Electronic Supplementary Information (ESI)

A multifaceted ferrocene-benzobisimidazole derivative: fluorogenic probe for Pb^{2+} and Zn^{2+} cations and unconventional fluorescence behaviour toward Cu^{2+} metal cations

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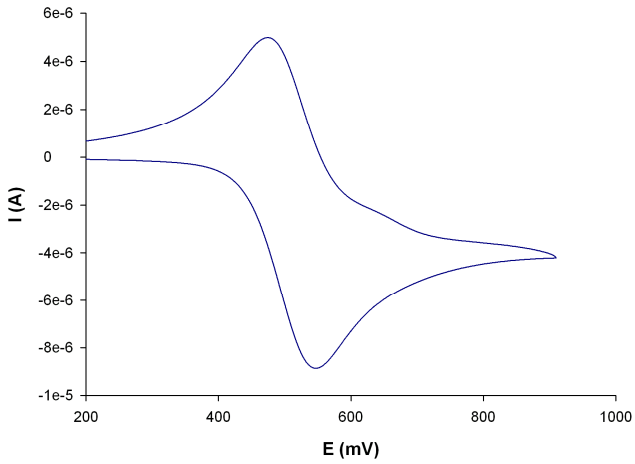

Figure ESI 1. Cyclic Voltammogran of **1** (1 mM, in DMSO/[(*n*-Bu)$_4$N]PF$_6$) scanned at 0.1 V s^{-1}.

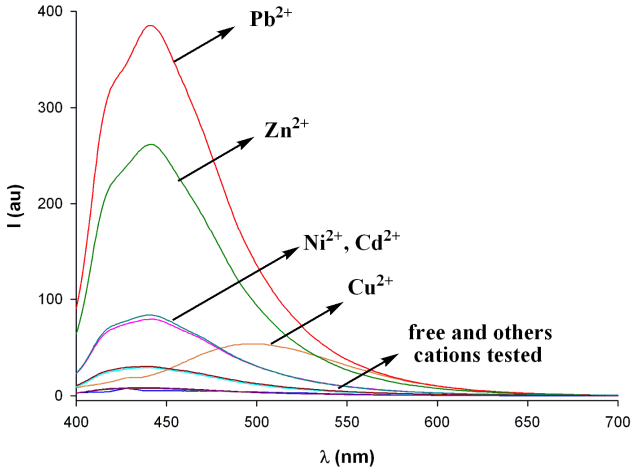

Figure ESI 2. Changes in the fluorescence emission spectrum of **1** (c = 1x10^{-5} M in DMSO) upon addition of several cations.

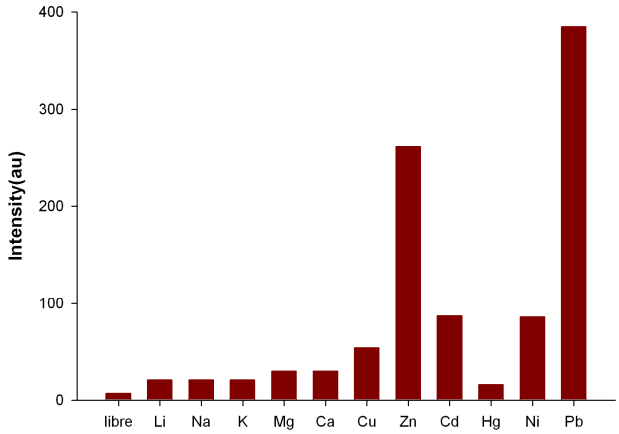

Figure ESI 3. Fluorescence intensity of ligand **1,** in DMSO, in relation to the free ligand, after addition of 1 equivalent of several cations.

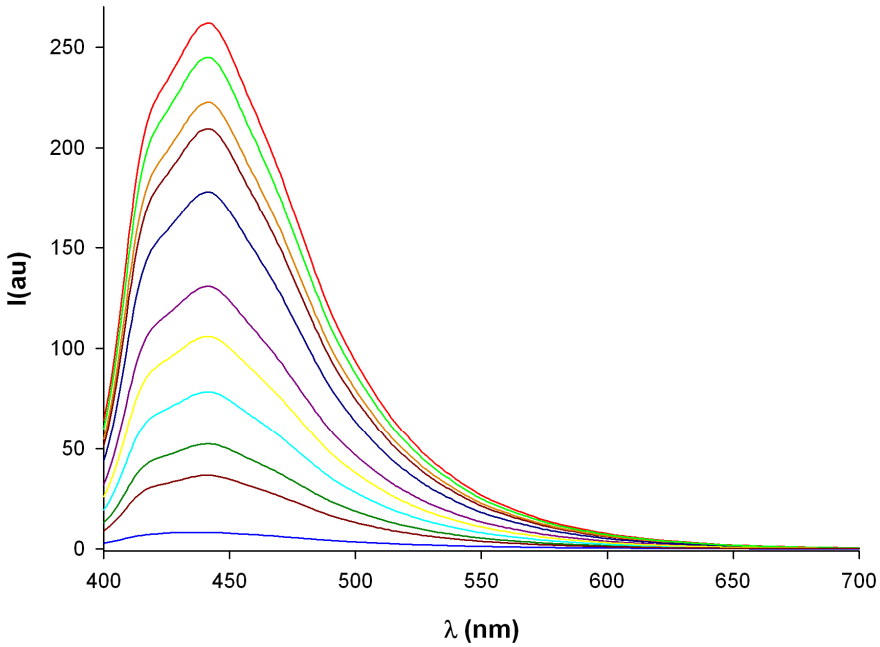

Figure ESI 4. Changes in the fluorescence emission spectrum of **1** (c = 1x10^{-5} M in DMSO) upon titration with Zn^{2+}: the initial (blue) is that of **1** and the final one (red), after addition of 1 equivalent of Zn^{2+}.

