

Large Structural Changes upon Protonation of Fe₄S₄ Clusters: the Consequences for Reactivity.

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Supplementary information

Table S1. Summary of Elementary Rate and Equilibrium Constants for the Acid Catalysed Substitution Mechanisms (shown in Figs. 3 and 5) for the Reactions between [Fe₄S₄X₄]²⁻ and PhSH in the presence of mixtures of NH₄⁺ and NEt₃ (solvent = MeCN, T = 25.0 °C)

parent cluster	K_0' ^a	K_0	$K_D k_e / s^{-1}$ ^b	$k_f K_D K_e' / dm^3 mol^{-1} s^{-1}$ ^b	Reference
[Fe ₄ S ₄ (SPh) ₄] ²⁻	≥ 20	1.58	0.0042		1
[Fe ₄ S ₄ (SEt) ₄] ²⁻	≥ 20	0.40	0.13		1
[Fe ₄ S ₄ (S ^t Bu) ₄] ²⁻	≥ 20	0.32	0.011		1
[Fe ₄ S ₄ (OPh) ₄] ²⁻	≥ 10	0.26	0.063		2
[Fe ₄ S ₄ Cl ₄] ²⁻		2.2		7.81 x 10 ²	3
[Fe ₄ S ₄ Br ₄] ²⁻		2.51		1.46 x 10 ³	3

footnotes:

^a Estimated assuming $K_0' [NH_4^+] / [NEt_3] \leq 0.1$

^b $K_D' = K_D [MeCN]$, $[MeCN] = 19.2 mol dm^{-3}$

References

- 1 R. A. Henderson and K. E. Oglieve, *J. Chem. Soc., Dalton Trans.*, 1993, 1467-1472.
- 2 A. Alwaaly, I. Dance and R. A. Henderson, *Chemical Communications*, 2014, **50**, 4799-4802.
- 3 R. A. Henderson and K. E. Oglieve, *Journal of the Chemical Society, Chemical Communications*, 1994, 377-379.

Pictures and Cartesian coordinates (Å) of intermediates and transition states.

In structural pictures, added protons are marked black.

With $X = \text{Cl}$

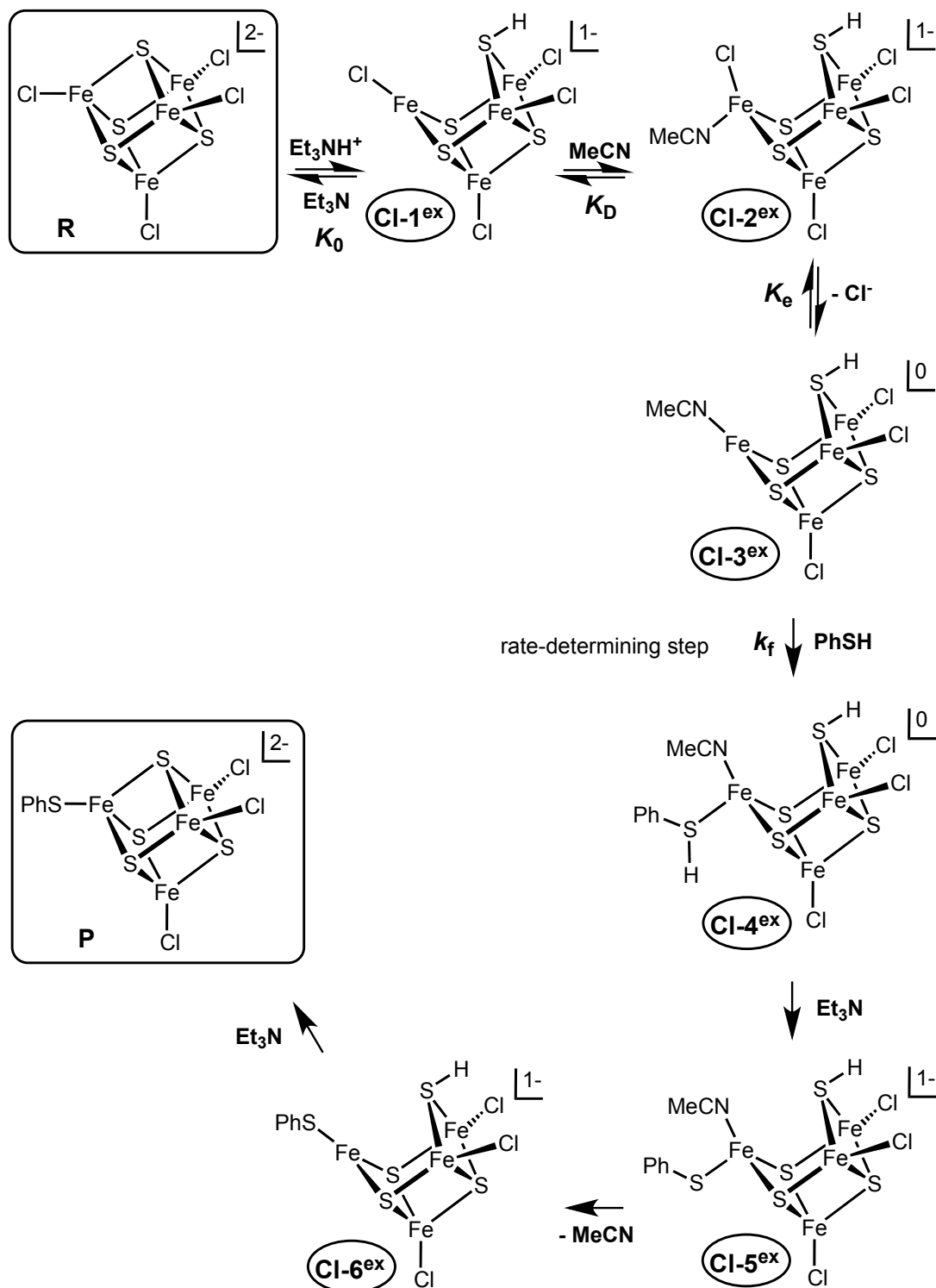
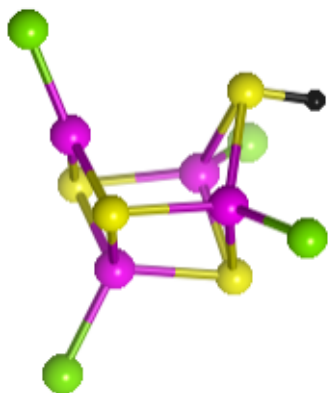


Fig. 5. The mechanism proposed for the substitution of $[\text{Fe}_4\text{S}_4\text{Cl}_4]^{2-}$ by PhSH , as catalysed by the acid Et_3NH^+ . Intermediates are drawn with the *exo* conformation of SH: an analogous set of intermediates exists for *endo*-SH.



fe4s4cl4pHd.car_3

CI-1ex

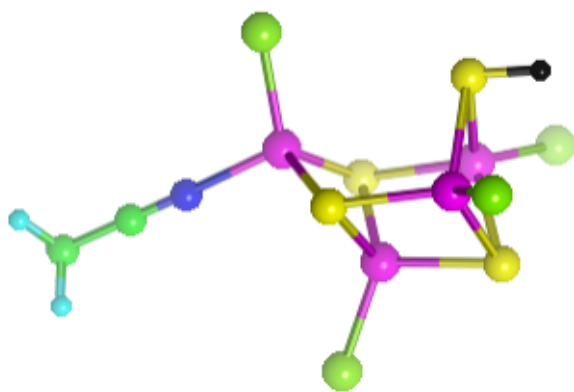
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Cl	2	2.774	-0.742	2.659
Cl	3	1.654	1.045	-3.574
Cl	4	-1.838	-3.327	-0.363
Fe	5	-1.671	1.177	0.304
Fe	6	1.316	-0.146	1.097
Fe	7	0.761	0.488	-1.615
Fe	8	-0.843	-1.343	-0.314
H	9	2.926	1.827	-0.285
S	10	-0.925	-0.289	1.784
S	11	1.628	2.016	0.083
S	12	-1.584	0.244	-1.765
S	13	1.416	-1.492	-0.795



fe4s3shcl4cxa.car_4

CI-1en

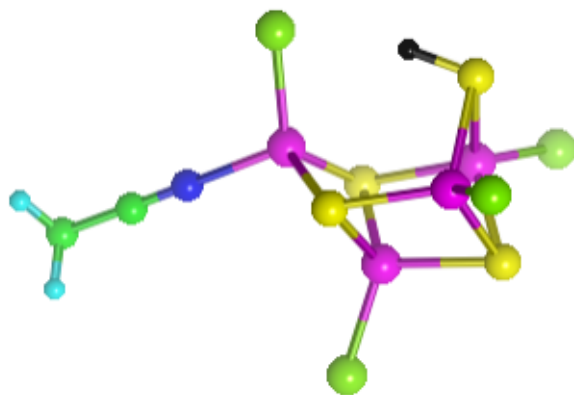
Cl	1	1.375	1.438	-3.385
Cl	2	-2.693	2.784	0.802
Cl	3	2.736	-0.102	3.007
Cl	4	-1.016	-3.665	-0.145
Fe	5	0.659	0.631	-1.441
Fe	6	-1.376	1.021	0.438
Fe	7	1.280	0.167	1.361
Fe	8	-0.483	-1.513	-0.103
H	9	0.025	2.924	0.769
S	10	-1.541	-0.124	-1.550
S	11	1.162	2.327	0.296
S	12	1.787	-1.081	-0.535
S	13	-0.855	-0.468	1.986



xfe4s3shcl4ncme.car_2

CI-2ex

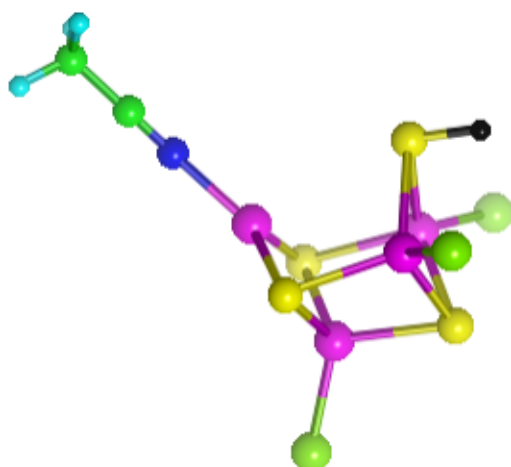
C	1	-4.721	-1.004	-1.152
C	2	-3.440	-0.422	-0.794
Cl	3	4.549	0.960	-2.344
Cl	4	-1.002	3.102	0.372
Cl	5	0.557	-3.297	-0.510
Cl	6	3.342	0.045	4.183
Fe	7	3.048	0.645	-0.699
Fe	8	2.607	0.117	2.067
Fe	9	1.267	-1.235	0.107
Fe	10	-0.602	0.916	-0.029
H	11	4.273	2.374	1.189
H	12	-5.528	-0.427	-0.681
H	13	-4.843	-0.977	-2.242
H	14	-4.763	-2.044	-0.804
N	15	-2.411	0.044	-0.516
S	16	0.309	-0.170	1.854
S	17	0.909	0.348	-1.587
S	18	2.923	2.288	1.026
S	19	3.525	-1.264	0.559



ffe4s3shcl4ncme.car_2

CI-2en

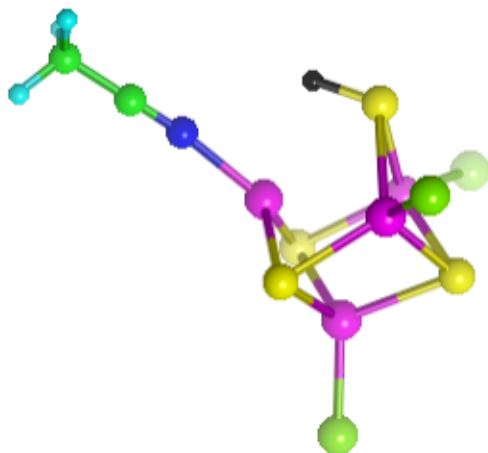
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C	2	-3.326	-0.303	-0.819
Cl	3	4.665	0.818	-2.321
Cl	4	-0.632	3.051	0.426
Cl	5	0.726	-3.461	-0.375
Cl	6	3.433	-0.075	4.209
Fe	7	3.152	0.537	-0.681
Fe	8	2.697	0.047	2.097
Fe	9	1.394	-1.366	0.164
Fe	10	-0.421	0.828	-0.010
H	11	1.878	2.662	0.959
H	12	-5.409	-0.155	-0.756
H	13	-4.732	-0.766	-2.297
H	14	-4.766	-1.825	-0.851
N	15	-2.277	0.099	-0.515
S	16	0.413	-0.300	1.890
S	17	1.036	0.154	-1.582
S	18	3.154	2.185	1.049
S	19	3.651	-1.335	0.617



xfe4s3shcl3ncme.car_2

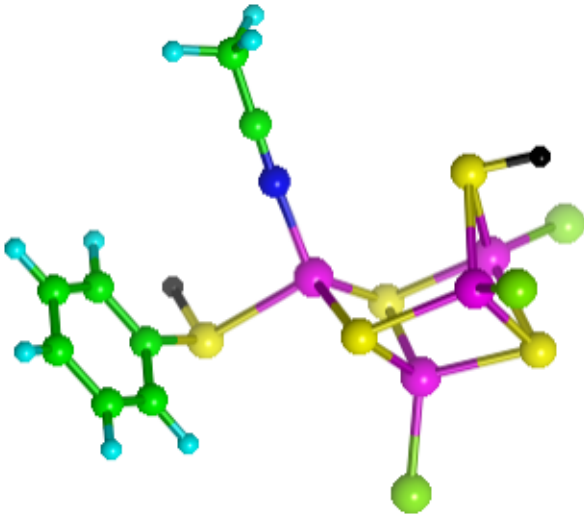
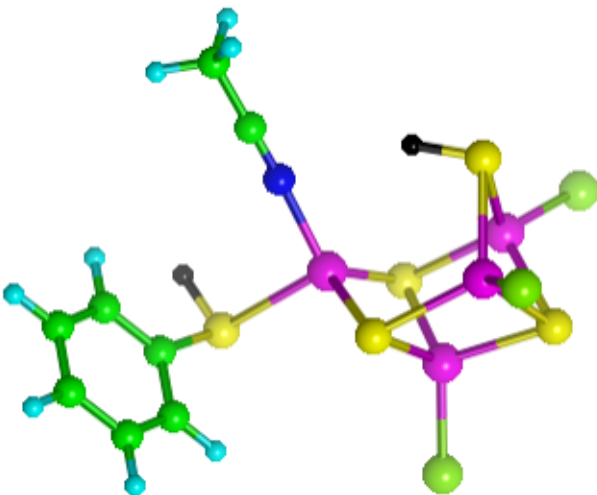
CI-3ex

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Cl	4	0.499	-4.762	-0.801
Cl	5	3.138	-0.991	3.572
Fe	6	2.510	-0.604	-1.226
Fe	7	2.205	-1.029	1.566
Fe	8	0.936	-2.655	-0.230
Fe	9	-0.663	-0.488	-0.102
H	10	3.670	1.301	0.590
H	11	-3.887	3.310	0.741
H	12	-4.002	3.204	-1.044
H	13	-5.002	2.128	-0.017
N	14	-2.128	0.844	-0.124
S	15	-0.025	-1.798	1.631
S	16	0.338	-1.190	-1.929
S	17	2.331	1.108	0.432
S	18	3.192	-2.385	0.094

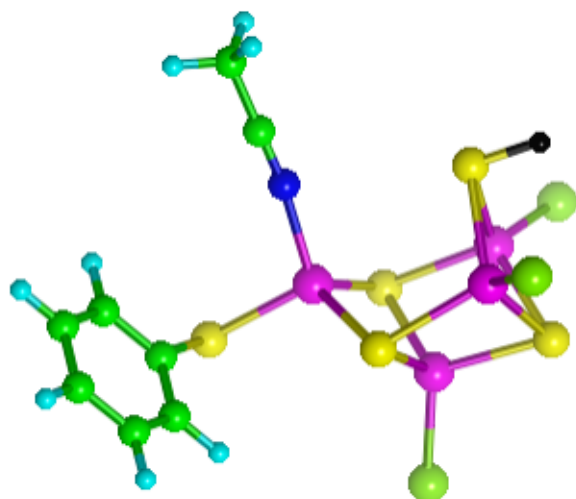


ffe4s3shcl3ncme.car_3

C	1	-3.885	2.209	0.055
C	2	-2.667	1.428	0.042
Cl	3	3.747	0.095	-3.080
Cl	4	1.277	-4.887	-0.723
Cl	5	2.972	-0.384	3.541
Fe	6	2.484	-0.375	-1.328
Fe	7	2.159	-0.779	1.509
Fe	8	1.327	-2.724	-0.240
Fe	9	-0.147	-0.462	-0.058
H	10	0.775	1.791	0.072
H	11	-3.859	2.917	0.892
H	12	-3.974	2.760	-0.890
H	13	-4.745	1.537	0.170
N	14	-1.689	0.798	0.022
S	15	0.195	-2.013	1.584

