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Electronic Supplementary Information for

Reactions of the μ_3-sulfido triiron cluster $[SFe_3(CO)_9]^{2-}$ with functionalized organic halides and mercury salts: selective reactivity, electrochemistry, and theoretical calculations

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Table S1 Cyclic Voltammetry (CV) of $[Et_4N]_2[SFe_3(CO)_9]$, $[Et_4N]$[**1**], $[Et_4N]$[**2**], $[Et_4N]$[**3**], $[Et_4N]_2$[**4**], and $[Et_4N]$[**5**]

	Oxidation process				Reduction process			
Complex	Ep^{ox}/V^a	Ep^{red}/V^b	$E_{1/2}$/V	ΔE/mV	Ep^{ox}/V^a	Ep^{red}/V^b	$E_{1/2}$/V	ΔE/mV
$[Et_4N]_2[SFe_3(CO)_9]$	0.048	- [c]			−0.156	−0.268	−0.106	112
	0.385	- [c]				−0.606		
$[Et_4N]$[**1**]	0.325				−0.014	−0.106	−0.060	92
	0.490	- [c]			~ −0.203	−0.359	−0.281	156
						−0.623		
$[Et_4N]$[**2**]	0.290	- [c]			−0.152	−0.239	−0.196	87
$[Et_4N]$[**3**]	0.339	- [c]			~ −0.014	−0.186	−0.100	172
						−0.593		
$[Et_4N]_2$[**4**]	~ 0.371	- [c]						
$[Et_4N]$[**5**]	- [c]	- [c]						

[a] Ep^{ox} = oxidative peak potential. [b] Ep^{red} = reductive peak potential. [c] Difficult to determine.

Table S2 Selected bond distances (Å) and bond angles (deg) for $[Et_4N][SFe_3(CO)_8(\mu\text{-}CO)(CH_2C(O)OCH_3)]$ ($[Et_4N][\mathbf{1}]$), $[Et_4N][(CH_2)_3ClSFe_3(CO)_9]$ ($[Et_4N][\mathbf{2}]$), $[Et_4N][(CH_2)_4ISFe_3(CO)_9]$ ($[Et_4N][\mathbf{3}]$), $[Et_4N]_2[\{SFe_3(CO)_9\}_2(\mu_4\text{-}Hg)]$ ($[Et_4N]_2[\mathbf{4}]$), and $[Et_4N][SFe_3(CO)_9(\mu\text{-}HgI)]$ ($[Et_4N][\mathbf{5}]$)

Complex **1**

S─Fe(1)	2.1771(8)	S─Fe(2)	2.203(1)
S─Fe(3)	2.195(1)	Fe(1)─Fe(2)	2.5705(6)
Fe(1)─Fe(3)	2.6057(5)	Fe(2)─Fe(3)	2.6277(5)
Fe(3)─C(10)	2.137(2)	C(11)─O(10)	1.206(3)
C(11)─O(11)	1.342(3)		
Fe(1)─S─Fe(2)	71.87(3)	Fe(1)─S─Fe(3)	73.17(3)
Fe(2)─S─Fe(3)	73.39(4)	S─Fe(1)─Fe(2)	54.53(3)
S─Fe(1)─Fe(3)	53.72(2)	S─Fe(2)─Fe(1)	53.60(2)
S─Fe(2)─Fe(3)	53.16(3)	S─Fe(3)─Fe(1)	53.11(2)
S─Fe(3)─Fe(2)	53.45(3)	Fe(2)─Fe(1)─Fe(3)	61.01(2)
Fe(1)─Fe(2)─Fe(3)	60.16(2)	Fe(1)─Fe(3)─Fe(2)	58.83(2)
Fe(3)─C(7)─O(7)	154.8(2)	Fe(2)─C(7)─O(7)	126.3(2)
Fe(3)─C(8)─O(8)	172.9(2)	Fe(3)─C(9)─O9)	179.8(3)
C(10)─Fe(3)─S	87.07(8)	C(10)─Fe(3)─Fe(1)	99.87(7)
C(10)─Fe(3)─Fe(2)	140.52(8)	C(10)─Fe(3)─C(8)	87.4(1)
C(10)─Fe(3)─C(7)	160.8(1)	C(10)─Fe(3)─C(9)	82.3(1)
Fe(3)─C(10)─C(11)	114.6(2)		

