Electronic Supplementary Information for

Synthesis, Characterization, DFT Calculations, and Electrochemical Comparison of Novel Iron(II) Complexes with Thione and Selone Ligands

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X-ray structural data. Crystal packing diagrams for **1**, **2**, **5b**, and **6b** are provided in Figs. S1-S4. Additional discussion of the crystallization and structure of **7** is also provided. The crystal structure diagram for **7** is given in Fig. S5, and the crystal packing diagram for **7** is shown in Fig. S6. Crystallographic data for **7** are provided in Table S1, and selected bond lengths and angles are given in Table S2.

Crystallization attempts with $\{Fe(ebit)Cl_2\}_n$ (7) and $\{Fe(ebis)Cl_2\}_n$ (8) and X-ray structure of 7. Crystal growth for the polymeric complexes **7** and **8** was attempted by vapor diffusion of ether into acetonitrile, dichloromethane, and mixtures of these solvents at both room and low temperatures as well as evaporation of acetonitrile and dichloromethane solutions. Small crystals were obtained only in low yields for $\{Fe(ebit)Cl_2\}_n$ (**7**), and its structure was determined using the best available crystal of the limited selection. Complex **7** crystallizes in space group $P2_1/c$ with a = 7.717(3), b = 16.526 (5), c = 15.059(5) Å, and β = 104.36(1)°, and the structure and crystal data are provided in Fig. S5 and Tables S1 and S2. Fe(II) ions are in a distorted tetrahedral coordination environment with angles ranging from 93.0(1)° to 114.4(1)°, an average Fe-Cl distance of 2.275(3) Å, and an average Fe-S distance of 2.366(3) Å, similar to values observed in complex **1** and slightly shorter than $\{Fe(L^1/L^2)Cl_2\}_n$ complexes (L^1 = 1,1'-methylenebis(3-methyl-imidazole-2-thione and L^2 = 1,1'-methylenebis(3-tertbutyl-imidazole-2-thione) with average Fe-S bond lengths of 2.3725(5) Å and 2.3819(5) Å, respectively.[1] The ebit ligands bridge symmetry-related Fe atoms through the Fe-S bonds, propagating the structure in a chain-like fashion, similar to the polymeric $\{Fe(L^1/L^2)Cl_2\}_n$ complexes.[1] The chains are connected by C-H---Cl intermolecular hydrogen bonding (Fig. S6) as well as hydrogen bonding with a crystallized acetonitrile molecule. The average bond lengths for ebit in complex **7** do not differ from those of the unbound ebit ligand.[2]

^{1}H NMR data. ^{1}H NMR spectra of iron complexes **1**-**8** are shown in Figs. S7-S15. Chemical shifts for these spectra are provided in Table 4.

Electrochemical data. Cyclic voltammograms of ebit and ebis are provided in Fig. S16 and voltammograms for iron complexes **1**, **2**, **3**, **4**, **7**, **8**, and $FeCl_2{\cdot}4H_2O$ are given in Figs. S17-S19. Negative and positive differential pulse voltammograms of dmit, dmise, ebit, and ebis and iron complexes **1**, **2**, **3**, **4**, **7**, and **8** are shown in Figs. S20-S31.

DFT calculation data. DFT Cartesian coordinates for iron-thione and -selone complexes 1-6 are provided on pages S18-S22.

References

(1) Meyer, S.; Demeshko, S.; Dechert, S.; Meyer, F. *Inorg. Chim. Acta* **2010**, *363*, 3088-3092.

(2) Liu, Q.; Shi, D.; Yu, K.; Xu, J. *Acta Cryst.* **2003**, *E59*, o356-o357.

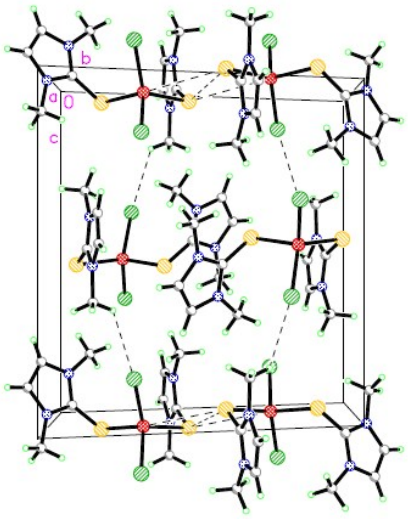

Fig. S1. Crystal packing diagram for $Fe(dmit)_2Cl_2$ (**1**) showing short Cl-Cl and Cl-H interactions as viewed along the *a*-axis with 50% probability density ellipsoids.

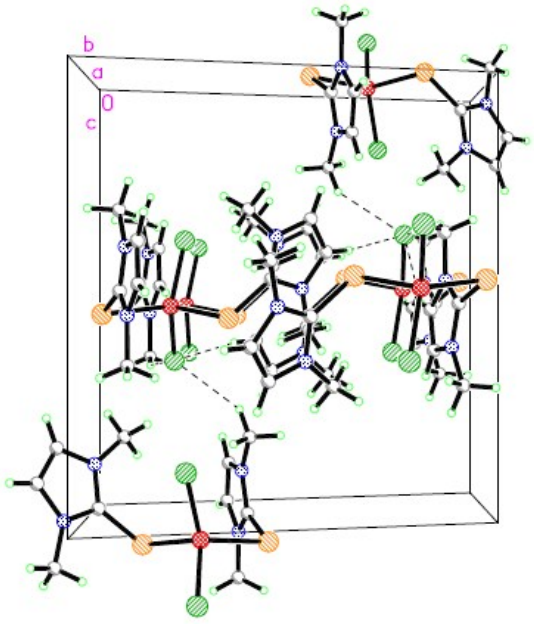

Fig. S2. Crystal packing diagram for $Fe(dmise)_2Cl_2$ (**2**) showing short Cl-H interactions as viewed along the *a*-axis with 50% probability density ellipsoids.

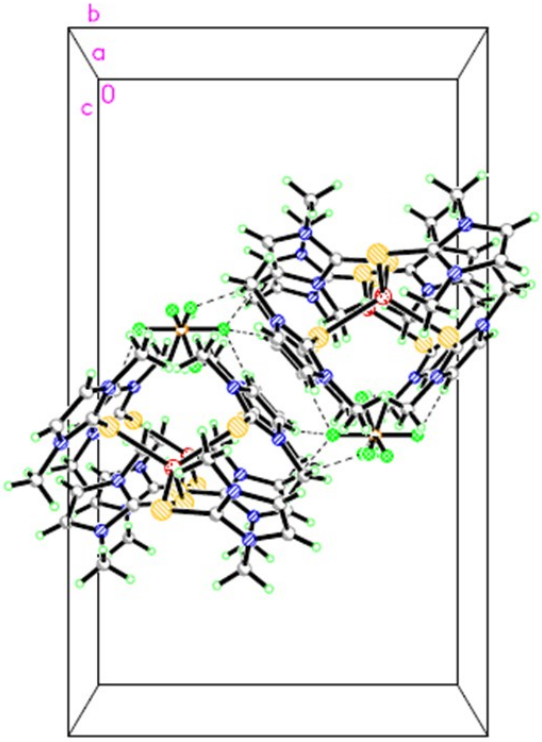

Fig. S3. Crystal packing diagram for $[Fe(dmit)_4][BF_4]_2$ (**5b**) showing short F-H interactions as viewed along the *a*-axis with 50% probability density ellipsoids

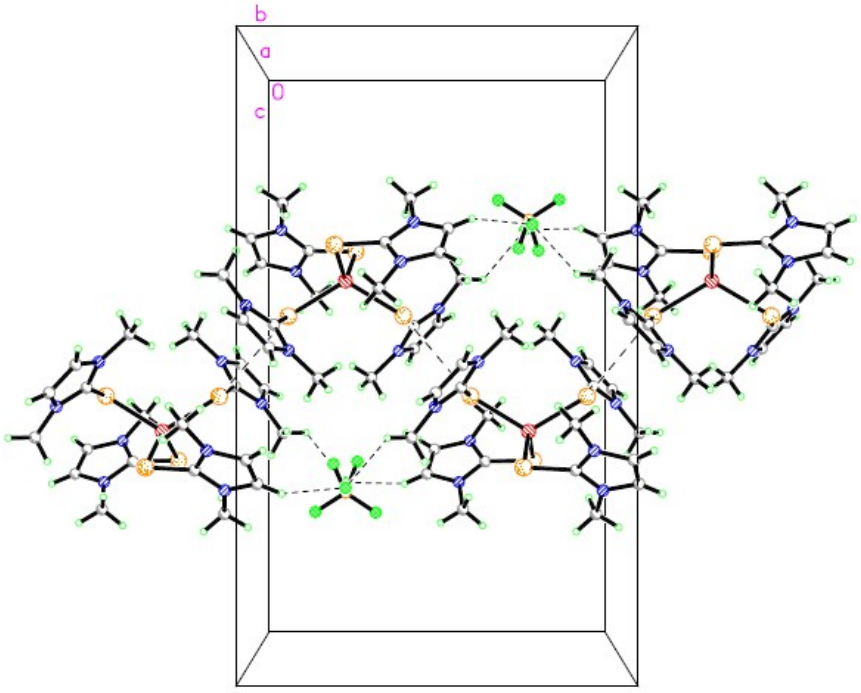

Fig. S4. Crystal packing diagram for $[Fe(dmise)_4][BF_4]_2$ (**6b**) showing short F-H interactions as viewed along the *a*-axis with 50% probability density ellipsoids.

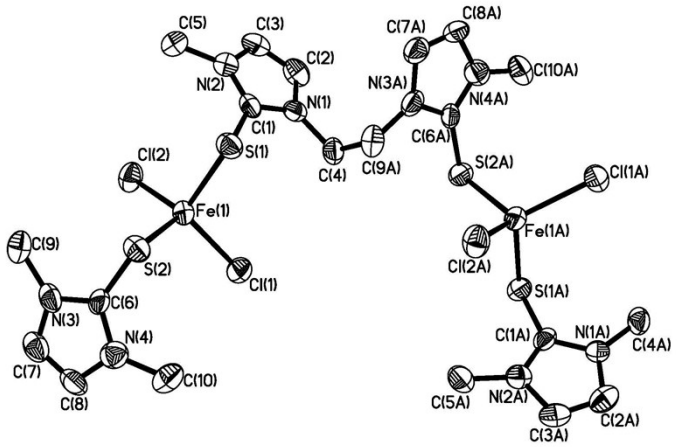

Fig. S5. Crystal structure diagram with 50% probability density ellipsoids for $\{Fe(ebit)Cl_2\}_n$ (**7**). Hydrogen atoms are omitted for clarity.

