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Supplementary Information

Nitrogen-Rich Multinuclear Ferrocenophanes as Multichannel Chemosensor Molecules for Transition and Heavy-Metal Cations. *Sensors* 2014, *14*, 14339-14355

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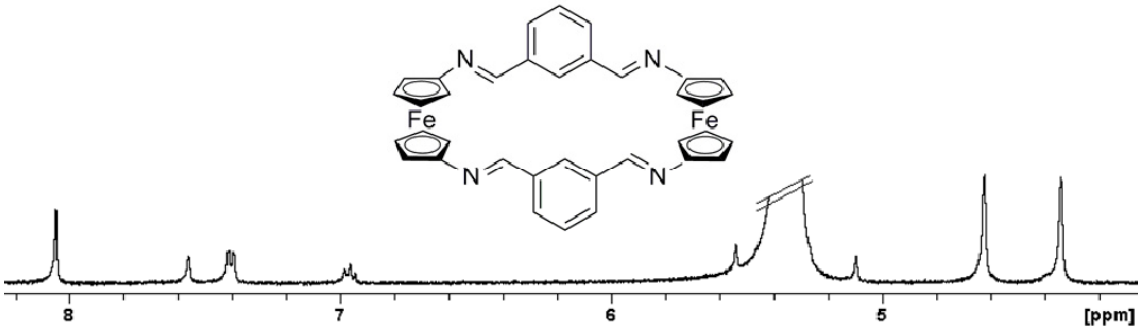
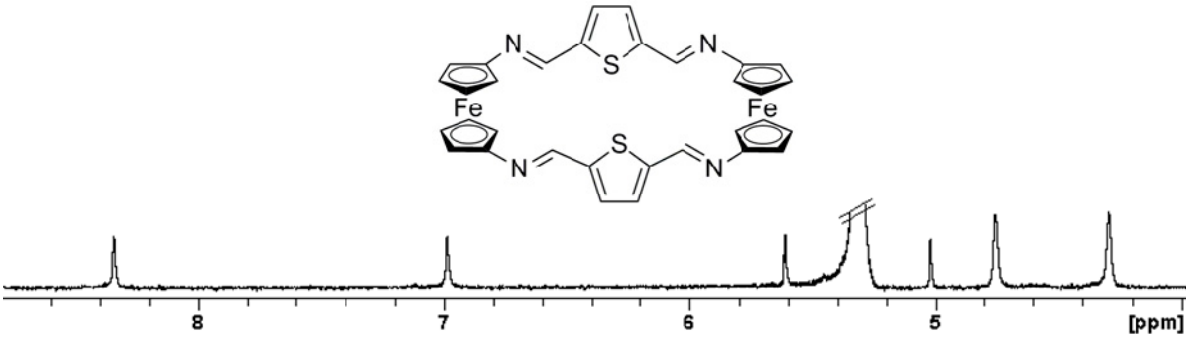
Bis[1,3-phenylene-bis(methylimino)][7.7]ferrocenophane (**3**)

^{1}H-NMR (400 MHz, CD_2Cl_2)



Bis[thiophene-2,5-diylbis(methylimino)][7.7]ferrocenophane (**4**)
^{1}H-NMR (300 MHz, CD_2Cl_2)



Bis[1,10-phenanthroline-2,9-diylbis(methylimino)][7.7]ferrocenophane (**5**)
^{1}H-NMR (400 MHz, CD_2Cl_2)

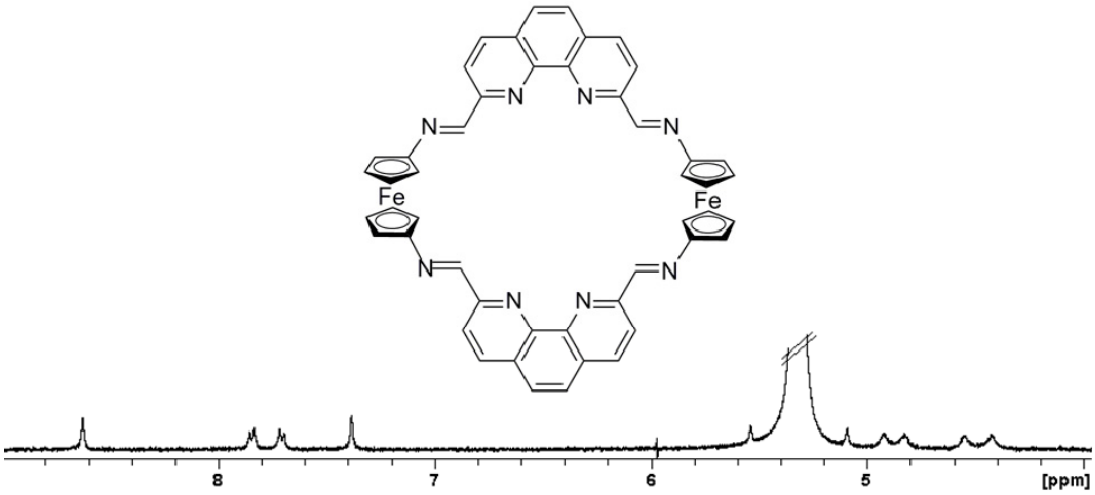


Figure S1. Evolution of the OSWV of receptor **3** in CH_2Cl_2 (c = $1\cdot\times 10^{-4}$ M) (black line) upon addition of 1.4 equiv of (**a**) Hg^{2+} and (**b**) Zn^{2+} ($2.5\cdot\times 10^{-2}$ M en CH_3CN) (red line), using [*n*-Bu_4N]PF_6 as supporting electrolyte.

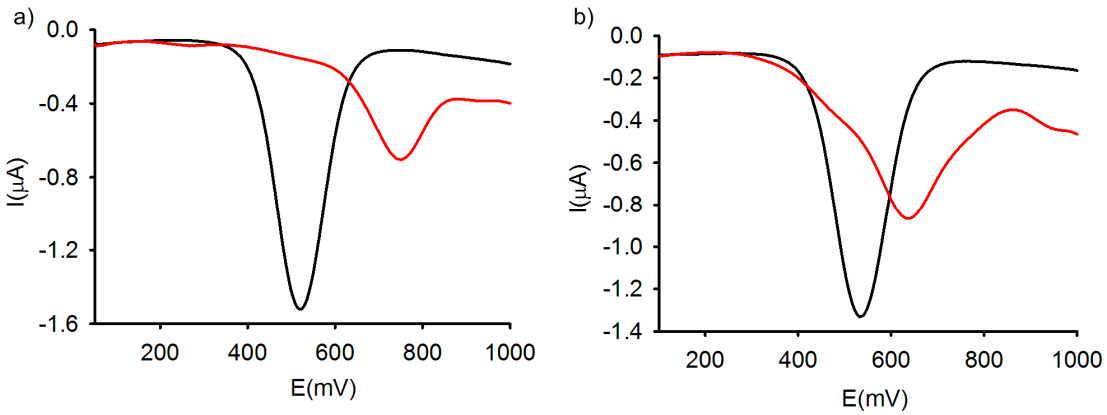


Figure S2. Evolution of the CV of receptor 3 in CH2Cl2 (c = 1·× 10^{-4} M) (black line) upon addition of 1.4 equiv of (**a**) Pb^{2+}, (**b**) Hg^{2+} and (**c**) Zn^{2+} (2.5·× 10^{-2} M en CH3CN) (red line), using [n-Bu4N]PF6 as supporting electrolyte.