Complex **2**

S(1)─Fe(1)	2.122(1)	S(1)─Fe(2)	2.122(1)
S(1)─Fe(3)	2.133(1)	Fe(1)─Fe(2)	2.6333(8)
Fe(1)─Fe(3)	2.6495(7)	Fe(2)─Fe(3)	2.6380(8)
S(1)─C(10)	1.827(3)	C(10)─C(11)	1.513(5)
C(11)─C(12)	1.514(5)	C(12)─Cl(1)	1.780(4)
Fe(1)─S(1)─Fe(2)	76.69(4)	Fe(1)─S(1)─Fe(3)	77.03(4)
Fe(2)─S(1)─Fe(3)	76.63(4)	S(1)─Fe(1)─Fe(2)	51.66(3)
S(1)─Fe(1)─Fe(3)	51.67(3)	S(1)─Fe(2)─Fe(1)	51.65(3)
S(1)─Fe(2)─Fe(3)	51.86(3)	S(1)─Fe(3)─Fe(1)	51.30(3)
S(1)─Fe(3)─Fe(2)	51.51(3)	Fe(2)─Fe(1)─Fe(3)	59.92(2)
Fe(1)─Fe(2)─Fe(3)	60.35(2)	Fe(1)─Fe(3)─Fe(2)	59.74(2)
S(1)─C(10)─C(11)	111.3(1)	C(10)─C(11)─C(12)	115.2(3)

C(11)─C(12)─Cl(1)	111.7(3)	C(10)─S(1)─Fe(1)	132.2(1)
C(10)─S(1)─Fe(2)	131.6(1)	C(10)─S(1)─Fe(3)	138.5(1)

Complex **3**

S(1)─Fe(1)	2.132(1)	S(1)─Fe(2)	2.126(1)
S(1)─Fe(3)	2.127(1)	Fe(1)─Fe(2)	2.6372(8)
Fe(2)─Fe(3)	2.6420(8)	Fe(1)─Fe(3)	2.6403(8)
S(1)─C(10)	1.813(4)	C(10)─C(11)	1.467(7)
C(11)─C(12)	1.565(8)	C(12)─C(13)	1.472(8)
C(13)─I(1)	2.141(8)		

Fe(1)─S(1)─Fe(2)	76.54(4)	Fe(1)─S(1)─Fe(3)	76.63(4)
Fe(2)─S(1)─Fe(3)	76.82(4)	S(1)─Fe(2)─Fe(1)	51.83(3)
S(1)─Fe(2)─Fe(3)	51.61(3)	S(1)─Fe(3)─Fe(1)	51.77(3)
S(1)─Fe(3)─Fe(2)	51.57(3)	S(1)─Fe(1)─Fe(2)	51.62(3)
S(1)─Fe(1)─Fe(3)	51.60(3)	Fe(1)─Fe(2)─Fe(3)	60.02(2)
Fe(1)─Fe(3)─Fe(2)	59.90(2)	Fe(2)─Fe(1)─Fe(3)	60.08(2)
S(1)─C(10)─C(11)	113.3(3)	C(10)─C(11)─C(12)	105.0(4)
C(11)─C(12)─C(13)	110.7(5)	C(12)─C(13)─I(1)	111.7(5)
C(10)─S(1)─Fe(2)	136.5(2)	C(10)─S(1)─Fe(3)	130.9(2)
C(10)─S(1)─Fe(1)	135.3(2)		

Complex **4**

S(1)─Fe(1)	2.200(1)	S(1)─Fe(2)	2.185(1)
S(1)─Fe(3)	2.194(1)	Fe(1)─Fe(2)	2.6020(9)
Fe(1)─Fe(3)	2.7842(9)	Fe(2)─Fe(3)	2.597(1)
Fe(1)─Hg(1)	2.7318(7)	Fe(3)─Hg(1)	2.7430(7)

