018130
S36	0.072377996	4.064749631	2.187348546
S37	0.175693242	1.358132959	-3.136104320
S38	1.911957625	4.054366789	-0.971584643
S39	-1.569255438	-1.105313201	-0.787116963
S40	-3.841974274	0.955673290	0.609213171
S41	0.292111728	-1.040847090	2.388628990
S42	2.097885419	-1.124209198	-0.835605175
S43	3.097786179	1.506921199	1.810225465

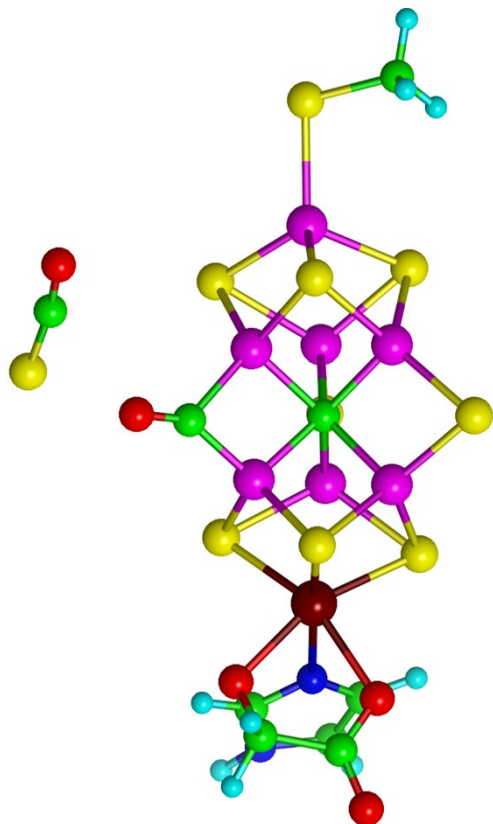
TS 8-2



Fe (10) 3.057
 Fe (11) -2.228
 Fe (12) 2.935
 Fe (13) -2.640
 Fe (14) 2.375
 Fe (15) -0.760
 Fe (16) -2.462
 Mo (26) 0.149
 S=1/2

C1	1.927410617	7.810645995	0.628308289
C2	1.159656048	-4.031942057	-2.574172861
C3	0.598145705	-4.836545471	-3.541925731
C4	-0.960138702	-4.090872388	-2.132073583
C5	-0.789618168	-4.656941542	1.605343457
C6	0.718666765	-4.955999047	1.507346384
C7	-1.776714992	1.203216415	2.261337500
C8	0.412757259	1.372199567	0.278529904
C9	-3.957660560	2.702156026	0.972210108
Fe10	0.180434331	4.943878911	0.275432498
Fe11	-1.002739735	2.617764222	1.043837863
Fe12	1.686648556	2.703810198	1.084647176
Fe13	0.377189512	2.694419426	-1.228288094
Fe14	0.398866170	0.099476033	-1.246006562
Fe15	-0.779769576	0.138826679	1.117051853
Fe16	1.758680299	0.064698082	1.018278552
H17	2.672071954	7.285695970	0.007983843
H18	2.045178741	8.902719749	0.485004683
H19	2.135805424	7.572338267	1.683855865
H20	2.191425738	-3.727983549	-2.425251237
H21	1.017675583	-5.378524239	-4.385646122
H22	-1.909924422	-3.928760971	-1.630538646
H23	-1.485831949	-5.318761001	-3.792580724
H24	-1.333402943	-5.608168715	1.386025295
H25	-0.981597002	-4.439439981	2.688527784
Mo26	0.254145805	-2.177638843	0.291608486
N27	0.183827167	-3.583939516	-1.717806464
N28	-0.761564190	-4.869543874	-3.242811553
O29	-2.412728747	1.225650401	3.287670114
O30	1.176028504	-6.051125092	1.930117477
O31	1.411829790	-4.000831626	0.981362439
O32	-1.222407073	-3.621762812	0.789618429
O33	-4.139611798	3.571254046	1.776518671
S34	0.215794104	7.299399951	0.155723429
S35	-1.531170058	3.917850930	-0.770671693
S36	0.222703848	3.967799561	2.384020110
S37	0.405702417	1.399160224	-3.039100396
S38	2.078085499	4.081808372	-0.755033616
S39	-1.531880421	-0.907117620	-0.676811048
S40	-4.568594657	1.595096898	-0.066906691
S41	0.446057729	-1.142268236	2.430039236
S42	2.197773067	-1.227055048	-0.795317368
S43	3.272794362	1.385355707	1.950542945

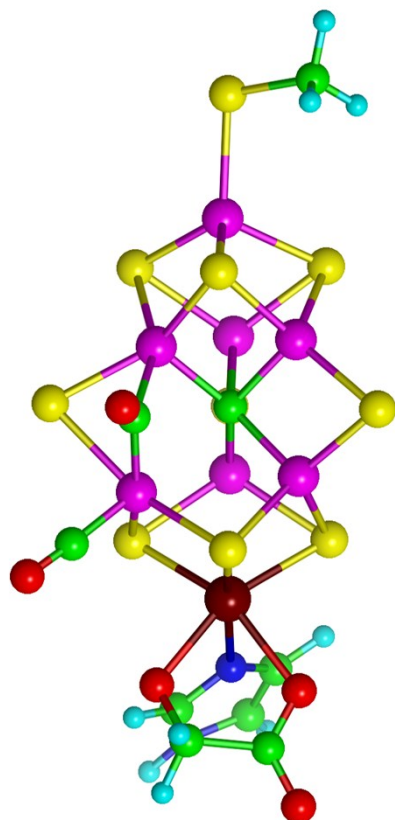
2 + SCO



S=1/2

C1	1.910656858	7.678847050	0.703813404
C2	1.120813086	-3.969280557	-2.651067691
C3	0.500208575	-4.757290326	-3.595424977
C4	-0.933102969	-4.178999650	-1.985824351
C5	-0.610301077	-4.712888691	1.679743831
C6	0.896918328	-4.991676061	1.506868320
C7	-1.942455340	1.210762976	1.970091741
C8	0.515345530	1.312743332	0.291966272
C9	-4.606386773	3.273210218	0.850145469
Fe10	0.205143762	4.884472712	0.351315744
Fe11	-0.803177699	2.563325365	1.106556663
Fe12	1.836520770	2.638486164	1.049469958
Fe13	0.399632843	2.654943604	-1.198726673
Fe14	0.483036352	0.051680789	-1.242255512
Fe15	-0.756887798	0.096641102	1.091348094
Fe16	1.836180190	0.008897445	1.025579545
H17	2.612120628	7.106875346	0.077212721
H18	2.083466071	8.761670513	0.551142511
H19	2.117665725	7.430018635	1.756408092
H20	2.141894086	-3.596889664	-2.606781785
H21	0.853092631	-5.227159417	-4.510464733
H22	-1.830759789	-4.080061901	-1.379512484
H23	-1.575050131	-5.333983403	-3.655835400
H24	-1.151074974	-5.676237652	1.507187263
H25	-0.747263305	-4.475767607	2.768997682
Mo26	0.333488557	-2.220187488	0.314185469
N27	0.220845503	-3.622310149	-1.673127116
N28	-0.813752974	-4.892634442	-3.151531638
O29	-2.904024565	1.306905032	2.713299431
O30	1.383323743	-6.095766770	1.874172928
O31	1.554211612	-4.011139401	0.987114897
O32	-1.102816285	-3.698476740	0.868103620
O33	-4.413107774	4.128972031	1.634827478
S34	0.170928976	7.237086958	0.261910168
S35	-1.551403943	3.836562463	-0.625492222
S36	0.430506908	3.887825000	2.438201862
S37	0.403265209	1.369988142	-3.030408103
S38	2.083069907	4.088125666	-0.777288925
S39	-1.450985847	-0.980868752	-0.703051001
S40	-5.065506790	2.136431321	-0.159567877
S41	0.481225184	-1.142860265	2.447580360
S42	2.272134808	-1.290304191	-0.782280199
S43	3.412369167	1.290311229	1.901377025

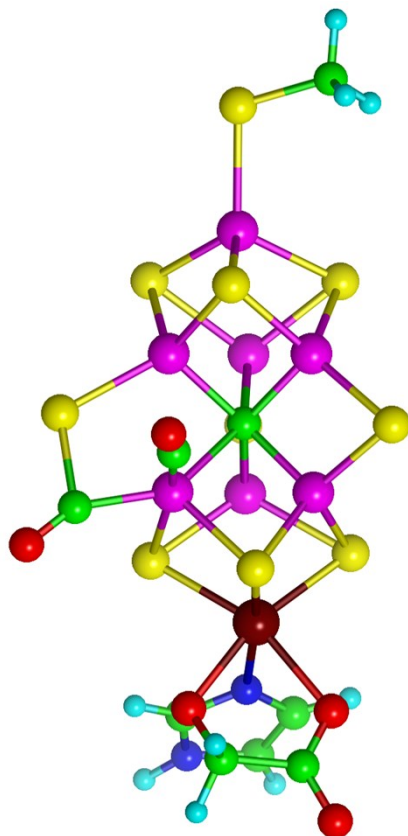
9



Fe (10) 3.038
 Fe (11) -2.147
 Fe (12) 2.733
 Fe (13) -2.626
 Fe (14) 2.234
 Fe (15) 0.083
 Fe (16) -2.621
 Mo (26) 0.092
 S=1/2

C1	1.905207438	7.825526587	0.630713326
C2	0.844875570	-3.487499648	-2.853092290
C3	0.276082388	-4.390313454	-3.725406662
C4	-0.988694962	-4.155682893	-1.900998117
C5	-0.646858713	-4.536864228	1.569727012
C6	0.861644039	-4.721290969	1.319705748
C7	-1.489838501	1.629389732	2.498285597
C8	0.221088107	1.645118492	0.093849878
C9	-2.713698223	-0.765390142	2.152316913
Fe10	0.137517657	5.181193086	-0.093384884
Fe11	-1.114488106	2.850622702	0.887158324
Fe12	1.510739734	2.939768210	0.841592531
Fe13	0.230255708	2.877140113	-1.464973279
Fe14	0.125549112	0.305911316	-1.277220252
Fe15	-1.520725243	0.132014717	1.269051442
Fe16	1.509293189	0.366140435	0.899508619
H17	2.697635903	7.284360869	0.090914583
H18	2.140642800	8.908552061	0.629875462
H19	1.897385957	7.465867745	1.671345243
H20	1.752635828	-2.893967732	-2.940187792
H21	0.577275818	-4.758004837	-4.702394885
H22	-1.762252646	-4.248284143	-1.136221673
H23	-1.605186079	-5.418752832	-3.496396212
H24	-1.138184725	-5.523660643	1.385284957
H25	-0.745062489	-4.343901076	2.669316013
Mo26	0.108881986	-1.958176954	0.240845849
N27	0.053991339	-3.365006784	-1.739036962
N28	-0.894384138	-4.815938024	-3.098213107
O29	-1.652551287	1.883420517	3.663298957
O30	1.429490672	-5.804473685	1.617518023
O31	1.444568599	-3.682077999	0.815166915
O32	-1.235260127	-3.528710022	0.816088486
O33	-3.539335725	-1.325721787	2.783170506
S34	0.267345204	7.521600296	-0.166197237
S35	-1.579329318	4.213576781	-1.076654617
S36	0.133899076	4.320285853	2.073291845
S37	0.060583320	1.466062118	-3.169422979
S38	2.022883829	4.193506242	-1.035284156
S39	-1.723688271	-0.895614372	-0.784360932
S40	-3.135913613	1.809790345	0.783264381
S41	0.223942864	-0.904394276	2.342350967
S42	1.987058418	-0.947208222	-0.870061725
S43	3.064992080	1.651064800	1.785860609

TS 9-10

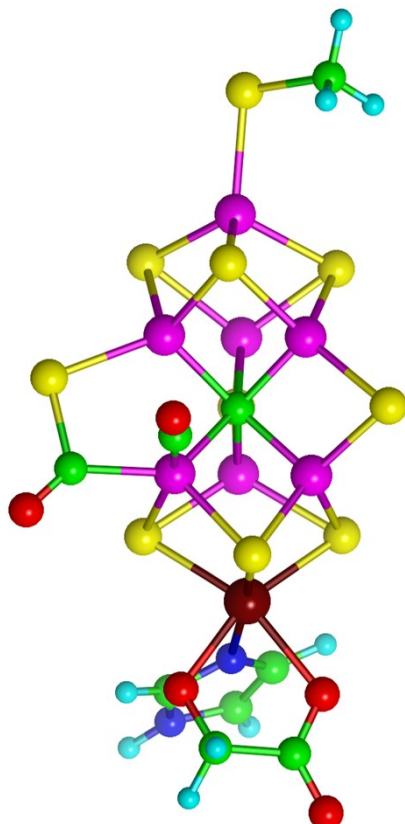


Fe (10) 3.034
Fe (11) -2.581
Fe (12) 2.827
Fe (13) -2.610
Fe (14) 2.674
Fe (15) -0.063
Fe (16) -1.624
Mo (26) -1.028

S=1/2

C1	1.878306374	8.003712017	0.735305962
C2	0.998281019	-3.830471396	-2.863869100
C3	0.338505927	-4.587760732	-3.807261633
C4	-1.089215521	-3.822512324	-2.270363902
C5	-0.498318374	-4.683259187	1.447121396
C6	1.017772172	-4.863652799	1.252463144
C7	-1.293704925	1.052596626	3.038158991
C8	0.118543634	1.588149513	0.253925513
C9	-3.112889086	0.087246345	1.671351715
Fe10	0.084759639	5.199931310	0.196176724
Fe11	-1.265408194	2.920402771	0.787056893
Fe12	1.376188269	2.851705323	1.115127271
Fe13	0.279871405	2.895838830	-1.283931561
Fe14	0.150555283	0.292165045	-1.275887385
Fe15	-1.277561722	0.335409405	1.432783578
Fe16	1.351511103	0.264918609	0.965485815
H17	2.614134658	7.538901136	0.061528106
H18	2.000293072	9.104784538	0.691235946
H19	2.100227391	7.669246141	1.761959062
H20	2.051991546	-3.580177241	-2.781258867
H21	0.673159253	-5.125235810	-4.691809660
H22	-1.995348969	-3.628370179	-1.707067771
H23	-1.775903094	-4.997010768	-3.904764466
H24	-0.981629588	-5.680215583	1.299182161
H25	-0.636440177	-4.430484598	2.531427996
Mo26	0.260199064	-2.139252441	0.094097833
N27	0.105109075	-3.368073496	-1.931272617
N28	-0.998547175	-4.573209578	-3.412698550
O29	-1.412379593	1.384340692	4.159344311
O30	1.592633250	-5.918175546	1.629428570
O31	1.597404669	-3.847371043	0.697072435
O32	-1.059199537	-3.722671490	0.619847682
O33	-4.042769276	-0.603711905	2.020134855
S34	0.162927836	7.546258038	0.223834710
S35	-1.539330526	4.315280946	-1.032965213
S36	-0.117398728	4.178602887	2.280464575
S37	0.210043464	1.592159597	-3.078990989
S38	2.012711947	4.209004123	-0.666737825
S39	-1.652924587	-0.929104825	-0.679441354
S40	-3.323781762	1.860099020	0.905289299
S41	0.202243410	-1.157636200	2.272588514
S42	2.074482277	-0.880970986	-0.839694922
S43	2.820895099	1.478575215	2.085622758