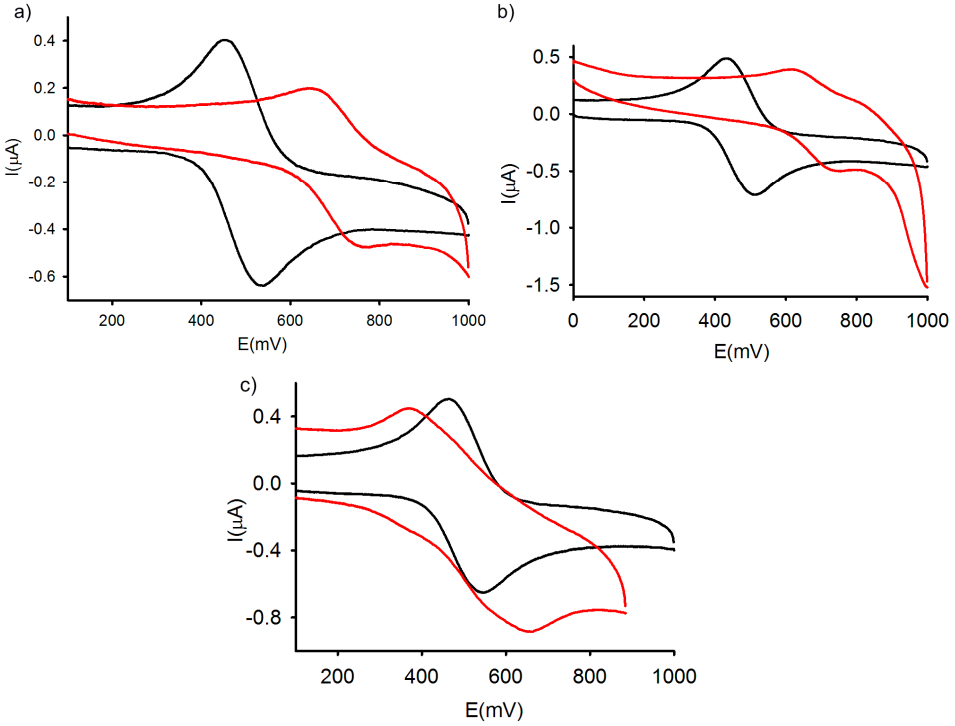


Figure S3. Evolution of the LSV of **3** in CH_2Cl_2 (c = 1·× 10^{-4} M) (black line), obtained using a rotating disk electrode at 100 m Vs^{-1} and 1000 rpm, upon addition of 1.4 equiv of (**a**) Pb^{2+}, (**b**) Hg^{2+}, (**c**) Zn^{2+} and (**d**) Cu^{2+} (2.5·× 10^{-2} M en CH_3CN) (red line), using [*n*-Bu_4N]PF_6 as supporting electrolyte.

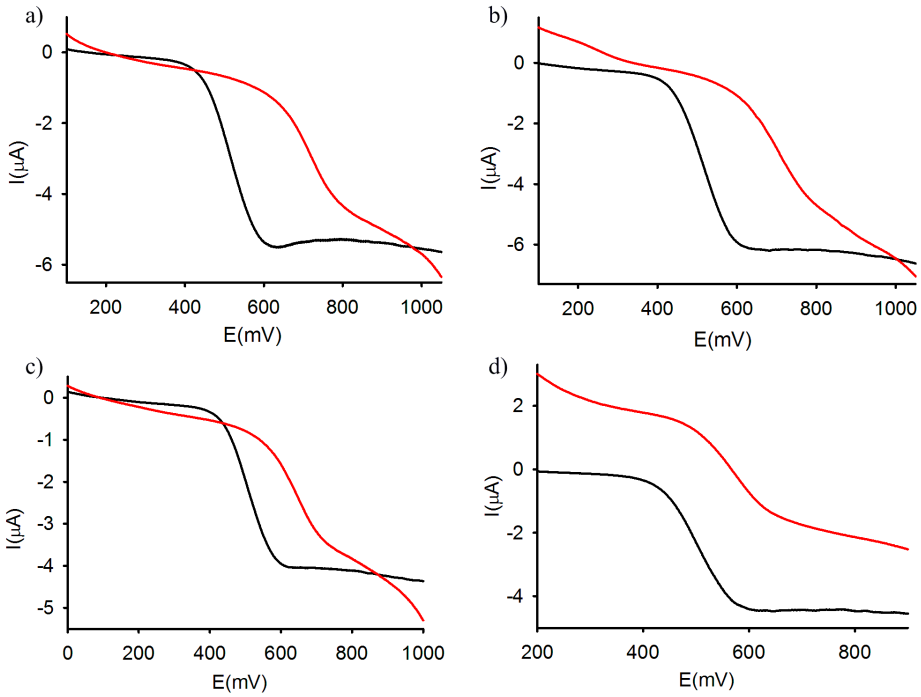


Figure S4. Evolution of the OSWV of **4** in CH_2Cl_2 (c = 1·× 10^{-4} M) (black line) upon addition of 1.4 equiv of (**a**) Hg^{2+} and (**b**) Zn^{2+} (2.5·× 10^{-2} M en CH_3CN) (red line), using [*n*-Bu_4N]PF_6 as supporting electrolyte.

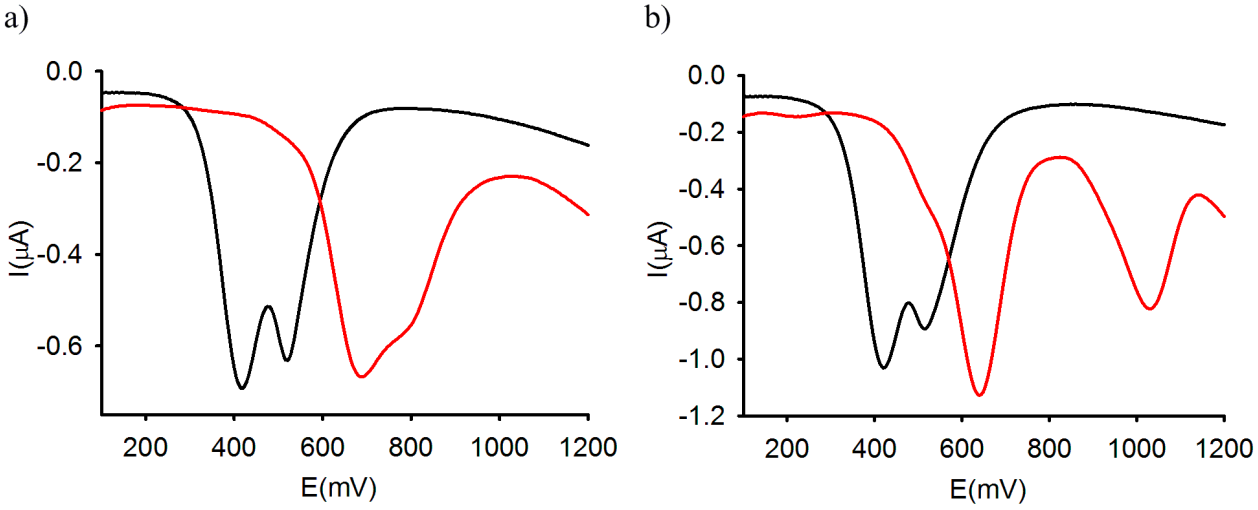


Figure S5. Changes in the absorption spectra of **3** (c =5 × 10^{-5} M) in CH_2Cl_2 upon addition of increasing amounts Zn^{2+} (c = 2.5·× 10^{-2} M in CH_3CN) until 2 equiv. The arrows indicate the absorptions that increase or decrease during the experiment. Inset: Titration profile showing the 1:1 (M^{+2}/receptor) stoichiometry for the complex formed with Zn^{2+}.

