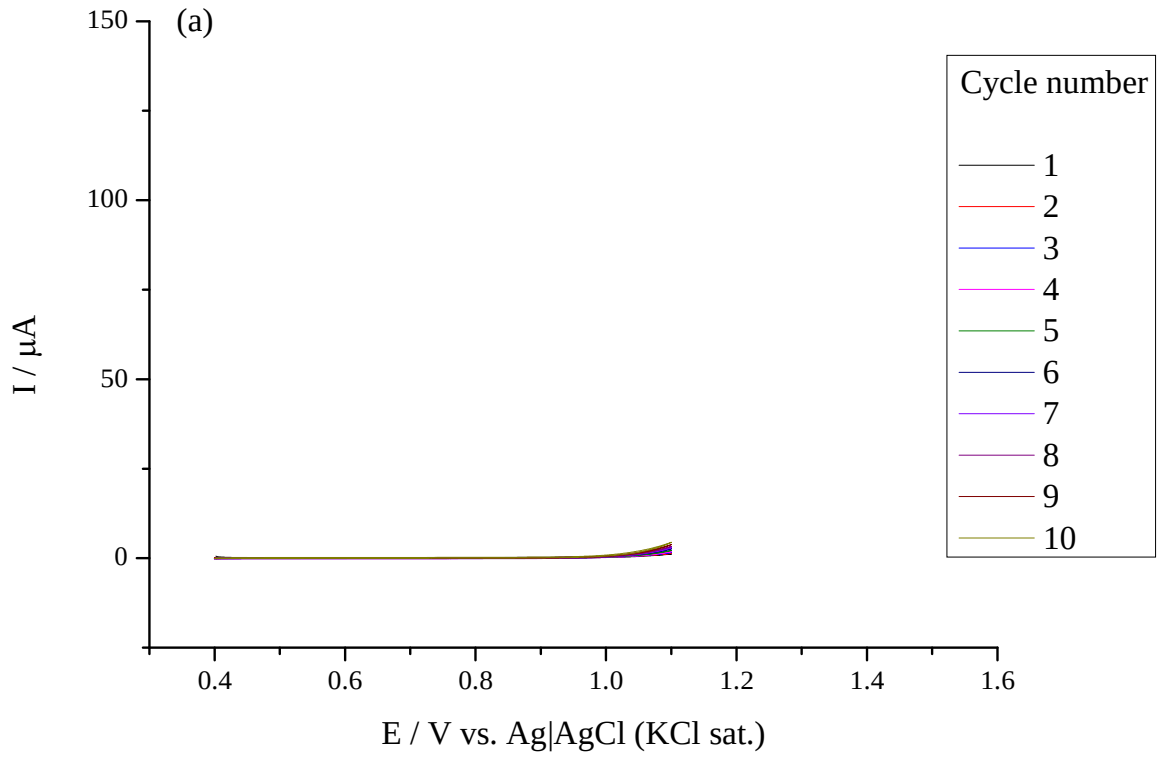
Supporting information for "Water-stable [Ni(salen)]-type electrode material based on phenylazosubstituted salicylic aldehyde imine ligand" published in New Journal of Chemistry

Anatoly A. Vereschagin, Vladimir V. Sizov, Petr S. Vlasov, Elena V. Alekseeva, Alexander S. Konev and Oleg V. Levin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0.6
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E / V vs. Ag|AgCl (KCl sat.)
Cycle number
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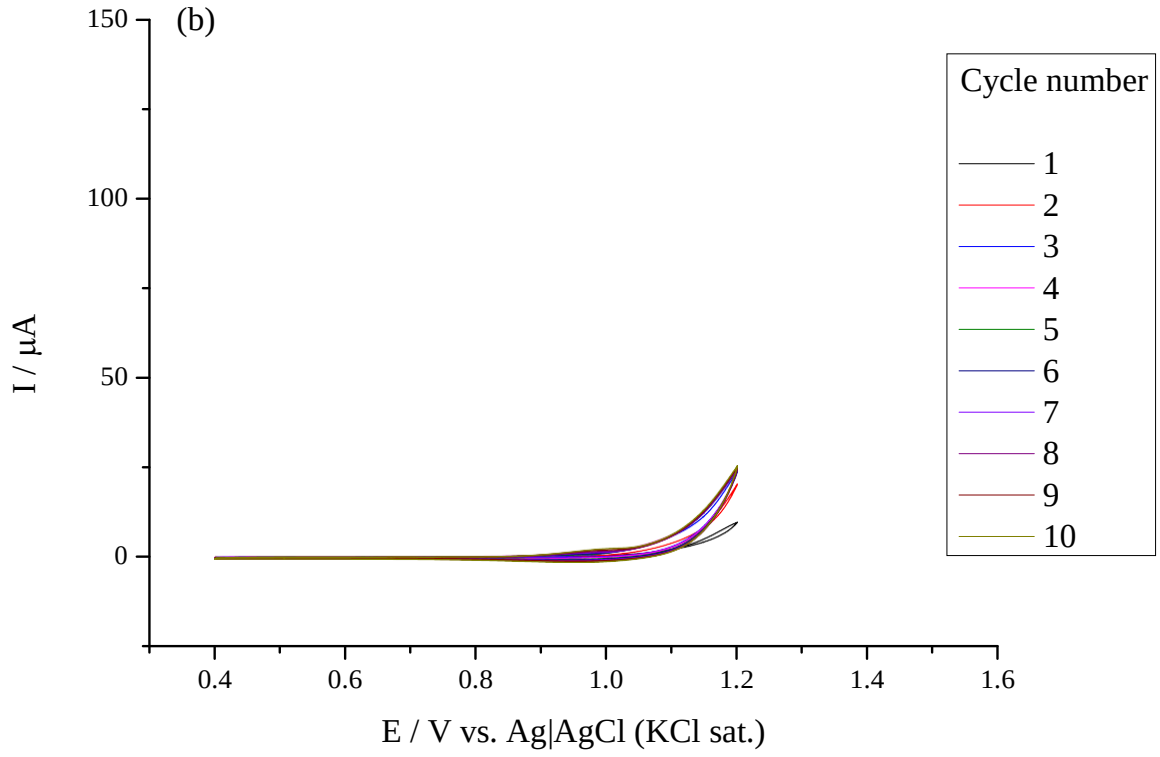
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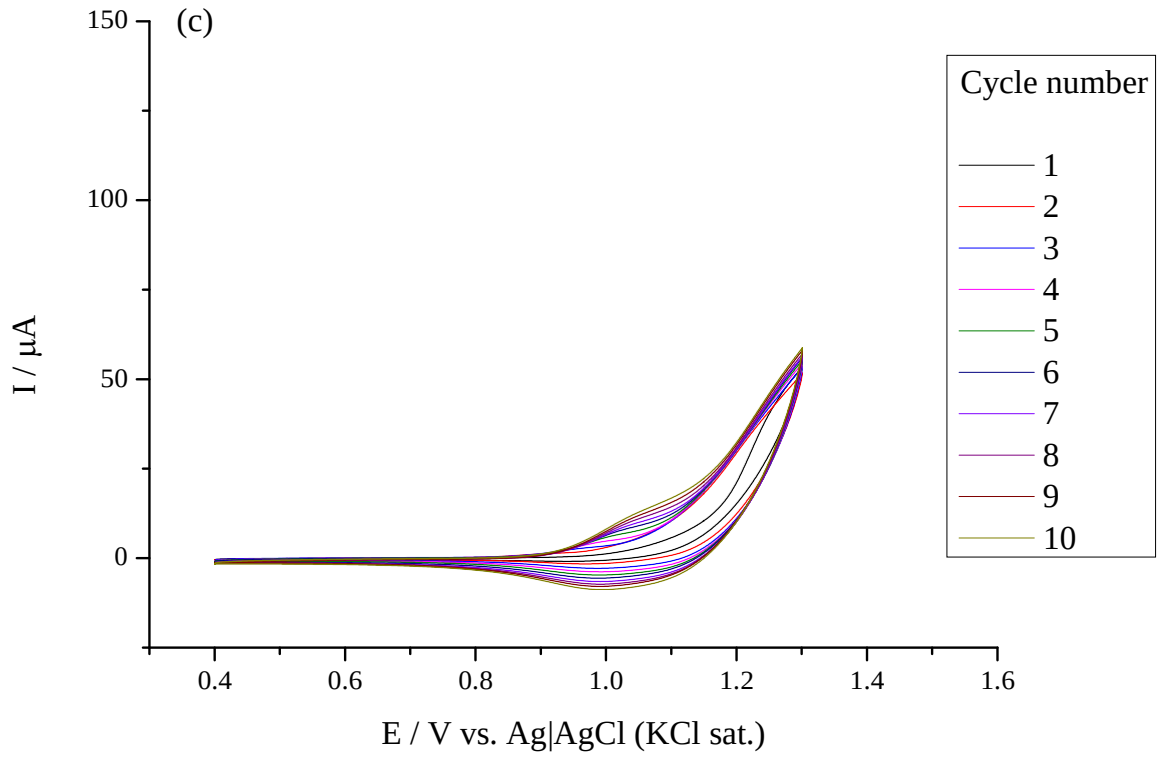
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Cycle number
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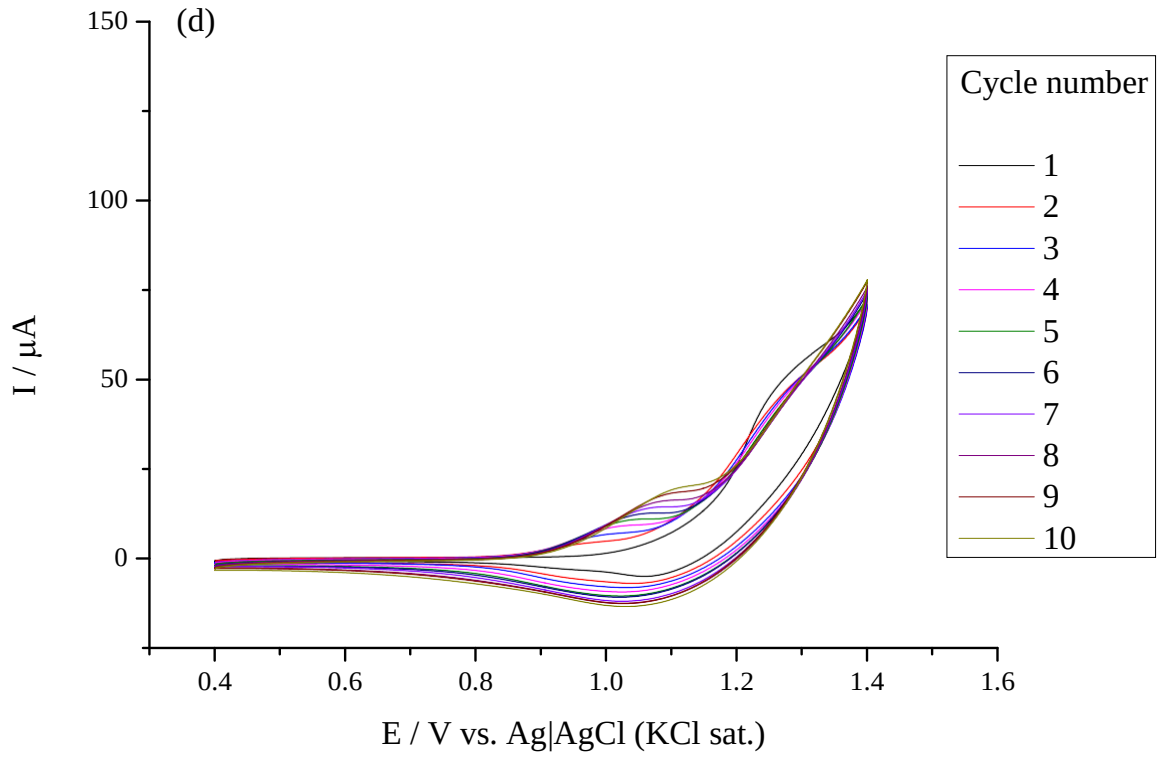
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I / µA
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E / V vs. Ag|AgCl (KCl sat.)
Cycle number
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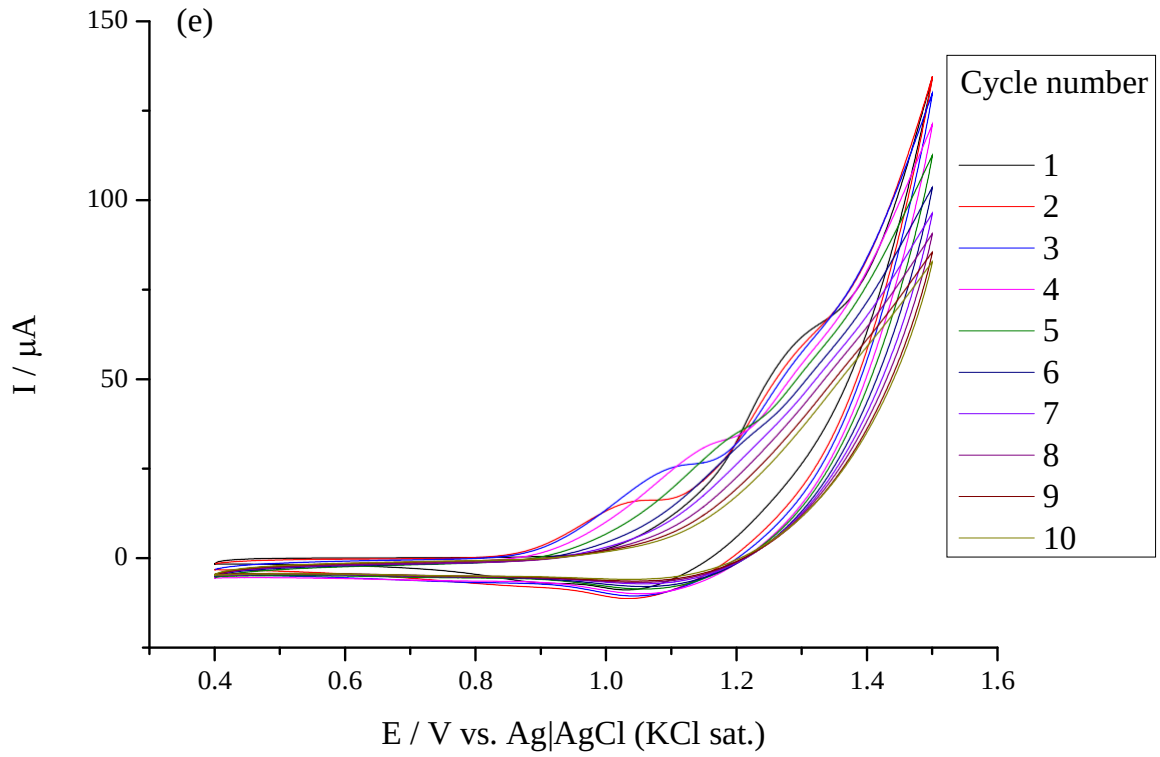