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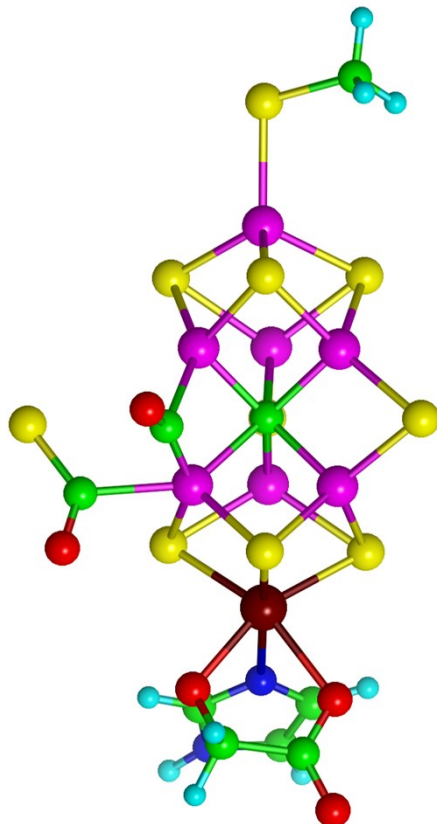


Fe (10)	2.987
Fe (11)	-2.764
Fe (12)	2.844
Fe (13)	-2.688
Fe (14)	2.549
Fe (15)	0.511
Fe (16)	-2.159
Mo (26)	-0.635

S=1/2

C1	2.058124666	7.730201826	0.478892116
C2	0.974413214	-3.731822408	-2.611283172
C3	0.374752362	-4.553795551	-3.540312720
C4	-1.072309926	-3.990227309	-1.935822527
C5	-0.706360163	-4.713961290	1.603352806
C6	0.804427717	-4.923253941	1.403444292
C7	-1.414144056	1.388070429	2.875849205
C8	0.124941849	1.532009891	0.248114191
C9	-3.220412237	0.686453544	1.388483629
Fe10	0.294415692	5.131914211	-0.367608423
Fe11	-1.237113355	3.015035556	0.431180021
Fe12	1.355649230	2.900436567	1.005944491
Fe13	0.476090133	2.678759853	-1.460284404
Fe14	0.273915018	0.130003932	-1.159748423
Fe15	-1.264273489	0.493300484	1.369913653
Fe16	1.349802592	0.294809166	1.166762520
H17	2.913066528	7.133958129	0.122318347
H18	2.329624400	8.804364891	0.474098448
H19	1.842553566	7.424168612	1.514730290
H20	1.987067672	-3.338955848	-2.570200218
H21	0.738813170	-5.037959569	-4.442904881
H22	-1.970119135	-3.911565648	-1.326861376
H23	-1.674825581	-5.216579876	-3.566795062
H24	-1.219493913	-5.670890488	1.342626282
H25	-0.842320421	-4.583827168	2.708853987
Mo26	0.149703670	-2.105949308	0.409891585
N27	0.070834952	-3.402360682	-1.632057220
N28	-0.934714659	-4.712529670	-3.092985741
O29	-1.583849882	1.833397469	3.952563425
O30	1.332606033	-6.039783260	1.649669201
O31	1.428094126	-3.865304457	0.998258673
O32	-1.233664804	-3.645659376	0.893265502
O33	-4.149205684	-0.009114833	1.781329501
S34	0.590164520	7.432424297	-0.603682591
S35	-1.278627845	4.178933011	-1.603465324
S36	-0.156657294	4.474997184	1.810862220
S37	0.532478765	1.180243082	-3.092200329
S38	2.229341969	3.955652622	-0.878567394
S39	-1.645789759	-0.893311318	-0.607451655
S40	-3.465060800	2.331781254	0.616051226
S41	0.014617157	-0.991773102	2.488704838
S42	2.100951847	-1.056037363	-0.485595244
S43	2.722478030	1.663741845	2.242647345

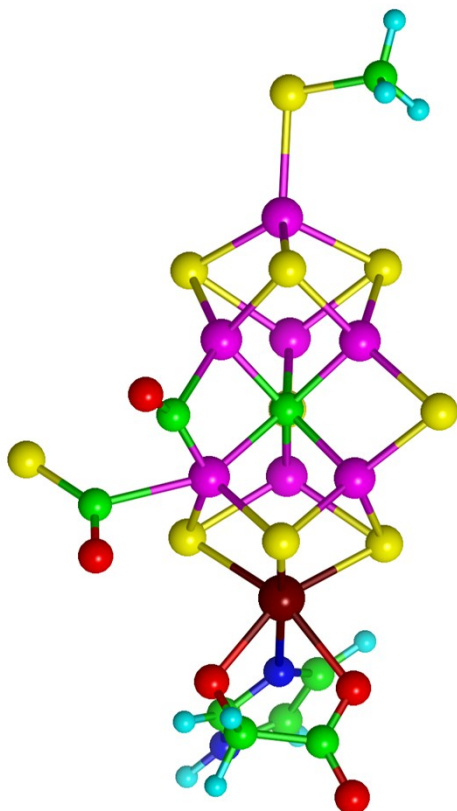
TS 10-11



Fe (10) 3.028
Fe (11) -2.617
Fe (12) 2.796
Fe (13) -2.582
Fe (14) 2.358
Fe (15) 0.400
Fe (16) -2.448
Mo (26) -0.118
S=1/2

C1	1.869358525	7.967484798	0.635295019
C2	1.071616277	-3.829706956	-2.630792094
C3	0.486833020	-4.622315780	-3.594457060
C4	-1.039666776	-3.886751380	-2.143744940
C5	-0.617154062	-4.575806481	1.573424749
C6	0.896701424	-4.773570165	1.376924598
C7	-1.647307838	1.378734962	2.488677018
C8	0.223429786	1.553256827	0.244924327
C9	-3.262551396	0.126474925	1.295735677
Fe10	0.153588407	5.158362281	0.144272731
Fe11	-1.048840251	2.863959170	0.952615858
Fe12	1.580702279	2.841675064	1.009319451
Fe13	0.303141972	2.867132610	-1.275525319
Fe14	0.247579544	0.286256279	-1.236759639
Fe15	-1.167152363	0.277993037	1.139914180
Fe16	1.544862468	0.259121616	1.027484024
H17	2.626358244	7.470002999	0.010065450
H18	1.998056617	9.063984770	0.556930089
H19	2.041780430	7.667143698	1.680917869
H20	2.108488911	-3.533560649	-2.498452824
H21	0.885489586	-5.154378928	-4.454312935
H22	-1.979623934	-3.721406416	-1.626215468
H23	-1.605215901	-5.100802642	-3.795994033
H24	-1.116996549	-5.554682337	1.380195568
H25	-0.755520606	-4.372820806	2.666371417
Mo26	0.166076889	-2.021263904	0.266606030
N27	0.115879000	-3.389635204	-1.749765177
N28	-0.867007407	-4.651502711	-3.267226007
O29	-2.011439115	1.707072258	3.574447396
O30	1.457300524	-5.840708321	1.738522101
O31	1.490963174	-3.756285995	0.842354676
O32	-1.161858996	-3.565901637	0.791709496
O33	-3.590430206	-0.910355676	1.859995775
S34	0.171755064	7.496612310	0.081505620
S35	-1.565876843	4.167410014	-0.878263027
S36	0.196380025	4.212991552	2.256421084
S37	0.239301874	1.545581190	-3.058349442
S38	2.051493629	4.212160431	-0.807376250
S39	-1.618038206	-0.852289589	-0.803670737
S40	-4.244536035	1.415675508	0.672613297
S41	0.192368152	-0.970085885	2.379023295
S42	2.076319847	-0.984201895	-0.772856654
S43	3.103390737	1.528946973	1.947494695

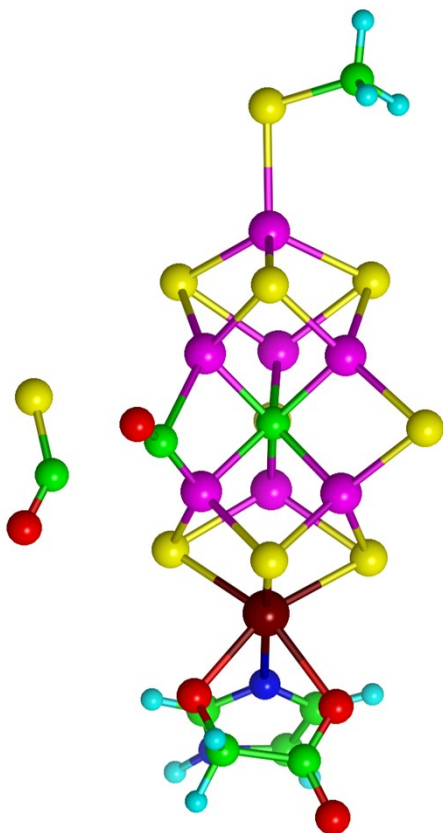
11



Fe (10) 3.025
 Fe (11) -2.494
 Fe (12) 2.792
 Fe (13) -2.620
 Fe (14) 2.300
 Fe (15) 0.383
 Fe (16) -2.440
 Mo (26) -0.077
 S=1/2

C1	2.083608743	7.803156090	0.67237215
C2	0.845063567	-3.451306039	-2.92244293
C3	0.237936767	-4.318620821	-3.80488349
C4	-0.927888321	-4.180383472	-1.90815294
C5	-0.647414712	-4.478839772	1.68421530
C6	0.873967261	-4.669654981	1.55026764
C7	-1.853118516	1.515331740	2.24124053
C8	0.279726775	1.576168690	0.20214440
C9	-3.334438304	-0.180352703	1.32829439
Fe10	0.235698091	5.175708639	0.11005007
Fe11	-0.932739628	2.907928344	0.92043283
Fe12	1.656780505	2.859346854	0.97402470
Fe13	0.366957743	2.882611547	-1.32036775
Fe14	0.288717970	0.296141038	-1.25323078
Fe15	-1.180573689	0.325458857	1.04624074
Fe16	1.540048276	0.280945007	1.04525665
H17	2.791398483	7.176464136	0.10822975
H18	2.364723092	8.868407773	0.55507122
H19	2.162315334	7.532260408	1.73730043
H20	1.741589766	-2.847575063	-3.03763012
H21	0.478852448	-4.630785397	-4.81705567
H22	-1.673636312	-4.304324264	-1.11974285
H23	-1.622811135	-5.368562886	-3.52905934
H24	-1.127912380	-5.474771079	1.53732481
H25	-0.831813123	-4.196509401	2.75038987
Mo26	0.158540569	-1.978487072	0.28665494
N27	0.115670710	-3.387126360	-1.76065380
N28	-0.891927773	-4.785207850	-3.13759708
O29	-2.384420119	1.915423336	3.23689729
O30	1.427490885	-5.713594078	1.98405183
O31	1.474690536	-3.675520232	0.98412571
O32	-1.171175731	-3.533368937	0.80962387
O33	-3.332821083	-1.122850250	2.10092269
S34	0.370738400	7.511835417	0.05191366
S35	-1.512474383	4.187421679	-0.87784609
S36	0.304859361	4.238896381	2.23486102
S37	0.327265702	1.535682700	-3.08965360
S38	2.122820658	4.214174301	-0.85573273
S39	-1.588001740	-0.832632830	-0.85687740
S40	-4.597126589	0.670861901	0.54257617
S41	0.137364361	-0.883626616	2.37679490
S42	2.095290830	-0.980515001	-0.73745696
S43	3.128171282	1.520379189	1.95708411

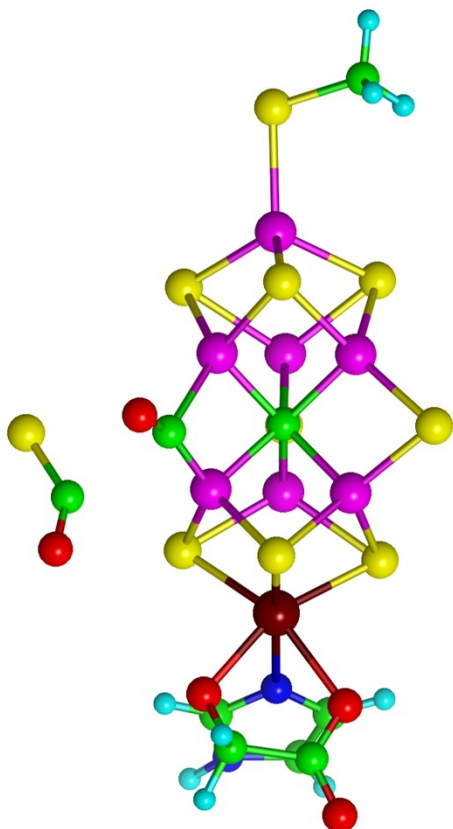
TS 10-2



Fe (10) 3.048
Fe (11) -2.680
Fe (12) 2.842
Fe (13) -2.594
Fe (14) 2.314
Fe (15) 0.413
Fe (16) -2.408
Mo (26) -0.081
S=1/2

C1	1.883984701	7.983581369	0.808735075
C2	1.129104104	-3.858885791	-2.634576463
C3	0.567510082	-4.630776512	-3.627437353
C4	-0.998844310	-3.877179278	-2.229999956
C5	-0.634130560	-4.628517468	1.524167438
C6	0.881405963	-4.836529673	1.344068842
C7	-1.788008835	1.175886943	2.418511101
C8	0.306429427	1.517893902	0.301163082
C9	-3.834385200	0.539910842	1.052164474
Fe10	0.238899870	5.127495174	0.282026057
Fe11	-0.967149133	2.824361710	1.014726899
Fe12	1.661467257	2.785471867	1.107699755
Fe13	0.407108189	2.863501597	-1.202222818
Fe14	0.275052339	0.267694412	-1.205943613
Fe15	-1.038943922	0.233263036	1.099805857
Fe16	1.585147085	0.188337757	1.074652102
H17	2.655720595	7.503410783	0.187139037
H18	1.990958266	9.083458766	0.731174673
H19	2.059250881	7.688231932	1.855737156
H20	2.165116727	-3.586326679	-2.458222297
H21	0.989205851	-5.168168067	-4.472609387
H22	-1.956193724	-3.691434146	-1.753189910
H23	-1.523844685	-5.051595855	-3.925971851
H24	-1.135720514	-5.606427252	1.327196566
H25	-0.776696362	-4.426329568	2.617872951
Mo26	0.183751660	-2.064347643	0.247221498
N27	0.148348763	-3.403457811	-1.789245595
N28	-0.798177875	-4.638035664	-3.352326995
O29	-2.234680257	1.490598602	3.484838777
O30	1.424610445	-5.912705608	1.708539087
O31	1.490275237	-3.821989965	0.823818982
O32	-1.167780489	-3.614940574	0.739688534
O33	-4.342143517	-0.450831579	1.509811518
S34	0.203054927	7.473018804	0.245544259
S35	-1.458877227	4.162197302	-0.799274598
S36	0.251168311	4.120316497	2.381143164
S37	0.302271549	1.558542877	-3.000036009
S38	2.149704306	4.201025408	-0.676963843
S39	-1.614408176	-0.861416597	-0.769290014
S40	-4.164044427	2.006584191	0.356971927
S41	0.233027558	-1.063699665	2.386027020
S42	2.100524507	-1.018699985	-0.770587171
S43	3.150930612	1.417511609	2.037452043

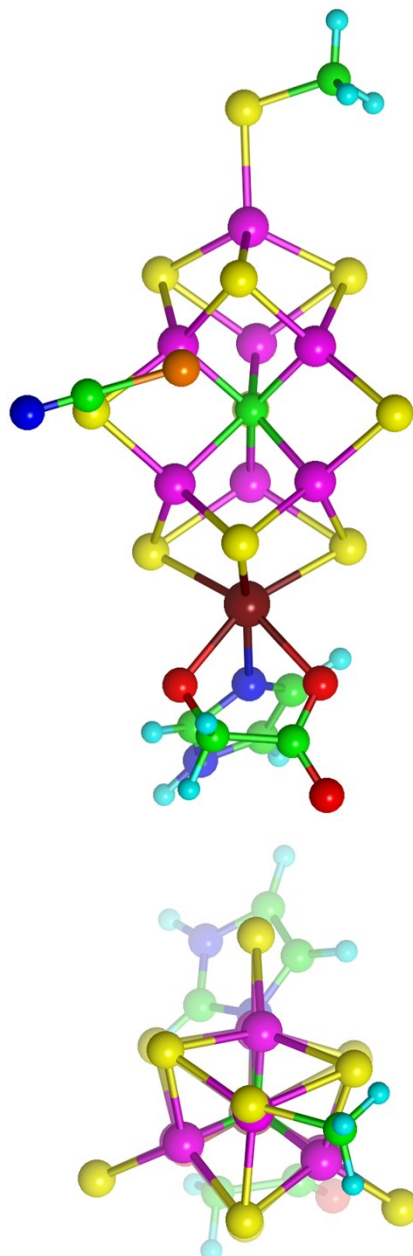
TS 11-2



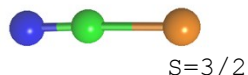
Fe (10) 3.040
 Fe (11) -2.526
 Fe (12) 2.837
 Fe (13) -2.636
 Fe (14) 2.302
 Fe (15) 0.241
 Fe (16) -2.385
 Mo (26) -0.041
 S=1/2

