

Supplementary Information

The role of conformational changes on the fluorescence enhancement of a selective chemosensor of Pb²⁺.

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Cartesian coordinates of the chemosensor 1- M²⁺ conformers with M=Ca, Hg and Pb by using PBE and PBE0 exchange correlation functionals

We made the calculations with PBE and PBE0 with TZVP basis set, the main finding discussed in the paper is the orientation of the Pb²⁺ since it point out of the chemosensor. For the other ions this conformation was not the most stable. This characteristic was preserved in the structures found with both functionals. In this way the main conclusions in the manuscript are independent of the exchange-correlation functionals tested. Besides PBE with 6-311++G** optimizations were performed for the more stable conformers, these structures are also listed below.

We use the Gaussian 09 code since it contains several proposals for inclusion of solvent effects. However, the asymptotic corrections on the exchange-correlation potential, which are important in the TDDFT calculations, are not included in the G09 program for that reason we use the NWChem code. We have added in Table 3 the values without the LB94 correction showing in this way the importance of this correction on the relative intensities. Besides we have performed the gas phase computations for the free chemosensor and the Ca complex with Gaussian 09 and we did not find any difference with NWChem gas phase without LB94 correction results. Thus, we have confidence that the use of different programs do not change our conclusions. The discussion of the solvent effect is addressed in the manuscript, anyway we are including here the structures obtained with G09 for the solvent correction for the more stable conformers.

Complex Ca-chemosensor A1

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PBE/TZVP CRENL ECP (Ca) E=-1836.69900172 a.u.

Ca	2.51020096	3.93677136	0.21063967
N	0.93548895	3.68045048	2.13212583
C	0.64665424	5.06485077	2.61563564
C	0.22987616	6.01308748	1.49038785
O	1.22921573	5.98826388	0.41604080
C	0.77179711	6.61179051	-0.82137222
C	1.71037900	6.22638765	-1.95987014
O	1.84675452	4.77768011	-1.92903030
C	2.48049073	4.10972761	-3.05945393
C	2.35951624	2.61103997	-2.81441861
O	2.93448089	2.29454379	-1.51423866
C	2.61114150	0.94276798	-1.03367711
C	3.25952816	0.73562452	0.32940590
O	2.94392542	1.85385763	1.22270081
C	2.24538713	1.55157340	2.46869217
C	1.75567764	2.86760286	3.08463271
H	1.56077198	5.44329390	3.10387241

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H	-0.15467324	5.08212073	3.37737958
H	0.14682265	7.03740379	1.88757843
H	-0.74350887	5.71699282	1.06624579
H	-0.25136189	6.25946987	-1.03616319
H	0.75476769	7.70857374	-0.71037003
H	1.26640308	6.55293169	-2.91433922
H	2.70425483	6.69914646	-1.85850794
H	1.95901360	4.36828674	-3.99527074
H	3.53470534	4.42919915	-3.14024842
H	1.29970539	2.30331699	-2.82480285
H	2.89811614	2.06582396	-3.60715132
H	1.51570773	0.82383242	-0.96877598
H	3.01322280	0.19540636	-1.73740756
H	2.87429054	-0.20628760	0.74730365
H	4.35644790	0.68208027	0.25985519
H	2.94143639	1.06561043	3.17145305
H	1.41094308	0.86931358	2.24720660
H	1.22318573	2.62621507	4.02204794
H	2.62121212	3.48559297	3.38425265
C	-1.98318674	1.15174881	0.34903637
C	-1.43773826	2.21254706	-0.38035355
C	-0.52697096	3.07947573	0.22619665
C	-0.20915739	2.94323324	1.58995182
C	-0.90599358	1.99755229	2.35385605
C	-1.76643425	1.09269869	1.73150526
O	-3.85272182	0.43853488	-0.91988356
N	-1.42046507	-7.64181830	-0.61016341
C	0.24747241	-8.00851213	1.25577930
C	-0.02781390	-7.96803342	-0.25101718
C	-3.16060543	-9.25410003	0.27499775
C	-2.32176390	-8.77286239	-0.91248443
C	-1.86544991	-6.35377534	-0.61330204
C	-3.23512415	-6.04332030	-0.92944644
C	-3.68117576	-4.74626841	-0.96535174
C	-2.81380191	-3.65279934	-0.68498114
C	-0.99149042	-5.26612702	-0.31797987
C	-1.46316267	-3.96926803	-0.36560359
C	-3.19931492	-2.30854139	-0.67378800
C	-2.30499660	-1.28698086	-0.34819903
C	-0.91239362	-1.60155271	-0.09445760
C	-2.79981718	0.10218715	-0.36314280
O	0.02530217	-0.81626378	0.09272212
O	-0.56109221	-2.96188441	-0.09129726
H	-1.68789077	2.32080376	-1.43793476
H	-0.34544370	-8.78972412	1.75066709
H	1.31028094	-8.23251190	1.43051106
H	0.01619397	-7.04894938	1.74004165
H	0.19229029	-8.94766546	-0.69723441
H	0.64091817	-7.25026272	-0.75156189
H	-3.81509111	-10.07742123	-0.04715878
H	-2.52786121	-9.62954882	1.09100162
H	-3.79630733	-8.45269297	0.67808426
H	-2.96623242	-8.49291867	-1.75887227
H	-1.68514893	-9.59075385	-1.27805092
H	-4.72560800	-4.53796501	-1.20775339
H	0.05137279	-5.42310989	-0.05230885
H	-4.22867815	-2.02513596	-0.91332663

H	-0.09123193	3.87329314	-0.39001257
H	-0.73739261	1.91289948	3.42925377
H	-2.24041262	0.30670592	2.32331795
H	-3.94090741	-6.84385018	-1.13908462

Complex Ca-chemosensor A2

78

PBE/TZVP CRENL ECP (Ca) E=-1836.73663239 a.u.

Ca	1.74674158	1.33707940	0.87389975
N	3.93806122	0.86367879	2.61963717
C	4.04389736	1.95106216	3.62361270
C	2.81086741	2.85067665	3.81620576
O	2.17313368	3.12834337	2.54449541
C	1.06057926	4.05935871	2.67061660
C	0.74024778	4.60904344	1.29830573
O	0.50398010	3.50332935	0.39223157
C	0.39888692	3.93575121	-0.99125625
C	0.75239908	2.76566029	-1.89161744
O	2.02859749	2.27709820	-1.40961070
C	2.76313703	1.37811748	-2.26727487
C	4.13286039	1.20870368	-1.63246042
O	3.96023765	0.90906611	-0.21831578
C	5.16340695	0.36522190	0.37791120
C	5.21228853	0.56391944	1.91994829
H	4.86635681	2.59073952	3.28090416
H	4.33322382	1.56897302	4.62116496
H	3.16509916	3.79816381	4.25684924
H	2.06242364	2.42488013	4.50115418
H	0.19427181	3.54124344	3.12022271
H	1.34363865	4.89822087	3.32783642
H	-0.15283068	5.25465764	1.36138080
H	1.58843129	5.20688468	0.92140377
H	-0.62207006	4.29521294	-1.20217513
H	1.11331334	4.75890827	-1.15986710
H	-0.00266669	1.95944323	-1.84601968
H	0.83882630	3.12008614	-2.93220458
H	2.22980304	0.41320668	-2.35570755
H	2.88128354	1.80850868	-3.27631313
H	4.66693267	0.38589900	-2.13642087
H	4.72667412	2.13350742	-1.72282495
H	6.03728328	0.87694771	-0.05710441
H	5.23988839	-0.70026905	0.10247131
H	5.69553348	-0.32701720	2.35764210
H	5.87498005	1.41188258	2.12648482
C	0.67338923	-1.76638930	2.68310857
C	0.89836946	-0.93713588	3.78744174
C	2.05169522	-0.15241745	3.86262533
C	3.01642792	-0.19390784	2.82952273
C	2.90372468	-1.23906707	1.87581116
C	1.73208419	-1.98981660	1.79301440
O	-1.29437635	-2.94559790	3.32001141
N	-5.21862957	-1.81164485	-3.98783936
C	-3.68727125	-1.05140300	-5.85267609
C	-4.81677447	-0.70500519	-4.87686967
C	-6.03769645	-3.90032404	-5.16335678
C	-6.38770568	-2.61826054	-4.40337537
C	-4.52744155	-2.09027314	-2.85076700

C	-4.91871378	-3.18255123	-1.99589714
C	-4.26469840	-3.43863878	-0.81937759
C	-3.15854846	-2.64435551	-0.39824245
C	-3.40334303	-1.30483261	-2.45131323
C	-2.76552036	-1.58404335	-1.26172996
C	-2.43821138	-2.83631132	0.77919375
C	-1.33708413	-2.03804703	1.12291821
C	-0.97569395	-0.95235291	0.26213946
C	-0.69673898	-2.31606467	2.44480271
O	-0.08040984	-0.07798467	0.42560333
O	-1.69757053	-0.77509245	-0.90823291
H	0.13660254	-0.86605180	4.56720314
H	-3.98075950	-1.85910326	-6.53641017
H	-3.44690284	-0.16883146	-6.46384084
H	-2.77317310	-1.36673749	-5.32882942
H	-5.71459434	-0.40628864	-5.43512975
H	-4.54619699	0.16273543	-4.25561928
H	-6.96329078	-4.43621964	-5.41903067
H	-5.50790910	-3.68450724	-6.10110096
H	-5.41034008	-4.57532704	-4.56372425
H	-6.99353622	-2.84213876	-3.51363495
H	-7.00821075	-1.96447197	-5.03165437
H	-4.58688827	-4.26734450	-0.18561397
H	-3.03433590	-0.48188158	-3.05870761
H	-2.72150452	-3.62568609	1.48176412
H	2.18933979	0.49241023	4.72783009
H	3.70436363	-1.44016630	1.16599409
H	1.63115421	-2.73184364	0.99752282
H	-5.74796475	-3.82545202	-2.28218664

Complex Ca-chemosensor A3

78

PBE/TZVP CRENB L ECP (Ca) E=-1836.69808962 a.u.

Ca	3.51995560	3.02197808	1.00467163
N	3.57838369	1.20447911	2.73694743
C	2.87767623	1.92929309	3.84614762
C	1.44817043	2.32269677	3.46196149
O	1.45789565	3.10510662	2.22605033
C	0.23145636	2.97375032	1.43118465
C	0.42655705	3.69470714	0.10666335
O	1.66256398	3.19171822	-0.48399238
C	1.96371335	3.55101119	-1.85634943
C	3.10863758	2.65520849	-2.30900567
O	4.19025025	2.73633942	-1.33099657
C	5.24361573	1.74614257	-1.53743384
C	6.27709758	1.90453493	-0.42810551
O	5.64627328	1.91015189	0.88719230
C	5.80188301	0.71012629	1.71515955
C	5.02083116	0.92511347	3.00963419
H	3.47443238	2.82691889	4.09696510
H	2.81869489	1.34006993	4.77923908
H	1.00229363	2.92493372	4.26951347
H	0.83195622	1.42498128	3.30278426
H	0.01769007	1.90444658	1.26262686
H	-0.61258622	3.43463097	1.96997772
H	-0.42787888	3.45977085	-0.54805803

H	0.49905138	4.78987239	0.22899618
H	1.09060871	3.36751278	-2.50372435
H	2.22839658	4.62182545	-1.91818955
H	2.77048359	1.60693511	-2.37726856
H	3.47194846	2.98195854	-3.29703177
H	4.79205392	0.73790651	-1.53169902
H	5.72826556	1.91088659	-2.51448564
H	7.02105763	1.09673484	-0.49763943
H	6.80724060	2.86484331	-0.51948708
H	6.86936852	0.56619074	1.94441365
H	5.42565319	-0.16754569	1.16388800
H	5.15835256	0.03582187	3.65048756
H	5.44307551	1.78652325	3.55430919
C	0.98626596	-1.92402213	1.45436423
C	1.43550464	-1.89880416	2.78248233
C	2.33379639	-0.91823079	3.21039382
C	2.81991646	0.02733686	2.29784935
C	2.47957317	-0.09251937	0.94319008
C	1.56061041	-1.05246671	0.52265559
O	0.09726883	-4.10091585	1.42965510
N	-6.99468272	-2.22249700	-2.60183613
C	-6.79558715	-0.14840762	-4.03450147
C	-7.39138702	-0.81537373	-2.79015600
C	-7.63809454	-3.79719349	-4.47708724
C	-7.93529104	-3.25873133	-3.07448439
C	-5.79410482	-2.54855007	-2.04388543
C	-5.40284601	-3.92422733	-1.88079365
C	-4.21925971	-4.25984764	-1.27291129
C	-3.32382291	-3.26482966	-0.78878885
C	-4.89115575	-1.54413865	-1.58660799
C	-3.70678076	-1.90786454	-0.97563833
C	-2.11331232	-3.52581921	-0.14023342
C	-1.27143127	-2.50700821	0.31391127
C	-1.66268509	-1.12118648	0.12671064
C	-0.07157260	-2.92693900	1.06977106
O	-1.07052008	-0.09724961	0.48050401
O	-2.88455187	-0.89302819	-0.53861680
H	1.04047456	-2.63227138	3.48817799
H	-7.13300280	-0.64322041	-4.95559480
H	-7.11818897	0.90241084	-4.08026984
H	-5.69633846	-0.16947857	-4.02111026
H	-8.48854116	-0.80034175	-2.84785791
H	-7.12841964	-0.25214336	-1.88105254
H	-8.37091229	-4.57602740	-4.73478493
H	-7.70902206	-3.00630587	-5.23656931
H	-6.63427613	-4.24124063	-4.54004480
H	-7.95800560	-4.07615694	-2.33850577
H	-8.93655517	-2.80628500	-3.05136903
H	-3.94985036	-5.31136980	-1.15178391
H	-5.10805869	-0.48385281	-1.69423204
H	-1.79687783	-4.55665337	0.04477243
H	2.61891720	-0.87778369	4.26459550
H	2.90072554	0.57891889	0.18660200
H	1.25845670	-1.09805579	-0.52429375
H	-6.04920756	-4.72146965	-2.24085832

Complex Ca-chemosensor PBE0 A1

78

PBE0/TZVP CRENBL ECP (Ca) optimization E=-1836.79772854 a.u.

