Electronic Supplementary Information (ESI)

Aldimines generated from aza-Wittig reaction between *bis*(iminophosphoranes) derived from 1,1´diazidoferrocene and aromatic or heteroaromatic aldehydes: electrochemical and optical behaviour towards metal cations

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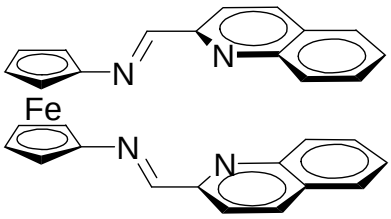
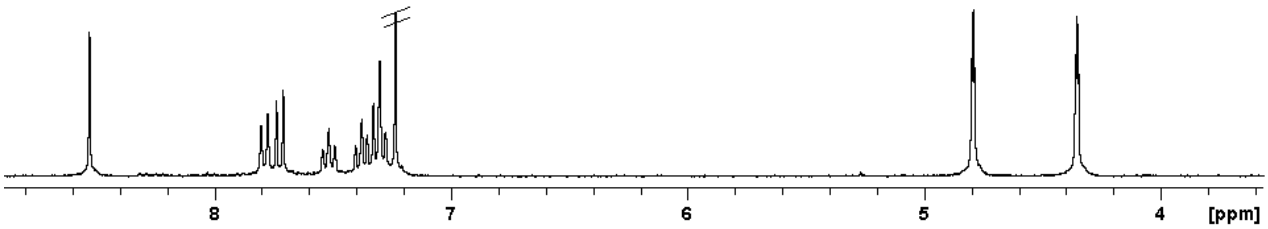
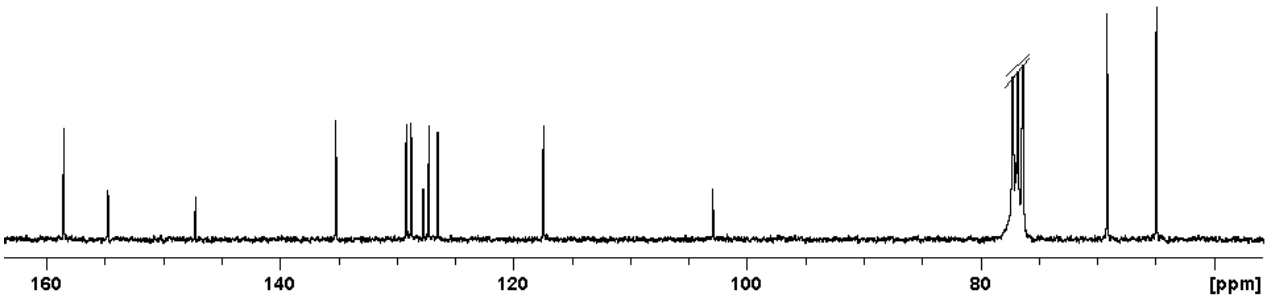
1,1,-Bis[(2-quinolyl)methyleneamino]ferrocene, 4

^{1}H NMR (400MHz, $CDCl_3$)



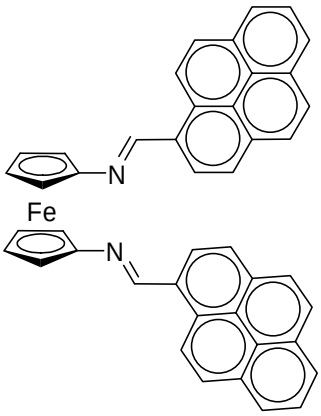


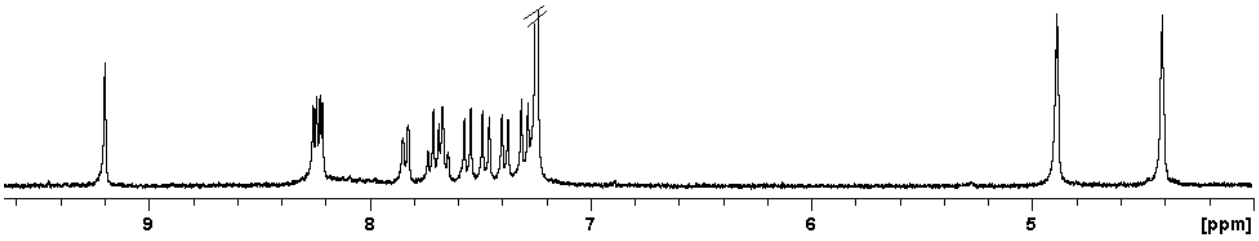
^{13}C NMR (100 MHz, $CDCl_3$)



1,1,-Bis[(1-pyrenyl)methyleneamino]ferrocene, 5

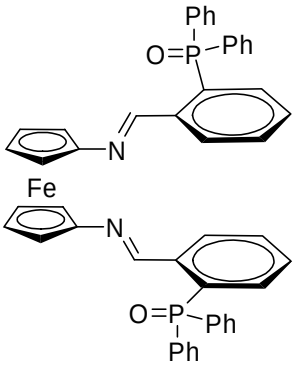
^{1}H NMR (300MHz, $CDCl_3$)

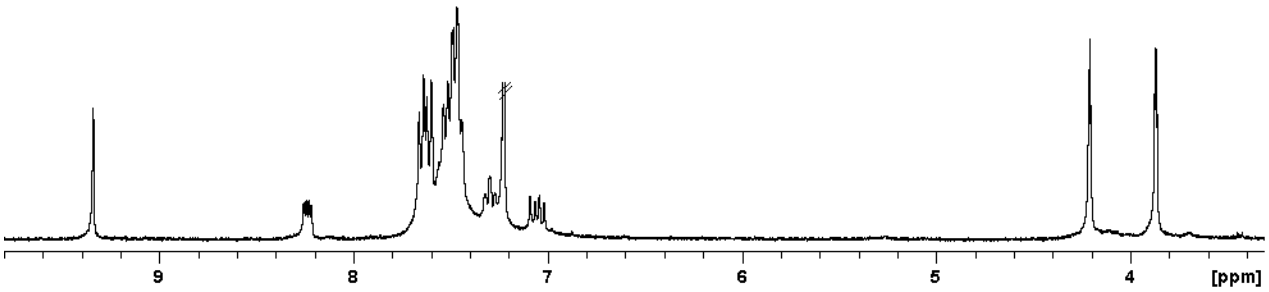




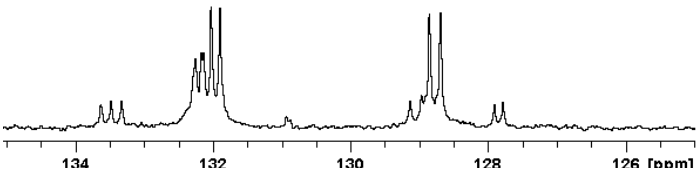
1,1,-Bis[(2-diphenylphosphoryl)benzylideneamino]ferrocene, 8

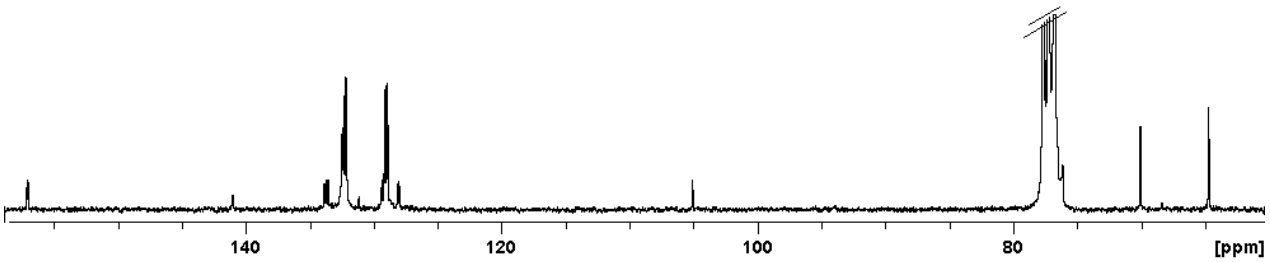
^{1}H NMR (300MHz, $CDCl_3$)



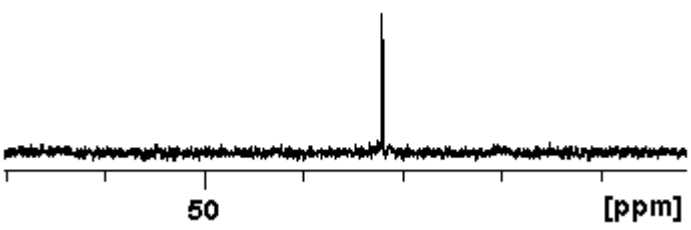


^{13}C NMR (75 MHz, $CDCl_3$)





^{31}P NMR (121 MHz, $CDCl_3$)



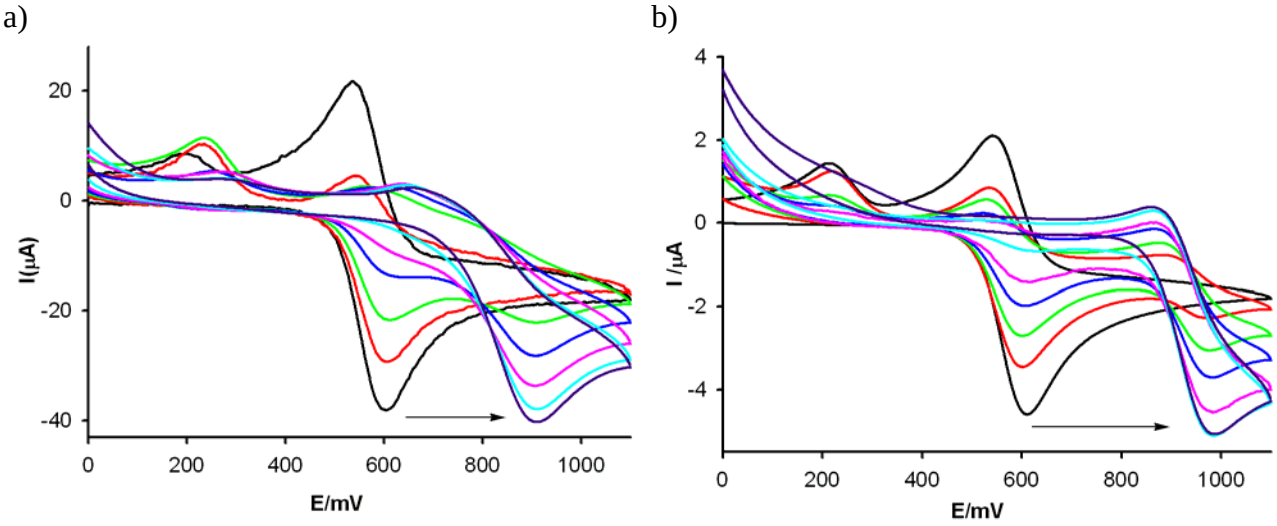
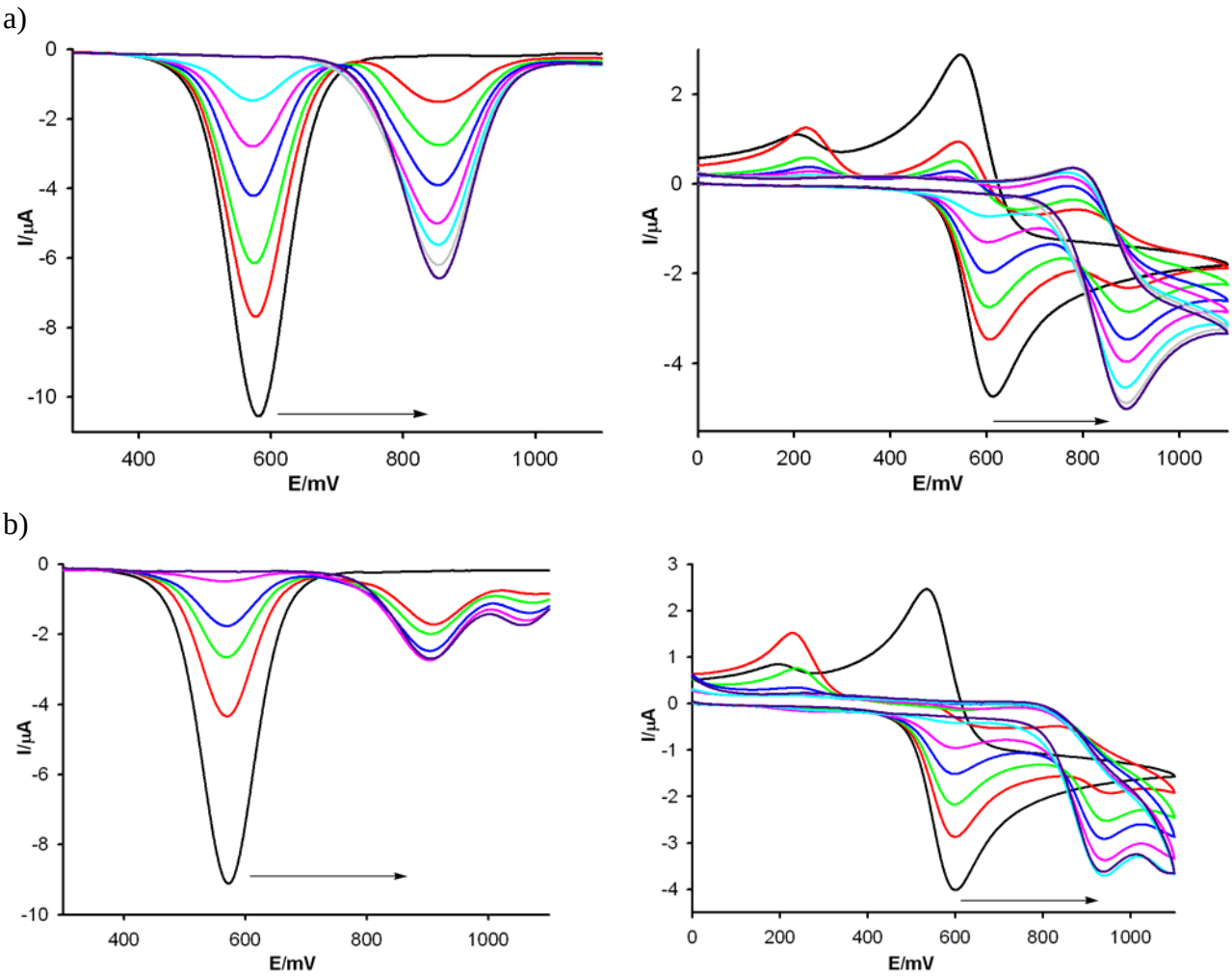


Figure ESI 1. Evolution of the CV of **4** (c = $1x10^{-4}$ M) in $CH_3CN/[(n\text{-}Bu)_4N]PF_6$ scanned at 0.1 V s^{-1} upon addition of increasing amounts (from 0 to 1.2 equiv) of **a)** Pb^{2+} and **b)** Hg^{2+}.



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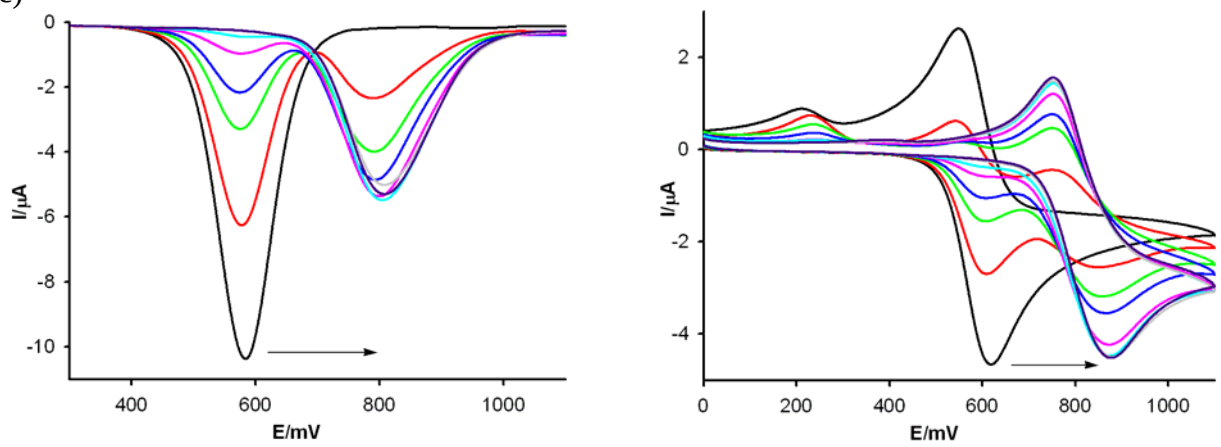


Figure ESI 2. Left: Evolution of the DPV of **4** (c = $1x10^{-4}$ M) in $CH_3CN/[(n\text{-}Bu)_4N]PF_6$ scanned at 0.1 V s^{-1} upon addition of increasing amounts (from 0 to 1.4 equiv) of: **a)** Cd^{2+}; **b)** Zn^{2+}; **c)** Ni^{2+}. **Right:** Evolution of the CV of **4** (c = $1x10^{-4}$ M) in $CH_3CN/[(n\text{-}Bu)_4N]PF_6$ scanned at 0.1 V s^{-1} upon addition of increasing amounts (from 0 to 1.4 equiv) of the same metals.