C1	1.853426039	8.003321340	0.767679558
C2	1.200985645	-3.867926590	-2.551933816
C3	0.669234001	-4.647173855	-3.554655668
C4	-0.939544726	-3.867608676	-2.221207226
C5	-0.718606978	-4.560995370	1.543608971
C6	0.800200747	-4.786273246	1.421026931
C7	-1.848554273	1.366102187	2.258481242
C8	0.333669568	1.530722362	0.285906621
C9	-3.748323070	0.174558750	0.987257949
Fe10	0.214222135	5.147319783	0.270622177
Fe11	-0.917386652	2.852442996	1.036616467
Fe12	1.680057615	2.816673311	1.099020617
Fe13	0.398560240	2.886622060	-1.206632690
Fe14	0.345154242	0.285700387	-1.218710112
Fe15	-1.050854421	0.296234930	1.035119435
Fe16	1.574671801	0.216617070	1.106517760
H17	2.630826594	7.512208227	0.160734925
H18	1.965454284	9.101765643	0.680959072
H19	2.017126518	7.720246970	1.820031988
H20	2.231002717	-3.597918433	-2.341815774
H21	1.117634063	-5.193399735	-4.380148031
H22	-1.912276901	-3.672361651	-1.780920926
H23	-1.412263494	-5.051733339	-3.926926688
H24	-1.222654643	-5.534795140	1.333803093
H25	-0.901557718	-4.352385412	2.629178279
Mo26	0.170341575	-2.021606143	0.269788410
N27	0.194599973	-3.396936014	-1.745427639
N28	-0.704866990	-4.643052518	-3.327182873
O29	-2.412360761	1.660114531	3.278718363
O30	1.315326154	-5.866703476	1.812286215
O31	1.440013530	-3.782120381	0.917623880
O32	-1.212345038	-3.546530292	0.733308255
O33	-3.986038240	-0.816052311	1.625841587
S34	0.174519168	7.489149977	0.197517572
S35	-1.510350132	4.135538631	-0.750141213
S36	0.299604735	4.166021969	2.381252568
S37	0.383882889	1.579160514	-3.013345652
S38	2.127728171	4.237009308	-0.697810090
S39	-1.564242440	-0.814607210	-0.842331727
S40	-4.503787542	1.395614565	0.147284497
S41	0.151276213	-0.979027823	2.395297962
S42	2.135093879	-1.020047318	-0.704324289
S43	3.141401524	1.446109426	2.068030017

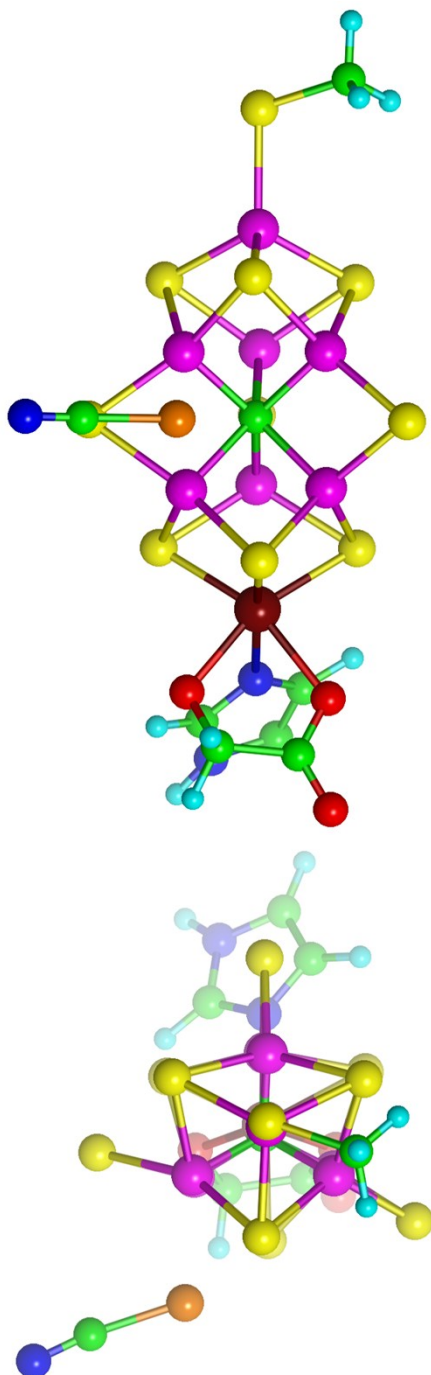
1 + SeCN⁻



C1	1.751199726	-0.317070881	7.777572479
C2	0.879686821	2.933696855	-3.713071589
C3	0.320980424	3.817867174	-4.607046682
C4	-0.966349284	2.012591620	-4.391056491
C5	-0.635729579	-1.493727013	-4.564996612
C6	0.878447156	-1.268097673	-4.674213756
C7	0.150802818	0.045963708	1.564424928
C8	-2.941734894	-5.392643833	1.859014696
Fe9	0.116309354	0.020317644	5.006141951
Fe10	-1.221184703	-0.561795611	2.783909940
Fe11	1.363514744	-0.887097773	2.753499777
Fe12	0.257438023	1.510610688	2.807284402
Fe13	0.122665955	1.540176620	0.197451158
Fe14	-1.304322106	-0.543229587	0.181182918
Fe15	1.340580416	-0.798897295	0.201277166
H16	2.488623569	0.356019186	7.317816541
H17	1.819871338	-0.232081051	8.874902414
H18	1.990042375	-1.348045124	7.482681614
H19	1.794699461	3.009760499	-3.134925732
H20	0.630085897	4.795804736	-4.957652783
H21	-1.767484357	1.282173451	-4.490952915
H22	-1.539219400	3.603336125	-5.666687882
H23	-1.086627609	-1.336909126	-5.569477244
H24	-0.760180385	-2.578403320	-4.330009570
Mo25	0.034165908	-0.000246031	-2.086865645
N26	0.070890654	1.832090356	-3.592748048
N27	-0.855173214	3.212145564	-5.030989738
N28	-4.087360919	-5.415984176	1.537830079
O29	1.508761335	-1.564999799	-5.706487456
O30	1.406062677	-0.773643590	-3.589829647
O31	-1.240082371	-0.674731455	-3.605497984
S32	0.056358560	0.156614653	7.234888833
S33	-1.543767611	1.178188158	4.119542786
S34	-0.072476476	-2.000807429	4.034841112
S35	0.147881674	3.303569731	1.569110579
S36	1.991416503	0.818570164	4.063326924
S37	-1.759470132	1.250551303	-1.088061515
S38	-2.860210798	-1.229882389	1.564013826
S39	-0.095805085	-2.076377038	-0.937483388
S40	1.949814947	0.996613583	-1.022587615
S41	2.846383037	-1.777247089	1.471210831
Se42	-1.179509569	-5.404735319	2.358708121



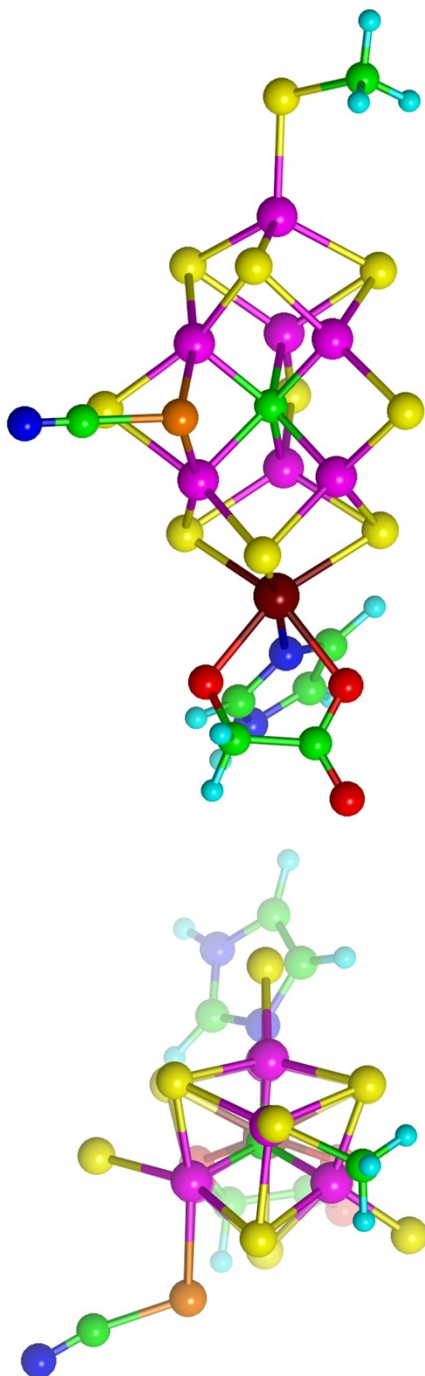
TS 1-12



C1	1.804793133	-0.635897073	7.880249343
C2	0.948976849	2.987167433	-3.559492952
C3	0.446811028	3.869032333	-4.490567571
C4	-0.958848471	2.168053565	-4.187491022
C5	-0.650364663	-1.355383170	-4.660517619
C6	0.862628032	-1.132448216	-4.807835327
C7	0.067567156	-0.332073407	1.535607345
C8	-3.198698354	-4.070465512	1.518585566
Fe9	0.118554345	-0.161295690	5.067852820
Fe10	-1.289688717	-1.077005890	2.761452501
Fe11	1.379215741	-1.092033736	2.771914689
Fe12	0.135002415	1.207716452	2.813628327
Fe13	0.083461254	1.220178461	0.257910356
Fe14	-1.248126623	-1.115973572	0.163934584
Fe15	1.385678339	-1.001046170	0.206525821
H16	2.589426612	0.018706971	7.473702950
H17	1.852944210	-0.615532201	8.983282275
H18	1.993311782	-1.663512595	7.538180958
H19	1.878635976	3.024249240	-2.998452748
H20	0.831034352	4.792873416	-4.911219285
H21	-1.792194035	1.476962378	-4.288249169
H22	-1.417562591	3.726757339	-5.554351135
H23	-1.126347648	-1.135847674	-5.642095958
H24	-0.781990730	-2.449592586	-4.483939998
Mo25	0.099904720	-0.133341090	-2.075291876
N26	0.067183779	1.946177309	-3.386738479
N27	-0.772981411	3.330768394	-4.880774723
N28	-4.266510702	-4.575903823	1.544903787
O29	1.467139675	-1.458590768	-5.848425285
O30	1.420339998	-0.599522389	-3.754628777
O31	-1.229727162	-0.607893491	-3.636581026
S32	0.134145775	-0.063846036	7.338707290
S33	-1.651139441	0.765314417	4.104404937
S34	0.020991800	-2.229079260	4.182152604
S35	0.085981144	2.996856785	1.566518701
S36	1.940601263	0.729171244	4.053381589
S37	-1.755146356	0.770144657	-0.929671774
S38	-3.067376253	-0.653130466	1.482755311
S39	0.141738862	-2.305390420	-1.167163640
S40	1.966206103	0.860031396	-0.932371229
S41	2.906414389	-1.946303675	1.455926199
Se42	-1.421985574	-3.479052877	1.494281638

Fe (9) 2.765
 Fe (10) -1.550
 Fe (11) 2.409
 Fe (12) -2.388
 Fe (13) 2.330
 Fe (14) 1.534
 Fe (15) -2.233
 Mo (25) -0.160
 S=3/2

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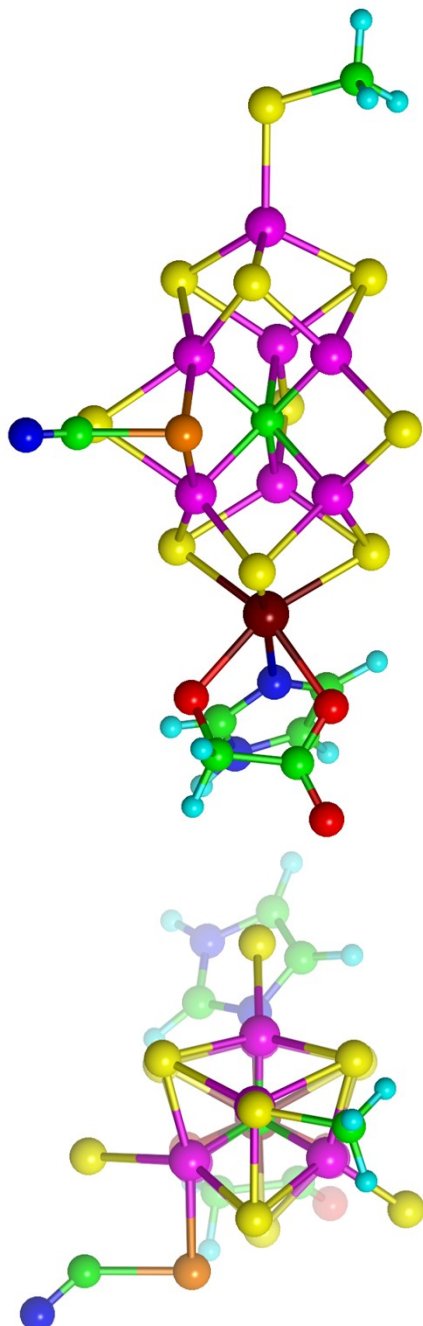


C1	2.082255241	-0.459164083	7.684645331
C2	0.609934892	2.978521224	-3.389882861
C3	0.058763924	3.846638752	-4.305442752
C4	-1.042882548	1.910534264	-4.304115474
C5	-0.656173517	-1.607943932	-4.631600578
C6	0.848928360	-1.346572346	-4.787833096
C7	0.080008522	-0.265480085	1.510829718
C8	-3.012794341	-3.862915842	1.676115819
Fe9	0.276054367	0.155736166	5.039782137
Fe10	-1.224233819	-0.981803220	2.798829087
Fe11	1.403739116	-0.952876188	2.820233599
Fe12	0.167509379	1.339041901	2.709208264
Fe13	0.071994009	1.211310293	0.168827387
Fe14	-1.237645665	-1.096247660	0.223392956
Fe15	1.382834070	-1.019883575	0.219557423
H16	2.878366605	0.109386842	7.183134633
H17	2.243225840	-0.426710848	8.775496992
H18	2.129991664	-1.503366246	7.346669896
H19	1.442042658	3.122041695	-2.706574858
H20	0.304634530	4.864279319	-4.591620727
H21	-1.743788564	1.105355761	-4.518083731
H22	-1.641880056	3.498750907	-5.575919019
H23	-1.134712594	-1.433620629	-5.621572471
H24	-0.761749259	-2.700335905	-4.423410455
Mo25	0.064527161	-0.255917903	-2.094910398
N26	-0.081160761	1.790734221	-3.408555771
N27	-0.995211739	3.147151067	-4.881203392
N28	-4.026973552	-4.465419064	1.716681081
O29	1.464840262	-1.699816269	-5.813077445
O30	1.385974481	-0.746526170	-3.760944357
O31	-1.257466363	-0.836480395	-3.638089018
S32	0.427098199	0.259927821	7.296752263
S33	-1.561597524	0.940507619	4.065206166
S34	0.092322567	-1.986437217	4.343730420
S35	0.042947285	3.051019184	1.350515864
S36	2.052726521	0.947444833	3.892836921
S37	-1.778315698	0.704207957	-0.981140754
S38	-3.036125837	-0.595306962	1.539901942
S39	0.117277902	-2.369326783	-1.092978826
S40	1.939815645	0.781170794	-1.008856351
S41	2.876016469	-1.934878518	1.535722956
Se42	-1.251109920	-3.216742894	1.637735767

