Electronic Supplementary Information for Dalton Transactions

Homoleptic Co(II), Ni(II), Cu(II), Zn(II) and Hg(II) complexes of bis-(phenyl)-diisoindol-aza-methene

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Supporting Information

1. **General remarks**
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1. General remarks:

Single crystals suitable for the X-ray diffraction study were obtained by slow evaporation from chloroform or toluene solution. The crystallographic data for were collected on a Bruker Nonius Kappa CCD diffractometer using graphite-mono-chromated Mo-Kα (λ = 0.71073 Å) radiation at 150 K. SADABS was used to perform area-detector scaling and absorption corrections.[1] The structures were solved by direct methods using Sir97[2] and were refined by full-matrix least-squares techniques against F_o^2 by using SHELXL-97.[3] All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were generated by their idealized geometry and refined within a riding model. Experimental details are given in Table 1. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-801539 (Co, 2a) & CCDC-801540 (Zn, 2d). Copies of the data can be obtained free of charge from www.ccdc.cam.ac.uk/conts/retrieving.html.

For all quantum chemical calculations, the Gaussian03 package was used. All *ab initio* calculations of the orbital energies and the absorption energies were performed with density functional theory with the b3lyp functional and the basis set 6-31g(d). No symmetry constrains were used for the optimization. All optimized structures were confirmed with subsequent frequency calculations to make sure that a true minimum was reached. The calculation of the absorption energies and the principal orbital contributions were done with time dependent DFT as implemented in the Gaussian package.

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1 *Bruker SADABS - Area Detector Absorption and Other Corrections, 2.03*, Delft, Netherlands, **2002**.

2 A. Altomare, M. C. Burla, M. Camalli, G. L. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna, *J. Appl. Cryst.* **1999**, *32*, 115–119.

3 G. M. Sheldrick, *SHELXL-97 Program for the Refinement of Crystal Structures*, Universität Göttingen, Göttingen (Germany), 1997.

2. Crystal Structure and refinement details

Table 1. Crystal data and structure refinement details for compounds **2a** and **2d**:

crystal	**2a**	**2d**
formula	$C_{56}H_{36}CoN_6 \cdot 0.5\ C_7H_8$	$C_{56}H_{36}N_6Zn \cdot C_6H_5Cl \cdot 0.5\ CH_2Cl_2$
M_W	897.91	1013.29
T [K]	198(2)	153(2)
crystal system	Triclinic	Triclinic
space group	$P\bar{1}$	$P\bar{1}$
unit cell parameter		
a [Å]	12.229(5)	13.239(5)
b [Å]	13.097(5)	13.699(5)
c [Å]	16.199(5)	16.251(5)
α [°]	113.080(5)	72.130(5)
β [°]	99.950(5)	68.380(5)
γ [°]	98.860(5)	68.570(5)
V [Å^3]	2279.4(15)	2499.5(15)
Z	2	2
$D_{calc.}$ [g cm^{-3}]	1.308	1.346
μ [mm^{-3}]	0.424	0.646
F_{000}	932	1046
Crystal size [mm^3]	0.14 x 0.12 x 0.08	0.25 x 0.12 x 0.06
θ_{min} / θ_{max} [°]	3.15 / 25.40	3.02 / 27.99
index ranges	$-14 \le h \le 14$	$-17 \le h \le 16$
	$-15 \le k \le 15$	$-18 \le k \le 18$
	$-19 \le l \le 19$	$-21 \le l \le 21$
reflections collected	59570	90345
independent reflections	8340	11995
R_{int}	0.0583	0.0799
completeness to θ [%]	99.3	99.4
T_{max} / T_{min}	0.9656 / 0.9449	0.9647 / 0.8567
data / restraints / parameters	8340 / 0 / 620	11995 / 0 / 631
GOF on F^2	1.202	1.079
final R indices [$I>\sigma_{(I)}$]	R_1 = 0.0482	R_1 = 0.0606
	wR_2 = 0.0938	wR_2 = 0.1484
R indices (all data)	R_1 = 0.0773	R_1 = 0.0807
	wR_2 = 0.1119	wR_2 = 0.1598
largest diff. peak and hole [e Å^{-3}]	0.261 / –0.332	1.023 / –0.935

Platon SQUEEZE proceedure was applied to a highly disordered molecule of dichloromethane. Although the atoms do not appear in the tables for atomic coordinates and equivalent isotropic/unisotropic displacement parameters they are considered in SFAC in order to get the correct values for M_W and density.