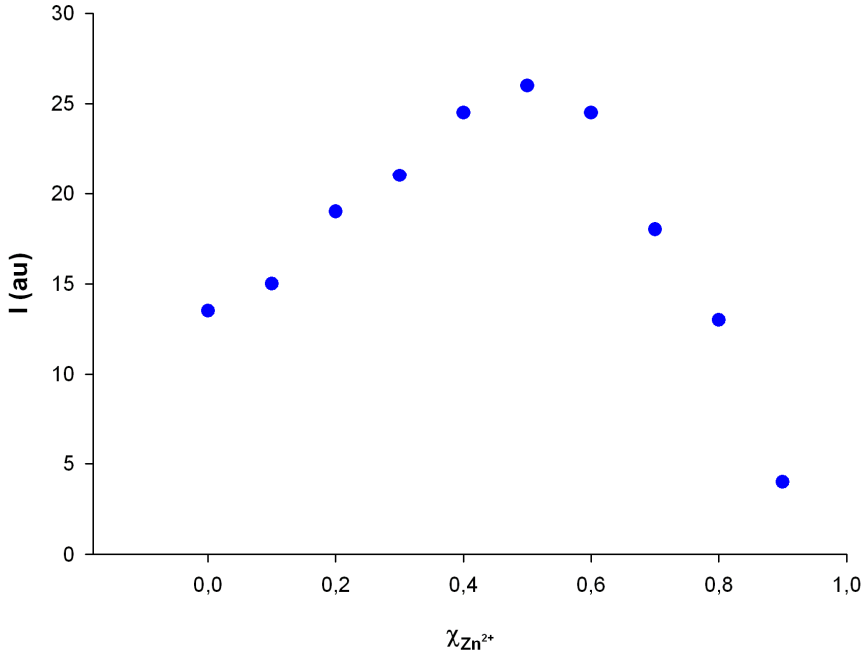

Figure ESI 5. Job´s plot for **1** and Zn^{2+}, indicating the formation of 1:1 complex. The total [**1**] + [Zn^{2+}] = 1·10^{-5}M.

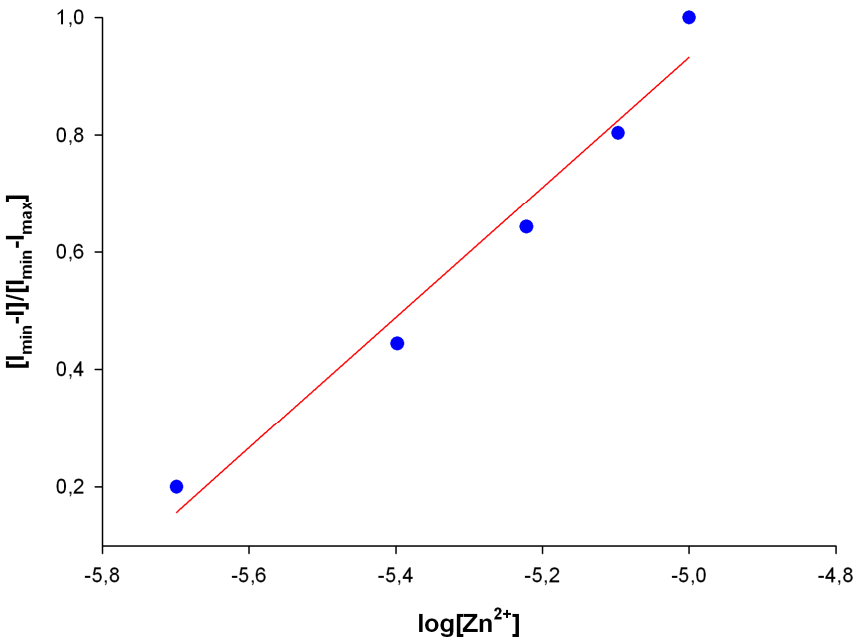

Figure ESI 6. Fluorescence intensity of **1** (in DMSO) at each concentration of Zn^{2+} added, normalized between the minimum fluorescence intensity, found at zero equiv of Zn^{2+}; and the maximum fluorescence intensity, found at $[Zn^{2+}]= 1.4\cdot10^{-6}$ M