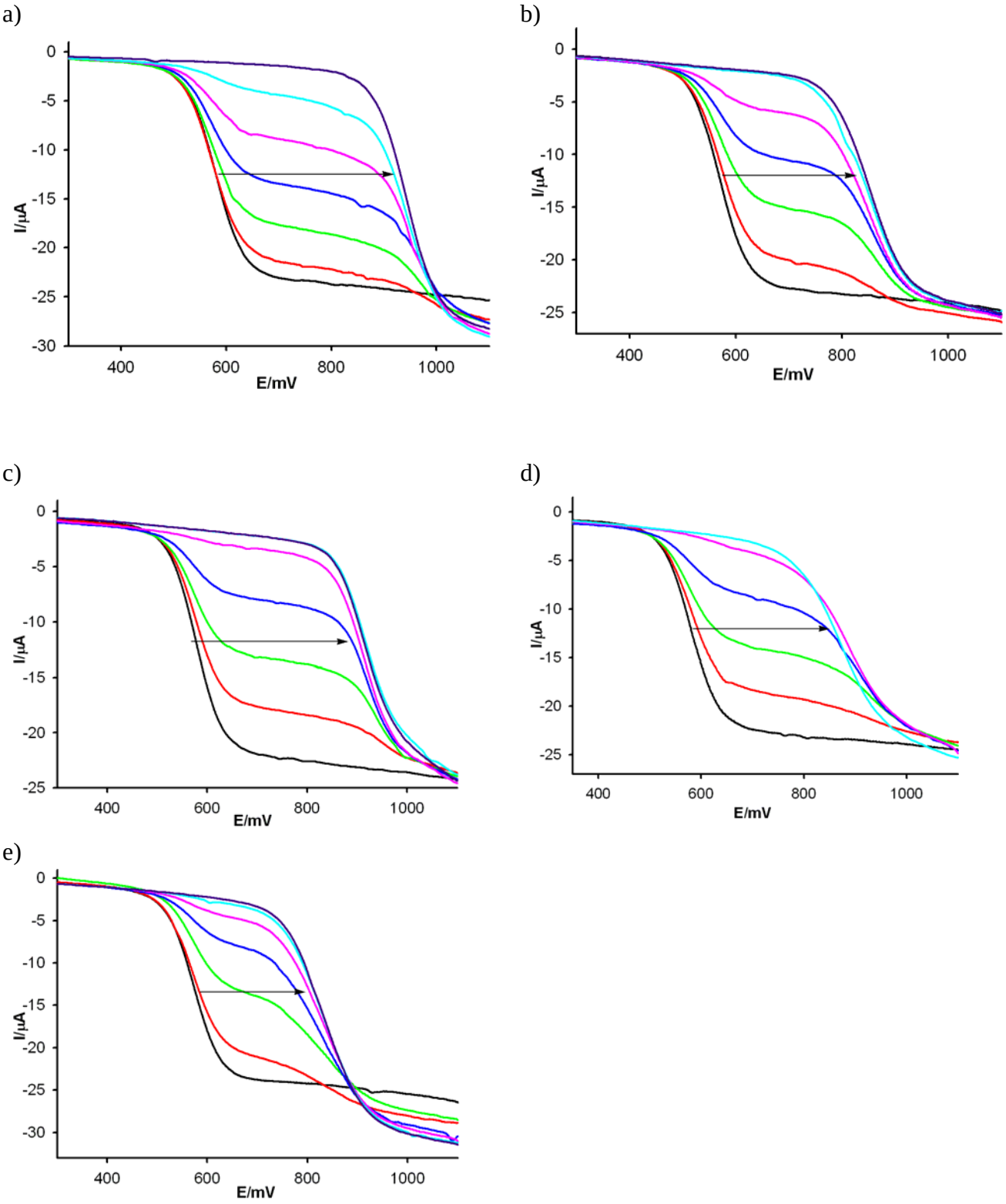
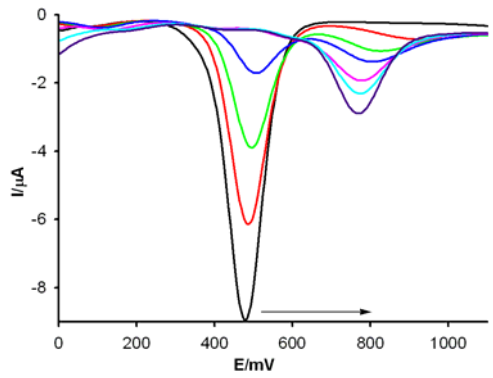
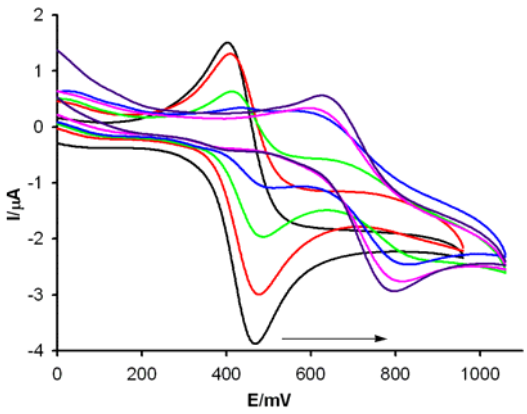


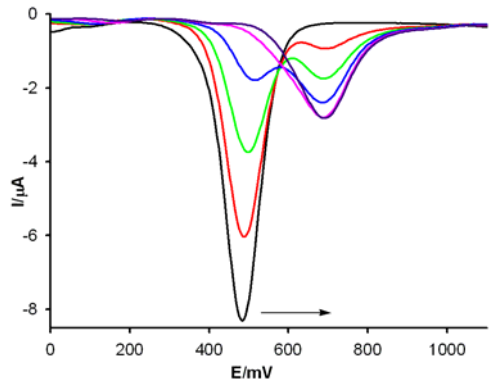
Figure ESI 3. Evolution of the LSW of **4** ($1x10^{-4}$ M) in $CH_3CN/[(n\text{-}Bu)_4N]PF_6$ obtained using a rotating disk electrode at 100 mVs^{-1} and 1000 rpm., upon addition of increasing amounts (from 0 to 1.4 equiv) of: a) Hg^{2+}; b) Cd^{2+}; c) Zn^{2+}; d) Pb^{2+}, e) Ni^{2+}.

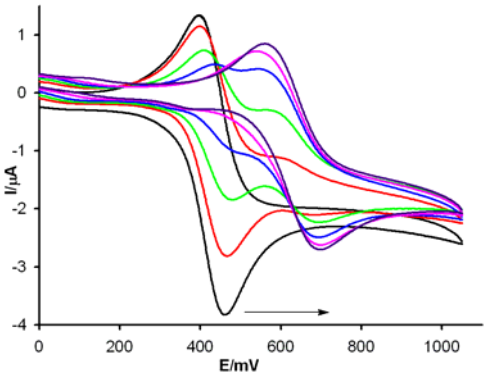
a)





b)





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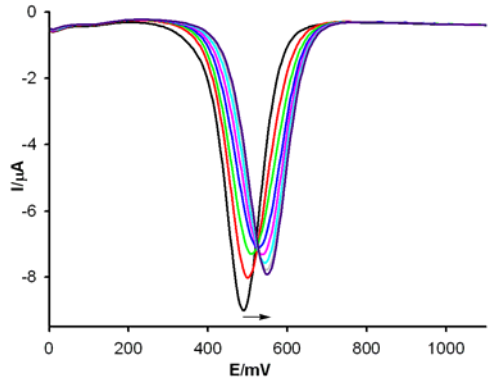
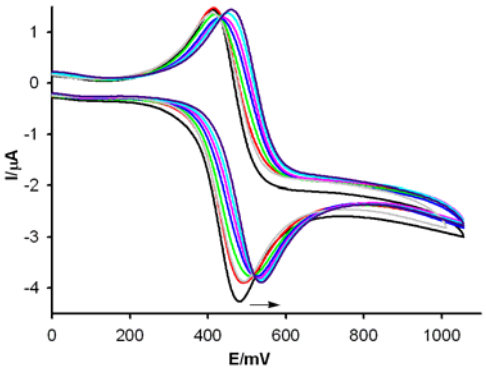
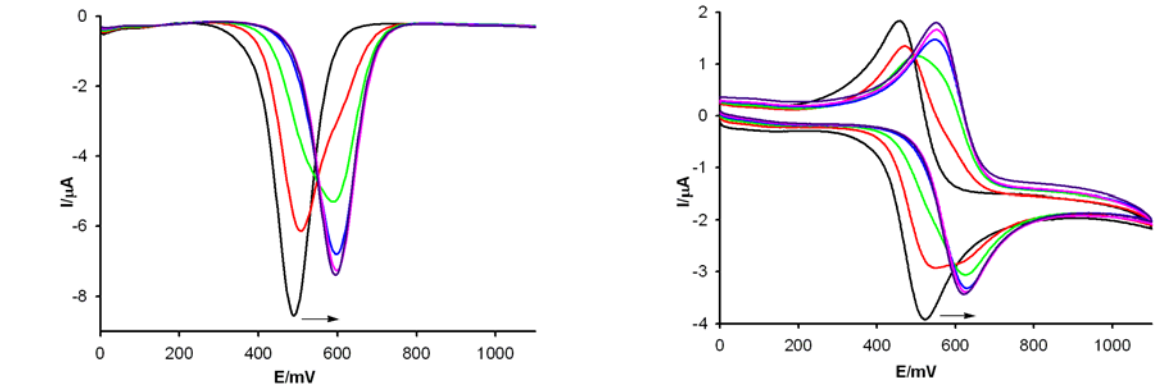




d)



e)

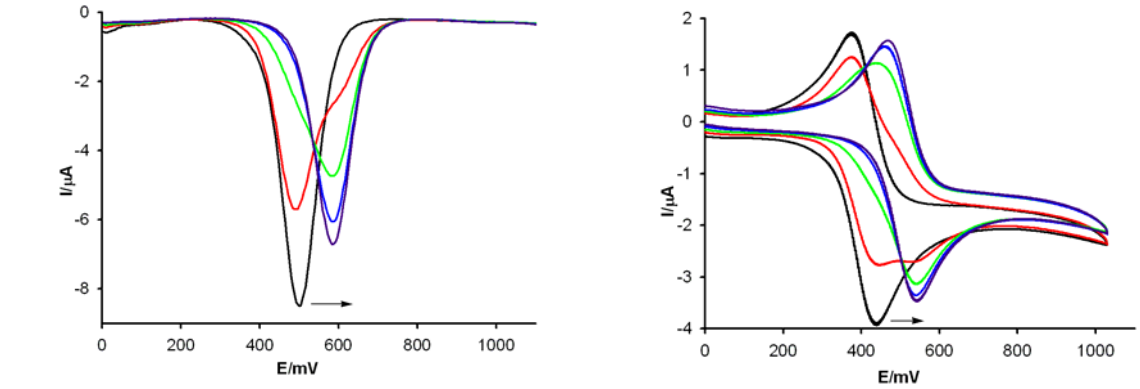


Figure ESI 4. Left: Evolution of the DPV of **8** (c = $1x10^{-4}$ M) in $CH_3CN/[(n\text{-}Bu)_4N]PF_6$ scanned at 0.1 V s^{-1} upon addition of increasing amounts (from 0 to 1 equiv) of: a) Pb^{2+}; b) Zn^{2+}; c) Li^{+}; d) Ca^{2+}, e) Mg^{2+} **. Right:** Evolution of the CV of **8** (c = $1x10^{-4}$ M) in $CH_3CN/[(n\text{-}Bu)_4N]PF_6$ scanned at 0.1 V s^{-1} upon addition of increasing amounts (from 0 to 1 equiv) of the same metals.

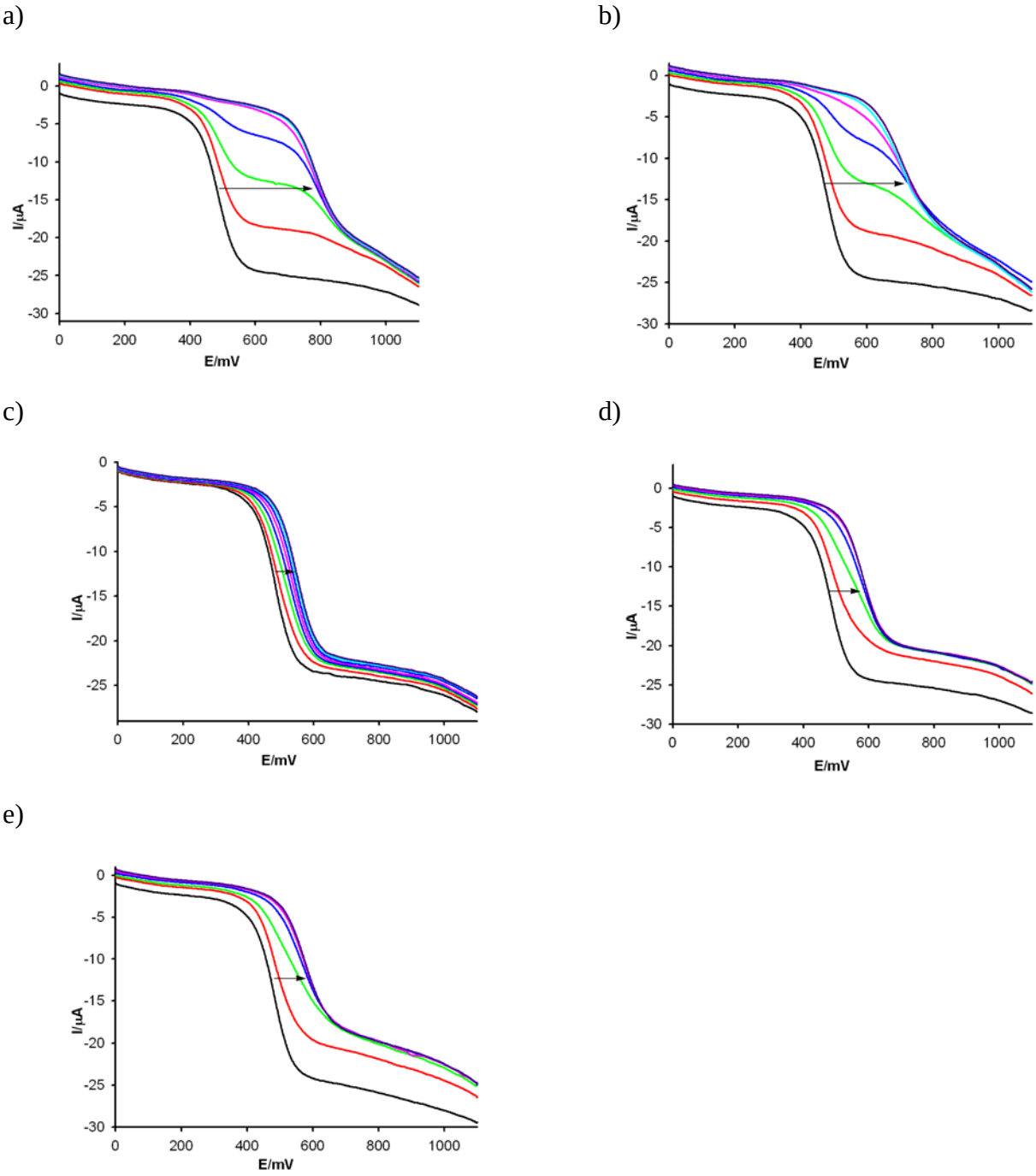


Figure ESI 5. Evolution of the LSW of **8** (c = $1x10^{-4}$ M) in $CH_3CN/[(n\text{-}Bu)_4N]PF_6$ obtained using a rotating disk electrode at 100 mVs^{-1} and 1000 rpm., upon addition of increasing amounts (from 0 to 1 equiv) of: a) Pb^{2+}; b) Zn^{2+}; c) Li^{+}; d) Ca^{2+}, e) Mg^{2+} .

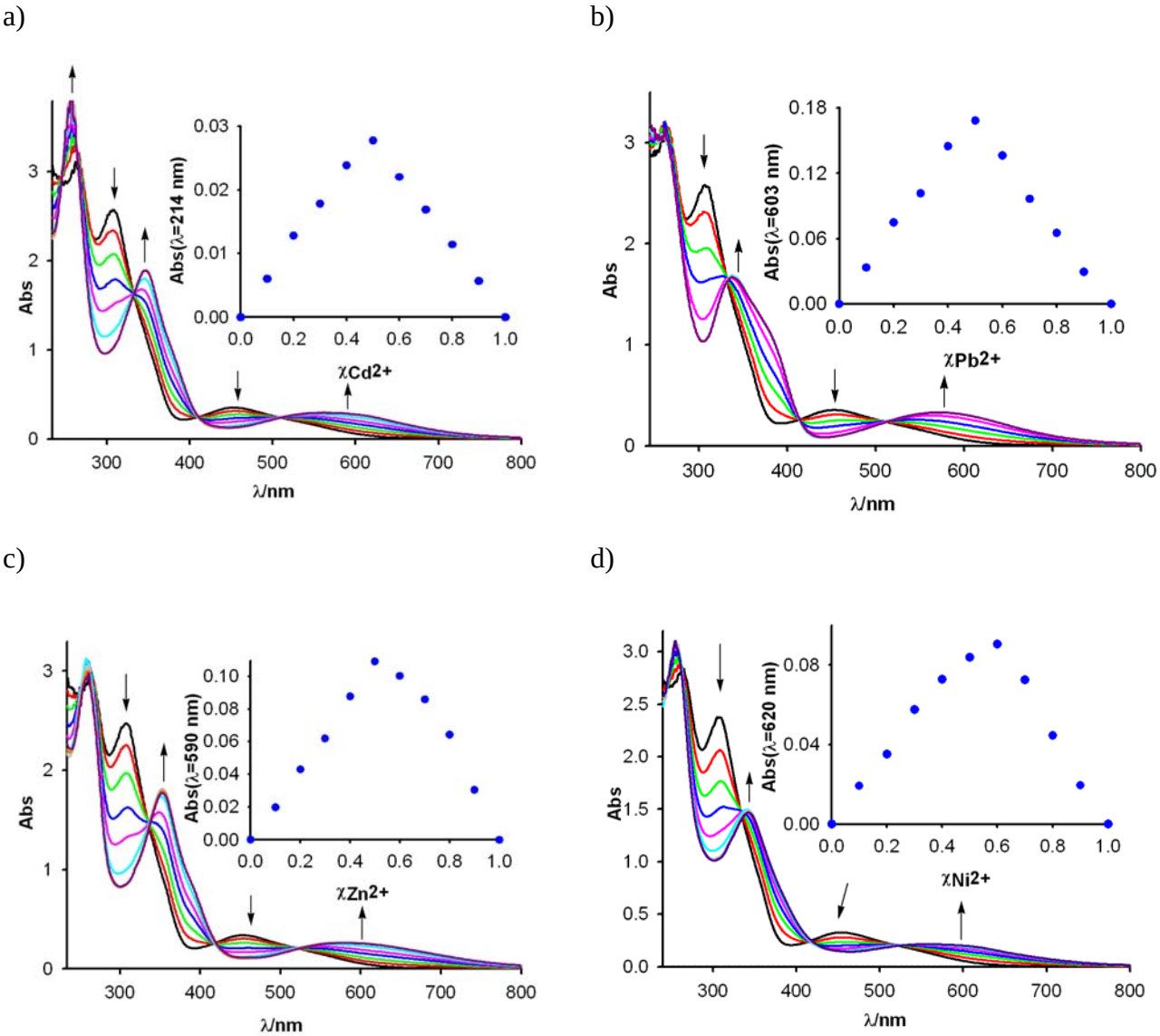
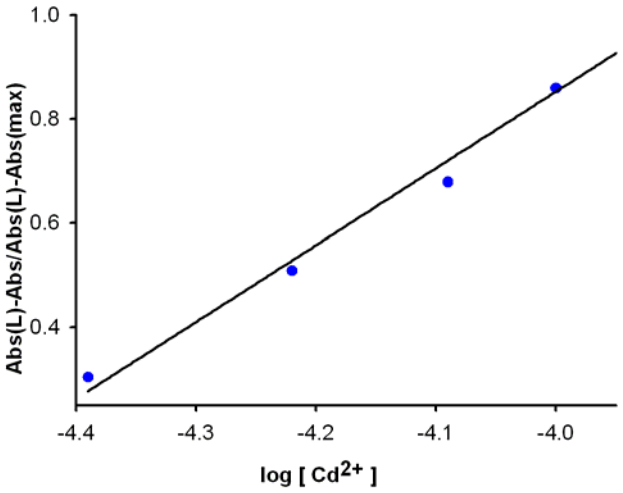
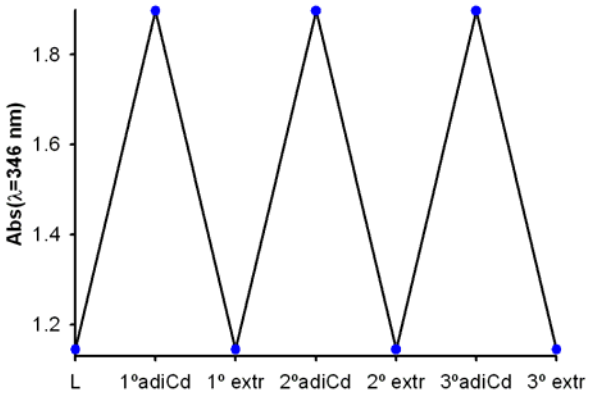


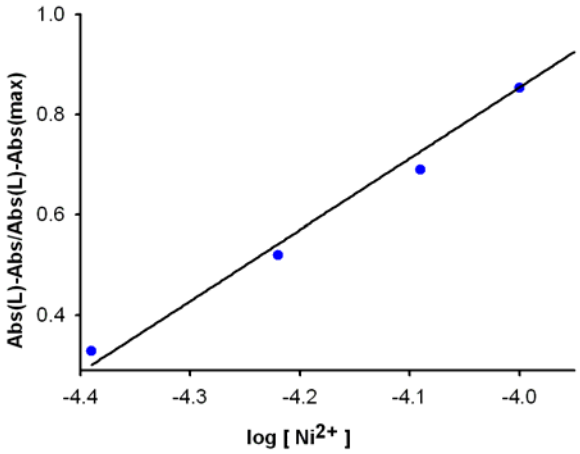
Figure ESI 6. Left: Changes in the absorption spectra of **4** (c =1x10^{-4} M) in CH_3CN upon addition of increasing amounts (from 0 to 1.6 equiv) of: a) Cd^{2+}; b) Pb^{2+}; c) Zn^{2+}; d) Ni^{2+}. **Inset:** Job´s plots indicating the formation of 1:1 complexes between **4** and Pb^{2+}, Cd^{2+}, Zn^{2+} and 2:1 complexes in the case of Ni^{2+} .The total [**4**] + [M^{2+}] =10^{-4} M.