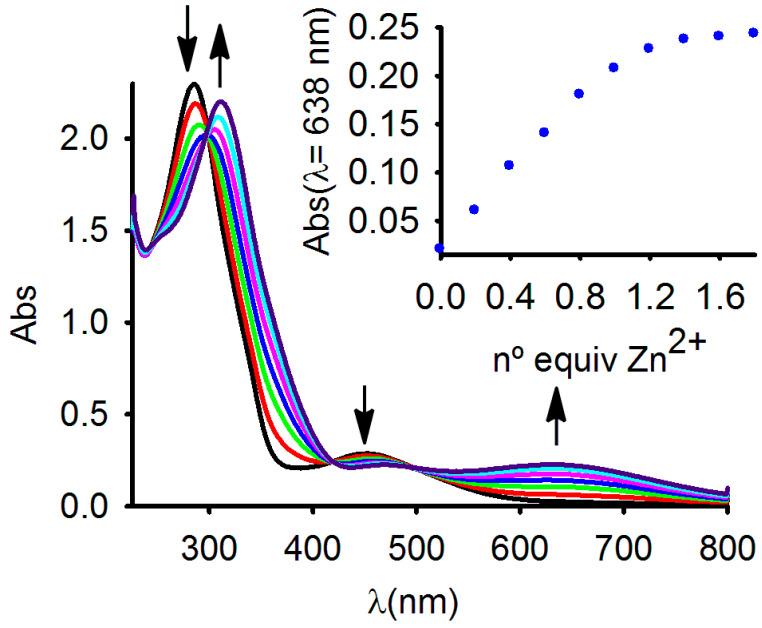


Figure S6. Absorbance of **3** (c = 5·× 10^{-5} M in CH_2Cl_2) at each concentration of (**a**) Pb^{2+}, (**b**) Hg^{2+} and (**c**) Zn^{2+} added, normalized between the minimum absorbance, found at zero equiv of cation, and the maximum absorbance.

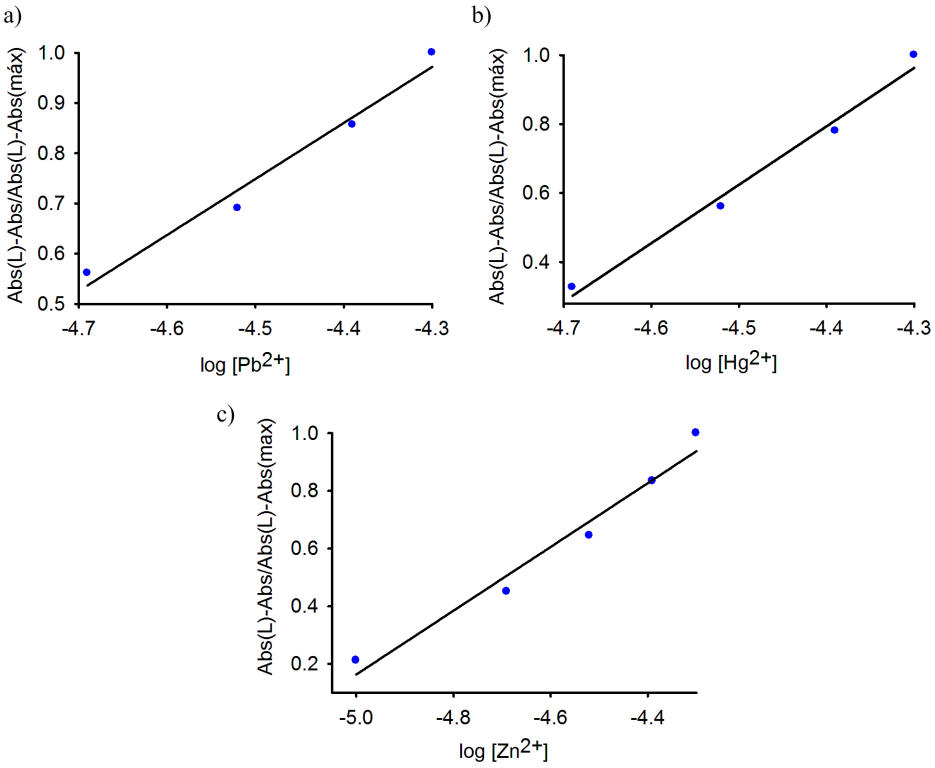


Figure S7. Changes in the absorption spectra of **4** (c =1 × 10^{-4} M) in CH_2Cl_2 upon addition of increasing amounts Zn^{2+} (c = 2.5·× 10^{-2}M in CH_3CN) until 2 equiv. The arrows indicate the absorptions that increase or decrease during the experiment. Inset: Titration profile showing the 1:1 (M^{+2}/receptor) stoichiometry for the complex formed with Zn^{2+}.

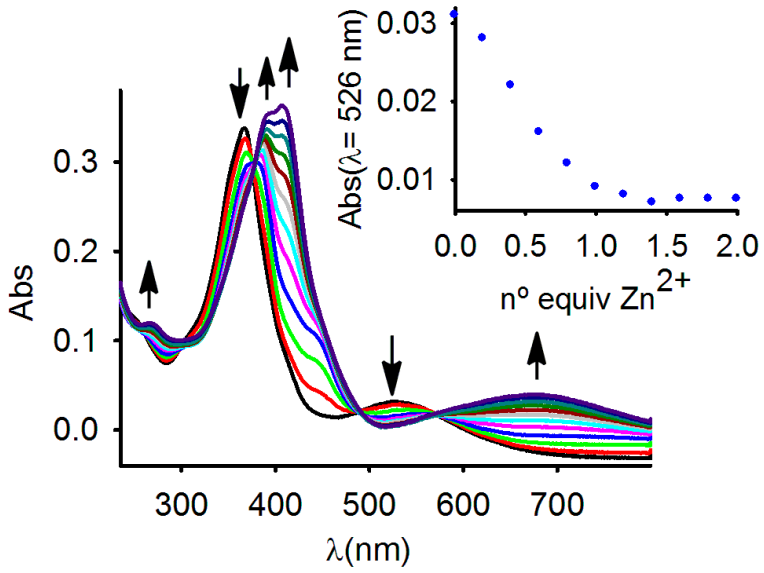


Figure S8. Absorbance of **4** (c = 1·× 10^{-4}M in CH_2Cl_2) at each concentration of (**a**) Pb^{2+}, (**b**) Hg^{2+} and (**c**) Zn^{2+} added, normalized between the minimum absorbance, found at zero equiv of cation, and the maximum absorbance.

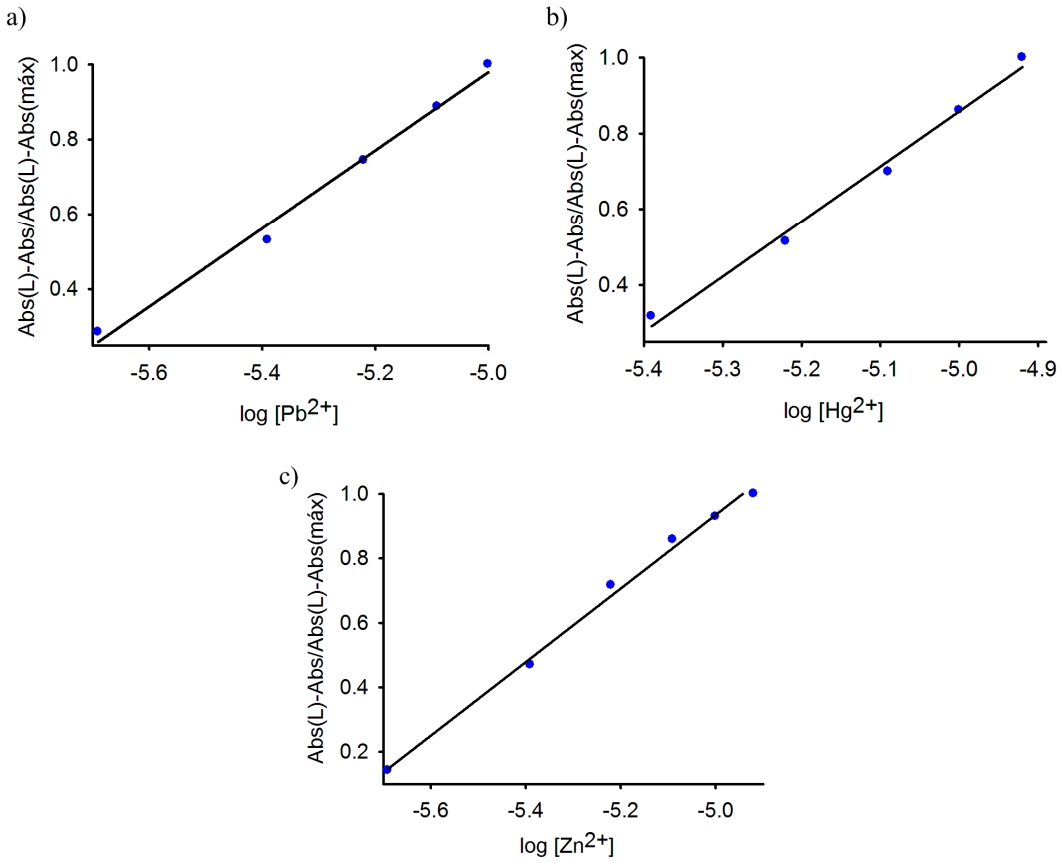


Figure S9. Evolution of the ^{1}H-NMR spectrum of the free ligand **3**, in CD_2Cl_2, upon addition of Hg^{2+}. The crossed signal corresponds to the solvent.