Ca	2.57485421	3.90644535	0.21329963
N	0.98770589	3.62108090	2.10181812
C	0.69092517	4.98348465	2.59606584
C	0.27541230	5.93324427	1.48419112
O	1.25819548	5.91449891	0.42217851
C	0.80968572	6.54549128	-0.79158488
C	1.74760676	6.18072529	-1.92638498
O	1.90773138	4.75408763	-1.90032268
C	2.51179017	4.10032134	-3.03005928
C	2.38665688	2.60833077	-2.79797541
O	2.94490038	2.28368322	-1.51461070
C	2.63456897	0.94180821	-1.06087775
C	3.27356911	0.71847043	0.29438565
O	2.95670125	1.81436399	1.18248974
C	2.28279303	1.50553699	2.41731627
C	1.79558481	2.80821482	3.04119001
H	1.59449606	5.36282859	3.08636092
H	-0.10580066	4.98609214	3.35103694
H	0.19072759	6.94719191	1.88611793
H	-0.69294829	5.64077475	1.06633858
H	-0.20336958	6.19408965	-1.01599117
H	0.78498423	7.63270796	-0.66779279
H	1.30187302	6.50206386	-2.87259587
H	2.72522295	6.66854405	-1.82385478
H	1.98493834	4.36812135	-3.95083914
H	3.55989710	4.40936499	-3.12323891
H	1.33260870	2.30918445	-2.81615377
H	2.92025299	2.07038796	-3.58799871
H	1.54808900	0.81589340	-0.99703221
H	3.03684658	0.21073941	-1.76906419
H	2.88699902	-0.22067856	0.69688507
H	4.36269164	0.65977791	0.22600084
H	2.98058203	1.02125106	3.10716295
H	1.45500872	0.82510930	2.20367838
H	1.26469918	2.56483011	3.96926930
H	2.65764808	3.41575669	3.34509579
C	-1.91923916	1.14756078	0.30016331
C	-1.36144947	2.19602648	-0.41652465
C	-0.45064005	3.04337245	0.19631274
C	-0.14173024	2.89391552	1.54901458
C	-0.84327527	1.95514125	2.29832152
C	-1.70574526	1.07086195	1.67114049
O	-3.74600196	0.43734050	-1.00394457
N	-1.35495031	-7.57917619	-0.59542453
C	0.30640276	-7.91294296	1.25548717
C	0.02800711	-7.89354428	-0.24145172
C	-3.08729834	-9.16545117	0.29440340
C	-2.24690236	-8.70345119	-0.88733240
C	-1.79940524	-6.30473498	-0.60560581
C	-3.16219611	-6.00222241	-0.92009202
C	-3.60686903	-4.71587226	-0.96737174
C	-2.74573220	-3.62711170	-0.69970173
C	-0.93449350	-5.22035497	-0.32029760
C	-1.40723462	-3.93453072	-0.37898057
C	-3.12620574	-2.28756256	-0.70256604

C	-2.23716773	-1.27684427	-0.38998814
C	-0.85356309	-1.59787759	-0.13173912
C	-2.72418818	0.10885912	-0.42324226
O	0.07170652	-0.81676636	0.04814449
O	-0.51976175	-2.93189108	-0.11473449
H	-1.60198931	2.31054882	-1.46800815
H	-0.27710054	-8.68672459	1.75738698
H	1.36390492	-8.12536440	1.43135898
H	0.06897955	-6.95566177	1.72488515
H	0.25016565	-8.87177493	-0.67069758
H	0.69060358	-7.18735697	-0.75016593
H	-3.73992118	-9.98499169	-0.01620483
H	-2.46146105	-9.52951441	1.11128700
H	-3.71612591	-8.36170404	0.68393832
H	-2.88225752	-8.43895687	-1.73596840
H	-1.61521336	-9.52240732	-1.23566862
H	-4.64483888	-4.51336106	-1.20959391
H	0.10133648	-5.37058032	-0.05455663
H	-4.14777580	-2.00712651	-0.94510368
H	-0.00307738	3.82885101	-0.40780041
H	-0.67646185	1.85848038	3.36524703
H	-2.18431931	0.28859637	2.25053809
H	-3.86152994	-6.80075977	-1.11928191

Complex Ca-chemosensor PBE0 A2

78

PBE0/TZVP CRENBL ECP (Ca) optimization E=-1836.84404666 a.u.

Ca	1.73233615	1.24153882	0.86977224
N	3.98458766	0.68533475	2.62007540
C	4.16024159	1.78040776	3.57229881
C	2.97069283	2.71837733	3.77375572
O	2.30439996	2.98992682	2.53426742
C	1.23536652	3.93914470	2.69335583
C	0.86408008	4.49222881	1.34336936
O	0.56592686	3.40902595	0.45996969
C	0.37252122	3.82872362	-0.89866498
C	0.70810594	2.67143208	-1.81405940
O	1.97608350	2.18732129	-1.36328646
C	2.76854734	1.38763579	-2.23750187
C	4.13920154	1.33090051	-1.60668063
O	4.01286981	0.88124743	-0.24923240
C	5.22448270	1.09032499	0.49418376
C	5.16711350	0.35580265	1.81974879
H	4.99022323	2.37572948	3.18833758
H	4.46765376	1.42052838	4.56423729
H	3.36094901	3.65601618	4.18424667
H	2.23932655	2.32764556	4.48524062
H	0.38175664	3.45013031	3.17935455
H	1.56255891	4.76788553	3.32937130
H	-0.00392648	5.15208450	1.45161858
H	1.69847193	5.07199201	0.93183254
H	-0.66029930	4.15755279	-1.05022472
H	1.04718900	4.66548297	-1.10723568
H	-0.03964678	1.87102199	-1.75735737
H	0.77072082	3.03047403	-2.84592142
H	2.32699192	0.38912233	-2.35206786
H	2.84617170	1.84870131	-3.22750885

H	4.78769633	0.65016441	-2.16828973
H	4.58563170	2.33176327	-1.61269872
H	5.36091135	2.16936614	0.64409125
H	6.07878049	0.71733475	-0.08135378
H	5.21005442	-0.72135483	1.66193682
H	6.07210085	0.60816291	2.38173340
C	0.54773880	-1.65994297	2.66719201
C	0.87654309	-0.91444842	3.79317977
C	2.08515036	-0.23370637	3.86401051
C	2.99480475	-0.28698316	2.79724947
C	2.75639171	-1.24421252	1.78661361
C	1.53961035	-1.89991700	1.72204821
O	-1.49517938	-2.61040436	3.36704951
N	-5.19805399	-1.85865978	-4.03866851
C	-3.56662764	-1.28331034	-5.85538284
C	-4.73180289	-0.84121683	-4.98081381
C	-6.02661229	-3.99410780	-5.07167019
C	-6.36559279	-2.65487105	-4.43417119
C	-4.55585254	-2.07796956	-2.87652647
C	-5.00076405	-3.09617432	-1.97088351
C	-4.38666014	-3.29863872	-0.77495009
C	-3.27279622	-2.51866915	-0.37891039
C	-3.42862264	-1.30506313	-2.49561746
C	-2.83302229	-1.53012242	-1.28365886
C	-2.58192717	-2.66127313	0.81477477
C	-1.47269229	-1.88421736	1.12738556
C	-1.07799179	-0.86405543	0.21814006
C	-0.85593470	-2.10533170	2.46292695
O	-0.17204489	-0.01442326	0.35591721
O	-1.76377361	-0.74206090	-0.94937315
H	0.15500278	-0.82684331	4.59891032
H	-3.84444416	-2.12715007	-6.48894781
H	-3.26523657	-0.46159799	-6.50967002
H	-2.70075115	-1.58258600	-5.26020931
H	-5.58431772	-0.57636251	-5.60760766
H	-4.48030491	0.06523203	-4.42260569
H	-6.94895743	-4.52743477	-5.31334338
H	-5.46482289	-3.86530947	-5.99859967
H	-5.43681634	-4.62620697	-4.40404580
H	-7.01184536	-2.78834429	-3.56368501
H	-6.93660064	-2.04360965	-5.13457768
H	-4.74688994	-4.07270671	-0.10598182
H	-3.02529589	-0.53462098	-3.13550513
H	-2.89855551	-3.39715836	1.54872971
H	2.30782650	0.34816912	4.74733245
H	3.48144068	-1.41982161	1.00192219
H	1.34630500	-2.56995057	0.89045546
H	-5.83864479	-3.72375633	-2.23630616

Complex Ca-chemosensor PBE0 A3

78

PBE0/TZVP CRENL ECP (Ca) optimization E=-1836.79690566 a.u.

Ca	3.51156445	3.04099543	0.97439427
N	3.60824324	1.23397515	2.69637772
C	2.94662848	1.95575271	3.81036540
C	1.51604638	2.34582556	3.46442269
O	1.49226321	3.09258628	2.23062033

C	0.26074018	2.95205319	1.48277410
C	0.40961325	3.66293592	0.15596526
O	1.62902399	3.19453067	-0.44964701
C	1.87615640	3.51523322	-1.82241107
C	2.99990313	2.61618339	-2.29386123
O	4.09198247	2.69645589	-1.35750783
C	5.13074564	1.72654205	-1.59236776
C	6.18703497	1.88141598	-0.51637717
O	5.59018464	1.89136814	0.79346589
C	5.77962008	0.72278819	1.62350154
C	5.04044316	0.94849513	2.93019338
H	3.54323903	2.85064306	4.03741650
H	2.91749165	1.37639177	4.74131167
H	1.09935368	2.95805463	4.26944927
H	0.89739363	1.45300806	3.34455517
H	0.05202903	1.88874510	1.32229462
H	-0.56637262	3.40266308	2.03980963
H	-0.44724538	3.40458338	-0.47289745
H	0.45507483	4.75241736	0.27061334
H	0.98724546	3.31876032	-2.42957682
H	2.13609275	4.57631966	-1.92018146
H	2.65484032	1.57739469	-2.34485201
H	3.33510535	2.92872972	-3.28761723
H	4.68963708	0.72243646	-1.57647209
H	5.58521894	1.89266486	-2.57463137
H	6.91835404	1.07399336	-0.60160066
H	6.71864614	2.83002962	-0.62790429
H	6.84641914	0.58845081	1.82272862
H	5.39755223	-0.16100982	1.10227573
H	5.18800951	0.07039574	3.57048471
H	5.48136414	1.80529653	3.45164456
C	1.00664609	-1.86265292	1.47007761
C	1.46795314	-1.83390994	2.78255233
C	2.36967391	-0.86153043	3.19122471
C	2.83969113	0.07337108	2.27553972
C	2.48129541	-0.04746290	0.93634981
C	1.56248890	-1.00144784	0.53411292
O	0.08243850	-4.00581615	1.49809881
N	-6.87284284	-2.15224357	-2.63673703
C	-6.62538751	-0.10591925	-4.06649572
C	-7.25109562	-0.75545461	-2.83955783
C	-7.48092273	-3.73528705	-4.48952867
C	-7.80406719	-3.17806493	-3.11060268
C	-5.69451920	-2.47896974	-2.06354684
C	-5.31830618	-3.84775364	-1.88393055
C	-4.15551383	-4.18336560	-1.25917181
C	-3.26757183	-3.19583492	-0.77486752
C	-4.79717690	-1.48434230	-1.60521031
C	-3.63374310	-1.85039114	-0.97739448
C	-2.07310677	-3.45289238	-0.10830307
C	-1.24320011	-2.44098821	0.33988981
C	-1.63335199	-1.06453369	0.13357600
C	-0.05878756	-2.85505403	1.11128860
O	-1.04623047	-0.05345505	0.48786389
O	-2.81752491	-0.85066021	-0.54040185
H	1.08182610	-2.55819242	3.49116382
H	-6.94648149	-0.60099648	-4.98475934

H	-6.93187845	0.94142612	-4.12680226
H	-5.53415683	-0.14070582	-4.02993573
H	-8.33875771	-0.72993566	-2.92296837
H	-7.00828822	-0.19039578	-1.93500840
H	-8.20597651	-4.50918992	-4.75304277
H	-7.52951392	-2.95858215	-5.25509820
H	-6.48405090	-4.18058083	-4.52344369
H	-7.85343609	-3.97978031	-2.36974698
H	-8.79554103	-2.72207568	-3.11852151
H	-3.89766821	-5.22866164	-1.12542789
H	-5.00199324	-0.43083941	-1.72470782
H	-1.76641084	-4.47607565	0.09055770
H	2.66969895	-0.81926948	4.23333009
H	2.88956955	0.61691146	0.17834014
H	1.24672864	-1.04898971	-0.50086337
H	-5.96054905	-4.63744035	-2.24499288

Complex Hg-chemosensor B1

78

PBE/TZVP CRENL ECP (Hg) E=-1953.55371672 a.u.