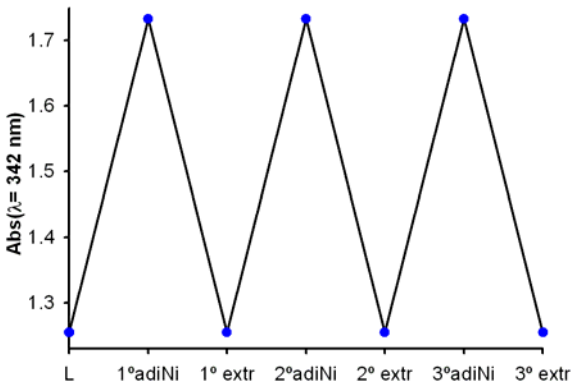
a)


Abs(L)-Abs/Abs(L)-Abs(max)
1.0
0.8
0.6
0.4
-4.4
-4.3
-4.2
-4.1
-4.0
log [Cd2+]

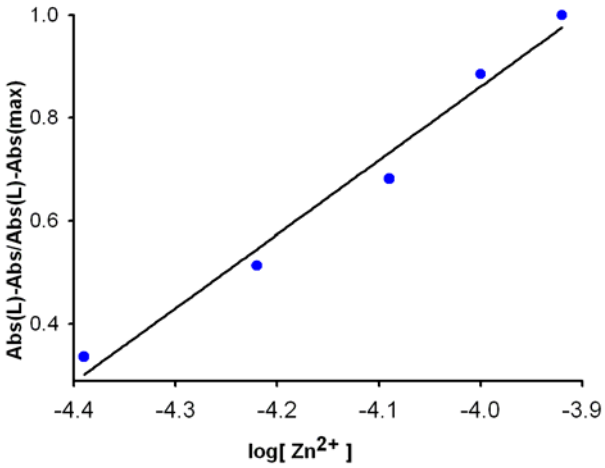

Abs(λ=346 nm)
1.8
1.6
1.4
1.2
L
1ºadiCd
1º extr
2ºadiCd
2º extr
3ºadiCd
3º extr

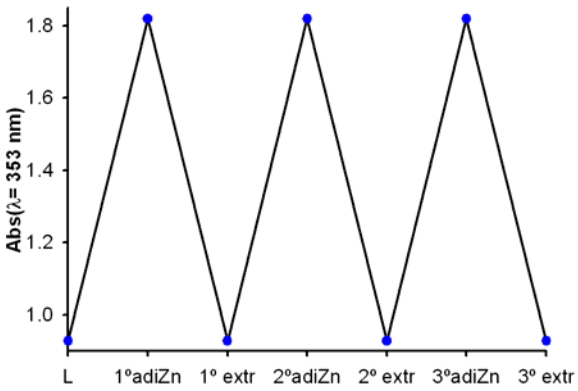
b)


Abs(L)-Abs/Abs(L)-Abs(max)
1.0
0.8
0.6
0.4
-4.4
-4.3
-4.2
-4.1
-4.0
log [Ni2+]

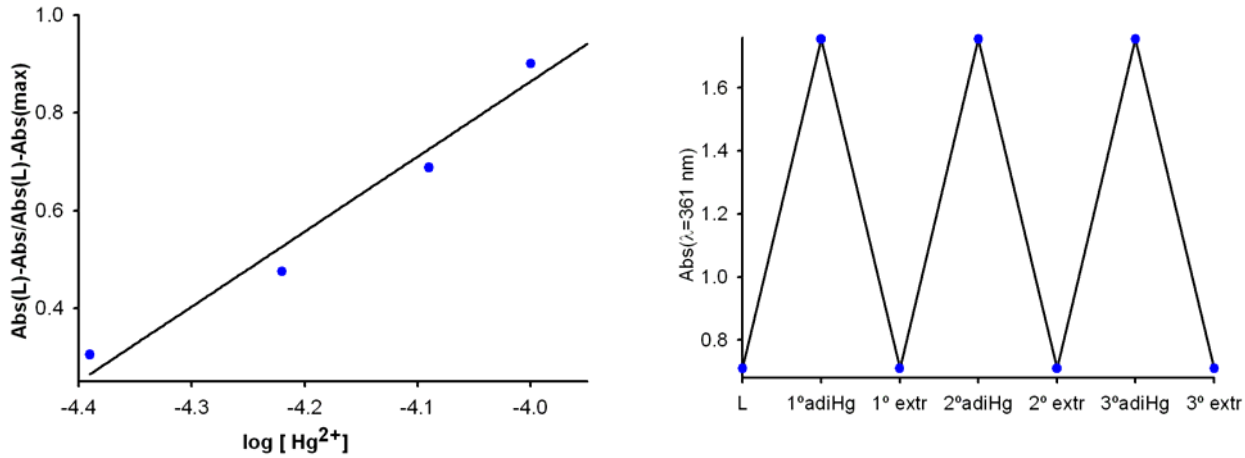

Abs(λ= 342 nm)
1.7
1.6
1.5
1.4
1.3
L
1ºadiNi
1º extr
2ºadiNi
2º extr
3ºadiNi
3º extr

c)


Abs(L)-Abs/Abs(L)-Abs(max)
1.0
0.8
0.6
0.4
-4.4
-4.3
-4.2
-4.1
-4.0
-3.9
log[Zn2+]


Abs(λ= 353 nm)
1.8
1.6
1.4
1.2
1.0
L
1ºadiZn
1º extr
2ºadiZn
2º extr
3ºadiZn
3º extr

d)



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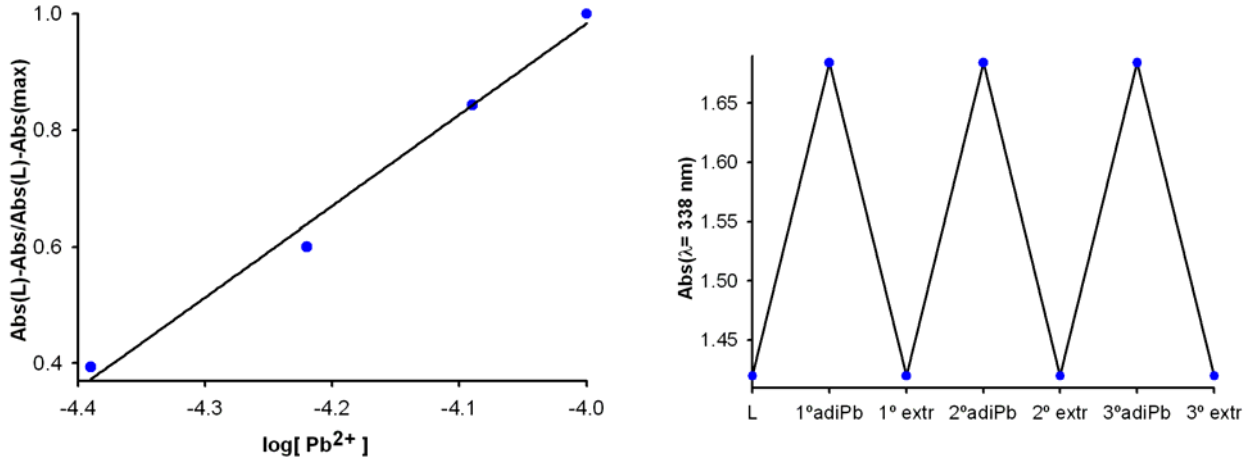
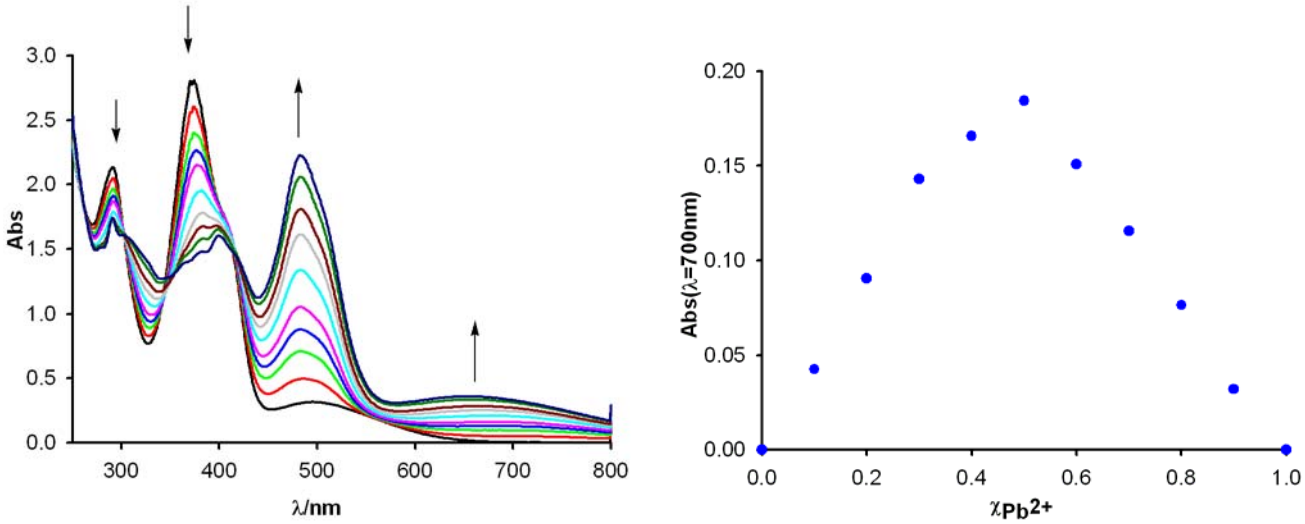


Figure ESI 7. Left: Absorbance of **4** (c = $1 \cdot 10^{-4}$M in CH_3CN) at each concentration of a) Cd^{2+}; b) Ni^{2+}; c) Zn^{2+}; d) Hg^{2+}, e) Pb^{2+} added, normalized between the minimum absorbance, found at zero equiv of M^{2+}, and the maximum absorbance. **Right:** Stepwise complexation [addition of a) Cd^{2+}; b) Ni^{2+}; c) Zn^{2+}; d) Hg^{2+}, e) Pb^{2+})]/decomplexation (extraction with H_2O) cycles of ligand **4** ($1 \cdot 10^{-4}$ M in CH_2Cl_2), carried out by UV/Vis analysis;

a)



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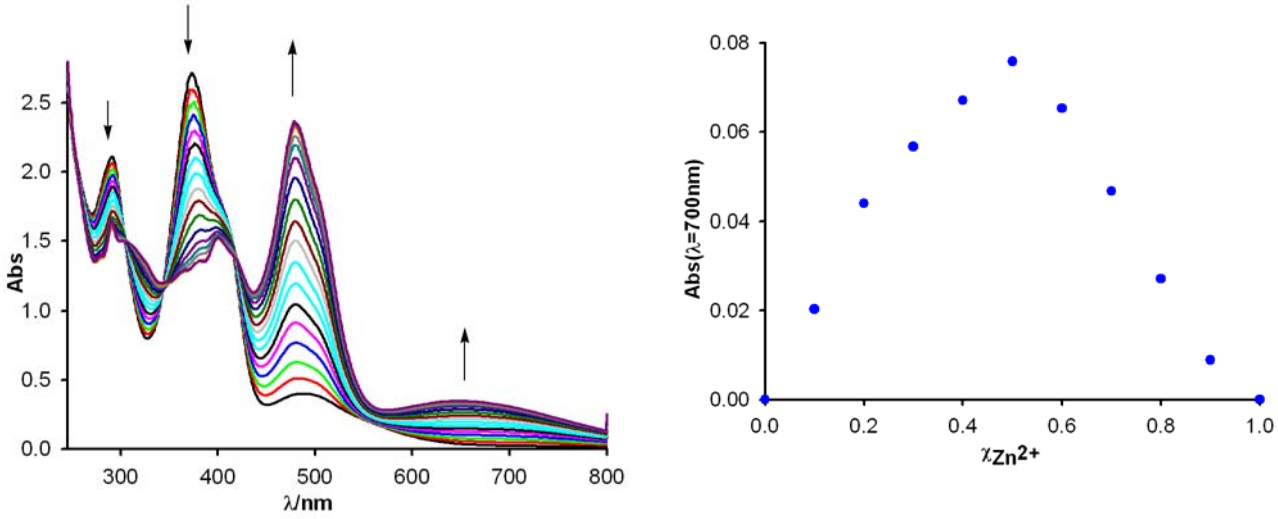
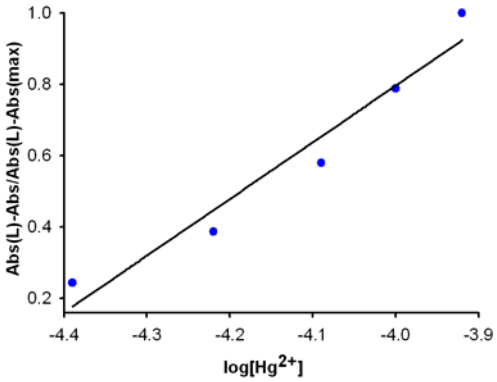
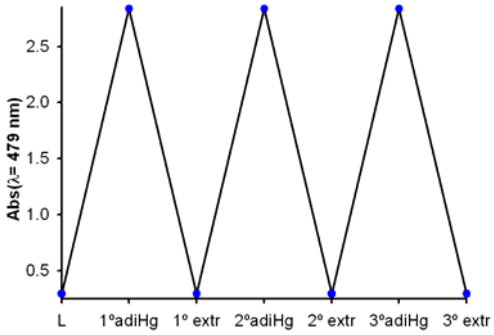


Figure ESI 8. Left: Changes in the absorption spectra of **5** (c =1x10^{-4} M) in $CHCl_3$ upon addition of increasing amounts, from 0 to 1.6 equiv, of: a) Pb^{2+}; b) Zn^{2+}. **Right:** Job´s Plot indicating the formation of 1:1 complexes between **5** and Pb^{2+}, Zn^{2+}.The total [**5**] + [M^{2+}] =10^{-4} M.

a)





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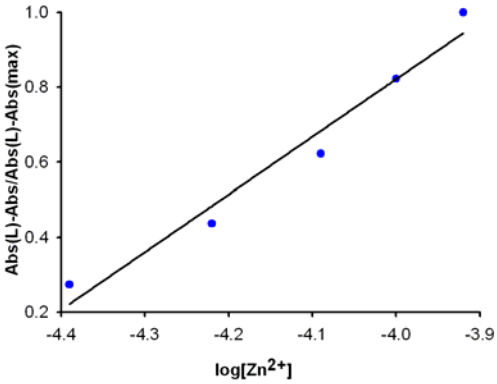
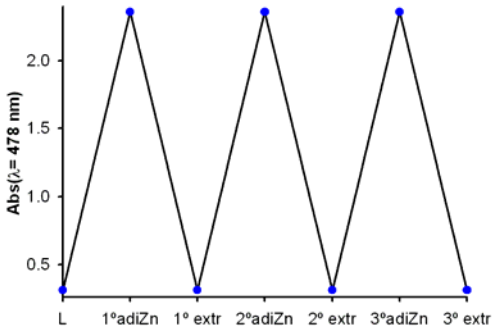
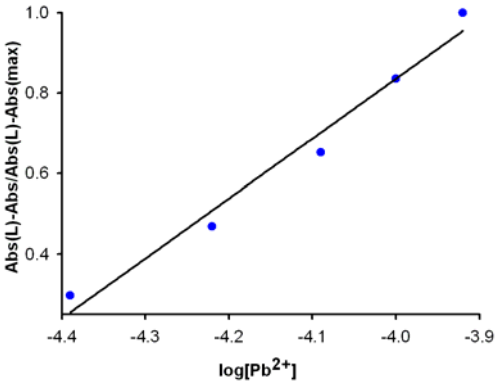




c)