Figure SI1. CVA synthesis of $[NiPhazoSalen]_n$ film in DCE containing 0.1M $[Bu_4N]^+[BF_4]^-$ as supporting electrolyte, scan rate - 50 mV/s. Figures a-e show CVA recorded at various anodic boundaries of the voltage range. All CVA's are presented at the same scale.

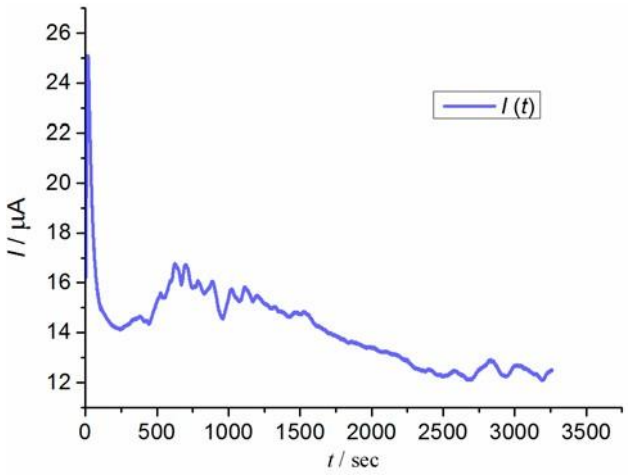

Figure SI2. Potentiostatic synthesis of $[NiPhazosalen]_n$ film in DCE containing 0.1M $[Bu_4N]^+[BF_4]^-$ as supporting electrolyte. The synthesis is terminated upon reaching the charging of 57 mC/cm^2

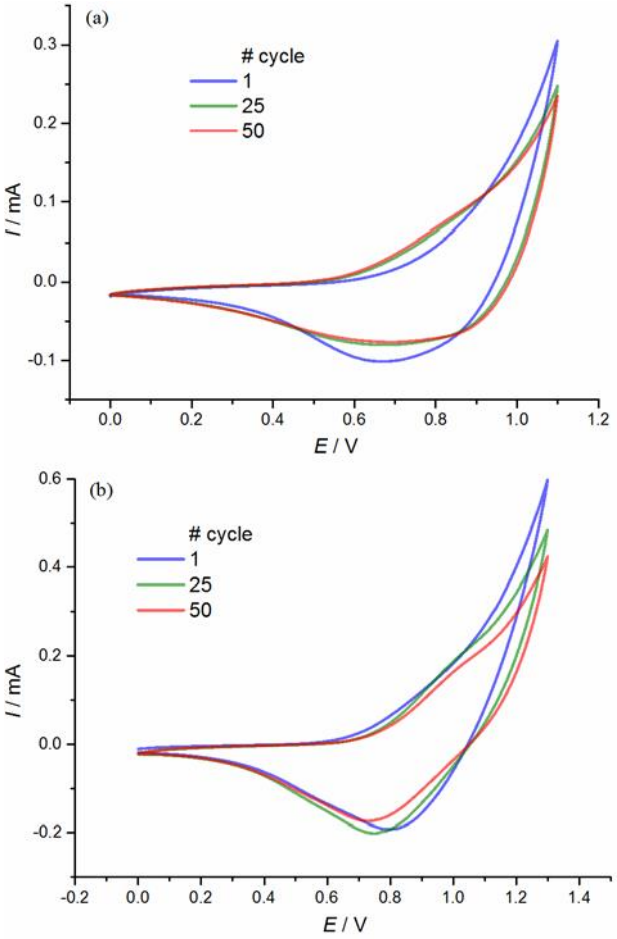

Figure SI3. CVA of $[Ni(Phazasalen)]_n$ film in 0.1 M aqueous solution of $LiClO_4$ as supporting electrolyte, with various potential ranges, scan rate - 50 mV/s.

Table SIA1. Numerical values of the elements of the equivalent circuit for the ITO electrode coated with the $[Ni(salen)]_n$ film in 0.1 M (TEA)BF4, in acetonitrile.