3. Thermogravimetric measurements

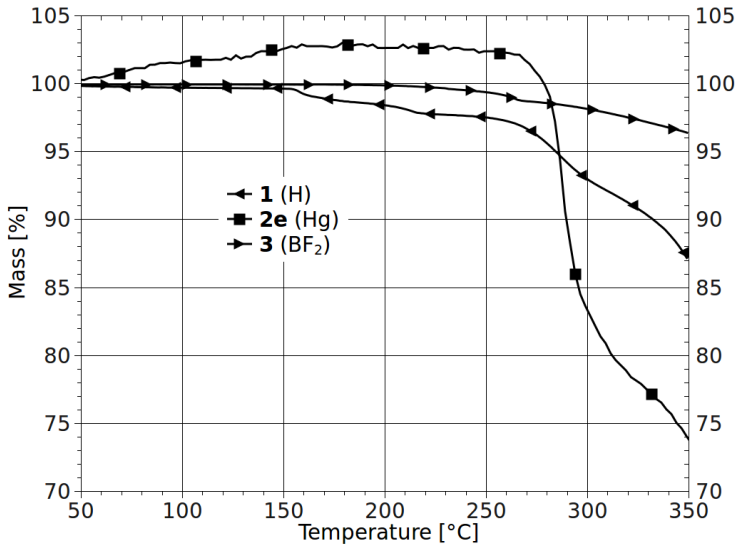


Figure 1: Thermogravimetric analysis in the lower temperature regime.

4. Absorption measurements

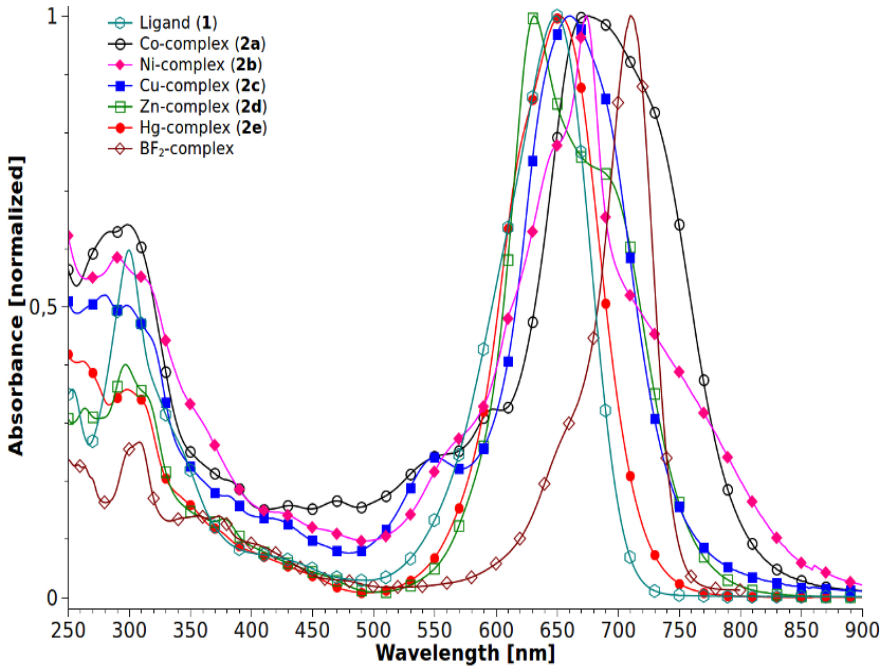
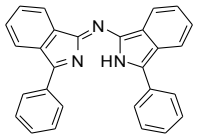


Figure 2: Normalized absorption spectra of the ligand, the metal complexes and the boron difluoride complex.