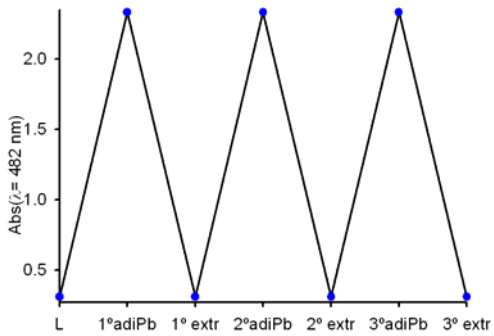
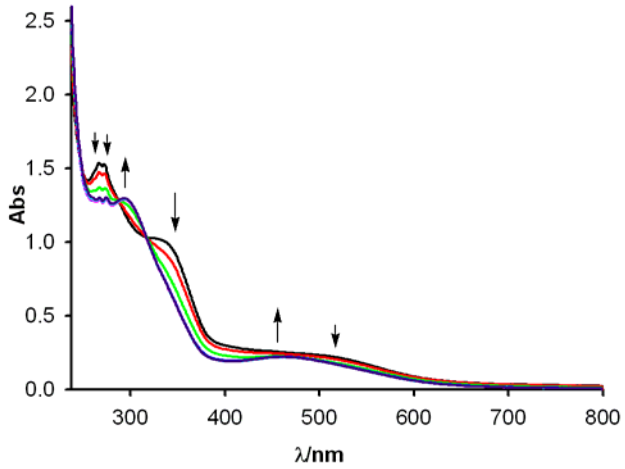
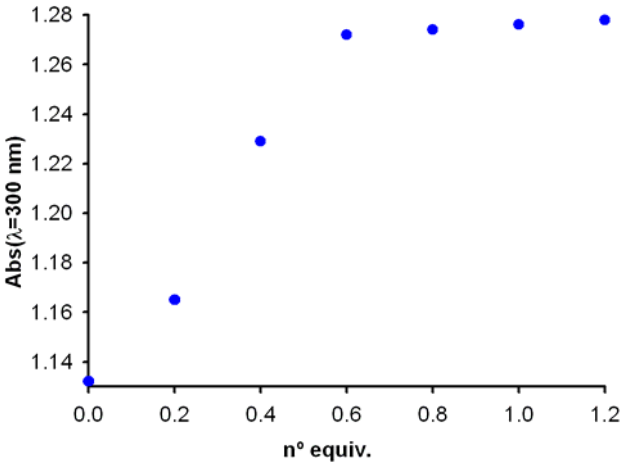


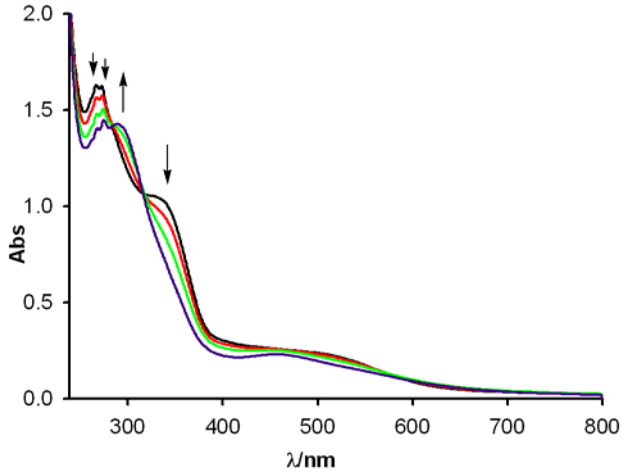
Figure ESI 9. Left: Absorbance of **5** (c = $1x10^{-4}$M in $CHCl_3$) at each concentration of a) Hg^{2+}; b) Zn^{2+}; c) Pb^{2+} added, normalized between the minimum absorbance, found at zero equiv of M^{2+}, and the maximum absorbance. **Right:** Stepwise complexation [addition of a) Hg^{2+}; b) Zn^{2+}; c) Pb^{2+}] /decomplexation (extraction with H_2O) cycles of ligand **5** ($1x10^{-4}$ M in $CHCl_3$), carried out by UV/Vis analysis;

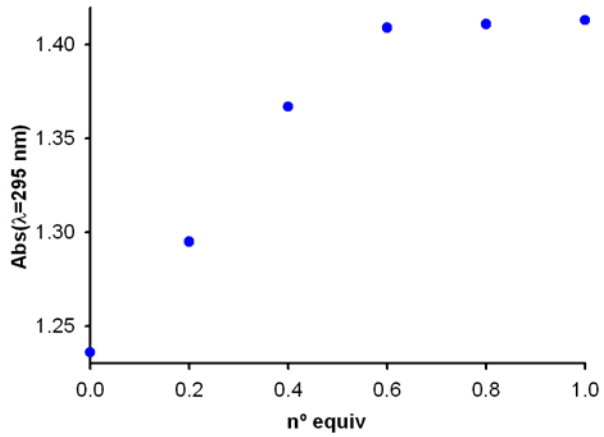
a)





b)





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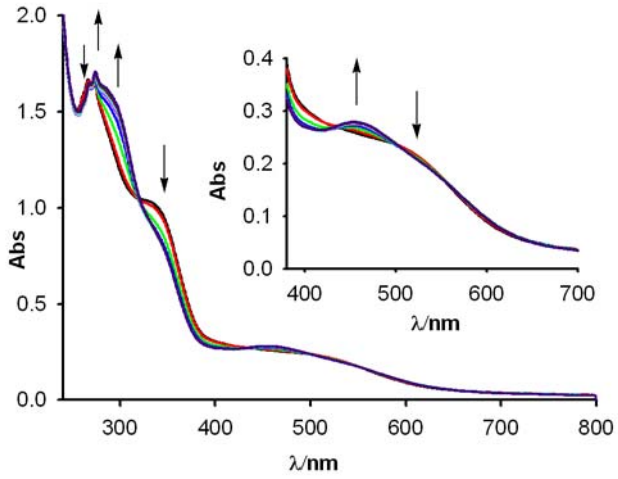
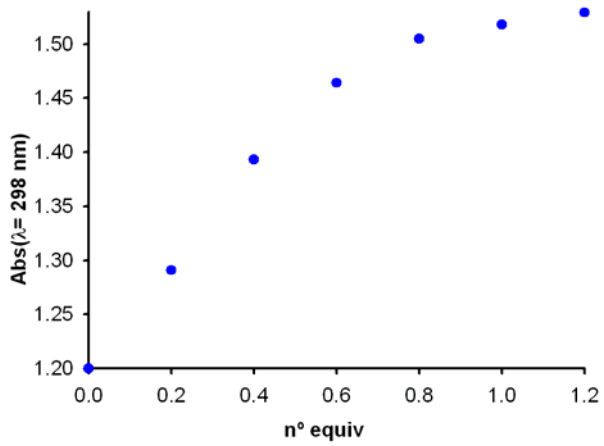




d)

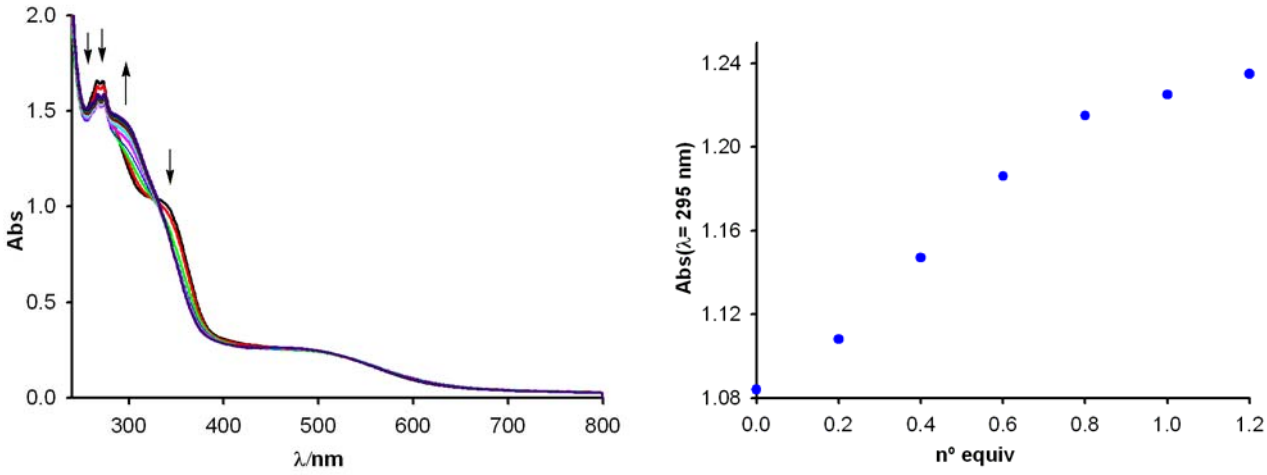
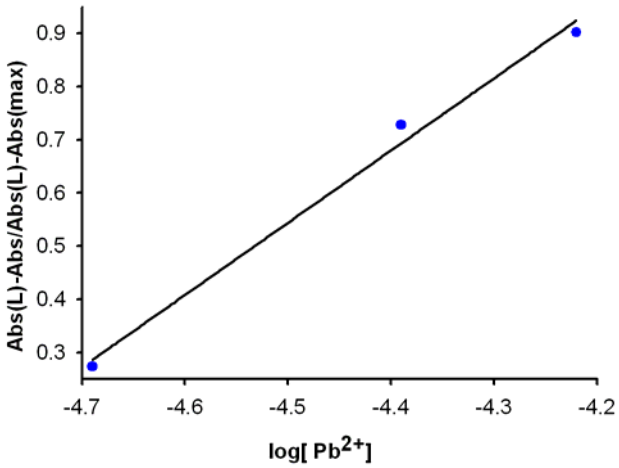
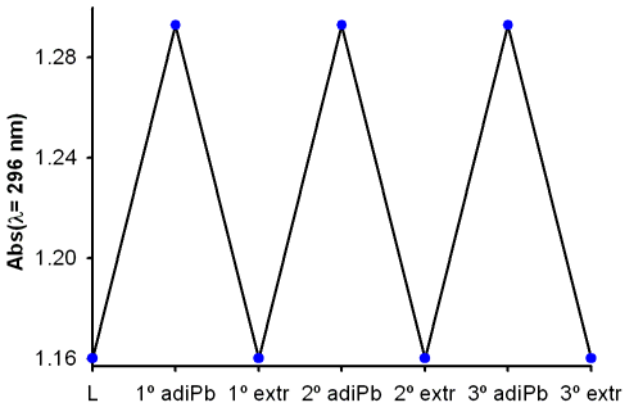


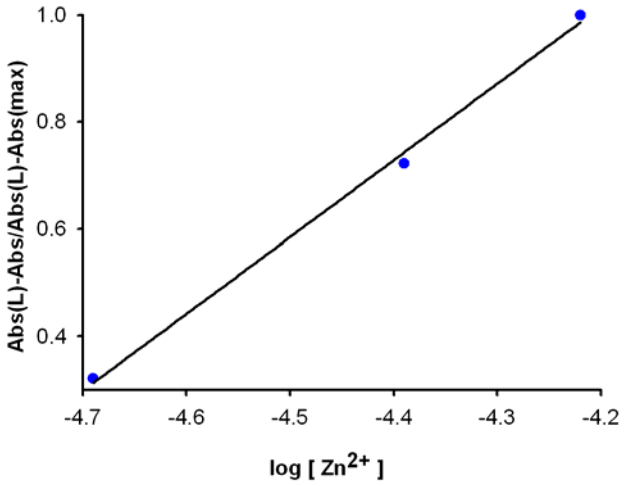
Figure ESI 10. Left: Changes in the absorption spectra of **8** (c =1x10^{-4} M) in CH_3CN upon addition of increasing amounts (from 0 to 1 equiv) of: a) Pb^{2+}; b) Zn^{2+}, c) Ca^{2+}; d) Mg^{2+}. **Right:** Binding profile associated with the observed maximum absorbance of ligand **8** (c = 1x10^{-4} M in CH_3CN), upon addition of increasing amounts of a) Pb^{2+}; b) Zn^{2+}, c) Ca^{2+}; d) Mg^{2+}, indicating the formation of 2:1 complex.

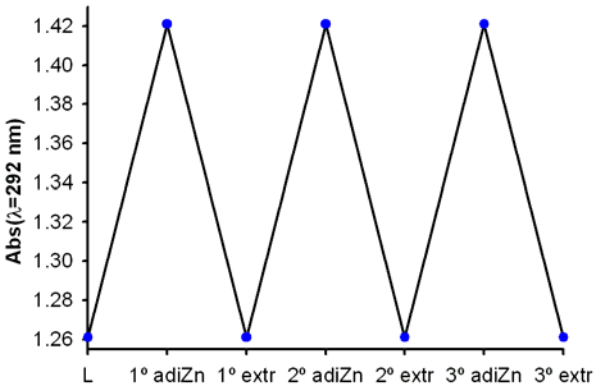
a)


Abs(L)-Abs/Abs(L)-Abs(max)
0.9
0.8
0.7
0.6
0.5
0.4
0.3
-4.7
-4.6
-4.5
-4.4
-4.3
-4.2
log[Pb2+]

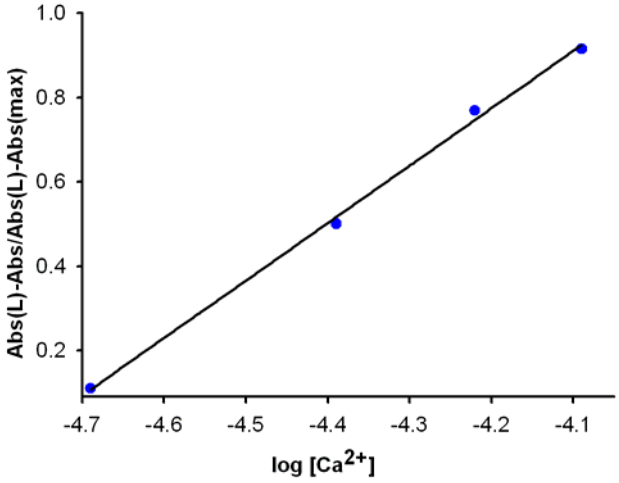

Abs(λ= 296 nm)
1.28
1.24
1.20
1.16
L
1º adiPb
1º extr
2º adiPb
2º extr
3º adiPb
3º extr

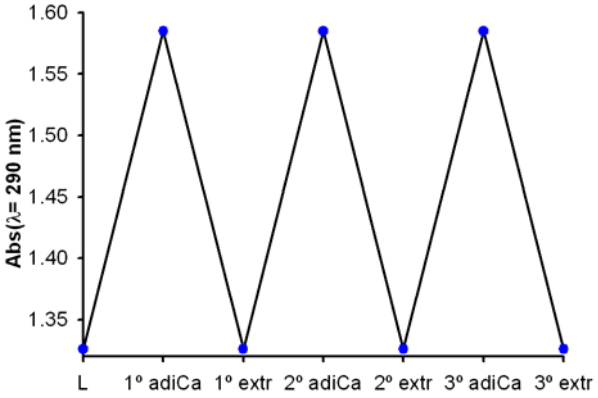
b)


Abs(L)-Abs/Abs(L)-Abs(max)
1.0
0.8
0.6
0.4
-4.7
-4.6
-4.5
-4.4
-4.3
-4.2
log [Zn2+]


Abs(λ=292 nm)
1.42
1.40
1.38
1.36
1.34
1.32
1.30
1.28
1.26
L
1º adiZn
1º extr
2º adiZn
2º extr
3º adiZn
3º extr

c)


Abs(L)-Abs/Abs(L)-Abs(max)
1.0
0.8
0.6
0.4
0.2
-4.7
-4.6
-4.5
-4.4
-4.3
-4.2
-4.1
log [Ca2+]


Abs(λ= 290 nm)
1.60
1.55
1.50
1.45
1.40
1.35
L
1º adiCa
1º extr
2º adiCa
2º extr
3º adiCa
3º extr

d)

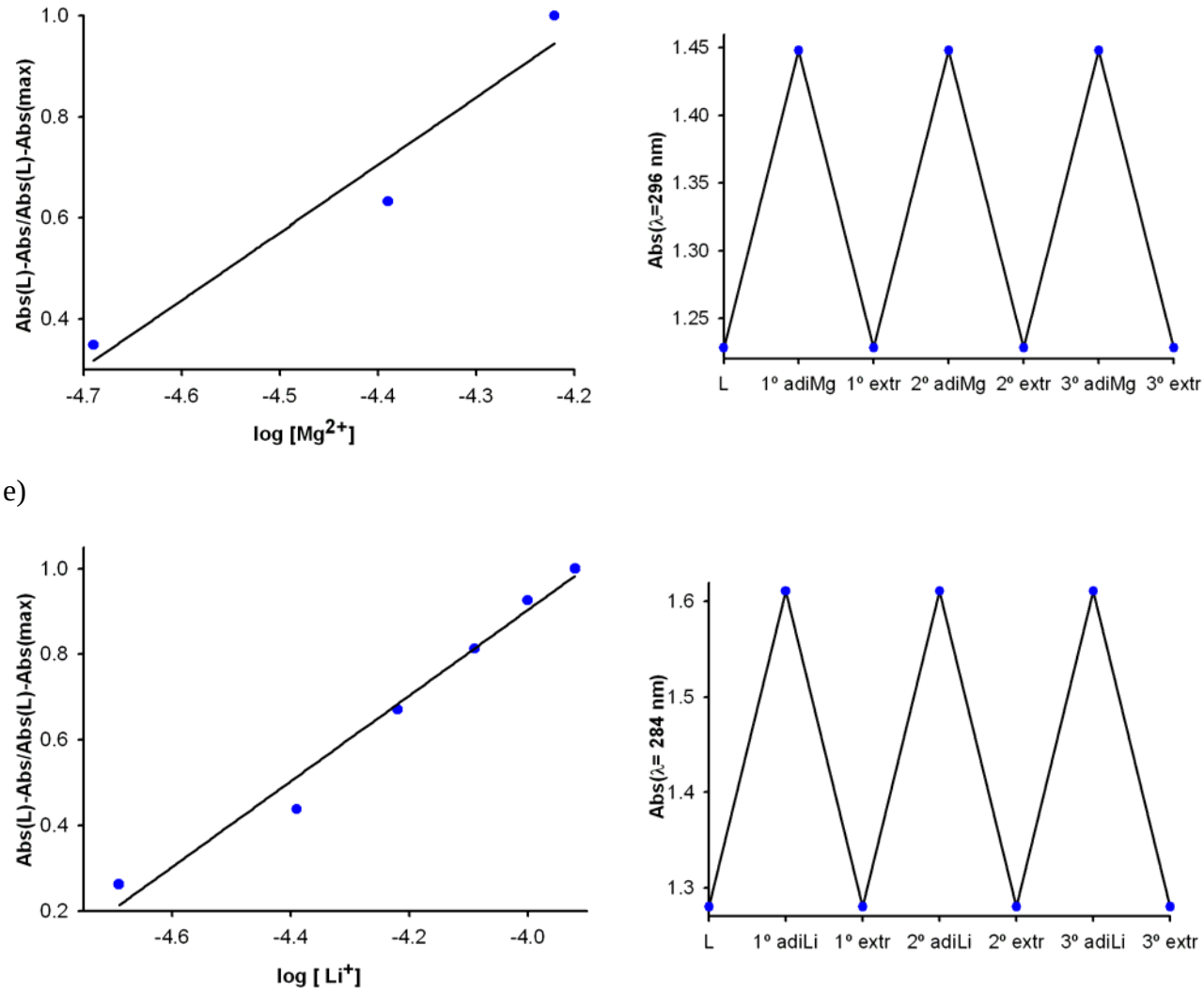


Figure ESI 11. Left: Absorbance of **8** (c = $1x10^{-4}$M in CH_3CN) at each concentration of a) Pb^{2+}; b) Zn^{2+}, c) Ca^{2+}; d) Mg^{2+}, e) Li^{+} added, normalized between the minimum absorbance, found at zero equiv of M^{2+}, and the maximum absorbance. **Right:** Stepwise complexation [addition of a) Pb^{2+}; b) Zn^{2+}, c) Ca^{2+}; d) Mg^{2+}, e) Li^{+}]/decomplexation (extraction with H_2O) cycles of ligand **8** ($1x10^{-4}$ M in CH_2Cl_2), carried out by UV/Vis analysis;

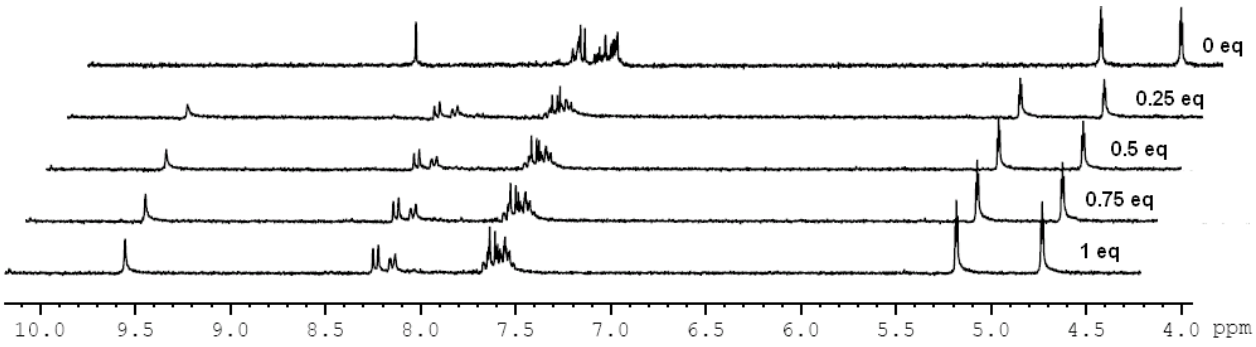


Figure ESI 12. Changes in the ^{1}H-NMR spectrum of **4** in CD_3CN upon addition of increasing amounts of Pb^{2+} from 0 equiv (top) to 1 equiv. (bottom).