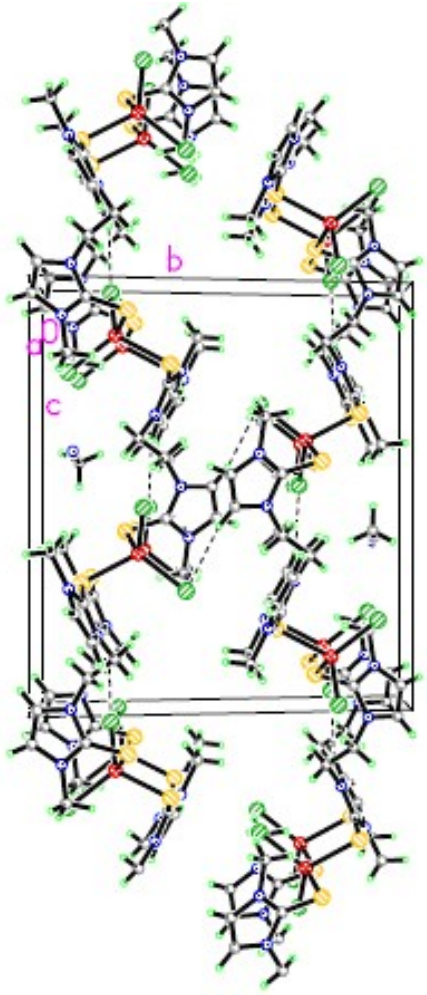

Fig. S6. Crystal packing diagram for $\{Fe(ebit)Cl_2\}_n$ (**7**) showing short Cl-H interactions as viewed along the *a*-axis with 50% probability density ellipsoids.

Table S1. Summary of crystallographic data for $\{Fe(ebit)Cl_2\}_n$ (**7**).

Parameter	**Value**
Chemical formula	$C_{12}H_{17}Cl_2FeN_5S_2$
F.W. (g/mol^{-1})	422.18
Space group	$P2_1/c$
Crystal system	monoclinic
*a,*Å	7.717 (3)
*b,*Å	16.526 (5)
*c,*Å	15.059 (5)
α, deg	90
β, deg	104.363 (12)
γ, deg	90
*V,*Å^{-3}	1860.5 (12)
Z	4
$D_{cal,}$ mg/m^3	1.507
indices (min)	[-9, -19, -17]
indices (max)	[6, 19, 17]
parameters	202
F(000)	864
μ, mm^{-1}	1.32
2θ range, deg	2.5-25.1
collected reflections	11826
unique reflections	3275
final R(obs. data)[a], R_1	0.097
wR_2	0.343
final R (all data), R_1	0.126
wR_2	0.393
goodness of fit (S)	1.49
largest diff. peak	3.00
largest diff. hole	-0.92

[a] $R_1 = \Sigma \| F_0| - |F_c\|/\Sigma|F_0|$; $wR_2 = \{\Sigma w(F_0^2 - F_c^2)^2\}^{1/2}$.

Table S2. Selected bond lengths and angles for $\{Fe(ebit)Cl_2\}_n$ (**7**).

Bond lengths (Å)		**Bond angles (°)**	
Fe1—S1	2.362 (3)	Cl1—Fe1—S1	111.23 (12)
Fe1—S2	2.371 (3)	Cl2—Fe1—S1	111.06 (13)
Fe1—Cl1	2.271 (3)	Cl1—Fe1—S2	111.48 (11)
Fe1—Cl2	2.281 (3)	Cl2—Fe1—S2	114.42 (12)
S1—C1	1.723 (10)	S1—Fe1—S2	92.95 (10)
S2—C6	1.737 (11)	C1—S1—Fe1	103.1 (3)
		C6—S2—Fe1	102.4 (3)
		Cl1—Fe1—Cl2	113.90 (12)

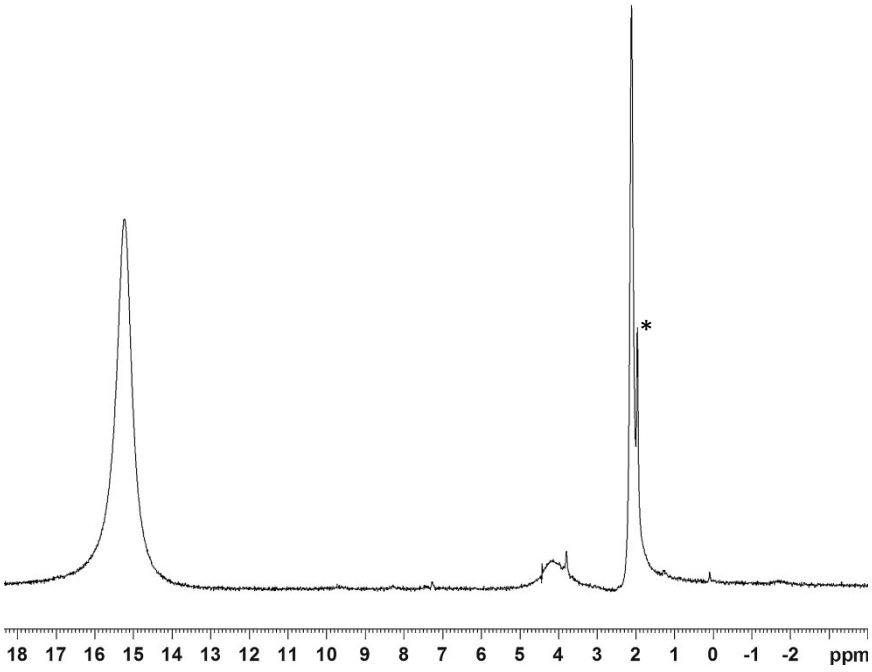

Fig. S7. ^{1}H NMR spectrum of $Fe(dmit)_2Cl_2$ (**1**) in CD_3CN. Spectra were acquired from δ -10 to 20 and no additional signals were observed. The asterisk indicates the resonance from residual CH_3CN solvent.

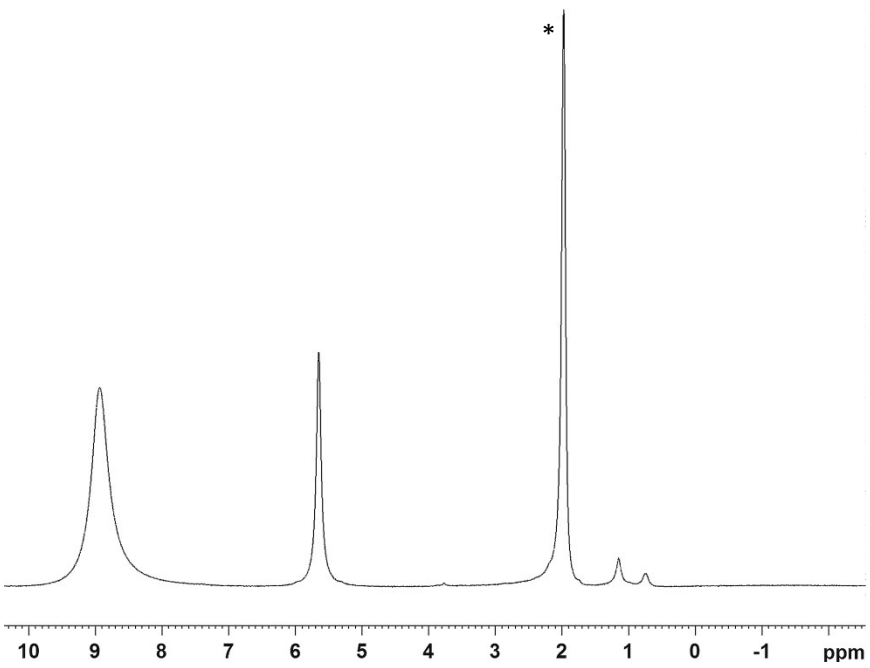

Fig. S8. ^{1}H NMR spectrum of $[Fe(dmit)_2(CH_3CN)_2][BF_4]_2$ (**3**) in CD_3CN. Spectra were acquired from δ -10 to 20 and no additional signals were observed. The asterisk indicates the residual CH_3CN solvent resonance.

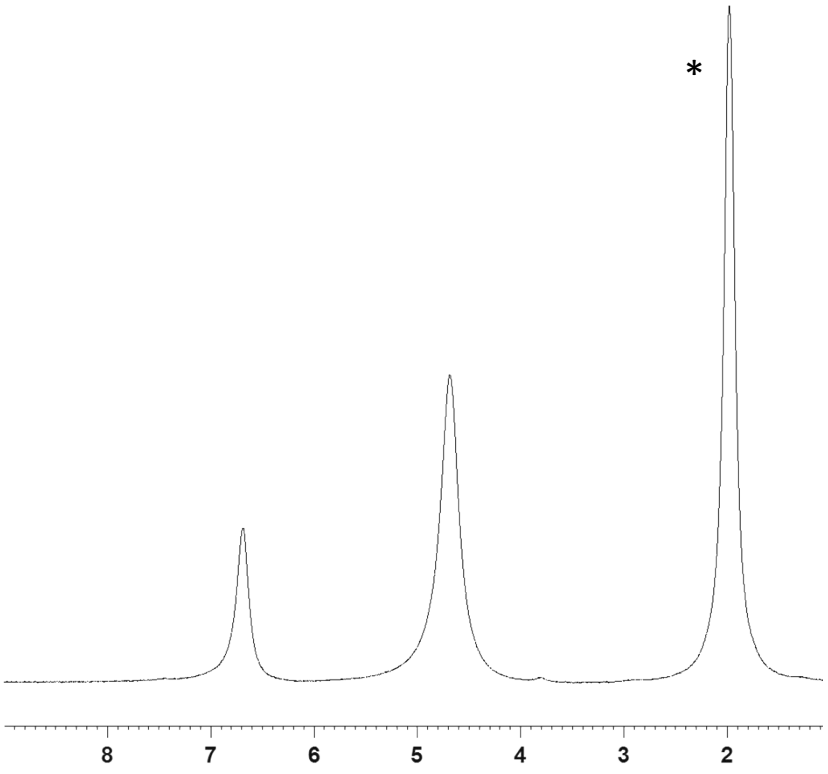

Fig. S9. ^{1}H NMR spectrum of $[Fe(dmise)_2(CH_3CN)_2][BF_4]_2$ (**4**) in CD_3CN. Spectra were acquired from δ -10 to 20 and no additional resonances were observed. The asterisk indicates the resonance from residual CH_3CN solvent.