Cl-3en		S	16	0.494	-1.357	-1.952
		S	17	2.049	1.343	0.279
		S	18	3.488	-1.898	0.105
 ffe4s3shcl3sphhxcme.car_2 Cl-4ex		C	1	-2.320	-1.322	-0.316
		C	2	-3.235	-0.288	-0.061
		C	3	-4.063	-0.370	1.068
		C	4	-3.973	-1.469	1.936
		C	5	-3.052	-2.494	1.672
		C	6	-2.225	-2.430	0.542
		C	7	-0.712	4.123	0.052
		C	8	-0.271	2.785	-0.292
		Cl	9	5.552	0.920	-3.352
		Cl	10	2.682	-4.166	-1.464
		Cl	11	4.680	-0.341	3.105
		Fe	12	4.170	0.289	-1.719
		Fe	13	3.869	-0.329	1.038
		Fe	14	2.867	-1.998	-0.907
		Fe	15	0.841	-0.106	-0.964
		H	16	5.087	2.176	0.187
		H	17	-3.308	0.567	-0.731
		H	18	-4.777	0.429	1.265
		H	19	-4.615	-1.525	2.814
		H	20	-2.980	-3.352	2.339
		H	21	-1.524	-3.236	0.332
		H	22	-0.335	4.382	1.050
		H	23	-0.320	4.838	-0.683
		H	24	-1.808	4.162	0.055
		H	25	-1.832	-0.273	-2.416
		N	26	0.089	1.713	-0.567
		S	27	1.701	-1.226	0.869
		S	28	2.210	-0.567	-2.639
		S	29	3.769	1.870	0.028
		S	30	5.054	-1.466	-0.474
		S	31	-1.222	-1.297	-1.765
 ffe4s3shcl3sphhncme.car_3 Cl-4en		C	1	-2.110	-1.419	-0.537
		C	2	-3.174	-0.574	-0.182
		C	3	-4.028	-0.954	0.864
		C	4	-3.817	-2.156	1.557
		C	5	-2.746	-2.988	1.197
		C	6	-1.889	-2.627	0.147
		C	7	-1.116	4.036	0.391
		C	8	-0.428	2.825	-0.011
		Cl	9	5.719	1.631	-3.013
		Cl	10	3.179	-3.711	-1.687
		Cl	11	4.634	-0.212	3.321
		Fe	12	4.312	0.826	-1.480
		Fe	13	3.935	-0.044	1.219
		Fe	14	3.157	-1.607	-0.910
		Fe	15	0.994	0.123	-0.879
		H	16	2.603	2.466	0.376
		H	17	-3.345	0.359	-0.715
		H	18	-4.863	-0.306	1.130

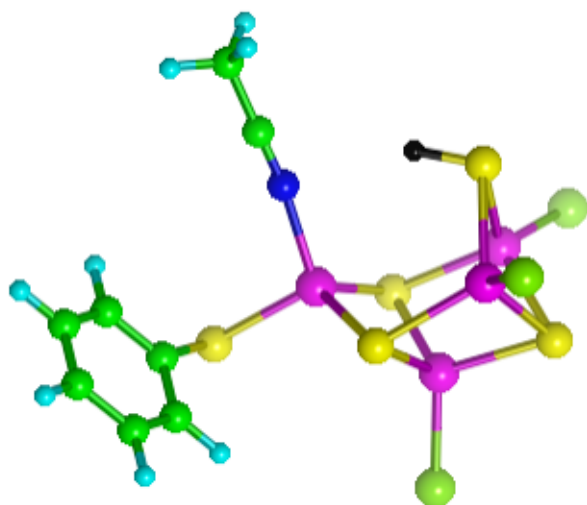
H	19	-4.485	-2.445	2.366
H	20	-2.577	-3.926	1.725
H	21	-1.067	-3.283	-0.136
H	22	-0.808	4.312	1.407
H	23	-0.863	4.850	-0.301
H	24	-2.199	3.865	0.370
H	25	-1.687	0.034	-2.397
N	26	0.122	1.853	-0.338
S	27	1.867	-1.106	0.875
S	28	2.452	-0.084	-2.536
S	29	3.941	2.237	0.413
S	30	5.273	-0.950	-0.321
S	31	-0.988	-1.024	-1.912



xfe4s3shcl3sphncme.car_1

CI-5ex

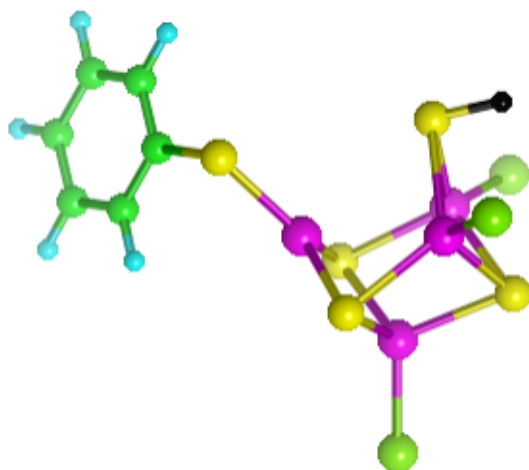
C	1	-2.276	-1.432	-0.178
C	2	-3.325	-0.571	0.208
C	3	-4.091	-0.864	1.346
C	4	-3.818	-2.008	2.112
C	5	-2.769	-2.861	1.732
C	6	-2.000	-2.578	0.595
C	7	-0.968	4.095	0.258
C	8	-0.409	2.811	-0.121
Cl	9	5.140	1.458	-3.893
Cl	10	2.732	-3.830	-2.306
Cl	11	4.688	0.049	2.632
Fe	12	3.970	0.648	-2.145
Fe	13	3.854	-0.077	0.534
Fe	14	2.838	-1.732	-1.447
Fe	15	0.595	-0.086	-1.077
H	16	4.816	2.578	-0.190
H	17	-3.544	0.315	-0.387
H	18	-4.902	-0.194	1.631
H	19	-4.418	-2.235	2.992
H	20	-2.547	-3.752	2.320
H	21	-1.193	-3.246	0.300
H	22	-0.571	4.398	1.235
H	23	-0.698	4.846	-0.495
H	24	-2.060	4.018	0.316
N	25	0.039	1.785	-0.437
S	26	1.798	-1.294	0.496
S	27	1.898	-0.142	-2.890
S	28	3.537	2.142	-0.350
S	29	5.043	-1.122	-1.082
S	30	-1.360	-1.119	-1.710



ffe4s3shcl3sphncme.car_2

Cl-5en

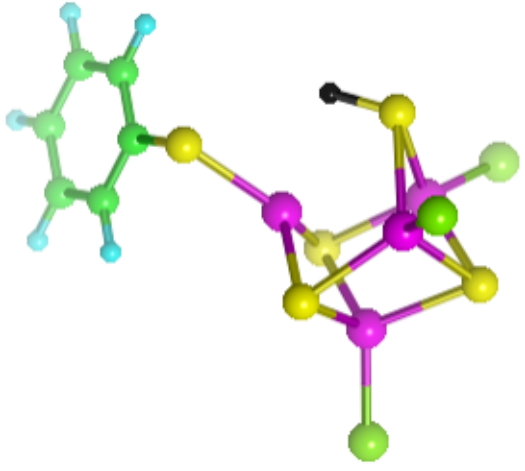
C	1	-2.189	-1.447	-0.238
C	2	-3.254	-0.583	0.095
C	3	-4.042	-0.841	1.226
C	4	-3.778	-1.956	2.038
C	5	-2.715	-2.813	1.711
C	6	-1.924	-2.565	0.581
C	7	-0.956	4.094	0.088
C	8	-0.379	2.811	-0.269
Cl	9	5.395	1.350	-3.718
Cl	10	2.938	-3.880	-2.008
Cl	11	4.564	0.089	2.899
Fe	12	4.153	0.633	-1.970
Fe	13	3.867	-0.032	0.753
Fe	14	2.980	-1.738	-1.246
Fe	15	0.692	-0.113	-1.087
H	16	2.507	2.438	-0.431
H	17	-3.467	0.281	-0.532
H	18	-4.863	-0.168	1.473
H	19	-4.393	-2.156	2.915
H	20	-2.499	-3.681	2.335
H	21	-1.105	-3.236	0.331
H	22	-0.597	4.391	1.081
H	23	-0.659	4.845	-0.654
H	24	-2.050	4.013	0.105
N	25	0.091	1.786	-0.556
S	26	1.813	-1.224	0.605
S	27	2.129	-0.210	-2.803
S	28	3.818	2.187	-0.197
S	29	5.157	-1.099	-0.775
S	30	-1.236	-1.176	-1.754



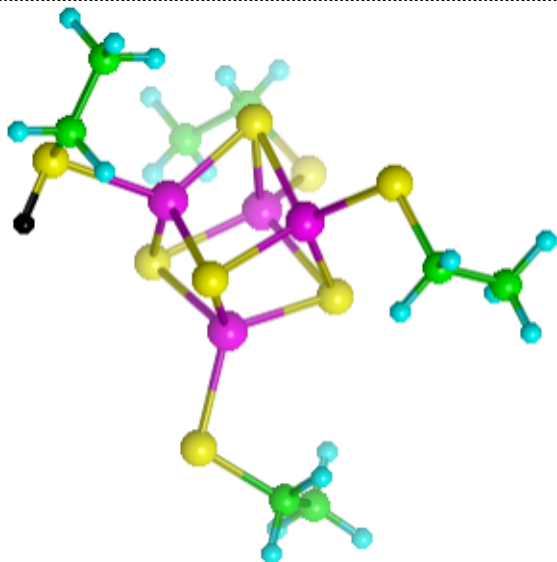
xfe4s3shcl3sph.car_2

Cl-6ex

C	1	-2.081	0.848	0.230
C	2	-2.728	-0.287	-0.299
C	3	-3.650	-0.147	-1.345
C	4	-3.942	1.123	-1.870
C	5	-3.305	2.254	-1.335
C	6	-2.379	2.123	-0.290
Cl	7	4.499	0.343	-2.405
Cl	8	4.206	-0.426	4.208
Cl	9	2.431	-4.872	-0.205
Fe	10	3.414	-0.263	-0.546
Fe	11	3.294	-0.777	2.184
Fe	12	2.430	-2.730	0.457
Fe	13	0.639	-0.779	0.970
H	14	4.375	1.714	1.342
H	15	-2.518	-1.272	0.111
H	16	-4.133	-1.037	-1.747
H	17	-4.658	1.230	-2.686
H	18	-3.521	3.244	-1.736
H	19	-1.890	3.006	0.116
S	20	1.465	-2.250	2.458
S	21	1.352	-1.279	-1.053
S	22	3.065	1.405	1.135
S	23	4.571	-1.860	0.683

 fe4s3shcl3sph.car_3 Cl-6en	S	24	-0.935	0.689	1.625
	C	1	-1.957	0.853	-0.028
	C	2	-2.541	-0.288	-0.613
	C	3	-3.330	-0.159	-1.764
	C	4	-3.549	1.105	-2.337
	C	5	-2.972	2.242	-1.751
	C	6	-2.178	2.122	-0.600
	Cl	7	4.858	0.404	-1.731
	Cl	8	3.734	-0.609	4.813
	Cl	9	2.409	-4.843	0.026
	Fe	10	3.521	-0.265	-0.069
	Fe	11	3.086	-0.889	2.681
	Fe	12	2.392	-2.720	0.744
	Fe	13	0.822	-0.524	1.103
	H	14	1.698	1.705	1.330
	H	15	-2.381	-1.269	-0.169
	H	16	-3.777	-1.046	-2.212
	H	17	-4.165	1.200	-3.231
	H	18	-3.140	3.228	-2.185
	H	19	-1.737	3.007	-0.146
	S	20	1.173	-2.222	2.584
	S	21	1.550	-1.206	-0.862
	S	22	2.982	1.334	1.632
	S	23	4.516	-1.886	1.270
	S	24	-1.014	0.726	1.517

With X = SEt

 fe4s4set3hset.car_6 1	C	1	-2.856	3.537	3.043
	C	2	-3.508	2.154	3.016
	C	3	-1.337	2.014	-5.141
	C	4	-0.201	2.625	-4.311
	C	5	1.105	-4.856	-1.728
	C	6	0.518	-4.770	-0.315
	C	7	4.725	-0.713	2.277
	C	8	3.441	-0.399	3.056
	Fe	9	-1.661	0.862	0.393
	Fe	10	0.089	0.682	-1.655
	Fe	11	-0.545	-1.574	-0.142
	Fe	12	0.915	0.463	1.113
	H	13	-3.507	4.300	2.595
	H	14	-1.959	1.352	-4.525
	H	15	-0.936	1.421	-5.976
	H	16	0.383	-5.301	-2.427
	H	17	5.452	0.107	2.372
	H	18	5.195	-1.636	2.659
	H	19	-2.852	1.389	3.442
	H	20	-4.476	2.149	3.530
	H	21	-1.981	2.808	-5.559
	H	22	0.410	3.297	-4.929

H	23	-0.598	3.214	-3.475
H	24	2.018	-5.478	-1.729
H	25	0.266	-5.773	0.060
H	26	1.236	-4.322	0.381
H	27	4.508	-0.850	1.211
H	28	2.727	-1.227	2.979
H	29	3.662	-0.250	4.122
H	30	1.370	-3.858	-2.099
H	31	-2.659	3.825	4.086
H	32	-1.899	3.531	2.506
H	33	-4.371	0.420	1.540
S	34	-3.850	1.637	1.236
S	35	1.002	1.355	-3.628
S	36	-1.084	-3.795	-0.221
S	37	2.606	1.178	2.469
S	38	1.517	-0.925	-0.701
S	39	-0.872	-0.617	2.021
S	40	-0.032	2.329	0.032
S	41	-1.963	-0.304	-1.577

Protonation of X and μ_3 -S, intermediate 2.

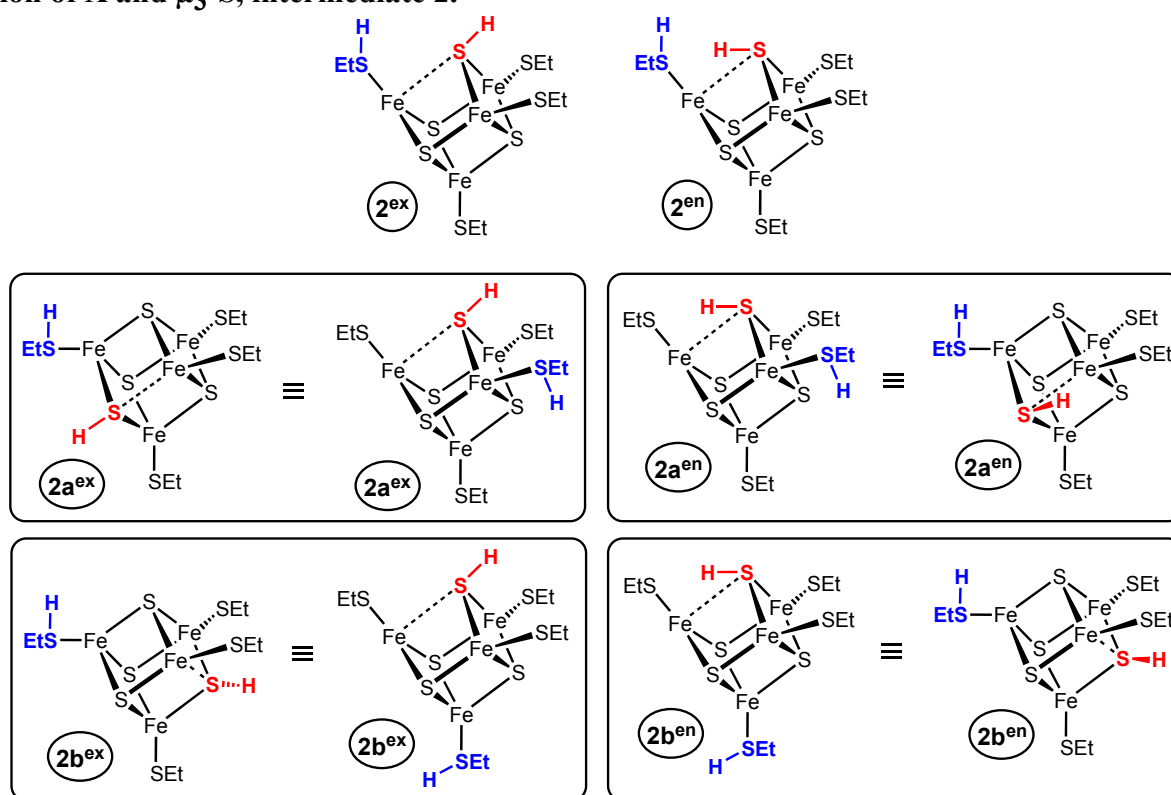
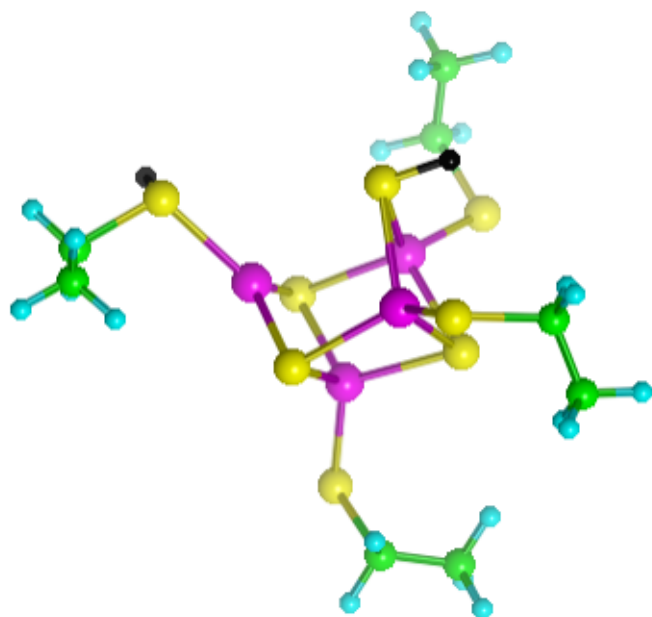
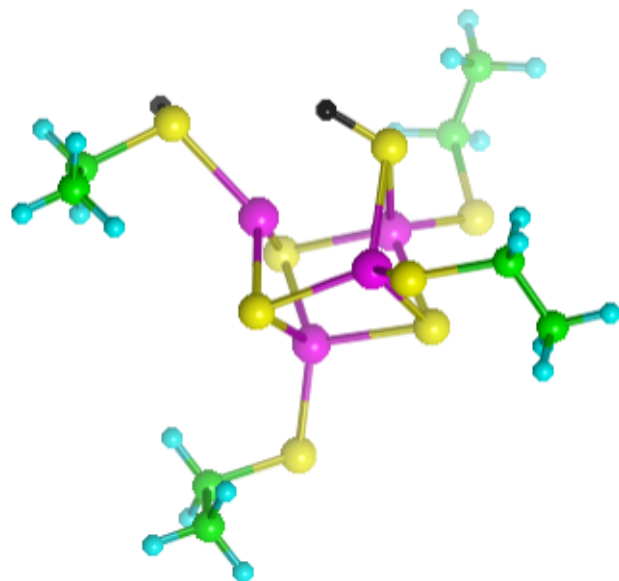


Fig. 6. The six isomers possible for $[\text{Fe}_4\text{S}_3(\text{SH})\text{X}_3(\text{XH})]^0$, drawn for $\text{X} = \text{SEt}$. Isomers **2a** have one Fe-S bond separating the protonation sites, while isomers **2b** have a three Fe-S bond separation. Isomers **2a** and **2b** are drawn in two orientations, to facilitate comparisons.