Fe (9) 2.738
 Fe (10) -1.109
 Fe (11) 2.378
 Fe (12) -2.405
 Fe (13) 2.228
 Fe (14) 1.190
 Fe (15) -2.259
 Mo (25) -0.082

S=3/2

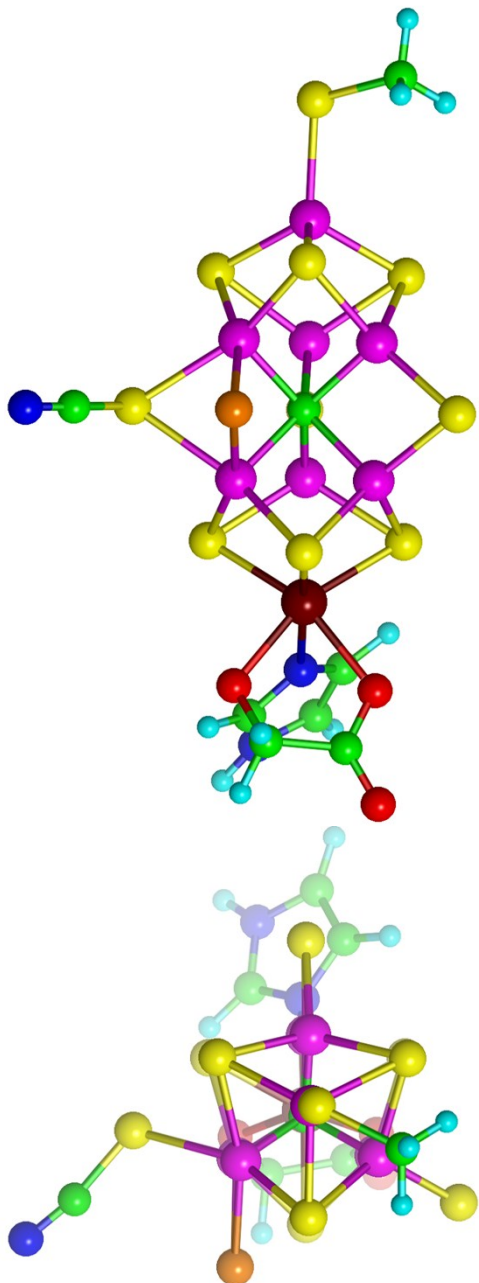
TS 12-13



C1	1.886597744	-0.443235810	7.983745934
C2	0.841349769	2.833834245	-3.770209777
C3	0.289481289	3.696594015	-4.689000946
C4	-1.078357387	1.980413417	-4.306878101
C5	-0.701894388	-1.587727376	-4.617481842
C6	0.812009851	-1.382831930	-4.783285864
C7	0.127537384	-0.238391509	1.546862744
C8	-3.107618507	-3.147816332	1.549577283
Fe9	0.090396683	-0.053781638	5.165980066
Fe10	-1.150230710	-1.058501271	2.826463686
Fe11	1.434316828	-0.981698262	2.861733371
Fe12	0.145404609	1.297179728	2.835787605
Fe13	0.115547915	1.261344966	0.240264960
Fe14	-1.131812649	-1.073602570	0.236545728
Fe15	1.446444869	-0.971632905	0.225673506
H16	2.559470306	0.281315490	7.504189615
H17	1.957136338	-0.326467207	9.079619008
H18	2.217458579	-1.459641262	7.720207229
H19	1.792701398	2.886821374	-3.249418000
H20	0.637005246	4.626639928	-5.128816091
H21	-1.912113299	1.282876605	-4.359452286
H22	-1.622916917	3.525463816	-5.660079875
H23	-1.179676076	-1.400722543	-5.605498874
H24	-0.845490658	-2.675256664	-4.409060298
Mo25	0.076941573	-0.197824838	-2.097511431
N26	-0.016387006	1.783774396	-3.546521483
N27	-0.937547937	3.135394942	-5.021568858
N28	-3.989494535	-3.958041004	1.570019947
O29	1.406338030	-1.774587008	-5.808506917
O30	1.374508488	-0.788863677	-3.768042878
O31	-1.264731625	-0.794651573	-3.616057528
S32	0.138900219	-0.139048420	7.457831319
S33	-1.654841756	0.842154546	4.091122239
S34	0.088735541	-2.145757906	4.304642093
S35	0.073733064	3.045123192	1.512421609
S36	1.925867144	0.863977637	4.147198110
S37	-1.730148590	0.773781117	-0.922744301
S38	-3.064410288	-0.992896283	1.520859002
S39	0.178914259	-2.305093089	-1.110092341
S40	1.955071760	0.851814775	-1.007990976
S41	2.910908772	-1.934826134	1.542425969
Se42	-1.095105327	-3.135606979	1.555047643

Fe (9) 2.844
 Fe (10) -1.305
 Fe (11) 2.679
 Fe (12) -2.508
 Fe (13) 2.324
 Fe (14) 1.109
 Fe (15) -2.363
 Mo (25) -0.096
 S=3/2

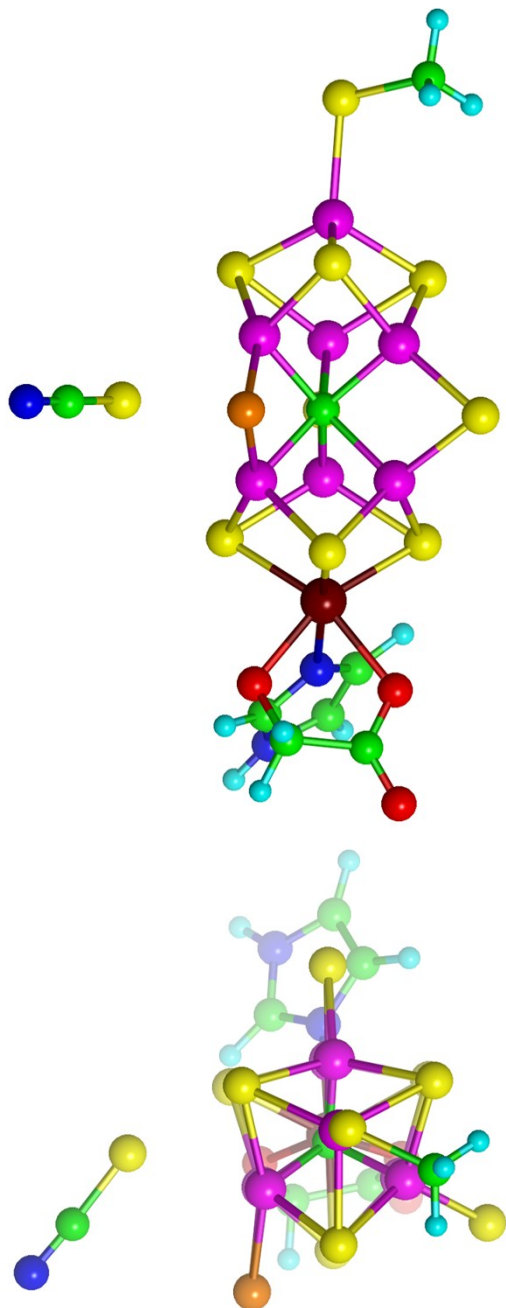
13



Fe (9) 2.614
 Fe (10) -1.460
 Fe (11) 2.783
 Fe (12) -2.394
 Fe (13) 2.266
 Fe (14) 1.321
 Fe (15) -2.410
 Mo (25) -0.106
 S=3/2

C1	1.980903720	-0.540550553	7.787009580
C2	0.643963189	2.851393056	-3.488269814
C3	0.078478467	3.705375110	-4.407801988
C4	-1.047031818	1.783675546	-4.330089456
C5	-0.494944228	-1.716913061	-4.657618075
C6	0.988951391	-1.349729643	-4.807436171
C7	0.142133102	-0.304045841	1.523080973
C8	-4.083469611	-2.157931645	1.642153195
Fe9	0.221521717	0.048560255	5.079254156
Fe10	-1.023262957	-1.164738574	2.887463732
Fe11	1.554118246	-0.930421100	2.809246814
Fe12	0.125765104	1.279676485	2.735950438
Fe13	0.062062397	1.155569550	0.178644266
Fe14	-1.085532703	-1.241412604	0.252230444
Fe15	1.497246163	-1.020147609	0.211524272
H16	2.784988825	0.011617968	7.280794282
H17	2.109960082	-0.448173947	8.877869737
H18	2.054986548	-1.600848094	7.507815086
H19	1.496589208	2.996797713	-2.830904871
H20	0.328728623	4.715730366	-4.716270639
H21	-1.762185483	0.983748038	-4.516908715
H22	-1.661436659	3.351023486	-5.624609810
H23	-0.988861905	-1.557498069	-5.642006674
H24	-0.522589126	-2.819265883	-4.472315494
Mo25	0.133424317	-0.345858424	-2.097040554
N26	-0.062822428	1.673457776	-3.458516672
N27	-1.000762739	3.007491400	-4.937967430
N28	-4.940353438	-2.972318963	1.670648715
O29	1.617637316	-1.592951181	-5.856390036
O30	1.494852992	-0.789473097	-3.743540008
O31	-1.141723560	-1.006900742	-3.646737192
S32	0.328420711	0.139825334	7.328993505
S33	-1.594018545	0.795860251	4.072821626
S34	0.324604085	-2.089151976	4.371342944
S35	-0.075606837	2.984750958	1.372063439
S36	1.974184070	1.009768532	3.977600229
S37	-1.740060290	0.553440609	-0.990014437
S38	-3.066839062	-0.798210203	1.602562956
S39	0.285421871	-2.447522989	-1.069329999
S40	1.937129090	0.817311707	-1.013016687
S41	3.118588581	-1.742365306	1.495543169
Se42	-0.993171284	-3.228658823	1.642187171

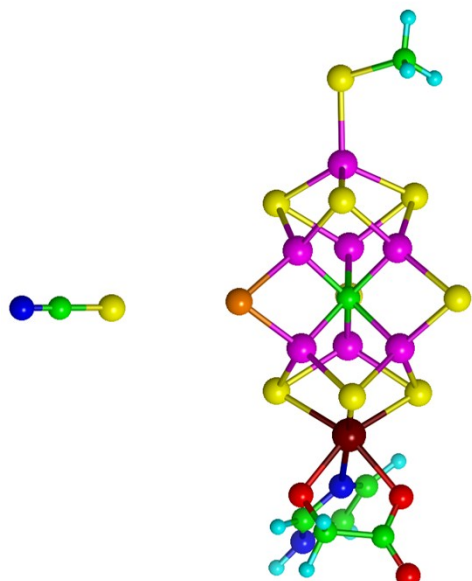
TS 13-14



C1	1.759101998	-0.793056966	7.828092077
C2	0.839560680	2.962679702	-3.359452075
C3	0.313695500	3.846706802	-4.273653296
C4	-0.816921699	1.928162593	-4.303182316
C5	-0.271041370	-1.556971380	-4.717152483
C6	1.220875610	-1.204006531	-4.795307555
C7	0.069645280	-0.378101441	1.509788350
C8	-4.676755978	-2.077713755	1.431698679
Fe9	0.075902289	-0.130888326	5.074119936
Fe10	-1.160207433	-1.295766727	2.833983419
Fe11	1.454887099	-1.036213338	2.819613295
Fe12	0.054454809	1.174850524	2.776012413
Fe13	0.093600330	1.135562331	0.217655972
Fe14	-1.079786942	-1.285984104	0.124538136
Fe15	1.502882880	-1.037691729	0.235716175
H16	2.579414782	-0.233811028	7.355752240
H17	1.867827132	-0.737543035	8.924592589
H18	1.826746919	-1.845500157	7.514434884
H19	1.669325652	3.085074702	-2.669972916
H20	0.579256971	4.862001169	-4.549046512
H21	-1.527612008	1.140497945	-4.545303436
H22	-1.375025476	3.537608193	-5.570288208
H23	-0.727785801	-1.362941673	-5.712549183
H24	-0.316543872	-2.661916579	-4.561572023
Mo25	0.249366341	-0.280220892	-2.096197843
N26	0.129475510	1.786188470	-3.394668791
N27	-0.742536614	3.169103083	-4.870189865
N28	-5.417808832	-3.006132130	1.402198593
O29	1.886956808	-1.426719562	-5.826018116
O30	1.689057851	-0.685797251	-3.694337714
O31	-0.952911267	-0.872972935	-3.709650085
S32	0.128043835	-0.070094908	7.355697378
S33	-1.722964397	0.646927049	4.024541628
S34	0.172228687	-2.285291599	4.295203568
S35	-0.052743291	2.928056260	1.462858227
S36	1.880372007	0.855920337	4.041609144
S37	-1.674299510	0.580112783	-1.015285170
S38	-3.696959896	-0.713672990	1.488751945
S39	0.351858442	-2.435111875	-1.142798312
S40	2.020963733	0.822707845	-0.909240754
S41	3.076848526	-1.809204393	1.548213246
Se42	-1.280445254	-3.238834481	1.450794753

Fe (9) 2.890
Fe (10) -1.948
Fe (11) 2.793
Fe (12) -2.462
Fe (13) 2.295
Fe (14) 1.570
Fe (15) -2.423
Mo (25) -0.115
S=3/2

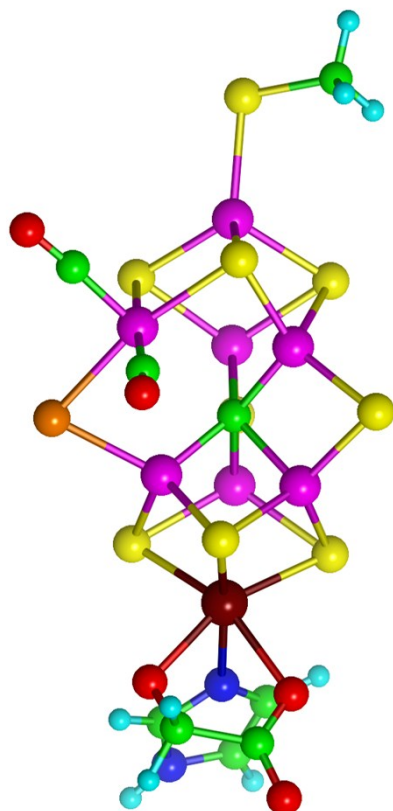
14 + SCN⁻



S=3/2

C1	1.972215979	-0.850747222	7.727348312
C2	0.810597771	3.044740031	-3.382614489
C3	0.166318289	3.852757112	-4.289961220
C4	-0.766827742	1.832288640	-4.254742282
C5	-0.048853060	-1.639713684	-4.575204823
C6	1.433103119	-1.256432495	-4.705019428
C7	0.483074709	-0.237468945	1.526817635
C8	-6.939892258	-2.454026684	1.255164768
Fe9	0.333730636	-0.256245972	5.003279107
Fe10	-0.791509534	-1.080565934	2.745640603
Fe11	1.804637541	-1.010948048	2.810997481
Fe12	0.440391650	1.236153363	2.838628769
Fe13	0.402199633	1.266099189	0.268070808
Fe14	-0.690990467	-1.085088581	0.209405589
Fe15	1.864428761	-0.889053924	0.207883397
H16	2.742934155	-0.239630531	7.236720299
H17	2.076606928	-0.766339169	8.820644932
H18	2.113750714	-1.901913320	7.437910268
H19	1.649989819	3.260970063	-2.729362998
H20	0.321737720	4.883326366	-4.590572603
H21	-1.390510247	0.961965484	-4.454794630
H22	-1.524338730	3.352043014	-5.521369325
H23	-0.530585548	-1.541934874	-5.572229061
H24	-0.063319614	-2.726936818	-4.323184665
Mo25	0.495730127	-0.179900423	-2.058027310
N26	0.221569485	1.802131930	-3.377958473
N27	-0.836226222	3.063650499	-4.836691844
N28	-7.895446025	-3.170996922	1.247831871
O29	2.103556318	-1.561309974	-5.708897429
O30	1.892091415	-0.616782025	-3.662880837
O31	-0.721985747	-0.885257100	-3.610601412
S32	0.292851834	-0.268649558	7.247966003
S33	-1.408029265	0.656104919	3.983806352
S34	0.410092607	-2.331938561	4.073634367
S35	0.365257588	3.011028162	1.573719272
S36	2.174084284	0.806656647	4.165773910
S37	-1.409801459	0.668613782	-0.911284765
S38	-5.627469358	-1.430972318	1.260826780
S39	0.679014557	-2.326978050	-1.051783171
S40	2.269531435	0.999213948	-0.949573698
S41	3.392887203	-1.768923142	1.502650846
Se42	-2.266588175	-2.218992526	1.422024287