Bias potential, V	Q_{dl}, μF cm^{-2}	N_{dl}	Q_{lf}, mF cm^{-2}	N_{lf}	R_s, Ω cm^2	R_{ct}, Ω cm^2	σ, Ω cm^2 $s^{-1/2}$
0.5	19±1	0.84±0.01	6.5±0.4	1.10±0.06	63.0±0.6	385±8	270±10
0.6	18±2	0.85±0.01	6.7±0.2	1.00±0.02	58.1±0.6	92.8±0.9	59±6
0.7	18±1	0.83±0.01	7.8±0.1	0.94±0.01	54.2±0.5	40.4±0.4	11±2
0.8	19±3	0.81±0.02	9.2±1	0.95±0.01	55.5±0.6	28.0±0.6	5±2
0.9	19±4	0.81±0.03	8.5±1	0.94±0.01	55.2±0.6	24.8±0.7	5±2

Table SIA2. Numerical values of the elements of the equivalent circuit for the ITO electrode coated with the [Ni(Phazosalen)]$_n$ film in 0.1 M (TEA)BF4, in acetonitrile.

Bias potential, V	Q_{dl}, μF cm^{-2}	N_{dl}	Q_{lf}, mF cm^{-2}	N_{lf}	R_s, Ω cm^2	R_{ct}, Ω cm^2	σ, Ω cm^2 s$^{-1/2}$
0.5	26.9±0.3	0.952±0.004	--		16.1±0.5	22000±1000	$1.2\cdot10^4\pm2\cdot10^3$
0.6	27±1	0.946±0.003	--	--	16.1±0.1	5400±100	$3.4\cdot10^3\pm6\cdot10^2$
0.7	25±1	0.97±0.01	1.0±0.1	0.75±0.04	16.0±0.2	1910±60	$5\cdot10^2\pm2\cdot10^2$
0.8	26.3±0.8	0.951±0.004	1.3±0.1	0.86±0.03	16.0±0.1	707±9	$2.4\cdot10^2\pm8\cdot10^1$
0.9	23.8±0.4	0.962±0.002	1.76±0.03	0.92±0.01	16.4±0.1	277±2	$2.0\cdot10^2\pm1\cdot10^1$
1.0	25±1	0.954±0.007	1.94±0.05	0.92±0.01	16.1±0.3	135±2	$1.0\cdot10^2\pm1\cdot10^1$

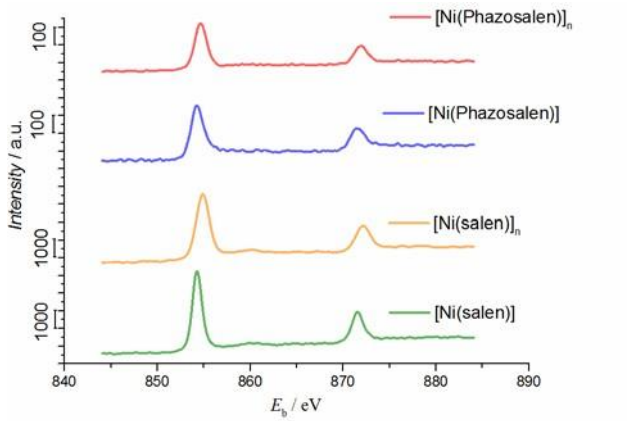

Figure SI4. XPS levels of Ni($2p_{3/2}$) and Ni($2p_{1/2}$) in different samples

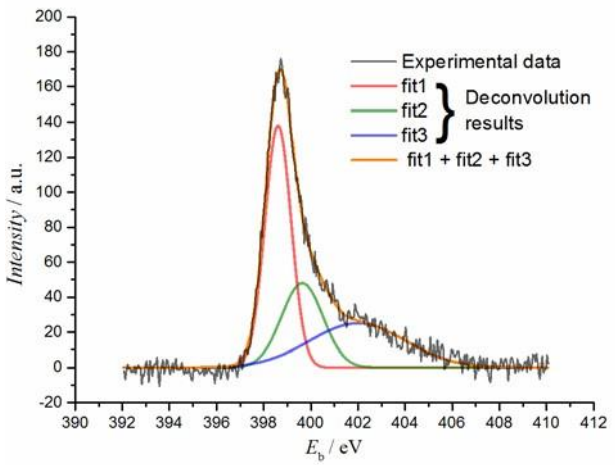

Figure SI5a. XPS levels of N(1s) in [Ni(Phazosalen)]

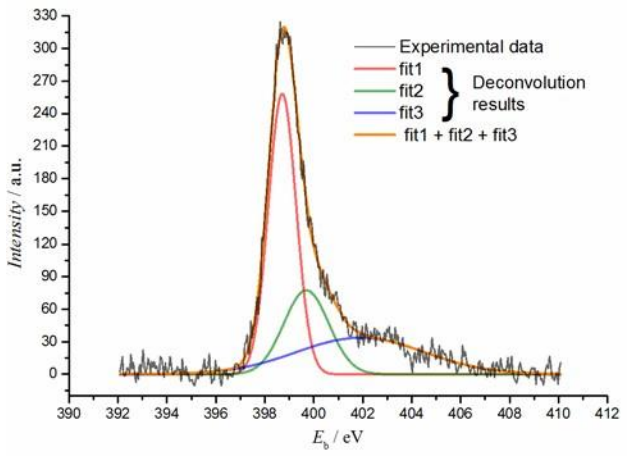

Figure SI5c. XPS levels of N(1s) in [Ni(Phazosalen)]$_n$

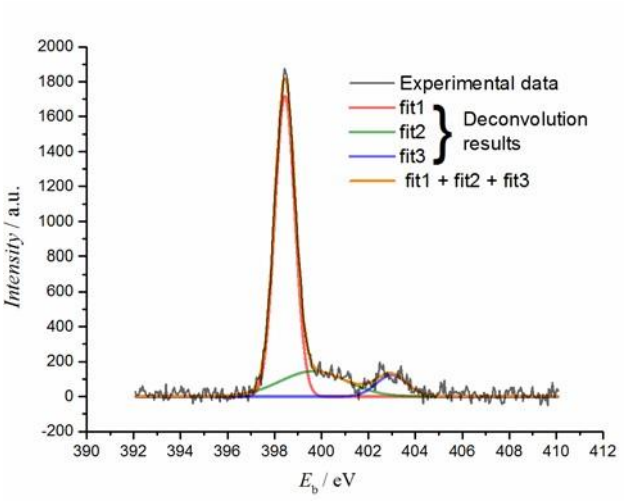

Figure SI5b. XPS levels of N(1s) in [Ni(salen)]

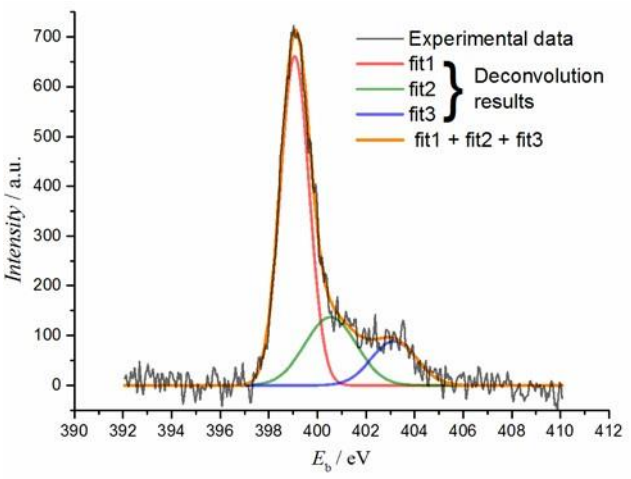

Figure SI5d. XPS levels of N(1s) in $[Ni(salen)]_n$

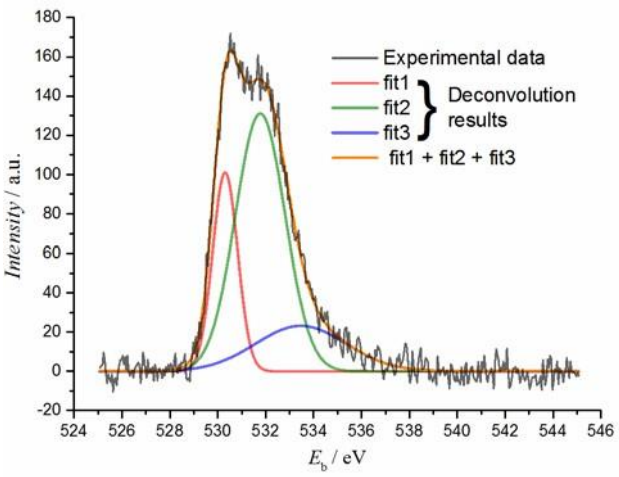

Figure SI6a. XPS levels of O(1s) in [Ni(Phazosalen)]