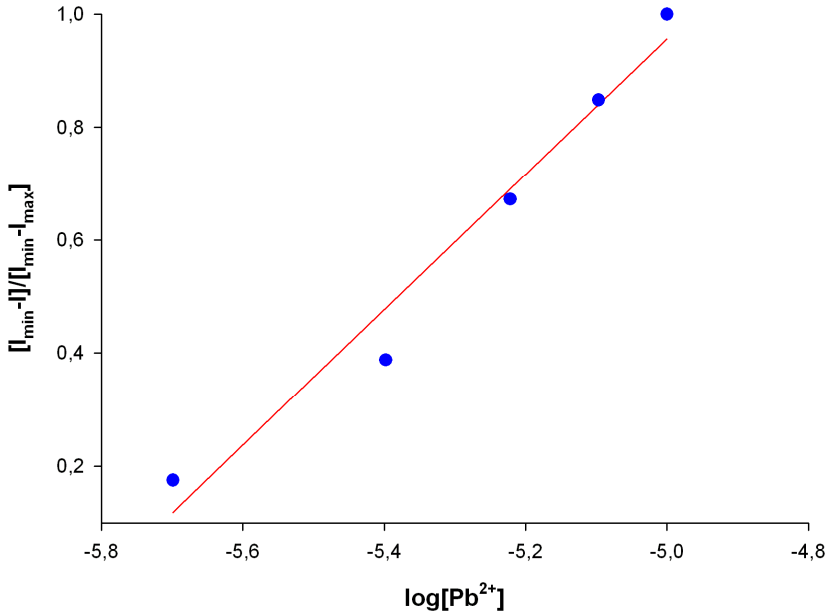

Figure ESI 7. Fluorescence intensity of **1** (in DMSO) at each concentration of Pb^{2+} added, normalized between the minimum fluorescence intensity, found at zero equiv of Pb^{2+}; and the maximum fluorescence intensity, found at $[Pb^{2+}]= 1.6\cdot10^{-6}$ M

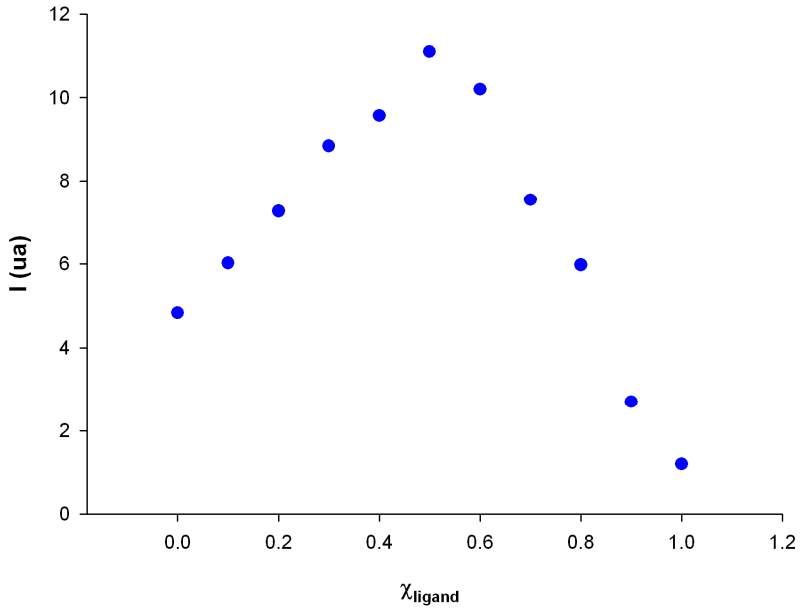

Figure ESI 8. Job´s plot for **1** and Cu^{2+}, indicating the formation of 1:1 complex. The total [**1**] + [Cu^{2+}] = $1 \cdot 10^{-5}$M.

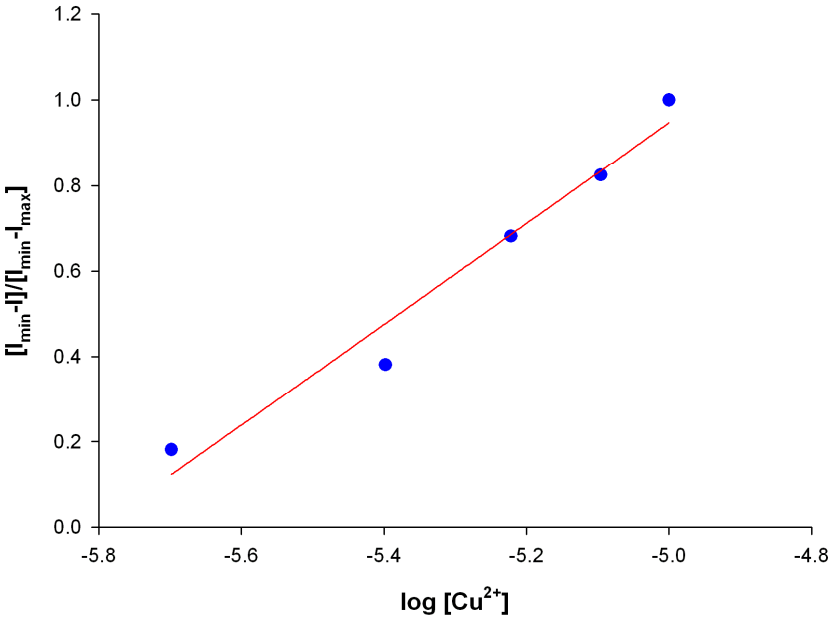

Figure ESI 9. Fluorescence intensity of **1** (in DMSO) at each concentration of Cu^{2+} added, normalized between the minimum fluorescence intensity, found at zero equiv of Cu^{2+}; and the maximum fluorescence intensity, found at [Cu^{2+}]= $1.6 \cdot 10^{-6}$ M

Experimental Section.-

General Comments.- Fluorescence spectra were carried out in a fluorescence spectrophotometer using a fluorescence cell 10 mm ($c \approx 10^{-5}$ M), as it is stated in the corresponding figure captions. Before recording the spectra, the samples were deoxygenated, to remove fluorescence quenching via oxygen, by bubbling nitrogen for at least 10 min. All the spectra were recorded before and after the sequential additions of aliquots of 0.1 equiv of a solution of cations in H_2O ($c = 2.5x\ 10^{-3}$ M). Quantum yield values were measured with respect to anthracene as standard ($\Phi = 0.27\pm0.01$)[1], using the equation $\Phi_x/\Phi_s = (S_x/S_s)\ [(1\text{-}10^{-As})/(1\text{-}10^{-Ax})]^2(n_s^2/n_x^2)$ where x and s indicate the unknown and standard solution, respectively, Φ is the quantum yield, S is the area under the emission curve, A is the absorbance at the excitation wavelength and n is the index of refraction.