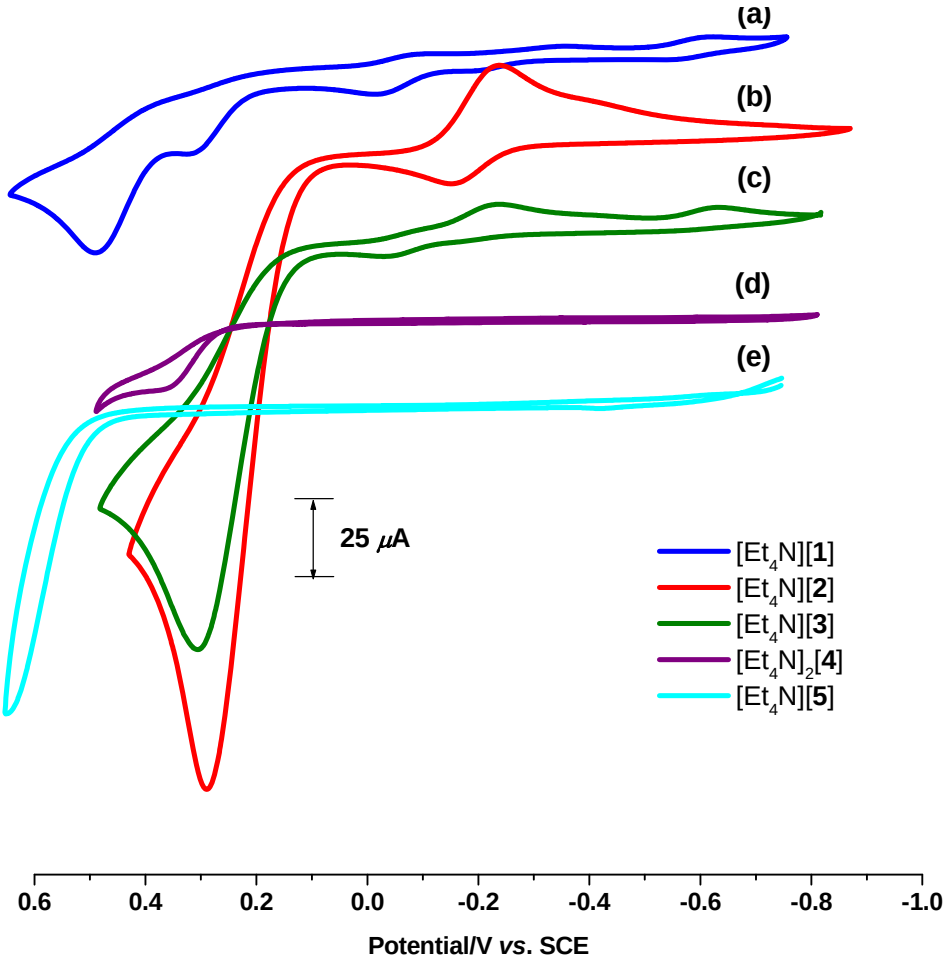
Fe(1)─S(1)─Fe(2)	72.80(4)	Fe(1)─S(1)─Fe(3)	78.65(5)
Fe(2)─S(1)─Fe(3)	72.75(5)	S(1)─Fe(1)─Fe(2)	53.34(4)
S(1)─Fe(1)─Fe(3)	50.58(4)	S(1)─Fe(2)─Fe(1)	53.86(4)
S(1)─Fe(2)─Fe(3)	53.77(4)	S(1)─Fe(3)─Fe(1)	50.77(4)
S(1)─Fe(3)─Fe(2)	53.48(4)	Fe(2)─Fe(1)─Fe(3)	57.53(2)
Fe(1)─Fe(2)─Fe(3)	64.76(2)	Fe(1)─Fe(3)─Fe(2)	57.71(2)
Fe(1)─Hg(1)─Fe(1a)	126.35(3)	Fe(1)─Hg(1)─Fe(3)	61.13(2)
Fe(1)─Hg(1)─Fe(3a)	156.30(2)	Fe(1a)─Hg(1)─Fe(3)	156.30(2)
Fe(3)─Hg(1)─Fe(3a)	122.67(3)	Fe(1)─C(1)─O(1)	173.5(5)
Fe(1)─C(3)─O(3)	175.3(5)	Fe(3)─C(7)─O(7)	175.4(4)

Fe(3)─C(9)─O(9)	174.5(4)		

Complex **5**

S(1)─Fe(1)	2.189(2)	S(1)─Fe(2)	2.191(2)
S(1)─Fe(3)	2.166(1)	Fe(1)─Fe(2)	2.805(1)
Fe(1)─Fe(3)	2.596(1)	Fe(2)─Fe(3)	2.602(1)
Fe(1)─Hg(1)	2.6384(8)	Fe(2)─Hg(1)	2.6385(7)
Hg(1)─I(1)	2.6985(4)		
Fe(1)─S(1)─Fe(2)	79.66(5)	Fe(1)─S(1)─Fe(3)	73.18(5)
Fe(2)─S(1)─Fe(3)	73.33(5)	S(1)─Fe(1)─Fe(2)	50.21(4)
S(1)─Fe(1)─Fe(3)	53.00(4)	S(1)─Fe(2)─Fe(1)	50.13(4)
S(1)─Fe(2)─Fe(3)	52.89(4)	S(1)─Fe(3)─Fe(1)	53.78(4)
S(1)─Fe(3)─Fe(2)	53.78(4)	Fe(2)─Fe(1)─Fe(3)	57.44(3)
Fe(1)─Fe(2)─Fe(3)	57.23(3)	Fe(1)─Fe(3)─Fe(2)	65.33(3)
I(1)─Hg(1)─Fe(1)	137.68(2)	I(1)─Hg(1)─Fe(2)	144.67(2)
Fe(1)─Hg(1)─Fe(2)	64.23(2)	Fe(1)─C(1)─O(1)	174.2(6)
Fe(1)─C(3)─O(3)	175.0(6)	Fe(2)─C(4)─O(4)	177.0(6)
Fe(2)─C(6)─O(6)	174.2(6)		