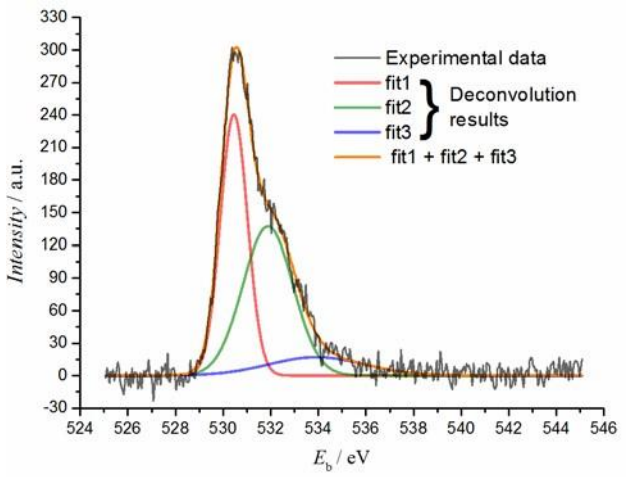

Figure SI6c. XPS levels of O(1s) in $[Ni(Phazosalen)]_n$

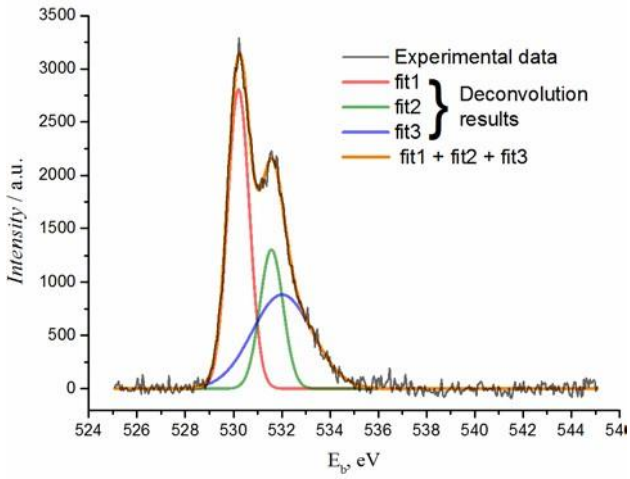

Figure SI6b. XPS levels of O(1s) in [Ni(salen)]

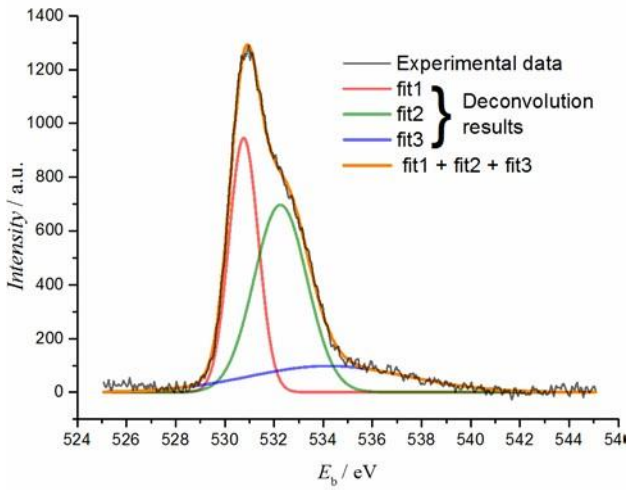

Figure SI6d. XPS levels of O(1s) in $[Ni(salen)]_n$

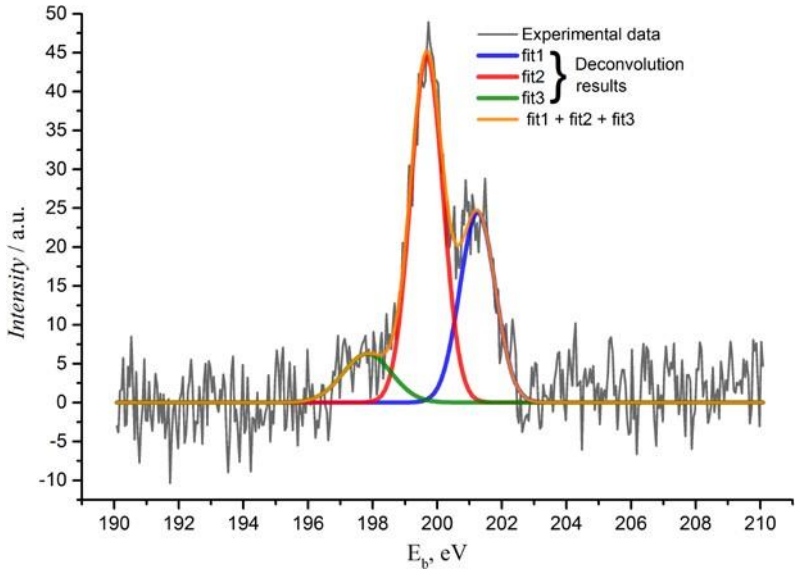

Figure SI7. XPS levels of Cl(2p) in $[Ni(Phazosalen)]_n$

Computational details

[Ni(Phazosalen)] charge = 0 E(DCBS) = -1727.64763638 Hartree

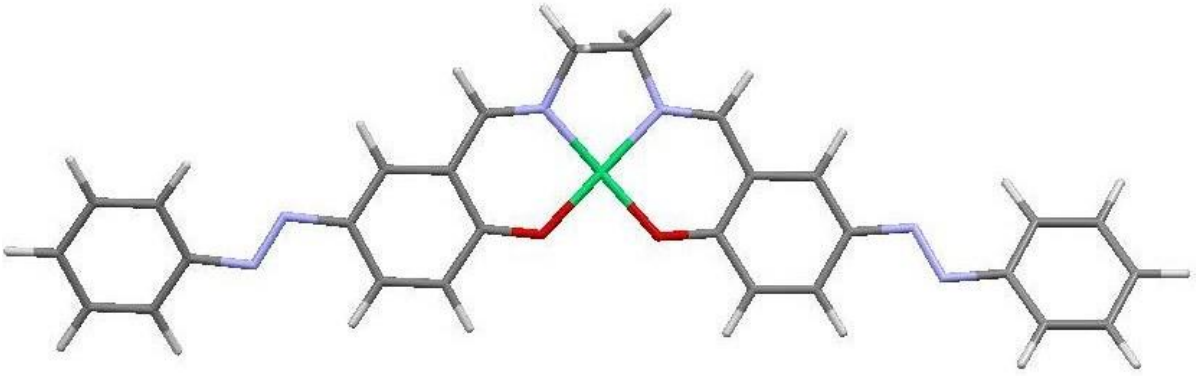

Table SI3. Cartesian coordinates of [Ni(Phazosalen)]

Atom	***x***	***y***	***z***	**Atom**	***x***	***y***	***z***
Ni	-1.720799	0.174987	1.652215	H	-0.852201	-3.428616	2.051547
N	-3.158201	-1.030124	1.639328	H	-3.471563	-3.071050	2.119406
N	-0.629165	-1.325180	1.889375	H	-2.645465	-2.745183	0.572918
O	-0.311618	1.351517	1.583461	N	5.115427	0.340058	1.197936
O	-2.801131	1.666009	1.550737	N	-8.316672	2.073146	1.445985
C	-4.411389	-0.734885	1.591331	C	7.235603	0.993780	0.833687
C	1.857316	2.162603	1.299514	C	8.049200	1.991511	0.301741
C	0.947472	1.081957	1.481501	C	7.796249	-0.211309	1.263118
C	1.497494	-0.229584	1.573569	C	9.417400	1.784619	0.178005
C	2.887192	-0.414187	1.489523	H	7.584735	2.920821	-0.011316
C	3.744436	0.647172	1.293688	C	9.162160	-0.409107	1.145949
C	3.205685	1.952624	1.203135	H	7.149045	-0.964750	1.694888
C	0.657471	-1.355536	1.832864	C	9.975781	0.583268	0.600393
C	-6.064953	3.154825	1.534935	H	10.047449	2.561861	-0.243379
C	-4.704956	3.014132	1.552117	H	9.601547	-1.339669	1.491678
C	-4.087744	1.727791	1.542397	H	11.045835	0.420493	0.513953
C	-4.947035	0.589934	1.537968	C	-10.218904	3.269036	1.423031
C	-6.340800	0.762610	1.508731	C	-10.825623	4.455170	1.832488
C	-6.910785	2.018518	1.504920	C	-10.994153	2.234839	0.891738
C	-1.384007	-2.506108	2.308498	C	-12.203485	4.603395	1.736993
C	-2.735928	-2.432979	1.619660	H	-10.196265	5.246397	2.226159
H	-5.132324	-1.555896	1.602339	C	-12.367670	2.393570	0.785911
H	1.430537	3.157579	1.230549	H	-10.503020	1.325340	0.567255
H	3.313254	-1.408821	1.583191	C	-12.976905	3.573295	1.211425
H	3.892423	2.778287	1.056002	H	-12.672985	5.525474	2.064859
H	1.154464	-2.309833	2.021824	H	-12.968970	1.594467	0.363064
H	-6.526452	4.135722	1.531558	H	-14.052612	3.690942	1.124074
H	-4.044546	3.874884	1.551320	N	-8.806331	3.219417	1.547987
H	-7.000045	-0.100807	1.506494	N	5.855107	1.308764	0.920421
H	-1.509951	-2.455847	3.393401				