Hg	3.12725794	2.29232284	0.50533275
N	2.43344638	0.88490584	2.39027213
C	1.79107695	1.83761308	3.36191849
C	0.86390825	2.85588271	2.70746895
O	1.69615457	3.79268222	1.98774483
C	1.01343508	4.67085058	1.06168838
C	2.07114283	5.49404065	0.35176242
O	2.93202511	4.62896852	-0.44019250
C	4.22672482	5.21972340	-0.73059027
C	5.19459723	4.14628096	-1.18666611
O	5.37715090	3.20970043	-0.09301589
C	6.31119862	2.13209686	-0.36413871
C	6.21745518	1.12110704	0.76214214
O	4.92184402	0.47043241	0.68278827
C	4.56297784	-0.35863153	1.81256180
C	3.75407663	0.38087329	2.88365095
H	2.59323339	2.37946313	3.88489298
H	1.22494851	1.26198704	4.11193852
H	0.30818590	3.39019205	3.49628580
H	0.13651861	2.37339285	2.03035931
H	0.40709142	4.08336784	0.34885815
H	0.34510092	5.35418707	1.61329520
H	1.58456439	6.22594868	-0.31468612
H	2.68057706	6.03417850	1.09595598
H	4.11349884	5.97050273	-1.53123262
H	4.61573906	5.71628523	0.17481593
H	4.82533751	3.61718935	-2.08276210
H	6.15982891	4.62324061	-1.42783831
H	6.07714098	1.65737904	-1.33271338
H	7.33380581	2.54418586	-0.40243656
H	7.00858191	0.36289660	0.63509515
H	6.35181047	1.62002105	1.73765155
H	5.47052318	-0.77337329	2.27932667
H	3.98063043	-1.19302138	1.39482381
H	3.60978875	-0.30667424	3.73504104
H	4.31577631	1.24924978	3.26147749
C	-0.34696123	-2.15954303	1.24135018

C	0.29805170	-2.21271505	2.48769972
C	1.20490509	-1.22568177	2.86858688
C	1.51218138	-0.18313383	1.97961922
C	0.89799479	-0.14652847	0.72434755
C	-0.03654161	-1.11650062	0.35708633
O	-0.90437527	-4.44291074	1.26240290
N	-8.09494124	-4.03472427	-2.93419956
C	-8.49402254	-1.86003695	-4.16010487
C	-8.85231988	-2.76830500	-2.97764823
C	-8.18764814	-5.50656030	-4.98921518
C	-8.71541162	-5.21092319	-3.58066481
C	-6.85878954	-4.10300797	-2.35955895
C	-6.14860690	-5.35382019	-2.28575116
C	-4.92350417	-5.43365955	-1.67029969
C	-4.30875538	-4.28846750	-1.09345019
C	-6.24028769	-2.94566107	-1.80366694
C	-5.00498932	-3.05118775	-1.19009578
C	-3.06992217	-4.30408868	-0.42355190
C	-2.50745693	-3.15296912	0.10602004
C	-3.21711141	-1.87978614	0.00318248
C	-1.24374375	-3.31512509	0.88311724
O	-2.87261625	-0.79373002	0.43868324
O	-4.46548502	-1.90685826	-0.66885451
H	0.07561096	-3.04217964	3.16108200
H	-8.72843278	-2.33659521	-5.12146790
H	-9.08203928	-0.93317827	-4.09301392
H	-7.42825687	-1.59109623	-4.15970383
H	-9.91595248	-3.03974704	-3.02136229
H	-8.70709822	-2.24381748	-2.02211602
H	-8.69332472	-6.40033742	-5.38263804
H	-8.38886275	-4.67514148	-5.67790621
H	-7.10556434	-5.69888198	-4.98963829
H	-8.58716338	-6.08318121	-2.92248369
H	-9.79451465	-5.01174554	-3.61817055
H	-4.40703049	-6.39395349	-1.61087584
H	-6.70560474	-1.96358893	-1.84553560
H	-2.52524557	-5.24399790	-0.29566963
H	1.65788468	-1.27400409	3.86122722
H	1.14674951	0.65815338	0.02026005
H	-0.50983691	-1.05864991	-0.62247115
H	-6.58271221	-6.25652828	-2.70925232

Complex Hg-chemosensor B2

78

PBE/TZVP CRENL ECP (Hg) E=-1953.55051248 a.u.

Hg	1.89611715	4.20441803	0.22984328
N	0.89110509	2.54546606	1.66794372
C	-0.02275387	3.40515785	2.49038380
C	-1.01874264	4.19696453	1.64119733
O	-0.31953584	5.17299308	0.82506269
C	-1.02612759	5.59113543	-0.37560200
C	-0.04772971	6.20931564	-1.35997325
O	0.86863305	5.17215540	-1.80892002
C	1.94727417	5.61297357	-2.67716626
C	2.90657372	4.45008504	-2.86602890
O	3.56288274	4.15610329	-1.60110306
C	4.16947713	2.83765535	-1.52264310

C	4.78194527	2.66183616	-0.13674535
O	3.82992201	2.81973513	0.95058155
C	3.23120901	1.61345234	1.49647281
C	2.08253483	2.02664430	2.41740379
H	0.60084824	4.09453697	3.08027948
H	-0.60083213	2.78643248	3.19784229
H	-1.70978975	4.72760269	2.31646589
H	-1.60353312	3.52022864	0.99543855
H	-1.52824029	4.72172569	-0.83376574
H	-1.78620512	6.34274819	-0.10426848
H	-0.61239877	6.59521724	-2.22534120
H	0.51454462	7.04082356	-0.90055612
H	1.53204174	5.89906274	-3.65804091
H	2.46118985	6.48505073	-2.23698828
H	2.36262903	3.55882327	-3.22460128
H	3.67289146	4.72474204	-3.60962205
H	3.41097213	2.06419298	-1.74410110
H	4.97746686	2.76135618	-2.27044591
H	5.26580699	1.67419937	-0.07645969
H	5.54301393	3.43622298	0.03732092
H	3.99216714	1.08597861	2.09424495
H	2.87933845	0.94326725	0.69340137
H	1.79678264	1.15738165	3.03149969
H	2.43162019	2.81911275	3.09681111
C	-1.17159617	-0.59381764	-0.38202973
C	-0.61983473	0.47456971	-1.10138829
C	0.06485898	1.49381243	-0.43649779
C	0.17257714	1.47654007	0.95807921
C	-0.42172938	0.43548192	1.68807532
C	-1.07388861	-0.59950596	1.01717688
O	-2.63155565	-1.24356643	-2.11449826
N	-2.99496578	-9.34770806	0.01450233
C	-2.04692718	-9.75014541	2.32393079
C	-1.90238619	-9.94315802	0.80962491
C	-5.29272225	-10.28198358	0.51107378
C	-4.07791855	-10.25232391	-0.42338609
C	-3.01966535	-8.01176397	-0.26554983
C	-4.10973549	-7.43128215	-1.00539867
C	-4.11976699	-6.09270926	-1.31352833
C	-3.06141680	-5.23153326	-0.91345519
C	-1.96262878	-7.15330667	0.15441696
C	-1.99245364	-5.80965325	-0.17291070
C	-3.00707062	-3.85240020	-1.19497230
C	-1.96064760	-3.05882830	-0.75104872
C	-0.83465873	-3.65961577	-0.04121343
C	-1.95922466	-1.62573059	-1.14823929
O	0.19523426	-3.11157099	0.31752912
O	-0.93613614	-5.04272485	0.24328301
H	-0.73819697	0.49658787	-2.18616788
H	-2.95247929	-10.23889956	2.70760416
H	-1.18071230	-10.20142785	2.82933224
H	-2.08752128	-8.68701168	2.59963312
H	-1.88586087	-11.01426358	0.56807705
H	-0.94599824	-9.53221881	0.45213826
H	-6.05145092	-10.96067514	0.09497974
H	-5.02555368	-10.65064993	1.51060666
H	-5.74755313	-9.28743677	0.62177351

H	-4.37551598	-9.97489247	-1.44477051
H	-3.63567611	-11.25527790	-0.49596765
H	-4.95452484	-5.67248778	-1.87845550
H	-1.11341124	-7.51876905	0.72711549
H	-3.80218660	-3.37832819	-1.77776084
H	0.49566777	2.31960472	-1.01305246
H	-0.36927959	0.41284457	2.77897472
H	-1.51484023	-1.41225531	1.59589472
H	-4.94488981	-8.04899289	-1.32748468

Complex Hg-chemosensor B3

78

PBE/TZVP CRENBL ECP (Hg) E=-1953.54944690 a.u.

Hg	3.19698887	2.07655230	0.62041917
N	2.68968101	0.48950126	2.31350196
C	2.10200559	1.35753784	3.39782527
C	1.01677579	2.30927098	2.89728286
O	1.63934579	3.33101406	2.07283298
C	0.74309315	4.07252802	1.20130979
C	1.57328205	4.83284472	0.18089496
O	2.23113823	3.88234854	-0.70946087
C	3.24826241	4.45700374	-1.57853283
C	4.05321924	3.33079720	-2.20490427
O	4.79648929	2.65892052	-1.15065144
C	5.38482283	1.37804863	-1.51495380
C	6.13682641	0.83769066	-0.29978976
O	5.32433526	0.84815174	0.90494497
C	4.91201961	-0.41693130	1.48411086
C	4.02711365	-0.09203166	2.68712145
H	2.92111144	1.94239106	3.84295372
H	1.67099109	0.72107989	4.18754992
H	0.54296313	2.79186844	3.76752258
H	0.24190166	1.77268453	2.32270917
H	0.04003604	3.38208015	0.70364390
H	0.16691243	4.79648822	1.80145202
H	0.90868867	5.47828254	-0.41681323
H	2.33034628	5.45987557	0.68218806
H	2.75382244	5.03734795	-2.37499012
H	3.90482016	5.12684152	-0.99736336
H	3.39266328	2.61358948	-2.72281874
H	4.76389644	3.75496495	-2.93327133
H	4.59108700	0.68869287	-1.85645312
H	6.10513950	1.52311029	-2.33775306
H	6.49809480	-0.17884576	-0.52012103
H	7.00203791	1.47968473	-0.07735046
H	5.80289132	-0.95820135	1.84183198
H	4.38366757	-1.04314095	0.74396493
H	3.88094546	-1.00985716	3.27740980
H	4.55015514	0.63891630	3.32092055
C	-0.18865579	-2.40548334	1.02136037
C	0.41858501	-2.51093001	2.28258380
C	1.35694126	-1.57191026	2.70781219
C	1.73385804	-0.52974528	1.84719755
C	1.16679581	-0.44978806	0.57200528
C	0.20068449	-1.37030916	0.16098885
O	-0.80488867	-4.66389679	0.89849964
N	-8.26933268	-3.65323983	-2.71280971

C	-8.43636619	-1.48415519	-4.00062821
C	-8.88311047	-2.31319174	-2.79091018
C	-8.77496787	-5.16901405	-4.67488645
C	-9.06671698	-4.78944002	-3.21893399
C	-7.00548077	-3.82529510	-2.22699078
C	-6.39876277	-5.13034873	-2.19237713
C	-5.14404377	-5.31282287	-1.66507314
C	-4.39489912	-4.22356901	-1.14019675
C	-6.25230214	-2.72386765	-1.72660729
C	-4.99184841	-2.93340449	-1.19756923
C	-3.12072663	-4.33978108	-0.55929597
C	-2.43087856	-3.23849861	-0.06630245
C	-3.03848630	-1.91345096	-0.12846153
C	-1.14103072	-3.50511100	0.61808651
O	-2.57984370	-0.85449197	0.27536586
O	-4.32383005	-1.83706719	-0.71783421
H	0.14080686	-3.34083791	2.93460414
H	-8.72539303	-1.96367654	-4.94558369
H	-8.91958852	-0.49693641	-3.96229207
H	-7.34788032	-1.33194130	-4.01276958
H	-9.97019528	-2.46618997	-2.82263891
H	-8.67620334	-1.77806814	-1.85147418
H	-9.39537536	-6.03263919	-4.95556352
H	-9.01420823	-4.34689250	-5.36301942
H	-7.72076255	-5.44381465	-4.82187062
H	-8.91404119	-5.65006361	-2.55177388
H	-10.12178621	-4.50317875	-3.10983440
H	-4.70540699	-6.31259841	-1.64069966
H	-6.63865965	-1.70734288	-1.73549245
H	-2.64368714	-5.32002365	-0.46847682
H	1.78256025	-1.65964665	3.71024259
H	1.46289606	0.35766801	-0.11177137
H	-0.24709804	-1.27463878	-0.82764327
H	-6.93140061	-5.99222694	-2.58763745

Complex Hg-chemosensor PBE0 B1

78

PBE0/TZVP CRENBL ECP (Hg) optimization E=-1953.59747493 a.u.