Computational details.- The reliably accurate description of weak interactions like hydrogen bonds and other found in supramolecular complexes generally requires a treatment of electron correlation. Density functional theory[2] (DFT) has proved quite useful in this regard offering an electron correlation correction frequently comparable to the second-order Møller–Plesset theory (MP2) or in certain cases, and for certain purposes, even superior to MP2, but at considerably lower computational cost. Due to the size of the systems investigated in the present study the cost advantage that offers mPW1B95 method in comparison with MP2 was significant. Calculated geometries at the DFT level were fully optimized in the gas-phase with tight convergence criteria using the Gaussian 03 package,[3] employing the hybrid meta functional mPW1B95 and the 6-31G** basis set for all atoms except Cu, Zn and Pb for which the Lanl2DZ with effective core potential (ecp) was used. Ultrafine grids (99 radial shells and 590 angular

points per shell) were employed for numerical integrations. Only 2:2 ligand-metal stoichiometries, in agreement with the experimental observations, were explored. Several different conformations, roughtly representing the full conformational space, were cheked initially at a slightly lower calculation level (mPW1B95/6-31G*/Lanl2Dzecp) with loose convergence criteria. Only those most stable complexes for every metal were thereafter refined at the final level. From these gas-phase optimized geometries all reported data were obtained by means of single-point (SP) calculations at the same mPW1B95/6-31G**/Lanl2DZ-ecp level. Energy values are uncorrected for the zero-point vibrational energy. Bond orders were characterized by the Wiberg's bond index (WBI) and calculated with the natural bond orbital (NBO) method as the sum of squares of the off-diagonal density matrix elements between atoms.[4] The topological analysis of the electronic charge density was conducted by means of the Bader's AIM methodology using the AIM2000 software[5] and the wavefunction at the working level of theory.

Calculated structures: cartesian coordinates (in Å) and energies computed for receptor **1**, and its complexes $[\mathbf{1}_2 \cdot M_2]\ (ClO_4)_4$, (M: Cu, Zn, Pb)**.-**

Compound **1** (C_i): E = -3826.79274101 au

C	0.00000000	0.00000000	0.00000000	C	6.51288518	-2.32828848	-3.35013945
C	1.40462616	0.00000000	0.00000000	C	6.00154570	-3.62649550	-3.01206121
C	2.13963329	1.23649361	0.00000000	C	4.58125914	-3.51098863	-2.83339389
C	1.55110160	2.50022934	0.00330449	H	3.21407304	-1.72771760	-2.95367946
C	0.14647544	2.50022934	0.00330449	H	5.46477422	-0.34743417	-3.60134692
C	-0.58853169	1.26373573	0.00330449	H	7.55495749	-2.08267919	-3.54539997
H	-0.56519369	-0.93292357	0.00002624	H	6.58811054	-4.53666161	-2.90302883
H	2.11629529	3.43315292	0.00327825	H	3.90252886	-4.31408173	-2.55392731
N	3.46740732	0.83318802	-0.00528778	C	-3.17950671	3.80934945	-0.00285056
C	3.48760453	-0.55424932	0.00217514	C	-4.51170580	3.31990058	0.27251073
N	2.26879594	-1.08335655	0.00065336	C	-5.42368934	4.42169161	0.16007097
N	-0.71769434	3.58358589	0.00265113	C	-4.66462328	5.59522359	-0.16911689
C	-1.93650293	3.05447866	0.00112935	C	-3.28321336	5.22576935	-0.25840733
N	-1.91630572	1.66704132	0.00859227	H	-4.78375486	2.29619236	0.52692354
H	4.27862937	1.43858563	0.06317257	H	-6.50065358	4.37401552	0.30773020
H	-2.72752777	1.06164370	-0.05986808	H	-5.06760873	6.59548783	-0.31427540
C	4.73060831	-1.30912011	0.00615504	H	-2.43961897	5.87132469	-0.48915000
C	4.83431495	-2.72554002	0.26171182	Fe	-4.01511532	4.78343703	1.56495657
C	6.21572488	-3.09499425	0.17242138	C	-2.66336256	4.64369492	3.06472714
C	6.97479093	-1.92146227	-0.15676648	C	-3.03015754	6.01121796	2.83669838
C	6.06280740	-0.81967125	-0.26920625	C	-4.45044410	6.12672483	3.01536570
H	3.99072057	-3.37109535	0.49245449	C	-4.96178359	4.82851781	3.35344394
H	6.61871033	-4.09525849	0.31757989	C	-3.85613399	3.91181484	3.38401949
H	8.05175518	-1.87378619	-0.30442571	H	-1.66297145	4.22794693	2.95698395
H	6.33485646	0.20403697	-0.52361905	H	-2.35142726	6.81431106	2.55723180
Fe	5.56621691	-2.28320769	-1.56165208	H	-5.03700895	7.03689094	2.90633332
C	4.21446415	-2.14346559	-3.06142265	H	-6.00385589	4.58290853	3.54870446
C	5.40723558	-1.41158550	-3.38071500	H	-3.91367263	2.84766350	3.60465141