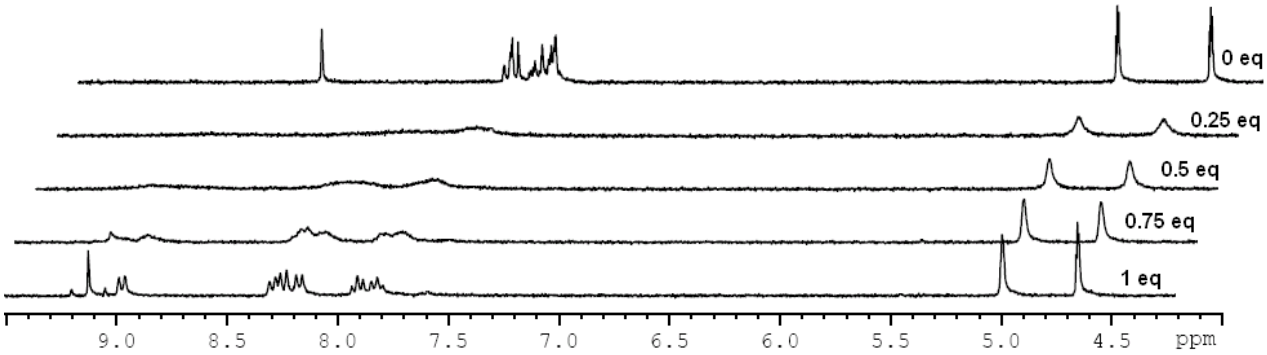


Figure ESI 13. Changes in the ^{1}H-NMR spectrum of **4** in CD_3CN upon addition of increasing amounts of Cd^{2+} from 0 equiv (top) to 1 equiv. (bottom).

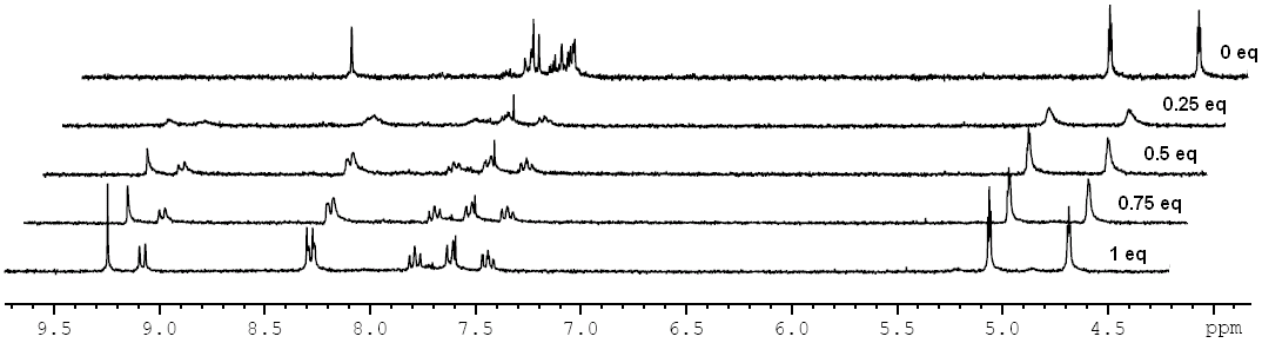


Figure ESI 14. Changes in the ^{1}H-NMR spectrum of **4** in CD_3CN upon addition of increasing amounts of Zn^{2+} from 0 equiv (top) to 1 equiv. (bottom).

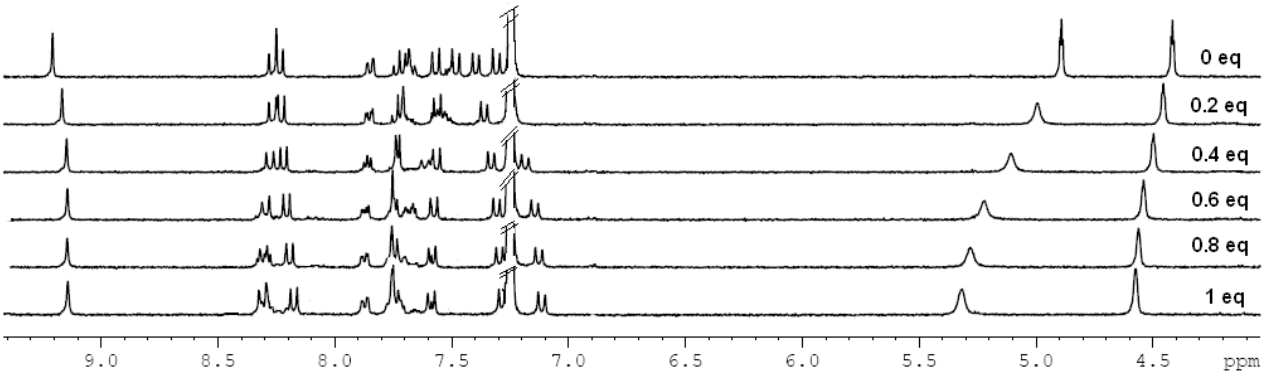


Figure ESI 15. Changes in the ^{1}H-NMR spectrum of **5** in $CDCl_3$ upon addition of increasing amounts of Pb^{2+} from 0 equiv (top) to 1 equiv. (bottom).

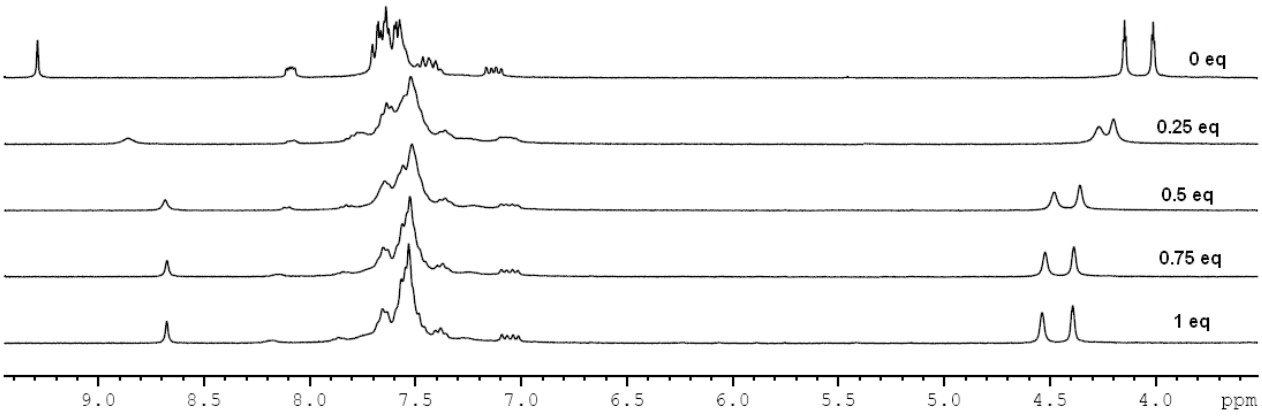


Figure ESI 16. Changes in the ^{1}H-NMR spectrum of **8** in CD_3CN upon addition of increasing amounts of Pb^{2+} from 0 equiv (top) to 1 equiv. (bottom).

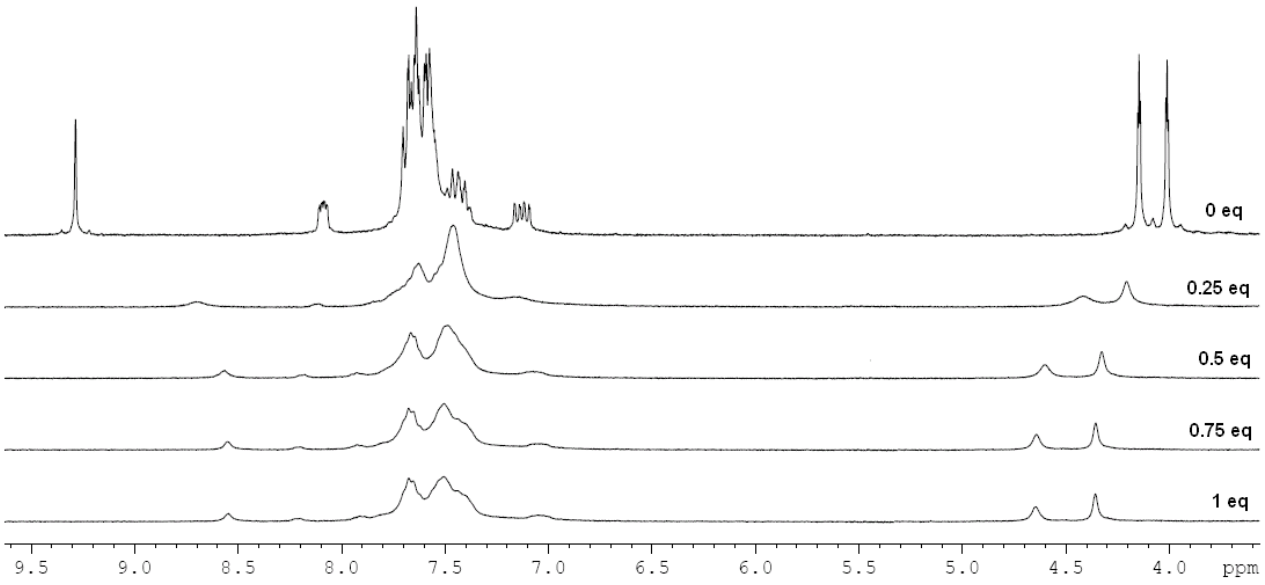


Figure ESI 17. Changes in the ^{1}H-NMR spectrum of **8** in CD_3CN upon addition of increasing amounts of Zn^{2+} from 0 equiv (top) to 1 equiv. (bottom).

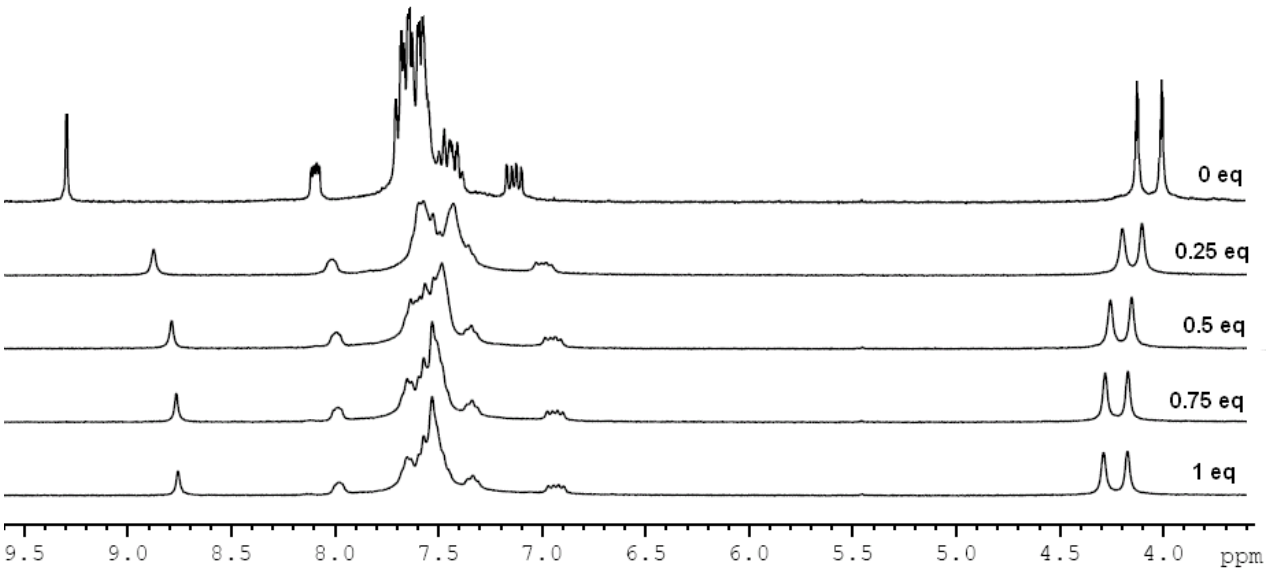


Figure ESI 18. Changes in the ^{1}H-NMR spectrum of **8** in CD_3CN upon addition of increasing amounts of Ca^{2+} from 0 equiv (top) to 1 equiv. (bottom).

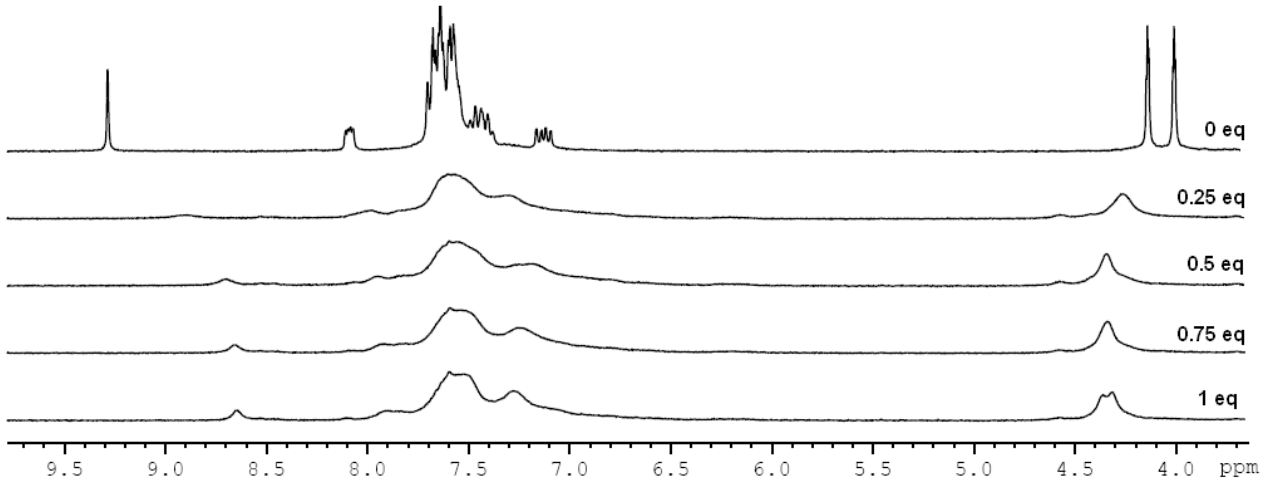


Figure ESI 19. Changes in the ^{1}H-NMR spectrum of **8** in CD_3CN upon addition of increasing amounts of Mg^{2+} from 0 equiv (top) to 1 equiv. (bottom).

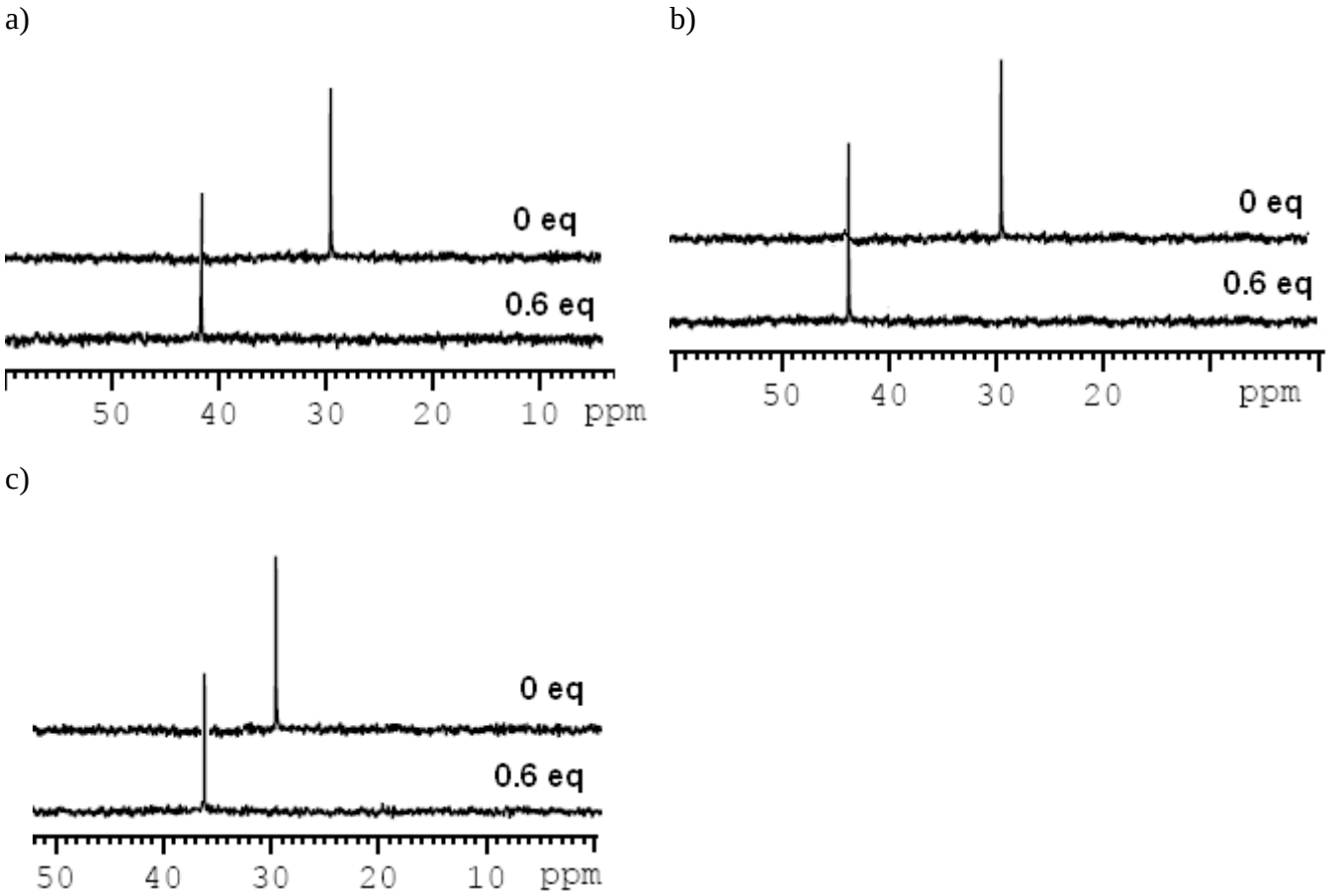


Figure ESI 20. Changes in the ^{31}P-NMR spectrum of **8** in CD_3CN upon addition of increasing amounts of a) Pb^{2+}, b) Zn^{2+}, c) $Ca^{2+}$from 0 equiv (top) to 0.6 equiv. (bottom).