[Ni(Phazosalen)]$^{+}$ charge = +1 E(DCBS) = -1727.40170630 Hartree

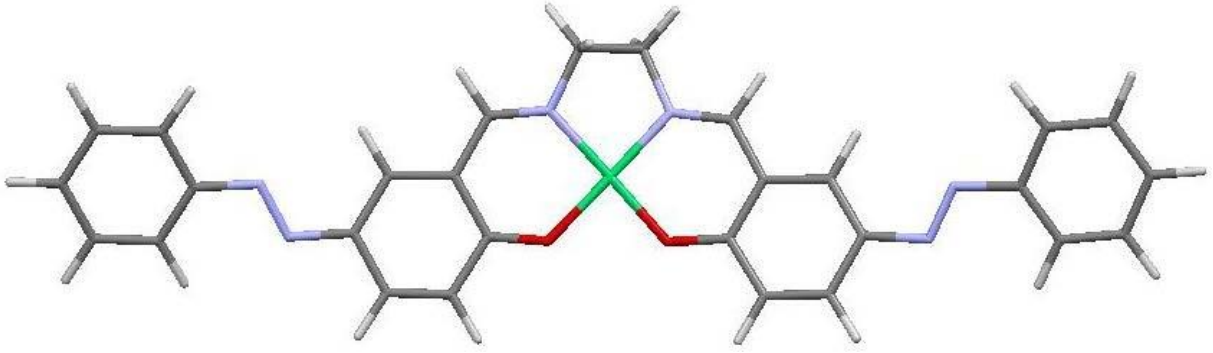

Table SI4. Cartesian coordinates of [Ni(Phazosalen)]$^{+}$

Atom	***x***	***y***	***z***	**Atom**	***x***	***y***	***z***
Ni	-1.678642	-0.010624	4.821777	H	-3.536787	3.173335	4.402345
N	-0.624578	1.529537	4.538312	H	-0.937912	3.626400	4.394178
N	-3.140979	1.131723	4.802436	H	-1.596235	2.609591	3.072913
O	-2.665642	-1.523528	4.993768	N	5.194673	-0.235395	4.860568
O	-0.191320	-1.138232	4.913243	N	-8.075571	-2.384131	4.146658
C	0.652583	1.611477	4.537721	C	-10.106710	-1.652387	3.481279
C	-4.494949	-2.965524	4.802628	C	-10.807930	-0.577141	2.937881
C	-3.951478	-1.658447	4.845296	C	-10.760043	-2.856643	3.762333
C	-4.851289	-0.565516	4.706690	C	-12.165855	-0.700124	2.672679
C	-6.218818	-0.793631	4.493593	H	-10.268521	0.340190	2.726281
C	-6.717193	-2.076918	4.405522	C	-12.113985	-2.971964	3.493564
C	-5.838868	-3.162349	4.591674	H	-10.195554	-3.676553	4.190168
C	-4.379938	0.780228	4.731178	C	-12.818631	-1.896140	2.950357
C	3.322350	-1.680016	5.047100	H	-12.709339	0.140606	2.255366
C	1.985577	-1.924032	5.065877	H	-12.629754	-3.901892	3.711104
C	1.039327	-0.851848	4.908143	H	-13.880608	-1.994512	2.747956
C	1.552300	0.495338	4.737752	C	7.005769	1.066015	4.609198
C	2.912676	0.707675	4.702275	C	7.876377	0.127344	5.191432
C	3.819800	-0.362327	4.850999	C	7.510780	2.252802	4.062490
C	-2.771815	2.546122	4.869639	C	9.231988	0.386216	5.215075
C	-1.441268	2.685154	4.152987	H	7.465344	-0.781628	5.612608
H	1.117509	2.576904	4.330969	C	8.873973	2.496973	4.078768
H	-3.814899	-3.798220	4.944354	H	6.811925	2.952229	3.617657
H	-6.900469	0.039654	4.361147	C	9.733314	1.565646	4.654966
H	-6.255012	-4.164218	4.551934	H	9.911947	-0.328282	5.666944
H	-5.130818	1.570006	4.669483	H	9.269380	3.407360	3.642205
H	4.048997	-2.474842	5.174963	H	10.801477	1.756693	4.672833
H	1.576746	-2.917064	5.212796	N	-8.733635	-1.411097	3.721187
H	3.319629	1.701000	4.551908	N	5.625441	0.909426	4.526399
H	-2.675285	2.829111	5.923374				

[Ni(salen)] charge = 0 E(DCBS) = -1046.97287517 Hartree

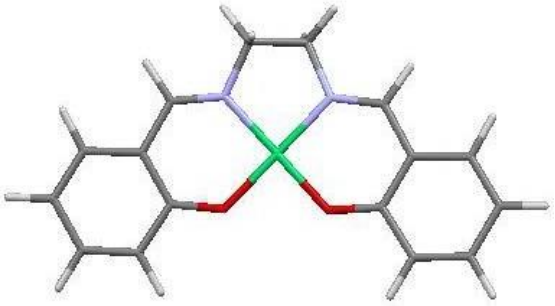

Table SI5. Cartesian coordinates of [Ni(salen)]

Atom	***x***	***y***	***z***	**Atom**	***x***	***y***	***z***
Ni	-1.717682	-0.218888	4.806665	C	3.759011	-0.638682	5.182444
N	-0.630049	1.277661	4.520037	C	-2.757239	2.373286	4.667660
N	-3.164314	0.967630	4.677103	C	-1.377069	2.439511	4.037238
O	-2.788827	-1.711772	4.952659	H	1.150105	2.254287	4.321676
O	-0.306638	-1.377402	4.989392	H	-4.018209	-3.931913	4.963269
C	0.657006	1.309934	4.565215	H	-6.961980	0.018999	4.465083
C	-4.677987	-3.078532	4.847091	H	-7.961312	-2.247382	4.496964
C	-4.074175	-1.791385	4.842255	H	-6.465305	-4.228513	4.731555
C	-4.939036	-0.669996	4.697088	H	-5.137602	1.468602	4.517579
C	-6.331586	-0.858734	4.581039	H	3.896000	-2.760527	5.559608
C	-6.888976	-2.114408	4.588375	H	1.452678	-3.147181	5.448794
C	-6.038402	-3.229224	4.722479	H	3.283681	1.403596	4.767571
C	-4.413836	0.657396	4.629460	H	4.829973	-0.474406	5.223150
C	3.225261	-1.927463	5.366585	H	-2.716678	2.720815	5.706637
C	1.870679	-2.156448	5.305221	H	-3.475772	2.987255	4.114948
C	0.956836	-1.098818	5.059746	H	-0.864752	3.373472	4.293455
C	1.502448	0.203044	4.878394	H	-1.455792	2.360993	2.949905
C	2.896722	0.401899	4.936681				

$[Ni(salen)]^+$ charge = +1 E(DCBS) = -1046.72473547 Hartree

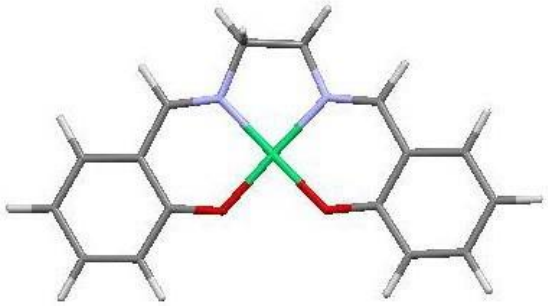

Table SI6. Cartesian coordinates of $[Ni(salen)]^+$

Atom	***x***	***y***	***z***	**Atom**	***x***	***y***	***z***
Ni	-1.692716	-0.157903	1.526098	C	-6.743268	1.991308	1.485792
N	-3.181481	-1.275135	1.493997	C	-1.524209	-2.853993	2.205229
N	-0.679830	-1.718122	1.829106	C	-2.837087	-2.697766	1.458189
O	-0.185985	0.936774	1.482035	H	-5.181595	-1.682128	1.506227
O	-2.654738	1.374791	1.339898	H	1.650822	2.654593	1.184896
C	-4.417418	-0.902520	1.479682	H	3.239463	-2.015499	1.777432
C	2.023783	1.646785	1.329501	H	4.085920	2.156500	1.220679
C	1.046648	0.610876	1.478178	H	1.034006	-2.810988	2.029018
C	1.519445	-0.741500	1.638521	H	-6.202527	4.080538	1.402206
C	2.894239	-0.994457	1.646948	H	-3.766698	3.660302	1.288441
C	3.812758	0.030452	1.517440	H	-6.941792	-0.136504	1.543936
C	3.360340	1.358818	1.344318	H	-7.809562	2.182300	1.522316
C	0.598417	-1.829633	1.829275	H	-1.700490	-2.768378	3.281963
C	-5.829644	3.060680	1.417150	H	-1.034901	-3.807176	1.982041
C	-4.472656	2.839850	1.360473	H	-3.623687	-3.304282	1.916782
C	-3.947753	1.524604	1.373060	H	-2.720338	-2.998740	0.411417
C	-4.871310	0.447879	1.441146	H	4.874906	-0.185312	1.521467
C	-6.258714	0.706829	1.490749				