Fig. S1 Cyclic votalmetry in MeCN for $[Et_4N][\mathbf{1}]$ (a), $[Et_4N][\mathbf{2}]$ (b), $[Et_4N][\mathbf{3}]$ (c), $[Et_4N]_2[\mathbf{4}]$ (d), and $[Et_4N][\mathbf{5}]$ (e). Conditions: electrolyte, 0.1 M Bu_4NClO_4; working electrode, glassy carbon; scan rate, 100 mv/s. Potentials are versus SCE.



Computational details:

All geometry optimizations were fully performed at the Becke's three-parameter (B3) exchange function and the Lee-Yang-Parr (LYP) correlation function (B3LYP) DFT level with the LanL2DZ ECP basis set for Cl, I, Fe and Hg atoms and 6-31+(G)* basis set for C, H, O, and S atoms using the Gaussian 03 program..

$[SFe_3(CO)_9]^{2-}$ (the optimized geometry)
G = -1788.773089 a.u.

	x	y	z
Fe	1.224396	-0.853435	-0.111776
Fe	0.126719	1.486102	-0.110536
Fe	-1.350884	-0.632843	-0.112703
S	0.000828	0.000703	-1.795904
C	0.914430	-2.569337	-0.210274
C	2.816586	-0.772082	-0.827093
C	1.636601	-0.695245	1.590091
C	1.767078	2.077470	-0.209054
C	-0.738595	2.825041	-0.825950
C	-0.217137	1.759696	1.591701
C	-1.417988	-1.068246	1.589231
C	-2.079224	-2.050925	-0.828303
C	-2.682287	0.493295	-0.208777
O	0.810344	-3.736175	-0.260682
O	3.887014	-0.805612	-1.302685
O	1.983070	-0.632132	2.705772
O	2.829046	2.571865	-0.260631
O	-1.243798	3.769388	-1.301438
O	-0.445099	2.025215	2.708092
O	-1.535492	-1.398708	2.705373
O	-2.645921	-2.960819	-1.301692
O	-3.641167	1.166394	-0.257683

$[SFe_3(CO)_8(\mu\text{-}CO)(CH_2C(O)OCH_3)]^-$ (**1**) (the optimized geometry)
G = -2056.487509 a.u.

	x	y	z
Fe	-0.719744	-1.463259	-0.173433

Fe	-1.848854	0.832302	-0.074781
Fe	0.840731	0.632278	0.019117
S	-0.502165	0.130955	-1.708966
C	0.506499	-2.643845	-0.650567
C	-0.899764	-1.908033	1.538875
C	-2.090134	-2.372096	-0.808726
C	-2.663113	0.527529	1.483331
C	-3.261861	0.390029	-1.019728
C	-2.042054	2.586141	-0.346579
C	-0.047682	1.384101	1.394405
C	1.489362	2.257773	-0.341715
C	1.650393	-0.371847	1.241875
C	2.471643	0.027007	-1.275024
H	2.317821	0.600441	-2.186705
H	2.319063	-1.032837	-1.452530
O	1.276173	-3.450128	-0.963271
O	-1.022527	-2.244893	2.640263
O	-2.965713	-3.007617	-1.224228
O	-3.264328	0.355632	2.456669
O	-4.192861	0.129958	-1.654813
O	-2.207696	3.716782	-0.518771
O	-0.206034	1.928007	2.416307
O	1.880908	3.321460	-0.561058
O	2.233284	-0.942064	2.067433
C	3.831432	0.292279	-0.754462
O	4.456336	1.341150	-0.834428
O	4.369286	-0.806606	-0.139734
C	5.649045	-0.616574	0.469058
H	5.906757	-1.578299	0.916068
H	5.601239	0.159241	1.239300
H	6.397102	-0.326421	-0.275563