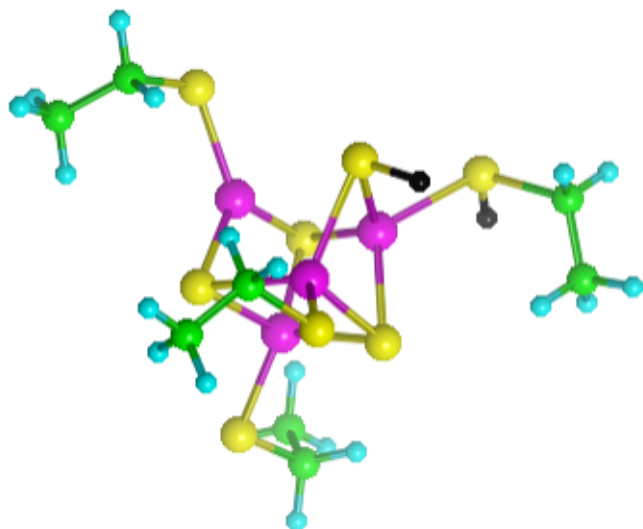
fe4s3shset4axa.car_3
2ex

C	1	1.457	4.571	-2.829
C	2	1.304	3.260	-3.606
C	3	4.053	-1.597	3.017
C	4	3.495	-0.179	3.160
C	5	1.718	-4.802	-1.229
C	6	0.249	-4.607	-0.838
C	7	-5.565	0.555	2.032
C	8	-5.524	1.150	0.625
Fe	9	0.715	1.036	-1.259
Fe	10	0.621	0.026	1.388
Fe	11	-0.425	-1.384	-0.732
Fe	12	-2.188	0.496	-0.090
H	13	2.516	4.815	-2.671
H	14	3.681	-2.078	2.104
H	15	3.772	-2.222	3.875
H	16	1.814	-5.066	-2.290
H	17	-4.163	2.491	-0.908
H	18	-5.500	1.334	2.803
H	19	-6.514	0.019	2.167
H	20	0.249	3.003	-3.757
H	21	1.770	3.335	-4.596
H	22	5.152	-1.561	2.963
H	23	3.883	0.307	4.064
H	24	3.758	0.444	2.300
H	25	2.159	-5.615	-0.631
H	26	-0.329	-5.524	-1.009
H	27	0.146	-4.341	0.220
H	28	-4.750	-0.162	2.191
H	29	-5.586	0.380	-0.149
H	30	-6.320	1.888	0.473
H	31	2.300	-3.890	-1.052
H	32	0.995	5.398	-3.391
H	33	0.973	4.510	-1.845
H	34	1.554	2.810	0.856
S	35	2.161	1.792	-2.801
S	36	1.629	-0.139	3.376
S	37	-0.619	-3.301	-1.875
S	38	-3.903	2.090	0.364
S	39	-1.437	-1.095	1.312
S	40	1.764	-0.791	-0.336
S	41	0.278	2.369	0.694
S	42	-1.341	0.274	-2.089



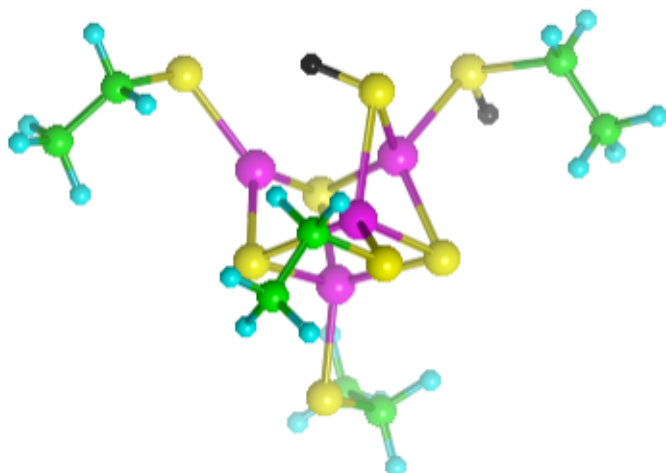
fe4s3shset4an.car_4
2en

C	1	2.968	3.655	-3.268
C	2	2.488	2.380	-3.967
C	3	4.373	-1.238	3.096
C	4	3.524	-0.011	3.438
C	5	-2.145	-4.984	0.266
C	6	-2.144	-4.216	-1.060
C	7	-4.656	1.347	1.863
C	8	-4.490	1.737	0.394
Fe	9	1.337	0.576	-1.466
Fe	10	0.967	-0.161	1.292
Fe	11	-0.172	-1.574	-0.778
Fe	12	-1.179	0.825	-0.238
H	13	4.048	3.615	-3.076
H	14	4.169	-1.592	2.078
H	15	4.174	-2.064	3.792
H	16	-1.477	-5.854	0.217
H	17	-3.013	2.912	-1.171
H	18	-4.602	2.225	2.521
H	19	-5.642	0.881	1.998
H	20	1.408	2.399	-4.154
H	21	2.987	2.254	-4.937
H	22	5.443	-0.982	3.162
H	23	3.721	0.331	4.462
H	24	3.731	0.825	2.761
H	25	-3.162	-5.344	0.490
H	26	-2.478	-4.856	-1.887
H	27	-2.806	-3.345	-1.021
H	28	-3.893	0.624	2.177
H	29	-4.535	0.870	-0.272
H	30	-5.233	2.479	0.084
H	31	-1.814	-4.345	1.093
H	32	2.764	4.532	-3.902
H	33	2.460	3.799	-2.306
H	34	0.123	2.837	0.442
S	35	2.900	0.799	-3.039
S	36	1.673	-0.336	3.407
S	37	-0.427	-3.645	-1.571
S	38	-2.812	2.569	0.128
S	39	-1.217	-0.960	1.146
S	40	2.092	-1.239	-0.307
S	41	1.289	2.130	0.384
S	42	-0.744	0.146	-2.274



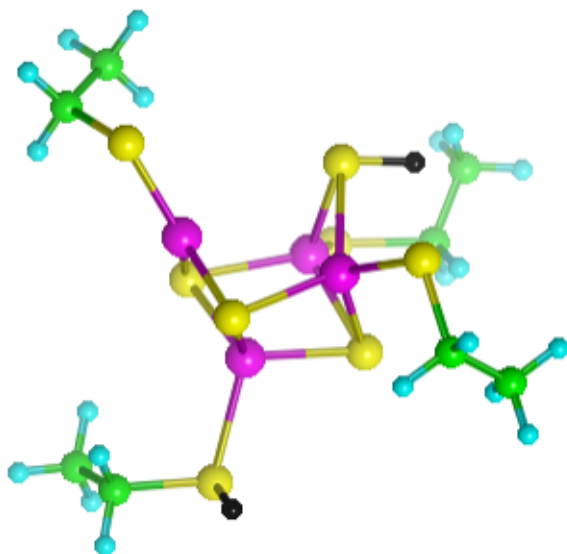
fe4s3shset4hbn.car_3.cmmf
2aex

C	1	5.226	-0.230	-0.849
C	2	4.952	1.268	-0.943
C	3	-0.317	-3.042	-4.640
C	4	-0.041	-3.688	-3.279
C	5	-4.635	2.813	0.346
C	6	-3.316	3.537	0.631
C	7	-2.236	-1.282	4.937
C	8	-1.083	-0.335	4.587
Fe	9	1.386	0.679	-0.648
Fe	10	-0.451	-1.240	-1.100
Fe	11	-1.325	1.269	-0.820
Fe	12	0.070	-0.227	1.503
H	13	5.322	-0.684	-1.844
H	14	-0.209	-1.951	-4.592
H	15	-1.334	-3.266	-4.986
H	16	-5.083	3.161	-0.594
H	17	-1.865	-2.181	5.447
H	18	-2.950	-0.777	5.605
H	19	4.885	1.739	0.045
H	20	5.720	1.797	-1.517
H	21	0.393	-3.427	-5.389
H	22	-0.157	-4.778	-3.330
H	23	0.977	-3.480	-2.931
H	24	-5.350	3.007	1.161
H	25	-3.472	4.619	0.722
H	26	-2.853	3.182	1.559
H	27	-2.773	-1.600	4.035
H	28	-1.444	0.562	4.073
H	29	2.181	1.598	2.003
H	30	-0.546	-0.012	5.488
H	31	-4.482	1.730	0.274
H	32	6.175	-0.392	-0.316
H	33	4.432	-0.755	-0.306
H	34	3.429	0.926	-2.834
S	35	3.318	1.739	-1.751
S	36	-1.242	-3.155	-1.935
S	37	-2.039	3.370	-0.738
S	38	0.215	-1.178	3.516
S	39	-2.004	-0.397	0.437
S	40	1.044	1.980	1.355
S	41	1.503	-1.412	0.129
S	42	-0.025	0.515	-2.511



fe4s3shset4hbx.car_4
2aen

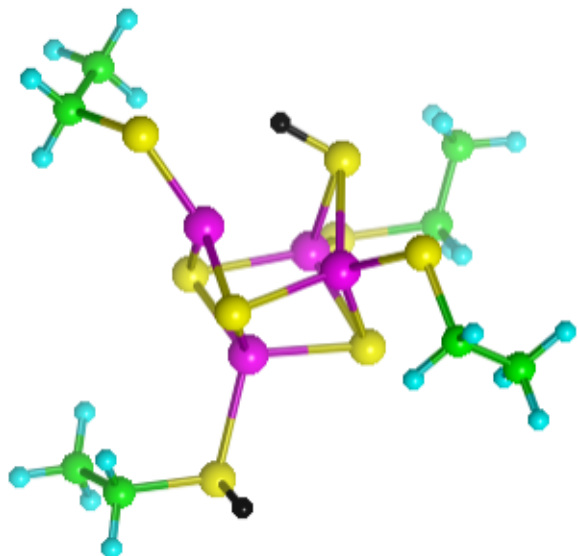
C	1	5.046	1.521	-1.316
C	2	4.223	2.801	-1.429
C	3	0.152	-3.412	-4.444
C	4	0.851	-3.776	-3.130
C	5	-5.237	1.297	0.532
C	6	-4.132	2.298	0.879
C	7	-1.224	-1.627	5.268
C	8	-0.459	-0.439	4.675
Fe	9	1.159	0.992	-0.800
Fe	10	-0.032	-1.422	-0.970
Fe	11	-1.548	0.770	-0.617
Fe	12	0.403	-0.166	1.522
H	13	5.239	1.080	-2.304
H	14	-0.124	-2.350	-4.465
H	15	-0.762	-4.003	-4.581
H	16	-5.775	1.597	-0.376
H	17	-0.548	-2.299	5.812
H	18	-1.990	-1.267	5.972
H	19	4.032	3.258	-0.451
H	20	4.705	3.550	-2.067
H	21	0.823	-3.613	-5.295
H	22	1.123	-4.839	-3.111
H	23	1.769	-3.196	-2.986
H	24	-5.962	1.241	1.359
H	25	-4.549	3.297	1.060
H	26	-3.582	1.992	1.775
H	27	-1.723	-2.209	4.483
H	28	-1.129	0.232	4.127
H	29	-0.486	2.727	1.016
H	30	0.036	0.149	5.458
H	31	-4.824	0.293	0.372
H	32	6.019	1.754	-0.860
H	33	4.544	0.772	-0.695
H	34	2.839	1.788	-3.183
S	35	2.493	2.581	-2.137
S	36	-0.242	-3.549	-1.618
S	37	-2.885	2.558	-0.507
S	38	0.921	-1.000	3.525
S	39	-1.613	-0.984	0.703
S	40	0.759	2.216	1.240
S	41	2.005	-0.897	0.029
S	42	-0.312	0.284	-2.466



fe4s3shset4hox.car_8

2bex

C	1	4.354	-1.847	2.967
C	2	3.223	-1.247	3.807
C	3	3.462	2.214	-3.625
C	4	2.912	0.797	-3.430
C	5	-3.265	4.158	-0.537
C	6	-4.013	3.353	0.528
C	7	-3.837	-3.432	-1.204
C	8	-3.125	-3.840	0.086
Fe	9	1.144	0.227	1.626
Fe	10	0.567	0.559	-1.074
Fe	11	-1.844	0.884	1.082
Fe	12	-0.655	-1.367	0.401
H	13	5.235	-1.191	2.964
H	14	3.260	2.846	-2.751
H	15	3.011	2.697	-4.501
H	16	-2.681	4.969	-0.083
H	17	-0.908	-4.225	1.060
H	18	-3.535	-4.067	-2.047
H	19	-4.921	-3.542	-1.066
H	20	2.340	-1.895	3.821
H	21	3.544	-1.095	4.846
H	22	4.552	2.176	-3.779
H	23	3.127	0.170	-4.304
H	24	3.353	0.310	-2.555
H	25	-3.984	4.603	-1.241
H	26	-4.724	3.989	1.072
H	27	-4.573	2.523	0.085
H	28	-3.632	-2.386	-1.464
H	29	-3.407	-3.205	0.932
H	30	-3.314	-4.889	0.339
H	31	-2.578	3.519	-1.107
H	32	4.654	-2.822	3.383
H	33	4.036	-2.001	1.928
H	34	2.526	2.298	0.205
S	35	2.688	0.460	3.235
S	36	1.040	0.761	-3.263
S	37	-2.903	2.656	1.878
S	38	-1.257	-3.699	-0.143
S	39	-1.762	0.122	-0.993
S	40	1.184	2.320	0.438
S	41	1.608	-1.258	-0.007
S	42	-0.904	-0.603	2.493



fe4s3shset4hon.car_6

2ben

C	1	4.538	-1.704	2.902
C	2	3.363	-1.190	3.739
C	3	3.371	2.473	-3.317
C	4	2.971	0.995	-3.382
C	5	-3.390	3.978	-0.687
C	6	-3.932	3.172	0.495
C	7	-3.809	-3.584	-1.139
C	8	-3.010	-4.018	0.091
Fe	9	1.172	0.128	1.607
Fe	10	0.612	0.489	-1.132
Fe	11	-1.441	0.985	0.938
Fe	12	-0.606	-1.450	0.337
H	13	5.373	-0.992	2.914
H	14	3.074	2.923	-2.361
H	15	2.902	3.049	-4.126
H	16	-2.863	4.878	-0.347
H	17	-0.717	-4.319	0.927
H	18	-3.536	-4.174	-2.024
H	19	-4.880	-3.737	-0.944
H	20	2.524	-1.895	3.736
H	21	3.663	-1.034	4.783
H	22	4.463	2.567	-3.418
H	23	3.273	0.547	-4.337
H	24	3.436	0.415	-2.579
H	25	-4.221	4.294	-1.336
H	26	-4.653	3.763	1.074
H	27	-4.434	2.258	0.162
H	28	-3.653	-2.522	-1.365
H	29	-3.274	-3.438	0.980
H	30	-3.135	-5.086	0.299
H	31	-2.697	3.379	-1.292
H	32	4.899	-2.662	3.310
H	33	4.240	-1.864	1.858
H	34	0.006	2.901	0.541
S	35	2.725	0.486	3.179
S	36	1.111	0.721	-3.305
S	37	-2.629	2.686	1.762
S	38	-1.165	-3.772	-0.233
S	39	-1.685	0.056	-1.064
S	40	1.201	2.248	0.392
S	41	1.682	-1.295	-0.053
S	42	-0.871	-0.657	2.413