[Ni(Phazosalen)]$_2$ charge = 0 E(DCBS) = -3455.35256321 Hartree

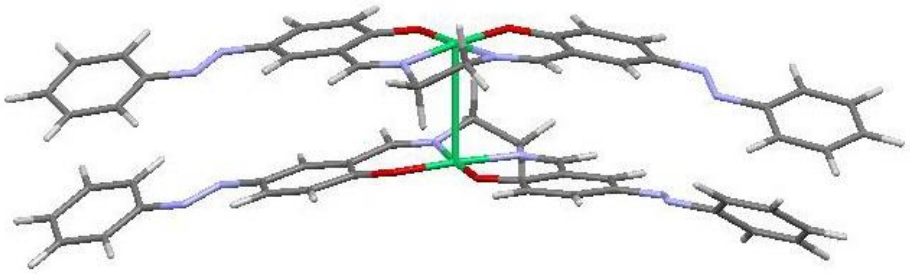

Table SI7. Cartesian coordinates of [Ni(Phazosalen)]$_2$

Atom	***x***	***y***	***z***	**Atom**	***x***	***y***	***z***
Ni	-1.718062	0.146978	1.976712	H	3.849942	-2.618140	5.279824
N	-3.161394	-1.049693	1.922806	H	1.392862	-3.026499	5.521062
N	-0.636447	-1.361976	2.180832	H	3.148751	1.551637	4.778012
O	-0.295606	1.317283	1.933881	H	-2.884791	2.731474	6.334765
O	-2.794077	1.647248	1.888788	H	-3.665068	3.119813	4.779317
C	-4.411629	-0.748794	1.839771	H	-1.058479	3.539893	4.960469
C	1.873553	2.108016	1.590531	H	-1.645145	2.618004	3.545895
C	0.956295	1.034606	1.774201	N	5.038332	-0.395539	4.855871
C	1.491090	-0.286187	1.808141	N	-8.198494	-2.379690	4.055418
C	2.873470	-0.486270	1.661218	C	-10.161251	-1.629010	3.231272
C	3.736446	0.568787	1.452061	C	-10.815055	-0.545535	2.647865
C	3.213824	1.882973	1.427085	C	-10.839178	-2.833329	3.442691
C	0.646937	-1.407223	2.080569	C	-12.148821	-0.659820	2.275416
C	-6.050844	3.148671	1.794668	H	-10.254839	0.370589	2.490659
C	-4.692555	3.002277	1.860754	C	-12.167938	-2.941346	3.064353
C	-4.080262	1.714065	1.841744	H	-10.311093	-3.659889	3.903103
C	-4.942542	0.579755	1.784021	C	-12.825860	-1.856637	2.482861
C	-6.335039	0.757278	1.708673	H	-12.654713	0.190087	1.829950
C	-6.898627	2.017306	1.706410	H	-12.700358	-3.873597	3.226892
C	-1.398991	-2.537051	2.600441	H	-13.869011	-1.948047	2.195553
C	-2.746215	-2.455876	1.902822	C	6.851940	0.848275	4.389697
H	-5.136171	-1.566536	1.824718	C	7.761064	-0.140915	4.776630
H	1.459495	3.110631	1.572793	C	7.311077	2.037295	3.829385
H	3.288831	-1.488606	1.709169	C	9.117593	0.066681	4.587380
H	3.904974	2.703762	1.273884	H	7.382349	-1.055504	5.216965
H	1.138519	-2.369414	2.240493	C	8.671787	2.235368	3.631311
H	-6.507779	4.131653	1.792528	H	6.579545	2.779566	3.528834
H	-4.029953	3.860416	1.901910	C	9.576414	1.250935	4.009841
H	-6.998478	-0.102805	1.677612	H	9.826670	-0.699291	4.886878
H	-1.528962	-2.479519	3.684548	H	9.024093	3.152284	3.170640
H	-0.871487	-3.463465	2.348433	H	10.639885	1.401307	3.852887
H	-3.489425	-3.090015	2.395853	N	-8.810351	-1.394883	3.587860
H	-2.649578	-2.765441	0.855828	N	5.445661	0.740444	4.531316
Ni	-1.834524	-0.090823	5.249465	N	5.093939	0.244396	1.266683
N	-0.780333	1.436915	5.014199	N	-8.299846	2.088488	1.571749
N	-3.304151	1.066710	5.160817	C	7.190977	0.866462	0.745009
O	-2.875223	-1.615309	5.351192	C	7.973447	1.842941	0.132398
O	-0.402882	-1.236538	5.368080	C	7.769383	-0.334355	1.161884
C	0.504112	1.475468	4.949240	C	9.327708	1.619571	-0.081515
C	-4.699429	-3.028351	4.990443	H	7.496308	2.769884	-0.168423
C	-4.136918	-1.726632	5.105855	C	9.122932	-0.547832	0.955427
C	-5.017817	-0.616954	4.928616	H	7.148437	-1.069966	1.658076
C	-6.363508	-0.824731	4.605365	C	9.904989	0.423500	0.331529

C	-6.869789	-2.100643	4.440044	H	9.933037	2.380114	-0.565002
C	-6.022022	-3.203465	4.668534	H	9.577544	-1.474445	1.292314
C	-4.536131	0.730218	5.005716	H	10.965127	0.248434	0.175312
C	3.136910	-1.800731	5.231907	C	-10.179639	3.311828	1.451743
C	1.790257	-2.030149	5.361790	C	-10.836448	4.418051	1.988221
C	0.856957	-0.962603	5.288169	C	-10.886501	2.384266	0.681982
C	1.379070	0.353897	5.102092	C	-12.201512	4.581045	1.790636
C	2.756705	0.556836	4.961557	H	-10.257913	5.134311	2.562105
C	3.642514	-0.503719	5.016484	C	-12.246493	2.563381	0.471291
C	-2.927825	2.475916	5.270035	H	-10.354352	1.544440	0.250885
C	-1.556012	2.620015	4.635530	C	-12.909040	3.654836	1.030498
H	0.975347	2.433356	4.717735	H	-12.712067	5.436690	2.221046
H	-4.037046	-3.870329	5.159280	H	-12.792908	1.852113	-0.140970
H	-7.023135	0.021384	4.444342	H	-13.972906	3.788850	0.861589
H	-6.444400	-4.198426	4.565773	N	-8.783290	3.236231	1.684916
H	-5.278771	1.524972	4.902402	N	5.824392	1.201095	0.929491

$[Ni(Phazosalen)]_2^+$ charge = 1 E(DCBS) = -3455.12235487 Hartree

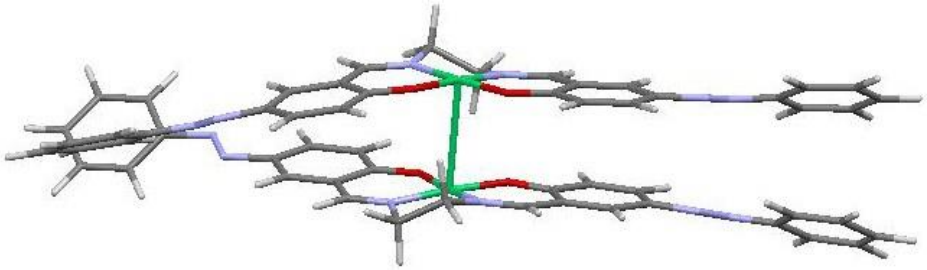

Table SI8. Cartesian coordinates of $[Ni(Phazosalen)]_2^+$

Atom	***x***	***y***	***z***	**Atom**	***x***	***y***	***z***
Ni	-1.893804	-0.030720	1.686942	H	4.048555	-2.433104	5.136087
N	-3.353931	-1.187511	1.608544	H	1.580179	-2.888018	5.208586
N	-0.836471	-1.570381	1.909269	H	3.291106	1.740421	4.549748
O	-0.422180	1.103267	1.637760	H	-2.710165	2.843121	5.955730
O	-2.907705	1.492777	1.610168	H	-3.573303	3.179820	4.433638
C	-4.598773	-0.849736	1.558724	H	-0.976090	3.645294	4.428195
C	1.764773	1.872294	1.445699	H	-1.630582	2.625796	3.106221
C	0.819812	0.805573	1.584872	N	5.182270	-0.185904	4.805565
C	1.333271	-0.532347	1.689463	N	-8.077012	-2.386638	4.110332
C	2.713557	-0.745845	1.661983	C	-10.071722	-1.656644	3.337475
C	3.606247	0.306155	1.518507	C	-10.743891	-0.582381	2.756715
C	3.105615	1.631517	1.406321	C	-10.748766	-2.844492	3.631860
C	0.445214	-1.647290	1.875767	C	-12.099252	-0.689495	2.471093
C	-6.130398	3.079738	1.682798	H	-10.184460	0.321275	2.536353
C	-4.771989	2.897973	1.674875	C	-12.098491	-2.945188	3.337653
C	-4.200764	1.597616	1.610348	H	-10.205980	-3.663363	4.088764
C	-5.092160	0.489455	1.564674	C	-12.775655	-1.869523	2.760111
C	-6.484565	0.702467	1.564070	H	-12.622930	0.152373	2.031278
C	-7.011009	1.973792	1.623904	H	-12.632710	-3.862731	3.563036
C	-1.646578	-2.736526	2.268620	H	-13.835131	-1.955556	2.539729
C	-2.968057	-2.599199	1.532224	C	6.986271	1.112504	4.495434
H	-5.342610	-1.648616	1.527719	C	7.858503	0.219855	5.141448
H	1.359596	2.874226	1.353845	C	7.488254	2.255199	3.861347
H	3.117339	-1.749681	1.752407	C	9.215510	0.476540	5.135909
H	3.821086	2.436303	1.286643	H	7.449140	-0.653658	5.633570
H	0.909293	-2.623377	2.035951	C	8.852979	2.495737	3.847029
H	-6.560488	4.074108	1.721426	H	6.787644	2.919956	3.368466
H	-4.088801	3.740754	1.689869	C	9.715476	1.607728	4.483165
H	-7.170153	-0.140022	1.551348	H	9.896863	-0.202753	5.637404
H	-1.813252	-2.683322	3.348876	H	9.246053	3.369114	3.338701
H	-1.135385	-3.671763	2.019092	H	10.784164	1.796522	4.477653
H	-3.735104	-3.240595	1.975865	N	-8.700853	-1.430215	3.603420
H	-2.844863	-2.866952	0.477101	N	5.603076	0.945382	4.426255
Ni	-1.697698	0.002692	4.853291	N	4.968767	-0.022323	1.474697
N	-0.652023	1.549617	4.569361	N	-8.420472	2.081895	1.583987
N	-3.168533	1.141108	4.839755	C	7.083839	0.626429	1.049009
O	-2.683137	-1.520182	5.041176	C	7.877718	1.563230	0.383217
O	-0.204293	-1.121321	4.932919	C	7.671142	-0.479489	1.676499
C	0.625641	1.635581	4.562390	C	9.253118	1.392451	0.327854
C	-4.507455	-2.966551	4.829372	H	7.390815	2.411851	-0.085300
C	-3.967921	-1.657530	4.884207	C	9.045575	-0.634620	1.630444
C	-4.870434	-0.566550	4.749449	H	7.038331	-1.183890	2.202773
C	-6.234567	-0.799055	4.516561	C	9.837644	0.296183	0.956031
C	-6.725064	-2.083360	4.401172	H	9.870110	2.113552	-0.197848