Complex $[\mathbf{1}_2 \cdot Cu_2]\ (ClO_4)_4$ (C_i): E = -11089.3757763 au

C	0.00000000	0.00000000	0.00000000	C	6.21759906	-3.12857516	-0.35829295
C	1.39782943	0.00000000	0.00000000	C	7.01244717	-1.93347022	-0.34587683
C	2.19161618	1.19029631	0.00000000	C	6.13934535	-0.80803536	-0.20817837
C	1.61235405	2.46161199	-0.01513352	H	4.00003258	-3.43921458	-0.18288060
C	0.21681388	2.48351656	0.02684452	H	6.58806808	-4.14686177	-0.45499367
C	-0.55755869	1.28149889	0.02734864	H	8.09448074	-1.88340602	-0.44583643
H	-0.59767244	-0.91183431	-0.01647744	H	6.43309372	0.23993223	-0.20976932
H	2.20117247	3.37384260	-0.10569369	Fe	5.65778673	-1.87479667	-1.85033012
N	3.53735064	0.83955296	-0.00591280	C	4.53478649	-1.08652208	-3.36144034
C	3.59273742	-0.49575110	-0.02620435	C	5.86149285	-0.54462179	-3.37748003
N	2.32178686	-1.03309391	-0.02719365	C	6.77763107	-1.64212371	-3.51837765
N	-0.63758409	3.58200635	0.06053458	C	6.01553851	-2.85915387	-3.58420979
C	-1.88400534	3.09521667	0.06535384	C	4.62475208	-2.51295511	-3.48440764
N	-1.87104165	1.71698613	0.02775634	H	3.62083579	-0.50794779	-3.23589734
H	2.11470719	-2.02616476	-0.01679411	H	6.11975199	0.50845120	-3.27921429
H	-2.70013925	1.13348297	0.06028862	H	7.86225466	-1.56408412	-3.55793838
C	4.78880646	-1.30730953	-0.10550510	H	6.41951466	-3.86409992	-3.69063534
C	4.84185663	-2.74917187	-0.22340766	H	3.78926660	-3.21022642	-3.50428070

C	-3.11411487	3.85835396	0.07419644
C	-3.23055924	5.26774687	-0.20324158
C	-4.62101613	5.60338358	-0.16583224
C	-5.37280883	4.41102284	0.10614611
C	-4.44774254	3.32563024	0.24614279
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H	-5.03728782	6.59295038	-0.34271828
H	-6.45451538	4.33699684	0.19594228
H	-4.71155438	2.29779469	0.49115116
Fe	-4.26145289	4.18334547	-1.57283687
C	-3.18755308	3.55765214	-3.18879947
C	-4.33591038	2.72171824	-2.97457119
C	-5.50710308	3.55412796	-3.04017976
C	-5.07424313	4.90026521	-3.29304109
C	-3.64250279	4.90069281	-3.38219576
H	-2.14340988	3.25191283	-3.15657016
H	-4.32634988	1.64640047	-2.80549149
H	-6.53735870	3.22369396	-2.92239712
H	-5.71937341	5.77211165	-3.38311205
H	-2.99544735	5.76284794	-3.52504123
Cu	0.12872992	5.28577229	0.97640030
Cl	0.42229634	6.21765824	-1.83543407
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Cl	-0.94942825	4.03359442	3.38858761
O	-1.77274163	5.10147003	2.66811366
O	0.46435997	4.08458433	2.70428527
O	-0.79423611	4.36041174	4.83501977
O	-1.54489521	2.68038824	3.17344463
C	5.02059972	7.47143708	1.70297702
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C	2.82898354	6.28114076	1.70297702
C	3.40824567	5.00982509	1.71811054
C	4.80378584	4.98792052	1.67613250
C	5.57815841	6.18993819	1.67562838
H	5.61827216	8.38327139	1.71945446
H	2.81942725	4.09759448	1.80867071
N	1.48324908	6.63188411	1.70888982
C	1.42786229	7.96718817	1.72918137
N	2.69881286	8.50453098	1.73017066
N	5.65818381	3.88943073	1.64244244
C	6.90460506	4.37622041	1.63762318
N	6.89164137	5.75445095	1.67522068
H	2.90589253	9.49760183	1.71977112
H	7.72073897	6.33795410	1.64268840
C	0.23179326	8.77874660	1.80848212
C	-1.11874563	8.27947244	1.91115538
C	-1.99184746	9.40490729	2.04885385
C	-1.19699935	10.60001223	2.06126997
C	0.17874308	10.22060895	1.92638468
H	-1.41249401	7.23150485	1.91274634
H	-3.07388102	9.35484309	2.14881344
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H	1.02056714	10.91065166	1.88585762
Fe	-0.63718702	9.34623375	3.55330713
C	0.48581322	8.55795916	5.06441735
C	0.39584764	9.98439219	5.18738466
C	-0.99493879	10.33059094	5.28718680
C	-1.75703135	9.11356079	5.22135467
C	-0.84089314	8.01605886	5.08045704
H	1.39976393	7.97938486	4.93887435
H	1.23133311	10.68166350	5.20725772
H	-1.39891494	11.33553700	5.39361236
H	-2.84165495	9.03552119	5.26091539
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C	8.13471458	3.61308311	1.62878057
C	9.46834224	4.14580684	1.45683422
C	10.39340854	3.06041424	1.59683091
C	9.64161584	1.86805350	1.86880926
C	8.25115895	2.20369021	1.90621860
H	9.73215409	5.17364240	1.21182586
H	11.47511508	3.13444024	1.50703474
H	10.05788752	0.87848670	2.04569530
H	7.41637256	1.54003962	2.12898428
Fe	9.28205259	3.28809162	3.27581389
C	8.20815279	3.91378495	4.89177649
C	8.66310250	2.57074427	5.08517278
C	10.09484283	2.57117188	4.99601810
C	10.52770278	3.91730913	4.74315678
C	9.35651009	4.74971885	4.67754821
H	7.16400959	4.21952426	4.85954718
H	8.01604706	1.70858915	5.22801825
H	10.73997311	1.69932545	5.08608906
H	11.55795840	4.24774313	4.62537413
H	9.34694959	5.82503661	4.50846850
Cu	4.89186979	2.18566479	0.72657671
Cl	4.59830337	1.25377883	3.53841108
O	5.38592449	0.81951847	2.21779220
O	3.40784309	2.04286148	3.06028297
O	4.20872236	-0.00666161	4.22708633
O	5.52002101	2.09171210	4.36975020
Cl	5.97002796	3.43784265	-1.68561059
O	6.79334134	2.36996704	-0.96513665
O	4.55623974	3.38685275	-1.00130825
O	5.81483582	3.11102533	-3.13204276
O	6.56549493	4.79104884	-1.47046762