Association of solvent MeCN to attain four coordination at the unique Fe atom

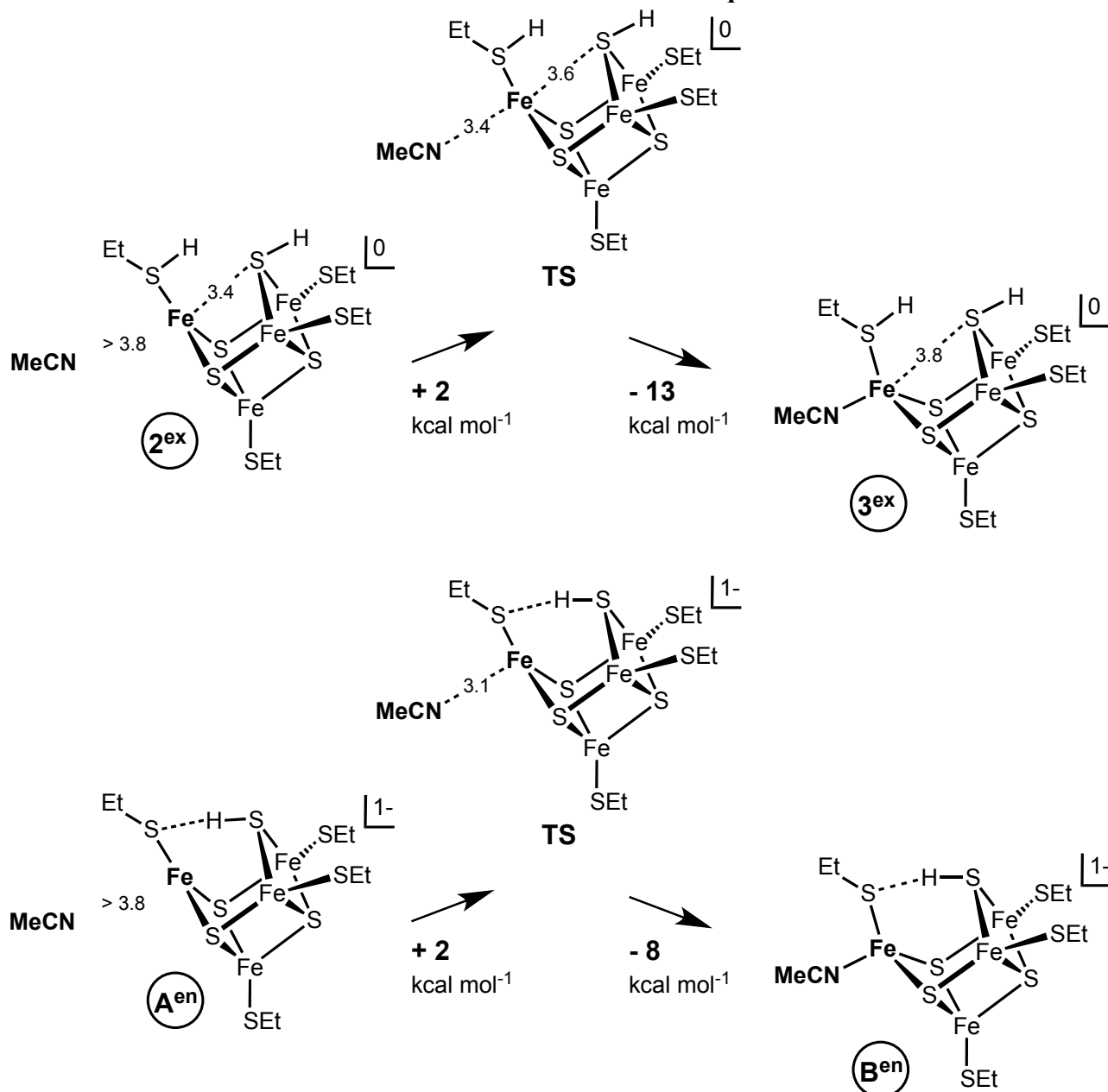
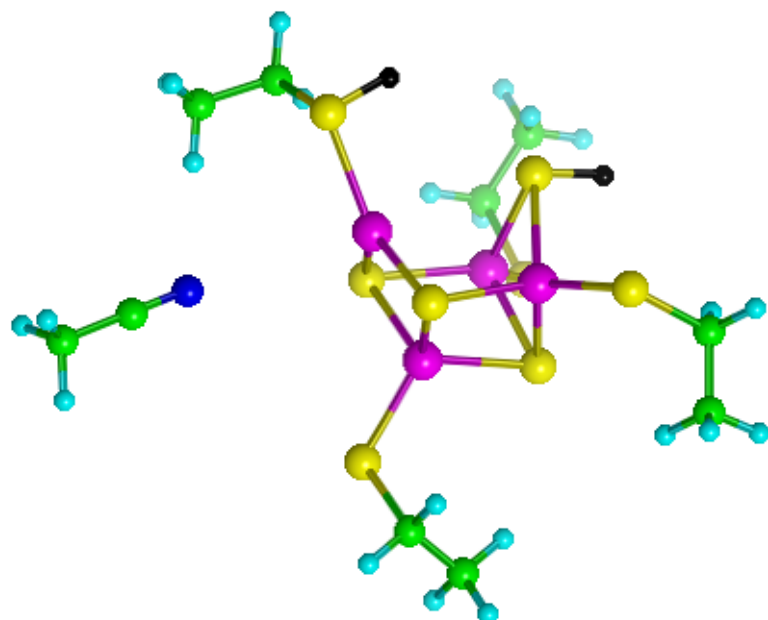


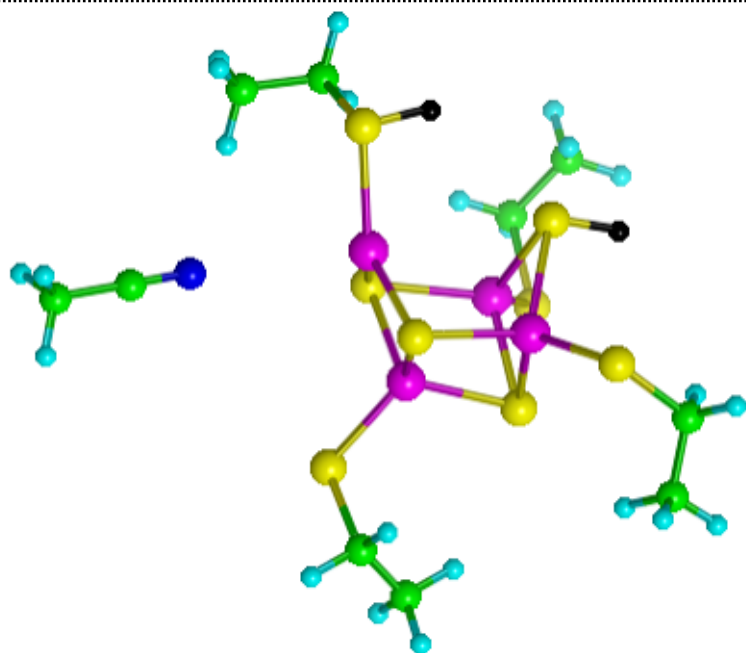
Fig. 7. Two examples of the reaction profile for addition of solvent MeCN to the three-coordinate Fe atom (COSMO energies included). Selected MeCN-Fe and Fe-S interatomic distances (Å) are marked.



s3shset4hancmecoste.car_1

2ex + MeCN

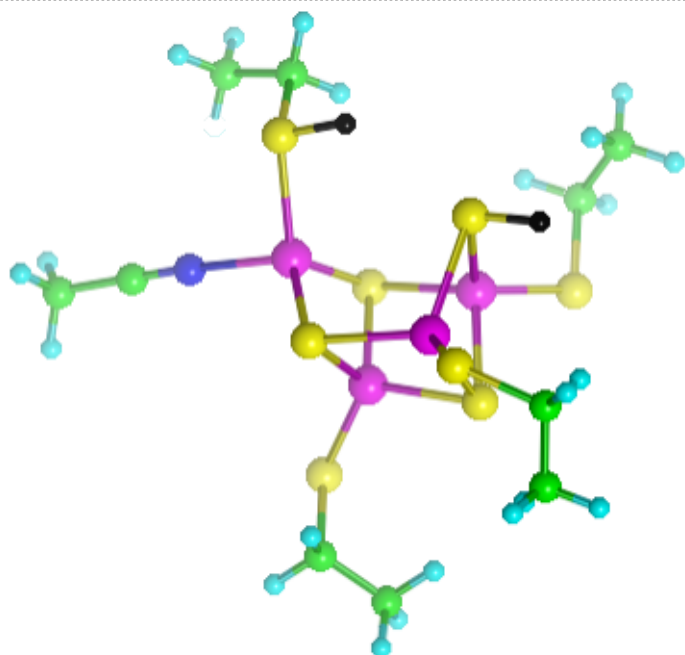
C	1	-6.739	1.169	2.672
C	2	2.806	2.236	-4.407
C	3	-5.339	1.270	2.263
C	4	1.629	1.268	-4.559
C	5	4.432	-3.837	1.784
C	6	4.900	-2.382	1.705
C	7	-0.916	-5.281	0.174
C	8	-1.603	-4.203	1.019
C	9	-2.951	4.634	-0.051
C	10	-1.427	4.632	-0.151
Fe	11	1.302	0.018	-1.517
Fe	12	2.110	-0.539	1.130
Fe	13	-0.394	-1.219	0.260
Fe	14	-0.585	1.377	0.877
H	15	-6.874	1.645	3.651
H	16	-7.380	1.673	1.938
H	17	-7.035	0.114	2.742
H	18	3.738	1.792	-4.781
H	19	3.483	-3.978	1.250
H	20	4.297	-4.158	2.826
H	21	-1.562	-5.607	-0.652
H	22	0.608	4.013	1.102
H	23	-3.289	5.149	0.858
H	24	-3.360	5.168	-0.920
H	25	0.695	1.713	-4.201
H	26	1.487	0.986	-5.609
H	27	5.188	-4.489	1.318
H	28	5.851	-2.244	2.235
H	29	5.032	-2.052	0.670
H	30	-0.688	-6.157	0.801
H	31	-2.548	-4.573	1.435
H	32	-0.971	-3.883	1.854
H	33	-3.358	3.615	-0.052
H	34	-1.056	4.118	-1.040
H	35	-1.009	5.643	-0.105
H	36	0.026	-4.909	-0.251
H	37	2.606	3.151	-4.986
H	38	2.954	2.520	-3.357
H	39	3.903	1.032	-0.620
N	40	-4.220	1.352	1.939
S	41	1.873	-0.375	-3.668
S	42	3.727	-1.176	2.552
S	43	-2.079	-2.685	0.014
S	44	-0.700	3.738	1.352
S	45	0.079	-0.260	2.281
S	46	1.634	-2.016	-0.468
S	47	2.685	1.444	-0.182
S	48	-0.962	0.556	-1.126



s3shset4hancmecostc_2_4312.88.cmmf

TS

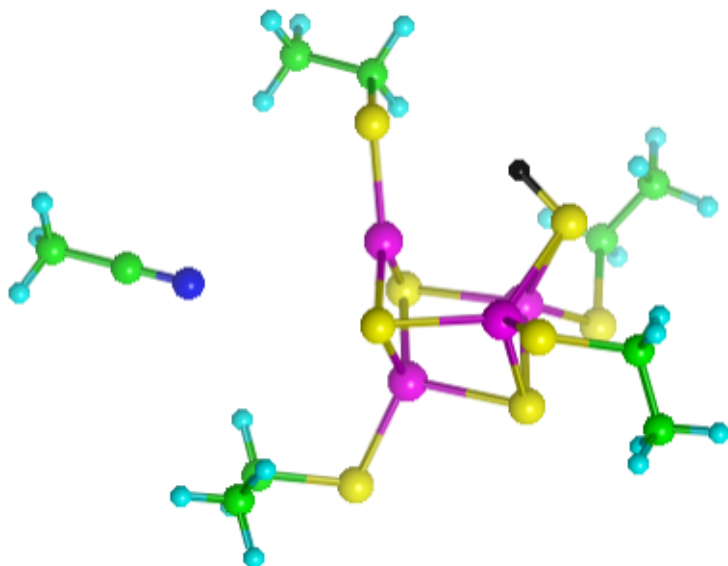
C	1	-6.873	0.276	2.273
C	2	2.737	2.889	-3.994
C	3	-5.469	0.525	1.942
C	4	1.698	1.806	-4.291
C	5	4.708	-3.445	1.793
C	6	5.012	-1.948	1.859
C	7	-0.296	-5.326	-0.308
C	8	-1.173	-4.432	0.570
C	9	-3.398	4.207	0.092
C	10	-1.884	4.398	0.073
Fe	11	1.332	0.293	-1.382
Fe	12	2.046	-0.393	1.262
Fe	13	-0.311	-1.274	0.155
Fe	14	-1.016	1.172	0.962
H	15	-7.099	0.691	3.262
H	16	-7.522	0.755	1.528
H	17	-7.073	-0.802	2.281
H	18	3.742	2.571	-4.301
H	19	3.818	-3.641	1.183
H	20	4.542	-3.864	2.794
H	21	-0.830	-5.640	-1.215
H	22	0.180	3.816	1.297
H	23	-3.839	4.600	1.016
H	24	-3.834	4.751	-0.755
H	25	0.697	2.109	-3.964
H	26	1.648	1.592	-5.366
H	27	5.559	-3.973	1.337
H	28	5.912	-1.754	2.455
H	29	5.164	-1.519	0.865
H	30	-0.009	-6.229	0.251
H	31	-2.087	-4.955	0.876
H	32	-0.647	-4.117	1.477
H	33	-3.675	3.151	-0.003
H	34	-1.418	3.987	-0.826
H	35	-1.599	5.448	0.191
H	36	0.622	-4.806	-0.613
H	37	2.484	3.806	-4.547
H	38	2.766	3.131	-2.923
H	39	3.723	1.542	-0.239
N	40	-4.350	0.735	1.684
S	41	2.090	0.140	-3.502
S	42	3.663	-0.949	2.716
S	43	-1.787	-2.897	-0.329
S	44	-1.117	3.502	1.553
S	45	-0.096	-0.433	2.267
S	46	1.831	-1.774	-0.473
S	47	2.438	1.760	0.156
S	48	-1.005	0.520	-1.138



s3shset4hancmecostca.car_5

3ex

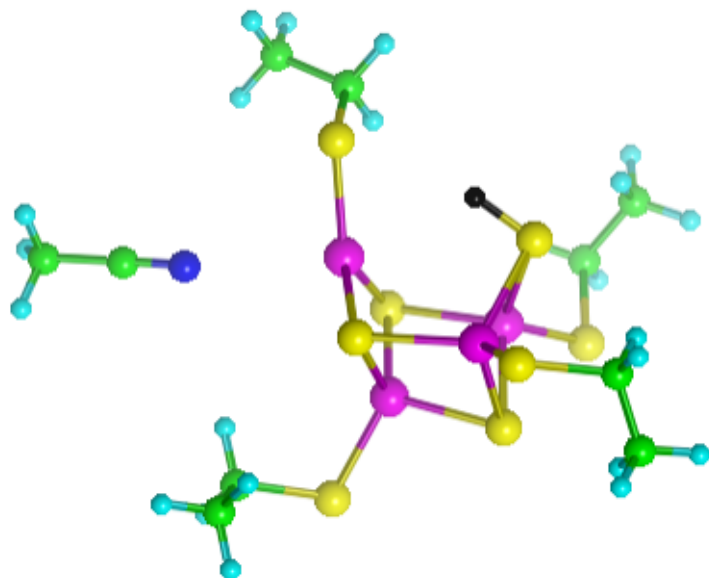
C	1	-6.185	0.291	-1.618
C	2	4.358	3.061	-1.680
C	3	-4.817	0.531	-1.188
C	4	3.609	2.055	-2.560
C	5	2.971	-3.377	4.017
C	6	2.992	-1.862	4.230
C	7	0.003	-5.509	-0.440
C	8	-1.261	-4.649	-0.364
C	9	-3.052	4.389	-1.729
C	10	-1.801	4.379	-0.853
Fe	11	1.683	0.307	-0.513
Fe	12	0.809	-0.506	2.041
Fe	13	-0.388	-1.438	-0.253
Fe	14	-1.802	0.915	-0.115
H	15	-6.880	0.636	-0.842
H	16	-6.378	0.840	-2.548
H	17	-6.335	-0.782	-1.791
H	18	5.382	2.722	-1.475
H	19	2.583	-3.631	3.022
H	20	2.349	-3.879	4.770
H	21	0.189	-5.849	-1.467
H	22	-0.804	3.454	1.180
H	23	-3.933	4.732	-1.171
H	24	-2.887	5.082	-2.566
H	25	2.587	2.387	-2.769
H	26	4.122	1.920	-3.520
H	27	3.995	-3.774	4.096
H	28	3.371	-1.609	5.228
H	29	3.620	-1.360	3.489
H	30	-0.110	-6.399	0.199
H	31	-2.140	-5.213	-0.700
H	32	-1.453	-4.305	0.657
H	33	-3.265	3.399	-2.149
H	34	-0.918	4.039	-1.399
H	35	-1.607	5.362	-0.414
H	36	0.884	-4.952	-0.097
H	37	4.415	4.032	-2.197
H	38	3.846	3.211	-0.721
H	39	2.871	1.599	1.813
N	40	-3.720	0.719	-0.846
S	41	3.528	0.325	-1.816
S	42	1.280	-1.080	4.162
S	43	-1.201	-3.145	-1.497
S	44	-2.022	3.224	0.624
S	45	-1.487	-0.631	1.588
S	46	1.751	-1.790	0.476
S	47	1.581	1.726	1.402
S	48	-0.331	0.402	-1.694



fe41n2ntfcos.car_2

Aen

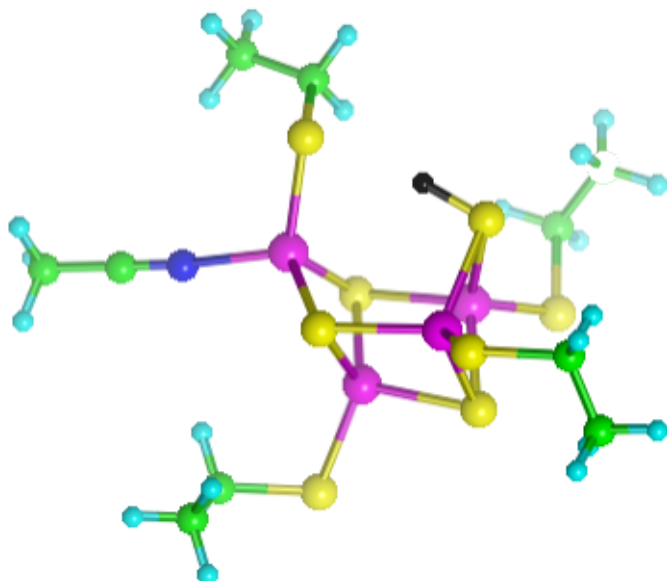
C	1	4.469	1.924	-3.153
C	2	3.490	0.883	-3.707
C	3	4.587	-2.660	3.639
C	4	4.174	-1.206	3.890
C	5	-3.353	-4.027	1.245
C	6	-2.984	-3.532	-0.157
C	7	-6.837	0.703	-0.486
C	8	-2.249	4.362	-1.291
C	9	-0.835	3.992	-0.837
C	10	-5.423	0.349	-0.411
Fe	11	2.037	-0.321	-0.957
Fe	12	1.632	-0.605	1.787
Fe	13	-0.150	-1.763	0.032
Fe	14	-0.603	0.869	0.393
H	15	5.486	1.514	-3.086
H	16	4.225	-3.010	2.664
H	17	4.189	-3.328	4.415
H	18	-3.071	-5.080	1.380
H	19	-7.032	1.590	0.128
H	20	-2.752	4.997	-0.549
H	21	-2.201	4.919	-2.239
H	22	-7.109	0.920	-1.526
H	23	2.473	1.286	-3.771
H	24	3.790	0.568	-4.714
H	25	5.685	-2.741	3.648
H	26	4.523	-0.865	4.874
H	27	4.594	-0.536	3.132
H	28	-4.440	-3.941	1.399
H	29	-3.499	-4.123	-0.925
H	30	-3.258	-2.482	-0.294
H	31	-2.862	3.466	-1.449
H	32	-7.449	-0.130	-0.121
H	33	-0.330	3.364	-1.577
H	34	-0.226	4.890	-0.676
H	35	-2.850	-3.432	2.019
H	36	4.495	2.800	-3.820
H	37	4.168	2.263	-2.153
H	38	1.945	2.194	0.672
N	39	-4.292	0.064	-0.357
S	40	3.428	-0.717	-2.714
S	41	2.312	-0.943	3.930
S	42	-1.149	-3.720	-0.548
S	43	-0.809	3.072	0.814
S	44	-0.708	-0.730	1.986
S	45	-0.206	-0.040	-1.577
S	46	2.875	1.197	0.719
S	47	2.102	-2.253	0.331