C	-5.847526	-3.167652	4.596709	H	9.509524	-1.480878	2.126313
C	-4.405768	0.783259	4.774612	H	10.914494	0.164463	0.923316
C	3.316754	-1.640971	5.020301	C	-10.266653	3.359478	1.673187
C	1.980714	-1.892175	5.057391	C	-10.835651	4.471147	2.291823
C	1.027012	-0.826302	4.915364	C	-11.066086	2.472857	0.945884
C	1.530935	0.522649	4.746693	C	-12.206957	4.679888	2.219972
C	2.893099	0.742591	4.695209	H	-10.186830	5.154381	2.829486
C	3.804958	-0.321381	4.817980	C	-12.432076	2.698457	0.861282
C	-2.805288	2.557273	4.902601	H	-10.602280	1.631637	0.444287
C	-1.474632	2.701611	4.186149	C	-13.006443	3.794527	1.504231
H	1.085100	2.604255	4.356754	H	-12.650552	5.538743	2.712826
H	-3.826272	-3.797622	4.975691	H	-13.053744	2.023358	0.280994
H	-6.917611	0.033514	4.387080	H	-14.075979	3.964490	1.433463
H	-6.258813	-4.170915	4.544028	N	-8.860456	3.231791	1.792791
H	-5.161791	1.568391	4.711113	N	5.705997	0.907752	1.066120

$[Ni(Phazosalen)]_2^{2+}$ charge = +2 E(DCBS) = -3454.79000069 Hartree

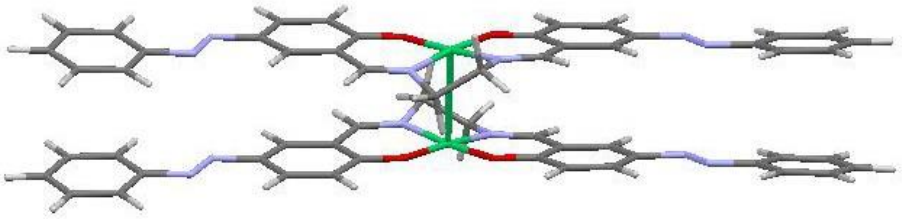

Table SI9. Cartesian coordinates of $[Ni(Phazosalen)]_2^{2+}$

Atom	***x***	***y***	***z***	**Atom**	***x***	***y***	***z***
Ni	-1.656420	-0.326606	1.356252	H	3.621913	-2.910312	4.625854
N	-2.948964	-1.649162	1.093053	H	1.124319	-3.049942	4.535576
N	-0.427747	-1.727687	1.463303	H	3.425541	1.358857	4.650258
O	-0.355464	0.979332	1.475823	H	-2.289989	3.040356	5.963726
O	-2.877951	1.051728	1.422221	H	-3.152930	3.698967	4.553141
C	-4.224381	-1.484495	1.051656	H	-0.531502	3.788831	4.412629
C	1.720175	2.035155	1.438712	H	-1.350407	2.959124	3.052946
C	0.915630	0.848203	1.429483	N	5.056799	-0.811014	4.658289
C	1.593768	-0.420047	1.397918	N	-8.449351	-1.165946	4.153980
C	2.986074	-0.458525	1.409160	C	-10.454219	-0.149687	4.245411
C	3.744906	0.707364	1.443623	C	-11.126725	1.055762	4.487255
C	3.080364	1.968812	1.445363	C	-11.179168	-1.328579	3.995192
C	0.854775	-1.647664	1.443596	C	-12.511497	1.087949	4.492938
C	-6.269961	2.198545	1.521432	H	-10.536604	1.945275	4.676156
C	-4.906137	2.198797	1.536820	C	-12.559233	-1.285746	3.997531
C	-4.158657	0.987001	1.385750	H	-10.640620	-2.250306	3.813101
C	-4.895971	-0.231032	1.207795	C	-13.226868	-0.081072	4.247553
C	-6.290504	-0.201665	1.184807	H	-13.034245	2.018258	4.684020
C	-6.993522	0.984489	1.350731	H	-13.129588	-2.189582	3.811175
C	-1.093879	-3.006063	1.709394	H	-14.311957	-0.061003	4.254251
C	-2.371378	-2.980790	0.892619	C	7.009912	0.298570	4.693077
H	-4.853148	-2.362194	0.892336	C	7.782484	-0.868872	4.842415
H	1.194309	2.983694	1.424911	C	7.631078	1.555185	4.641951
H	3.514423	-1.406551	1.401750	C	9.154589	-0.762167	4.941156
H	3.689715	2.864613	1.447586	H	7.283913	-1.829150	4.885182
H	1.433544	-2.570050	1.513768	C	9.008842	1.651946	4.742856
H	-6.835244	3.116956	1.627506	H	7.005806	2.433581	4.529283
H	-4.337575	3.116204	1.644111	C	9.769691	0.495117	4.890926
H	-6.861136	-1.113806	1.042242	H	9.760202	-1.653844	5.063519
H	-1.332795	-3.034054	2.777917	H	9.491695	2.621804	4.705312
H	-0.453614	-3.854892	1.451288	H	10.849254	0.567122	4.975757
H	-3.066765	-3.767974	1.198175	N	-9.061458	-0.072551	4.294067
H	-2.143554	-3.104293	-0.171142	N	5.619549	0.318853	4.606228
Ni	-1.732646	0.259240	4.468108	N	5.125546	0.540470	1.458459
N	-0.501747	1.661559	4.411620	N	-8.383332	0.883983	1.307314
N	-3.037571	1.580662	4.670147	C	7.162982	1.485573	1.411980
O	-2.945546	-1.120926	4.356293	C	7.881611	2.687342	1.316030
O	-0.427013	-1.044511	4.407407	C	7.843821	0.256637	1.501056
C	0.777805	1.584078	4.490035	C	9.265328	2.667122	1.307447
C	-4.962879	-2.271940	4.149548	H	7.324990	3.615222	1.242527
C	-4.227146	-1.061751	4.330976	C	9.223968	0.247270	1.493948
C	-4.976281	0.158284	4.470008	H	7.270947	-0.659306	1.570264
C	-6.366258	0.138613	4.424203	C	9.935876	1.447491	1.398554
C	-7.060463	-1.054040	4.226554	H	9.825049	3.592406	1.225843
C	-6.328671	-2.261483	4.099564	H	9.759438	-0.693250	1.562772
C	-4.312507	1.414488	4.654155	H	11.020958	1.428015	1.387534

C	3.005003	-2.018259	4.595805	C	-10.379914	1.909225	1.383431
C	1.644131	-2.098501	4.540816	C	-11.053753	3.119998	1.596223
C	0.841169	-0.915258	4.509587	C	-11.101209	0.738927	1.086469
C	1.518291	0.356591	4.570494	C	-12.435537	3.166606	1.516529
C	2.905324	0.407946	4.620280	H	-10.466255	4.005200	1.814248
C	3.667853	-0.762439	4.615879	C	-12.478307	0.795662	1.006514
C	-2.470682	2.913682	4.891346	H	-10.562025	-0.184735	0.919562
C	-1.158650	2.937677	4.131095	C	-13.147186	2.004828	1.221288
H	1.358456	2.506697	4.443254	H	-12.960366	4.102374	1.675044
H	-4.393885	-3.191584	4.072459	H	-13.044109	-0.100378	0.776024
H	-6.938722	1.053077	4.533258	H	-14.229580	2.039809	1.149875
H	-6.893584	-3.178601	3.967985	N	-8.988442	1.978413	1.469319
H	-4.950021	2.290920	4.781868	N	5.777692	1.621186	1.404647