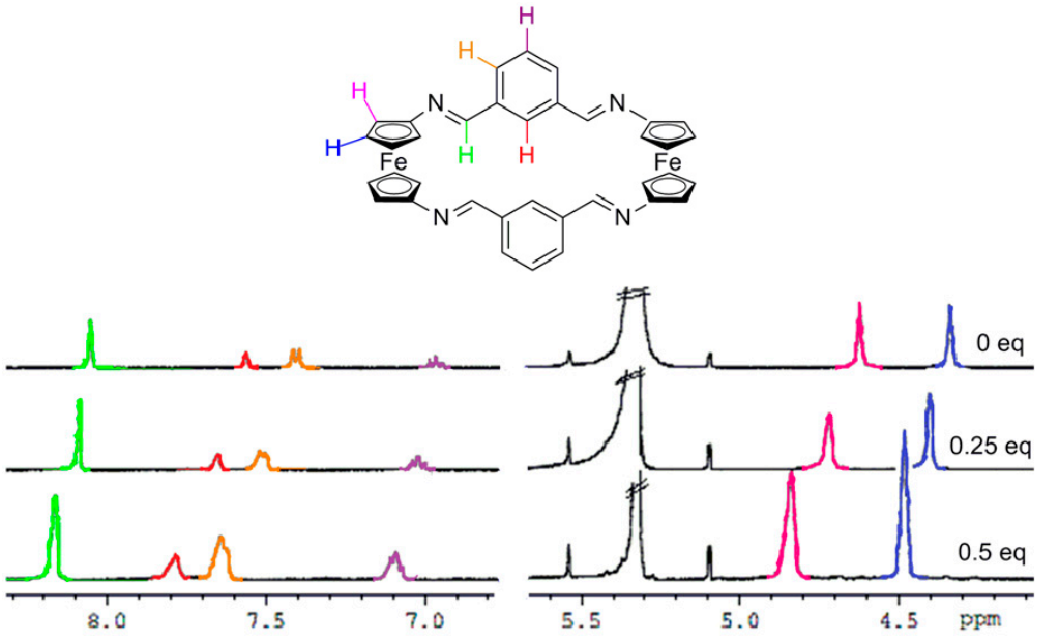


Figure S10. Evolution of the ^{1}H-NMR spectrum of the free ligand **3**, in CD_2Cl_2, upon addition of Pb^{2+}. The crossed signal corresponds to the solvent.

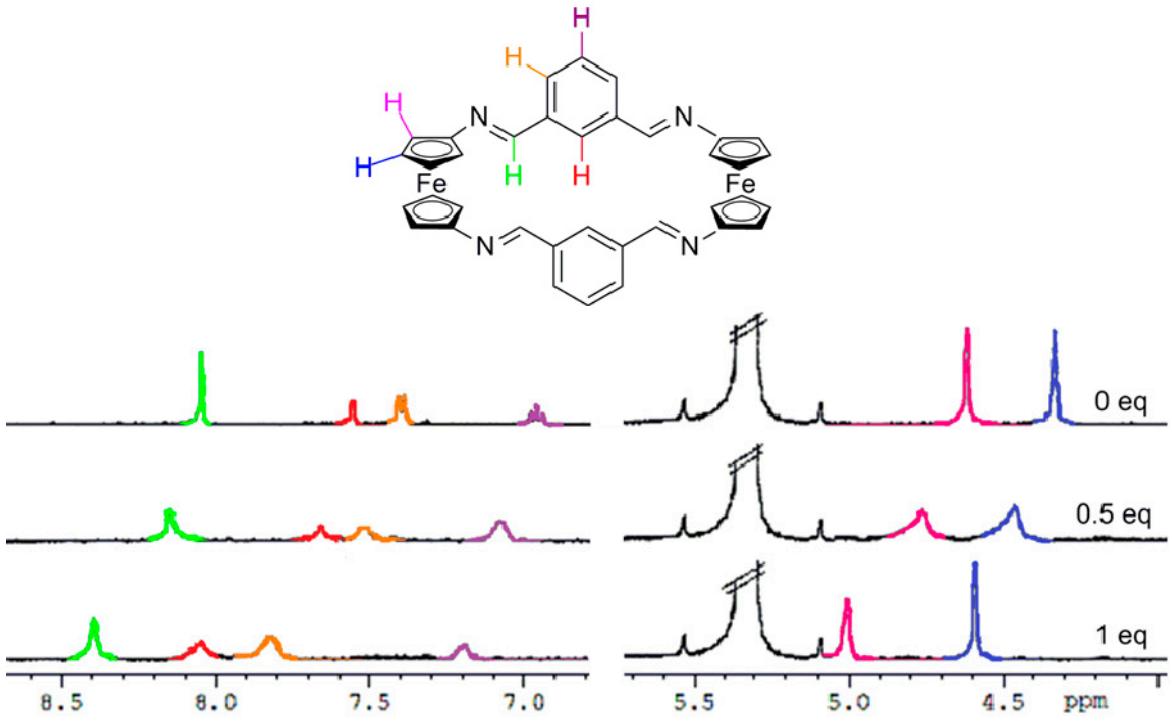


Figure S11. Evolution of the ^{1}H-NMR spectrum of the free ligand **4**, in CD_2Cl_2, upon addition of Hg^{2+}. The crossed signal corresponds to the solvent.