Complex [$\mathbf{1}_2$·Zn_2] $(ClO_4)_4$ (C_i): E = -10829.3415735 au

C	0.00000000	0.00000000	0.00000000
C	1.39640796	0.00000000	0.00000000
C	2.19343389	1.18527837	0.00000000
C	1.61048589	2.45646203	-0.01659068
C	0.21269766	2.48415591	0.01869386
C	-0.55656370	1.28059115	0.02094817
H	-0.59787241	-0.91176786	-0.00098759
H	2.20568187	3.36440624	-0.10322606
N	3.54361001	0.82912057	0.02765475
C	3.58657255	-0.51074510	0.01699453
N	2.31355092	-1.03588578	-0.00003064
N	-0.65161125	3.58005232	0.06653490
C	-1.89720929	3.08502332	0.07327320
N	-1.87173233	1.70865226	0.04416744
H	2.10560210	-2.02821993	-0.03324555
H	-2.70000863	1.12347478	0.01793382
C	4.75515896	-1.36717527	-0.01298216
C	4.74797507	-2.80460654	0.17577739
C	6.09069901	-3.27608372	0.01025687
C	6.92553727	-2.14826175	-0.28893375
C	6.10943447	-0.97300740	-0.32125990
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H	6.41528341	-4.31029519	0.10267572	N	5.72584630	4.13822314	1.42972819
H	7.99515344	-2.17911088	-0.48488846	C	6.97144405	4.63325356	1.42298819
H	6.44060972	0.03524143	-0.55931520	N	6.94596588	6.00962456	1.45209704
Fe	5.43749832	-2.32374591	-1.65502816	H	2.96862816	9.74649321	1.52952938
C	4.16291081	-1.85769748	-3.16663248	H	7.77424153	6.59480284	1.47833204
C	5.46998620	-1.32026638	-3.41627715	C	0.31907216	9.08544611	1.50927438
C	6.39742234	-2.41745630	-3.43176523	C	-1.03520229	8.69127430	1.81755276
C	5.66411568	-3.62883710	-3.18736069	C	-1.85130692	9.86652750	1.78523946
C	4.27996319	-3.28117554	-3.02276059	C	-1.01647006	10.99435274	1.48605711
H	3.24652550	-1.27597364	-3.07740065	C	0.32625431	10.52287820	1.32052872
H	5.71182258	-0.26681587	-3.54576745	H	-1.36637700	7.68302273	2.05559980
H	7.47141315	-2.34204051	-3.58976411	H	-2.92092224	9.89737422	1.98119672
H	6.08271496	-4.63206012	-3.13603702	H	-1.34105519	12.02856480	1.39364770
H	3.46566294	-3.97741349	-2.83019766	H	1.18097704	11.13843675	1.04280255
C	-3.14954413	3.81431080	0.07620845	Fe	-0.36326392	10.04200134	3.15133103
C	-3.34091096	5.20915162	-0.24304490	C	0.91132773	9.57594094	4.66292700
C	-4.74195593	5.48906005	-0.15684201	C	0.79427333	10.99941937	4.51906987
C	-5.42968991	4.27775932	0.18727490	C	-0.58987894	11.34707749	4.68367645
C	-4.45527909	3.23698923	0.32733285	C	-1.32318309	10.13569331	4.92807187
H	-2.55834682	5.91140312	-0.52181152	C	-0.39574596	9.03850509	4.91257094
H	-5.20542236	6.45465528	-0.34747481	H	1.82771320	8.99421929	4.57368815
H	-6.50275105	4.16430710	0.32592990	H	1.60857236	11.69566092	4.32651075
H	-4.66505743	2.21200201	0.63044138	H	-1.00848007	12.35030121	4.63236308
Fe	-4.36542185	4.03628934	-1.52028424	H	-2.39717435	10.06027494	5.08607279
C	-3.48517861	3.04605631	-3.06010281	H	-0.63757992	7.98505291	5.04205178
C	-4.82445520	2.57269564	-2.85202830	C	8.22377999	3.90396785	1.42004952
C	-5.71448658	3.69196250	-2.99057693	C	9.52951345	4.48129083	1.16892068
C	-4.92067676	4.85342106	-3.28365671	C	10.50392556	3.44052277	1.30897658
C	-3.54073926	4.45557216	-3.32397851	C	9.81619494	2.22922169	1.65309674
H	-2.57623594	2.44873197	-3.00397915	C	8.41515017	2.50912854	1.73930357
H	-5.11823385	1.54709366	-2.63567733	H	9.73928918	5.50627769	0.86581112
H	-6.79788547	3.66449869	-2.89168392	H	11.57698668	3.55397685	1.17031903
H	-5.29789673	5.86252946	-3.43704900	H	10.27966295	1.26362708	1.84372920
H	-2.68454446	5.10499241	-3.49717765	H	7.63258820	1.80687482	2.01807325
Zn	5.01416123	2.23190775	0.72876026	Fe	9.43966217	3.68199259	3.01653950
Cl	4.58912949	1.05283906	3.28973479	C	8.55942239	4.67222544	4.55635909
O	5.71672807	0.82513732	2.21279206	C	8.61498565	3.26270994	4.82023581
O	3.75485465	2.19840541	2.68635545	C	9.99492296	2.86486263	4.77991008
O	5.21112837	1.46061123	4.57719547	C	10.78873071	4.02632171	4.48682757
O	3.77991464	-0.18890088	3.40989000	C	9.89869877	5.14558769	4.34828064
Cl	5.91592614	3.18866519	-1.79893402	H	7.65047888	5.26954845	4.50023799
O	6.56764580	2.18268950	-0.77712197	H	7.75879290	2.61328917	4.99343768
O	4.51333149	3.42841292	-1.21029836	H	10.37214562	1.85575475	4.93330117
O	5.83683931	2.54977935	-3.13867514	H	11.87213023	4.05378657	4.38793062
O	6.70944318	4.44742805	-1.80644322	H	10.19247509	6.17118976	4.13192780
C	5.07423189	7.71827598	1.49627288	Zn	0.06007423	5.48636455	0.76751069
C	3.67782414	7.71827440	1.49627681	Cl	0.48511376	6.66544346	-1.79345605
C	2.88079914	6.53299566	1.49627457	O	-0.64248724	6.89314330	-0.71651625
C	3.46374843	5.26181222	1.51285993	O	1.31938497	5.51987334	-1.19007981
C	4.86153619	5.23411949	1.47757232	O	-0.13688375	6.25767716	-3.08092028
C	5.63079661	6.43768463	1.47532024	O	1.29433031	7.90718226	-1.91360543
H	5.67210290	8.63004350	1.49726219	Cl	-0.84169453	4.52959007	3.29519728
H	2.86855423	4.35386710	1.59949307	O	-1.49341357	5.53557224	2.27339112
N	1.53062294	6.88915143	1.46862461	O	0.56090343	4.28985120	2.70656375
C	1.48765938	8.22901731	1.47928929	O	-0.76261287	5.16846595	4.63494330
N	2.76068046	8.75415897	1.49631361	O	-1.63520750	3.27082632	3.30269446