$[Ni(salen)]_2$ charge = 0 E(DCBS) = -2093.99420786 Hartree

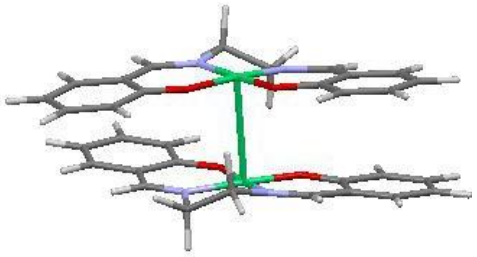

Table SI10. Cartesian coordinates of $[Ni(salen)]_2$

Atom	***x***	***y***	***z***	**Atom**	***x***	***y***	***z***
Ni	-1.671812	-0.049231	1.479241	N	-0.632849	1.321914	4.478300
N	-3.122260	-1.233887	1.553522	N	-3.165974	1.005477	4.634919
N	-0.594066	-1.547662	1.778914	O	-2.786195	-1.678641	4.888319
O	-0.253836	1.112820	1.339848	O	-0.301975	-1.338190	4.927266
O	-2.738632	1.450880	1.312522	C	0.654123	1.355160	4.516822
C	-4.372520	-0.923246	1.555936	C	-4.674079	-3.047017	4.767484
C	1.934755	1.897036	1.132196	C	-4.072375	-1.758869	4.782255
C	1.012624	0.835355	1.319204	C	-4.938798	-0.636478	4.658847
C	1.550437	-0.469240	1.503719	C	-6.331421	-0.825376	4.543106
C	2.945855	-0.666538	1.506146	C	-6.887112	-2.082543	4.527573
C	3.817647	0.378898	1.316900	C	-6.034909	-3.198123	4.640453
C	3.291840	1.669743	1.129797	C	-4.415224	0.693340	4.595679
C	0.693523	-1.579591	1.775243	C	3.237353	-1.891252	5.233487
C	-5.995430	2.965954	1.461070	C	1.881085	-2.120049	5.194142
C	-4.631148	2.816712	1.375805	C	0.963210	-1.059401	4.981956
C	-4.027554	1.529378	1.379272	C	1.504478	0.245721	4.811759
C	-4.895772	0.405814	1.476549	C	2.899236	0.444544	4.847375
C	-6.291561	0.592816	1.549541	C	3.766683	-0.599889	5.060558
C	-6.849179	1.849221	1.547758	C	-2.762500	2.412737	4.630621
C	-1.354491	-2.711822	2.234859	C	-1.381974	2.485271	4.002121
C	-2.717709	-2.640816	1.569499	H	1.144858	2.301512	4.276663
H	-5.100445	-1.734041	1.641278	H	-4.012689	-3.901202	4.868107
H	1.522562	2.889992	0.986830	H	-6.963139	0.053090	4.441300
H	3.326313	-1.669507	1.681478	H	-7.959435	-2.215091	4.436010
H	3.969575	2.506381	0.982206	H	-6.459887	-4.198154	4.631977
H	1.178552	-2.525507	2.028396	H	-5.141390	1.503247	4.489379
H	-6.421812	3.965411	1.456450	H	3.911719	-2.727127	5.399681
H	-3.968167	3.671810	1.295438	H	1.466222	-3.113443	5.328527
H	-6.924930	-0.286502	1.631970	H	3.283225	1.447915	4.682317
H	-7.923985	1.980305	1.606325	H	4.838131	-0.435447	5.081857
H	-1.461281	-2.634601	3.319824	H	-2.725052	2.756034	5.671109
H	-0.836050	-3.644483	1.986267	H	-3.482988	3.025330	4.078903
H	-3.452209	-3.253806	2.101945	H	-0.871424	3.418485	4.264537
H	-2.652064	-2.984684	0.530582	H	-1.459722	2.407864	2.914721
Ni	-1.716861	-0.177636	4.749282	H	4.889456	0.215608	1.324895

$[Ni(salen)]_2^+$ charge = 1 E(DCBS) = -2093.76232361 Hartree

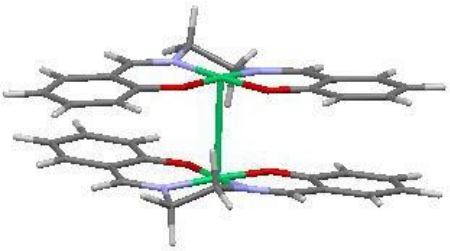

Table SI11. Cartesian coordinates of $[Ni(salen)]_2^+$

Atom	***x***	***y***	***z***	**Atom**	***x***	***y***	***z***
Ni	-1.694426	-0.175617	1.562269	N	-0.704437	1.504381	4.402854
N	-3.175915	-1.300961	1.527919	N	-3.217240	1.072197	4.656635
N	-0.670622	-1.730373	1.851012	O	-2.709323	-1.584114	4.823025
O	-0.191749	0.931295	1.512844	O	-0.231799	-1.156638	4.757342
O	-2.666652	1.355982	1.377539	C	0.573438	1.610218	4.446539
C	-4.413981	-0.935391	1.510720	C	-4.534638	-3.038799	4.734837
C	2.013779	1.654281	1.360661	C	-4.002195	-1.726536	4.750427
C	1.042619	0.611688	1.504818	C	-4.916848	-0.643853	4.665163
C	1.522738	-0.739602	1.654356	C	-6.303635	-0.894130	4.569465
C	2.899067	-0.984903	1.658094	C	-6.795575	-2.176053	4.543872
C	3.812093	0.046534	1.535334	C	-5.890704	-3.251380	4.630578
C	3.352237	1.373765	1.371553	C	-4.454865	0.705240	4.639081
C	0.608130	-1.834614	1.842792	C	3.307698	-1.594929	4.991884
C	-5.854103	3.019530	1.479948	C	1.969759	-1.877013	4.967974
C	-4.495369	2.808549	1.414543	C	1.001490	-0.835611	4.797472
C	-3.961180	1.496901	1.413329	C	1.483852	0.516247	4.659845
C	-4.876666	0.413140	1.471996	C	2.859449	0.763105	4.692093
C	-6.265923	0.661780	1.528068	C	3.770119	-0.267230	4.839490
C	-6.759872	1.943134	1.540018	C	-2.868799	2.493943	4.701555
C	-1.505937	-2.872108	2.230232	C	-1.530411	2.644904	4.000276
C	-2.824807	-2.722357	1.492539	H	1.020064	2.590252	4.265413
H	-5.173887	-1.719143	1.540702	H	-3.836042	-3.864204	4.821557
H	1.634600	2.660795	1.223068	H	-6.979462	-0.046153	4.500923
H	3.250475	-2.004849	1.780612	H	-7.861232	-2.360042	4.471263
H	4.073270	2.176107	1.251547	H	-6.269213	-4.269207	4.622526
H	1.050714	-2.814145	2.036190	H	-5.214562	1.488071	4.587526
H	-6.233839	4.036927	1.477768	H	4.026296	-2.396328	5.131205
H	-3.795534	3.634803	1.348337	H	1.588239	-2.883871	5.096179
H	-6.942408	-0.187050	1.577020	H	3.212783	1.783345	4.577970
H	-7.827379	2.125879	1.582174	H	4.832819	-0.055784	4.866489
H	-1.674791	-2.787664	3.308147	H	-2.787817	2.796081	5.751385
H	-1.012435	-3.821835	2.001540	H	-3.637400	3.101513	4.214617
H	-3.605876	-3.330726	1.958168	H	-1.044503	3.595356	4.241807
H	-2.714714	-3.024339	0.445311	H	-1.669781	2.559568	2.918239
Ni	-1.733989	-0.051624	4.664116	H	4.875383	-0.163647	1.536046

$[Ni(salen)]_2^{2+}$ charge = +2 E(DCBS) = -2093.40029378 Hartree

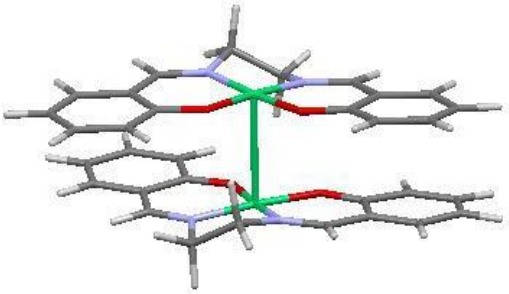

Table SI12. Cartesian coordinates of $[Ni(salen)]_2^{2+}$

Atom	***x***	***y***	***z***	**Atom**	***x***	***y***	***z***
Ni	-1.705417	-0.214782	1.593318	N	-0.732632	1.554500	4.391093
N	-3.187921	-1.311599	1.500679	N	-3.231527	1.083284	4.681445
N	-0.697786	-1.780687	1.861441	O	-2.681095	-1.552072	4.755295
O	-0.175952	0.872649	1.574505	O	-0.216949	-1.098397	4.694902
O	-2.638017	1.324087	1.443904	C	0.543984	1.685221	4.431176
C	-4.422972	-0.927698	1.463649	C	-4.475969	-3.047068	4.731665
C	2.029638	1.599771	1.432401	C	-3.976088	-1.724806	4.730921
C	1.043755	0.554776	1.580640	C	-4.909501	-0.653536	4.684502
C	1.511840	-0.818437	1.733935	C	-6.294678	-0.927814	4.638541
C	2.881673	-1.070336	1.742104	C	-6.757545	-2.220952	4.627924
C	3.798278	-0.033187	1.665307	C	-5.831375	-3.282431	4.679845
C	3.356952	1.308729	1.469851	C	-4.466777	0.698275	4.684274
C	0.579558	-1.910280	1.858045	C	3.312085	-1.531563	4.896226
C	-5.790583	3.051814	1.432242	C	1.984466	-1.823602	4.898236
C	-4.434060	2.817605	1.418183	C	1.002190	-0.779474	4.722318
C	-3.933306	1.495746	1.432160	C	1.473222	0.594063	4.581284
C	-4.866764	0.423693	1.451844	C	2.842619	0.847002	4.609961
C	-6.252898	0.696780	1.459288	C	3.757535	-0.189440	4.711794
C	-6.716955	1.989541	1.457652	C	-2.902817	2.508799	4.769846
C	-1.554114	-2.926189	2.178766	C	-1.580586	2.699258	4.049500
C	-2.855485	-2.736764	1.421082	H	0.973903	2.678817	4.291843
H	-5.190267	-1.703560	1.443506	H	-3.761722	-3.860610	4.797375
H	1.656002	2.603874	1.264820	H	-6.991932	-0.095503	4.608879
H	3.234047	-2.091841	1.841789	H	-7.821072	-2.426790	4.597293
H	4.094196	2.095161	1.346007	H	-6.194223	-4.305412	4.688854
H	1.006098	-2.903500	2.009861	H	-5.235052	1.473418	4.682444
H	-6.153904	4.074495	1.413682	H	4.046314	-2.317346	5.040417
H	-3.718925	3.631762	1.372941	H	1.607198	-2.827880	5.056339
H	-6.949987	-0.136139	1.468938	H	3.196750	1.868718	4.519063
H	-7.781095	2.194488	1.458653	H	4.819330	0.029387	4.739013
H	-1.745369	-2.861164	3.255806	H	-2.809585	2.780927	5.826093
H	-1.064203	-3.874121	1.939353	H	-3.687065	3.120316	4.314746
H	-3.651812	-3.349199	1.853420	H	-1.098535	3.647602	4.302828
H	-2.731886	-3.008372	0.367822	H	-1.741128	2.634298	2.967460
Ni	-1.746090	-0.012342	4.631324	H	4.860565	-0.251278	1.666525