Calculated structures: cartesian coordinates (in Å) and energies for all computed species.-

Compound **4** (C_i): E = -2638.847478176 au

C	0.00000000	0.00000000	0.00000000	C	-4.46483094	-4.55746048	0.00092426
C	1.43095764	0.00000000	0.00000000	C	-3.08076989	-4.70331046	-0.25972065
C	1.87446517	1.34833252	0.00000000	C	-2.26368538	-3.61254362	-0.19732101
C	0.72546609	2.19220800	-0.01250144	H	-6.65763503	-2.06983744	0.83701841
C	-0.43268181	1.37048814	-0.01731074	H	-8.23342937	-3.98625380	0.75023476
H	2.04074925	-0.88831653	-0.02100727	H	-7.40635634	-6.25598269	0.18693054
H	2.89927056	1.68089403	-0.03421160	H	-5.01059586	-6.62329990	-0.28939552
H	0.73756562	3.26865300	-0.07056236	H	-2.68888009	-5.68398268	-0.50552689
H	-1.45237654	1.71402513	-0.07258547	H	-1.20129350	-3.67017191	-0.38748865
Fe	0.72652266	0.96777665	-1.67449503	N	2.19805891	3.10927897	-3.30636111
C	1.45304533	1.93555330	-3.34899005	C	3.44863359	3.07923364	-3.55151679
C	1.88572714	0.56506516	-3.33167932	H	3.98780541	2.16698323	-3.82438837
C	0.72757924	-0.25665470	-3.33648862	C	4.28231885	4.28441730	-3.47973302
C	-0.42141984	0.58722078	-3.34899006	N	5.56643653	4.10890173	-3.73156410
C	0.02208769	1.93555330	-3.34899005	C	6.39199368	5.18469499	-3.67269233
H	2.90542187	0.22152818	-3.27640459	C	7.77026072	5.00344652	-3.94193551
H	0.71547971	-1.33309970	-3.27842770	C	8.63389728	6.06913915	-3.89121175
H	-1.44622523	0.25465927	-3.31477845	C	8.16350435	7.36259766	-3.57042391
H	-0.58770392	2.82386983	-3.32798279	C	6.83195233	7.56926322	-3.30515272
N	-0.74501358	-1.17372567	-0.04262894	C	5.91787627	6.49301378	-3.34991432
C	-1.99558826	-1.14368035	0.20252674	C	4.53381522	6.63886376	-3.08926940
H	-2.53476008	-0.23142993	0.47539832	C	3.71673070	5.54809691	-3.15166904
C	-2.82927353	-2.34886401	0.13074296	H	8.11068036	4.00539074	-4.18600846
N	-4.11339120	-2.17334843	0.38257405	H	9.68647470	5.92180710	-4.09922482
C	-4.93894835	-3.24914169	0.32370228	H	8.85940167	8.19153599	-3.53592059
C	-6.31721539	-3.06789322	0.59294545	H	6.46364119	8.55885320	-3.05959453
C	-7.18085195	-4.13358585	0.54222170	H	4.14192542	7.61953598	-2.84346316
C	-6.71045902	-5.42704436	0.22143386	H	2.65433882	5.60572521	-2.96150140
C	-5.37890700	-5.63370992	-0.04383734				

Complex **4**·2Ni(ClO_4)$_2$ (C_i): E = -8698.837027966 au

C	0.00000000	0.00000000	0.00000000	H	-2.38978203	-0.17507296	0.94210607
C	1.43346720	0.00000000	0.00000000	C	-2.78247363	-2.30867317	0.60335888
C	1.85332019	1.35128107	0.00000000	N	-2.22343273	-3.41738979	0.12581702
C	0.70044178	2.18721177	-0.02432386	C	-2.87161136	-4.60439182	0.23202820
C	-0.44796332	1.36385892	-0.03194530	C	-2.23819395	-5.79668679	-0.18669395
H	2.06038439	-0.87285987	0.00376497	C	-2.90135268	-6.99056923	-0.07920939
H	2.87066190	1.70197076	-0.02360369	C	-4.21494276	-7.05330979	0.44204131
H	0.70257874	3.26019539	-0.07411221	C	-4.84482539	-5.91452112	0.87065092
H	-1.46916841	1.70022652	-0.10306985	C	-4.18918965	-4.66476903	0.78851671
Fe	0.71365476	0.93350172	-1.68962235	C	-4.77224043	-3.46674777	1.24737679
C	1.42730951	1.86700343	-3.37924471	C	-4.06910815	-2.29271716	1.17461913
C	1.87527282	0.50314450	-3.34729941	H	-1.23630439	-5.74650961	-0.58258676
C	0.72686772	-0.32020835	-3.35492085	H	-2.41245905	-7.90168945	-0.39911096
C	-0.42601069	0.51572236	-3.37924471	H	-4.71807739	-8.00948990	0.50647029
C	-0.00615770	1.86700343	-3.37924471	H	-5.84560011	-5.95217797	1.28346647
H	2.89647791	0.16677690	-3.27617486	H	-5.77084917	-3.49142640	1.66683884
H	0.72473077	-1.39319197	-3.30513250	H	-4.47775320	-1.35985743	1.53909341
H	-1.44335240	0.16503267	-3.35564102	Ni	-0.48478572	-2.97398356	-0.88757752
H	-0.63307489	2.73986330	-3.38300968	O	0.84750789	-4.07587453	0.28481816
N	-0.78720054	-1.14714458	0.05655655	Cl	2.08978510	-3.71981567	-0.48150414
C	-1.97553168	-1.09732904	0.54146615	O	1.56159789	-2.78130831	-1.51845278

O	3.01089517	-3.03520947	0.37178015
O	2.65514187	-4.87862014	-1.08240944
O	-1.56488500	-2.25024801	-2.54648749
Cl	-1.61025180	-3.54226558	-3.31635893
O	-0.74082765	-4.43097628	-2.50136785
O	-1.06330397	-3.34868920	-4.61816368
O	-2.94965471	-4.03885446	-3.34398833
N	2.21451005	3.01414801	-3.43580127
C	3.40284119	2.96433247	-3.92071087
H	3.81709154	2.04207640	-4.32135079
C	4.20978314	4.17567660	-3.98260360
N	3.65074225	5.28439322	-3.50506174
C	4.29892087	6.47139526	-3.61127292
C	3.66550347	7.66369022	-3.19255076
C	4.32866219	8.85757267	-3.30003532
C	5.64225227	8.92031322	-3.82128603
C	6.27213490	7.78152455	-4.24989563
C	5.61649916	6.53177247	-4.16776142
C	6.19954994	5.33375120	-4.62662151
C	5.49641766	4.15972059	-4.55386384
H	2.66361390	7.61351305	-2.79665795
H	3.83976857	9.76869288	-2.98013376
H	6.14538691	9.87649334	-3.88571500
H	7.27290962	7.81918140	-4.66271118
H	7.19815868	5.35842984	-5.04608356
H	5.90506271	3.22686086	-4.91833813
Ni	1.91209524	4.84098700	-2.49166719
O	0.57980162	5.94287796	-3.66406288
Cl	-0.66247559	5.58681910	-2.89774057
O	-0.13428837	4.64831174	-1.86079194
O	-1.58358566	4.90221290	-3.75102486
O	-1.22783236	6.74562357	-2.29683527
O	2.99219451	4.11725144	-0.83275722
Cl	3.03756131	5.40926901	-0.06288578
O	2.16813716	6.29797971	-0.87787686
O	2.49061348	5.21569264	1.23891896
O	4.37696422	5.90585789	-0.03525639

Complex **4**·Ni(ClO_4)$_2$ (C_2): E = -5668.875628768 au

C	0.00000000	0.00000000	0.00000000
C	1.42915238	0.00000000	0.00000000
C	1.84171284	1.36214680	0.00000000
C	0.67999536	2.18763355	-0.02107845
C	-0.46908911	1.34621282	-0.01334750
H	2.04648290	-0.88169425	-0.02138544
H	2.86309814	1.70590948	-0.02428662
H	0.66813369	3.26409586	-0.07568915
H	-1.50374726	1.63846798	-0.09001263
Fe	0.72909457	0.91922655	-1.66322068
C	0.13623145	-0.20545784	-3.25270416
C	-0.45066053	1.09678145	-3.29968443
C	0.62110248	2.02958329	-3.38247820
C	1.85104426	1.30957980	-3.36520522
C	1.55597015	-0.08184820	-3.29238275
H	-1.50686599	1.29992049	-3.25381907
H	0.51569694	3.10203921	-3.40928383
H	2.83857973	1.74163049	-3.36501643
H	2.24968237	-0.90124815	-3.19670006
N	-0.78290056	-1.17240097	0.04433878
C	-1.42536520	-1.43484218	1.11004091
H	-1.41774292	-0.76265639	1.96765625
C	-2.08922834	-2.73396109	1.24411900
N	-1.96658442	-3.55488845	0.21046154
C	-2.31983451	-4.85463613	0.34869493
C	-2.00482692	-5.78205465	-0.67191913
C	-2.36839754	-7.09455429	-0.53563088
C	-3.07458457	-7.54059092	0.60600098
C	-3.36854163	-6.66986346	1.62242192
C	-2.97858973	-5.31257652	1.53323902
C	-3.18204651	-4.38814034	2.57756111
C	-2.70534840	-3.10908487	2.45243988
H	-1.44143559	-5.43394237	-1.52275628
H	-2.10829371	-7.80426410	-1.31037658
H	-3.36365118	-8.58102783	0.68270387
H	-3.88163451	-7.00732350	2.51500410
H	-3.68557681	-4.71022812	3.48138332
H	-2.79133458	-2.38677965	3.25314163
N	-0.61201039	-1.40039338	-3.21163766
C	-0.62234580	-2.14726222	-4.24092740
H	-0.04117453	-1.90909999	-5.13138492
C	-1.53788621	-3.29009758	-4.28690826
N	-2.30229811	-3.46142332	-3.21745375
C	-3.34610360	-4.32169726	-3.27776107
C	-4.28697426	-4.36194087	-2.22223712
C	-5.33809715	-5.23673329	-2.27961547
C	-5.49205211	-6.12058312	-3.37326965
C	-4.61134488	-6.08412187	-4.42241881
C	-3.53179410	-5.16937495	-4.41520300
C	-2.64022944	-5.02991081	-5.49790692
C	-1.66640452	-4.06627730	-5.45369411
H	-4.17316680	-3.66301963	-1.40917331
H	-6.06612805	-5.25049691	-1.47876936
H	-6.32390915	-6.81323355	-3.38744877
H	-4.73747375	-6.73497814	-5.27934596
H	-2.75664760	-5.66634041	-6.36714915
H	-0.99925266	-3.89002813	-6.28681258
Ni	-1.43120170	-2.42086009	-1.54272196
O	0.19256755	-3.75332612	-1.79119139
Cl	1.49040958	-3.74918073	-1.02726555
O	1.19984956	-3.42764733	0.34994389
O	2.05294365	-5.06122278	-1.16205546
O	2.34158473	-2.74036078	-1.61576921
O	-3.30398565	-1.47340172	-1.28036279
Cl	-3.85828920	-0.32794417	-2.08576231
O	-3.49126108	-0.53124839	-3.46723704
O	-5.28039576	-0.34490807	-1.90302649
O	-3.26925112	0.88998460	-1.57759201

Complex $[\mathbf{4}\cdot Zn]^{2+}$ (C_2): E = -4417.795529985 au

C	0.00000000	0.00000000	0.00000000	C	-2.97114262	-5.43847390	-1.24834766
C	1.43433586	0.00000000	0.00000000	C	-1.94101989	-5.72547561	-0.33302036
C	1.85407675	1.35402807	0.00000000	C	-1.13167334	-4.71534787	0.13513446
C	0.70191818	2.18822550	0.00112982	H	-4.28123801	-2.73288266	-2.91494472
C	-0.44924657	1.36334554	-0.01678424	H	-5.74014837	-4.50912014	-3.80487482
H	2.07523289	-0.86551135	-0.04250550	H	-5.45506539	-6.85934009	-3.08308001
H	2.87633102	1.69394643	-0.03174869	H	-3.69301142	-7.46011002	-1.45913664
H	0.70465881	3.26570653	-0.01828767	H	-1.79134190	-6.74716747	-0.00553355
H	-1.47745567	1.68911537	-0.02291811	H	-0.33234373	-4.91022206	0.83734085
Fe	0.66094078	0.92874280	-1.67630547	N	-1.90619916	0.29346696	-2.95336239
C	-0.58006458	0.61941445	-3.24908250	C	-2.89406555	1.06699709	-3.23460588
C	-0.00369391	1.92828313	-3.35853108	H	-2.77086191	1.95386402	-3.85120968
C	1.40055966	1.76158360	-3.45781638	C	-4.21060680	0.77613224	-2.66803465
C	1.69871914	0.37147577	-3.41246056	N	-4.25730217	-0.18758825	-1.73795428
C	0.48477997	-0.34320780	-3.26580704	C	-5.43793614	-0.51015158	-1.14515108
H	-0.53271526	2.86661992	-3.32211530	C	-5.48358963	-1.51753089	-0.15902279
H	2.12394723	2.55799015	-3.52108804	C	-6.67632006	-1.82943489	0.44160740
H	2.68453149	-0.06250706	-3.44685287	C	-7.86973638	-1.15555317	0.08637383
H	0.36934795	-1.41343040	-3.19742148	C	-7.85332514	-0.17252692	-0.86817524
N	-0.85289207	-1.09248910	-0.17710938	C	-6.64147458	0.17815153	-1.50906683
C	-0.52252743	-2.29401976	0.13992384	C	-6.55927368	1.18921990	-2.48494113
H	0.38332018	-2.51102615	0.70051340	C	-5.34800278	1.49441236	-3.06308401
C	-1.36021831	-3.40545152	-0.30938630	H	-4.57182700	-2.03300947	0.11618560
N	-2.32937305	-3.10299829	-1.18417101	H	-6.71102831	-2.59896148	1.20197134
C	-3.14337856	-4.07884480	-1.66840020	H	-8.79618516	-1.42049895	0.57815977
C	-4.15623123	-3.76049968	-2.59691093	H	-8.76025982	0.35066495	-1.14365282
C	-4.96596789	-4.75210090	-3.08854104	H	-7.45643694	1.72433650	-2.77174016
C	-4.80348690	-6.09706959	-2.67719067	H	-5.25821215	2.26805905	-3.81368779
C	-3.82701736	-6.43378047	-1.77668698	Zn	-2.44549195	-1.09338845	-1.50721334

Complex $[\mathbf{4}\cdot Hg]^{2+}$ (C_2): E = -2791.823434220 au

C	0.00000000	0.00000000	0.00000000	C	-2.87906761	-5.65954374	-0.61543459
C	1.43660288	0.00000000	0.00000000	C	-1.76662875	-5.78473810	0.23854083
C	1.85940102	1.35234986	0.00000000	C	-0.99311792	-4.68639325	0.52530996
C	0.70788723	2.18824311	0.00062714	H	-4.50159485	-3.25212879	-2.45603568
C	-0.44450333	1.36589012	-0.01703412	H	-5.89092895	-5.19546536	-3.01629771
H	2.07619924	-0.86664180	-0.03917453	H	-5.38922975	-7.43115032	-2.07412105
H	2.88224161	1.69056966	-0.03199874	H	-3.47022453	-7.73090648	-0.54523250
H	0.71229162	3.26573795	-0.02063437	H	-1.52794878	-6.75340497	0.66041535
H	-1.47080893	1.69652261	-0.02229733	H	-0.13171436	-4.75460985	1.17616684
Fe	0.68046052	0.91835926	-1.66469716	N	-1.88501247	0.41507742	-3.07777084
C	-0.52782815	0.67416826	-3.26408334	C	-2.79452714	1.24587208	-3.42189429
C	0.11752316	1.95563878	-3.33607515	H	-2.55978629	2.14402466	-3.99050471
C	1.51376832	1.72293429	-3.39897578	C	-4.19622082	1.03955996	-3.05425164
C	1.74208226	0.31879925	-3.36767963	N	-4.50024192	0.06702071	-2.19328183
C	0.49173923	-0.33776228	-3.26693434	C	-5.79012419	-0.15086393	-1.80916379
H	-0.36625098	2.91819124	-3.30228880	C	-6.11364187	-1.17104862	-0.89036908
H	2.27654966	2.48378856	-3.42872200	C	-7.41719122	-1.36229440	-0.50567942
H	2.70626724	-0.16251595	-3.37991094	C	-8.45495647	-0.54860312	-1.01668817
H	0.32589454	-1.40217915	-3.22044781	C	-8.17059430	0.45034254	-1.91065629
N	-0.85012424	-1.09953696	-0.10998606	C	-6.83871782	0.67717096	-2.33086957
C	-0.50037105	-2.27487226	0.25349336	C	-6.49345765	1.69959848	-3.23525071
H	0.43473892	-2.45296609	0.78165155	C	-5.18061206	1.88543378	-3.59416388
C	-1.33249733	-3.44350606	-0.03690612	H	-5.32790405	-1.79900512	-0.48640554
N	-2.37973425	-3.30268411	-0.85115083	H	-7.65742941	-2.14467604	0.20245078
C	-3.17278104	-4.36687004	-1.16324335	H	-9.47353403	-0.71802513	-0.69427511
C	-4.27417440	-4.22373707	-2.03276612	H	-8.95548106	1.08177280	-2.30743460
C	-5.04962713	-5.31214474	-2.34556604	H	-7.27144378	2.33631522	-3.63847659
C	-4.76438013	-6.58902101	-1.80853599	H	-4.88711830	2.66450505	-4.28495591
C	-3.70076587	-6.75826924	-0.96117950	Hg	-2.77425108	-1.20806171	-1.54523683