fe4ln2ntgcos_1_4353.22

TS

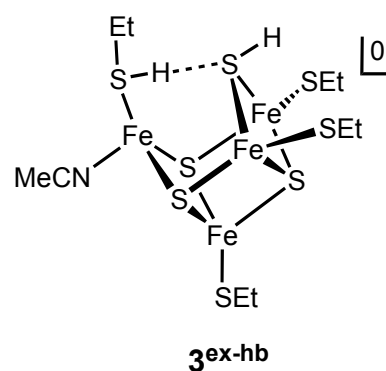
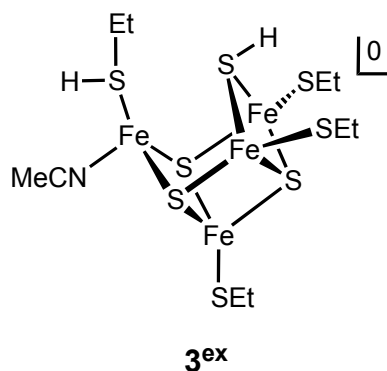
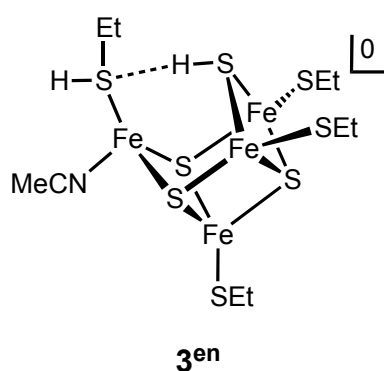
C	1	4.487	1.867	-3.053
C	2	3.538	0.757	-3.519
C	3	4.600	-2.810	3.654
C	4	4.159	-1.371	3.943
C	5	-3.349	-3.965	1.209
C	6	-3.001	-3.445	-0.190
C	7	-6.608	0.806	-0.555
C	8	-2.250	4.604	-1.439
C	9	-0.927	4.027	-0.920
C	10	-5.150	0.731	-0.521
Fe	11	2.026	-0.428	-0.836
Fe	12	1.577	-0.800	1.928
Fe	13	-0.139	-1.787	0.003
Fe	14	-0.982	0.833	0.162
H	15	5.530	1.518	-3.041
H	16	4.213	-3.150	2.684
H	17	4.237	-3.497	4.430
H	18	-3.129	-5.038	1.298
H	19	-6.961	1.627	0.081
H	20	-2.725	5.242	-0.681
H	21	-2.069	5.218	-2.337
H	22	-6.945	0.981	-1.585
H	23	2.501	1.112	-3.553
H	24	3.807	0.411	-4.525
H	25	5.700	-2.869	3.626
H	26	4.542	-1.030	4.914
H	27	4.525	-0.677	3.177
H	28	-4.422	-3.817	1.412
H	29	-3.567	-3.983	-0.961
H	30	-3.234	-2.379	-0.287
H	31	-2.951	3.801	-1.703
H	32	-7.037	-0.138	-0.195
H	33	-0.455	3.379	-1.664
H	34	-0.223	4.830	-0.669
H	35	-2.777	-3.430	1.979
H	36	4.423	2.725	-3.743
H	37	4.228	2.217	-2.046
H	38	1.499	1.951	0.895
N	39	-3.985	0.662	-0.500
S	40	3.594	-0.787	-2.446
S	41	2.290	-1.180	4.049
S	42	-1.193	-3.702	-0.642
S	43	-1.144	3.035	0.666
S	44	-0.761	-0.677	1.878
S	45	-0.149	-0.128	-1.669
S	46	2.603	1.148	0.891
S	47	2.050	-2.394	0.403



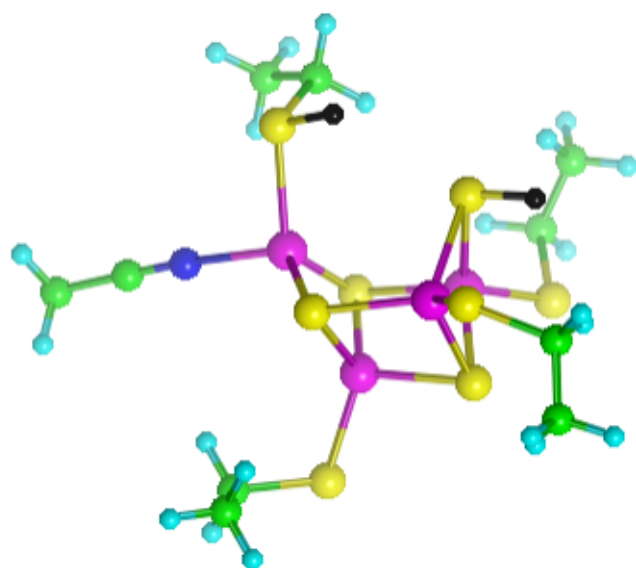
ffe4s3shset4ncme.car_2

2

C	1	4.447	2.300	-2.650
C	2	3.601	1.202	-3.300
C	3	4.377	-2.624	4.023
C	4	3.799	-1.237	4.318
C	5	-3.299	-4.282	0.695
C	6	-2.788	-3.704	-0.629
C	7	-6.052	0.417	-0.973
C	8	-2.344	4.437	-1.404
C	9	-1.002	3.953	-0.846
C	10	-4.616	0.447	-0.740
Fe	11	1.973	-0.232	-0.738
Fe	12	1.429	-0.746	1.986
Fe	13	-0.091	-1.775	-0.075
Fe	14	-1.470	0.711	-0.009
H	15	5.489	1.975	-2.521
H	16	4.176	-2.925	2.986
H	17	3.949	-3.384	4.691
H	18	-2.990	-5.329	0.815
H	19	-6.538	1.175	-0.345
H	20	-2.906	5.007	-0.651
H	21	-2.171	5.094	-2.271
H	22	-6.264	0.629	-2.029
H	23	2.562	1.524	-3.430
H	24	3.997	0.939	-4.289
H	25	5.469	-2.613	4.172
H	26	4.007	-0.944	5.355
H	27	4.236	-0.477	3.661
H	28	-4.399	-4.244	0.720
H	29	-3.186	-4.270	-1.480
H	30	-3.098	-2.660	-0.748
H	31	-2.968	3.596	-1.733
H	32	-6.447	-0.574	-0.714
H	33	-0.446	3.375	-1.591
H	34	-0.380	4.804	-0.541
H	35	-2.917	-3.710	1.550
H	36	4.446	3.199	-3.287
H	37	4.049	2.578	-1.665
H	38	1.080	2.013	0.953
N	39	-3.469	0.479	-0.538
S	40	3.591	-0.420	-2.340
S	41	1.924	-1.138	4.154
S	42	-0.915	-3.788	-0.809
S	43	-1.172	2.884	0.697
S	44	-0.888	-0.703	1.758
S	45	-0.169	-0.058	-1.665
S	46	2.275	1.326	1.038
S	47	2.109	-2.231	0.440



Scheme 2.

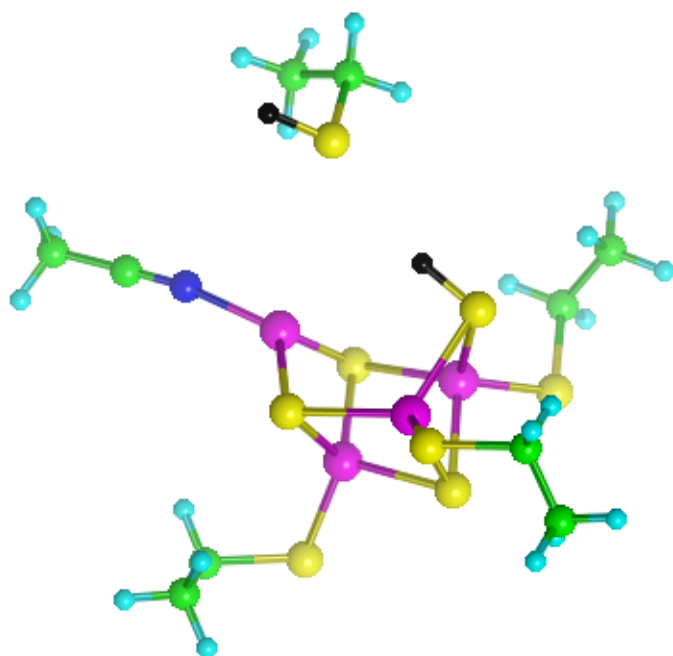
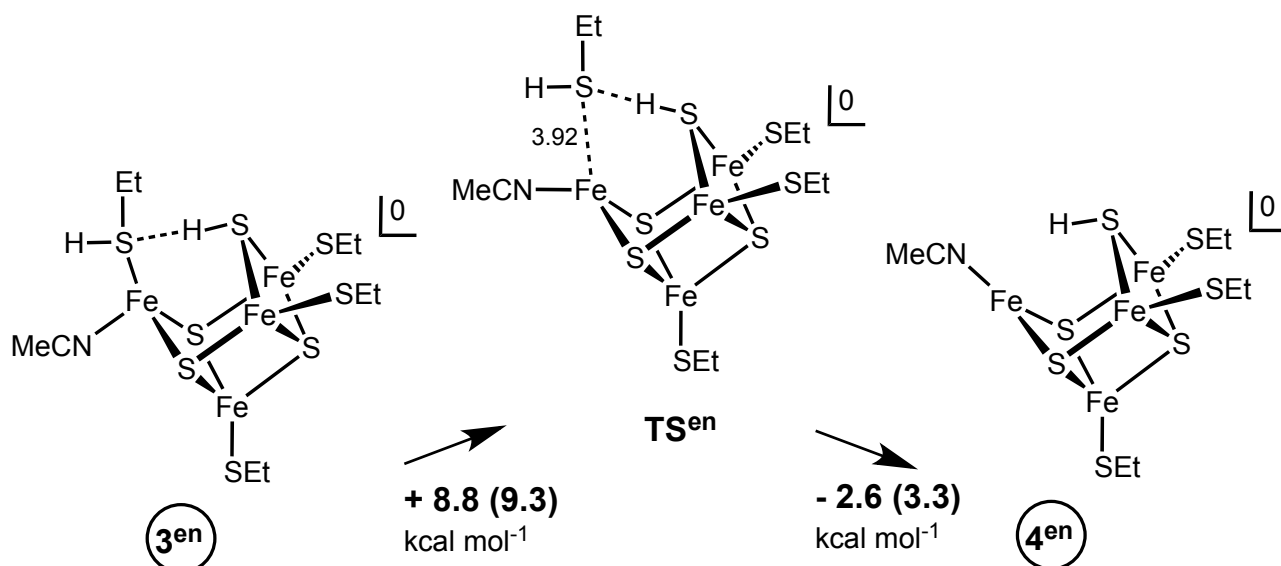


fe43xacos.car_1
3^{ex-hb}

C	1	3.994	2.406	-3.061
C	2	3.372	1.067	-3.466
C	3	3.735	-2.585	4.395
C	4	3.691	-1.063	4.257
C	5	-2.726	-4.370	1.539
C	6	-2.565	-3.980	0.068
C	7	-5.985	-0.136	-1.325
C	8	-1.938	4.017	-2.342
C	9	-0.976	4.015	-1.157
C	10	-4.610	0.179	-0.978
Fe	11	1.914	-0.060	-0.689
Fe	12	1.274	-0.278	2.048
Fe	13	-0.113	-1.701	0.121
Fe	14	-1.545	0.663	-0.104
H	15	5.069	2.302	-2.860
H	16	3.261	-3.075	3.534
H	17	3.222	-2.917	5.308
H	18	-2.199	-5.307	1.764
H	19	-6.663	0.592	-0.863
H	20	-2.898	4.482	-2.082
H	21	-1.488	4.598	-3.158
H	22	-6.104	-0.100	-2.415
H	23	2.301	1.169	-3.670
H	24	3.852	0.672	-4.370
H	25	4.782	-2.921	4.448
H	26	4.151	-0.574	5.124
H	27	4.215	-0.724	3.358
H	28	-3.793	-4.516	1.769
H	29	-2.964	-4.761	-0.591
H	30	-3.094	-3.048	-0.159
H	31	-2.127	3.002	-2.716
H	32	-6.234	-1.143	-0.967
H	33	-0.026	3.531	-1.397
H	34	-0.788	5.027	-0.786
H	35	-2.337	-3.586	2.201
H	36	3.867	3.132	-3.880
H	37	3.513	2.815	-2.163
H	38	3.284	1.684	1.214
H	39	-0.664	3.283	1.148
N	40	-3.504	0.416	-0.699
S	41	3.593	-0.300	-2.187
S	42	1.937	-0.375	4.195

S	43	-0.773	-3.785	-0.481
S	44	-1.715	3.088	0.312
S	45	-1.053	-0.531	1.822
S	46	-0.198	-0.164	-1.657
S	47	1.969	1.748	0.876
S	48	2.086	-1.886	0.724

Dissociation of XH or X⁻

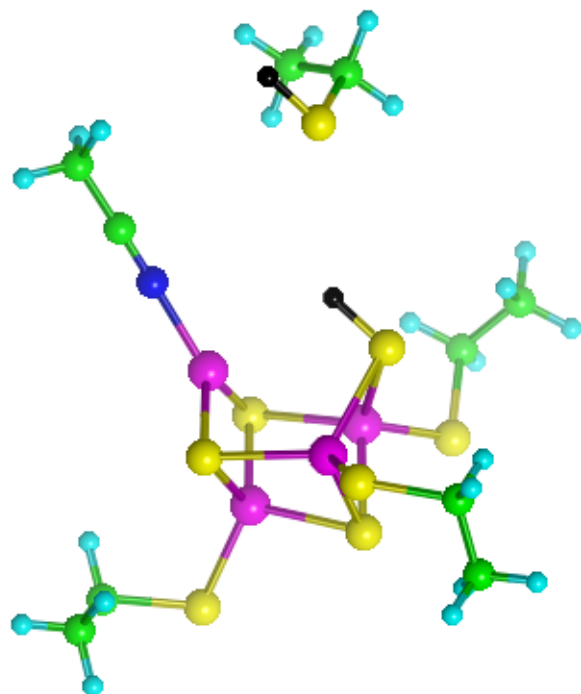


fe43n4ntf429363cos_1_4314.36

TS^{en}

C	1	3.344	1.483	-4.029
C	2	2.502	0.210	-4.151
C	3	5.369	-1.572	3.246
C	4	4.592	-0.258	3.360
C	5	-2.170	-4.777	2.466
C	6	-2.321	-4.550	0.961
C	7	-6.148	0.637	0.360
C	8	-2.625	4.232	-2.065
C	9	-1.303	4.657	-1.425
C	10	-4.701	0.548	0.278
Fe	11	1.647	-0.689	-1.093
Fe	12	1.690	-0.617	1.741
Fe	13	-0.020	-2.233	0.320
Fe	14	-1.593	-0.014	0.234
H	15	4.413	1.261	-4.139
H	16	5.008	-2.178	2.405
H	17	5.279	-2.167	4.164
H	18	-1.539	-5.651	2.673
H	19	-6.438	1.567	0.864
H	20	-3.481	4.557	-1.456
H	21	-2.722	4.691	-3.059
H	22	-6.576	0.621	-0.649
H	23	1.431	0.422	-4.053
H	24	2.660	-0.278	-5.121
H	25	6.435	-1.355	3.079

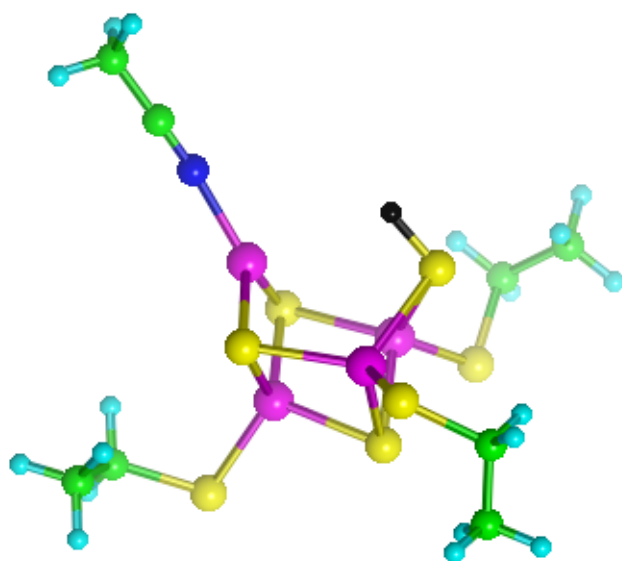
H	26	4.953	0.343	4.204
H	27	4.681	0.347	2.451
H	28	-3.159	-4.951	2.917
H	29	-2.793	-5.416	0.476
H	30	-2.933	-3.667	0.741
H	31	-2.674	3.143	-2.178
H	32	-6.530	-0.219	0.929
H	33	-0.444	4.351	-2.034
H	34	-1.247	5.742	-1.281
H	35	-1.722	-3.902	2.955
H	36	3.056	2.193	-4.819
H	37	3.190	1.970	-3.057
H	38	1.149	1.909	0.368
H	39	-2.063	4.340	0.874
N	40	-3.542	0.449	0.218
S	41	2.957	-1.111	-2.887
S	42	2.758	-0.504	3.716
S	43	-0.682	-4.372	0.054
S	44	-0.969	3.854	0.234
S	45	-0.630	-0.960	2.087
S	46	-0.632	-0.937	-1.533
S	47	2.296	1.193	0.247
S	48	2.248	-2.343	0.409



fe43n4npcos.car_1
4en + EtSH

C	1	4.127	1.147	-2.838
C	2	3.041	0.272	-3.468
C	3	3.344	-3.981	3.370
C	4	2.947	-2.555	3.756
C	5	-4.180	-4.999	0.302
C	6	-3.731	-4.423	-1.042
C	7	-4.198	3.722	0.125
C	8	-0.202	5.578	-1.038
C	9	0.878	5.432	0.035
C	10	-3.415	2.507	0.008
Fe	11	1.167	-1.149	-1.135
Fe	12	0.515	-1.717	1.577
Fe	13	-0.983	-2.677	-0.516
Fe	14	-1.776	-0.160	-0.200
H	15	5.101	0.639	-2.843
H	16	3.073	-4.203	2.330
H	17	2.858	-4.721	4.021
H	18	-3.924	-6.063	0.384
H	19	-3.781	4.356	0.918
H	20	-1.060	6.149	-0.661
H	21	0.209	6.116	-1.906
H	22	-4.176	4.266	-0.828
H	23	2.067	0.773	-3.463
H	24	3.287	0.025	-4.508
H	25	4.434	-4.095	3.472
H	26	3.209	-2.341	4.800
H	27	3.441	-1.811	3.123
H	28	-5.273	-4.901	0.398
H	29	-4.188	-4.966	-1.878
H	30	-4.001	-3.367	-1.140