5. Cartesian coordinates for the optimized structures

Ligand



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C	4.415737	1.844327	-0.537184
C	3.186793	1.489503	0.053887
C	2.413826	2.507886	0.649051
C	2.857337	3.827165	0.655139
C	4.082304	4.162880	0.073119
C	4.856940	3.164791	-0.522471
C	2.714316	0.110501	0.034590
C	3.419443	-1.131415	0.034888
C	2.438857	-2.176186	0.024587
C	1.153965	-1.558601	0.021772
N	1.388609	-0.192342	0.037824
C	4.792488	-1.464687	0.095151
C	5.151152	-2.798976	0.103824
C	4.173268	-3.826728	0.064767
C	2.823849	-3.528619	0.033223
N	-0.039292	-2.161541	0.001484
C	-1.181500	-1.517849	-0.021885
C	-2.490019	-2.160989	-0.020622
C	-3.438828	-1.113349	-0.035006
C	-2.647655	0.126800	-0.036947
N	-1.348462	-0.126997	-0.041639
C	-2.883210	-3.497493	-0.031206
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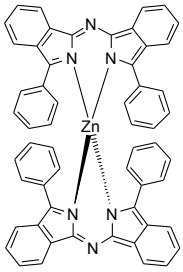
C	-5.198577	-2.745027	-0.110536
C	-4.805603	-1.405668	-0.100052
C	-3.151556	1.505139	-0.050937
C	-4.374591	1.848491	0.553524
C	-4.826869	3.166846	0.543451
C	-4.070840	4.165038	-0.073547
C	-2.850616	3.837807	-0.672492
C	-2.392922	2.523995	-0.657824
H	-2.140589	-4.289650	-0.018641
H	-4.585696	-4.812953	-0.078723
H	-6.255807	-2.991417	-0.158553
H	-5.552362	-0.620555	-0.160513
H	-1.451677	2.262416	-1.130210
H	-2.257584	4.609576	-1.156131
H	-4.427759	5.191344	-0.086169
H	-5.768947	3.415594	1.024660
H	-4.952366	1.087551	1.067242
H	5.553185	-0.692915	0.152437
H	6.202215	-3.070723	0.149561
H	4.496745	-4.864149	0.071555
H	2.068075	-4.307881	0.021226
H	5.004969	1.086082	-1.041667
H	5.804950	3.417514	-0.989746
H	4.428878	5.192442	0.082682
H	2.249002	4.594410	1.126417
H	1.475930	2.256701	1.137232
H	0.593089	0.446777	-0.002635

Zn-complex



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C	-2.033664	-1.124537	2.662580
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C	-4.285535	-0.368022	2.229650
C	-4.771105	-1.635942	2.545115
C	-3.892647	-2.673226	2.894455
C	-2.522610	-2.391216	2.977470
C	-2.345657	1.203987	1.774327
C	-2.881382	2.511553	2.067835
C	-2.012469	3.452642	1.437459
C	-0.978013	2.697504	0.748394
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C	-3.973044	2.925215	2.851452
C	-4.200847	4.288160	3.001539
C	-3.354887	5.231183	2.382227
C	-2.261659	4.826084	1.613013
N	-0.000550	3.208547	-0.000065
C	0.977100	2.697784	-0.748500
N	1.240572	1.331017	-1.007489
C	2.345249	1.204665	-1.774362
C	2.880534	2.512399	-2.067939
C	2.011310	3.453232	-1.437591
C	2.260057	4.826747	-1.613197
C	3.353145	5.232169	-2.382434
C	4.199411	4.289395	-3.001717
C	3.972052	2.926382	-2.851580
Zn	0.000017	0.126999	0.000042
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C	0.914535	-2.697484	0.706081
C	1.927804	-3.431449	1.395178
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C	2.197519	-1.182790	1.647325
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C	3.227843	-5.209989	2.255350
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N	0.000570	-3.314369	-0.000036
C	-0.913591	-2.697782	-0.706130
N	-1.092428	-1.331017	-0.901597
C	-2.197109	-1.183515	-1.647299
C	-2.753527	-2.470091	-2.004402
C	-1.926608	-3.432077	-1.395246
C	-3.823869	-2.905256	-2.809213
C	-4.051185	-4.268275	-2.917047
C	-3.226056	-5.211037	-2.255454
C	-2.154141	-4.805597	-1.486214
C	-2.725679	0.113691	-2.029726
C	-1.907216	1.166339	-2.471955
C	-2.481323	2.348173	-2.956074
C	-3.872603	2.481486	-2.999967
C	-4.687145	1.465024	-2.502467
C	-4.116415	0.281950	-2.017769
C	2.725608	0.114594	2.029811
C	4.116266	0.283350	2.017948
C	4.686530	1.466600	2.502719