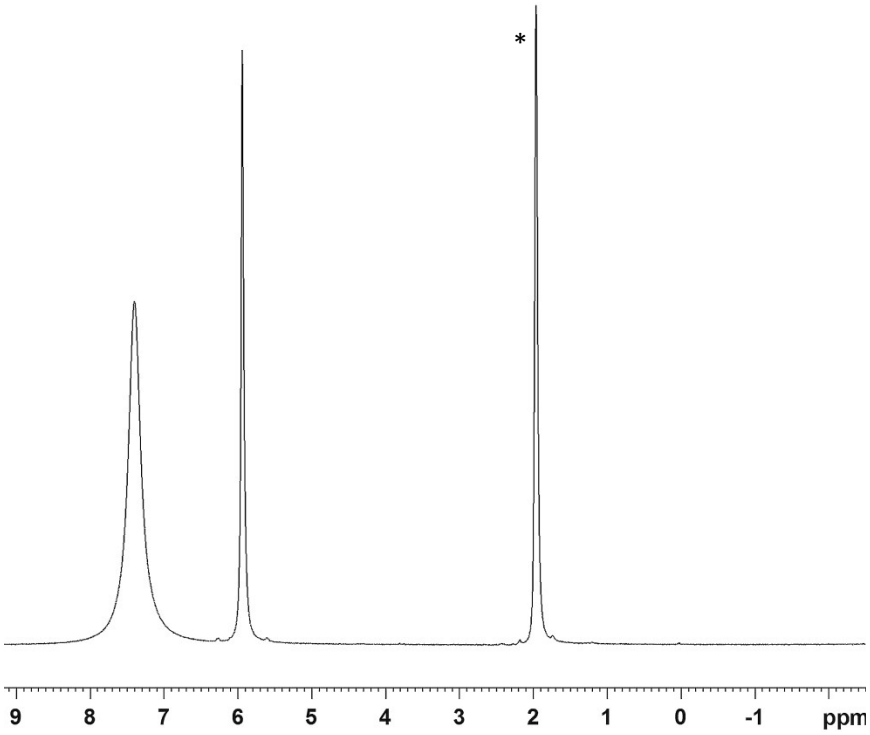

Fig. S10. ^{1}H NMR spectrum of $[Fe(dmit)_4][OTf]_2$ (**5a**) in CD_3CN. Spectra were acquired from δ -10 to 20 and no additional signals were observed. The asterisk indicates the residual CH_3CN solvent resonance.

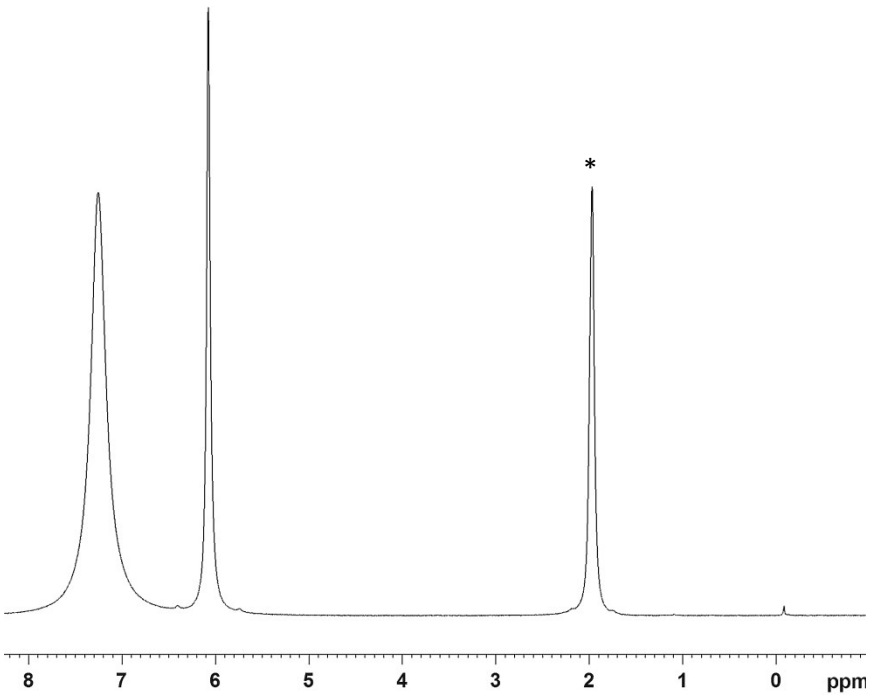

Fig. S11. ^{1}H NMR spectrum of $[Fe(dmise)_4][OTf]_2$ (**6a**) in CD_3CN. Spectra were acquired from δ -10 to 20 and no additional signals were observed. The asterisk indicates the residual CH_3CN solvent resonance.

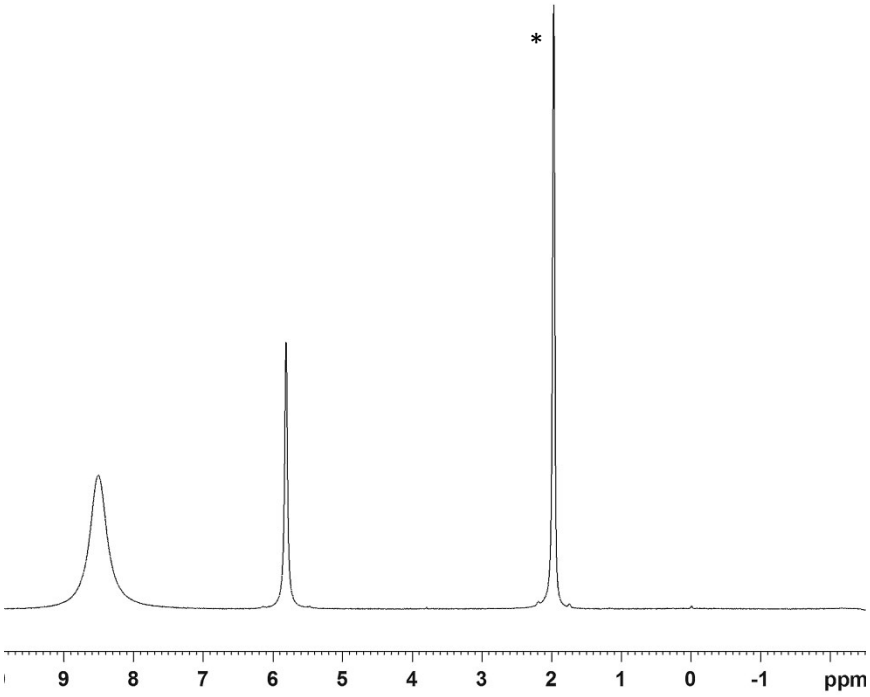

Fig. S12. ^{1}H NMR spectrum of $[Fe(dmit)_4][BF_4]_2$ (**5b**) in CD_3CN. Spectra were acquired from δ-10 to 20 and no additional signals were observed. The asterisk indicates the residual CH_3CN solvent resonance.

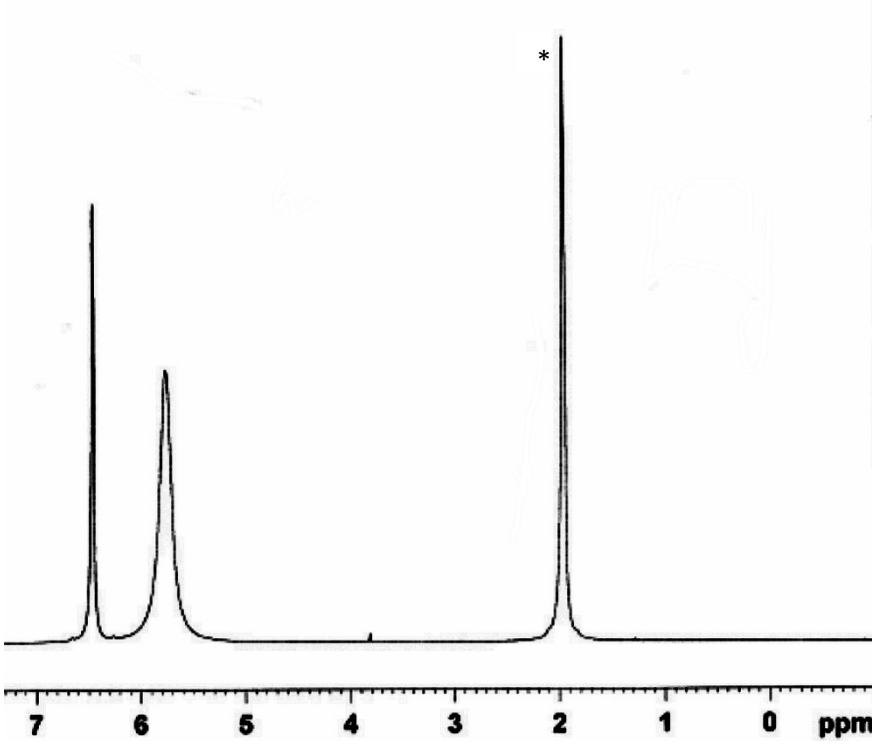

Fig. S13. ^{1}H NMR spectrum of $[Fe(dmise)_4][BF_4]_2$ (**6b**) in CD_3CN. Spectra were acquired from δ -10 to 20 and no additional signals were observed. The asterisk indicates the residual CH_3CN solvent resonance.

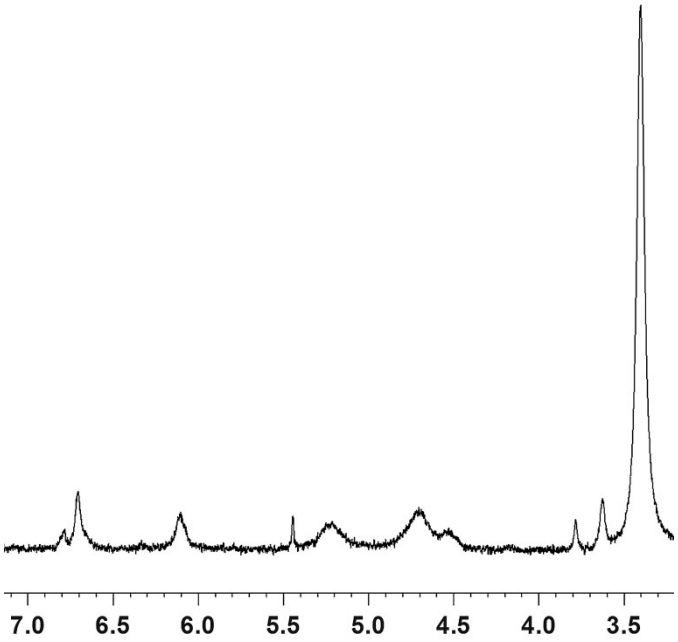

Fig. S14. ^{1}H NMR spectrum of $\{Fe(ebit)Cl_2\}_n$ (**7**) in CD_3CN. Spectra were acquired from δ -10 to 20 and no additional signals were observed except a residual CH_3CN resonance at δ 1.94.