H	31	-0.561	4.597	-1.376
H	32	-5.236	3.464	0.372
H	33	1.725	4.840	-0.331
H	34	1.263	6.405	0.359
H	35	-3.715	-4.465	1.140
H	36	4.226	2.079	-3.416
H	37	3.878	1.409	-1.802
H	38	0.617	1.215	0.724
H	39	-0.637	5.383	1.944
N	40	-2.798	1.525	-0.093
S	41	2.851	-1.403	-2.621
S	42	1.091	-2.236	3.684
S	43	-1.872	-4.579	-1.335
S	44	0.324	4.501	1.562
S	45	-1.821	-1.770	1.384
S	46	-0.964	-0.959	-2.079
S	47	1.621	0.296	0.729
S	48	1.197	-3.156	0.001

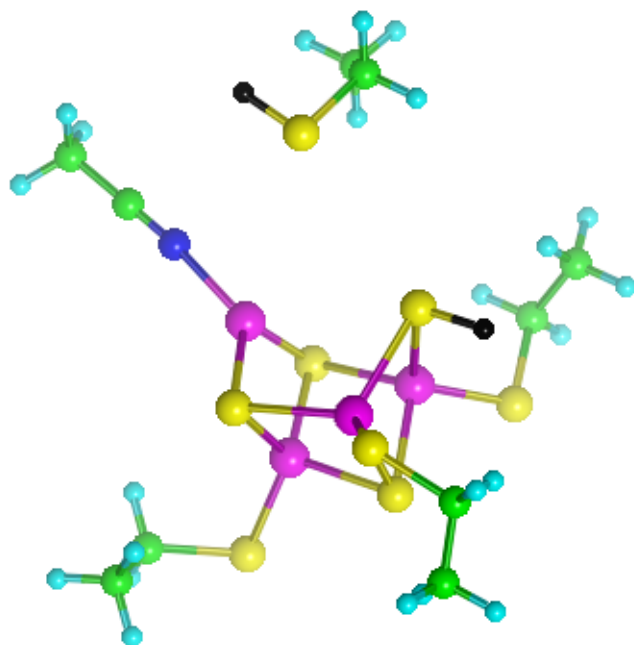
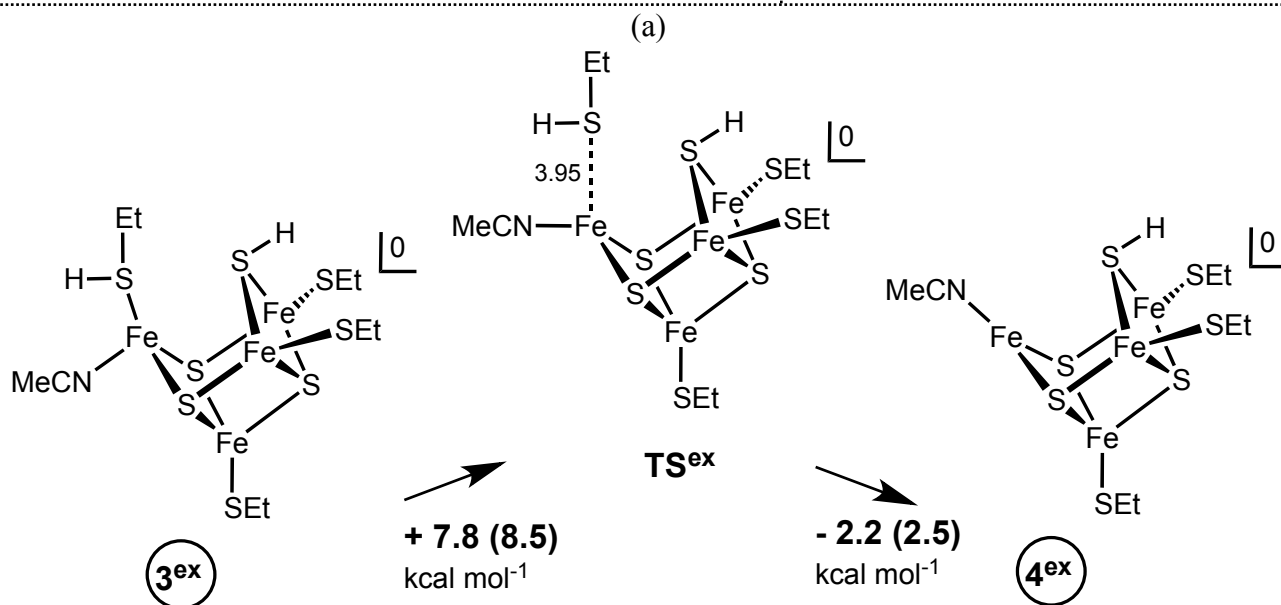


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4en

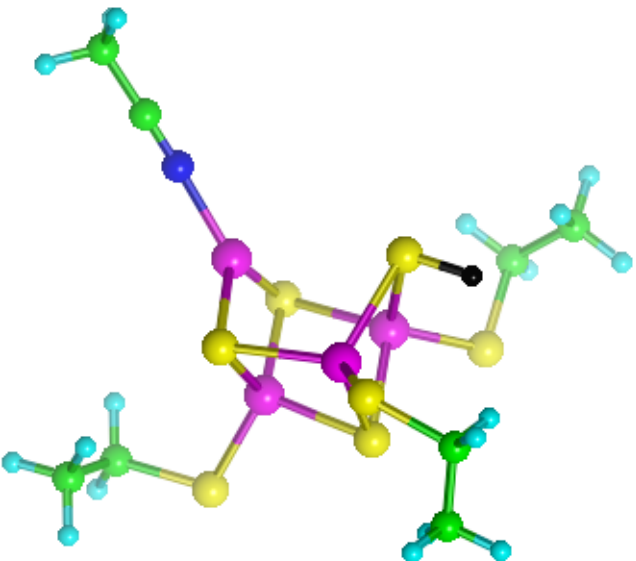
C	1	4.555	1.754	-2.902
C	2	3.306	1.142	-3.541
C	3	3.034	-3.482	3.192
C	4	3.092	-1.994	3.540
C	5	-4.694	-2.680	0.231
C	6	-4.017	-2.351	-1.101
C	7	-4.031	5.258	0.221
C	8	-3.174	4.091	0.130
Fe	9	1.302	0.022	-1.155
Fe	10	0.757	-0.514	1.586
Fe	11	-1.017	-1.159	-0.410
Fe	12	-1.501	1.436	-0.052
H	13	5.417	1.078	-2.980
H	14	2.613	-3.642	2.192
H	15	2.423	-4.035	3.917
H	16	-4.670	-3.759	0.435
H	17	-3.683	5.911	1.031
H	18	-4.004	5.807	-0.728
H	19	2.452	1.825	-3.488
H	20	3.480	0.901	-4.597
H	21	4.050	-3.903	3.208
H	22	3.518	-1.839	4.538
H	23	3.697	-1.430	2.822
H	24	-5.747	-2.360	0.198
H	25	-4.502	-2.877	-1.932
H	26	-4.057	-1.279	-1.318
H	27	-5.060	4.937	0.427
H	28	-4.205	-2.160	1.065
H	29	4.808	2.691	-3.421
H	30	4.388	1.982	-1.842
H	31	1.214	2.344	0.777
N	32	-2.503	3.143	0.048
S	33	2.804	-0.501	-2.762
S	34	1.394	-1.179	3.635
S	35	-2.215	-2.904	-1.190

S	36	-1.571	-0.161	1.551
S	37	-0.839	0.563	-1.959
S	38	2.106	1.323	0.690
S	39	1.081	-1.996	-0.058



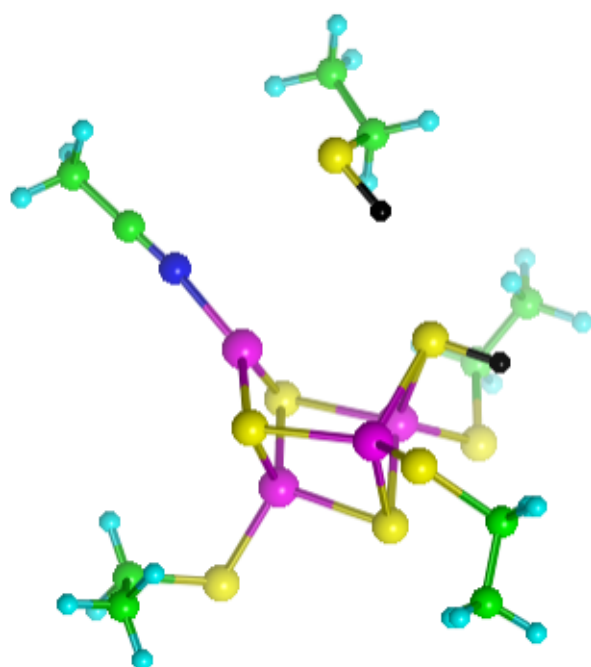
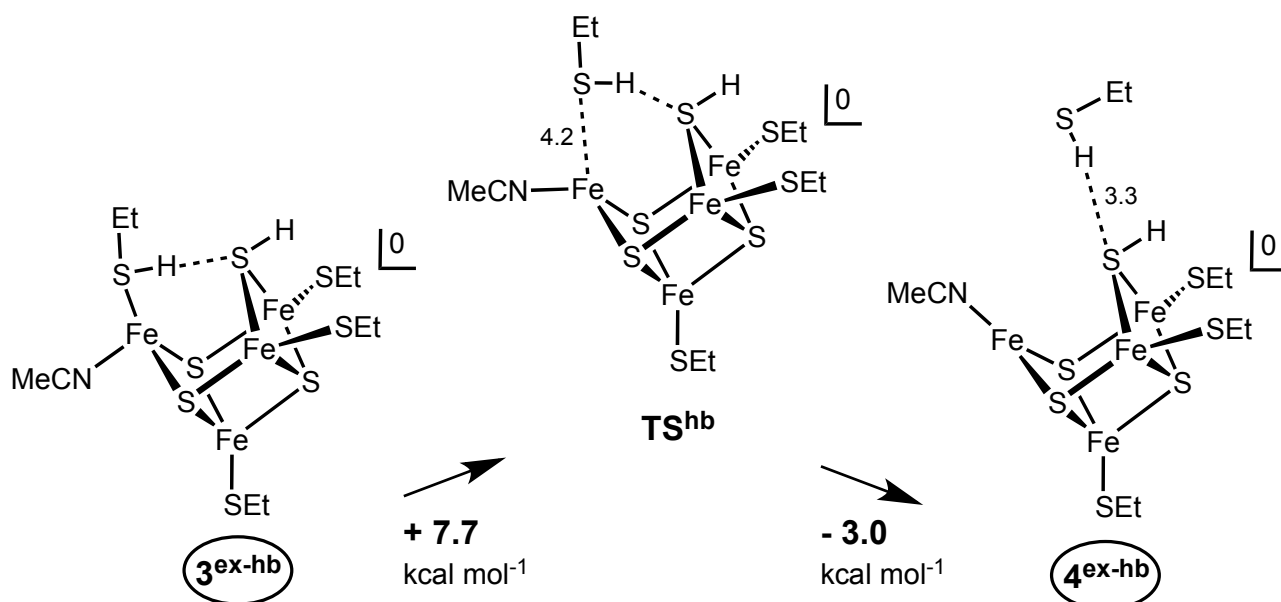
fe43x4xtecos.car_1
TS^{ex}

C	1	4.610	1.452	-2.033
C	2	3.794	0.444	-2.849
C	3	2.137	-4.525	3.890
C	4	2.360	-3.022	4.067
C	5	-4.052	-4.493	-0.259
C	6	-3.450	-3.876	-1.524
C	7	-4.892	3.479	-1.235
C	8	0.458	5.180	-1.088
C	9	0.659	5.034	0.422
C	10	-3.811	2.567	-0.911
Fe	11	1.573	-0.829	-0.724
Fe	12	0.447	-1.400	1.818
Fe	13	-0.776	-2.176	-0.521
Fe	14	-1.618	0.388	-0.341
H	15	5.566	1.018	-1.710
H	16	1.740	-4.754	2.892
H	17	1.440	-4.917	4.641
H	18	-3.764	-5.549	-0.157
H	19	-4.964	4.264	-0.471
H	20	-0.516	5.632	-1.321
H	21	1.240	5.836	-1.498
H	22	-4.698	3.939	-2.212
H	23	2.836	0.868	-3.170
H	24	4.343	0.131	-3.746
H	25	3.098	-5.050	4.006
H	26	2.751	-2.794	5.066
H	27	3.060	-2.625	3.326
H	28	-5.150	-4.438	-0.308
H	29	-3.787	-4.407	-2.424
H	30	-3.728	-2.823	-1.632
H	31	0.520	4.209	-1.594

					H	32	-5.837	2.924	-1.279
					H	33	1.623	4.568	0.652
					H	34	0.623	6.003	0.931
					H	35	-3.723	-3.956	0.640
					H	36	4.825	2.336	-2.653
					H	37	4.060	1.783	-1.142
					H	38	2.872	0.237	1.636
					H	39	-1.675	4.660	1.011
					N	40	-2.951	1.824	-0.661
					S	41	3.451	-1.168	-1.933
					S	42	0.769	-2.015	3.953
					S	43	-1.570	-3.997	-1.593
					S	44	-0.574	3.907	1.271
					S	45	-1.837	-1.231	1.246
					S	46	-0.368	-0.403	-1.976
					S	47	1.652	0.624	1.178
					S	48	1.232	-2.860	0.322
 xfe4s3shset3ncme.car_3 4ex					C	1	4.846	2.010	-2.181
					C	2	3.678	1.382	-2.946
					C	3	2.463	-3.605	3.442
					C	4	2.591	-2.114	3.759
					C	5	-4.688	-2.702	-0.609
					C	6	-3.798	-2.385	-1.812
					C	7	-4.036	5.318	-0.078
					C	8	-3.243	4.106	-0.115
					Fe	9	1.388	0.085	-0.939
					Fe	10	0.465	-0.537	1.662
					Fe	11	-0.998	-1.161	-0.569
					Fe	12	-1.615	1.412	-0.183
					H	13	5.721	1.345	-2.178
					H	14	2.080	-3.766	2.426
					H	15	1.789	-4.104	4.151
					H	16	-4.673	-3.774	-0.374
					H	17	-3.767	5.913	0.803
					H	18	-3.850	5.907	-0.985
					H	19	2.800	2.036	-2.945
					H	20	3.950	1.185	-3.989
					H	21	3.453	-4.081	3.515
					H	22	2.975	-1.957	4.774
					H	23	3.261	-1.606	3.058
					H	24	-5.727	-2.414	-0.831
					H	25	-4.127	-2.937	-2.700
					H	26	-3.814	-1.318	-2.056
					H	27	-5.101	5.056	-0.029
					H	28	-4.363	-2.148	0.281
					H	29	5.136	2.958	-2.661
					H	30	4.575	2.223	-1.139
					H	31	2.919	1.078	1.321
					N	32	-2.621	3.122	-0.152
					S	33	3.174	-0.301	-2.261
					S	34	0.942	-1.202	3.751
					S	35	-2.002	-2.909	-1.582
					S	36	-1.848	-0.255	1.337

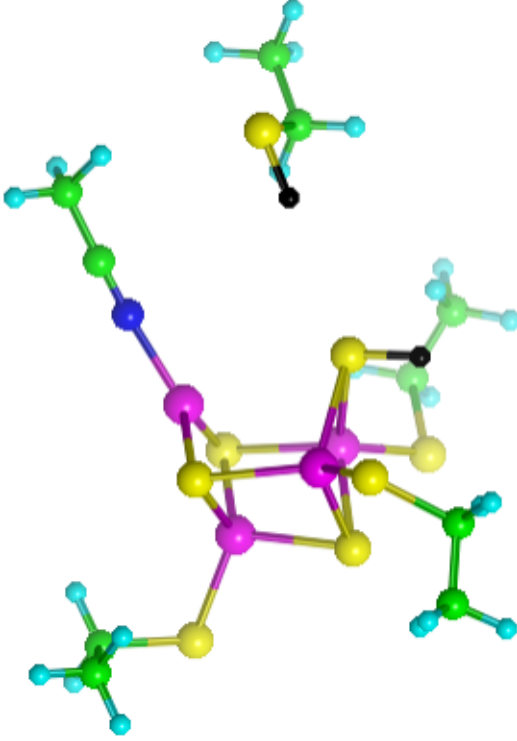
S	37	-0.647	0.632	-2.002
S	38	1.663	1.481	0.981
S	39	1.048	-1.973	0.057