$[(CH_2C(O)OCH_3)SFe_3(CO)_9]^-$ (**1a**) (the optimized geometry)
G = -2056.485430 a.u.

	x	y	z
Fe	-1.568009	0.135424	-0.981121
Fe	-0.027535	1.200788	0.894446
Fe	0.009430	-1.420197	0.477448

S	0.599302	0.151437	-0.895403
C	-1.960151	-0.864713	-2.382897
C	-2.969978	-0.275376	0.015808
C	-2.085557	1.718331	-1.568681
C	-1.380747	1.262647	2.031700
C	0.013019	2.918041	0.472543
C	1.319141	1.126115	2.033469
C	-1.083753	-1.709199	1.837425
C	1.504059	-1.943730	1.260591
C	-0.349688	-2.846921	-0.499284
C	1.910801	0.388956	-2.190227
H	1.651025	1.285831	-2.752109
H	1.870221	-0.496754	-2.828850
O	-2.240501	-1.479848	-3.327433
O	-3.939023	-0.538305	0.597830
O	-2.471893	2.733312	-1.980316
O	-2.234512	1.374441	2.809793
O	0.068164	4.052562	0.236780
O	2.193234	1.122644	2.798671
O	-1.759225	-1.974068	2.743158
O	2.474353	-2.339245	1.761546
O	-0.565512	-3.816473	-1.101219
C	3.285387	0.564352	-1.587599
O	3.927386	1.596491	-1.622771
O	3.714062	-0.568446	-1.000964
C	4.964851	-0.487354	-0.293475
H	5.097966	-1.466404	0.165221
H	4.914067	0.290066	0.472319
H	5.780279	-0.263561	-0.987059

$[Cl(CH_2)_3SFe_3(CO)_9]^-$ (**2**) (the optimized geometry)

G = -1921.580010 a.u.

	x	y	z
Fe	1.251978	-0.931845	-0.938020
Fe	-0.225478	-0.644752	1.240236
Fe	0.792815	1.481816	0.032288
S	-0.664266	0.077240	-0.768445
C	1.738297	-0.643561	-2.609837

C	2.868564	-0.973733	-0.219199
C	0.918817	-2.664122	-1.007560
C	1.172307	-1.066243	2.234132
C	-1.088832	-2.179871	1.398877
C	-1.111061	0.352682	2.392692
C	-0.162190	2.824666	0.658897
C	1.560238	2.255917	-1.354359
C	2.128855	1.569437	1.188902
C	-2.100697	0.263769	-1.914490
O	2.052677	-0.505755	-3.719475
O	3.955234	-1.044446	0.181528
O	0.746518	-3.809699	-1.087216
O	2.032570	-1.378546	2.948230
O	-1.674090	-3.170161	1.552147
O	-1.699002	0.963489	3.188790
O	-0.766876	3.743912	1.035890
O	2.068528	2.814129	-2.237716
O	3.001522	1.712743	1.940301
H	-1.667447	0.599727	-2.860055
H	-2.528684	-0.732138	-2.057176
C	-3.145362	1.263259	-1.412023
Cl	-5.199739	-0.560507	-0.815436
H	-2.640149	2.179936	-1.079161
H	-3.796241	1.546831	-2.248472
C	-3.999532	0.777490	-0.255709
H	-3.419397	0.316269	0.541031
H	-4.639542	1.563003	0.142486

$[SFe_3(CO)_8(\mu\text{-}CO)(CH_2)_3Cl]^-$ (**2a**) (the optimized geometry)
G = -1921.568207 a.u.

	x	y	z
Fe	1.147606	1.364193	-0.228006
Fe	1.644068	-1.148326	-0.171142
Fe	-0.850735	-0.249218	0.259364
S	0.312612	-0.132591	-1.652368
C	0.220216	2.828094	-0.569396
C	1.700745	1.742083	1.419276
C	2.598258	1.862947	-1.093829