Hg	3.00549013	2.22633344	0.82466156
N	2.55648432	0.84946510	2.54027557
C	1.82994914	1.70047774	3.53356618
C	0.65609374	2.43143930	2.91244675
O	1.18529077	3.37222846	1.97052854
C	0.29236426	3.82924825	0.94989811
C	1.10026960	4.68275912	0.00455341
O	2.17079397	3.89628694	-0.56850779
C	3.20087505	4.68749607	-1.18796388
C	4.34201832	3.78305145	-1.57662904
O	4.79673388	3.10666860	-0.39245691
C	5.89389870	2.19384956	-0.60509637
C	6.07036129	1.34416105	0.62918001
O	4.85596970	0.60781798	0.80294038
C	4.73638171	-0.22957132	1.95877204
C	3.89040424	0.41694045	3.04727175
H	2.53997185	2.42412996	3.94377001
H	1.47035704	1.07699080	4.35575442
H	0.11217114	2.96746862	3.69553862

H	-0.02920936	1.73554278	2.41568118
H	-0.16711705	2.97544226	0.43671136
H	-0.50226036	4.44389929	1.38530484
H	0.46323020	5.05069553	-0.80466928
H	1.53560293	5.53192703	0.54107030
H	2.79860280	5.17158638	-2.08301598
H	3.53801846	5.45539732	-0.48341171
H	4.03230179	3.04479104	-2.32487868
H	5.15499122	4.38929194	-1.98764846
H	5.67539465	1.56155876	-1.47198160
H	6.80239038	2.77283983	-0.79481302
H	6.90702134	0.65672275	0.46848663
H	6.28535487	1.96463286	1.50754193
H	5.72294240	-0.46625600	2.36541176
H	4.27449975	-1.15704652	1.61441383
H	3.76435210	-0.30381149	3.86147796
H	4.38866512	1.29972741	3.45966714
C	-0.04641251	-2.26729577	1.30027711
C	0.40926398	-2.21180147	2.61363845
C	1.27384799	-1.20815835	3.02424264
C	1.72109399	-0.27355752	2.09750778
C	1.33490640	-0.37856404	0.76847959
C	0.44355014	-1.35981348	0.36896660
O	-0.69837027	-4.49888439	1.33315421
N	-7.74765284	-3.46685038	-2.96510037
C	-7.66929609	-1.42755211	-4.42424418
C	-8.26067112	-2.11929499	-3.20344907
C	-8.12912394	-5.13366646	-4.80472517
C	-8.55298992	-4.58974937	-3.44769310
C	-6.55862878	-3.66208217	-2.35466788
C	-6.04915258	-4.98184428	-2.14076717
C	-4.87373204	-5.18493487	-1.48310035
C	-4.10434844	-4.10368029	-0.99614773
C	-5.78210441	-2.57338437	-1.89131626
C	-4.60300314	-2.80534301	-1.22976737
C	-2.90360545	-4.22705132	-0.30271285
C	-2.19582715	-3.12494640	0.14071586
C	-2.72242538	-1.79685479	-0.09405423
C	-0.98995446	-3.38013573	0.93114185
O	-2.24354905	-0.73596918	0.25880444
O	-3.91019332	-1.71850100	-0.79347282
H	0.06281575	-2.95609023	3.32158724
H	-7.91055489	-1.96742023	-5.34171414
H	-8.07999997	-0.41858067	-4.51193101
H	-6.58205543	-1.34749287	-4.35662596
H	-9.34237492	-2.20744246	-3.31688286
H	-8.10311824	-1.51837394	-2.30330907
H	-8.76122164	-5.98310755	-5.07501004
H	-8.23220015	-4.37908637	-5.58684095
H	-7.09093871	-5.47316617	-4.79862834
H	-8.54496870	-5.38038841	-2.69332952
H	-9.58492792	-4.23798662	-3.49604544
H	-4.51251706	-6.19570257	-1.32514687
H	-6.08977952	-1.54829973	-2.03493417
H	-2.49585960	-5.20990653	-0.08330250
H	1.57712643	-1.16355254	4.06524620
H	1.71592099	0.31324383	0.01280651

H	0.11937111	-1.40602956	-0.66263505
H	-6.59729021	-5.83914909	-2.50265260

Complex Hg-chemosensor PBE0 B1

78

PBE0/TZVP CRENBL ECP (Hg) optimization E=-1953.59674113 a.u.

Hg	1.69072199	3.76989761	-0.02154692
N	0.67211323	2.52987071	1.56465084
C	-0.13071623	3.49535454	2.37656347
C	-0.95947023	4.43179495	1.52022965
O	-0.06464234	5.24319323	0.74740185
C	-0.65185867	5.93576454	-0.36112687
C	0.46172077	6.44551550	-1.24328970
O	1.22447647	5.31593299	-1.71264905
C	2.37132895	5.63782708	-2.51703120
C	3.11979372	4.35568788	-2.78933706
O	3.49401765	3.79429152	-1.52157638
C	4.06786895	2.47359943	-1.56588960
C	4.51398331	2.11620834	-0.16023740
O	3.47862290	2.39600758	0.79072387
C	2.86377936	1.31045561	1.49821413
C	1.77945659	1.91878823	2.36502892
H	0.56240676	4.07858629	2.98825939
H	-0.79674961	2.94585207	3.04767719
H	-1.56020342	5.07194488	2.17300323
H	-1.62963891	3.87418445	0.85619209
H	-1.30797636	5.25752504	-0.91871648
H	-1.24237922	6.78409323	-0.00086417
H	0.03328609	6.97019473	-2.10237269
H	1.11985094	7.12828609	-0.69490873
H	2.04095668	6.07790740	-3.46262389
H	3.00518708	6.35590098	-1.98540832
H	2.49598482	3.64478406	-3.34314913
H	4.01954868	4.57342158	-3.37230962
H	3.32419914	1.76773390	-1.95582317
H	4.93708738	2.47470901	-2.23042428
H	4.80072870	1.06198930	-0.12636730
H	5.37339384	2.72392932	0.13123198
H	3.60334970	0.83161870	2.14618185
H	2.45877796	0.56597929	0.80362924
H	1.37724746	1.14935577	3.02740177
H	2.21821233	2.70443037	2.98497439
C	-1.66746972	-0.51002897	-0.27230991
C	-1.10829122	0.49814391	-1.04567462
C	-0.34342332	1.48818512	-0.44607098
C	-0.16761836	1.50590234	0.92989235
C	-0.78974504	0.53956289	1.71571584
C	-1.51807779	-0.47047852	1.11128956
O	-3.31694452	-1.13682270	-1.79303262
N	-2.74354201	-9.28500453	-0.00773438
C	-1.62003243	-9.64991568	2.20645621
C	-1.55787435	-9.77897516	0.69056511
C	-4.91364667	-10.39728089	0.59182133
C	-3.75783572	-10.26827844	-0.39035262
C	-2.91309101	-7.96635676	-0.24559009
C	-4.08394555	-7.48153499	-0.90985661
C	-4.23929058	-6.15658106	-1.18597659

C	-3.25937007	-5.20557334	-0.82043010
C	-1.93541567	-7.01850143	0.13926721
C	-2.11454512	-5.69045487	-0.15250383
C	-3.34818217	-3.83574381	-1.05721381
C	-2.36149057	-2.96201420	-0.64200752
C	-1.16954314	-3.47500756	-0.00009541
C	-2.50966646	-1.54691044	-0.96842699
O	-0.19274356	-2.83939600	0.34302687
O	-1.12897537	-4.83407393	0.23149140
H	-1.27206892	0.49378347	-2.11705951
H	-2.43662188	-10.24299841	2.62207357
H	-0.68690920	-10.01094921	2.64596205
H	-1.76354325	-8.61329033	2.51907220
H	-1.44128506	-10.82797349	0.41332668
H	-0.67733836	-9.26592206	0.29392356
H	-5.63309833	-11.13104033	0.22016083
H	-4.56834053	-10.73454881	1.57090372
H	-5.43765938	-9.44855367	0.72766641
H	-4.12450419	-10.02730775	-1.39128544
H	-3.24496641	-11.22680199	-0.48602314
H	-5.13427454	-5.81448561	-1.69497632
H	-1.03499530	-7.30401945	0.66245037
H	-4.20829206	-3.42362054	-1.57765585
H	0.09569825	2.26037787	-1.08304598
H	-0.69616427	0.54578362	2.79656510
H	-1.96761283	-1.24069512	1.72626647
H	-4.86568912	-8.16817417	-1.19953934

Complex Hg-chemosensor PBE0 B3

78

PBE0/TZVP CRENBL ECP (Hg) optimization E=-1953.59662717 a.u.

Hg	3.08410974	2.18968816	0.74148804
N	2.77757381	0.68680327	2.39352853
C	2.10490292	1.47895993	3.47272155
C	0.88240427	2.22075651	2.97013933
O	1.31281804	3.20150586	2.01387206
C	0.29781313	3.69101034	1.12582591
C	0.97619927	4.47405815	0.02848919
O	1.86793391	3.59019345	-0.68132692
C	2.68030278	4.21295842	-1.68880305
C	3.63432889	3.17188122	-2.22199327
O	4.41888783	2.69238076	-1.11789518
C	5.26891173	1.56459504	-1.39965472
C	6.09984229	1.28977535	-0.16072704
O	5.28268713	1.22987118	1.01537502
C	5.05457779	-0.04149528	1.63780350
C	4.13019622	0.20942332	2.81294097
H	2.83303845	2.19154810	3.86976917
H	1.80416717	0.81496116	4.28733396
H	0.40161833	2.72561927	3.81297052
H	0.16351918	1.53537907	2.50778568
H	-0.27439076	2.85136096	0.71442411
H	-0.38357124	4.35343143	1.66887924
H	0.22253443	4.85461386	-0.66713361
H	1.54772279	5.31365315	0.43886010
H	2.04240633	4.57433999	-2.50101084
H	3.22532981	5.05813377	-1.25416120

H	3.09093180	2.33865957	-2.68203244
H	4.29399761	3.62590204	-2.96732255
H	4.64938759	0.70518370	-1.68470667
H	5.93614313	1.80907261	-2.23184604
H	6.66024850	0.36071746	-0.29433187
H	6.80855334	2.10384634	0.00511971
H	6.00175747	-0.43947578	2.01312864
H	4.62249621	-0.75646490	0.92773148
H	4.02890724	-0.70884881	3.39639411
H	4.57513727	0.97416086	3.45394889
C	0.07831882	-2.32864259	1.10370095
C	0.61030627	-2.36168843	2.38900019
C	1.50882144	-1.39361375	2.81107915
C	1.91425243	-0.40337793	1.92299350
C	1.45019588	-0.42174827	0.61474184
C	0.52681693	-1.36920376	0.20521576
O	-0.60733087	-4.54899761	1.01452472
N	-7.96350613	-3.10425257	-2.59108992
C	-7.95586856	-0.97744477	-3.92121322
C	-8.46179428	-1.73468926	-2.70091614
C	-8.54796700	-4.63920703	-4.49119610
C	-8.83518345	-4.17868549	-3.06912721
C	-6.73204481	-3.36042224	-2.09928987
C	-6.23683339	-4.70031106	-2.01622815
C	-5.01521256	-4.96737155	-1.47638868
C	-4.18270645	-3.93455053	-0.98783147
C	-5.89389976	-2.31868124	-1.63471615
C	-4.66895631	-2.61498254	-1.09332659
C	-2.93264752	-4.12508581	-0.40640682
C	-2.16550031	-3.06800246	0.04872210
C	-2.67705352	-1.71788680	-0.05795535
C	-0.90761018	-3.39915146	0.72177813
O	-2.14500671	-0.68995313	0.31713806
O	-3.91629235	-1.57215468	-0.64839967
H	0.29585164	-3.14612187	3.06804978
H	-8.28465040	-1.45253427	-4.84730983
H	-8.34765508	0.04274078	-3.91109553
H	-6.86507717	-0.92290271	-3.93964088
H	-9.55093677	-1.79494367	-2.72910074
H	-8.21645468	-1.19602768	-1.78118216
H	-9.22215932	-5.45717300	-4.75674621
H	-8.70256108	-3.83282435	-5.21062861
H	-7.52190762	-4.99736040	-4.60137792
H	-8.77753516	-5.01726483	-2.37088561
H	-9.85880939	-3.80655353	-3.00004614
H	-4.66546165	-5.99257669	-1.41595981
H	-6.18940359	-1.28119960	-1.68351048
H	-2.53142330	-5.12745971	-0.28537062
H	1.87147965	-1.41859433	3.83360298
H	1.77576093	0.32698179	-0.11148544
H	0.13991943	-1.34404504	-0.80534686
H	-6.83300141	-5.52186665	-2.38509705

Complex Pb-chemosensor C1

78

PBE/TZVP ECP CRENBL (Pb) E=-1861.56370556 a.u.