(b)



fe43x4xbtb.car_1
TS^{hb}

C	1	4.348	1.370	-2.418
C	2	3.502	0.301	-3.117
C	3	2.028	-4.628	3.780
C	4	2.353	-3.139	3.926
C	5	-4.166	-4.317	0.079
C	6	-3.749	-3.703	-1.262
C	7	-4.630	3.894	-0.923
C	8	0.393	5.689	-0.770
C	9	1.002	4.457	-0.100
C	10	-3.631	2.861	-0.701
Fe	11	1.446	-0.924	-0.847
Fe	12	0.410	-1.442	1.763
Fe	13	-0.958	-2.100	-0.535
Fe	14	-1.636	0.488	-0.287
H	15	5.338	0.980	-2.149
H	16	1.573	-4.839	2.805
H	17	1.333	-4.960	4.563
H	18	-3.845	-5.364	0.149
H	19	-4.556	4.658	-0.138
H	20	0.371	6.541	-0.080
H	21	0.987	5.975	-1.648
H	22	-4.462	4.362	-1.901
H	23	2.514	0.687	-3.389
H	24	3.990	-0.039	-4.039
H	25	2.952	-5.221	3.865
H	26	2.810	-2.928	4.901
H	27	3.046	-2.802	3.148
H	28	-5.262	-4.283	0.183
H	29	-4.208	-4.243	-2.101
H	30	-4.052	-2.653	-1.335

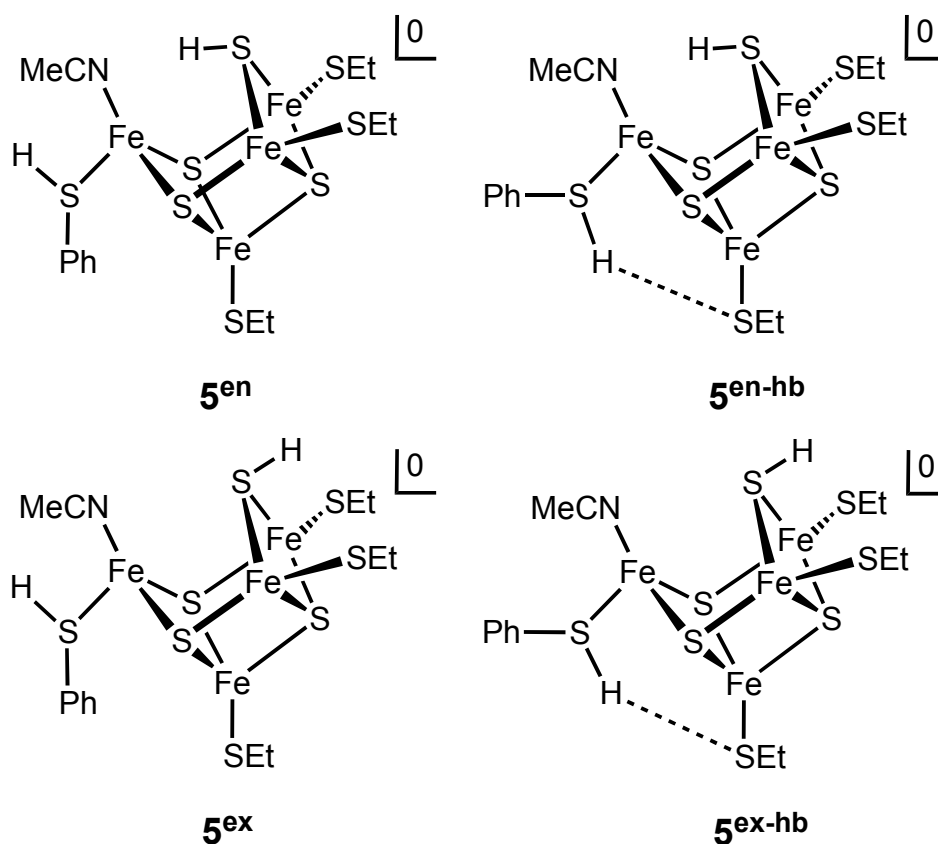
	H	31	-0.633	5.486	-1.104
	H	32	-5.639	3.462	-0.909
	H	33	1.024	3.603	-0.785
	H	34	2.019	4.657	0.252
	H	35	-3.724	-3.765	0.918
	H	36	4.491	2.232	-3.089
	H	37	3.862	1.725	-1.499
	H	38	2.953	0.010	1.438
	H	39	0.723	2.914	1.752
	N	40	-2.821	2.041	-0.530
	S	41	3.275	-1.271	-2.109
	S	42	0.827	-2.043	3.881
	S	43	-1.907	-3.826	-1.604
	S	44	-0.036	3.985	1.390
	S	45	-1.888	-1.109	1.282
	S	46	-0.526	-0.347	-1.985
	S	47	1.743	0.497	1.063
	S	48	1.020	-2.929	0.214
 fe43x4xbp.car_2 4ex-hb + EtSH	C	1	3.214	1.536	-3.490
	C	2	2.449	0.266	-3.875
	C	3	3.222	-4.009	3.565
	C	4	3.322	-2.484	3.468
	C	5	-3.513	-5.277	1.229
	C	6	-3.416	-4.776	-0.217
	C	7	-4.076	3.774	0.182
	C	8	-0.171	6.314	-1.210
	C	9	0.298	5.010	-0.558
	C	10	-3.437	2.477	0.037
	Fe	11	1.096	-1.042	-1.156
	Fe	12	0.695	-1.426	1.630
	Fe	13	-0.887	-2.680	-0.251
	Fe	14	-1.875	-0.228	-0.096
	H	15	4.294	1.349	-3.433
	H	16	2.612	-4.417	2.750
	H	17	2.768	-4.317	4.516
	H	18	-3.063	-6.274	1.332
	H	19	-3.410	4.430	0.762
	H	20	0.195	7.191	-0.661
	H	21	0.207	6.380	-2.240
	H	22	-4.249	4.220	-0.807
	H	23	1.371	0.450	-3.937
	H	24	2.778	-0.104	-4.855
	H	25	4.226	-4.458	3.499
	H	26	3.927	-2.080	4.290
	H	27	3.778	-2.168	2.524
	H	28	-4.571	-5.341	1.530
	H	29	-3.929	-5.464	-0.902
	H	30	-3.875	-3.788	-0.331
	H	31	-1.268	6.371	-1.248
	H	32	-5.038	3.663	0.699
	H	33	-0.056	4.138	-1.117
	H	34	1.390	4.973	-0.501
	H	35	-2.999	-4.596	1.920

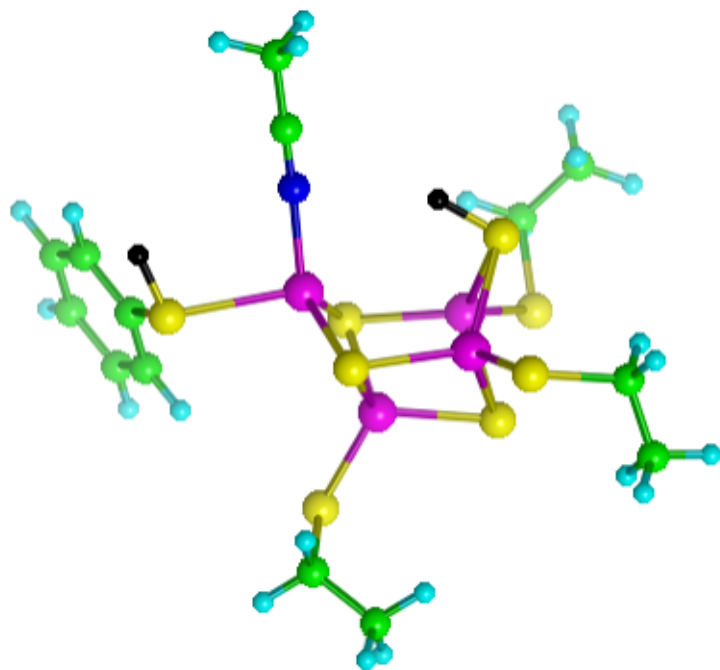
H	36	3.046	2.323	-4.243
H	37	2.883	1.911	-2.512
H	38	2.624	0.654	0.717
H	39	0.116	3.655	1.453
N	40	-2.905	1.444	-0.056
S	41	2.738	-1.166	-2.691
S	42	1.660	-1.621	3.636
S	43	-1.656	-4.689	-0.873
S	44	-0.376	4.895	1.191
S	45	-1.653	-1.659	1.624
S	46	-1.113	-1.120	-1.945
S	47	1.279	0.693	0.516
S	48	1.348	-2.937	0.132

(c)

Fig. 8. Reaction energy profiles for dissociation of EtSH from (a) **3^{en}**, (b) **3^{ex}** and (c) **3^{ex-hb}**. Energies with COSMO solvation contributions included are in parentheses. Selected interatomic distances are marked in Å.

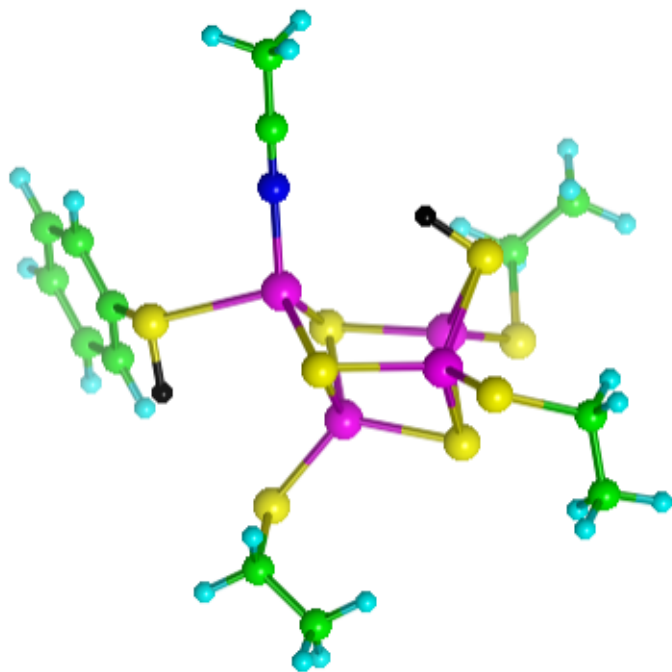
Association of PhSH.





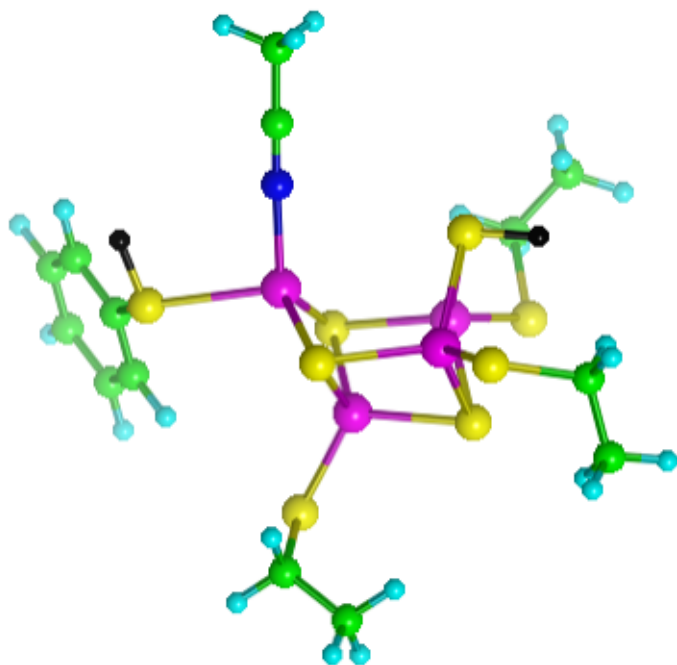
fe45nacos.car_2
5en

C	1	4.004	3.050	-2.965
C	2	2.932	2.046	-3.400
C	3	5.408	-2.403	3.112
C	4	4.942	-0.987	3.458
C	5	0.181	-5.533	1.048
C	6	-1.014	-4.587	0.899
C	7	-1.707	5.133	1.915
C	8	-4.439	0.298	-0.930
C	9	-4.141	-0.739	-1.828
C	10	-4.692	-0.711	-3.117
C	11	-5.540	0.337	-3.507
C	12	-5.835	1.365	-2.599
C	13	-5.285	1.354	-1.308
C	14	-1.525	3.741	1.544
Fe	15	1.892	0.273	-0.794
Fe	16	1.998	-0.430	1.943
Fe	17	0.199	-1.572	0.217
Fe	18	-1.198	0.696	0.732
H	19	5.010	2.700	-3.233
H	20	4.903	-2.778	2.212
H	21	5.211	-3.099	3.937
H	22	0.332	-6.127	0.137
H	23	-1.292	5.302	2.916
H	24	-1.185	5.777	1.195
H	25	1.927	2.395	-3.141
H	26	2.962	1.884	-4.485
H	27	6.492	-2.396	2.920
H	28	5.441	-0.618	4.363
H	29	5.154	-0.284	2.645
H	30	0.000	-6.228	1.883
H	31	-1.935	-5.149	0.701
H	32	-1.169	-3.990	1.804
H	33	-2.776	5.381	1.917
H	34	1.106	-4.981	1.257
H	35	3.832	4.015	-3.466
H	36	3.974	3.219	-1.881
H	37	1.386	2.401	1.244
H	38	-3.486	-1.558	-1.535
H	39	-4.455	-1.514	-3.815
H	40	-5.967	0.352	-4.508
H	41	-6.490	2.185	-2.890
H	42	-5.517	2.157	-0.611
H	43	-4.272	1.370	1.200
N	44	-1.379	2.623	1.247
S	45	3.177	0.330	-2.657
S	46	3.103	-0.879	3.852
S	47	-0.868	-3.403	-0.557
S	48	-0.304	-0.766	2.271
S	49	-0.386	0.128	-1.246
S	50	2.544	1.743	0.978
S	51	2.481	-1.736	0.185
S	52	-3.734	0.210	0.744



fe45nbcos.car_2
5en-hb

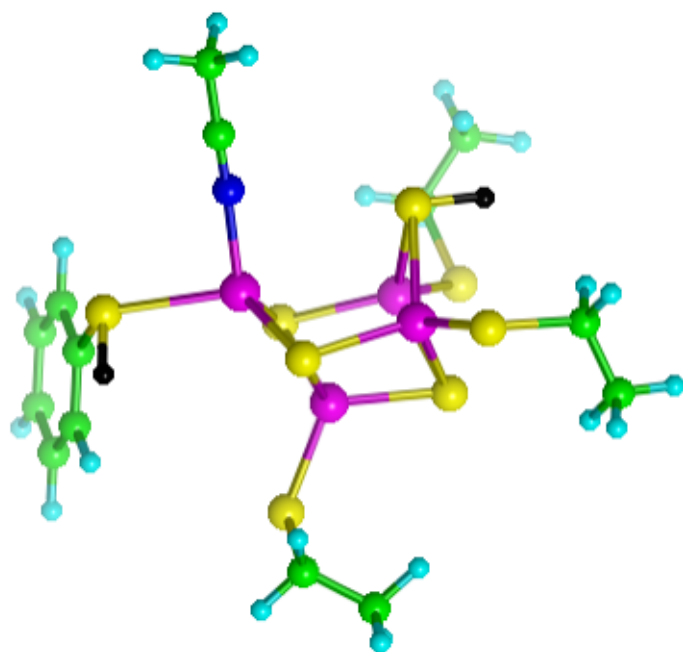
C	1	4.384	2.604	-2.900
C	2	3.254	1.663	-3.327
C	3	4.974	-2.914	3.337
C	4	4.722	-1.447	3.692
C	5	-0.480	-5.380	1.161
C	6	-1.567	-4.311	1.017
C	7	-1.373	5.351	1.894
C	8	-4.288	0.614	-1.190
C	9	-4.194	-0.352	-2.206
C	10	-4.765	-0.087	-3.459
C	11	-5.419	1.131	-3.700
C	12	-5.503	2.090	-2.679
C	13	-4.941	1.836	-1.419
C	14	-1.303	3.959	1.484
Fe	15	2.013	0.094	-0.696
Fe	16	1.934	-0.528	2.051
Fe	17	0.080	-1.501	0.294
Fe	18	-1.124	0.907	0.665
H	19	5.368	2.168	-3.120
H	20	4.459	-3.193	2.409
H	21	4.630	-3.582	4.139
H	22	-0.388	-5.980	0.246
H	23	-0.974	5.450	2.912
H	24	-0.774	5.967	1.210
H	25	2.271	2.094	-3.111
H	26	3.300	1.455	-4.404
H	27	6.053	-3.079	3.194
H	28	5.231	-1.178	4.626
H	29	5.082	-0.775	2.906
H	30	-0.736	-6.057	1.990
H	31	-2.544	-4.772	0.821
H	32	-1.657	-3.705	1.926
H	33	-2.415	5.694	1.876
H	34	0.496	-4.928	1.377
H	35	4.301	3.556	-3.447
H	36	4.335	2.821	-1.825
H	37	1.616	2.311	1.264
H	38	-3.683	-1.297	-2.027
H	39	-4.691	-0.834	-4.249
H	40	-5.862	1.331	-4.675
H	41	-6.012	3.037	-2.857
H	42	-5.020	2.578	-0.625
H	43	-3.341	-1.015	0.273
N	44	-1.244	2.842	1.157
S	45	3.352	-0.034	-2.511
S	46	2.909	-1.047	4.010
S	47	-1.304	-3.140	-0.432
S	48	-0.389	-0.559	2.301
S	49	-0.237	0.219	-1.243
S	50	2.725	1.554	1.060
S	51	2.322	-1.944	0.351
S	52	-3.585	0.311	0.458