C	2.710938	-1.076636	1.255986
C	2.980785	-1.108871	-1.311733
C	1.321031	-2.889468	-0.383040
C	-0.024083	-1.189508	1.549762
C	-1.967484	-1.604213	0.056636
C	-1.183401	0.990408	1.463643
O	-0.353653	3.810959	-0.787416
O	2.073684	2.035013	2.476208
O	3.537843	2.234253	-1.661881
O	3.460898	-1.074758	2.136979
O	3.853345	-1.115891	-2.071077
O	1.148271	-4.023937	-0.520485
O	0.119340	-1.739770	2.571903
O	-2.695062	-2.498451	-0.065555
O	-1.520828	1.750772	2.280801
C	-2.444319	0.777470	-0.820376
H	-1.910509	1.608144	-1.278133
H	-2.733817	0.096983	-1.623329
C	-3.691711	1.324880	-0.121694
H	-3.416553	1.980497	0.714952
H	-4.240891	1.965910	-0.828770
C	-4.675591	0.325524	0.453157
Cl	-5.633143	-0.584058	-0.897055
H	-4.204607	-0.464524	1.035469
H	-5.459387	0.808769	1.035832

$[I(CH_2)_4SFe_3(CO)_9]^-$ (**3**) (the optimized geometry)

G = -1957.312590 a.u.

	x	y	z
I	-6.810002	0.014496	0.209785
C	-4.718744	-0.066482	-0.516224
H	-4.649888	0.761785	-1.221053
H	-4.659104	-1.013211	-1.052338
C	-3.706780	0.034696	0.613030
C	-2.269630	-0.025610	0.056477
H	-3.854787	0.972291	1.161446
H	-3.864895	-0.782895	1.326140
C	-1.228177	0.060814	1.172684

H	-2.107385	0.796149	-0.650995
H	-2.124222	-0.957651	-0.501718
S	0.492901	0.021484	0.517475
H	-1.317541	0.993889	1.737997
H	-1.309686	-0.779683	1.869202
Fe	1.646031	1.278119	-0.828390
Fe	1.661020	-1.364118	-0.682124
Fe	2.485402	0.081765	1.377643
C	3.319350	1.572210	-1.321274
C	1.236627	2.924481	-0.343558
C	0.871276	1.208565	-2.411063
C	0.565074	-1.913651	-1.950612
C	1.827875	-2.847953	0.257444
C	3.160596	-1.421181	-1.618148
C	2.403714	-0.999498	2.771393
C	4.172085	-0.215659	0.936599
C	2.658860	1.637973	2.191383
O	4.390597	1.838933	-1.679626
O	0.938958	4.014357	-0.072122
O	0.377023	1.219321	-3.463221
O	-0.152743	-2.329658	-2.764961
O	1.937053	-3.855320	0.826137
O	4.115547	-1.531079	-2.268597
O	2.358145	-1.666897	3.720951
O	5.297333	-0.412061	0.731094
O	2.809917	2.636795	2.765219

$[SFe_3(CO)_8(\mu\text{-}CO)(CH_2)_4I]^-$ (**3a**) (the optimized geometry)
G = -1957.302442 a.u.

	x	y	z
Fe	2.005292	1.480229	-0.063847
Fe	3.216192	-0.750503	-0.423844
Fe	0.649967	-0.718288	0.354290
S	1.467327	-0.025124	-1.612722
C	0.664989	2.627695	-0.156494
C	2.599019	1.833577	1.575425
C	3.153511	2.475999	-0.954208
C	4.379947	-0.496576	0.902687

C	4.326016	-0.191769	-1.666700
C	3.388279	-2.473912	-0.844809
C	1.865260	-1.503609	1.418920
C	-0.073106	-2.296995	0.045950
C	0.107649	0.226766	1.741601
O	-0.186311	3.410917	-0.219663
O	2.982747	2.110550	2.632557
O	3.884335	3.166408	-1.530697
O	5.197016	-0.351291	1.709097
O	5.056253	0.143761	-2.498705
O	3.532067	-3.587323	-1.121031
O	2.292498	-2.100545	2.329180
O	-0.591318	-3.317282	-0.150528
O	-0.356065	0.762060	2.666485
I	-6.996551	0.130398	-0.319562
C	-5.056645	-0.486038	0.583127
H	-5.153558	-1.567168	0.680582
H	-5.073932	-0.021175	1.568570
C	-3.853443	-0.072724	-0.243220
C	-2.545142	-0.544060	0.439881
H	-3.921800	-0.505237	-1.248134
H	-3.835467	1.016654	-0.361991
C	-1.308133	-0.141799	-0.365578
H	-2.589765	-1.633509	0.563086
H	-2.503747	-0.118286	1.449400
H	-1.362737	-0.558117	-1.374751
H	-1.255742	0.942996	-0.461045

$[\{SFe_3(CO)_9\}_2(\mu_4\text{-Hg})]^{2-}$ (**4**) (the optimized geometry)
G = -3620.280538 a.u.