Pb	3.07982315	2.85408549	0.96076270
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N	2.85935663	0.75702289	2.51446635
C	2.08627101	1.41729991	3.61947276
C	0.66870973	1.78229665	3.18407097
O	0.71886713	2.62605039	1.99665765
C	-0.42533780	2.46093252	1.09802413
C	-0.10183118	3.13095665	-0.22290845
O	1.14124899	2.54546256	-0.71408486
C	1.53858785	2.86949357	-2.07142019
C	2.65896946	1.91442871	-2.44221797
O	3.72611969	2.03130333	-1.45734461
C	4.70817806	0.95731336	-1.53541311
C	5.76318963	1.19606215	-0.46858037
O	5.17699336	1.33538030	0.85696791
C	5.12424222	0.13101952	1.67946481
C	4.26980753	0.43800612	2.90044200
H	2.64376914	2.31604395	3.94298785
H	2.01141666	0.76672334	4.50797218
H	0.16595551	2.33107932	3.99655089
H	0.09068554	0.87440347	2.95403422
H	-0.63187411	1.38783196	0.94945091
H	-1.31125901	2.94462509	1.54153720
H	-0.91494609	2.91693599	-0.93515007
H	0.01283241	4.22504741	-0.12542112
H	0.69104309	2.71090304	-2.75814035
H	1.85441694	3.92585476	-2.14120489
H	2.28765164	0.87546627	-2.45220258
H	3.05174873	2.16658367	-3.44110405
H	4.19618018	-0.01187570	-1.40067674
H	5.18987389	0.97064280	-2.52787561
H	6.49665081	0.37504427	-0.47622203
H	6.30118875	2.13716787	-0.65630791
H	6.14711379	-0.12621307	1.99774616
H	4.70012650	-0.70650168	1.10160719
H	4.30512067	-0.42766364	3.58402539
H	4.69026195	1.30120160	3.44409393
C	0.41194514	-2.40863353	1.04619823
C	0.88457772	-2.44842061	2.36611105
C	1.73015703	-1.44717585	2.84967756
C	2.13673768	-0.41479219	1.99256596
C	1.77410404	-0.45077279	0.64425420
C	0.90744585	-1.43523921	0.17176455
O	-0.32053444	-4.63355257	0.84969328
N	-7.70616453	-2.89390409	-2.69716485
C	-7.69470146	-0.71316123	-3.97725672
C	-8.18994711	-1.50264682	-2.76086360
C	-8.34877839	-4.36325946	-4.65626837
C	-8.60902664	-3.94688582	-3.20554606
C	-6.46403506	-3.18807049	-2.21846836
C	-5.98922159	-4.54652206	-2.17675645
C	-4.76087757	-4.85479864	-1.64843848
C	-3.89986462	-3.84616789	-1.13059760
C	-5.59747591	-2.16769865	-1.72716387
C	-4.36668992	-2.50407151	-1.19819271
C	-2.64732540	-4.08123400	-0.55683718
C	-1.84394791	-3.04917285	-0.06309272
C	-2.32000082	-1.67856046	-0.13136234
C	-0.58847855	-3.44800034	0.60565358

O	-1.76801345	-0.64953502	0.26823998
O	-3.58228110	-1.47637183	-0.72402388
H	0.55019125	-3.25217769	3.02482854
H	-8.04808112	-1.15992402	-4.91666755
H	-8.07859116	0.31668869	-3.92981806
H	-6.59677394	-0.66829300	-4.01458342
H	-9.28767353	-1.54906134	-2.76753495
H	-7.91425629	-0.99219399	-1.82486986
H	-9.04833562	-5.16323787	-4.94009383
H	-8.49956367	-3.52482153	-5.35017963
H	-7.32584513	-4.74133195	-4.79558013
H	-8.55115231	-4.81554270	-2.53293884
H	-9.63160707	-3.55712414	-3.10528187
H	-4.42790698	-5.89452151	-1.61874194
H	-5.87756088	-1.11701626	-1.74559059
H	-2.26471178	-5.10196472	-0.46449104
H	2.03433299	-1.46692161	3.89910523
H	2.10324619	0.33831487	-0.03520880
H	0.57722635	-1.41894399	-0.86757716
H	-6.60682230	-5.35213938	-2.56724943

Complex Pb-chemosensor C2

78

PBE/TZVP CRENL ECP (Pb) E=-1861.56398110 a.u.

Pb	2.56597191	3.40292223	0.32692350
N	0.61471608	2.88407888	1.98465358
C	0.23952991	4.24037002	2.49992219
C	-0.28677673	5.15756241	1.40309794
O	0.71700398	5.28743920	0.35385261
C	0.18711491	5.75727797	-0.91759207
C	1.14309819	5.36130258	-2.03145985
O	1.34613015	3.92540138	-1.91561719
C	1.99723709	3.23614684	-3.01747855
C	1.91898569	1.75113405	-2.70963706
O	2.56059686	1.49506688	-1.42867245
C	2.28245643	0.15720300	-0.89328067
C	3.07914863	-0.00950448	0.38611779
O	2.80447976	1.07038435	1.33389929
C	1.88292772	0.76515285	2.42357586
C	1.37327632	2.08080810	2.99956700
H	1.13157387	4.68447807	2.97520892
H	-0.53793214	4.16140282	3.28079526
H	-0.50130049	6.15022358	1.83132199
H	-1.21293190	4.74962977	0.96621904
H	-0.79983053	5.29547354	-1.08684618
H	0.07198770	6.85368711	-0.89532608
H	0.68302276	5.60028715	-3.00416923
H	2.11029242	5.89130950	-1.96304526
H	1.45927572	3.44077188	-3.95764643
H	3.04097873	3.58195426	-3.12485673
H	0.86789246	1.42139948	-2.66129676
H	2.43953825	1.18247001	-3.49805329
H	1.19945751	0.03533854	-0.72302443
H	2.61932858	-0.59761896	-1.62333039
H	2.83584794	-0.98111253	0.84095265
H	4.16144414	0.03204941	0.19394276
H	2.43219055	0.21513753	3.20462738

H	1.05670561	0.14224965	2.04708811
H	0.75803730	1.86051640	3.88777182
H	2.21977425	2.69254903	3.35984176
C	-2.36681865	0.35656524	0.29038596
C	-1.67592459	1.26423033	-0.51835275
C	-0.73408837	2.12457071	0.04755347
C	-0.52097733	2.12692270	1.43028743
C	-1.34064828	1.34517889	2.25612988
C	-2.24518168	0.45031970	1.68298326
O	-4.33443736	-0.37181405	-0.80782174
N	-1.87665217	-8.44491687	-0.69363156
C	-0.20060023	-8.85157988	1.15652210
C	-0.48274514	-8.77983272	-0.34789160
C	-3.63746273	-10.04340813	0.17469704
C	-2.78435216	-9.56850075	-1.00526227
C	-2.31713340	-7.15543967	-0.67892016
C	-3.68577612	-6.83678369	-0.99223358
C	-4.12783177	-5.53810279	-1.01048053
C	-3.25739882	-4.45128258	-0.71312506
C	-1.44019349	-6.07478269	-0.36681355
C	-1.90797112	-4.77595215	-0.39559945
C	-3.63818741	-3.10654055	-0.68650517
C	-2.73994766	-2.09034787	-0.35210017
C	-1.35150862	-2.41365575	-0.08217668
C	-3.23717118	-0.70397497	-0.34151061
O	-0.41563857	-1.63774314	0.14197075
O	-1.00495961	-3.77614926	-0.10064408
H	-1.83317562	1.25066015	-1.59913589
H	-0.78975019	-9.64382319	1.63821448
H	0.86333700	-9.07727838	1.32168667
H	-0.43141133	-7.90247261	1.66114735
H	-0.26523973	-9.74985682	-0.81594248
H	0.18387803	-8.05197536	-0.83624051
H	-4.29737470	-10.85974770	-0.15393710
H	-3.01473314	-10.42575327	0.99507996
H	-4.26827826	-9.23625900	0.57370119
H	-3.41914578	-9.28249307	-1.85722987
H	-2.15085869	-10.39109992	-1.36508186
H	-5.17102636	-5.32299054	-1.25193056
H	-0.39882967	-6.23863515	-0.09952542
H	-4.66661169	-2.81591778	-0.92150351
H	-0.15519819	2.78089291	-0.60635694
H	-1.24861489	1.37610773	3.34370604
H	-2.82802365	-0.21118023	2.32708702
H	-4.39338466	-7.63242903	-1.21407802

Complex Pb-chemosensor C3

78

PBE/TZVP CRENBL ECP (Pb) E=-1861.56000207 a.u.

Pb	3.22537423	1.90372622	0.01299844
N	2.19819490	1.04167111	2.28695345
C	1.37142764	2.08236169	2.99430234
C	0.64164784	3.04229107	2.06572574
O	1.64017275	3.60676788	1.17356740
C	1.20913888	4.68680595	0.30101206
C	2.44972635	5.47585984	-0.06987352
O	3.45271513	4.56433898	-0.59215630

C	4.78622368	5.13794345	-0.57042321
C	5.80963930	4.03244496	-0.71727723
O	5.57506109	3.06950772	0.34848509
C	6.63991406	2.09899074	0.53688482
C	6.24077027	1.21017332	1.69354249
O	4.99447450	0.54135267	1.34525668
C	4.38078288	-0.21960104	2.42947466
C	3.32632035	0.60085794	3.16455071
H	2.05890193	2.66759527	3.62240054
H	0.63571036	1.59427576	3.65607451
H	0.19897975	3.84907407	2.67309920
H	-0.16459286	2.55696314	1.49286064
H	0.69084302	4.27554960	-0.58305418
H	0.50939821	5.34896908	0.83585495
H	2.19976802	6.23911410	-0.82634016
H	2.85387889	5.97678715	0.82606563
H	4.90115611	5.86098578	-1.39600027
H	4.93699898	5.66245281	0.38843854
H	5.74631081	3.53278566	-1.70099550
H	6.81845420	4.46512921	-0.61313688
H	6.79373217	1.51262604	-0.38653945
H	7.57867773	2.62189760	0.78535131
H	7.02198919	0.45102666	1.86304490
H	6.10807190	1.80794055	2.61112418
H	5.15809856	-0.54475283	3.13748006
H	3.95057945	-1.11470421	1.95874573
H	2.96162950	0.02295646	4.03169929
H	3.78839297	1.51270709	3.57290894
C	-0.19932398	-2.08572243	0.56730147
C	0.53722099	-2.32133422	1.73706889
C	1.30381221	-1.31532711	2.33125418
C	1.38562400	-0.05219870	1.73119552
C	0.66991369	0.17683058	0.53583357
C	-0.12682742	-0.82228155	-0.03058758
O	-0.26002812	-4.30970118	-0.13491574
N	-8.28100018	-4.32963590	-2.59483624
C	-9.11221790	-2.04216270	-3.28529940
C	-9.15403513	-3.18715830	-2.26783338
C	-8.69972077	-5.44940028	-4.82533046
C	-8.89676550	-5.46760006	-3.30647842
C	-6.95211675	-4.31296443	-2.28967792
C	-6.10460698	-5.43252592	-2.60808096
C	-4.77735670	-5.44043466	-2.25929439
C	-4.17886969	-4.34062761	-1.58156921
C	-6.35749807	-3.19742594	-1.63177820
C	-5.01910106	-3.22805059	-1.29157338
C	-2.84199275	-4.28336045	-1.17638630
C	-2.31221113	-3.17075355	-0.51708824
C	-3.16640759	-2.02777740	-0.23099767
C	-0.92327996	-3.26032817	-0.05426992
O	-2.86737590	-0.98226848	0.33751235
O	-4.51065480	-2.12385799	-0.65101345
H	0.50139715	-3.31453596	2.18856130
H	-9.46560160	-2.36912911	-4.27290627
H	-9.76721981	-1.22538068	-2.94757417
H	-8.09651425	-1.63829739	-3.40338070
H	-10.17661438	-3.58244738	-2.19165281

H	-8.89372114	-2.82461828	-1.26156310
H	-9.17235387	-6.33826470	-5.26878428
H	-9.16040068	-4.56170991	-5.28029197
H	-7.63493637	-5.45839960	-5.09899370
H	-8.51394937	-6.40420620	-2.87383921
H	-9.96910007	-5.44255701	-3.06786945
H	-4.15778033	-6.30677560	-2.50152497
H	-6.92635143	-2.30524123	-1.38033285
H	-2.17306078	-5.12952801	-1.35862623
H	1.82250753	-1.53885642	3.26415109
H	0.61453612	1.17523184	0.08468962
H	-0.70470094	-0.60502343	-0.92825064
H	-6.51315463	-6.29452240	-3.13062393

Complex Pb-chemosensor PBE0 C1

78

PBE0/TZVP CRENBL ECP optimization (Pb) E=-1861.31924579 a.u.