Complex [$\mathbf{1}_2$·Pb_2] $(ClO_4)_4$ (C_i): E = -10703.8420275 au

C	0.00000000	0.00000000	0.00000000	C	0.22713124	2.48201964	-0.04221163
C	1.39480568	0.00000000	0.00000000	C	-0.55159883	1.28147126	-0.02229996
C	2.20694785	1.18025104	0.00000000	H	-0.59836152	-0.91270274	0.00945824
C	1.62704983	2.45515710	-0.01759053	H	2.21903882	3.36950970	0.02893482

N	3.55375374	0.80337933	0.00093523
C	3.57480458	-0.53546006	-0.00099147
N	2.29653367	-1.04712572	0.01616387
N	-0.63170674	3.58154376	-0.06645479
C	-1.87352495	3.09276736	-0.07601441
N	-1.86694063	1.71528650	-0.02623542
H	2.07270633	-2.03066839	-0.10542134
H	-2.69776223	1.13790353	-0.12736983
C	4.71587048	-1.43205334	0.04328259
C	6.11659006	-1.12652179	-0.14433923
C	6.86141611	-2.34702302	-0.05004185
C	5.94251968	-3.41724967	0.20535908
C	4.62430375	-2.86204544	0.27302573
H	6.54654542	-0.14445411	-0.33129910
H	7.94176881	-2.43913338	-0.15077922
H	6.19879023	-4.46700088	0.33944088
H	3.71393330	-3.42778457	0.47361726
Fe	5.81291821	-1.99286827	1.64334691
C	5.26478917	-0.77078532	3.17581849
C	4.85901731	-2.12518396	3.42734449
C	6.03456906	-2.95250112	3.41222394
C	7.16508459	-2.10503575	3.15112136
C	6.68710642	-0.75941884	3.00656544
H	4.61429313	0.09950462	3.08785372
H	3.83850309	-2.46576677	3.59869587
H	6.06400437	-4.03045980	3.56771657
H	8.20169908	-2.42939626	3.06688594
H	7.27871622	0.12616544	2.78222871
C	-3.13328622	3.82419578	-0.13163216
C	-4.35176580	3.43575186	0.54765850
C	-5.38571146	4.35049349	0.16200406
C	-4.82380517	5.29791413	-0.75666920
C	-3.44414422	4.97359785	-0.95706264
H	-4.45001860	2.61266666	1.25610190
H	-6.41476852	4.33724575	0.51830035
H	-5.35742953	6.11792919	-1.23496015
H	-2.77396690	5.44976643	-1.67268728
Fe	-3.82519058	5.32709247	1.01022378
C	-2.29919633	5.92026267	2.23336441
C	-2.85716034	7.04690960	1.54441735
C	-4.25553296	7.11581827	1.86082329
C	-4.55984719	6.03514639	2.75681727
C	-3.34946515	5.29511033	2.98250546
H	-1.25979067	5.59018773	2.20898506
H	-2.30331161	7.74645550	0.91806862
H	-4.96134672	7.85891391	1.49190426
H	-5.53650978	5.81155633	3.18462669
H	-3.24352548	4.41437244	3.61425224
Pb	5.41016201	2.27248665	-0.94040680
Cl	5.20970142	3.24575652	2.09130148
O	6.25716256	2.22410881	1.60336710
O	4.45735169	3.67650524	0.78079006
O	5.87334339	4.43605014	2.67575064
O	4.24814908	2.60071283	3.02422144
Cl	3.78349744	1.08368098	-3.39795550
O	4.96640586	0.33398025	-2.77689368
O	3.79928043	2.50112094	-2.68691441
O	2.50525573	0.38917740	-3.08693003
O	3.98816317	1.30672858	-4.84957886
C	5.30814488	8.31198221	-1.66532635
C	3.91333920	8.31198221	-1.66532635
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C	3.68109505	5.85682511	-1.64773582
C	5.08101364	5.82996257	-1.62311472
C	5.85974371	7.03051095	-1.64302639
H	5.90650639	9.22468495	-1.67478459
H	3.08910606	4.94247251	-1.69426117
N	1.75439113	7.50860289	-1.66626158