C	3.871593	2.482749	3.000195
C	2.480386	2.348945	2.956200
C	1.906746	1.166932	2.472010
C	2.894934	-0.092548	-2.241498
C	2.034095	-1.123976	-2.662610
C	2.523482	-2.390486	-2.977436
C	3.893587	-2.672031	-2.894324
C	4.771671	-1.634455	-2.544944
C	4.285660	-0.366707	-2.229536
H	1.605150	5.565913	-1.150045
H	3.538589	6.292283	-2.515396
H	5.039720	4.640456	-3.609244
H	4.608137	2.199475	-3.351870
H	0.972305	-0.934413	-2.726615
H	1.823898	-3.171280	-3.273846
H	4.275005	-3.670179	-3.119765
H	5.836177	-1.833351	-2.484907
H	4.977578	0.405629	-1.901772
H	-4.608901	2.198122	3.351764
H	-5.041273	4.638972	3.609050
H	-3.540682	6.291234	2.515145
H	-1.606983	5.565444	1.149836
H	-4.977738	0.404091	1.901923
H	-5.835560	-1.835199	2.485156
H	-4.273720	-3.671509	3.119941
H	-1.822742	-3.171781	3.273855
H	-0.971925	-0.934606	2.726510
H	1.501129	-5.501920	0.980595
H	3.455954	-6.270040	2.367127
H	4.871870	-4.617769	3.524540
H	4.460700	-2.198091	3.330690
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H	1.844036	3.150702	3.316058
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H	-4.744799	-0.511600	-1.626545
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H	-4.317563	3.394961	-3.394710
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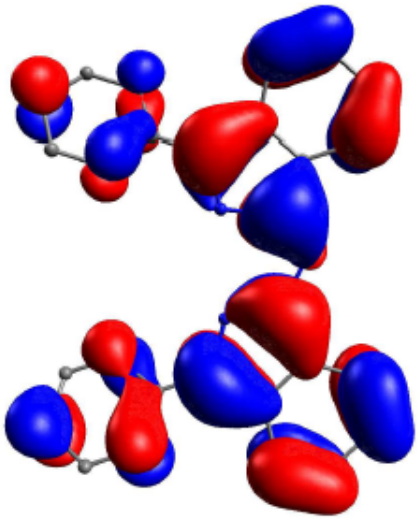
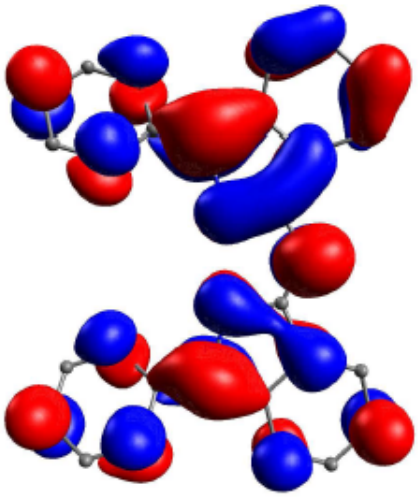
H	-0.824250	1.040329	-2.493621

7. Additional frontier orbitals for 1



(a) HOMO



(b) LUMO