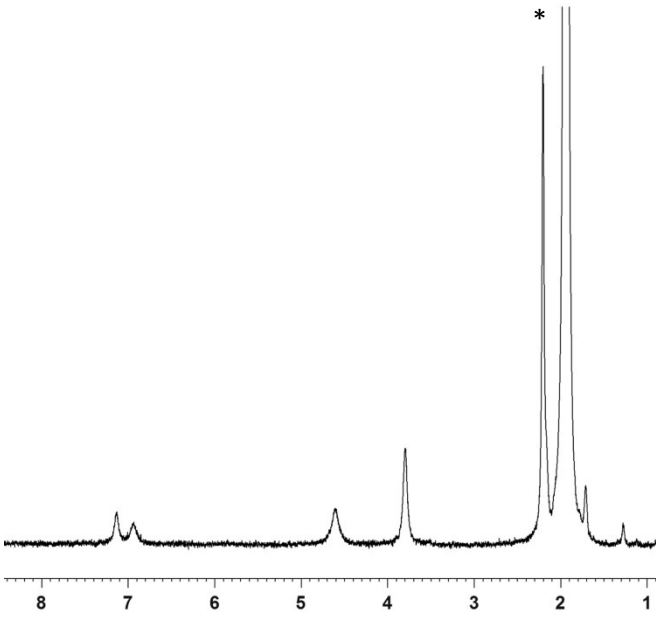

Fig. S15. ^{1}H NMR spectrum of $\{Fe(ebis)Cl_2\}_n$ (**8**) in CD_3CN. Spectra were acquired from δ -10 to 20 and no additional signals were observed. The asterisk indicates the residual CH_3CN solvent resonance..

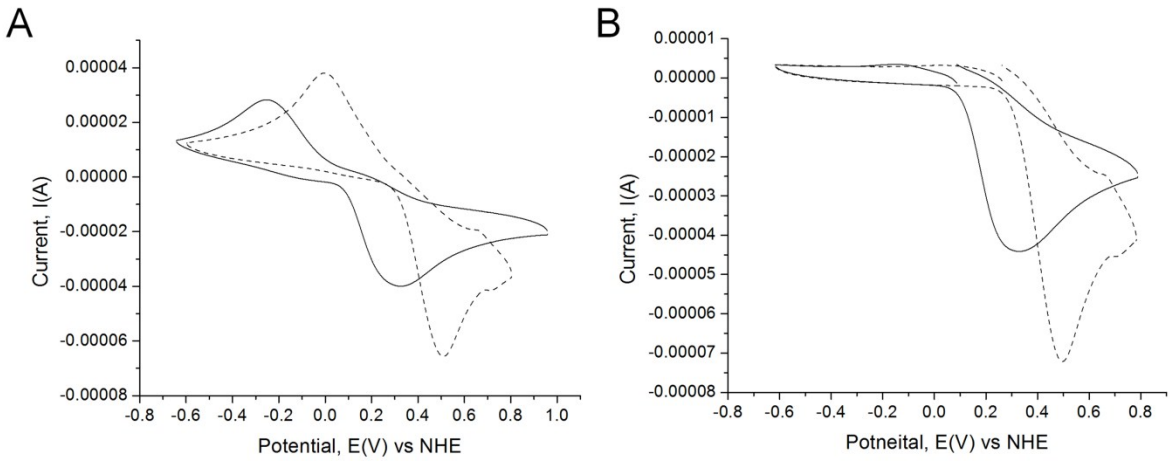

Fig. S16. Cyclic voltammetry with initial starting potential at A) 0.94 V for ebis (solid) and 0.80 V for ebit (dashed) and B) 0.09 V for ebis (solid) and 0.26 V for ebit (dashed).

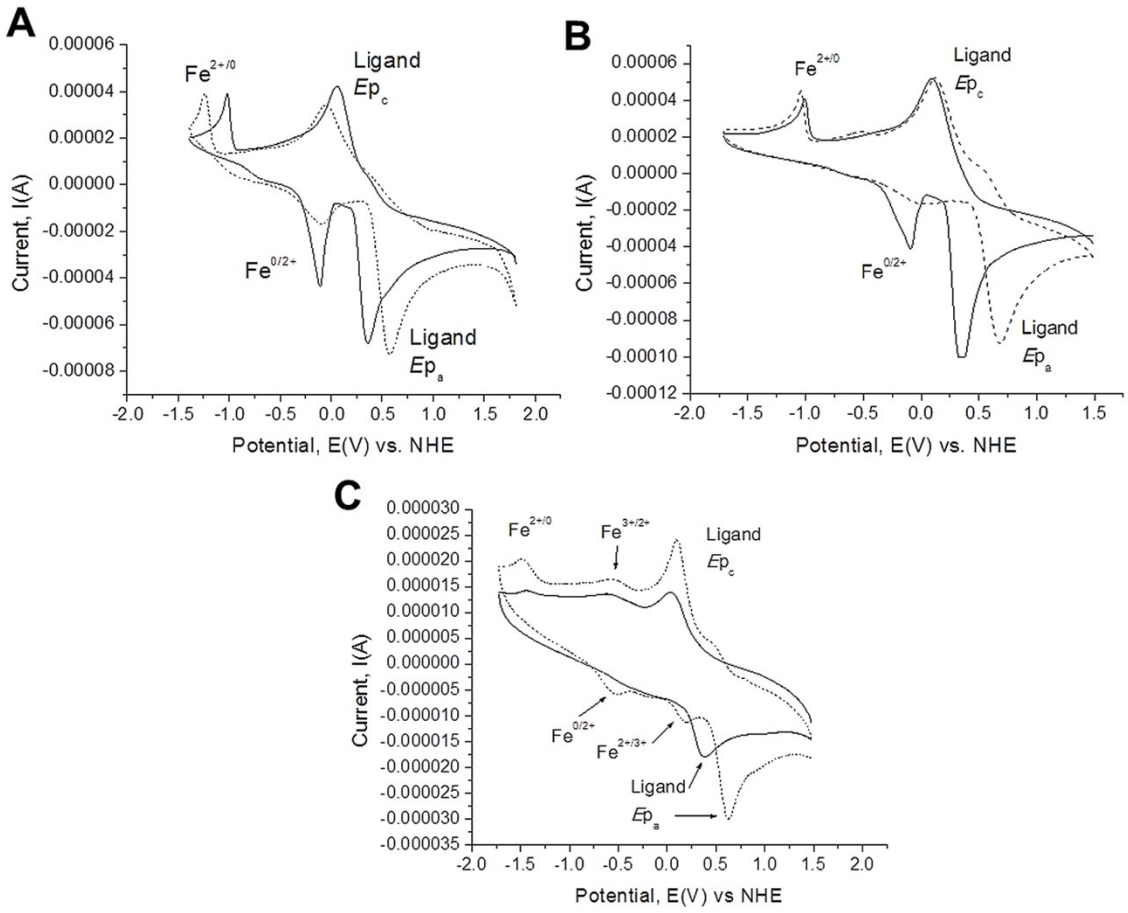

Fig. S17. Cyclic voltammograms of A) $[Fe(dmit)_2(CH_3CN)_2][OTf]_2$ (**3**; dashed line) and $[Fe(dmise)_2(CH_3CN)_2][OTf]_2$ (**4**; solid line) starting at 1.53 V; B) $[Fe(dmit)_4][OTf]_2$ (**5a**; dashed) and $[Fe(dmise)_4][OTf]_2$ (**6a**; solid) starting at 1.49 V; and C) $\{Fe(ebit)Cl_2\}_n$ (**7**; dashed) and $\{Fe(ebis)Cl_2\}_n$ (**8**; solid) starting at 1.48 V. All data were collected with 10 mM complex in acetonitrile.

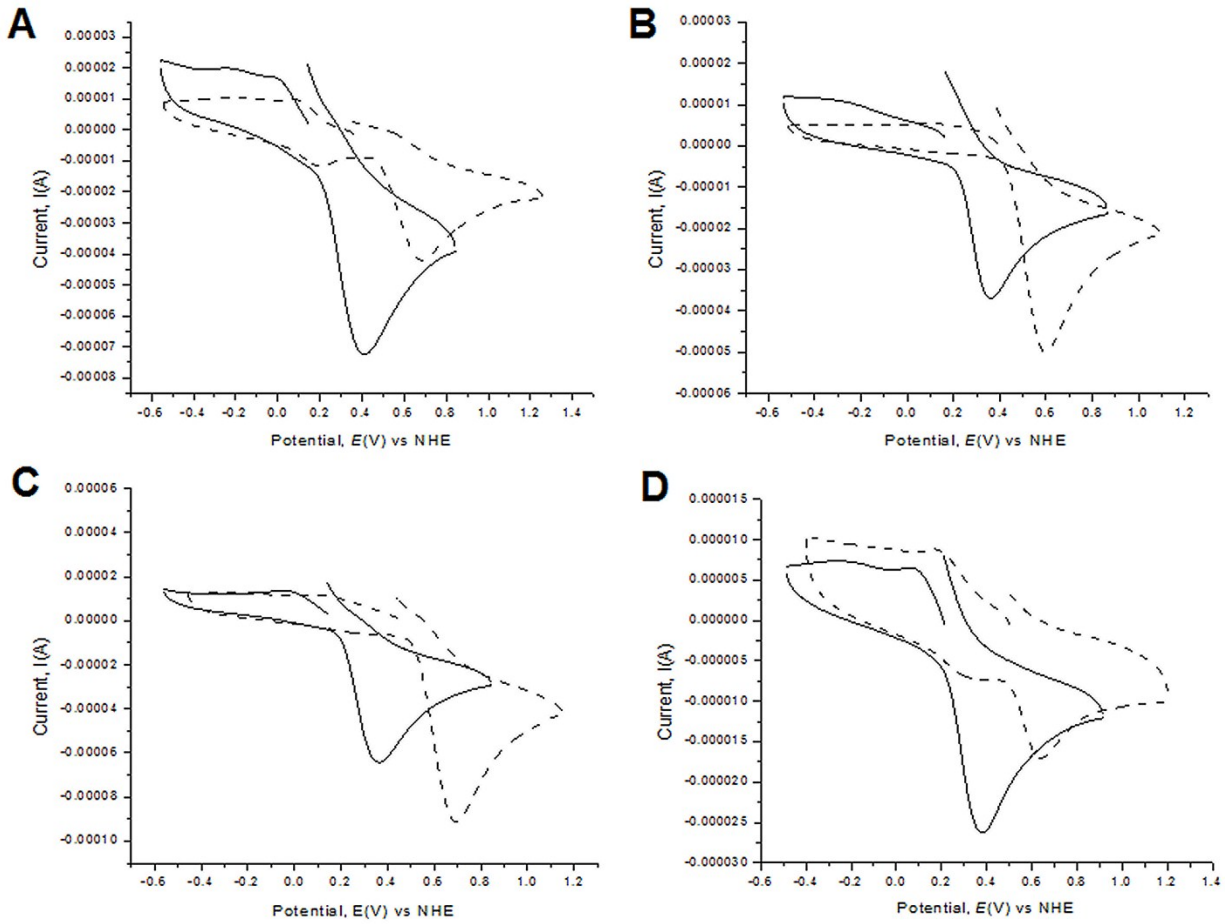

Fig. S18. Cyclic voltammograms of A) $Fe(dmit)_2Cl_2$ (**1**; dashed) and $Fe(dmise)_2Cl_2$ (**2**; solid) starting at 0.5 V for **1** and 0.15 V for **2**, respectively; B) $[Fe(dmit)_2(CH_3CN)_2][OTf]_2$ (**3**; dashed) and $[Fe(dmise)_2(CH_3CN)_2[OTf]_2$ (**4**; solid) starting at 0.4 V for **3** and 0.15 V for **4**, respectively; C) $[Fe(dmit)_4][OTf]_2$ (**5a**; dashed) and $[Fe(dmise)_4][OTf]_2$ (**6a**; solid) starting at 0.45 V for **5a** and 0.15 V for **6a**, respectively; and D) $\{Fe(ebit)Cl_2\}_n$ (**7**; dashed) and $\{Fe(ebis)Cl_2\}_n$ (**8**; solid) starting at 0.25 V for **7** and 0.10 V for **8**. All data were collected with 10 mM complex in acetonitrile.