Compound **5** (*quasi*-C_2): E = -3066.426426575 au

C	0.00000000	0.00000000	0.00000000	H	-1.23832962	-2.29712377	-2.14103165
C	1.43301898	0.00000000	0.00000000	H	-2.69814476	-2.66566307	-4.03303021
C	1.86958914	1.35483664	0.00000000	H	-4.82931694	-3.53782875	-4.94152990
C	0.71894502	2.19450479	0.00115390	H	-6.88410327	-4.88484539	-4.66114162
C	-0.43451529	1.36315638	-0.01938746	H	-7.29893770	-6.10041025	-2.54749381
H	2.06116956	-0.87436135	-0.05388895	H	-6.58890721	-6.74310286	-0.27540620
H	2.89472495	1.68781446	-0.03492958	H	-5.00317015	-6.53280399	1.59157675
H	0.72299566	3.27232998	-0.02367421	H	-2.96731405	-5.52309506	2.55807765
H	-1.46511385	1.67661590	-0.05806127	H	-1.12765223	-3.88504639	2.40534265
Fe	0.70987733	0.98305248	-1.67492369	N	-1.78009594	0.04791886	-3.20937210
C	-0.49279898	0.56238345	-3.31089947	C	-2.74919385	0.62296526	-3.80580353
C	-0.06400554	1.92852445	-3.35055220	H	-2.57343018	1.48165170	-4.46931273
C	1.35908313	1.94097322	-3.38960835	C	-4.13622628	0.15337275	-3.75521731
C	1.81603384	0.59196100	-3.37454717	C	-4.72073450	-0.52937189	-2.65871711
C	0.67827729	-0.25941237	-3.30356380	C	-4.06087098	-0.70118918	-1.39812695
H	-0.71092821	2.78916135	-3.29710936	C	-4.64813449	-1.37942729	-0.38176269
H	1.98348251	2.82010028	-3.39071969	C	-5.93932930	-1.97424476	-0.52145044
H	2.84589096	0.27332757	-3.37170299	C	-6.52804361	-2.72995127	0.49749161
H	0.67425925	-1.33590889	-3.24648399	C	-7.78261615	-3.29986862	0.32379621
N	-0.88393180	-1.06796094	-0.07777963	C	-8.47779648	-3.12323706	-0.86554120
C	-0.61723000	-2.18826977	0.46922830	C	-7.92466543	-2.37747641	-1.91257200
H	0.27240417	-2.32576639	1.09876410	C	-8.61267832	-2.18576725	-3.15226858
C	-1.54934032	-3.31705363	0.38223224	C	-8.05629926	-1.46593691	-4.15898426
C	-2.32539602	-3.58232695	-0.77128136	C	-6.75692980	-0.88199363	-4.02374048
C	-2.06676608	-2.97738010	-2.04177720	C	-6.17191798	-0.13954441	-5.05661681
C	-2.89382286	-3.17249208	-3.09659139	C	-4.89720506	0.37379851	-4.91184681
C	-4.07359094	-3.96891116	-2.98196183	C	-6.03761309	-1.05999542	-2.80770581
C	-5.00706378	-4.07614308	-4.01838215	C	-6.63589556	-1.79708860	-1.74724300
C	-6.15932393	-4.83355027	-3.85872060	H	-3.05584640	-0.33210915	-1.27243016
C	-6.39541534	-5.51527089	-2.67107628	H	-4.11467181	-1.51328091	0.55138662
C	-5.48598220	-5.44274289	-1.61151339	H	-5.98130466	-2.87985191	1.42041314
C	-5.70176015	-6.12815936	-0.37323444	H	-8.21827911	-3.89171886	1.11916951
C	-4.82868462	-6.00989238	0.65827435	H	-9.45560773	-3.57099810	-0.99994488
C	-3.67503695	-5.16765251	0.56018908	H	-9.59405846	-2.63079467	-3.27035416
C	-2.79839177	-4.97924229	1.63613245	H	-8.58644656	-1.32197596	-5.09336727
C	-1.75943375	-4.06879650	1.54338006	H	-6.72532798	0.01920801	-5.97458493
C	-3.42381850	-4.48156745	-0.66180277	H	-4.44977577	0.93261952	-5.72631490
C	-4.31813072	-4.64385128	-1.75575918				

Complex **5**·$Zn(OTf)_2$ (C_2) E = -6768.899702002 au

C	0.00000000	0.00000000	0.00000000	H	0.74322163	-1.38643964	-3.22835838
C	1.42923143	0.00000000	0.00000000	N	-0.85899583	-1.12177047	-0.00965651
C	1.85334158	1.35737557	0.00000000	C	-0.54772406	-2.13968686	0.71773680
C	0.69576313	2.18583556	0.00282865	H	0.40620029	-2.12565793	1.24412345
C	-0.45621065	1.35292620	-0.00531220	C	-1.41680920	-3.27668857	0.92718020
H	2.05820186	-0.87336228	-0.05655577	C	-0.88226489	-4.57352194	1.10282969
H	2.87544928	1.69728031	-0.04100654	C	0.51142246	-4.86626833	0.95968468
H	0.68838704	3.26316894	-0.02529251	C	0.98827046	-6.12709212	1.11924734
H	-1.48614262	1.66917686	-0.01886628	C	0.11856637	-7.22202531	1.41483339
Fe	0.68313336	0.95990310	-1.67036542	C	0.59129588	-8.53022646	1.57469436
C	-0.50637462	0.46633527	-3.25771142	C	-0.28568568	-9.57384070	1.84183159
C	-0.15395638	1.84918203	-3.33669692	C	-1.65120098	-9.33612773	1.94876658
C	1.26394314	1.92150229	-3.41835834	C	-2.16798460	-8.04503960	1.79365466
C	1.77992538	0.59506043	-3.39274324	C	-3.57010695	-7.76998650	1.88647059
C	0.69044503	-0.31175921	-3.28523248	C	-4.05191633	-6.51133375	1.72459403
H	-0.84075801	2.67765800	-3.27757733	C	-3.17710738	-5.41085840	1.45943068
H	1.84711285	2.82755107	-3.44851823	C	-3.66215024	-4.10762992	1.28682284
H	2.82202999	0.32084284	-3.41049448	C	-2.79947126	-3.06309552	1.02964721

C	-1.77554807	-5.64754080	1.37205629	C	-6.48426691	0.09595901	-4.28603609
C	-1.27535930	-6.96844841	1.53031707	C	-7.64771563	0.90207020	-4.41489271
H	1.19101029	-4.07519413	0.67617866	H	-4.19300189	2.60452914	-3.82325243
H	2.04636987	-6.32867805	1.00134529	H	-6.18040715	3.97936349	-4.09823232
H	1.65415291	-8.72012516	1.48285249	H	-8.61756415	4.17476123	-4.45430549
H	0.09582157	-10.57989051	1.96321259	H	-10.82777048	3.10953509	-4.76759581
H	-2.33297481	-10.15347117	2.15230354	H	-11.02453004	0.64526195	-4.84028855
H	-4.24361226	-8.59539373	2.08590538	H	-9.98447221	-1.58852532	-4.73529517
H	-5.11515693	-6.31395635	1.79067728	H	-7.97566612	-2.98726489	-4.49048504
H	-4.72521128	-3.91969710	1.37222177	H	-5.53983282	-3.18826507	-4.19730417
H	-3.18564232	-2.05686948	0.95078838	H	-3.33454655	-2.14448259	-3.94189065
N	-1.80301537	-0.08501504	-3.15248953	Zn	-2.20958869	-1.28531458	-1.54212298
C	-2.75134189	0.43844438	-3.85164044	O	-2.13584052	-3.18429570	-2.11927196
H	-2.53164110	1.33533737	-4.43005715	S	-0.95785138	-3.72693060	-2.87234448
C	-4.07731578	-0.12827285	-3.96377075	O	-0.96350565	-3.34911482	-4.26145505
C	-5.20996120	0.70433784	-4.11290475	O	0.27793469	-3.57883939	-2.13915604
C	-5.14164209	2.13183644	-4.03457457	C	-1.36116275	-5.54776638	-2.84500809
C	-6.25278425	2.90034592	-4.16601720	F	-2.53166295	-5.77391102	-3.45100086
C	-7.54296817	2.31885855	-4.36584938	F	-1.43619542	-6.00364300	-1.59078099
C	-8.70098211	3.09516873	-4.49532979	F	-0.40561742	-6.22359192	-3.48910313
C	-9.94173486	2.49508046	-4.66858195	O	-3.99685928	-0.71630251	-0.88900879
C	-10.05435356	1.11009771	-4.70998715	S	-4.18979812	0.59088989	-0.17960629
C	-8.92402252	0.29522108	-4.58207549	O	-3.74887006	0.55091660	1.19020738
C	-9.00875918	-1.13387380	-4.60897482	O	-3.78231356	1.71824105	-0.98564550
C	-7.90081309	-1.90654374	-4.47485664	C	-6.05249877	0.65293580	-0.10648405
C	-6.60568942	-1.32280230	-4.30589246	F	-6.52643486	-0.39726667	0.57241117
C	-5.45481853	-2.10924111	-4.16280262	F	-6.58139571	0.64006588	-1.33393727
C	-4.21725272	-1.52364767	-3.99873670	F	-6.43517815	1.77339748	0.51221425

Complex $[\mathbf{5}\cdot Hg]^{2+}$: E = -3219.356652745 au

C	0.00000000	0.00000000	0.00000000	C	-4.67992188	-4.32165477	1.33198528
C	1.42907446	0.00000000	0.00000000	C	-4.66943123	-3.16062570	2.11611511
C	1.85290010	1.35603134	0.00000000	C	-3.65467755	-2.23829374	1.98468362
C	0.69943271	2.18751010	-0.03462340	C	-3.59942590	-4.55221168	0.42680455
C	-0.45242766	1.35606036	-0.03432903	C	-3.61909181	-5.71997727	-0.38570186
H	2.06085388	-0.87299165	0.02260357	H	-0.38661151	-3.69807072	-0.10449905
H	2.87639135	1.69368019	-0.01102823	H	-0.50179209	-5.52001508	-1.74123319
H	0.69926457	3.26407767	-0.08662137	H	-1.74403209	-7.39370750	-2.73268702
H	-1.47966116	1.68035492	-0.07658264	H	-3.69476990	-8.91623980	-2.62898913
Fe	0.74056551	0.93395122	-1.68751072	H	-5.54712002	-8.44126659	-1.07059456
C	0.04489899	0.09796373	-3.43605109	H	-6.56887814	-7.09173915	0.70194212
C	-0.18484956	1.50996795	-3.45432493	H	-6.53514922	-5.09124529	2.13349289
C	1.08022533	2.14204959	-3.34293600	H	-5.47362301	-2.98870987	2.82009298
C	2.07979305	1.13425328	-3.24609964	H	-3.67953184	-1.33061957	2.57569191
C	1.44719940	-0.13783419	-3.28813210	N	-0.95126104	-0.89073901	-3.61243822
H	-1.14682182	1.99079513	-3.52982040	C	-1.66781140	-0.88409463	-4.69610885
H	1.25058830	3.20538610	-3.30072060	H	-1.34607406	-0.19400364	-5.47728478
H	3.13733205	1.30236665	-3.12582610	C	-2.77238186	-1.74868749	-5.00499300
H	1.93525142	-1.09847316	-3.25014485	C	-3.71951997	-2.22514114	-4.05602363
N	-0.78234482	-1.16980547	0.03277649	C	-3.88669131	-1.65121241	-2.74743526
C	-1.66460094	-1.31278381	0.95760542	C	-4.82909880	-2.12063568	-1.87944486
H	-1.77698588	-0.52530176	1.70716613	C	-5.69521242	-3.19472102	-2.23418143
C	-2.58245517	-2.43337880	1.09247527	C	-6.68415676	-3.66978630	-1.36475528
C	-2.51779228	-3.63469219	0.35367902	C	-7.54718059	-4.68061561	-1.76084704
C	-1.36341864	-4.01568285	-0.46036004	C	-7.44944279	-5.23006106	-3.03390606
C	-1.40029010	-5.19923476	-1.22574429	C	-6.48926946	-4.77164776	-3.94363529
C	-2.53660066	-6.01715460	-1.27322611	C	-6.40488754	-5.28267527	-5.27704659
C	-2.57774952	-7.17568552	-2.07679359	C	-5.50748685	-4.78439664	-6.16735280
C	-3.66340015	-8.02709154	-2.01375127	C	-4.60335005	-3.74415463	-5.79626643
C	-4.71003154	-7.75590882	-1.13232250	C	-3.72333648	-3.16975277	-6.72741731
C	-4.70658320	-6.62582346	-0.30383159	C	-2.84764119	-2.17874808	-6.34462906
C	-5.75858345	-6.37686674	0.63317958	C	-4.62597535	-3.24491078	-4.45833163
C	-5.73950817	-5.27467612	1.42238567	C	-5.59235555	-3.74378190	-3.54188922

H	-3.33939130	-0.75177874	-2.49347267	H	-7.09375899	-6.06423632	-5.57430484
H	-4.96135039	-1.64757904	-0.91388767	H	-5.47354598	-5.15772931	-7.18301159
H	-6.77327216	-3.23031710	-0.38040551	H	-3.73988469	-3.51330912	-7.75364013
H	-8.31180308	-5.03329948	-1.08133248	H	-2.16519164	-1.75537462	-7.07179987
H	-8.13540131	-6.00926726	-3.34356883	Hg	-1.19638160	-2.40335362	-2.07465286

Complex $[\mathbf{8}\cdot Zn]^{2+}$ (quasi-C_2): E = -5836.934257281 au

C	0.00000000	0.00000000	0.00000000	C	-8.32860681	-2.58531612	1.64988202
C	1.42687622	0.00000000	0.00000000	C	-7.43427528	-2.52945076	2.71673009
C	1.84537490	1.35823449	0.00000000	C	-6.10164959	-2.21034195	2.48939563
C	0.69108777	2.18810240	0.01050640	H	-6.22133869	-1.77148789	-0.88504486
C	-0.45942166	1.35512030	-0.00414445	H	-8.59792982	-2.35132868	-0.46890761
H	2.06329885	-0.86887160	-0.04821067	H	-9.36735655	-2.82955192	1.83165072
H	2.86671880	1.69977897	-0.04000070	H	-7.77755838	-2.72503096	3.72406903
H	0.68863868	3.26562249	-0.00574954	H	-5.41038908	-2.15052545	3.32050974
H	-1.49097084	1.66668287	0.00608564	O	-3.85414772	-0.79225958	-0.45548995
Fe	0.65312051	0.96241005	-1.66794337	N	-1.90053272	0.19621640	-3.13815124
C	-0.56168549	0.63328987	-3.26450589	C	-2.82638053	0.68816337	-3.87503611
C	-0.05839452	1.96595905	-3.33934388	H	-2.58763154	1.50883410	-4.55316601
C	1.35846894	1.87540797	-3.40893946	C	-4.21534865	0.22386434	-3.84854810
C	1.72594606	0.50216336	-3.38708805	C	-4.60955565	-1.13799923	-3.76957149
C	0.54272182	-0.27676358	-3.28347972	C	-5.97203664	-1.42946357	-3.70318258
H	-0.64275761	2.87061958	-3.29480861	C	-6.93243592	-0.41964080	-3.70904031
H	2.03925615	2.71038422	-3.43462768	C	-6.54410222	0.90719423	-3.82843919
H	2.73252724	0.11783468	-3.40743929	C	-5.19277680	1.21965947	-3.91840577
H	0.46776374	-1.35100166	-3.25027944	H	-6.29561089	-2.46061135	-3.67473216
N	-0.88391274	-1.10317783	-0.04542415	H	-7.98180068	-0.67850004	-3.65574512
C	-0.70995936	-2.11654986	0.71949993	H	-7.28460853	1.69519952	-3.86613040
H	0.17213118	-2.15437484	1.35990671	H	-4.88719319	2.25377718	-4.02325815
C	-1.62287802	-3.26119053	0.77085178	P	-3.43867121	-2.53954778	-3.87531071
C	-3.03881421	-3.16661993	0.75439372	C	-2.41481503	-2.23048436	-5.31260535
C	-3.78133387	-4.34713524	0.75763548	C	-1.11198509	-2.73591380	-5.32102467
C	-3.16166480	-5.59462828	0.77330671	C	-0.30283557	-2.54070369	-6.43321290
C	-1.77832122	-5.68173757	0.83134830	C	-0.79103825	-1.84660508	-7.53734425
C	-1.01925118	-4.51821772	0.85076453	C	-2.09086082	-1.34674543	-7.53389835
H	-4.86151200	-4.29707879	0.77678886	C	-2.90454293	-1.53684858	-6.42363678
H	-3.76517166	-6.49291020	0.77450652	H	-0.73863845	-3.27888863	-4.46167197
H	-1.29015742	-6.64629638	0.87524853	H	0.70590478	-2.93256357	-6.44212255
H	0.06090094	-4.58381917	0.90789117	H	-0.15890854	-1.69782195	-8.40338285
P	-3.94803781	-1.58327592	0.85102220	H	-2.46925892	-0.81158937	-8.39520680
C	-3.24611709	-0.68223697	2.23143563	H	-3.91331829	-1.14373661	-6.42275870
C	-3.30440155	0.71433999	2.20736331	C	-4.38731755	-4.03355216	-4.12400022
C	-2.80498591	1.44499519	3.27813618	C	-4.77761725	-4.77429754	-3.00254013
C	-2.25204032	0.78696813	4.37397714	C	-5.54991836	-5.91647223	-3.17043296
C	-2.19718428	-0.60430248	4.40273357	C	-5.93028489	-6.32084687	-4.44844499
C	-2.69324422	-1.34127703	3.33364382	C	-5.53557915	-5.58764373	-5.56471855
H	-3.73916085	1.22171344	1.35520628	C	-4.76422889	-4.44283047	-5.40618291
H	-2.85117077	2.52619076	3.26220103	H	-4.46040755	-4.46467097	-2.01504114
H	-1.86727935	1.35867408	5.20870393	H	-5.85118359	-6.49696891	-2.30801030
H	-1.77158911	-1.11353823	5.25768627	H	-6.52753958	-7.21462210	-4.57543302
H	-2.64625393	-2.42262692	3.35818821	H	-5.82138262	-5.91219273	-6.55663726
C	-5.66472643	-1.94933464	1.18749028	H	-4.44609799	-3.88101793	-6.27507162
C	-6.56340538	-1.99923527	0.11639540	O	-2.60556136	-2.68304709	-2.59902835
C	-7.89506202	-2.31711855	0.35354337	Zn	-2.25484761	-1.05440308	-1.56033635