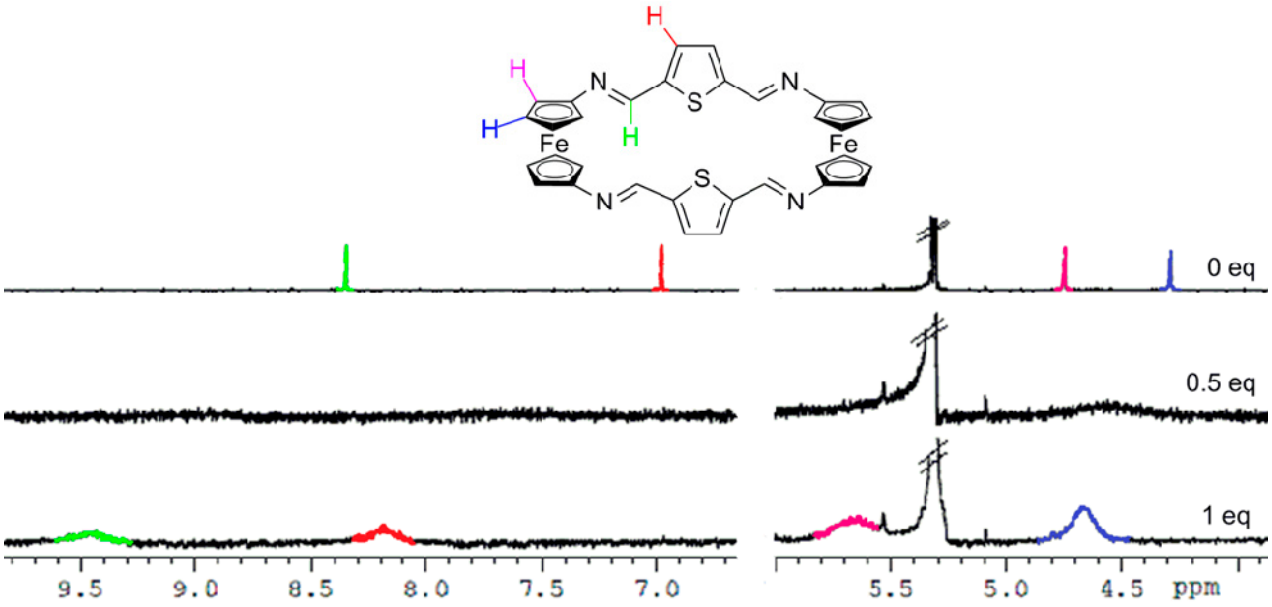
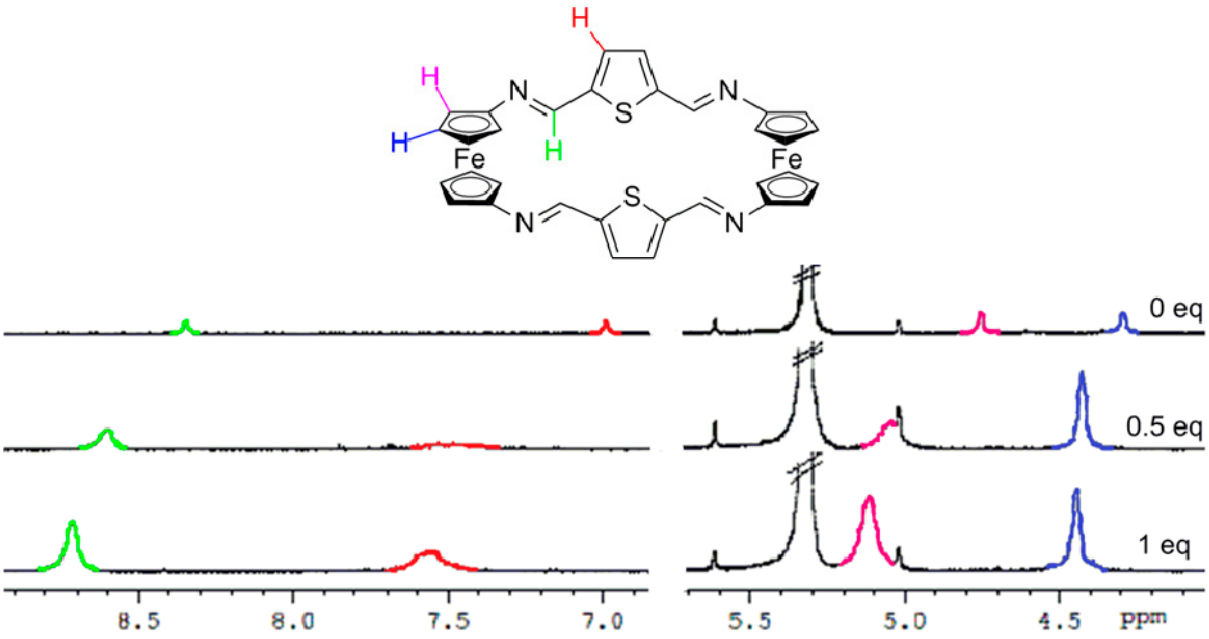
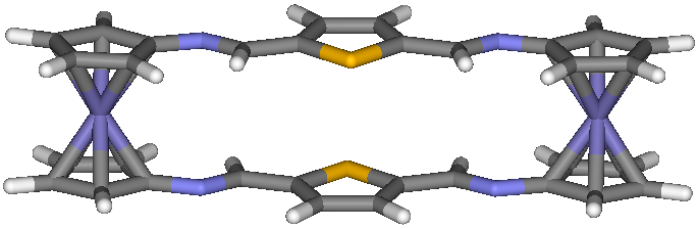


Figure S12. Evolution of the ^{1}H-NMR spectrum of the free ligand **4**, in CD_2Cl_2, upon addition of Zn^{2+}. The crossed signal corresponds to the solvent.



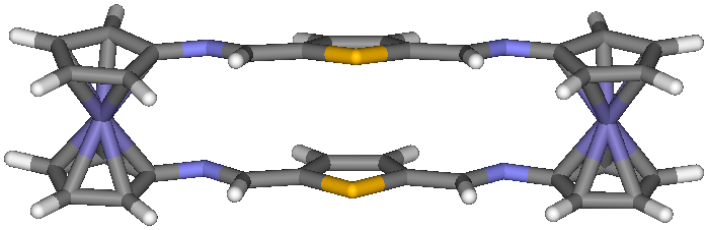
Cartesian coordinates (Å) and energies (hartree) for all computed species.



Ligand **4**$^{EE\text{-}anti}$: E = −4774.006078797 au (B3LYP-D3/def2-SVP)

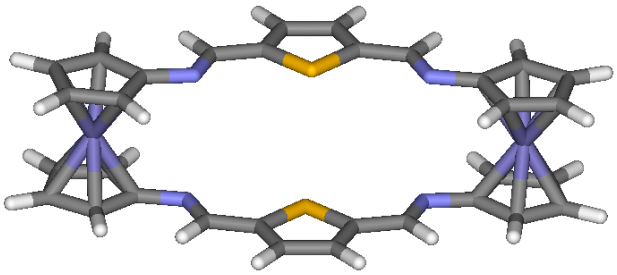
C	0.016013	−0.026762	−0.007001	C	−2.485895	0.085248	−2.688193
C	0.126924	−0.104121	1.423007	C	−3.801611	0.068783	−2.233956
C	1.508598	−0.081006	1.768593	C	−4.746834	0.089563	−3.280301
C	2.265982	0.016468	0.557936	C	−4.161686	0.120332	−4.542118
C	1.359919	0.034895	−0.539584	S	−2.429107	0.140569	−4.422304
H	−0.723752	−0.186839	2.096631	H	−4.036477	0.038961	−1.168840
H	1.921271	−0.141132	2.774616	H	−5.830989	0.080136	−3.155191
H	3.352801	0.037904	0.479847	C	−4.775940	0.138064	−5.853082
H	1.641598	0.071264	−1.590306	H	−4.071847	0.214357	−6.702367
Fe	1.100470	−1.693542	0.538332	N	−6.047700	0.087652	−6.028463
C	0.601294	−3.275489	−0.687861	C	−6.560989	0.177981	−7.316435
C	2.011692	−3.282627	−0.411359	C	−5.875301	0.277992	−8.586460
C	2.192651	−3.389985	0.997448	C	−6.858322	0.358199	−9.611593
C	0.898344	−3.452853	1.607539	C	−8.152475	0.290321	−9.001767
C	−0.084538	−3.371334	0.582388	C	−7.971279	0.181487	−7.593158
H	2.785093	−3.200188	−1.173067	H	−4.798538	0.270268	−8.746608
H	3.146609	−3.406126	1.522071	H	−6.649253	0.427234	−10.679018
H	0.689316	−3.519435	2.675133	H	−9.106446	0.304248	−9.526433
H	−1.161279	−3.359523	0.742502	H	−8.744447	0.095373	−6.831638
N	−1.208424	−0.041450	−0.662967	Fe	−7.055176	−1.403441	−8.545773
C	−1.244130	0.054652	−1.943089	C	−5.968431	−3.070092	−8.003730
H	−0.322902	0.126889	−2.550222	C	−7.313236	−3.136072	−7.473840