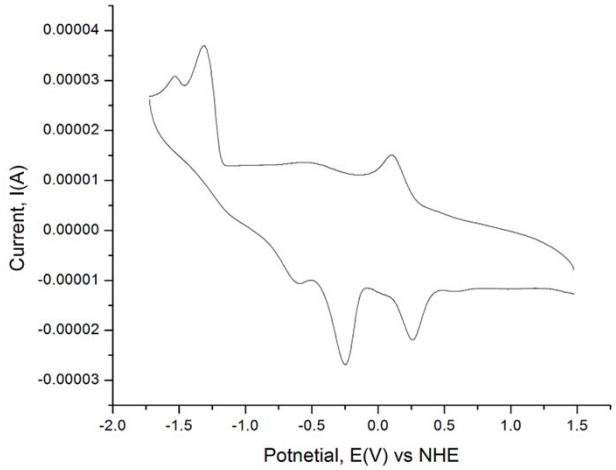

Fig. S19. Cyclic voltammogram for $FeCl_2{\cdot}4H_2O$ (10 mM) in acetonitrile starting at 1.48 V.

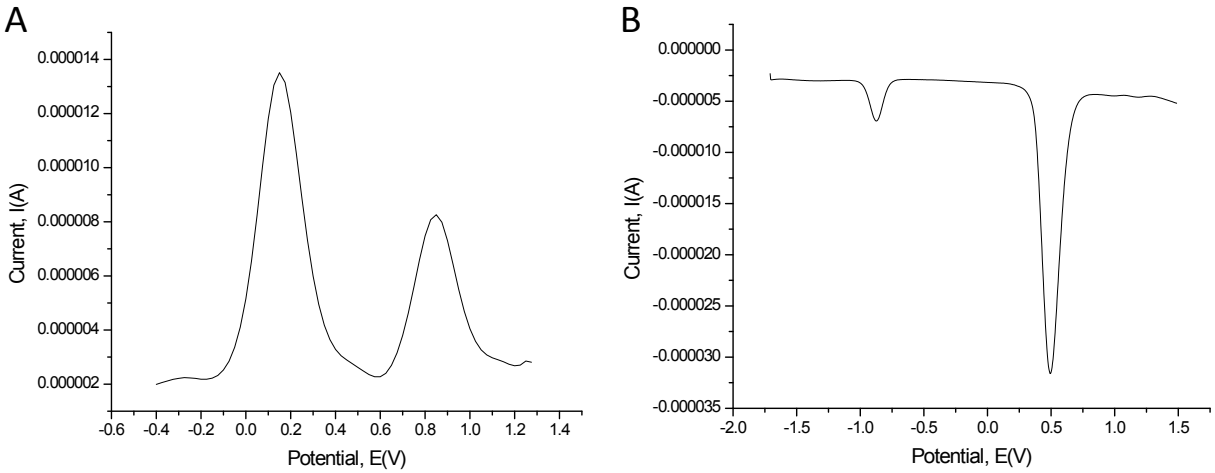

Fig. S20. Differential pulse voltammograms of dmit (10 mM) in acetonitrile: A) negative mode and B) positive mode; potentials are reported vs. NHE.

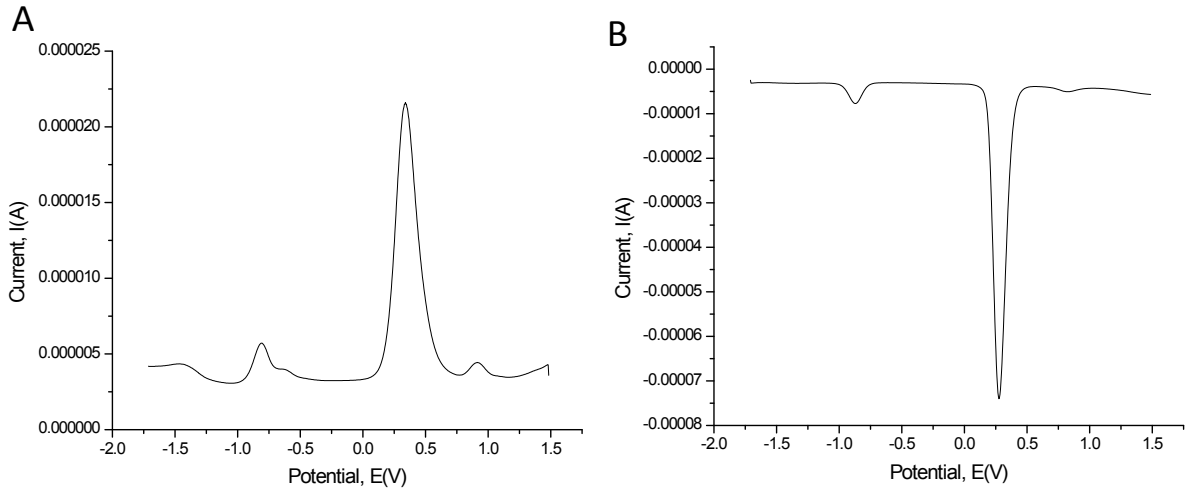

Fig. S21. Differential pulse voltammograms of dmise (10 mM) in acetonitrile: A) negative mode and B) positive mode; potentials are reported vs. NHE.

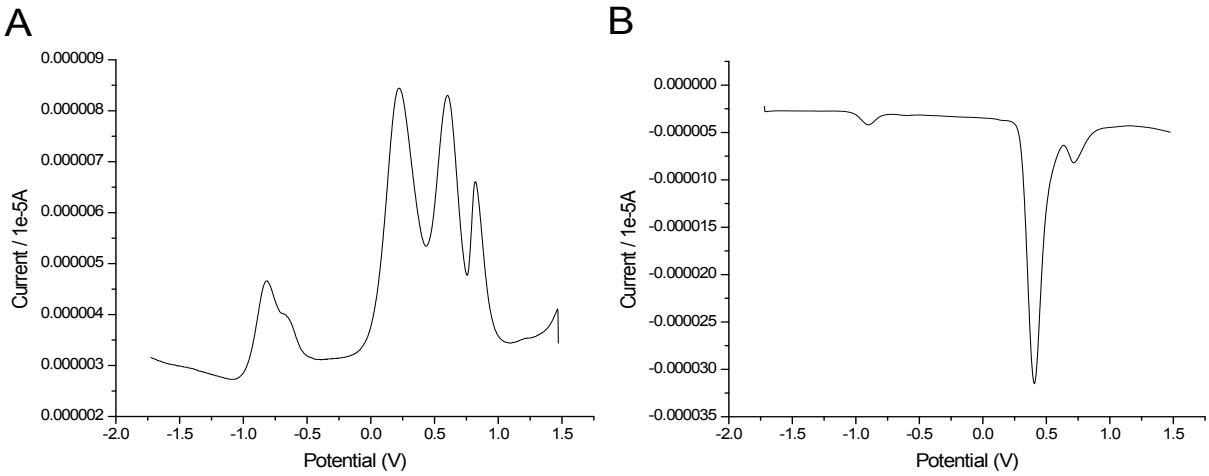

Fig. S22. Differential pulse voltammograms of ebit (10 mM) in acetonitrile: A) negative mode and B) positive mode; potentials are reported vs. NHE.

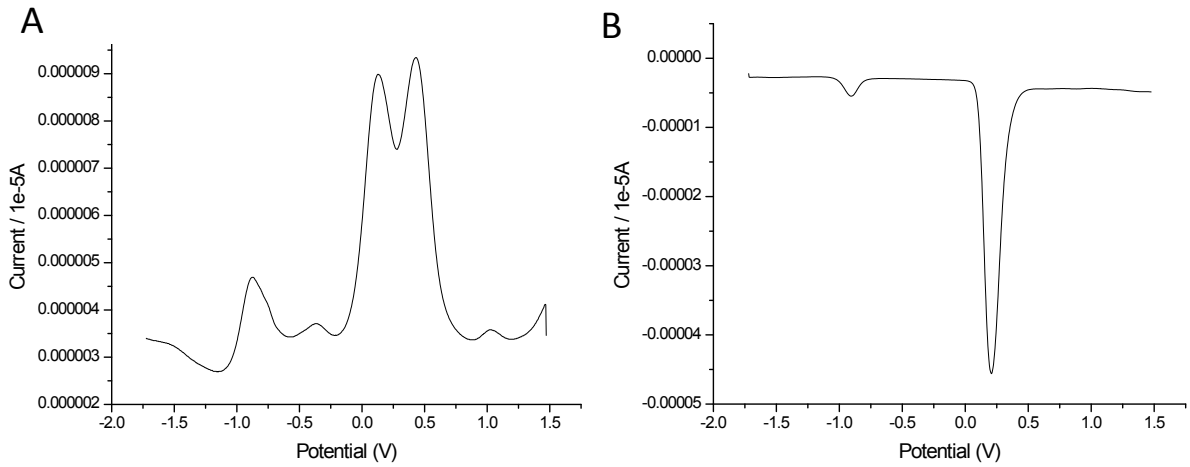

Fig. S23. Differential pulse voltammograms of ebis (10 mM) in acetonitrile: A) negative mode and B) positive mode; potentials are reported vs. NHE.