Pb	3.07320613	2.83196728	0.94985347
N	2.87837443	0.76207898	2.48438492
C	2.14145129	1.41266899	3.59971573
C	0.72336077	1.77827224	3.19850754
O	0.75320602	2.58492602	2.00996401
C	-0.40179441	2.43189430	1.15730698
C	-0.11193936	3.10278709	-0.16199886
O	1.11776735	2.54869431	-0.66494423
C	1.46980395	2.84441988	-2.02078519
C	2.56556156	1.88182387	-2.41200613
O	3.63107802	1.97384908	-1.45273386
C	4.60518484	0.92335899	-1.57163981
C	5.67837767	1.15118057	-0.53277650
O	5.11518074	1.28823639	0.78120579
C	5.09906781	0.11380650	1.61145143
C	4.27848507	0.43229239	2.84183360
H	2.70122206	2.30608968	3.90833941
H	2.09097524	0.76572764	4.48245407
H	0.24887428	2.33937577	4.00907275
H	0.13789558	0.87611359	3.00372580
H	-0.61376099	1.36804210	1.00719855
H	-1.26901952	2.91057477	1.62293666
H	-0.92761797	2.87903861	-0.85579217
H	-0.01591528	4.19072015	-0.06349126
H	0.60713047	2.68761882	-2.67550084
H	1.79162507	3.88889774	-2.11445516
H	2.17998739	0.85625126	-2.42426797
H	2.94319495	2.13169156	-3.40866162
H	4.10814646	-0.04467488	-1.43620255
H	5.05799979	0.95036052	-2.56855199
H	6.40000714	0.33029633	-0.55505510
H	6.21672008	2.08056024	-0.73304978
H	6.12354614	-0.13131529	1.90656702
H	4.66977356	-0.73142644	1.06388454
H	4.31770536	-0.42210056	3.52651755
H	4.71705224	1.28901372	3.36595695
C	0.41948778	-2.37789374	1.07725849
C	0.91047379	-2.41514800	2.37904456
C	1.75962304	-1.41987297	2.84061793
C	2.14445171	-0.39555394	1.98116300

C	1.75679401	-0.43117259	0.65051954
C	0.89014069	-1.41198531	0.19887613
O	-0.34682609	-4.57745506	0.94017044
N	-7.60437186	-2.85585371	-2.71115777
C	-7.53978131	-0.70340681	-3.99787350
C	-8.06977276	-1.47296332	-2.79554264
C	-8.21127280	-4.33852214	-4.64563988
C	-8.49854297	-3.89946907	-3.21693188
C	-6.38356122	-3.15135915	-2.21601329
C	-5.92241416	-4.50468971	-2.15440029
C	-4.71339208	-4.81352168	-1.60887781
C	-3.85978496	-3.81124877	-1.09342064
C	-5.52272091	-2.13967585	-1.72568235
C	-4.31129665	-2.47890520	-1.17938001
C	-2.62173881	-4.04275476	-0.50233726
C	-1.83021852	-3.01660239	-0.01688835
C	-2.30721266	-1.65438898	-0.10463662
C	-0.58814304	-3.41076077	0.66614317
O	-1.76039167	-0.63784306	0.29410827
O	-3.53284579	-1.46550068	-0.70724153
H	0.58975402	-3.21235066	3.04026935
H	-7.87443199	-1.15205202	-4.93493502
H	-7.90810599	0.32514228	-3.96946049
H	-6.44788016	-0.67447393	-4.01009888
H	-9.15980692	-1.50666013	-2.83031538
H	-7.81698014	-0.95914450	-1.86364165
H	-8.90409149	-5.13325903	-4.93270716
H	-8.33950416	-3.51423488	-5.34975284
H	-7.19400600	-4.72100179	-4.75548319
H	-8.46711247	-4.75256992	-2.53483603
H	-9.51312184	-3.50347678	-3.14808017
H	-4.39069986	-5.84831145	-1.56422830
H	-5.79220304	-1.09450028	-1.75773103
H	-2.24730331	-5.05697656	-0.39467627
H	2.08374963	-1.43834593	3.87619025
H	2.06941882	0.34922325	-0.03356843
H	0.54164004	-1.39725558	-0.82651203
H	-6.53603148	-5.30364874	-2.54367536

Complex Pb-chemosensor PBE0 C2

78

PBE0/TZVP CRENL ECP (Pb) optimization E=-1861.31942107 a.u.

Pb	2.48494937	3.43929797	0.29852077
N	0.55358353	2.91237166	1.92147991
C	0.17250428	4.24606324	2.44946295
C	-0.35375009	5.16608571	1.36727483
O	0.62951429	5.28504567	0.32621763
C	0.11662898	5.78227666	-0.91842768
C	1.07560209	5.40857665	-2.02646241
O	1.29536191	3.99441773	-1.92115917
C	1.92078473	3.31950220	-3.02071031
C	1.82743395	1.83994779	-2.73141573
O	2.43124886	1.57177393	-1.45716499
C	2.16939888	0.23689719	-0.96261133
C	2.95488666	0.04832984	0.31126684
O	2.67952832	1.11006924	1.24832144
C	1.80156167	0.80239882	2.34539320

C	1.29887641	2.10959340	2.92497915
H	1.05573925	4.68915143	2.92486511
H	-0.59733479	4.15248801	3.22494777
H	-0.55772816	6.15094400	1.79870296
H	-1.28093987	4.76880029	0.94239910
H	-0.86275747	5.32993731	-1.10685531
H	0.00291238	6.87011781	-0.87364339
H	0.62168322	5.65003516	-2.99241980
H	2.02792171	5.94776114	-1.94791064
H	1.38716492	3.54020389	-3.95035471
H	2.96166140	3.64863841	-3.12876933
H	0.77988960	1.52202333	-2.70736446
H	2.35231661	1.27864387	-3.51113005
H	1.09531304	0.10146242	-0.79759125
H	2.51149258	-0.49418578	-1.70230786
H	2.70073596	-0.91879040	0.75090236
H	4.03054367	0.07783798	0.12297225
H	2.36485524	0.26170902	3.11190024
H	0.97663529	0.17745967	1.99246349
H	0.68780672	1.89330496	3.80694101
H	2.14411380	2.71039480	3.28405436
C	-2.41892002	0.44247365	0.20824991
C	-1.73077577	1.35003338	-0.58329876
C	-0.78777702	2.18953511	-0.01072339
C	-0.57049616	2.16665615	1.36040524
C	-1.38293803	1.37899563	2.17038744
C	-2.28795219	0.50454874	1.59065342
O	-4.34430593	-0.28391043	-0.93481020
N	-1.92170350	-8.29155392	-0.70820620
C	-0.26081684	-8.66401012	1.13538353
C	-0.53878201	-8.61427740	-0.36087388
C	-3.67207684	-9.86834961	0.16292868
C	-2.81852968	-9.40948646	-1.01072495
C	-2.36229576	-7.01579935	-0.70276967
C	-3.72330271	-6.70578740	-1.01863657
C	-4.16448810	-5.41790706	-1.04965790
C	-3.30153419	-4.33521465	-0.76294460
C	-1.49564435	-5.93770758	-0.39868537
C	-1.96489975	-4.65006191	-0.44064209
C	-3.67813983	-2.99558777	-0.75092267
C	-2.78670376	-1.98948426	-0.42714483
C	-1.40762854	-2.31826093	-0.15195597
C	-3.27740657	-0.60664269	-0.43815016
O	-0.48423044	-1.54529817	0.06339820
O	-1.07759904	-3.65399758	-0.15520746
H	-1.89188012	1.35482051	-1.65600939
H	-0.84343498	-9.44855557	1.62136504
H	0.79684821	-8.87871191	1.30730341
H	-0.49975498	-7.71658488	1.62367438
H	-0.31730373	-9.58353973	-0.81051597
H	0.12377913	-7.89804628	-0.85514480
H	-4.32843888	-10.68189356	-0.15537498
H	-3.05556424	-10.23926752	0.98378156
H	-4.29771800	-9.06074786	0.54948014
H	-3.44489758	-9.13854595	-1.86427428
H	-2.18888768	-10.23160073	-1.35492785
H	-5.20069780	-5.20914481	-1.29373443

H	-0.46186871	-6.09439121	-0.12881090
H	-4.69825687	-2.70837651	-0.99131995
H	-0.21321504	2.84972190	-0.65132854
H	-1.28487360	1.38914619	3.25014050
H	-2.86472881	-0.16328096	2.22108277
H	-4.42333656	-7.49998934	-1.23236698

Complex Pb-chemosensor PBE0 C3

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PBE0/TZVP CRENL ECP (Pb) optimization E=-1861.31383923 a.u.

Pb	3.10921244	1.95620208	0.13291763
N	2.12294026	1.11012592	2.39376348
C	1.28688097	2.12620618	3.09512179
C	0.52741150	3.05294733	2.17060092
O	1.48295878	3.59829206	1.25071973
C	1.05076824	4.67522115	0.40679963
C	2.27688799	5.48303657	0.06076779
O	3.29033991	4.59978530	-0.43453633
C	4.59267062	5.19528613	-0.43113673
C	5.63044734	4.11659701	-0.59364868
O	5.41812490	3.14581638	0.44279404
C	6.49312088	2.21610138	0.63031952
C	6.12337095	1.32704752	1.78640650
O	4.88826411	0.66648252	1.46688284
C	4.30854608	-0.10188123	2.53791054
C	3.24679957	0.69746738	3.26661205
H	1.96212892	2.73271827	3.70265628
H	0.57872558	1.63030580	3.76808292
H	0.09486684	3.86096000	2.76922105
H	-0.28389557	2.55047546	1.63642651
H	0.55178643	4.27654317	-0.48419494
H	0.34034350	5.31305693	0.94051008
H	2.02926806	6.23853181	-0.69263998
H	2.65118647	5.98640146	0.95891896
H	4.68177444	5.91867132	-1.24887633
H	4.74694175	5.71563450	0.52056057
H	5.57137480	3.63531752	-1.57809138
H	6.62475797	4.56234547	-0.48955978
H	6.65515485	1.63138567	-0.28347115
H	7.41511180	2.75641356	0.86865966
H	6.90680242	0.57836710	1.93986398
H	6.00754508	1.92019285	2.70008578
H	5.08911761	-0.40280253	3.24120555
H	3.89941347	-1.00466653	2.08126241
H	2.89367111	0.12779032	4.13342136
H	3.69499976	1.61274773	3.66231191
C	-0.23671784	-2.03624319	0.74501864
C	0.51690688	-2.25525602	1.89336465
C	1.27968761	-1.24390721	2.46131073
C	1.33035177	0.00759768	1.85832302
C	0.59740841	0.21841982	0.68321299
C	-0.18744592	-0.78815977	0.13868934
O	-0.36383741	-4.26819912	0.12806371
N	-8.27003801	-4.13484495	-2.45121370
C	-9.00526243	-1.84453391	-3.16670215
C	-9.10983677	-2.97619242	-2.15324966
C	-8.66681741	-5.26279904	-4.65897939