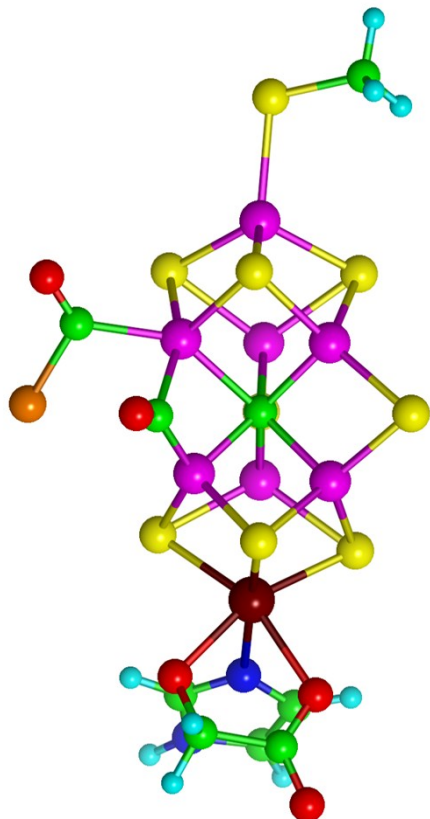
15



Fe (10) 3.079
 Fe (11) -0.094
 Fe (12) 0.192
 Fe (13) -2.818
 Fe (14) 2.354
 Fe (15) 0.554
 Fe (16) -2.230
 Mo (26) -0.183
 S=1/2

C1	1.831335533	7.671461351	0.708155461
C2	1.221414874	-3.830643100	-2.986834759
C3	0.721934473	-4.737248812	-3.897882763
C4	-0.758615438	-4.354903450	-2.272946268
C5	-0.740744109	-4.754879708	1.342890030
C6	0.783923876	-4.964751092	1.279865882
C7	-1.744406633	1.805508034	3.096192296
C8	0.196726832	1.274455271	0.208134099
C9	-3.075786568	3.788869171	2.132396154
Fe10	0.032427004	4.977654500	0.224398882
Fe11	-1.782436599	2.754384279	1.607177336
Fe12	1.188172838	2.545314937	1.200057103
Fe13	0.200628869	2.711462907	-1.188049892
Fe14	0.356964366	0.097130905	-1.406365999
Fe15	-1.166778081	0.065389508	0.632231294
Fe16	1.425277271	-0.062356443	0.990345717
H17	2.591013299	7.152207693	0.102927159
H18	2.029374373	8.761277310	0.686296806
H19	1.925130948	7.314708375	1.745713422
H20	2.173576098	-3.308014463	-2.965939758
H21	1.135270753	-5.184838281	-4.797456001
H22	-1.623830281	-4.400284533	-1.611119494
H23	-1.218163382	-5.676462690	-3.875784984
H24	-1.227091104	-5.751357840	1.206480080
H25	-0.950654178	-4.444327075	2.399514031
Mo26	0.163674840	-2.244306332	-0.001240309
N27	0.297826394	-3.614927861	-1.995094709
N28	-0.546105909	-5.065694020	-3.424610165
O29	-1.812236473	1.304108616	4.158792333
O30	1.300639568	-6.022949951	1.727874920
O31	1.424935724	-3.969915794	0.760087178
O32	-1.224294731	-3.826586849	0.429040295
O33	-3.989565180	4.419477529	2.548524291
S34	0.139078326	7.315604291	0.056572119
S35	-1.688158342	3.867075592	-0.651653662
S36	0.040019762	4.044235038	2.358225664
S37	0.439589525	1.553971588	-3.074459056
S38	1.952395298	3.943767507	-0.388003806
S39	-1.542253351	-1.106087900	-1.201032918
S40	-0.102869514	-1.227000728	2.139204381
S41	2.160466037	-1.167383134	-0.824312486
S42	2.724914837	1.302872538	2.142052142
Se43	-3.262710755	1.043978595	0.679658181

TS 15-16

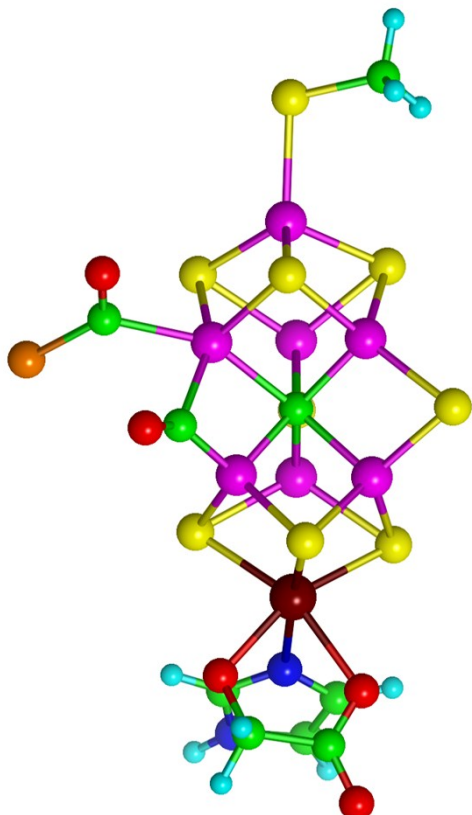


Fe (10) 3.000
Fe (11) -1.984
Fe (12) 2.874
Fe (13) -2.527
Fe (14) 2.413
Fe (15) -0.798
Fe (16) -2.276
Mo (26) 0.090

S=1/2

C1	2.240200449	7.670013023	0.514942510
C2	0.937621816	-4.180886106	-2.464059421
C3	0.331009562	-4.911175375	-3.461854134
C4	-1.194186360	-3.959868635	-2.141620445
C5	-0.823698939	-4.676287618	1.636755431
C6	0.683973833	-4.943572560	1.471400793
C7	-1.649209638	1.291471115	2.407090258
C8	0.296506405	1.364079066	0.212374266
C9	-3.149285760	3.019572339	1.290889763
Fe10	0.293550722	4.946430484	0.144137549
Fe11	-1.200915425	2.731084708	0.991676580
Fe12	1.600548356	2.655781831	1.029573613
Fe13	0.364860550	2.659120997	-1.287917823
Fe14	0.287675472	0.072257686	-1.297091201
Fe15	-0.943234572	0.190248255	1.037703424
Fe16	1.615812601	0.048620065	0.965892088
H17	2.947506199	7.106206492	-0.114976266
H18	2.430657019	8.752230477	0.388926919
H19	2.431394276	7.401905249	1.565692969
H20	1.989980553	-4.012674616	-2.252648395
H21	0.719593271	-5.508497191	-4.281169888
H22	-2.144336126	-3.648264575	-1.720728042
H23	-1.780729042	-5.104190962	-3.837610564
H24	-1.353625726	-5.632195849	1.397327205
H25	-0.979990528	-4.511245546	2.734581784
Mo26	0.128531523	-2.180278716	0.283295898
N27	-0.019236822	-3.600417421	-1.667489915
N28	-1.035962577	-4.767538349	-3.236262551
O29	-2.034634803	1.322754568	3.537032857
O30	1.181685710	-6.032044685	1.860001972
O31	1.337691893	-3.966005740	0.931090834
O32	-1.309972766	-3.623908662	0.876804545
O33	-3.714814476	3.897510195	1.912249294
S34	0.497208291	7.283011388	0.035632460
S35	-1.411991529	4.003654625	-0.945899843
S36	0.187850484	4.000287536	2.251485771
S37	0.316662389	1.360743125	-3.087206984
S38	2.150338932	3.949608180	-0.804935843
S39	-1.627240602	-0.958139441	-0.754865254
S40	0.267964657	-1.078211168	2.377241337
S41	2.074876851	-1.254652613	-0.818267012
S42	3.134819708	1.321293027	1.942538358
Se43	-4.075455828	1.502171394	0.378265103

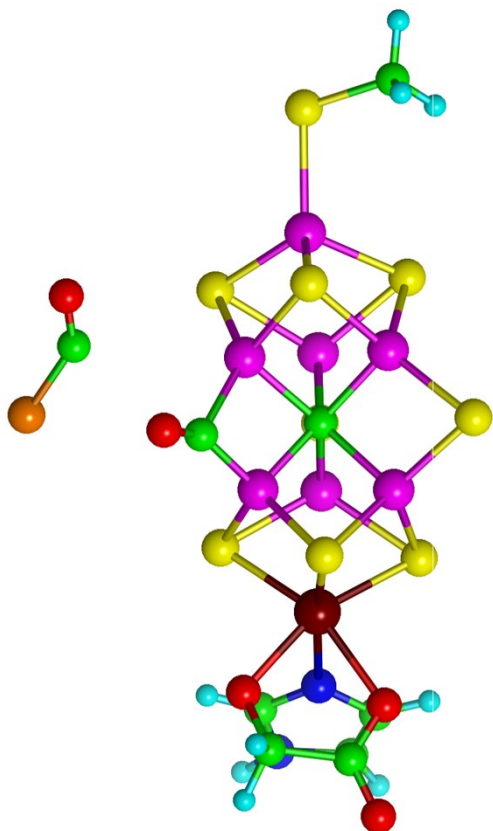
16



Fe (10) 3.026
 Fe (11) -2.226
 Fe (12) 2.916
 Fe (13) -2.591
 Fe (14) 2.258
 Fe (15) -0.646
 Fe (16) -2.418
 Mo (26) 0.142
 S=1/2

C1	1.926092162	7.596272808	0.734376963
C2	1.082426383	-4.045640155	-2.516735422
C3	0.510399041	-4.783712208	-3.528295920
C4	-1.059782366	-3.899456739	-2.215842944
C5	-0.618846163	-4.752462917	1.525920342
C6	0.889936136	-4.976081575	1.311924744
C7	-1.904593830	1.025099117	2.283832286
C8	0.302239244	1.358795214	0.260519372
C9	-3.319086098	3.040140117	1.262415727
Fe10	0.108943035	4.872903829	0.289207941
Fe11	-1.303167412	2.604588286	1.057691692
Fe12	1.583965273	2.670046591	1.060196499
Fe13	0.313392019	2.662405134	-1.238239663
Fe14	0.311238582	0.101564569	-1.259199952
Fe15	-0.836653123	0.100809552	1.106294629
Fe16	1.704294215	0.066685575	0.966731709
H17	2.632402336	7.033732379	0.103818824
H18	2.114100591	8.680666732	0.613602985
H19	2.117254830	7.322725624	1.784671673
H20	2.125070416	-3.845823993	-2.290004420
H21	0.930756271	-5.357803213	-4.348705328
H22	-2.024477699	-3.619384134	-1.804347288
H23	-1.589171887	-5.044117633	-3.929382980
H24	-1.135124662	-5.701986847	1.241761626
H25	-0.754465752	-4.656647086	2.634871772
Mo26	0.241979292	-2.179609682	0.259830557
N27	0.098759498	-3.508443992	-1.724565999
N28	-0.863195233	-4.687351550	-3.319014387
O29	-2.569434075	0.967015408	3.278221983
O30	1.416959934	-6.077523028	1.613982223
O31	1.511099859	-3.952216185	0.822469983
O32	-1.142949625	-3.666534373	0.841021629
O33	-3.363524394	3.875441035	2.149795041
S34	0.187161778	7.207142934	0.253824199
S35	-1.539871413	3.893986279	-0.851928706
S36	0.114779226	3.854450700	2.370421181
S37	0.346444671	1.384547053	-3.049144053
S38	2.007090274	4.052387979	-0.749910137
S39	-1.591712682	-0.945183581	-0.671396516
S40	0.447017364	-1.147561940	2.403518239
S41	2.135759527	-1.185716901	-0.859717214
S42	3.227635771	1.381286630	1.864712343
Se43	-4.771111533	2.280572774	0.260791714

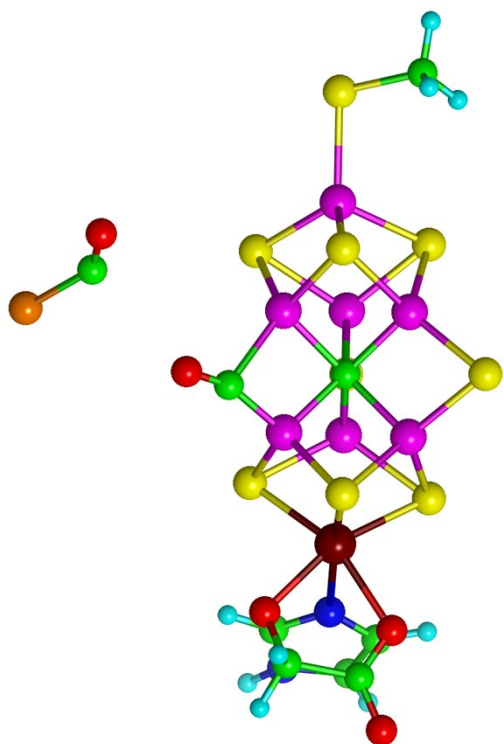
TS 16-2



Fe (10) 3.044
 Fe (11) -2.361
 Fe (12) 2.897
 Fe (13) -2.637
 Fe (14) 2.348
 Fe (15) -0.712
 Fe (16) -2.454
 Mo (26) 0.148
 S=1/2

C1	1.702944297	7.824889048	0.694213910
C2	1.383705224	-4.098027918	-2.392872294
C3	0.926392423	-4.865425448	-3.439693650
C4	-0.775349665	-4.006871055	-2.284198698
C5	-0.616201386	-4.762847985	1.546567868
C6	0.910118982	-4.950971901	1.473846867
C7	-1.889488156	1.141251946	2.227422212
C8	0.348395046	1.374983123	0.296875476
C9	-4.286289223	2.809659895	0.983540357
Fe10	0.060699049	4.938285609	0.237168936
Fe11	-1.074675542	2.603706655	1.038243278
Fe12	1.609794369	2.732861647	1.075343769
Fe13	0.302868566	2.681982806	-1.230452092
Fe14	0.365587089	0.092581074	-1.215398977
Fe15	-0.826680696	0.116645754	1.127967482
Fe16	1.721570633	0.111922927	1.058472855
H17	2.501593462	7.332102174	0.116209738
H18	1.799851780	8.922360852	0.577526520
H19	1.849136573	7.570793553	1.757690833
H20	2.398809345	-3.863807707	-2.086553139
H21	1.429298305	-5.440005015	-4.215220767
H22	-1.782796043	-3.756097590	-1.966013652
H23	-1.121788174	-5.195232388	-4.021929463
H24	-1.082443129	-5.722107044	1.212875894
H25	-0.859877090	-4.672202691	2.635607672
Mo26	0.291986101	-2.179377711	0.330769409
N27	0.320668428	-3.577269752	-1.693650550
N28	-0.464498832	-4.806447574	-3.354407577
O29	-2.593184708	1.224668410	3.201510251
O30	1.429432340	-6.027342990	1.870051774
O31	1.547151708	-3.932267287	0.996962067
O32	-1.104200095	-3.688546692	0.819789011
O33	-4.426618886	3.753025597	1.704520751
S34	0.036575120	7.281290620	0.105736352
S35	-1.628764255	3.861618779	-0.792403768
S36	0.131671616	3.989172192	2.354389795
S37	0.345734972	1.366593851	-3.024242239
S38	1.978290112	4.101141149	-0.773533355
S39	-1.535407537	-0.973682468	-0.653628719
S40	0.422873293	-1.122271866	2.466712470
S41	2.201204807	-1.168070388	-0.746665731
S42	3.221741336	1.464191756	1.955783879
Se43	-5.169831560	1.513144051	0.025065245