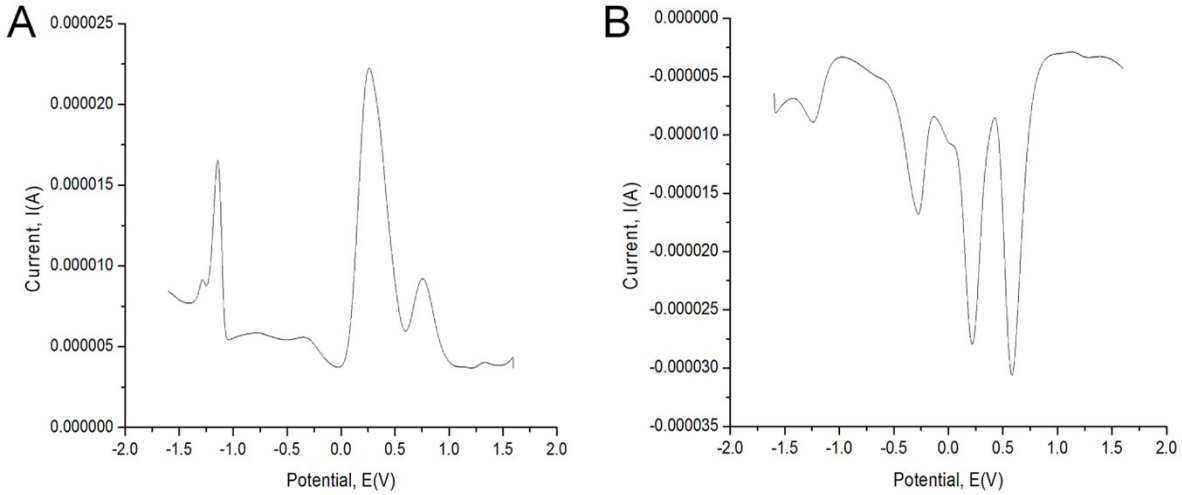

Fig. S24. Differential pulse voltammograms of $Fe(dmit)_2Cl_2$ (**1**; 10 mM) in acetonitrile: A) negative mode and B) positive mode; potentials are reported vs. NHE.

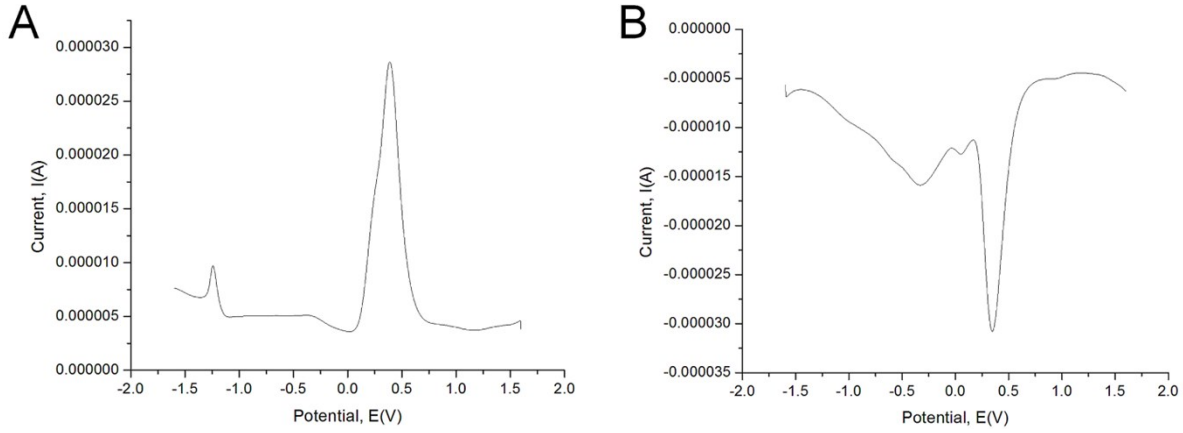

Fig. S25. Differential pulse voltammograms of $Fe(dmise)_2Cl_2$ (**2**; 10 mM) in acetonitrile: A) negative mode and B) positive mode; potentials are reported vs. NHE.

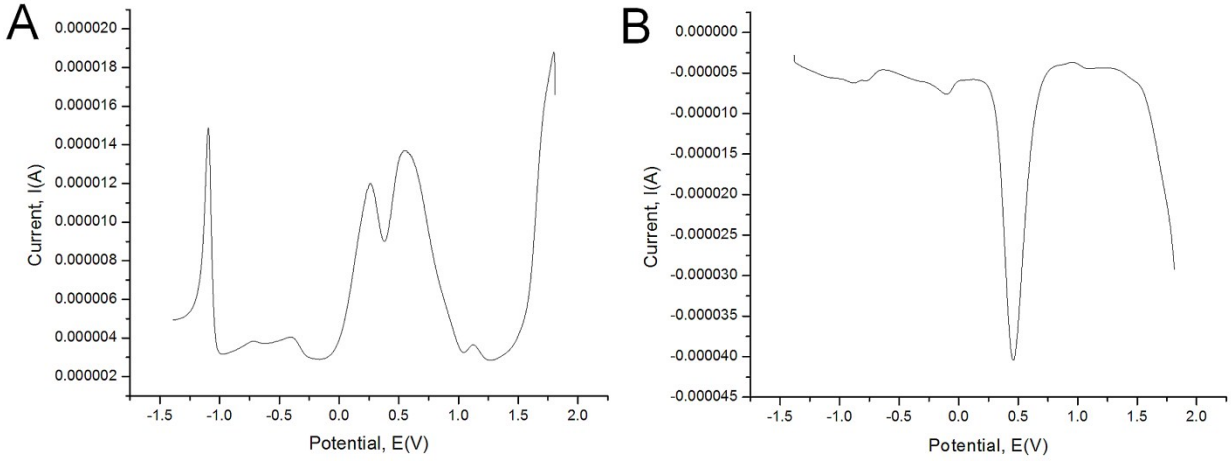

Fig. S26. Differential pulse voltammograms of $[Fe(dmit)_2(CH_3CN)_2][OTf]_2$ (**3**; 10 mM) in acetonitrile: A) negative mode and B) positive mode; potentials are reported vs. NHE.

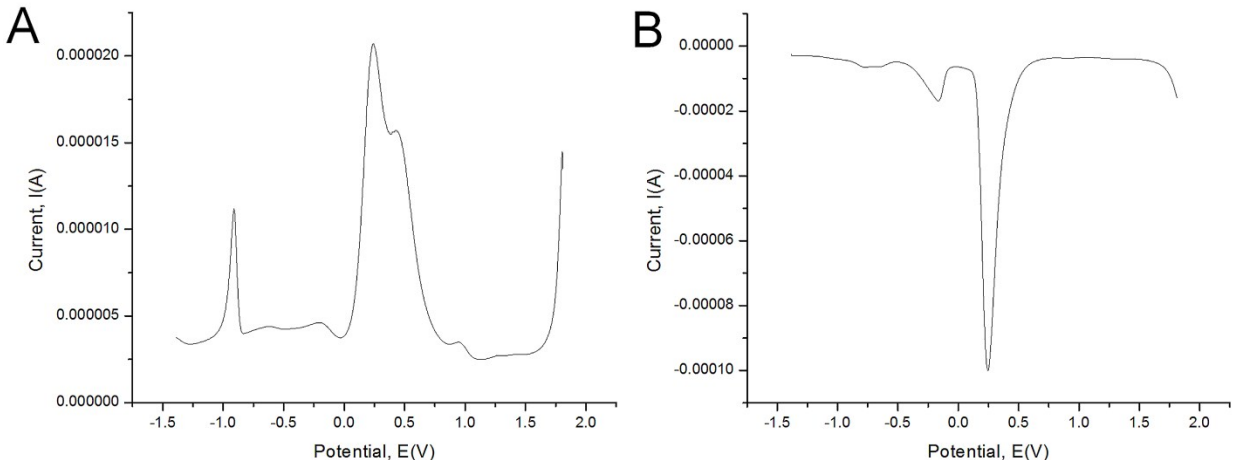

Fig. S27. Differential pulse voltammograms of $[Fe(dmise)_2(CH_3CN)_2][OTf]_2$ (**4**; 10 mM) in acetonitrile: A) negative mode and B) positive mode; potentials are reported vs. NHE.

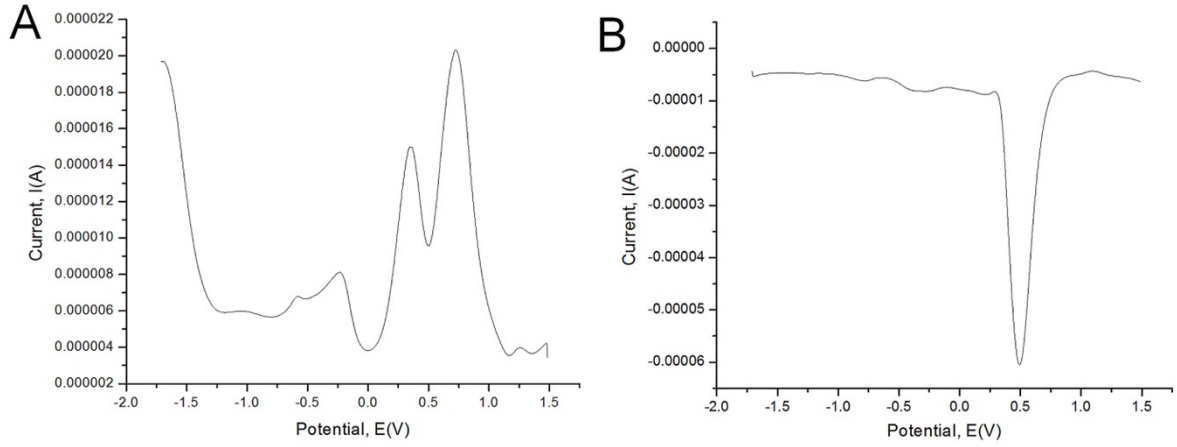

Fig. S28. Differential pulse voltammograms of $[Fe(dmit)_4][OTf]_2$ (**5a**; 10 mM) in acetonitrile: A) negative mode and B) positive mode; potentials are reported vs. NHE.

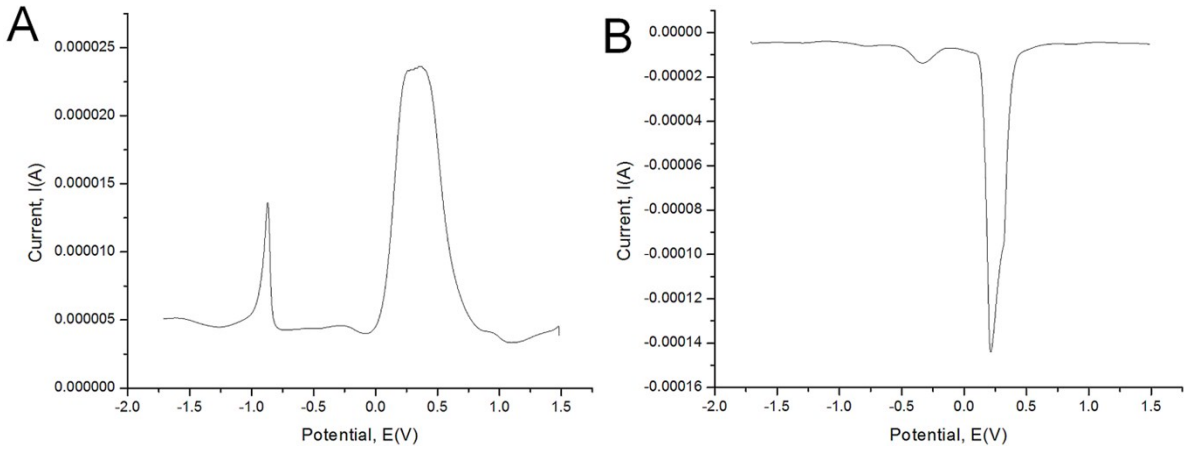

Fig. S29. Differential pulse voltammograms of $[Fe(dmise)_4][OTf]_2$ (**6a**; 10 mM) in acetonitrile: A) negative mode and B) positive mode; potentials are reported vs. NHE.