C	-8.89492346	-5.25634581	-3.15403174
C	-6.95879952	-4.14713927	-2.12738722
C	-6.13789707	-5.28141691	-2.42289167
C	-4.82685784	-5.31689074	-2.05496942
C	-4.21992810	-4.23297807	-1.38019385
C	-6.35298742	-3.04918345	-1.47190579
C	-5.03072242	-3.11009270	-1.11228988
C	-2.89427906	-4.19708536	-0.95701061
C	-2.36059843	-3.09885222	-0.30716324
C	-3.20270389	-1.95122033	-0.03712940
C	-0.98195887	-3.21042203	0.16797312
O	-2.89330554	-0.92564383	0.53490110
O	-4.51013790	-2.02773930	-0.47515859
H	0.49744978	-3.23845135	2.34984008
H	-9.34209830	-2.16362106	-4.15473678
H	-9.63523146	-1.00862446	-2.85247423
H	-7.97990121	-1.48017966	-3.26132945
H	-10.13932049	-3.33503285	-2.10464933
H	-8.87092130	-2.61870144	-1.14793405
H	-9.14453606	-6.14077633	-5.10074522
H	-9.09567355	-4.37640474	-5.13010683
H	-7.60363549	-5.29535084	-4.90734469
H	-8.55093279	-6.19179179	-2.70547659
H	-9.96409652	-5.20258466	-2.94238075
H	-4.22781373	-6.19294464	-2.28043296
H	-6.90039976	-2.14871696	-1.23609722
H	-2.24323503	-5.05095262	-1.12233151
H	1.81846069	-1.45594340	3.37627285
H	0.52439455	1.20456726	0.22763020
H	-0.77661349	-0.58631366	-0.74601594
H	-6.55510986	-6.13064501	-2.94361261

Complex Ca-chemosensor A2

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PBE/6-311++G** CRENL ECP (Ca)

Ca	1.71729016	1.37552381	0.97607557
N	4.01796583	0.82125079	2.58145782
C	4.22946430	1.90082443	3.57497344
C	3.05598954	2.86405496	3.84119632
O	2.30827309	3.12663071	2.63150717
C	1.23058530	4.07944166	2.84461940
C	0.80272669	4.63274903	1.50217131
O	0.47819013	3.53033556	0.62475892
C	0.23387349	3.95250557	-0.74267350
C	0.52210375	2.78187015	-1.66718920
O	1.84707442	2.32250804	-1.30901868
C	2.46802737	1.36163949	-2.18453917
C	3.88283285	1.16363615	-1.66767649
O	3.83004247	0.89372121	-0.24004357
C	5.08160127	0.36299203	0.25068692
C	5.22429103	0.46049685	1.80192284
H	5.06431948	2.49771824	3.18701172
H	4.55260750	1.49851052	4.55453965
H	3.48793558	3.81095200	4.20968580
H	2.36216522	2.49733987	4.61370336
H	0.39672001	3.57725751	3.36892530
H	1.58410830	4.91406789	3.47329652

H	-0.07466079	5.28864550	1.64065418
H	1.62186486	5.22100976	1.05136867
H	-0.81024932	4.28945112	-0.85549741
H	0.91184295	4.79001291	-0.98005380
H	-0.20481864	1.95834714	-1.54000011
H	0.50020155	3.12906624	-2.71422105
H	1.89278023	0.41602689	-2.17786967
H	2.50928535	1.74248732	-3.21983302
H	4.34808142	0.31485291	-2.19821326
H	4.49299027	2.06842572	-1.83038542
H	5.90772997	0.92946229	-0.21137180
H	5.17143161	-0.68410816	-0.08789959
H	5.63849846	-0.49547523	2.16677320
H	5.97588095	1.22736393	2.02209706
C	0.62719868	-1.64292114	2.67874333
C	0.88946033	-0.80447834	3.77067329
C	2.08106005	-0.07513413	3.83871983
C	3.05224849	-0.18538985	2.81189873
C	2.88706682	-1.23809419	1.87051040
C	1.67713472	-1.92853376	1.79288605
O	-1.39137729	-2.70316679	3.35306248
N	-5.13522665	-1.85378772	-4.10359427
C	-3.46261245	-1.29180750	-5.91460162
C	-4.65136353	-0.83923560	-5.05865113
C	-6.00317138	-3.96709005	-5.19466797
C	-6.32402069	-2.63905126	-4.50196325
C	-4.48886858	-2.08233428	-2.93053236
C	-4.92927269	-3.12045588	-2.03037727
C	-4.30694476	-3.33697105	-0.82778256
C	-3.19101439	-2.54927062	-0.41736121
C	-3.36058890	-1.29712165	-2.53543331
C	-2.75756953	-1.53354871	-1.31729588
C	-2.49705259	-2.70529883	0.78308328
C	-1.38456728	-1.91616107	1.11311836
C	-0.99249370	-0.86771168	0.21859222
C	-0.76597049	-2.14680860	2.45526547
O	-0.09274188	-0.00140477	0.36985295
O	-1.68843467	-0.72859990	-0.96884145
H	0.12986057	-0.68389970	4.54715402
H	-3.72613558	-2.15600616	-6.54005496
H	-3.15922751	-0.47317249	-6.58472113
H	-2.59485563	-1.57203018	-5.29901024
H	-5.50200298	-0.58499197	-5.70602286
H	-4.40958372	0.08095248	-4.50185708
H	-6.94075380	-4.49008032	-5.43554708
H	-5.45700959	-3.81089878	-6.13581214
H	-5.40016283	-4.62806787	-4.55452748
H	-6.95226423	-2.79878615	-3.61315507
H	-6.91156691	-1.99562115	-5.17251764
H	-4.66140739	-4.13003295	-0.16541426
H	-2.96368289	-0.50589693	-3.16818293
H	-2.80928393	-3.46043967	1.51119156
H	2.24843679	0.57619490	4.69413565
H	3.67710543	-1.48234739	1.16103775
H	1.54078417	-2.67458991	1.00577350
H	-5.76692165	-3.75816399	-2.30587316

Complex Hg-chemosensor B1

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PBE/6-311++G** CRENBL ECP (Hg)

Hg	3.10837990	2.28866781	0.45103903
N	2.41586729	0.88911870	2.35283507
C	1.76840601	1.84380813	3.31654562
C	0.83915478	2.85657813	2.65419664
O	1.67101115	3.78315690	1.92753479
C	0.99830481	4.67437300	1.01217011
C	2.06549259	5.50260454	0.32054055
O	2.93654066	4.64122024	-0.45693514
C	4.22640660	5.23276119	-0.74792225
C	5.19170948	4.15969077	-1.21329407
O	5.35951828	3.20946725	-0.13378033
C	6.30301433	2.14226334	-0.39268709
C	6.20672996	1.13533015	0.73813476
O	4.91211517	0.48999197	0.65958232
C	4.54993661	-0.34598522	1.77962202
C	3.73605603	0.39079756	2.85011475
H	2.56804090	2.39264721	3.83726459
H	1.20301394	1.27052027	4.06986187
H	0.28433235	3.39809649	3.43936153
H	0.11063889	2.36972140	1.98023975
H	0.39577305	4.09687495	0.28695817
H	0.32772965	5.35278184	1.56790510
H	1.58757857	6.23636484	-0.35094668
H	2.66458256	6.04069018	1.07569824
H	4.11186063	5.98874267	-1.54414113
H	4.61783719	5.72330662	0.16069005
H	4.82437189	3.64350777	-2.11845078
H	6.16172876	4.63381772	-1.44245009
H	6.07947969	1.66188162	-1.36173689
H	7.32322132	2.56207849	-0.42419594
H	6.99669593	0.37457975	0.61607251
H	6.33885902	1.63869515	1.71249447
H	5.45659395	-0.76291532	2.24743039
H	3.96884539	-1.17814244	1.35485808
H	3.59074776	-0.29643974	3.70232807
H	4.29426741	1.26216552	3.22776314
C	-0.34692978	-2.17060837	1.20020030
C	0.28560193	-2.21261497	2.45417649
C	1.18661313	-1.21921520	2.83677186
C	1.50073510	-0.18201537	1.94179473
C	0.89930695	-0.15801814	0.67863485
C	-0.03011884	-1.13357545	0.30947138
O	-0.89743214	-4.45423773	1.21576195
N	-8.10921447	-4.02509995	-2.95563315
C	-8.49092604	-1.85113111	-4.18677243
C	-8.85742583	-2.75428513	-3.00158517
C	-8.20540730	-5.48783486	-5.01642274
C	-8.73467572	-5.19506682	-3.60659961
C	-6.87277778	-4.09982637	-2.38437733
C	-6.16850873	-5.35593545	-2.31075790
C	-4.94062694	-5.44188535	-1.69957142
C	-4.31689001	-4.29837722	-1.12655329
C	-6.24583938	-2.94438114	-1.83050125
C	-5.00755082	-3.05586045	-1.22165593

C	-3.07508770	-4.31844405	-0.45933518
C	-2.50509045	-3.16792418	0.06531834
C	-3.21166459	-1.89017943	-0.03655479
C	-1.23858118	-3.33191397	0.84069927
O	-2.86403025	-0.80935962	0.39332757
O	-4.45973984	-1.91800909	-0.70563393
H	0.05793420	-3.03728257	3.13258445
H	-8.72659557	-2.33033877	-5.14718908
H	-9.07331395	-0.91986672	-4.12397804
H	-7.42274959	-1.58922374	-4.18474042
H	-9.92352248	-3.01828614	-3.04524469
H	-8.70913113	-2.22885827	-2.04637070
H	-8.71701363	-6.37612218	-5.41581527
H	-8.39921544	-4.65050007	-5.70105735
H	-7.12411288	-5.68815190	-5.01524052
H	-8.61226277	-6.07079962	-2.95098353
H	-9.81315550	-4.98979062	-3.64516580
H	-4.42889795	-6.40525453	-1.64098265
H	-6.70524064	-1.95882543	-1.87080310
H	-2.53346987	-5.26091927	-0.33217622
H	1.63045158	-1.25754849	3.83469538
H	1.15515555	0.64289136	-0.02893898
H	-0.49402767	-1.08514785	-0.67585851
H	-6.60970505	-6.25725991	-2.73142589

Complex Pb-chemosensor C2

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PBE/6-311++G** CRENBLECP (Pb)

Pb	2.51357431	3.47761345	0.27968035
N	0.56131230	2.98034643	1.95178029
C	0.19076650	4.34249432	2.45099947
C	-0.33933407	5.24720710	1.34417253
O	0.65174323	5.34818503	0.28423241
C	0.12084036	5.81406656	-0.98450494
C	1.07422064	5.41027505	-2.09935348
O	1.28807039	3.98101917	-1.96446265
C	1.90714842	3.26489969	-3.06364776
C	1.80957158	1.78608363	-2.72832553
O	2.45535092	1.54501763	-1.45045361
C	2.18788164	0.21388735	-0.89970614
C	2.99871274	0.06426612	0.37371935
O	2.72590239	1.15248144	1.30799792
C	1.82387316	0.86225669	2.41347239
C	1.31842274	2.18753673	2.97412034
H	1.08691774	4.79070717	2.91612157
H	-0.58322322	4.27460477	3.23712866
H	-0.54018807	6.24921286	1.75797634
H	-1.27399010	4.84006281	0.92309043
H	-0.86809114	5.35259000	-1.14804085
H	0.00751785	6.91115723	-0.96687838
H	0.60777731	5.63340655	-3.07320294
H	2.03865581	5.94777454	-2.04210945
H	1.35734146	3.46355983	-3.99867150
H	2.95525066	3.59137330	-3.19268922
H	0.75380634	1.47212800	-2.66426612
H	2.31526663	1.19524898	-3.51072032
H	1.10658305	0.09109273	-0.71731593