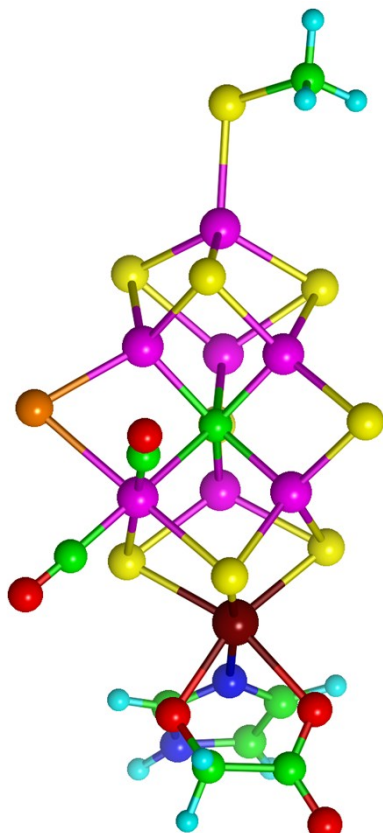
2 + SeCO



Fe (10) 2.999
 Fe (11) -2.546
 Fe (12) 2.750
 Fe (13) -2.634
 Fe (14) 2.302
 Fe (15) -0.567
 Fe (16) -2.434
 Mo (26) 0.124
 S=1/2

C1	1.739009735	7.676231994	0.674620584
C2	1.344312963	-4.167680032	-2.482403657
C3	0.788068372	-4.921287707	-3.491742015
C4	-0.793964632	-4.062161951	-2.180242232
C5	-0.466561387	-4.717224445	1.665150498
C6	1.050777858	-4.936717896	1.510560964
C7	-1.947601752	1.006288445	2.111833858
C8	0.452009205	1.342281277	0.331849191
C9	-4.906080670	3.250049897	0.821162947
Fe10	0.112605032	4.896091245	0.232334154
Fe11	-0.903370585	2.595846338	1.063527466
Fe12	1.725594817	2.705400142	1.053410765
Fe13	0.403432362	2.638865959	-1.213130679
Fe14	0.461871585	0.057138202	-1.183112238
Fe15	-0.755520633	0.069248964	1.151978766
Fe16	1.831559799	0.102221426	1.081997982
H17	2.494185052	7.152802035	0.067268224
H18	1.864734973	8.768493640	0.559655887
H19	1.904692160	7.405969079	1.730090366
H20	2.387482734	-3.951450297	-2.277012002
H21	1.217003870	-5.497065005	-4.306975274
H22	-1.764543184	-3.816829300	-1.761527628
H23	-1.306267862	-5.229658661	-3.884613023
H24	-0.981448434	-5.678123149	1.426033588
H25	-0.638272186	-4.539912046	2.757948497
Mo26	0.413310371	-2.198784231	0.353719679
N27	0.353729414	-3.643213643	-1.687817769
N28	-0.585343157	-4.857708149	-3.276807813
O29	-2.836515972	1.257720664	2.878214478
O30	1.578557531	-6.014181327	1.884678247
O31	1.678882504	-3.929731175	0.995654906
O32	-0.969579925	-3.678622573	0.894058682
O33	-4.754423663	4.013519098	1.728489032
S34	0.042821076	7.203934295	0.129167395
S35	-1.540331895	3.794168200	-0.777734646
S36	0.293807885	3.968994419	2.356558758
S37	0.436703486	1.303742641	-2.990958879
S38	2.043714181	4.100583145	-0.773217316
S39	-1.420669758	-1.030633746	-0.634784785
S40	0.532723730	-1.137152106	2.478354713
S41	2.309089186	-1.171748628	-0.730239474
S42	3.376014282	1.492887850	1.887509097
Se43	-6.266187672	2.377410701	-0.173497177

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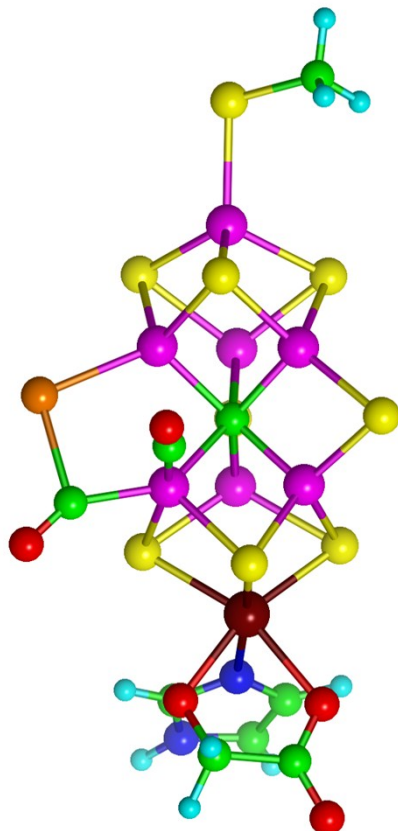


Fe (10) 3.036
 Fe (11) -2.923
 Fe (12) 2.820
 Fe (13) -2.662
 Fe (14) 2.403
 Fe (15) -0.022
 Fe (16) -2.653
 Mo (26) 1.021

S=1/2

C1	1.528405609	8.093408203	0.778728249
C2	1.422704996	-3.722529779	-2.690017133
C3	0.943094896	-4.521272554	-3.703834204
C4	-0.724396555	-3.814031094	-2.400074474
C5	-0.349783693	-4.761704382	1.382828984
C6	1.186245491	-4.805315572	1.295996882
C7	-1.758612466	1.147492444	2.947883326
C8	-0.131941451	1.589644456	0.328732826
C9	-3.021908210	-0.804229475	1.843757041
Fe10	-0.023553692	5.248859086	-0.086145766
Fe11	-1.540405696	3.067372462	0.565054490
Fe12	1.053639882	2.954918531	1.151829355
Fe13	0.172435697	2.849981465	-1.312376325
Fe14	0.102404809	0.300839862	-1.132021027
Fe15	-1.715002698	0.291388748	1.393922156
Fe16	1.203967182	0.369439191	1.173699340
H17	2.480532915	7.667203651	0.423052937
H18	1.617248165	9.197182077	0.787067526
H19	1.367285130	7.747232614	1.811777724
H20	2.438760504	-3.418356473	-2.458828058
H21	1.427570422	-5.050693063	-4.519358743
H22	-1.713426575	-3.658201786	-1.980884667
H23	-1.108746740	-5.045690860	-4.094914732
H24	-0.729574282	-5.790791980	1.171308698
H25	-0.579635753	-4.565999890	2.463435546
Mo26	0.271343102	-2.108661640	0.176283553
N27	0.383254557	-3.298459700	-1.899281460
N28	-0.434765193	-4.569308707	-3.507392396
O29	-1.848328931	1.557335472	4.041800608
O30	1.820732809	-5.826207708	1.670879392
O31	1.712776565	-3.717442018	0.831388409
O32	-0.936080472	-3.820138671	0.551907103
O33	-3.907720439	-1.505213812	2.168721310
S34	0.124434112	7.584749759	-0.306496747
S35	-1.586432721	4.347031287	-1.379557798
S36	-0.485230485	4.447769942	2.054190378
S37	0.232964990	1.450067183	-3.022910044
S38	1.918240663	4.117755958	-0.666993096
S39	-1.694602124	-1.010135419	-0.693848167
S40	-0.060154173	-1.150248180	2.324115314
S41	2.061315991	-0.739578370	-0.631134951
S42	2.492916453	1.740964757	2.331118589
Se43	-3.611990233	1.933577541	0.816611124

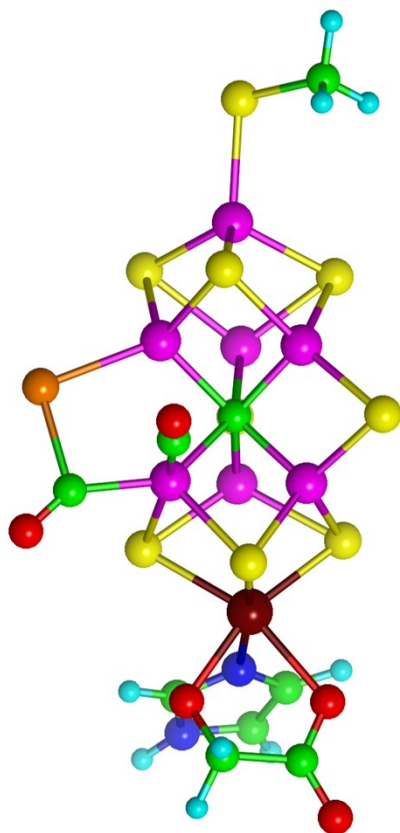
TS 17-18



Fe (10) 2.999
 Fe (11) -2.773
 Fe (12) 2.833
 Fe (13) -2.668
 Fe (14) 2.625
 Fe (15) 0.342
 Fe (16) -1.914
 Mo (26) -0.782
 S=1/2

C1	1.640896558	7.956656419	0.786542663
C2	1.040964856	-3.731916790	-2.837671502
C3	0.416968950	-4.453449781	-3.831493837
C4	-1.067103621	-3.741950517	-2.323913476
C5	-0.306113536	-4.765774634	1.368325721
C6	1.201045131	-4.886643208	1.070822606
C7	-1.157634473	1.037095157	3.095233741
C8	0.029709741	1.534888266	0.308296408
C9	-3.017229276	-0.036890212	1.851938513
Fe10	-0.072693443	5.175296019	0.139154017
Fe11	-1.386420709	2.905297278	0.838322620
Fe12	1.282719303	2.880033867	1.072725420
Fe13	0.113125793	2.858369462	-1.271846519
Fe14	0.094750142	0.273577532	-1.245025455
Fe15	-1.165205138	0.263254349	1.516874005
Fe16	1.390435516	0.296424301	0.954712596
H17	2.428424523	7.491764936	0.173622656
H18	1.773884206	9.055540651	0.769937292
H19	1.764578992	7.600927144	1.822063811
H20	2.088568606	-3.482879713	-2.699860032
H21	0.788057724	-4.954908654	-4.721053846
H22	-1.998269337	-3.557030247	-1.797235013
H23	-1.689877972	-4.864109902	-4.022501391
H24	-0.774233791	-5.759108515	1.160410301
H25	-0.379629334	-4.621297437	2.479532863
Mo26	0.302094106	-2.123990410	0.129126897
N27	0.112409141	-3.299935528	-1.925040494
N28	-0.933328066	-4.453366935	-3.488270986
O29	-1.204410985	1.386755465	4.215690523
O30	1.821456310	-5.949423860	1.335413747
O31	1.719663430	-3.815117613	0.563322983
O32	-0.941379507	-3.749142643	0.672009284
O33	-3.861378627	-0.811062433	2.222775665
S34	-0.025283052	7.514992828	0.125025224
S35	-1.718950539	4.248714393	-1.019306722
S36	-0.188702258	4.223914569	2.255377855
S37	0.047962091	1.546062441	-3.059028353
S38	1.844644958	4.209856528	-0.756647823
S39	-1.667601271	-0.958043616	-0.583836396
S40	0.348780770	-1.177943777	2.304852804
S41	2.060296319	-0.843119222	-0.871902553
S42	2.847721827	1.596249514	1.984151062
Se43	-3.603714061	1.981434529	1.238373122

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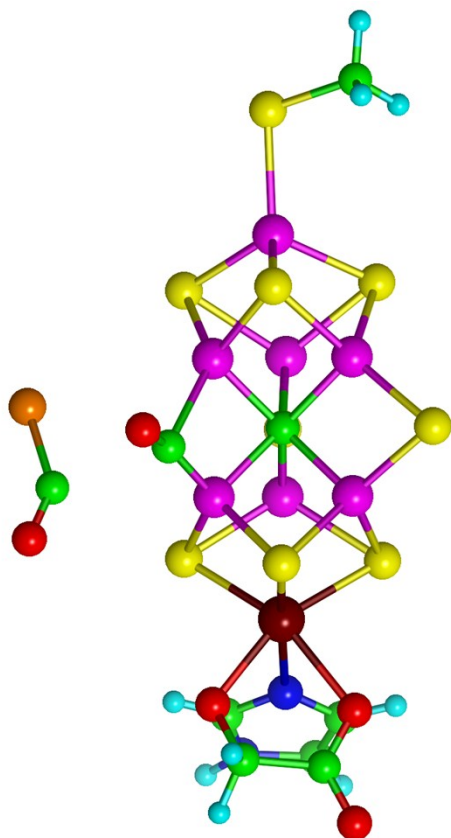


Fe (10) 2.972
 Fe (11) -2.768
 Fe (12) 2.836
 Fe (13) -2.649
 Fe (14) 2.596
 Fe (15) 0.431
 Fe (16) -1.986
 Mo (26) -0.813

S=1/2

C1	1.856207772	7.816925157	0.828211720
C2	1.204100056	-3.727319394	-2.707091140
C3	0.660938792	-4.495112893	-3.713160196
C4	-0.925543045	-3.801519759	-2.304132102
C5	-0.570702866	-4.780520471	1.402701181
C6	0.950255405	-4.944716784	1.228954265
C7	-1.474264317	1.242305320	2.936756195
C8	0.019324276	1.541273288	0.318816937
C9	-3.291452172	0.312876840	1.493095933
Fe10	0.155703722	5.163175871	-0.077063007
Fe11	-1.366863309	3.018189864	0.577056476
Fe12	1.228551097	2.861924883	1.186722106
Fe13	0.389742171	2.773008871	-1.292644672
Fe14	0.204038827	0.204515640	-1.157177789
Fe15	-1.380345065	0.416320992	1.384667922
Fe16	1.232971493	0.264877051	1.176509324
H17	2.752927823	7.322949121	0.421862320
H18	2.038917419	8.908186094	0.879389983
H19	1.691970806	7.434839573	1.847934000
H20	2.234140123	-3.435083039	-2.527683696
H21	1.096069884	-5.001748968	-4.570181632
H22	-1.887624734	-3.641662982	-1.827352219
H23	-1.414200747	-5.013646669	-3.983524356
H24	-1.060044638	-5.761404790	1.189781424
H25	-0.717943684	-4.593224084	2.499429588
Mo26	0.195628243	-2.146614624	0.240836346
N27	0.214200964	-3.312549974	-1.850858281
N28	-0.705903277	-4.529165450	-3.445327859
O29	-1.593225925	1.643270591	4.035646263
O30	1.519532965	-6.030677507	1.515846015
O31	1.538858337	-3.875217371	0.799067693
O32	-1.117238100	-3.765366084	0.630109057
O33	-4.200836401	-0.409939786	1.826214568
S34	0.384492002	7.473085996	-0.233021121
S35	-1.375054996	4.261427553	-1.390380115
S36	-0.297262706	4.377209200	2.057095161
S37	0.443730268	1.382942628	-3.015294343
S38	2.120816264	4.044906610	-0.613258006
S39	-1.669672916	-0.937560309	-0.668993744
S40	-0.068906311	-1.135878235	2.382060991
S41	2.096255432	-0.923387225	-0.541138563
S42	2.576908609	1.551825371	2.364793663
Se43	-3.689220081	2.246289375	0.694733940