C	1.73334030	8.84744227	-1.66433487
N	3.01161120	9.35910794	-1.68149022
N	5.93985162	4.73043845	-1.59887156
C	7.18166982	5.21921485	-1.58931194
N	7.17508551	6.59669571	-1.63909093
H	3.23543855	10.34265060	-1.55990501
H	8.00590711	7.17407868	-1.53795652
C	0.59227440	9.74403555	-1.70860894
C	0.68384113	11.17402765	-1.93835208
C	-0.63437481	11.72923188	-1.87068543
C	-1.55327123	10.65900523	-1.61528450
C	-0.80844518	9.43850401	-1.52098712
H	1.59421158	11.73976678	-2.13894361
H	-0.89064535	12.77898309	-2.00476723
H	-2.63362393	10.75111559	-1.51454713
H	-1.23840055	8.45643632	-1.33402725
Fe	-0.50477333	10.30485049	-3.30867326
C	0.04335571	9.08276753	-4.84114484
C	-1.37896155	9.07140105	-4.67189179
C	-1.85693972	10.41701797	-4.81644771
C	-0.72642419	11.26448334	-5.07755029
C	0.44912757	10.43716617	-5.09267084
H	0.69385175	8.21247760	-4.75318007
H	-1.97057134	8.18581677	-4.44755505
H	-2.89355421	10.74137847	-4.73221229
H	-0.75585950	12.34244202	-5.23304292
H	1.46964179	10.77774898	-5.26402221
C	8.44143110	4.48778643	-1.53369419
C	8.75228910	3.33838436	-0.70826372
C	10.13195005	3.01406809	-0.90865715
C	10.69385633	3.96148872	-1.82733041
C	9.65991068	4.87623035	-2.21298485
H	8.08211177	2.86221579	0.00736093
H	10.66557441	2.19405303	-0.43036621
H	11.72291340	3.97473647	-2.18362671
H	9.75816348	5.69931555	-2.92142825
Fe	9.13333546	2.98488974	-2.67555013
C	7.60734121	2.39171955	-3.89869076
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C	9.86799207	2.27683582	-4.42214362
C	9.56367784	1.19616394	-3.52614964
C	8.16530522	1.26507261	-3.20974370
H	6.56793554	2.72179448	-3.87431141
H	8.55167036	3.89760977	-5.27957859
H	10.84465465	2.50042588	-4.84995303
H	10.26949160	0.45306830	-3.15723061
H	7.61145649	0.56552671	-2.58339497
Pb	-0.10201713	6.03949556	-0.72491955
Cl	0.09844346	5.06622569	-3.75662783
O	-0.94901768	6.08787340	-3.26869345
O	0.85079319	4.63547697	-2.44611641
O	-0.56519852	3.87593208	-4.34107699
O	1.05999579	5.71126938	-4.68954779
Cl	1.52464744	7.22830123	1.73262915
O	0.34173902	7.97800196	1.11156733
O	1.50886444	5.81086127	1.02158806
O	2.80288914	7.92280482	1.42160368
O	1.31998171	7.00525363	3.18425251

References.-

1.- W. R. Dawson, M. W. Windsor, *J. Phys.Chem.* 1968, **72**, 3251-3260.

2.- L. J. Bartolottiand and K. Fluchick, in *Reviews in Computational Chemistry*, ed. K. B. Lipkowitz and B. D. Boyd, VCH, New York, 1996; vol. 7, pp. 187-216.

3.- Gaussian 03, Revision B.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

4.- K. Wiberg, *Tetrahedron,* 1968, **24**, 1083-1096.

5.- (a) AIM2000 v. 2.0, designed by F. W. Biegler-König, and J. Schönbohm, 2002. Home page http://www.aim2000.de/. F. Biegler-König, J. Schönbohm and D. J. Bayles, *Comp. Chem.,* 2001, **22**, 545-559. (b) F. Biegler-König and J. Schönbohm, *J. Comp. Chem.,* 2002, **23**, 1489-1494.