H	2.51967100	-0.54741903	-1.62609143
H	2.76517189	-0.90309806	0.84349868
H	4.07932999	0.10879856	0.17081752
H	2.38518700	0.32632337	3.19627375
H	0.99470585	0.23097193	2.05632688
H	0.70435264	1.98156375	3.86732660
H	2.16828791	2.80216318	3.32271369
C	-2.42920756	0.45847182	0.25999601
C	-1.74375787	1.37294951	-0.54761276
C	-0.79772351	2.23063211	0.01822484
C	-0.57406939	2.22260409	1.40071817
C	-1.38707914	1.43219297	2.22723481
C	-2.29547974	0.53988490	1.65330745
O	-4.39980203	-0.26772314	-0.83343352
N	-1.92566020	-8.34027194	-0.75741408
C	-0.25976697	-8.74321154	1.10226496
C	-0.53375129	-8.67265468	-0.40476640
C	-3.68158792	-9.94319319	0.11120117
C	-2.82955728	-9.46553510	-1.06983425
C	-2.36959256	-7.05263173	-0.73996342
C	-3.73999961	-6.73593769	-1.05503010
C	-4.18663147	-5.43766146	-1.06742778
C	-3.31949196	-4.34878152	-0.76356616
C	-1.49519236	-5.96938193	-0.42351652
C	-1.96737684	-4.67093097	-0.44727988
C	-3.70315012	-3.00359448	-0.73157335
C	-2.80653994	-1.98665402	-0.39150154
C	-1.41573529	-2.31035443	-0.12307731
C	-3.30579382	-0.59898078	-0.37385516
O	-0.48430331	-1.53819516	0.10405132
O	-1.07127272	-3.67073135	-0.14957945
H	-1.90869510	1.36725063	-1.62794537
H	-0.85327069	-9.53481641	1.58098893
H	0.80349918	-8.97002789	1.27384584
H	-0.49261690	-7.79280748	1.60493584
H	-0.31239055	-9.64310538	-0.87148107
H	0.13476874	-7.94374548	-0.89047880
H	-4.33868845	-10.76284471	-0.21653146
H	-3.05644014	-10.32221731	0.93215602
H	-4.31556288	-9.13732298	0.50955431
H	-3.46533746	-9.18059326	-1.92220083
H	-2.19349501	-10.28660408	-1.43052776
H	-5.23073790	-5.22476958	-1.30908110
H	-0.45253769	-6.12952044	-0.15641172
H	-4.73276435	-2.71395279	-0.96538642
H	-0.22185827	2.89247461	-0.63361246
H	-1.28496924	1.45425539	3.31474185
H	-2.87248833	-0.12830987	2.29678155
H	-4.44531829	-7.53300989	-1.28208489

Complex Ca-chemosensor A2 optimized with acetonitrile

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PBE/TZVP CRENL ECP(Ca) solvent acetonitrile optimization

Ca	2.170712	-0.696646	-0.152121
N	4.443444	1.055210	0.792635
C	5.457435	1.080692	-0.288909
C	4.948563	0.719622	-1.683656

O	4.266382	-0.556209	-1.637575
C	3.945015	-1.049674	-2.964583
C	3.518041	-2.494839	-2.851257
O	2.378970	-2.585196	-1.967506
C	2.080407	-3.947734	-1.579778
C	1.328719	-3.916552	-0.263494
O	2.135666	-3.111377	0.624874
C	1.798472	-3.161570	2.024115
C	2.928885	-2.475655	2.768455
O	3.225613	-1.206808	2.126071
C	4.077360	-0.372830	2.939423
C	4.968948	0.553283	2.088927
H	6.220694	0.341591	-0.016809
H	5.972568	2.056789	-0.350380
H	5.829599	0.640356	-2.343226
H	4.268827	1.474199	-2.110349
H	3.153120	-0.423602	-3.413860
H	4.838166	-0.998148	-3.609384
H	3.260332	-2.878109	-3.853896
H	4.343645	-3.101454	-2.440480
H	1.479194	-4.446561	-2.358339
H	3.026883	-4.499022	-1.449925
H	0.321827	-3.472664	-0.369202
H	1.224501	-4.942128	0.126481
H	0.829328	-2.662627	2.200909
H	1.723214	-4.205945	2.370457
H	2.624182	-2.312005	3.815465
H	3.841671	-3.093991	2.749697
H	4.757602	-1.010875	3.527104
H	3.454681	0.181276	3.660842
H	5.278982	1.394198	2.734786
H	5.875417	-0.008128	1.837263
C	0.962652	3.313180	0.229537
C	2.105727	3.618757	-0.525271
C	3.318362	2.984838	-0.261545
C	3.415754	2.019333	0.770104
C	2.340272	1.947840	1.693497
C	1.125467	2.552289	1.397649
O	-0.665987	4.764164	-0.758382
N	-6.697299	-1.101291	-0.326117
C	-5.979698	-3.169724	0.939994
C	-6.320194	-2.523527	-0.406961
C	-8.655621	-0.539172	1.173527
C	-8.136600	-0.787492	-0.246428
C	-5.750234	-0.120065	-0.284499
C	-6.122224	1.268668	-0.216033
C	-5.173984	2.263283	-0.216851
C	-3.784445	1.964246	-0.273274
C	-4.360550	-0.430555	-0.323346
C	-3.429581	0.590082	-0.323956
C	-2.752652	2.913103	-0.262267
C	-1.406478	2.553366	-0.275239
C	-1.055247	1.153573	-0.375331
C	-0.385817	3.644632	-0.291134
O	0.072136	0.644334	-0.498725
O	-2.100265	0.226505	-0.379707
H	2.023529	4.290362	-1.382543

H	-6.845792	-3.163904	1.616275
H	-5.682503	-4.216500	0.777807
H	-5.148480	-2.653525	1.441692
H	-7.167059	-3.049140	-0.869097
H	-5.478832	-2.624548	-1.108915
H	-9.730227	-0.306823	1.133545
H	-8.522533	-1.425640	1.809045
H	-8.142810	0.307104	1.652892
H	-8.349033	0.076595	-0.893505
H	-8.667409	-1.639306	-0.692681
H	-5.485084	3.309007	-0.169928
H	-3.999174	-1.455919	-0.352334
H	-2.995350	3.978811	-0.231216
H	4.172187	3.203052	-0.899941
H	2.411533	1.347112	2.596595
H	0.276289	2.383483	2.063602
H	-7.171564	1.550420	-0.162540

Complex Hg-chemosensor B1 optimization with acetonitrile

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PBE/TZVP CRENBL ECP (Hg) solvent acetonitrile optimization

Hg	-3.810189	-0.541060	-0.324435
N	-2.907301	1.285976	0.976494
C	-3.152684	0.902259	2.419129
C	-2.867006	-0.557833	2.739367
O	-3.921956	-1.328072	2.131699
C	-3.731640	-2.759561	2.089772
C	-4.901341	-3.328521	1.312304
O	-4.888683	-2.821683	-0.048009
C	-6.183407	-2.902776	-0.693720
C	-6.189379	-2.044906	-1.941133
O	-5.985429	-0.670290	-1.534373
C	-6.029600	0.292661	-2.617466
C	-5.656665	1.655828	-2.071700
O	-4.236304	1.665140	-1.779158
C	-3.787022	2.735670	-0.921781
C	-3.837863	2.399976	0.568382
H	-4.210956	1.103143	2.637204
H	-2.544600	1.548973	3.069061
H	-2.893081	-0.691006	3.833757
H	-1.879144	-0.884101	2.369212
H	-2.765802	-3.001734	1.613572
H	-3.743075	-3.176540	3.110873
H	-4.835956	-4.428925	1.290230
H	-5.846074	-3.034695	1.799631
H	-6.390974	-3.950229	-0.970325
H	-6.963211	-2.555532	0.005014
H	-5.401663	-2.349535	-2.650847
H	-7.172266	-2.141225	-2.431676
H	-5.339423	-0.010712	-3.422848
H	-7.056707	0.328362	-3.016821
H	-5.870006	2.422562	-2.835302
H	-6.249245	1.878814	-1.168697
H	-4.393223	3.639026	-1.094344
H	-2.755689	2.952982	-1.236331
H	-3.607268	3.316429	1.134224
H	-4.850999	2.089368	0.860129

C	1.231086	2.360327	0.516105
C	0.319647	3.229129	1.136717
C	-1.016741	2.867078	1.287057
C	-1.486272	1.643704	0.775356
C	-0.585393	0.784685	0.136338
C	0.763503	1.134684	0.024908
O	2.841491	4.013364	0.001616
N	9.302699	-1.373973	-0.190694
C	8.591378	-3.776833	0.167434
C	9.291939	-2.531122	0.721083
C	10.330708	-1.744572	-2.469911
C	10.489970	-1.198782	-1.047172
C	8.231538	-0.529931	-0.272698
C	8.253203	0.616369	-1.141311
C	7.193326	1.491329	-1.191410
C	6.028696	1.295591	-0.400559
C	7.061272	-0.744684	0.509590
C	6.008397	0.149581	0.439007
C	4.902420	2.134404	-0.407109
C	3.770404	1.861907	0.352897
C	3.764003	0.721030	1.249953
C	2.640530	2.818636	0.293688
O	2.902360	0.396284	2.062362
O	4.911089	-0.109708	1.227540
H	0.668116	4.190998	1.516371
H	9.100860	-4.157196	-0.728796
H	8.603658	-4.571418	0.928356
H	7.543228	-3.571618	-0.093658
H	10.341384	-2.764375	0.948526
H	8.834139	-2.222029	1.672828
H	11.255543	-1.563238	-3.037636
H	10.141649	-2.826987	-2.462925
H	9.502923	-1.254358	-3.002423
H	10.760013	-0.132327	-1.070032
H	11.319631	-1.711645	-0.541783
H	7.237515	2.358801	-1.853744
H	6.959652	-1.603191	1.169712
H	4.897435	3.027029	-1.038575
H	-1.686492	3.551390	1.809188
H	-0.891756	-0.172579	-0.283637
H	1.448137	0.446489	-0.473574
H	9.118466	0.809365	-1.771854

Complex Pb-chemosensor C2 optimization with acetonitrile

78

PBE/TZVP CRENBLECP (Pb) solvent acetonitrile optimization

Pb	-5.018963	-0.522200	-0.275392
N	-2.642974	-0.620270	-1.590165
C	-3.071715	0.029594	-2.872321
C	-3.398349	1.504574	-2.688929
O	-4.434884	1.647917	-1.684305
C	-4.438561	2.936179	-1.015162
C	-5.220209	2.814981	0.278123
O	-4.630631	1.717967	1.027433
C	-5.052670	1.584966	2.410005
C	-4.184024	0.512159	3.033039
O	-4.328056	-0.711870	2.263917

C	-3.337025	-1.721610	2.597719
C	-3.605538	-2.947863	1.745924
O	-3.628552	-2.632877	0.326590
C	-2.374158	-2.796912	-0.391474
C	-2.508967	-2.104390	-1.737160
H	-3.953545	-0.513887	-3.249693
H	-2.288860	-0.055017	-3.646468
H	-3.750372	1.920623	-3.646493
H	-2.506030	2.066539	-2.369324
H	-3.398275	3.232526	-0.802986
H	-4.905495	3.697139	-1.661693
H	-5.118853	3.751690	0.848688
H	-6.291888	2.621500	0.101316
H	-4.888746	2.535982	2.940977
H	-6.123992	1.326876	2.457834
H	-3.125700	0.822291	3.030468
H	-4.503391	0.334045	4.072742
H	-2.327352	-1.311194	2.426673
H	-3.433980	-1.995346	3.661499
H	-2.848391	-3.719364	1.950106
H	-4.598602	-3.362957	1.970076
H	-2.194965	-3.872161	-0.548338
H	-1.540713	-2.376730	0.193872
H	-1.646507	-2.378144	-2.366628
H	-3.406492	-2.477620	-2.255498
C	0.951305	1.121644	-0.040242
C	-0.288260	1.390184	0.558084
C	-1.457221	0.813962	0.056570
C	-1.409414	-0.013346	-1.069786
C	-0.178749	-0.241607	-1.706493
C	0.991482	0.306900	-1.183950
O	2.085404	2.967611	0.913978
N	9.685243	-0.610768	0.285225
C	9.540118	-2.721743	-1.098328
C	9.792158	-2.080604	0.270902
C	11.363633	0.574437	-1.191132
C	10.939935	0.159861	0.221968
C	8.467511	0.008044	0.306886
C	8.361241	1.441088	0.247436
C	7.137226	2.066567	0.292835
C	5.927477	1.327502	0.397236
C	7.260620	-0.741415	0.400963
C	6.042846	-0.087512	0.452451
C	4.640697	1.890167	0.417032
C	3.490808	1.110193	0.474522
C	3.607253	-0.329512	0.617340
C	2.177694	1.797097	0.495693
O	2.715132	-1.149633	0.816053
O	4.915769	-0.868424	0.564845
H	-0.331314	2.042241	1.432097
H	10.286549	-2.395127	-1.835552
H	9.606097	-3.816188	-1.007698
H	8.542290	-2.472285	-1.486311
H	10.805055	-2.326661	0.616910
H	9.102839	-2.494279	1.023497
H	12.295071	1.157672	-1.137948
H	11.548205	-0.302080	-1.827775

H	10.598659	1.197096	-1.677188
H	10.845543	1.042336	0.871473
H	11.718484	-0.469480	0.675262
H	7.083382	3.156281	0.241611
H	7.259783	-1.828452	0.439803
H	4.524348	2.976344	0.369691
H	-2.410363	1.027196	0.543108
H	-0.118010	-0.853109	-2.608140
H	1.941939	0.110177	-1.682831
H	9.256311	2.052121	0.153021

Table S1. Main molecular orbitals involved in the electronic transitions of the Ca^{2+} , Hg^{2+} and Pb^{2+} complexes showed in this order.