TS 18-2

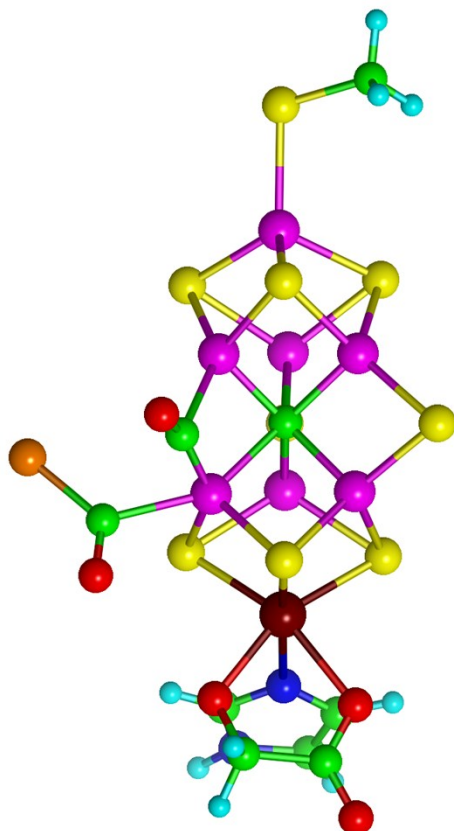


Fe (10) 3.049
 Fe (11) -2.645
 Fe (12) 2.846
 Fe (13) -2.617
 Fe (14) 2.320
 Fe (15) 0.383
 Fe (16) -2.375
 Mo (26) -0.074

S=1/2

C1	1.930932816	7.953508254	0.870643461
C2	1.242364937	-3.940184238	-2.479234039
C3	0.748782516	-4.649802362	-3.552794527
C4	-0.912075960	-3.788221232	-2.344231828
C5	-0.720066038	-4.671783778	1.488561792
C6	0.806170715	-4.863660394	1.386214912
C7	-1.879195353	1.238365449	2.333005585
C8	0.313625951	1.502748378	0.329011959
C9	-4.065083611	0.568990575	0.956958009
Fe10	0.283575064	5.119276985	0.241928131
Fe11	-0.954910781	2.847046168	0.986813527
Fe12	1.654234108	2.781442811	1.140876559
Fe13	0.456567125	2.839086615	-1.202357733
Fe14	0.291671769	0.235848107	-1.179138986
Fe15	-1.038262270	0.264019913	1.085058181
Fe16	1.555300117	0.181502373	1.145534146
H17	2.744224370	7.458764719	0.311101350
H18	2.058053944	9.047610541	0.801405696
H19	2.014945056	7.653234767	1.929301978
H20	2.268160602	-3.754743396	-2.175288493
H21	1.228962267	-5.201097679	-4.358500798
H22	-1.906018509	-3.509127650	-2.004570715
H23	-1.314146436	-4.889867431	-4.121743536
H24	-1.196273329	-5.639849558	1.182597863
H25	-0.935349787	-4.561651597	2.582451873
Mo26	0.147438849	-2.068169424	0.302716878
N27	0.203943232	-3.417993331	-1.751554417
N28	-0.635820637	-4.548748254	-3.450572326
O29	-2.363692015	1.555012934	3.384924479
O30	1.335172510	-5.945178083	1.757682731
O31	1.434307916	-3.834052712	0.923488672
O32	-1.223939641	-3.609100908	0.751144190
O33	-4.547794804	-0.374832261	1.511522257
S34	0.289392002	7.467955766	0.178400938
S35	-1.408771546	4.151426299	-0.856822176
S36	0.215104449	4.150482090	2.362716870
S37	0.372027617	1.506766466	-2.984941008
S38	2.210711438	4.161606643	-0.649105442
S39	-1.619966041	-0.856125302	-0.765749770
S40	0.156968491	-1.034925764	2.436023277
S41	2.103543259	-1.044927829	-0.671755753
S42	3.109682010	1.417974882	2.124578170
Se43	-4.454496373	2.101372447	0.043698064

TS 18-19

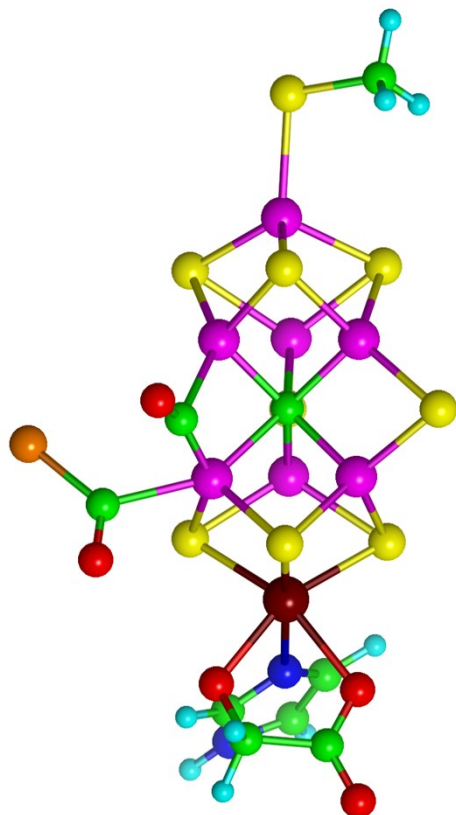


Fe (10) 3.022
 Fe (11) -2.589
 Fe (12) 2.792
 Fe (13) -2.588
 Fe (14) 2.342
 Fe (15) 0.430
 Fe (16) -2.448
 Mo (26) -0.108

S=1/2

C1	2.084210786	7.934741424	0.752833933
C2	1.060669801	-3.874166498	-2.603070080
C3	0.507107689	-4.581021398	-3.648897428
C4	-1.084768171	-3.684205540	-2.370516402
C5	-0.763664763	-4.598577731	1.432267210
C6	0.757362623	-4.793275689	1.293989538
C7	-1.706616868	1.413311375	2.475507786
C8	0.263531562	1.578848918	0.274834670
C9	-3.246077317	-0.132225923	1.519754539
Fe10	0.276036031	5.170879048	0.202602531
Fe11	-0.957617814	2.891469011	1.003580450
Fe12	1.653602956	2.814909409	1.061647891
Fe13	0.376031501	2.894612224	-1.234520117
Fe14	0.212037610	0.320273237	-1.197170486
Fe15	-1.197060610	0.289395097	1.161184823
Fe16	1.502561343	0.233845832	1.076568638
H17	2.855102134	7.423665664	0.154676405
H18	2.240456713	9.028765078	0.681189074
H19	2.211066399	7.629999000	1.804095469
H20	2.102273572	-3.711947480	-2.341927912
H21	0.941027244	-5.143194637	-4.471728093
H22	-2.057007642	-3.391458047	-1.985289750
H23	-1.584334641	-4.792123280	-4.118062487
H24	-1.253118132	-5.560861124	1.151109110
H25	-0.959055529	-4.459672963	2.524645937
Mo26	0.077722026	-2.012083366	0.250003672
N27	0.064546402	-3.328388895	-1.832348320
N28	-0.870084387	-4.453819069	-3.483885224
O29	-2.092048228	1.789330068	3.537436041
O30	1.300218401	-5.871164932	1.647183330
O31	1.375306896	-3.763396519	0.811152436
O32	-1.268948553	-3.542206383	0.686368392
O33	-3.418165661	-1.160001406	2.143721784
S34	0.395413110	7.506960033	0.138047013
S35	-1.478796153	4.207973370	-0.798666092
S36	0.305730973	4.209215637	2.315879176
S37	0.279040387	1.580334705	-3.015605014
S38	2.153670346	4.184468131	-0.753095534
S39	-1.685977966	-0.779230583	-0.795268401
S40	0.127514069	-1.011385135	2.381302180
S41	2.018222962	-0.988723398	-0.746212612
S42	3.096517814	1.438431803	2.028621285
Se43	-4.613638915	1.091700930	0.886060637

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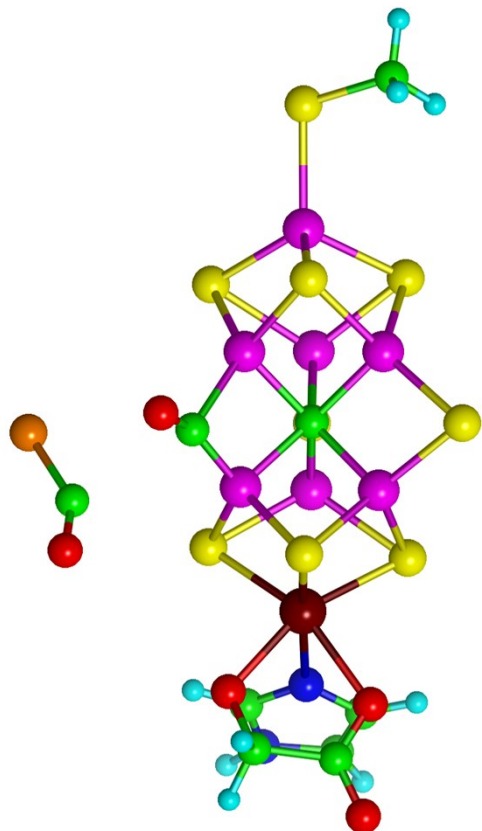


Fe (10) 3.017
 Fe (11) -2.587
 Fe (12) 2.792
 Fe (13) -2.586
 Fe (14) 2.319
 Fe (15) 0.433
 Fe (16) -2.442
 Mo (26) -0.100

S=1/2

C1	2.064214109	7.759319775	0.883169071
C2	0.940760964	-3.427858879	-2.948552343
C3	0.324600906	-4.234023472	-3.879998860
C4	-0.920372204	-4.066911156	-2.037355571
C5	-0.652808273	-4.594704957	1.485052349
C6	0.875215495	-4.744347225	1.387317569
C7	-1.790223357	1.415517197	2.391133246
C8	0.245486192	1.594524718	0.250701228
C9	-3.263549751	-0.163644135	1.351200227
Fe10	0.200448372	5.173382816	0.177163432
Fe11	-1.022616479	2.893406293	0.943328317
Fe12	1.593341533	2.864492103	1.061042974
Fe13	0.364357152	2.903146687	-1.259858761
Fe14	0.273925141	0.323696007	-1.213228957
Fe15	-1.203282140	0.294714528	1.103493229
Fe16	1.509727981	0.286002585	1.087703876
H17	2.811758122	7.256864802	0.251248051
H18	2.290266823	8.841061635	0.922234320
H19	2.143958231	7.341145167	1.898069829
H20	1.880446775	-2.884286955	-3.009071723
H21	0.594153145	-4.529754621	-4.889918240
H22	-1.710953196	-4.174865747	-1.292855458
H23	-1.614863028	-5.160223921	-3.719605912
H24	-1.100221101	-5.577026886	1.199887291
H25	-0.885558727	-4.452588236	2.569656306
Mo26	0.164500994	-1.990511597	0.265878078
N27	0.161196544	-3.342999425	-1.819877705
N28	-0.863266364	-4.642609124	-3.278674266
O29	-2.238488726	1.773907245	3.434592922
O30	1.436265709	-5.799795449	1.779455471
O31	1.473558931	-3.709270027	0.894635055
O32	-1.172171097	-3.562504938	0.712259132
O33	-3.433454849	-1.192487785	1.974265478
S34	0.368930808	7.497532570	0.195794294
S35	-1.517858623	4.199957372	-0.880480009
S36	0.190638287	4.224994574	2.289976782
S37	0.324154336	1.580089581	-3.035450430
S38	2.111750772	4.223758603	-0.753520035
S39	-1.593553574	-0.824949953	-0.845952365
S40	0.124654925	-0.955411368	2.381741915
S41	2.094755755	-0.942017424	-0.709111995
S42	3.060991105	1.529990481	2.053029952
Se43	-4.640843065	0.995277133	0.629482226

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Fe (10) 3.046
 Fe (11) -2.494
 Fe (12) 2.864
 Fe (13) -2.647
 Fe (14) 2.298
 Fe (15) 0.210
 Fe (16) -2.364
 Mo (26) -0.033
 S=1/2

C1	1.848583487	7.999898435	0.713279300
C2	1.294416582	-3.931518036	-2.413394598
C3	0.819367650	-4.659005904	-3.481396255
C4	-0.863274702	-3.781524900	-2.310033710
C5	-0.720561422	-4.594734519	1.536822782
C6	0.806178946	-4.792780542	1.464272173
C7	-1.871234591	1.393691394	2.218488261
C8	0.352092994	1.536660495	0.286150866
C9	-4.118036868	0.054494438	1.123381982
Fe10	0.204543996	5.153322388	0.188900571
Fe11	-0.908235738	2.860124840	1.007642372
Fe12	1.688771815	2.856301934	1.061780111
Fe13	0.386783065	2.864589527	-1.243104139
Fe14	0.341663341	0.261497788	-1.194292626
Fe15	-0.981714470	0.309457346	1.066553826
Fe16	1.606063323	0.249876973	1.120237776
H17	2.654049280	7.497325230	0.155317663
H18	1.976150419	9.097007355	0.618118718
H19	1.951426799	7.727418376	1.775641363
H20	2.314775482	-3.737053921	-2.097093136
H21	1.308207682	-5.221945684	-4.271845644
H22	-1.862146694	-3.501832539	-1.989586367
H23	-1.236660919	-4.909927741	-4.077427541
H24	-1.193674603	-5.558015784	1.231584545
H25	-0.954916209	-4.468739748	2.626238029
Mo26	0.186605517	-2.016673462	0.326274932
N27	0.243424955	-3.399915819	-1.706344242
N28	-0.568759112	-4.558064745	-3.400738337
O29	-2.466807913	1.704884872	3.217446187
O30	1.321676225	-5.872367530	1.857308809
O31	1.449782363	-3.773943618	0.995899998
O32	-1.199287441	-3.532891443	0.781399406
O33	-4.251087258	-0.875230114	1.852325668
S34	0.195866094	7.494496046	0.063422781
S35	-1.530722620	4.112159181	-0.793561571
S36	0.297285115	4.220470370	2.322210749
S37	0.355929092	1.514216994	-3.017431675
S38	2.114315605	4.228699817	-0.774203885
S39	-1.576364368	-0.820231383	-0.763024833
S40	0.207947553	-0.945249658	2.443384371
S41	2.139838617	-1.022792347	-0.678496875
S42	3.170247088	1.513739773	2.045314394
Se43	-4.932508156	1.324105867	0.112577801

2. Comparison of results without and with the COSMO continuum solvation model: dielectric constant 15, except where marked as dielectric constant 5

species	without COSMO	with COSMO
2	c26coalpbe.car_2	c26coalpbe15.car_1
	geometry	geometry
S=1/2	C7 -> Fe10 = 1.9707	C7 -> Fe10 = 1.9338
	C7 -> Fe14 = 1.8457	C7 -> Fe14 = 1.8476
	C8 -> Fe10 = 1.9923	C8 -> Fe10 = 1.9714
	C8 -> Fe14 = 1.9312	C8 -> Fe14 = 1.9326
	Fe14 -> Fe10 = 2.468	Fe14 -> Fe10 = 2.445
	spins	spins
	Fe (9) 3.055	Fe (9) 2.951
	Fe (10) -2.112	Fe (10) -1.935
	Fe (11) 2.950	Fe (11) 2.862
	Fe (12) -2.736	Fe (12) -2.612
	Fe (13) 2.411	Fe (13) 2.360
	Fe (14) -0.765	Fe (14) -0.931
	Fe (15) -2.433	Fe (15) -2.378
	Mo (25) 0.144	Mo (25) 0.167