	x	y	z
Hg	0.000000	0.172003	0.000000
Fe	2.417336	-1.123816	-1.104566
Fe	-2.417336	-1.123815	1.104567
Fe	2.666529	1.492979	-0.045914
Fe	-2.666529	1.492979	0.045913
Fe	4.436915	-0.367299	0.344328
S	3.875401	0.483816	-1.636621

C	1.246930	-1.003358	-2.436810
C	3.307585	-2.388305	-1.917495
C	1.837809	-2.217740	0.172923
Fe	-4.436915	-0.367299	-0.344328
S	-3.875400	0.483818	1.636620
C	-1.246930	-1.003355	2.436810
C	-3.307585	-2.388303	1.917498
C	-1.837808	-2.217742	-0.172920
C	2.138685	1.513178	1.653592
C	3.831953	2.769562	0.206527
C	1.603280	2.534019	-1.011312
C	-2.138684	1.513179	-1.653593
C	-3.831955	2.769560	-0.206529
C	-1.603281	2.534021	1.011312
C	5.467784	-1.737872	-0.040840
C	3.861537	-0.897611	1.935720
C	5.764332	0.659935	0.866092
O	0.574446	-0.998958	-3.381799
O	3.852547	-3.232339	-2.499163
O	1.509764	-3.017763	0.949132
C	-5.467784	-1.737872	0.040842
C	-3.861535	-0.897614	-1.935718
C	-5.764331	0.659934	-0.866097
O	-0.574445	-0.998953	3.381799
O	-3.852548	-3.232336	2.499167
O	-1.509763	-3.017766	-0.949127
O	1.863358	1.625155	2.776301
O	4.562228	3.660586	0.352474
O	1.009353	3.309757	-1.638364
O	-1.863356	1.625147	-2.776303
O	-4.562232	3.660582	-0.352477
O	-1.009355	3.309759	1.638365
O	6.195595	-2.622116	-0.241621
O	3.568178	-1.259319	2.998077
O	6.681544	1.277438	1.225702
O	-6.195594	-2.622115	0.241626
O	-3.568176	-1.259325	-2.998075
O	-6.681541	1.277437	-1.225711

$[SFe_3(CO)_9(\mu\text{-HgI})]^-$ (**5**) (the optimized geometry)
G = -1843.014814 a.u.

	x	y	z
Hg	1.448436	0.000556	0.044196
I	4.260079	-0.000386	-0.565102
Fe	-0.872662	1.470445	0.617791
Fe	-0.872158	-1.470243	0.618339
Fe	-2.568335	-0.000536	-0.694337
S	-2.311097	-0.000020	1.510687
C	-0.276166	2.227019	-0.881223
C	-1.994615	2.781577	0.917812
C	0.172677	1.933056	1.983677
C	0.172951	-1.931712	1.984813
C	-1.993581	-2.781839	0.918239
C	-0.274795	-2.226844	-0.880220
C	-3.727739	-1.298429	-0.988439
C	-1.756765	-0.001037	-2.276669
C	-3.727644	1.297241	-0.989329
O	0.060560	2.819131	-1.820658
O	-2.708494	3.661522	1.149722
O	0.790646	2.308636	2.888861
O	0.790829	-2.306507	2.890381
O	-2.707113	-3.662098	1.150054
O	0.062291	-2.819197	-1.819375
O	-4.512040	-2.120150	-1.214129
O	-1.278008	-0.001369	-3.331036
O	-4.511846	2.118877	-1.215673

$[\{SFe_3(CO)_9\}_2\{\mu\text{-}(CH_2)_3\}]^{2-}$ (the optimized geometry)
G = -3695.320182 a.u.

	x	y	z
Fe	-4.202727	-0.862244	1.172304
Fe	-3.433952	-0.687391	-1.355921
Fe	-4.237951	1.467399	-0.062018
S	-2.493049	0.235172	0.385148
C	-4.239690	-0.460277	2.890176