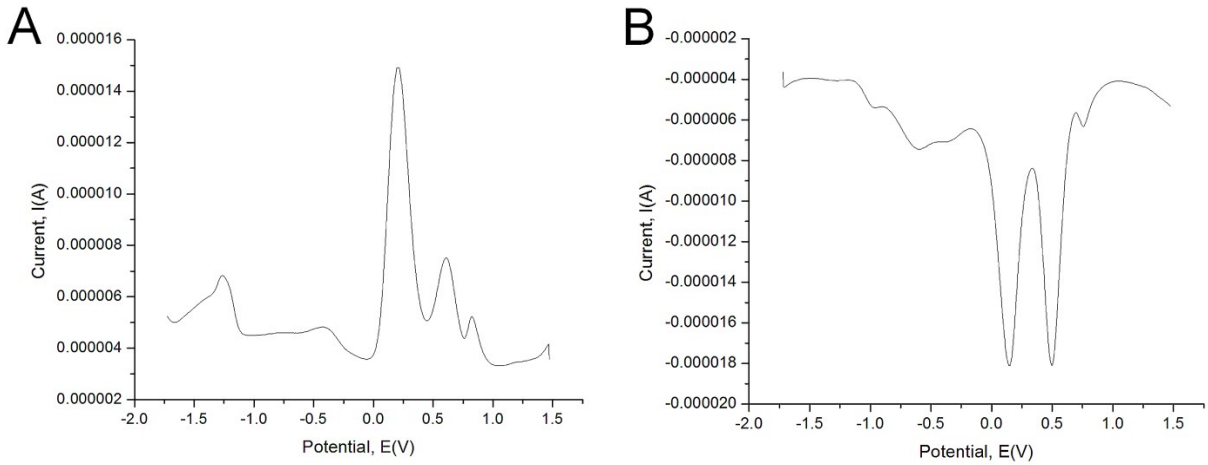

Fig. S30. Differential pulse voltammograms of $\{Fe(ebit)Cl_2\}_n$ (**7**; 10 mM) in acetonitrile: A) negative mode and B) positive mode; potentials are reported vs. NHE.

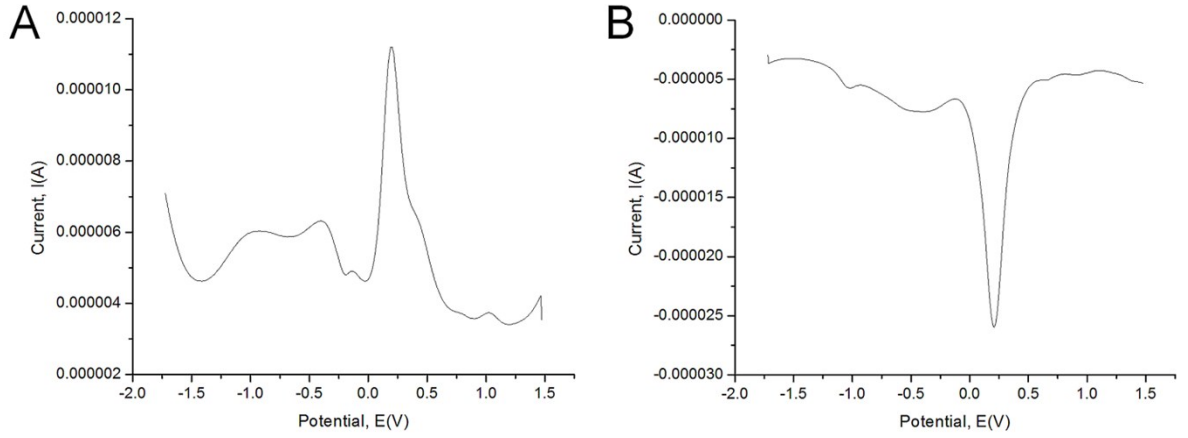

Fig. S31. Differential pulse voltammograms of $\{Fe(ebis)Cl_2\}_n$ (**8**; 10 mM) in acetonitrile: A) negative mode and B) positive mode; potentials are reported vs. NHE.

DFT Cartesian coordinates for iron-thione and -selone complexes **1-6**.

1

16	-1.824608	-0.000413	-1.627348
6	-4.722144	0.681042	0.899951
6	-4.721994	-0.681365	0.900256
1	-5.332197	1.384318	1.446172
1	-5.331898	-1.384529	1.446786
6	-3.113775	-0.000292	-0.487485
7	-3.732573	-1.084373	0.036488
7	-3.732813	1.083880	0.036003
6	-3.355155	2.456101	-0.255513
1	-2.364706	2.661267	0.160779
1	-3.330027	2.603321	-1.337628
1	-4.098078	3.118547	0.192503
6	-3.354639	-2.456642	-0.254439
1	-4.097428	-3.119044	0.193864
1	-3.329489	-2.604326	-1.336491
1	-2.364142	-2.661434	0.161924
16	1.824597	0.000314	-1.627403
6	4.722076	0.680709	0.900276
6	4.721931	-0.681695	0.899996
26	0.000041	0.000386	-0.012465
17	0.000249	-1.958296	1.173579
17	-0.000209	1.959234	1.173243
6	3.113809	-0.000035	-0.487568
7	3.732568	-1.084335	0.035987
7	3.732798	1.083916	0.036435
6	3.355150	2.456267	-0.254462
6	3.354572	-2.456481	-0.255409
1	5.332126	1.383755	1.446797
1	5.331817	-1.385093	1.446245
1	3.329948	2.603955	-1.336511
1	2.364728	2.661303	0.161961
1	4.098129	3.118498	0.193778
1	4.097880	-3.119054	0.191780
1	2.364463	-2.661663	0.161689
1	3.328440	-2.603475	-1.337530

2

34	1.937254	0.000056	1.523204
6	4.681701	0.681221	-1.383202
6	4.681707	-0.681335	-1.383144
1	5.231882	1.385158	-1.988931
1	5.231893	-1.385318	-1.988815
6	3.227232	0.000002	0.162271
7	3.786663	-1.082815	-0.421685
7	3.786653	1.082774	-0.421778
6	3.436336	2.458396	-0.108696
1	2.414087	2.660539	-0.441355
1	3.504351	2.613555	0.970154
1	4.138568	3.116079	-0.624379
6	3.436345	-2.458412	-0.108500
1	4.138586	-3.116135	-0.624120
1	3.504345	-2.613486	0.970363
1	2.414101	-2.660585	-0.441156
34	-1.937239	0.000061	1.523114
6	-4.681699	0.681154	-1.383296
6	-4.681620	-0.681402	-1.383283
26	0.000053	0.000033	-0.143289
17	0.000103	-1.950606	-1.348479
17	0.000104	1.950601	-1.348594
6	-3.227188	-0.000025	0.162150
7	-3.786694	-1.082858	-0.421706
7	-3.786818	1.082732	-0.421727
6	-3.436758	2.458373	-0.108439
6	-3.436457	-2.458451	-0.108408
1	-5.231905	1.385078	-1.989019
1	-5.231743	-1.385401	-1.988995
1	-3.504804	2.613375	0.970432
1	-2.414538	2.660730	-0.441059
1	-4.139098	3.116009	-0.624036
1	-4.138713	-3.116182	-0.623998
1	-2.414213	-2.660678	-0.441034
1	-3.504478	-2.613456	0.970464

3A

16	-1.607790	0.650769	-1.346705
6	-5.289047	0.538667	-0.000654
6	-5.264724	-0.585395	-0.769211
1	-6.093868	0.987054	0.563541
1	-6.047053	-1.292690	-1.003155
6	-3.234600	0.323752	-0.830572
7	-3.991380	-0.703594	-1.272210
7	-4.031193	1.092323	-0.056028
6	-3.638259	2.329266	0.598618
1	-3.304109	2.131751	1.621196
1	-2.831621	2.789637	0.026251
1	-4.495192	3.004139	0.620575
6	-3.553882	-1.719358	-2.221406
1	-4.274118	-2.537948	-2.208089
1	-3.499419	-1.294520	-3.226677
1	-2.568763	-2.090715	-1.935664
16	1.607261	-0.719018	-1.305700
6	5.271951	0.518645	-0.777470
6	5.292186	-0.580071	0.026993
26	0.000844	0.013835	0.235375
6	3.236894	-0.381273	-0.804810
7	4.031461	-1.128651	-0.007769
7	3.998048	0.627206	-1.281236
6	3.565797	1.611813	-2.264943
6	3.634549	-2.342757	0.686437
1	6.057352	1.213923	-1.035902
1	6.095898	-1.014075	0.603864
1	3.525190	1.157109	-3.257782
1	2.575277	1.985065	-2.001542
1	4.281008	2.434961	-2.267971
1	4.491492	-3.016132	0.735526
1	3.295362	-2.110795	1.700032
1	2.830952	-2.822749	0.126032
6	0.859492	2.475084	2.116383
6	-0.868860	-2.317148	2.270577
6	1.247176	3.606518	2.939562
1	1.050026	4.536871	2.398601
1	0.674438	3.599678	3.871483
1	2.314427	3.543354	3.171449
6	-1.261267	-3.390941	3.165593
1	-2.332874	-3.321791	3.374521
1	-1.047102	-4.355415	2.695509
1	-0.704768	-3.312483	4.104052
7	0.553051	1.580751	1.462095
7	-0.558621	-1.468430	1.559759

3B

16	1.543122	0.497346	1.290202
6	4.401462	1.870091	-1.031343
6	5.120432	1.308206	-0.021790
1	4.724751	2.407874	-1.910678
1	6.187083	1.270904	0.144892
6	2.964231	0.956140	0.402182
7	4.220025	0.746230	0.851502
7	3.071296	1.651602	-0.751163
6	1.969351	2.114528	-1.576743
1	1.730656	1.380355	-2.351651
1	1.093372	2.278355	-0.948334
1	2.252706	3.056560	-2.048678
6	4.565019	0.085632	2.103914
1	5.632306	-0.136708	2.093015
1	4.335672	0.737924	2.950115
1	3.998447	-0.842310	2.197480
16	-1.556211	0.431960	-1.338032
6	-5.104946	1.307417	0.014111
6	-4.363444	2.009907	0.913515
26	-0.008021	-0.705276	0.006969
6	-2.957645	0.956178	-0.453309
7	-3.039846	1.789833	0.606658
7	-4.223506	0.661077	-0.819074
6	-4.598424	-0.154268	-1.967421
6	-1.921611	2.385116	1.318603
1	-6.175775	1.224049	-0.101311
1	-4.667350	2.647094	1.731251
1	-4.433486	0.401290	-2.893858
1	-3.999684	-1.066347	-1.981268
1	-5.654392	-0.410500	-1.877925
1	-2.197958	3.393311	1.631516
1	-1.662665	1.790341	2.199035
1	-1.061401	2.439592	0.651016
6	1.307479	-2.806507	-2.038980
6	-1.322869	-2.660204	2.193039
6	1.847965	-3.766363	-2.983664
1	2.774489	-3.376024	-3.414932
1	2.058455	-4.708248	-2.468437
1	1.122030	-3.942877	-3.782815
6	-1.860894	-3.550748	3.204611
1	-1.103446	-3.732957	3.972646
1	-2.741438	-3.093659	3.665615
1	-2.146772	-4.500288	2.742550
7	0.874535	-2.047304	-1.292324
7	-0.891685	-1.955752	1.393617