C	−8.217322	−3.115312	−8.573013	C	−3.470524	−3.185640	−5.318955
C	−7.457794	−3.012192	−9.781945	C	−2.154375	−3.167364	−5.771774
C	−6.076797	−2.987817	−9.433700	C	−1.210296	−3.188631	−4.724453
H	−7.596862	−3.176518	−6.423764	C	−1.796725	−3.221516	−3.463269
H	−9.304253	−3.138865	−8.496957	S	−3.529177	−3.243196	−3.584935
H	−7.868670	−2.949015	−10.788534	H	−1.918362	−3.135823	−6.836557
H	−5.224986	−2.901468	−10.105447	H	−0.126012	−3.177929	−4.848279
N	−4.745236	−3.054770	−7.345520	C	−1.183304	−3.239832	−2.151931
C	−4.711369	−3.154831	−6.065602	H	−1.887595	−3.320681	−1.303207
H	−5.633367	−3.230558	−5.460013	N	0.088234	−3.185383	−1.975880



Ligand **4**$^{EE-syn}$: E = −4774.002850680 au (B3LYP−D3/def2−SVP)

C	−0.012113	−0.026487	0.002515	C	−7.745462	−6.102451	0.161834
C	1.423610	−0.043272	0.043297	C	−8.994201	−5.374394	0.180139
C	1.890139	1.302842	0.001318	C	−10.057088	−6.322995	0.175323
C	0.751012	2.164728	−0.073040	C	−9.486902	−7.636649	0.131002
C	−0.423476	1.356322	−0.096114	C	−8.068236	−7.501999	0.122651
H	2.019318	−0.952239	0.090998	H	−9.112465	−4.292502	0.207547
H	2.929890	1.626946	0.007613	H	−11.119553	−6.080511	0.183355
H	0.778346	3.252669	−0.130182	H	−10.041909	−8.572946	0.091653
H	−1.446031	1.724428	−0.157339	H	−7.328517	−8.299414	0.075194
Fe	−8.894657	−6.535802	−1.508969	Fe	0.782179	0.889118	−1.687462
C	−7.823868	−5.948482	−3.179481	C	0.010155	−0.064340	−3.348230
C	−8.081216	−7.364605	−3.201934	C	−0.271888	1.351872	−3.388024
C	−9.493156	−7.559662	−3.198647	C	0.976063	2.045221	−3.382469
C	−10.120182	−6.272658	−3.143570	C	2.028751	1.079482	−3.326099
C	−9.099918	−5.276961	−3.125033	C	1.439943	−0.217143	−3.290660
H	−7.305946	−8.128486	−3.222317	H	−1.258033	1.811688	−3.399503
H	−10.007125	−8.519766	−3.206275	H	1.113097	3.126406	−3.392309
H	−11.191826	−6.078649	−3.100642	H	3.092843	1.309885	−3.287977
H	−9.260789	−4.202125	−3.059280	H	1.948699	−1.176923	−3.228384
N	−0.775514	−1.184076	0.054325	N	−0.852602	−1.144426	−3.295557
C	−2.054000	−1.115254	−0.040536	C	−2.106132	−0.996915	−3.533068
H	−2.581551	−0.153888	−0.191210	H	−2.540868	−0.024970	−3.836811
C	−2.902304	−2.284464	0.058841	C	−3.019808	−2.114684	−3.420744
C	−2.556241	−3.608585	0.308794	C	−2.725074	−3.406228	−2.999699
C	−3.668237	−4.473422	0.337968	C	−3.851359	−4.247181	−2.972613
C	−4.875070	−3.820672	0.111720	C	−5.018742	−3.611402	−3.375691
S	−4.622254	−2.118469	−0.132050	S	−4.712822	−1.948245	−3.794156
H	−1.517850	−3.903949	0.464231	H	−1.713301	−3.685130	−2.706379
H	−3.634757	−5.548811	0.518266	H	−3.864249	−5.289300	−2.654442
C	−6.212965	−4.371575	0.055901	C	−6.346544	−4.183605	−3.441598
H	−7.027674	−3.637631	−0.094646	H	−7.167834	−3.509379	−3.752680
N	−6.441247	−5.628861	0.176638	N	−6.546045	−5.421473	−3.160413



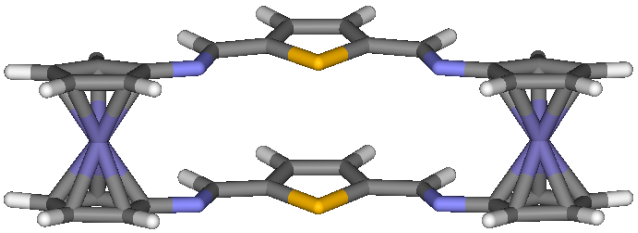
Ligand $\mathbf{4}^{ZZ-anti}$: E = −4774.001526826 au (B3LYP−D3/def2−SVP)

C	0.167479	0.080496	0.065598	C	−3.123470	−8.315485	0.168354
C	1.599922	0.157291	0.012247	C	−4.411808	−8.966611	0.231962
C	1.973002	1.532999	−0.035185	C	−4.188352	−10.374451	0.283968
C	0.776536	2.317233	−0.007583	C	−2.777152	−10.608042	0.235422
C	−0.339958	1.433505	0.038333	C	−2.123485	−9.343202	0.160676
H	2.256255	−0.710477	−0.005186	H	−5.383674	−8.477043	0.234003
H	2.987756	1.923473	−0.098761	H	−4.961000	−11.141325	0.326931
H	0.721992	3.404948	−0.049235	H	−2.292380	−11.583128	0.235320
H	−1.385596	1.735522	0.044286	H	−1.054630	−9.144433	0.102894
Fe	0.772527	1.060479	−1.647259	Fe	−3.397016	−9.582477	−1.447109
C	0.499215	−0.206584	−3.262736	C	−2.792232	−8.602377	−3.160003
C	−0.500744	0.821158	−3.255238	C	−2.284836	−9.955408	−3.132931
C	0.152962	2.085980	−3.329930	C	−3.401352	−10.839101	−3.086885
C	1.564166	1.852352	−3.378230	C	−4.597784	−10.054826	−3.059013
C	1.787578	0.444509	−3.326139	C	−4.224665	−8.679128	−3.106420
H	−1.569612	0.622398	−3.197638	H	−1.239208	−10.257450	−3.139130
H	−0.331782	3.061079	−3.329939	H	−3.346861	−11.926823	−3.045343
H	2.336839	2.619207	−3.421095	H	−5.612540	−10.445276	−2.995299
H	2.759432	−0.045086	−3.328000	H	−4.880958	−7.811333	−3.088815
N	−0.513042	−1.130696	0.090397	N	−2.111662	−7.391203	−3.184862
C	−1.794750	−1.140211	0.116357	C	−0.829949	−7.381743	−3.210623
H	−2.396704	−0.210837	0.125597	H	−0.228037	−8.311146	−3.219644
C	−3.491245	−4.660960	0.117586	C	0.866813	−3.861119	−3.211994
C	−4.488764	−3.694499	0.100344	C	1.864252	−4.827660	−3.194931
C	−3.976649	−2.380682	0.103058	C	1.352031	−6.141433	−3.197664
C	−2.588284	−2.346292	0.122890	C	−0.036338	−6.175713	−3.217344
S	−1.901170	−3.948050	0.138457	S	−0.723319	−4.573901	−3.233351
H	−5.550041	−3.952635	0.084780	H	2.925554	−4.569619	−3.179346
H	−4.582929	−1.472874	0.086661	H	1.958239	−7.049287	−3.181253
C	−3.728393	−6.084827	0.127825	C	1.104050	−2.437269	−3.222053
H	−4.802462	−6.353917	0.149915	H	2.178136	−2.168227	−3.243949
N	−2.796079	−6.965160	0.120483	N	0.171775	−1.556894	−3.214905

Ligand $\mathbf{4}^{ZZ-syn}$: E = −4774.007472877 au (B3LYP−D3/def2−SVP)