C	-5.941128	-1.058137	0.936587
C	-3.738101	-2.563040	1.256854
C	-5.014948	-1.251104	-1.898029
C	-2.544675	-2.188751	-1.645637
C	-2.969319	0.248583	-2.776775
C	-3.621668	2.801408	-1.035816
C	-4.620293	2.325785	1.428073
C	-5.853952	1.384777	-0.771389
C	-0.805489	0.677506	1.009447
O	-4.270203	-0.251104	4.032765
O	-7.088587	-1.230612	0.863608
O	-3.486992	-3.692286	1.358308
O	-6.014958	-1.660287	-2.327066
O	-1.968665	-3.164035	-1.896055
O	-2.680976	0.815702	-3.749568
O	-3.253281	3.722550	-1.642563
O	-4.896681	2.938509	2.377187
O	-6.918467	1.422503	-1.237110
H	-0.992501	1.236088	1.929704
H	-0.305049	-0.259263	1.268726
C	0.000068	1.507708	0.001725
H	-0.680146	2.168252	-0.548170
H	0.680530	2.166943	0.552885
C	0.805280	0.679145	-1.007643
H	0.304534	-0.257001	-1.268574
H	0.992360	1.239365	-1.926884
O	3.486775	-3.690694	-1.363480
C	3.737855	-2.561592	-1.260400
Fe	4.202453	-0.860899	-1.173445
S	2.492865	0.235289	-0.384439
C	5.940846	-1.057080	-0.938000
C	4.239621	-0.456441	-2.890721
Fe	4.237691	1.467338	0.063528
Fe	3.434532	-0.688944	1.355374
O	7.088302	-1.229678	-0.865277
O	4.270405	-0.245575	-4.032989
C	4.618696	2.327862	-1.425669
C	3.621379	2.799798	1.039419

C	5.854130	1.384501	0.771914
C	2.969558	0.244902	2.777517
C	2.545968	-2.191124	1.643310
C	5.015925	-1.252354	1.896636
O	4.894104	2.941916	-2.374202
O	3.252916	3.719954	1.647612
O	6.918878	1.422091	1.237104
O	2.680998	0.810563	3.751092
O	1.970408	-3.166978	1.892544
O	6.016225	-1.661411	2.325105

$[\{SFe_3(CO)_9\}_2\{\mu\text{-}(CH_2)_4\}]^{2-}$ (the optimized geometry)
G = -3734.619163 a.u.

	x	y	z
C	1.719704	0.070630	0.891060
H	1.615376	0.996616	1.464800
H	1.598300	-0.777122	1.572273
C	0.724613	0.014300	-0.268218
C	-0.731145	0.037700	0.238315
H	0.902632	0.864409	-0.937825
H	0.899255	-0.895311	-0.855381
C	-1.729221	0.000841	-0.919393
H	-0.905431	0.940752	0.835809
H	-0.908802	-0.819270	0.898991
S	-3.488433	0.002375	-0.358934
H	-1.624580	0.874622	-1.569884
H	-1.612215	-0.901950	-1.526641
Fe	-4.778960	1.308532	0.816030
Fe	-4.794532	-1.335123	0.763576
Fe	-5.398650	0.031681	-1.408381
C	-6.492764	1.613216	1.109450
C	-4.323359	2.942749	0.328934
C	-4.189001	1.291323	2.478417
C	-3.838314	-1.845712	2.157611
C	-4.888691	-2.851457	-0.131461
C	-6.377668	-1.351196	1.544583
C	-5.163101	-1.087627	-2.751404
C	-7.120195	-0.265566	-1.147689

C	-5.484020	1.559846	-2.282448
O	-7.597244	1.892515	1.340455
O	-4.014632	4.030383	0.061822
O	-3.832364	1.338166	3.583604
O	-3.224290	-2.239434	3.061596
O	-4.969005	-3.880110	-0.666845
O	-7.395289	-1.436899	2.099528
O	-5.022241	-1.781976	-3.672509
O	-8.262132	-0.466467	-1.065824
O	-5.581349	2.539617	-2.900941
O	5.027474	-3.762385	1.105596
C	4.932745	-2.805618	0.452227
Fe	4.816631	-1.409334	-0.618276
S	3.482302	0.023061	0.342880
C	6.403226	-1.492189	-1.388026
C	3.879452	-2.098076	-1.946781
Fe	4.771919	1.210887	-0.953068
Fe	5.381724	0.191963	1.399466
O	7.423991	-1.626506	-1.927285
O	3.280362	-2.608925	-2.800903
C	4.195258	1.003685	-2.607212
C	4.292049	2.882558	-0.650916
C	6.484353	1.501435	-1.268223
C	5.450075	1.812290	2.088810
C	5.144407	-0.763058	2.863807
C	7.107964	-0.115668	1.186639
O	3.845054	0.924616	-3.712620
O	3.967141	3.988477	-0.506432
O	7.587630	1.766492	-1.520531
O	5.538418	2.857361	2.590886
O	5.001727	-1.343946	3.860099
O	8.252241	-0.313468	1.135705