fe45xacos.car_2

5ex

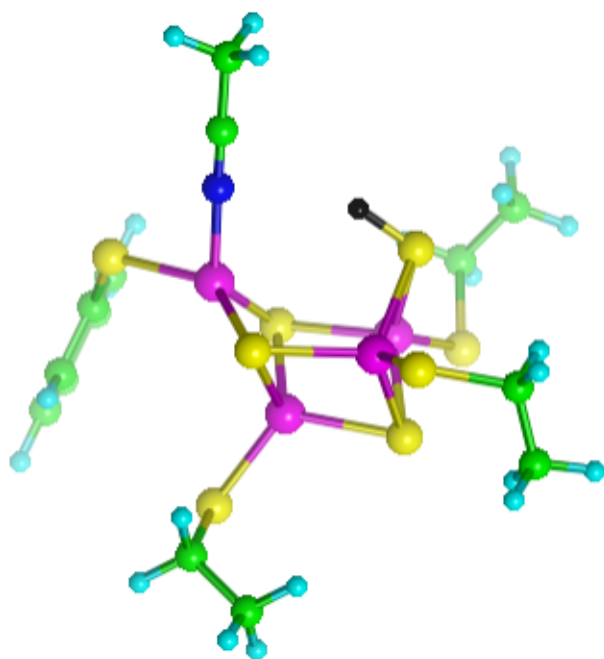
C	1	4.108	2.951	-2.828
C	2	3.104	1.862	-3.215
C	3	4.888	-2.362	3.743
C	4	4.505	-0.894	3.945
C	5	-0.041	-5.438	1.400
C	6	-1.218	-4.513	1.076
C	7	-1.376	5.326	1.428
C	8	-4.383	0.345	-1.340
C	9	-4.065	-0.819	-2.058
C	10	-4.516	-0.957	-3.379
C	11	-5.285	0.054	-3.976
C	12	-5.596	1.212	-3.248
C	13	-5.145	1.366	-1.929
C	14	-1.377	3.898	1.161
Fe	15	1.894	0.234	-0.607
Fe	16	1.722	-0.318	2.142
Fe	17	0.076	-1.548	0.327
Fe	18	-1.289	0.790	0.558
H	19	5.141	2.625	-3.010
H	20	4.430	-2.770	2.833
H	21	4.575	-2.979	4.597
H	22	0.209	-6.080	0.544
H	23	-1.052	5.504	2.461
H	24	-0.679	5.826	0.742
H	25	2.074	2.185	-3.033
H	26	3.193	1.604	-4.278
H	27	5.982	-2.445	3.642
H	28	4.951	-0.493	4.864
H	29	4.837	-0.273	3.108
H	30	-0.308	-6.087	2.248
H	31	-2.114	-5.094	0.823
H	32	-1.463	-3.864	1.924
H	33	-2.383	5.736	1.286
H	34	0.854	-4.867	1.677
H	35	3.923	3.852	-3.434
H	36	4.014	3.226	-1.769
H	37	3.560	1.761	1.171
H	38	-3.470	-1.608	-1.601
H	39	-4.263	-1.857	-3.938
H	40	-5.639	-0.062	-4.999
H	41	-6.192	2.003	-3.703
H	42	-5.389	2.269	-1.371
H	43	-4.321	1.701	0.630
N	44	-1.369	2.753	0.945
S	45	3.388	0.235	-2.302
S	46	2.652	-0.626	4.165
S	47	-0.938	-3.416	-0.428
S	48	-0.609	-0.598	2.267
S	49	-0.326	0.066	-1.294
S	50	2.203	1.852	1.121
S	51	2.349	-1.733	0.526
S	52	-3.821	0.464	0.385



ffe4s3shset3mecnxsphh.car_4
5ex-hb

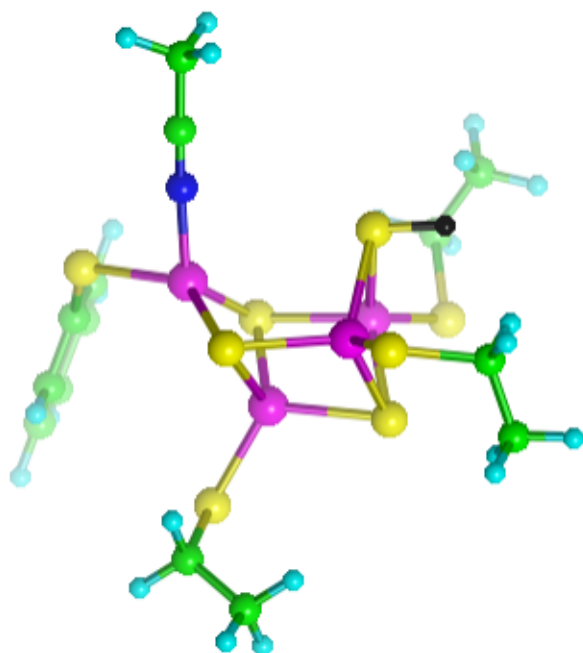
C	1	2.811	3.653	-3.418
C	2	1.999	2.387	-3.703
C	3	5.678	-1.199	2.763
C	4	5.043	0.161	3.059
C	5	1.131	-5.214	1.226
C	6	-0.236	-4.525	1.255
C	7	-2.032	5.007	2.409
C	8	-4.467	-0.406	-0.828
C	9	-4.529	-1.796	-1.010
C	10	-4.924	-2.308	-2.254
C	11	-5.242	-1.441	-3.311
C	12	-5.172	-0.053	-3.118
C	13	-4.788	0.472	-1.875
C	14	-1.834	3.683	1.847
Fe	15	1.551	0.661	-0.907
Fe	16	1.921	0.152	1.826
Fe	17	0.235	-1.387	0.310
Fe	18	-1.434	0.711	0.805
H	19	3.864	3.522	-3.702
H	20	5.164	-1.707	1.938
H	21	5.648	-1.854	3.644
H	22	1.254	-5.815	0.315
H	23	-1.315	5.168	3.223
H	24	-1.874	5.764	1.631
H	25	0.951	2.506	-3.405
H	26	2.018	2.144	-4.772
H	27	6.732	-1.060	2.475
H	28	5.560	0.668	3.883
H	29	5.077	0.818	2.183
H	30	1.223	-5.885	2.094
H	31	-1.046	-5.264	1.229
H	32	-0.361	-3.919	2.159
H	33	-3.053	5.095	2.800
H	34	1.948	-4.482	1.270
H	35	2.406	4.495	-3.999
H	36	2.775	3.920	-2.354
H	37	3.188	2.496	0.609
H	38	-4.269	-2.475	-0.201
H	39	-4.978	-3.387	-2.396
H	40	-5.546	-1.844	-4.276
H	41	-5.426	0.627	-3.931
H	42	-4.746	1.551	-1.729
H	43	-4.009	-0.827	1.475
N	44	-1.674	2.618	1.405
S	45	2.689	0.853	-2.849
S	46	3.251	0.044	3.634
S	47	-0.565	-3.424	-0.236
S	48	-0.263	-0.539	2.351
S	49	-0.695	0.130	-1.191
S	50	1.845	2.349	0.761
S	51	2.508	-1.174	0.122
S	52	-3.991	0.327	0.764

Scheme 3. The isomers of intermediate **5** for X = SET. The broken line is a hydrogen bond.



ffe4s3shset3mecnsph.car_3
6en

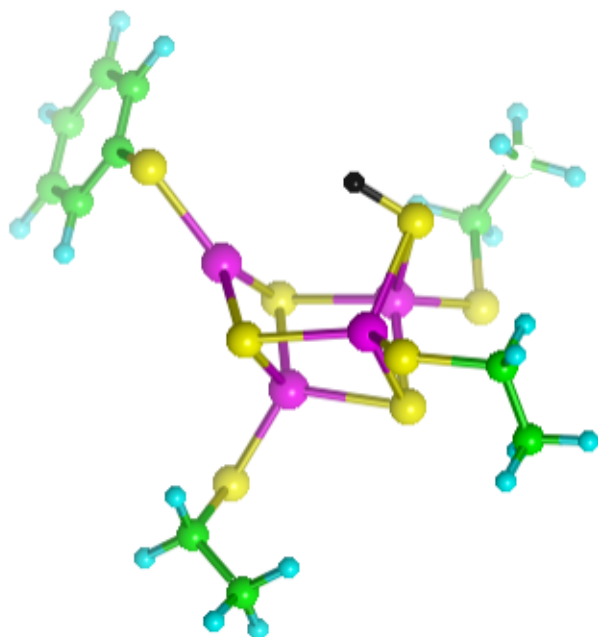
C	1	4.096	2.568	-2.788
C	2	3.089	1.539	-3.310
C	3	4.504	-2.282	3.807
C	4	4.154	-0.826	4.122
C	5	-0.935	-5.054	1.742
C	6	-1.979	-4.016	1.321
C	7	-1.299	5.379	2.211
C	8	-3.801	0.687	-1.987
C	9	-4.418	-0.580	-1.959
C	10	-4.700	-1.256	-3.156
C	11	-4.371	-0.678	-4.394
C	12	-3.765	0.588	-4.428
C	13	-3.487	1.266	-3.235
C	14	-1.386	4.011	1.722
Fe	15	1.808	0.126	-0.618
Fe	16	1.503	-0.214	2.154
Fe	17	-0.211	-1.331	0.400
Fe	18	-1.521	1.139	0.548
H	19	5.124	2.185	-2.850
H	20	4.108	-2.581	2.827
H	21	4.098	-2.963	4.567
H	22	-0.748	-5.779	0.939
H	23	-0.712	5.415	3.138
H	24	-0.815	6.011	1.455
H	25	2.065	1.927	-3.258
H	26	3.299	1.280	-4.355
H	27	5.598	-2.407	3.787
H	28	4.564	-0.531	5.097
H	29	4.567	-0.147	3.367
H	30	-1.292	-5.607	2.626
H	31	-2.935	-4.501	1.083
H	32	-2.163	-3.290	2.121
H	33	-2.306	5.768	2.407
H	34	0.017	-4.575	2.001
H	35	4.034	3.489	-3.390
H	36	3.889	2.830	-1.742
H	37	1.162	2.536	1.011
H	38	-4.667	-1.037	-1.002
H	39	-5.175	-2.238	-3.122
H	40	-4.588	-1.208	-5.320
H	41	-3.507	1.048	-5.381
H	42	-3.022	2.250	-3.259
N	43	-1.454	2.922	1.311
S	44	3.126	-0.104	-2.385
S	45	2.306	-0.490	4.246
S	46	-1.528	-3.062	-0.238
S	47	-0.813	-0.156	2.290
S	48	-0.346	0.333	-1.164
S	49	2.271	1.754	0.943
S	50	2.036	-1.765	0.574
S	51	-3.478	1.626	-0.475



xfe4s3shset3mecnsph.car_2

6ex

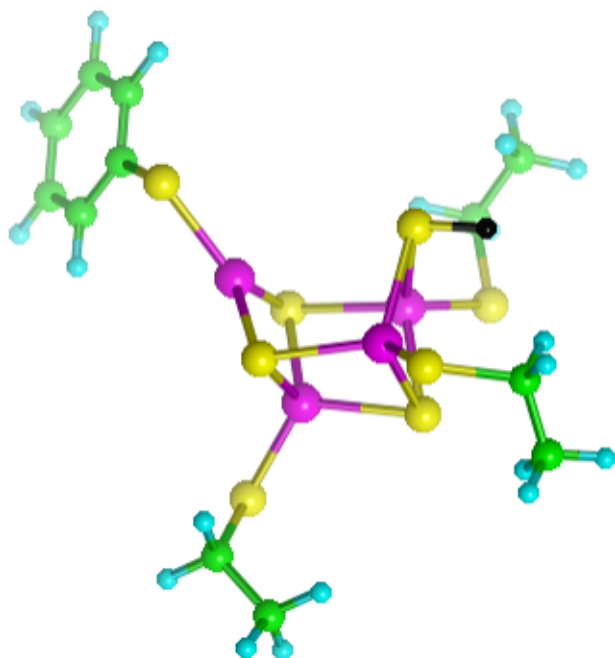
C	1	3.812	3.062	-2.557
C	2	2.976	1.915	-3.132
C	3	4.467	-1.911	4.051
C	4	3.978	-0.482	4.309
C	5	-0.582	-5.167	1.638
C	6	-1.677	-4.213	1.153
C	7	-1.795	5.238	2.136
C	8	-3.798	0.337	-2.152
C	9	-4.289	-0.983	-2.177
C	10	-4.456	-1.653	-3.397
C	11	-4.133	-1.020	-4.608
C	12	-3.639	0.296	-4.591
C	13	-3.478	0.970	-3.373
C	14	-1.807	3.865	1.651
Fe	15	1.756	0.305	-0.505
Fe	16	1.346	-0.088	2.213
Fe	17	-0.150	-1.349	0.379
Fe	18	-1.686	0.993	0.476
H	19	4.881	2.811	-2.546
H	20	4.133	-2.273	3.069
H	21	4.097	-2.603	4.820
H	22	-0.271	-5.856	0.841
H	23	-1.236	5.300	3.079
H	24	-1.315	5.886	1.391
H	25	1.908	2.158	-3.134
H	26	3.273	1.689	-4.164
H	27	5.568	-1.937	4.068
H	28	4.309	-0.138	5.297
H	29	4.378	0.212	3.561
H	30	-0.959	-5.768	2.480
H	31	-2.569	-4.775	0.847
H	32	-1.977	-3.516	1.944
H	33	-2.823	5.586	2.302
H	34	0.304	-4.618	1.981
H	35	3.682	3.968	-3.171
H	36	3.504	3.300	-1.531
H	37	3.172	2.053	1.260
H	38	-4.532	-1.486	-1.244
H	39	-4.834	-2.675	-3.405
H	40	-4.269	-1.540	-5.555
H	41	-3.378	0.800	-5.524
H	42	-3.100	1.993	-3.360
N	43	-1.798	2.773	1.242
S	44	3.178	0.286	-2.203
S	45	2.103	-0.294	4.333
S	46	-1.213	-3.205	-0.368
S	47	-0.970	-0.251	2.235
S	48	-0.374	0.307	-1.179
S	49	1.824	1.990	1.062
S	50	2.110	-1.571	0.673
S	51	-3.651	1.275	-0.614



fe4s3shset3sph.car_4

7en

C	1	3.960	2.693	-2.416
C	2	3.109	1.553	-2.983
C	3	4.146	-2.565	4.050
C	4	3.632	-1.188	4.478
C	5	-1.262	-5.428	1.393
C	6	-2.188	-4.355	0.814
C	7	-3.596	2.863	-1.101
C	8	-4.364	1.901	-1.789
C	9	-4.829	2.160	-3.086
C	10	-4.544	3.385	-3.712
C	11	-3.793	4.352	-3.024
C	12	-3.319	4.095	-1.729
Fe	13	1.607	0.062	-0.416
Fe	14	1.118	-0.550	2.303
Fe	15	-0.384	-1.613	0.290
Fe	16	-1.643	0.764	0.477
H	17	5.012	2.395	-2.319
H	18	3.911	-2.767	2.997
H	19	3.705	-3.363	4.662
H	20	-0.949	-6.145	0.622
H	21	2.053	1.835	-3.050
H	22	3.448	1.281	-3.991
H	23	5.239	-2.604	4.172
H	24	3.889	-0.983	5.525
H	25	4.064	-0.390	3.864
H	26	-1.797	-5.985	2.179
H	27	-3.095	-4.809	0.396
H	28	-2.491	-3.635	1.581
H	29	-0.362	-4.985	1.840
H	30	3.913	3.563	-3.091
H	31	3.599	3.007	-1.427
H	32	0.843	2.270	1.429
H	33	-4.592	0.952	-1.309
H	34	-5.418	1.404	-3.605
H	35	-4.904	3.582	-4.721
H	36	-3.570	5.309	-3.495
H	37	-2.729	4.847	-1.205
S	38	3.233	-0.049	-1.996
S	39	1.757	-1.012	4.418
S	40	-1.450	-3.386	-0.621
S	41	-1.226	-0.697	2.186
S	42	-0.554	0.064	-1.317
S	43	1.999	1.554	1.425
S	44	1.842	-1.952	0.709
S	45	-3.020	2.568	0.595



xfe4s3shset3sph.car_2

7ex

C	1	3.727	2.960	-2.504
C	2	2.900	1.792	-3.048
C	3	4.241	-2.656	3.747
C	4	3.817	-1.231	4.114
C	5	-0.961	-5.665	1.070
C	6	-1.955	-4.565	0.681
C	7	-3.758	2.859	-0.723
C	8	-4.500	1.901	-1.444
C	9	-5.110	2.243	-2.659
C	10	-4.999	3.548	-3.169
C	11	-4.272	4.509	-2.447
C	12	-3.653	4.170	-1.234
Fe	13	1.584	0.126	-0.509
Fe	14	1.158	-0.540	2.186
Fe	15	-0.351	-1.664	0.202
Fe	16	-1.634	0.678	0.530
H	17	4.802	2.733	-2.529
H	18	3.834	-2.952	2.772
H	19	3.903	-3.380	4.500
H	20	-0.731	-6.318	0.217
H	21	1.828	2.014	-3.021
H	22	3.170	1.575	-4.089
H	23	5.339	-2.708	3.690
H	24	4.201	-0.950	5.103
H	25	4.191	-0.501	3.389
H	26	-1.396	-6.287	1.868
H	27	-2.894	-4.999	0.315
H	28	-2.190	-3.921	1.535
H	29	-0.020	-5.239	1.442
H	30	3.554	3.857	-3.120
H	31	3.449	3.196	-1.468
H	32	3.097	1.604	1.516
H	33	-4.599	0.890	-1.052
H	34	-5.673	1.488	-3.207
H	35	-5.470	3.813	-4.115
H	36	-4.181	5.525	-2.831
H	37	-3.087	4.921	-0.684
S	38	3.184	0.173	-2.122
S	39	1.953	-0.997	4.250
S	40	-1.368	-3.462	-0.730
S	41	-1.173	-0.848	2.156
S	42	-0.617	0.080	-1.338
S	43	1.752	1.667	1.319
S	44	1.901	-1.900	0.570
S	45	-2.993	2.462	0.871