	4A				4B		
34	1.687212	-0.623857	-1.243479	34	-1.647853	-0.434177	1.338639
6	5.468145	-0.439579	0.262421	6	-4.442214	-1.842860	-1.282184
6	5.414814	0.745267	-0.406572	6	-5.231605	-1.227879	-0.359743
1	6.276406	-0.903386	0.809198	1	-4.700390	-2.401740	-2.170022
1	6.171124	1.501849	-0.557432	1	-6.307283	-1.155955	-0.290758
6	3.427004	-0.236432	-0.602516	6	-3.112159	-0.919154	0.244949
7	4.149701	0.854476	-0.932012	7	-4.395719	-0.661230	0.572284
7	4.236319	-1.034659	0.125398	7	-3.137547	-1.648655	-0.890291
6	3.895139	-2.339304	0.671550	6	-1.988828	-2.177264	-1.606799
1	3.719441	-2.263798	1.748074	1	-1.800013	-1.590058	-2.509585
1	2.996956	-2.704075	0.172083	1	-1.115210	-2.135530	-0.956124
1	4.718278	-3.030945	0.482952	1	-2.184984	-3.215299	-1.882450
6	3.707166	1.936606	-1.802895	6	-4.840909	0.050744	1.764319
1	4.330292	2.811507	-1.613250	1	-5.897285	0.293052	1.645420
1	3.802188	1.638872	-2.850098	1	-4.707671	-0.575655	2.649633
1	2.663970	2.172909	-1.590784	1	-4.265261	0.970525	1.880007
34	-1.687183	0.624386	-1.243600	34	1.674634	-0.349277	-1.392671
6	-5.414182	-0.746157	-0.406978	6	5.182098	-1.275936	0.402160
6	-5.468178	0.438623	0.262100	6	4.362863	-2.061802	1.153397
26	-0.000067	0.000107	0.442542	26	0.012732	0.819884	0.009790
6	-3.426892	0.236615	-0.602709	6	3.094403	-0.941683	-0.292038
7	-4.236649	1.034357	0.125212	7	3.079358	-1.849195	0.706927
7	-4.148993	-0.854644	-0.932364	7	4.383507	-0.590303	-0.481166
6	-3.705246	-1.936647	-1.802800	6	4.874849	0.315246	-1.512897
6	-3.896338	2.339386	0.670987	6	1.909085	-2.524503	1.244109
1	-6.170104	-1.503109	-0.557913	1	6.255884	-1.158973	0.421598
1	-6.276745	0.902023	0.808769	1	4.588270	-2.751175	1.954156
1	-3.793229	-1.636607	-2.849948	1	4.872080	-0.183662	-2.485075
1	-2.664138	-2.177260	-1.585220	1	4.238038	1.199980	-1.558129
1	-4.332642	-2.809597	-1.618403	1	5.893124	0.609239	-1.256601
1	-4.718824	3.031154	0.479972	1	2.156261	-3.571631	1.427910
1	-3.723043	2.264727	1.747953	1	1.590948	-2.054611	2.178531
1	-2.996949	2.703449	0.173179	1	1.101513	-2.466196	0.514396
6	-0.736739	-2.429615	2.417256	6	-1.239322	2.956263	-2.045805
6	0.736174	2.429397	2.417996	6	1.270493	2.792980	2.219644
6	-1.061415	-3.544469	3.289058	6	-1.747010	3.930683	-2.994099
1	-0.849506	-4.485901	2.773542	1	-2.662439	3.550760	-3.457062
1	-0.461197	-3.487175	4.201729	1	-1.967539	4.867542	-2.474045
1	-2.122511	-3.508155	3.552596	1	-0.997256	4.112863	-3.769628
6	1.060626	3.544060	3.290127	6	1.778957	3.690933	3.240248
1	0.853186	4.485656	2.773099	1	0.961390	3.994868	3.900565
1	0.456873	3.489101	4.200609	1	2.547200	3.180374	3.828393
1	2.120630	3.505057	3.557647	1	2.213748	4.576539	2.767693
7	-0.479828	-1.548622	1.724808	7	-0.831794	2.185549	-1.296639
7	0.479427	1.548582	1.725260	7	0.862354	2.082494	1.413475

5a

26	-0.000872	0.002066	0.000832
16	0.901702	-1.828165	1.226329
16	1.837569	0.917831	-1.204084
7	2.937042	-0.833513	2.800618
7	3.654097	-1.750432	0.972651
7	0.867451	2.974313	-2.766914
7	1.754166	3.665607	-0.914153
6	2.535112	-1.434658	1.660050
6	4.309987	-0.763222	2.826787
1	4.852087	-0.327700	3.653354
6	4.759779	-1.336299	1.676660
1	5.765732	-1.485903	1.312801
6	2.047573	-0.373911	3.854262
1	1.536977	-1.225995	4.309793
1	1.310091	0.316552	3.439094
1	2.643689	0.138625	4.609963
6	3.692807	-2.400581	-0.327008
1	2.828691	-3.059700	-0.418772
1	4.608878	-2.988935	-0.398098
1	3.672389	-1.651597	-1.123787
6	1.450188	2.556495	-1.622496
6	0.794967	4.347327	-2.773703
1	0.371665	4.900983	-3.598912
6	1.349691	4.780906	-1.608388
1	1.493073	5.781551	-1.228021
6	0.420727	2.099568	-3.838287
1	-0.327016	1.399571	-3.458359
1	1.270273	1.544870	-4.243735
1	-0.019704	2.713931	-4.624265
6	2.387058	3.684406	0.394427
1	3.073505	2.840058	0.468968
1	1.630008	3.615753	1.180791
1	2.943690	4.616620	0.500602
16	-0.932615	1.825256	1.216465
16	-1.814308	-0.917936	-1.236566
7	-3.003725	0.833801	2.746572
7	-3.676730	1.740150	0.896642
7	-0.774612	-2.964073	-2.769726
7	-1.751670	-3.666407	-0.967244
6	-2.574771	1.430089	1.613294
6	-4.376570	0.758718	2.737709
1	-4.938331	0.325153	3.552029
6	-4.798657	1.325642	1.573992
1	-5.795453	1.471463	1.184557
6	-2.139528	0.375966	3.821767
1	-1.581249	1.219811	4.234030
1	-1.442548	-0.375575	3.443661
1	-2.762466	-0.062627	4.601991
6	-3.681925	2.388828	-0.404301
1	-2.846473	3.088188	-0.456108
1	-4.620174	2.933230	-0.519834
1	-3.589014	1.642581	-1.198409
6	-1.409632	-2.553213	-1.651052
6	-0.708423	-4.337421	-2.784878
1	-0.248863	-4.886323	-3.593821
6	-1.319973	-4.777937	-1.650986
1	-1.485103	-5.781086	-1.286111
6	-0.281465	-2.082745	-3.815002
1	0.391913	-1.339171	-3.383046
1	-1.118977	-1.579236	-4.304452
1	0.258751	-2.683923	-4.547040
6	-2.442969	-3.689516	0.311513
1	-3.167412	-2.874419	0.340640
1	-1.726073	-3.575916	1.129595
1	-2.963440	-4.643089	0.409674

6a

26	0.000006	-0.000012	0.003658
34	-2.184670	0.066624	-1.213951
34	0.069177	2.174452	1.236006
7	-1.826148	2.486052	-2.794424
7	-3.347707	2.711936	-1.271028
7	2.459523	1.864461	2.849496
7	2.780445	3.227153	1.198426
6	-2.438507	1.851419	-1.774013
6	-2.348992	3.750046	-2.932716
1	-2.009170	4.437688	-3.693055
6	-3.306887	3.891460	-1.975014
1	-3.953666	4.725469	-1.745679
6	-0.810577	1.901876	-3.654996
1	-1.248983	1.097476	-4.251300
1	0.009067	1.504982	-3.051672
1	-0.431752	2.679725	-4.318981
6	-4.258492	2.424776	-0.173086
1	-4.986834	1.669257	-0.476824
1	-4.777668	3.345697	0.093689
1	-3.695216	2.060484	0.688008
6	1.867327	2.412411	1.768278
6	3.749113	2.328633	2.956902
1	4.408516	2.027194	3.757449
6	3.951207	3.183869	1.917556
1	4.820473	3.762212	1.640390
6	1.816552	0.958174	3.787349
1	1.425062	0.087755	3.255844
1	1.000183	1.472712	4.300313
1	2.558896	0.636626	4.518719
6	2.594100	4.025076	-0.003599
1	1.528180	4.081382	-0.224825
1	3.121511	3.564016	-0.843035
1	2.983194	5.030309	0.169574
34	2.184849	-0.066636	-1.213653
34	-0.069366	-2.174459	1.236011
7	1.826558	-2.486076	-2.794162
7	3.347882	-2.711954	-1.270530
7	-2.459903	-1.864438	2.849215
7	-2.780654	-3.227094	1.198083
6	2.438767	-1.851435	-1.773667
6	2.349405	-3.750081	-2.932350
1	2.009683	-4.437734	-3.692724
6	3.307175	-3.891478	-1.974521
1	3.953921	-4.725485	-1.745086
6	0.811132	-1.901898	-3.654905
1	1.249632	-1.097466	-4.251098
1	-0.008638	-1.505043	-3.051727
1	0.432456	-2.679734	-4.318990
6	4.258508	-2.424784	-0.172458
1	4.986896	-1.669272	-0.476101
1	4.777643	-3.345705	0.094401
1	3.695111	-2.060481	0.688551
6	-1.867592	-2.412372	1.768052
6	-3.749523	-2.328568	2.956445
1	-4.409018	-2.027128	3.756916
6	-3.951513	-3.183771	1.917052
1	-4.820762	-3.762082	1.639764
6	-1.817016	-0.958211	3.787185
1	-1.425424	-0.087786	3.255764
1	-1.000732	-1.472801	4.300231
1	-2.559441	-0.636663	4.518472
6	-2.594169	-4.025035	-0.003908
1	-1.528226	-4.081304	-0.225034
1	-3.121520	-3.564010	-0.843400
1	-2.983239	-5.030281	0.169247