C	0.032496	0.260651	−0.178992	C	−2.427126	−9.501342	−3.301141
C	1.449203	0.513187	−0.168697	H	0.869857	−8.964297	−2.879555
C	1.650482	1.923917	−0.170086	H	0.162050	−11.599362	−2.828185
C	0.365445	2.556508	−0.209931	H	−2.515866	−11.743256	−3.200950
C	−0.634234	1.540385	−0.226406	H	−3.465899	−9.218240	−3.459650
H	2.209135	−0.266110	−0.155804	N	−0.496712	−1.018733	−0.144364
H	2.612658	2.434056	−0.170846	C	−1.739660	−1.200767	0.122234
H	0.175068	3.629120	−0.246246	H	−2.432721	−0.362164	0.331848
H	−1.708814	1.708872	−0.275042	C	−2.837988	−4.945863	0.321838
Fe	−1.487994	−9.731817	−1.491991	C	−3.954251	−4.159383	0.579782
C	−1.309166	−8.591916	−3.215925	C	−3.671902	−2.777333	0.524746
C	−0.127394	−9.379468	−3.012473	C	−2.341572	−2.511376	0.224386
C	−0.505740	−10.753626	−2.984966	S	−1.425024	−3.976911	0.014067
C	−1.923034	−10.830081	−3.173786	H	−4.932887	−4.587159	0.808199

H	−4.402208	−1.985562	0.704436	C	1.572282	0.548685	−3.505822
C	−2.800976	−6.391318	0.316531	H	−1.648909	1.559772	−3.550060
H	−3.768085	−6.877081	0.553172	H	0.120349	3.586349	−3.511903
N	−1.729449	−7.062912	0.093127	H	2.622826	2.532719	−3.454589
C	−1.756696	−8.447805	0.113673	H	2.376515	−0.184362	−3.473499
C	−2.874961	−9.349394	−0.022432	N	−0.284169	−1.094631	−3.528129
C	−2.380051	−10.683148	0.098509	C	−1.528773	−1.336810	−3.335251
C	−0.962949	−10.619925	0.291505	H	−2.273453	−0.535249	−3.164370
C	−0.573267	−9.248526	0.281246	C	−2.481455	−5.116833	−3.180528
H	−3.908630	−9.062462	−0.206817	C	−3.622778	−4.373470	−2.913920
H	−2.973559	−11.593814	0.024978	C	−3.393313	−2.983324	−2.972397
H	−0.296465	−11.474822	0.393534	C	−2.077628	−2.669609	−3.282742
H	0.429600	−8.840510	0.388914	S	−1.109264	−4.099105	−3.521422
Fe	0.609091	1.342707	−1.853345	H	−4.577153	−4.837055	−2.657889
C	0.176060	0.213839	−3.534597	H	−4.146841	−2.219414	−2.772797
C	−0.565590	1.453876	−3.532366	C	−2.395015	−6.555067	−3.122417
C	0.372623	2.526144	−3.519710	H	−3.355695	−7.054381	−2.891902
C	1.692087	1.968516	−3.494927	N	−1.301728	−7.205400	−3.286560



Ligand **4** (**4**$^{ZZ-syn}$): E = −4776.180795312501 au

C	0.000136	0.236536	−0.072066	C	−1.632912	−8.381466	0.192249
C	1.417657	0.437000	−0.043084	C	−2.677303	−9.368762	0.153906
C	1.673139	1.830724	−0.081044	C	−2.070226	−10.650953	0.230401
C	0.421629	2.507402	−0.162241	C	−0.657596	−10.474110	0.291807
C	−0.612480	1.533416	−0.171623	C	−0.386274	−9.083427	0.252952
H	2.141593	−0.359501	0.003430	H	−3.734975	−9.180692	0.070551
H	2.644260	2.298303	−0.080747	H	−2.588853	−11.596127	0.213752
H	0.283582	3.574226	−0.236084	H	0.075880	−11.262872	0.330963
H	−1.666748	1.740712	−0.251995	H	0.578634	−8.604435	0.266575
Fe	−1.410253	−9.652770	−1.455086	Fe	0.648340	1.246762	−1.785503
C	−1.464310	−8.532232	−3.219672	C	0.169805	0.123095	−3.482349
C	−0.231351	−9.249590	−3.122397	C	−0.465579	1.413171	−3.515951
C	−0.522184	−10.634916	−3.050997	C	0.552961	2.402762	−3.497053
C	−1.937846	−10.791746	−3.096510	C	1.814638	1.744059	−3.426051
C	−2.526348	−9.502028	−3.184827	C	1.580322	0.346100	−3.413844
H	0.739666	−8.783710	−3.092069	H	−1.524460	1.605715	−3.563676
H	0.198036	−11.430863	−2.953764	H	0.395930	3.469390	−3.509910
H	−2.472700	−11.726677	−3.047421	H	2.776262	2.227406	−3.367680
H	−3.583153	−9.297921	−3.231298	H	2.315430	−0.438682	−3.346126
N	−0.562104	−1.028220	−0.020015	N	−0.376248	−1.151691	−3.490412
C	−1.818487	−1.194071	0.156735	C	−1.636664	−1.334512	−3.379385
H	−2.519566	−0.358987	0.274256	H	−2.350097	−0.511421	−3.254222
C	−2.873546	−4.935173	0.312681	C	−2.682326	−5.077333	−3.303176
C	−4.013069	−4.169109	0.470694	C	−3.817884	−4.313851	−3.117336
C	−3.750720	−2.789154	0.431345	C	−3.557850	−2.934344	−3.155446
C	−2.411623	−2.504160	0.242239	C	−2.224425	−2.647520	−3.370355
S	−1.464985	−3.948256	0.117359	S	−1.279642	−4.089522	−3.543849
H	−4.995183	−4.601449	0.605928	H	−4.790968	−4.747931	−2.933938
H	−4.504458	−2.020018	0.531922	H	−4.304337	−2.166713	−3.005653
C	−2.802345	−6.374217	0.305639	C	−2.613713	−6.512990	−3.237039
H	−3.761517	−6.886530	0.447661	H	−3.579516	−7.011472	−3.092774
N	−1.693744	−6.997961	0.168132	N	−1.506550	−7.148584	−3.305212

Complex **4**·$Zn(ClO_4)_2$: E_{ZPE} = −8077.196575232982 au

C	−0.158982	0.076393	−0.029000	H	−11.116270	−5.885563	0.336104
C	1.236956	0.357161	0.100074	H	−10.192400	−8.392672	0.011345
C	1.393245	1.765723	0.112760	H	−7.493830	−8.270076	−0.096660
C	0.110187	2.365893	−0.021703	Fe	0.479863	1.140291	−1.661315
C	−0.856664	1.329053	−0.107198	C	−0.009931	−0.019637	−3.281573
H	2.016545	−0.383266	0.146470	C	−0.604983	1.281364	−3.408008
H	2.333402	2.286387	0.186002	C	0.447750	2.234176	−3.431952
H	−0.101610	3.422047	−0.063432	C	1.682633	1.536168	−3.317841
H	−1.916020	1.472251	−0.246073	C	1.407840	0.148184	−3.227174
Fe	−8.998798	−6.311573	−1.499871	H	−1.656986	1.513867	−3.435799
C	−7.970498	−5.715929	−3.219030	H	0.320942	3.302726	−3.498879
C	−8.361604	−7.093277	−3.297794	H	2.663521	1.980835	−3.289868
C	−9.776114	−7.154290	−3.229624	H	2.127686	−0.648109	−3.128975
C	−10.271203	−5.827469	−3.061798	N	−0.670123	−1.265064	−3.127316
C	−9.164827	−4.937265	−3.048863	C	−1.861700	−1.355284	−3.631772
H	−7.675149	−7.916168	−3.408512	H	−2.233957	−0.486515	−4.173611
H	−10.372493	−8.050957	−3.264014	C	−2.787804	−2.440782	−3.551441
H	−11.305276	−5.546460	−2.941478	C	−2.634735	−3.767983	−3.185845
H	−9.217575	−3.869739	−2.908053	C	−3.833935	−4.482232	−3.186108
N	−0.726228	−1.220482	−0.141560	C	−4.929939	−3.717466	−3.548514
C	−1.950545	−1.348693	0.254542	S	−4.455889	−2.106023	−3.939494
H	−2.444761	−0.466087	0.658822	H	−1.680568	−4.200769	−2.937732
C	−2.760242	−2.525588	0.217672	H	−3.925507	−5.521974	−2.912771
C	−2.443242	−3.873908	0.220527	C	−6.320737	−4.123755	−3.569930
C	−3.572848	−4.702550	0.218224	H	−7.058011	−3.367047	−3.860630
C	−4.765054	−3.997690	0.211423	N	−6.645043	−5.320462	−3.257360
S	−4.479397	−2.298065	0.226211	Zn	0.254522	−2.422841	−1.579255
H	−1.430711	−4.242651	0.271471	Cl	0.293850	−5.567302	−1.369865
H	−3.533543	−5.781339	0.219190	O	0.188085	−4.279251	−2.204096
C	−6.133958	−4.457240	0.189449	O	0.552261	−5.162937	−0.010320
H	−6.893692	−3.667748	0.206235	O	−0.993588	−6.204241	−1.493829
N	−6.439834	−5.696415	0.154057	O	1.338229	−6.344553	−1.932994
C	−7.774047	−6.081076	0.168300	Cl	3.369409	−2.887422	−1.635172
C	−8.972384	−5.291148	0.293870	O	2.122506	−2.246492	−0.987603
C	−10.080102	−6.175495	0.266037	O	3.266499	−2.630118	−3.051532
C	−9.589835	−7.503613	0.098946	O	4.479557	−2.203889	−1.040283
C	−8.175861	−7.447030	0.038767	O	3.355265	−4.281091	−1.337070
H	−9.035154	−4.221544	0.407782				