Compound **9a** (C_i): E = -3133.887936626 au

C	0.00000000	0.00000000	0.00000000	C	1.43885810	0.00000000	0.00000000

C	1.86982224	1.35405448	0.00000000	H	-1.49231462	-6.58133405	-1.68499733
C	0.71917102	2.19618129	-0.01822339	H	-3.73969844	-6.45714049	-0.68198343
C	-0.42893572	1.36290300	-0.00720961	H	-4.47583912	-4.36781932	0.43957945
H	2.07239614	-0.87190582	-0.00390216	H	-2.94454000	-2.41780276	0.55001685
H	2.89418711	1.68935135	-0.02983832	P	0.69331323	-4.75547048	-1.88559684
H	0.71618106	3.27494937	-0.06806601	O	1.11420943	-3.73160314	-2.87245517
H	-1.45829764	1.67990314	-0.05007619	H	0.62255446	-6.08559132	-2.35712077
Fe	0.73664104	0.94890494	-1.67489222	H	1.57772697	-4.90076943	-0.79053117
C	1.47328209	1.89780987	-3.34978444	N	2.35676147	2.97638492	-3.31330899
C	0.03442399	1.89780987	-3.34978444	C	1.94284959	4.11631246	-2.92182619
C	-0.39654015	0.54375539	-3.34978444	H	0.92033437	4.25121474	-2.56038160
C	0.75411107	-0.29837142	-3.33156105	C	2.82666532	5.28565830	-2.86085366
C	1.90221781	0.53490687	-3.34257483	C	2.40947700	6.47787064	-2.23043672
H	-0.59911405	2.76971570	-3.34588228	C	3.27945151	7.56983747	-2.16432892
H	-1.42090502	0.20845853	-3.31994612	C	4.54842869	7.50228919	-2.72572818
H	0.75710103	-1.37713950	-3.28171843	C	4.95983618	6.32769458	-3.35307683
H	2.93157973	0.21790674	-3.29970825	C	4.11010655	5.23443040	-3.41900325
N	-0.88347937	-1.07857505	-0.03647545	H	2.96559671	8.47914392	-1.66478711
C	-0.46956750	-2.21850258	-0.42795825	H	5.21298054	8.35495036	-2.66780101
H	0.55294772	-2.35340487	-0.78940284	H	5.94912121	6.26562919	-3.78936389
C	-1.35338323	-3.38784843	-0.48893078	H	4.41782209	4.31561264	-3.89980129
C	-0.93619491	-4.58006077	-1.11934772	P	0.77996886	6.65328035	-1.46418760
C	-1.80616942	-5.67202760	-1.18545552	O	0.35907266	5.62941301	-0.47732927
C	-3.07514660	-5.60447932	-0.62405625	H	0.85072763	7.98340119	-0.99266367
C	-3.48655409	-4.42988471	0.00329239	H	-0.10444487	6.79857930	-2.55925327
C	-2.63682446	-3.33662052	0.06921881				

Compound **9a**’ with hampered internal H-bonds (C_i): E = -3133.883012482 au

C	0.00000000	0.00000000	0.00000000	C	-2.77245921	-3.22732877	-0.06224204
C	1.43855907	0.00000000	0.00000000	H	-1.35221188	-6.81045999	0.24497261
C	1.87290512	1.35189773	0.00000000	H	-3.79548325	-6.46197904	-0.03678825
C	0.72254516	2.19320820	-0.01002777	H	-4.69273664	-4.15741074	-0.23575184
C	-0.42917586	1.36464187	-0.01644521	H	-3.14984228	-2.21713717	-0.14656378
H	2.07915727	-0.86583052	-0.03786709	P	0.86596420	-5.13263278	0.41125794
H	2.89702293	1.68609562	-0.04460084	O	1.16025820	-6.58183907	0.46410345
H	0.73151353	3.27056426	-0.05006064	H	1.28232292	-4.37982975	1.53431733
H	-1.45958292	1.67773278	-0.05357784	H	1.50675710	-4.41123748	-0.62369474
Fe	0.72810898	0.96731869	-1.67317026	N	2.35401947	2.99499793	-3.30477877
C	1.45621795	1.93463738	-3.34634052	C	1.95008207	4.18774658	-3.50373827
C	0.01765888	1.93463738	-3.34634052	H	0.89767499	4.39315480	-3.72749022
C	-0.41668717	0.58273965	-3.34634052	C	2.84999791	5.34270402	-3.44903375
C	0.73367279	-0.25857082	-3.33631274	C	2.34704641	6.65530807	-3.56214363
C	1.88539381	0.56999551	-3.32989531	C	3.21694823	7.74558482	-3.50816092
H	-0.62293932	2.80046790	-3.30847343	C	4.58305735	7.54587187	-3.34785295
H	-1.44080498	0.24854176	-3.30173968	C	5.08497142	6.25090428	-3.23551951
H	0.72470442	-1.33592689	-3.29627988	C	4.22867715	5.16196616	-3.28409848
H	2.91580087	0.25690459	-3.29276268	H	2.80842980	8.74509737	-3.59131313
N	-0.89780153	-1.06036055	-0.04156175	H	5.25170118	8.39661643	-3.30955227
C	-0.49386413	-2.25310920	0.15739775	H	6.14895457	6.09204814	-3.11058868
H	0.55854295	-2.45851742	0.38114970	H	4.60606022	4.15177455	-3.19977674
C	-1.39377998	-3.40806664	0.10269324	P	0.59025373	7.06727015	-3.75759846
C	-0.89082848	-4.72067069	0.21580311	O	0.29595973	8.51647645	-3.81044396
C	-1.76073030	-5.81094744	0.16182041	H	0.17389502	6.31446713	-4.88065785
C	-3.12683942	-5.61123448	0.00151243	H	-0.05053917	6.34587485	-2.72264577
C	-3.62875348	-4.31626689	-0.11082100				

Complex [**9a**·Zn]$^{2+}$ (quasi-C_2): E = -4912.824472327 au

C	0.00000000	0.00000000	0.00000000	C	-1.05843718	-4.53691208	0.96340190
C	1.42778462	0.00000000	0.00000000	H	-4.89455959	-4.12650770	1.06065473
C	1.84435613	1.35817555	0.00000000	H	-3.90263490	-6.36752196	1.18220354
C	0.69158589	2.18914384	0.01245179	H	-1.43723971	-6.63878131	1.16354650
C	-0.45948481	1.35865519	-0.00065509	H	0.01805007	-4.65773507	0.97190279
H	2.06867855	-0.86564514	-0.04760434	P	-3.84606602	-1.51050167	0.90682642
H	2.86617121	1.69856704	-0.04299140	O	-3.85575516	-0.72975736	-0.39861705
H	0.69000817	3.26671291	-0.00311094	H	-3.27400310	-0.77754524	1.95750788
H	-1.49055594	1.67618155	0.01288336	H	-5.14237807	-1.81280453	1.33913936
Fe	0.64329386	0.95617031	-1.66464462	N	-1.91021107	0.24359481	-3.17557789
C	-0.55832950	0.65850307	-3.26859683	C	-2.81176331	0.81798525	-3.89299512
C	-0.03054061	1.98348729	-3.33567949	H	-2.52832748	1.67789596	-4.50100435
C	1.38395781	1.86636464	-3.39482561	C	-4.20577733	0.39334731	-3.97085893
C	1.72774803	0.48746062	-3.37741415	C	-4.63609364	-0.95964220	-3.91479946
C	0.53177398	-0.27228174	-3.28548987	C	-5.99980193	-1.24437101	-4.00172396
H	-0.59606566	2.90044351	-3.29289118	C	-6.93738690	-0.22324971	-4.14464628
H	2.07962108	2.68956842	-3.40971922	C	-6.51497171	1.09581666	-4.23490747
H	2.72790013	0.08636214	-3.39262169	C	-5.15833448	1.39588048	-4.16772112
H	0.44561378	-1.34733378	-3.25830610	H	-6.34398666	-2.27144553	-3.98423419
N	-0.89398248	-1.09664921	-0.02479688	H	-7.98956840	-0.46652069	-4.21211192
C	-0.66196436	-2.14781470	0.68104608	H	-7.23559139	1.89124037	-4.37180278
H	0.27931397	-2.22158995	1.22683251	H	-4.83156184	2.42487466	-4.25593161
C	-1.59924561	-3.25726659	0.82199804	P	-3.52938330	-2.37174030	-3.88501787
C	-3.01034043	-3.09908993	0.87072333	O	-2.75718231	-2.59625845	-2.59478614
C	-3.81783986	-4.23005060	0.99940759	H	-2.67731176	-2.23739544	-4.99217378
C	-3.25858063	-5.50377492	1.08235224	H	-4.35355855	-3.45992271	-4.19376884
C	-1.87861437	-5.65501042	1.07298461	Zn	-2.26193006	-0.97444300	-1.55898874

Compound **9b** (C_i): E = -3291.169029152 au

C	0.00000000	0.00000000	0.00000000	O	1.19741482	-3.57756700	-2.53619203
C	1.43730335	0.00000000	0.00000000	C	-0.56297932	-5.12943617	-3.98940123
C	1.86969265	1.35552418	0.00000000	H	-1.23849168	-5.98057748	-3.89131121
C	0.71862531	2.19679402	-0.02037296	H	-1.12881684	-4.25647378	-4.31965774
C	-0.42968964	1.36098656	-0.00896958	H	0.20808173	-5.35396158	-4.73006395
H	2.06618723	-0.87539035	-0.00786855	C	1.08441015	-6.26425528	-1.90707509
H	2.89515772	1.68805862	-0.03192628	H	0.38516646	-7.09928356	-1.83824785
H	0.70938364	3.27377057	-0.08975817	H	1.86183811	-6.49566432	-2.63878172
H	-1.45857807	1.67855778	-0.05591828	H	1.54987986	-6.10292744	-0.93290358
Fe	0.76430752	0.95104580	-1.67289299	N	2.40937844	2.98564620	-3.33847951
C	1.52861504	1.90209160	-3.34578599	C	2.01072032	4.10908301	-2.88415040
C	0.09131169	1.90209160	-3.34578599	H	1.02692239	4.23900963	-2.43894810
C	-0.34107761	0.54656742	-3.34578599	C	2.89729023	5.28534336	-2.89867238
C	0.80998974	-0.29470241	-3.32541304	C	2.64906041	6.43526605	-2.11840049
C	1.95830469	0.54110504	-3.33681641	C	3.53629656	7.51746779	-2.20254046
H	-0.53757219	2.77748195	-3.33791744	C	4.64736016	7.48389760	-3.02976231
H	-1.36654267	0.21403298	-3.31385971	C	4.89527282	6.34498382	-3.79450387
H	0.81923141	-1.37167897	-3.25602782	C	4.03149742	5.26743843	-3.72733598
H	2.98719311	0.22353382	-3.28986771	H	3.36058941	8.40505664	-1.60666485
N	-0.88076339	-1.08355460	-0.00730648	H	5.31376110	8.33597939	-3.07825145
C	-0.48210526	-2.20699141	-0.46163559	H	5.75913801	6.30459695	-4.44667261
H	0.50169267	-2.33691802	-0.90683789	H	4.20579913	4.37808610	-4.31778091
C	-1.36867517	-3.38325177	-0.44711361	P	1.27082977	6.62650135	-0.92965178
C	-1.12044534	-4.53317445	-1.22738550	O	0.33120024	5.47965861	-0.80959396
C	-2.00768148	-5.61537620	-1.14324553	C	2.09159439	7.03152777	0.64361524
C	-3.11874508	-5.58180601	-0.31602369	H	2.65743191	6.15856537	0.97387174
C	-3.36665775	-4.44289223	0.44871788	H	2.76710676	7.88266907	0.54552521
C	-2.50288236	-3.36534684	0.38154998	H	1.32053334	7.25605318	1.38427795
H	-1.83197433	-6.50296505	-1.73912115	C	0.44420493	8.16634689	-1.43871090
H	-3.78514602	-6.43388781	-0.26753455	H	-0.02126478	8.00501905	-2.41288242
H	-4.23052294	-4.40250537	1.10088661	H	-0.33322303	8.39775593	-0.70700428
H	-2.67718407	-2.47599451	0.97199491	H	1.14344862	9.00137516	-1.50753815
P	0.25778530	-4.72440975	-2.41613422				

Compound **9b**' with hampered internal H-bonds (C_i): E = -3291.165442514 au

C	0.00000000	0.00000000	0.00000000	O	0.96774265	-6.57749074	-1.28181648
C	1.43919472	0.00000000	0.00000000	C	1.89047017	-4.82354307	0.62315696
C	1.87549667	1.35174959	0.00000000	H	1.83587683	-3.79190180	0.97318185
C	0.72622389	2.19287793	-0.01170238	H	1.55792559	-5.48822853	1.42289623
C	-0.42656326	1.36404024	-0.01314214	H	2.92509452	-5.06938192	0.37169742
H	2.08181258	-0.86435849	-0.02484415	C	1.41747743	-3.99389183	-2.12987182
H	2.89986144	1.68539558	-0.04073532	H	1.40434370	-2.95348000	-1.80445194
H	0.73394573	3.26976401	-0.05008843	H	2.43262373	-4.27424041	-2.42071712
H	-1.45672636	1.67840093	-0.05042953	H	0.76195648	-4.10936031	-2.99551711
Fe	0.73404008	0.96316943	-1.67288661	N	2.36879198	2.98789780	-3.29021865
C	1.46808015	1.92633886	-3.34577322	C	1.93524819	4.18649381	-3.32881938
C	0.02888543	1.92633886	-3.34577322	H	0.86895770	4.38919676	-3.41843050
C	-0.40741651	0.57458926	-3.34577322	C	2.81960127	5.35213834	-3.24443365
C	0.74185626	-0.26653908	-3.33407085	C	2.32973200	6.63781050	-2.92419201
C	1.89464341	0.56229862	-3.33263108	C	3.22619848	7.70864305	-2.85320100
H	-0.61373242	2.79069735	-3.32092907	C	4.58081407	7.52628991	-3.10413177
H	-1.43178129	0.24094328	-3.30503790	C	5.06272637	6.25853135	-3.41831929
H	0.73413442	-1.34342515	-3.29568479	C	4.19029511	5.18435577	-3.48350912
H	2.92480652	0.24793793	-3.29534370	H	2.84458512	8.68627907	-2.58802812
N	-0.90071183	-1.06155895	-0.05555457	H	5.25631460	8.37101192	-3.05077426
C	-0.46716802	-2.26015495	-0.01695385	H	6.11722413	6.10842061	-3.61468663
H	0.59912247	-2.46285790	0.07265728	H	4.54650375	4.19223911	-3.72561069
C	-1.35152111	-3.42579949	-0.10133958	P	0.60216493	7.08827188	-2.50163115
C	-0.86165183	-4.71147165	-0.42158121	O	0.50033752	8.50382960	-2.06395674
C	-1.75811831	-5.78230420	-0.49257222	C	-0.42239000	6.74988193	-3.96893018
C	-3.11273390	-5.59995107	-0.24164145	H	-0.08984542	7.41456739	-4.76866945
C	-3.59464620	-4.33219250	0.07254607	H	-0.36779666	5.71824066	-4.31895507
C	-2.72221494	-3.25801692	0.13773589	H	-1.45701435	6.99572079	-3.71747065
H	-1.37650495	-6.75994021	-0.75774510	C	0.05060273	5.92023069	-1.21590141
H	-3.78823442	-6.44467307	-0.29499896	H	0.70612369	6.03569917	-0.35025611
H	-4.64914396	-4.18208177	0.26891340	H	-0.96454356	6.20057928	-0.92505610
H	-3.07842359	-2.26590026	0.37983746	H	0.06373646	4.87981886	-1.54132128
P	0.86591524	-5.16193302	-0.84414208				

Complex [**9b**·Zn]$^{2+}$ (C_2): E = -5070.134040599 au

C	0.00000000	0.00000000	0.00000000	C	-0.69074695	-2.10707483	0.74934190
C	1.42759582	0.00000000	0.00000000	H	0.22491275	-2.14499264	1.34211557
C	1.84569908	1.35805914	0.00000000	C	-1.61566008	-3.22844405	0.89879048
C	0.69316496	2.18906496	0.01275112	C	-3.03246757	-3.11686992	0.93232864
C	-0.45915702	1.35778998	0.00010371	C	-3.78044134	-4.28849663	1.05493845
H	2.06549877	-0.86755334	-0.04889977	C	-3.17207646	-5.53858207	1.14472763
H	2.86736714	1.69848848	-0.04270919	C	-1.78860989	-5.63795492	1.15223815
H	0.69093563	3.26652683	-0.00366528	C	-1.02160591	-4.48502478	1.05083776
H	-1.48997515	1.67528779	0.00500308	H	-4.85906879	-4.24308341	1.10592467
Fe	0.64790015	0.95299618	-1.64325984	H	-3.78455202	-6.42582902	1.23814207
C	-0.54354139	0.63291466	-3.22638780	H	-1.30712417	-6.60187748	1.25046607
C	-0.04211443	1.96806402	-3.28945155	H	0.05936486	-4.55742438	1.07187757
C	1.37485527	1.88012802	-3.34944389	P	-3.93486848	-1.53155764	0.95656872
C	1.74666994	0.50875686	-3.33667167	O	-3.84708486	-0.79249979	-0.37941795
C	0.56504421	-0.27538133	-3.24772267	C	-3.28263536	-0.54804961	2.32073995
H	-0.62727148	2.87212479	-3.24227615	H	-3.37663224	-1.09946794	3.25891798
H	2.05397558	2.71687840	-3.36233700	H	-2.23702515	-0.29540539	2.14954304
H	2.75430104	0.12717144	-3.35312393	H	-3.86354531	0.37499789	2.38753752
H	0.49970220	-1.35157287	-3.21678630	C	-5.65855510	-1.85841656	1.35265159
N	-0.89089452	-1.09954375	-0.02075566	H	-5.75841971	-2.35995436	2.31643040

H	-6.16302554	-0.89032527	1.39782523	H	-7.23225446	1.70057189	-4.21545338
H	-6.12338170	-2.45826382	0.56938496	H	-4.83234051	2.26298822	-4.15999640
N	-1.88388206	0.18813646	-3.13268843	P	-3.40025481	-2.53623745	-3.96092563
C	-2.78988801	0.70711635	-3.87971002	O	-2.61920599	-2.67394363	-2.65334289
H	-2.52992088	1.55872979	-4.51091737	C	-2.31160801	-2.31481688	-5.38200983
C	-4.17010819	0.23301595	-3.95379901	H	-2.90177744	-2.23693584	-6.29782104
C	-4.56487846	-1.13241941	-3.92811294	H	-1.70050281	-1.42078595	-5.26497438
C	-5.92876805	-1.42249291	-3.98168156	H	-1.65532291	-3.18569441	-5.45127157
C	-6.88818712	-0.41538531	-4.05999405	C	-4.32886980	-4.04513642	-4.27029926
C	-6.49552963	0.91330993	-4.12556975	H	-4.87558070	-3.99111789	-5.21294018
C	-5.14337865	1.22712680	-4.09344893	H	-3.60265405	-4.85974943	-4.32272221
H	-6.26740370	-2.44884733	-3.98633451	H	-5.01853737	-4.24435808	-3.44928982
H	-7.93723056	-0.67813826	-4.09908999	Zn	-2.27772248	-1.07193748	-1.54761518