3	cfe26copbe3.car_2	cfe26copbe315.car_1
	geometry	geometry
S=3/2	C7 -> Fe10 = 2.0337	C7 -> Fe10 = 1.9953
	C7 -> Fe14 = 1.9965	C7 -> Fe14 = 1.9691
	C8 -> Fe10 = 1.9965	C8 -> Fe10 = 1.9800
	C8 -> Fe14 = 2.0117	C8 -> Fe14 = 1.9966
	S38 -> Fe10 = 2.3374	S38 -> Fe10 = 2.315
	S38 -> Fe14 = 2.3319	S38 -> Fe14 = 2.313
	Fe14 -> Fe10 = 2.546	Fe14 -> Fe10 = 2.52
	C7 -> S38 = 2.0111	C7 -> S38 = 2.0483
	spins	spins
	Fe(9) 3.060	Fe(9) 2.950
	Fe(10) -2.020	Fe(10) -1.809
	Fe(11) 2.845	Fe(11) 2.768
	Fe(12) -2.590	Fe(12) -2.480
	Fe(13) 2.367	Fe(13) 2.304
	Fe(14) 1.491	Fe(14) 1.277
	Fe(15) -2.438	Fe(15) -2.369
	Mo(25) -0.170	Mo(25) -0.126
6	cfe26co2coxpb1.car_2	csc2pbatotss15ta_3_5162.56
	geometry	geometry
S=1/2	C8 -> Fe11 = 2.9311	C8 -> Fe11 = 2.5718
	C8 -> Fe15 = 1.8890	C8 -> Fe15 = 1.9189
	C7 -> Fe11 = 1.7622	C7 -> Fe11 = 1.8848
	C7 -> Fe15 = 3.3185	C7 -> Fe15 = 2.0357
	spins	spins
	Fe(10) 1.105	Fe(10) 2.660
	Fe(11) -0.142	Fe(11) 0.034
	Fe(12) 1.752	Fe(12) 0.311
	Fe(13) -2.756	Fe(13) -2.351
	Fe(14) 2.073	Fe(14) 2.361
	Fe(15) 1.329	Fe(15) 0.084
	Fe(16) -2.331	Fe(16) -2.205
	Mo(26) -0.093	Mo(26) -0.089
	energy to TS 6-7	energy to TS 6-7
	16.9 kcal mol ⁻¹	12.4 kcal mol ⁻¹
TS 6-7	csc2pbatot_1_4692.04	csc2pbatotss15tb_1_5150.19
	geometry	geometry
S=1/2	C7 -> Fe11 = 1.9494	C7 -> Fe11 = 1.9359
	C7 -> Fe15 = 1.9820	C7 -> Fe15 = 1.9667
	S40 -> Fe11 = 2.605	S40 -> Fe11 = 2.5856
	S40 -> Fe15 = 2.321	S40 -> Fe15 = 2.3145
	C9 -> Fe11 = 1.8845	C9 -> Fe11 = 1.8623
	C9 -> S40 = 1.9700	C9 -> S40 = 1.9476
	S40 -- C9 -- O33 = 121.74	S40 -- C9 -- O33 = 122.140
	C9 -- Fe11 -- C8 = 141.82	C9 -- Fe11 -- C8 = 142.072
	C9 -- Fe11 -- Fe13 = 130.65	C9 -- Fe11 -- Fe13 = 131.399
	spins	spins
	Fe(10) 2.955	Fe(10) 2.766
	Fe(11) -1.319	Fe(11) -1.071
	Fe(12) 2.262	Fe(12) 2.078
	Fe(13) -2.742	Fe(13) -2.610
	Fe(14) 2.295	Fe(14) 2.283
	Fe(15) -0.254	Fe(15) -0.434
	Fe(16) -2.358	Fe(16) -2.264
	Mo(26) -0.012	Mo(26) 0.039
7	cscocycpb1.car_2	csc2pbatotss15tb.car_2
	geometry	geometry
S=1/2	C8 -> Fe11 = 2.0963	C8 -> Fe11 = 2.0710
	C8 -> Fe15 = 1.9891	C8 -> Fe15 = 1.9917
	C7 -> Fe11 = 1.8626	C7 -> Fe11 = 1.8814

	C7 -> Fe15 = 2.1061 S40 -> Fe11 = 2.7945 S40 -> Fe15 = 2.3015 C9 -> Fe11 = 1.9266 C9 -> S40 = 1.8747 spins Fe(10) 3.123 Fe(11) -0.928 Fe(12) 1.086 Fe(13) -2.675 Fe(14) 2.406 Fe(15) 0.225 Fe(16) -2.309 Mo(26) -0.113 energy to TS 6-7 2.2 kcal mol ⁻¹	C7 -> Fe15 = 2.0233 S40 -> Fe11 = 2.8156 S40 -> Fe15 = 2.2948 C9 -> Fe11 = 1.9124 C9 -> S40 = 1.8718 spins Fe(10) 2.970 Fe(11) -0.859 Fe(12) 0.965 Fe(13) -2.533 Fe(14) 2.378 Fe(15) 0.149 Fe(16) -2.225 Mo(26) -0.068 energy to TS 6-7 1.6 kcal mol ⁻¹
7	cscocycpbe1.car_2 geometry C8 -> Fe11 = 2.0963 C8 -> Fe15 = 1.9891 C7 -> Fe11 = 1.8626 C7 -> Fe15 = 2.1061 S40 -> Fe11 = 2.7945 S40 -> Fe15 = 2.3015 C9 -> Fe11 = 1.9266 C9 -> S40 = 1.8747 spins Fe(10) 3.123 Fe(11) -0.928 Fe(12) 1.086 Fe(13) -2.675 Fe(14) 2.406 Fe(15) 0.225 Fe(16) -2.309 Mo(26) -0.113 energy to TS 7-8 9.0 kcal mol ⁻¹	dielectric constant 5 cscoc2pbccti5tg.car_2 geometry C8 -> Fe11 = 2.0669 C8 -> Fe15 = 1.9889 C7 -> Fe11 = 1.8774 C7 -> Fe15 = 2.0354 S40 -> Fe11 = 2.8036 S40 -> Fe15 = 2.2945 C9 -> Fe11 = 1.9143 C9 -> S40 = 1.8711 spins Fe(10) 2.982 Fe(11) -0.893 Fe(12) 1.060 Fe(13) -2.547 Fe(14) 2.355 Fe(15) 0.134 Fe(16) -2.226 Mo(26) -0.066 energy to TS 7-8 9.7 kcal mol ⁻¹
TS 7-8	cscoc2pbccti_1_4685.27 geometry C7 -> Fe11 = 1.9106 C7 -> Fe15 = 2.0105 S40 -> Fe11 = 3.093 S40 -> Fe15 = 2.898 C9 -> Fe11 = 2.0183 C9 -> S40 = 1.7692	dielectric constant 5 cscoc2pbccti5th_1_5049.78 geometry C7 -> Fe11 = 2.0009 C7 -> Fe15 = 1.9146 S40 -> Fe11 = 3.169 S40 -> Fe15 = 3.355 C9 -> Fe11 = 2.0098 C9 -> S40 = 1.7496
8	cscopbetp.outmol_2 geometry C8 -> Fe11 = 2.1778 C8 -> Fe15 = 1.9005 C7 -> Fe11 = 2.1123 C7 -> Fe15 = 1.8265 Fe11 -> C9 = 2.0928 spins Fe(10) 3.049 Fe(11) -2.258 Fe(12) 2.926 Fe(13) -2.629	dielectric constant 5 cscoc2pbccti5th.car_2 geometry C8 -> Fe11 = 2.1107 C8 -> Fe15 = 1.8984 C7 -> Fe11 = 2.0691 C7 -> Fe15 = 1.8250 C9 -> Fe11 = 2.0348 spins Fe(10) 2.937 Fe(11) -2.053 Fe(12) 2.863 Fe(13) -2.531

	Fe(14) 2.267 Fe(15) -0.689 Fe(16) -2.398 Mo(26) 0.151 energy to TS 7-8 8.9 kcal mol ⁻¹	Fe(14) 2.217 Fe(15) -0.775 Fe(16) -2.348 Mo(26) 0.162 energy to TS 7-8 7.8 kcal mol ⁻¹
12 S=3/2	fe26secnpbec.outmol_3 geometry C7 -> Fe10 = 1.9680 C7 -> Fe14 = 2.0209 S38 -> Fe10 = 2.2399 S38 -> Fe14 = 2.2844 Se42 -> Fe10 = 2.5187 Se42 -> Fe14 = 2.5489 Se42 -> S38 = 3.1730 spins Fe(9) 2.738 Fe(10) -1.109 Fe(11) 2.378 Fe(12) -2.405 Fe(13) 2.228 Fe(14) 1.190 Fe(15) -2.259 Mo(25) -0.082 energy to TS 12-13 10.3 kcal mol ⁻¹	fe26secnpbestel15tg.car_2 geometry C7 -> Fe10 = 1.9520 C7 -> Fe14 = 2.0113 S38 -> Fe10 = 2.2499 S38 -> Fe14 = 2.2892 Se42 -> Fe10 = 2.4864 Se42 -> Fe14 = 2.5242 Se42 -> S38 = 3.1545 spins Fe(9) 2.470 Fe(10) -0.825 Fe(11) 2.344 Fe(12) -2.318 Fe(13) 2.187 Fe(14) 1.070 Fe(15) -2.232 Mo(25) -0.067 energy to TS 12-13 5.3 kcal mol ⁻¹
TS 12-13 S=3/2	fe26secnpbestel_1_4565.66 geometry C8 -> Se42 = 2.0126 C8 -> S38 = 2.1555 spins Fe(9) 2.844 Fe(10) -1.305 Fe(11) 2.679 Fe(12) -2.508 Fe(13) 2.324 Fe(14) 1.109 Fe(15) -2.363 Mo(25) -0.096	fe26secnpbestel15ti_1_4836.0 geometry C8 -> Se42 = 2.0158 C8 -> S38 = 2.0968 spins Fe(9) 2.411 Fe(10) -0.662 Fe(11) 2.465 Fe(12) -2.270 Fe(13) 2.193 Fe(14) 0.828 Fe(15) -2.299 Mo(25) -0.034
13 S=3/2	fe26secnpbea.outmol_2 geometry C7 -> Fe10 = 1.9901 C7 -> Fe14 = 2.0002 S38 -> Fe10 = 2.4416 S38 -> Fe14 = 2.4383 Se42 -> Fe10 = 2.4107 Se42 -> Fe14 = 2.4269 C8 -> Se42 = 3.2705 spins Fe(9) 2.614 Fe(10) -1.460 Fe(11) 2.783 Fe(12) -2.394 Fe(13) 2.266 Fe(14) 1.321 Fe(15) -2.410 Mo(25) -0.106 energy to TS 12-13	fe26secnpbestel15ti.car_2 geometry C7 -> Fe10 = 1.9333 C7 -> Fe14 = 1.9831 Se42 -> Fe10 = 2.4095 Se42 -> Fe14 = 2.4534 S38 -> Fe10 = 2.3564 S38 -> Fe14 = 2.3910 S38 -> Se42 = 3.1854 spins Fe(9) 2.465 Fe(10) -0.598 Fe(11) 2.455 Fe(12) -2.288 Fe(13) 2.179 Fe(14) 0.894 Fe(15) -2.370 Mo(25) -0.065 energy to TS 12-13

	15.2 kcal mol ⁻¹	10.6 kcal mol ⁻¹
TS 13-14	fe26secnpbesdtd_1_4576.16	fe26secnpbesdtd15ti_1_4839.03
	geometry	geometry
S=3/2	S38 -> Fe10 = 2.9298	S38 -> Fe10 = 3.1604
	S38 -> Fe14 = 3.0064	S38 -> Fe14 = 3.1743
	S38 -> Se42 = 3.4953	S38 -> Se42 = 3.6291
	spins	spins
	Fe (9) 2.890	Fe (9) 2.714
	Fe (10) -1.948	Fe (10) -1.764
	Fe (11) 2.793	Fe (11) 2.772
	Fe (12) -2.462	Fe (12) -2.376
	Fe (13) 2.295	Fe (13) 2.275
	Fe (14) 1.570	Fe (14) 1.407
	Fe (15) -2.423	Fe (15) -2.422
	Mo (25) -0.115	Mo (25) -0.092
14	fe26secnpbesdtb3.car_1	fe26secnpbesdtd15td
S=3/2	energy to TS 13-14	energy to TS 13-14
	27.3 kcal mol ⁻¹	16.0 kcal mol ⁻¹
15	cseco2pbtc.outmol_4	cseco2pbcctx15tf.car_3
	geometry	geometry
S=1/2	C8 -> Fe11 = 2.8398	C8 -> Fe11 = 2.3455
	C8 -> Fe15 = 1.8711	C8 -> Fe15 = 1.9674
	C7 -> Fe11 = 1.7661	C7 -> Fe11 = 1.9262
	C7 -> Fe15 = 3.0713	C7 -> Fe15 = 2.0211
	Se43 -> Fe11 = 2.444	Se43 -> Fe11 = 2.53
	Se43 -> Fe15 = 2.313	Se43 -> Fe15 = 2.42
	spins	spins
	Fe (10) 3.079	Fe (10) 2.628
	Fe (11) -0.094	Fe (11) -0.189
	Fe (12) 0.192	Fe (12) 2.524
	Fe (13) -2.818	Fe (13) -2.633
	Fe (14) 2.354	Fe (14) 2.151
	Fe (15) 0.554	Fe (15) -1.596
	Fe (16) -2.230	Fe (16) -2.344
	Mo (26) -0.183	Mo (26) 0.209
	energy to TS 15-16	energy to TS 15-16
	25.3 kcal mol ⁻¹	21.7 kcal mol ⁻¹
TS 15-16	cseco2pbcctx_1_4670.08	cseco2pbcctx15tf_1_5126.181
	geometry	geometry
S=1/2	C7 -> Fe11 = 2.0681	C7 -> Fe11 = 2.0548
	C7 -> Fe15 = 1.8938	C7 -> Fe15 = 1.8854
	Se43 -> Fe11 = 3.185	Se43 -> Fe11 = 3.115
	Se43 -> Fe15 = 3.459	Se43 -> Fe15 = 3.427
	C9 -> Fe11 = 1.9922	C9 -> Fe11 = 1.9426
	C9 -> Se43 = 1.9983	C9 -> Se43 = 1.9940
	Se43 -- C9 -- O33 = 124.50	Se43 -- C9 -- O33 = 123.733
	C9 -- Fe11 -- C8 = 145.006	C9 -- Fe11 -- C8 = 147.211
	C9 -- Fe11 -- Fe13 = 132.926	C9 -- Fe11 -- Fe13 = 132.611
	spins	spins
	Fe (10) 3.000	Fe (10) 2.827
	Fe (11) -1.984	Fe (11) -1.745
	Fe (12) 2.874	Fe (12) 2.767
	Fe (13) -2.527	Fe (13) -2.439
	Fe (14) 2.413	Fe (14) 2.344
	Fe (15) -0.798	Fe (15) -0.855
	Fe (16) -2.276	Fe (16) -2.193
	Mo (26) 0.090	Mo (26) 0.110
16	cseco2pbte.car_2	cseco2pbcctx15te.car_2

S=1/2

geometry
C8 -> Fe11 = 2.1828
C8 -> Fe15 = 1.8960
C7 -> Fe11 = 2.0880
C7 -> Fe15 = 1.8389
C9 -> Fe11 = 2.0726
Se43 -> Fe15 = 4.5767
C8 -- Fe11 -- C9 = 150.619

spins
Fe(10) 3.026
Fe(11) -2.226
Fe(12) 2.916
Fe(13) -2.591
Fe(14) 2.258
Fe(15) -0.646
Fe(16) -2.418
Mo(26) 0.142

energy to TS 15-16
5.4 kcal mol⁻¹

geometry
C8 -> Fe11 = 2.1202
C8 -> Fe15 = 1.8917
C7 -> Fe11 = 2.0770
C7 -> Fe15 = 1.8272
C9 -> Fe11 = 2.0098
Se43 -> Fe15 = 4.284
C9 -- Fe11 -- C8 = 149.366

spins
Fe(10) 2.891
Fe(11) -2.066
Fe(12) 2.825
Fe(13) -2.482
Fe(14) 2.196
Fe(15) -0.629
Fe(16) -2.360
Mo(26) 0.135

energy to TS 15-16
3.8 kcal mol⁻¹