Complex $[\mathbf{4}_2Pb]^{2+}$: E_{ZPE} = −9744.888164881964 au

C	−0.218133	−0.046367	−0.355008	H	−11.628778	−1.949490	−4.676416
C	−0.344215	0.051739	1.069445	H	−9.206194	−2.839802	−5.364928
C	0.954012	−0.011882	1.631849	N	−1.303726	−0.058895	−1.243010
C	1.891412	−0.143374	0.571966	C	−1.115550	−0.376372	−2.483960
C	1.181900	−0.172339	−0.654673	H	−0.135657	−0.702069	−2.832032
H	−1.262180	0.168536	1.618063	C	−4.365404	−0.274194	−4.623262
H	1.187471	0.018032	2.683138	C	−3.422541	−1.001787	−5.312525
H	2.960223	−0.227511	0.679826	C	−2.172269	−1.060642	−4.661986
H	1.630890	−0.257320	−1.629893	C	−2.150773	−0.379181	−3.465041
Fe	−9.366071	−0.466351	−3.841878	S	−3.669839	0.432692	−3.191635
C	−8.619762	−2.315610	−3.251436	H	−3.637487	−1.490625	−6.251802
C	−9.398084	−1.723333	−2.201268	H	−1.324807	−1.618859	−5.034324
C	−10.717120	−1.539360	−2.680469	C	−5.747570	−0.032594	−4.931817
C	−10.766378	−1.987522	−4.031024	H	−6.106282	−0.412103	−5.891630
C	−9.478904	−2.456185	−4.395896	N	−6.483107	0.578824	−4.079325
H	−9.022670	−1.476501	−1.223172	C	−7.820162	0.841884	−4.299300
H	−11.538040	−1.107277	−2.132148	C	−8.642643	0.595567	−5.455842

C	−9.953911	1.036585	−5.150236	H	−1.697085	−8.530690	0.681510
C	−9.966610	1.529270	−3.813247	H	−1.851771	−5.834180	0.551546
C	−8.661321	1.406077	−3.283838	N	−6.237056	−5.053926	0.360281
H	−8.326236	0.174172	−6.395420	C	−7.129225	−4.704860	1.210022
H	−10.804459	0.984654	−5.810129	H	−7.706585	−5.407115	1.817885
H	−10.830677	1.907631	−3.292274	C	−7.431359	−3.306902	1.383429
H	−8.327816	1.680506	−2.297235	C	−8.351809	−2.705557	2.217902
Fe	0.549717	−1.737025	0.528615	C	−8.379610	−1.303809	2.087641
C	−0.551845	−3.371072	−0.106004	C	−7.472019	−0.829842	1.159429
C	0.798737	−3.462507	−0.582669	S	−6.620960	−2.134638	0.400036
C	1.658180	−3.492060	0.548253	H	−8.990239	−3.265996	2.886260
C	0.855385	−3.417847	1.719611	H	−9.035919	−0.655939	2.652726
C	−0.502167	−3.325415	1.324055	C	−7.251077	0.537338	0.801037
H	1.114279	−3.472005	−1.613266	H	−7.977002	1.245182	1.207131
H	2.734881	−3.532486	0.520414	N	−6.301012	0.949309	0.031270
H	1.218488	−3.405575	2.734090	N	−3.536113	−4.691295	2.452672
H	−1.361590	−3.293183	1.967497	C	−4.375905	−4.261934	3.320194
N	−1.739049	−3.311350	−0.838682	H	−4.969194	−4.905503	3.974763
C	−1.790417	−3.904991	−1.976284	C	−4.560073	−2.843676	3.475331
H	−0.937173	−4.464273	−2.371710	C	−5.410049	−2.150795	4.309222
C	−5.248615	−3.635646	−3.755402	C	−5.289015	−0.750709	4.197420
C	−4.404408	−4.351866	−4.577768	C	−4.350523	−0.360708	3.266165
C	−3.112013	−4.513652	−4.036786	S	−3.542853	−1.748257	2.582019
C	−2.966425	−3.919436	−2.800097	H	−6.095976	−2.644939	4.982298
S	−4.448802	−3.189564	−2.284403	H	−5.890341	−0.046644	4.756024
H	−4.717173	−4.753679	−5.531482	C	−4.081471	0.963446	2.805118
H	−2.312241	−5.050325	−4.528762	H	−4.410656	1.772365	3.456524
C	−6.633029	−3.296510	−3.967326	N	−3.510061	1.219274	1.671679
H	−7.078320	−3.672682	−4.893225	C	−6.240335	2.321509	−0.264369
N	−7.280066	−2.622119	−3.091921	C	−6.627894	3.427463	0.562236
Pb	−3.813772	−0.510337	−0.261129	C	−6.382557	4.621228	−0.168724
C	−5.902956	−6.372606	0.132099	C	−5.846444	4.265395	−1.435854
C	−4.974209	−6.754873	−0.894214	C	−5.745473	2.853331	−1.496866
C	−4.823812	−8.160308	−0.846456	H	−7.002920	3.372728	1.571259
C	−5.631976	−8.660511	0.214629	H	−6.546822	5.623849	0.190943
C	−6.292168	−7.568456	0.831023	H	−5.547277	4.951027	−2.211342
H	−4.492438	−6.070707	−1.571516	H	−5.433357	2.269667	−2.342522
H	−4.185022	−8.752508	−1.480852	Fe	−4.622308	3.554316	0.096302
H	−5.706115	−9.692506	0.516764	C	−3.275392	2.537548	1.259404
H	−6.959857	−7.635412	1.673789	C	−2.668198	2.872564	0.003036
Fe	−4.246119	−7.302872	0.961899	C	−2.673837	4.282963	−0.121291
C	−3.255272	−6.028715	2.270674	C	−3.272171	4.830141	1.045098
C	−3.748215	−7.193565	2.961046	C	−3.650399	3.765092	1.901352
C	−3.127646	−8.327939	2.381602	H	−2.244819	2.178048	−0.702869
C	−2.279003	−7.890430	1.323898	H	−2.299274	4.842633	−0.962057
C	−2.360030	−6.481782	1.244944	H	−3.435506	5.877377	1.239364
H	−4.442889	−7.210506	3.784352	H	−4.140906	3.879198	2.8533
H	−3.289432	−9.352101	2.675947				