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Electronic Supporting Information

Experimental observation and theoretical investigation on a novel Cd(II) complex with π-hole interaction involving nitro groups

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Computational methods

The energies of the complex included in this study were computed at the BP86-D3/def2-TZVP level of theory. The geometries have been fully optimized unless otherwise noted. For instance to evaluate the noncovalent interactions observed in the solid state, we have used the crystallographic coordinates. The calculations have been performed by using the program TURBOMOLE version 6.5.[1] For the calculations we have used the BP86 functional with the latest available correction for dispersion (D3).[2]

1. R. Ahlrichs, M. Bär, M. Hacer, H. Horn and C. Kömel, *Chem. Phys. Lett.*, 1989, **162**, 165–169.
2. S. Grimme, J. Antony, S. Ehrlich, and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104-19.

Table S1. Crystal data and structure refinement for **1**.

Empirical formula	$C_{38}H_{22}CdN_8O_{12}$, C_3H_7NO, H_2O	
Formula weight	986.15	
Temperature	294(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 12.913(1) Å	a= 114.394(1)°.
	b = 13.7018(10) Å	b= 107.217(1)°.
	c = 14.1084(11) Å	g = 98.206(1)°.
Volume	2068.3(3) $Å^3$	
Z	2	
Density (calculated)	1.583 Mg/m^3	
Absorption coefficient	0.609 mm^{-1}	
F(000)	1000	
Crystal size	0.12 x 0.11 x 0.06 mm^3	
θ range for data collection	1.713 to 28.364°.	
Index ranges	-17<=h<=17, -18<=k<=17, -18<=l<=18	
Reflections collected	24444	
Independent reflections	9737 [R(int) = 0.0209]	
Completeness to θ = 25.000°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.97 and 0.93	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9737 / 2 / 594	
Goodness-of-fit on F^2	0.981	
Final R indices [I>2σ(I)]	R1 = 0.0332, wR2 = 0.0827	
R indices (all data)	R1 = 0.0376, wR2 = 0.0858	
Largest diff. peak and hole	0.628 and -0.350 e.$Å^{-3}$	

Table S2. Hydrogen bonds for **1** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1W)-H(1W)...O(1)	0.87(2)	1.99(4)	2.794(4)	153(6)
O(1W)-H(2W)...O(4)	0.84(2)	2.37(3)	3.178(5)	160(7)
C(24)-H(24)...O(2)	0.93	2.42	3.064(3)	126
C(27)-H(27)...O(4)	0.93	2.23	2.997(4)	139
C(39)-H(39A)...O(6)	0.96	2.58	3.372(7)	140
C(19)-H(19)...O(7)#1	0.93	2.55	3.384(3)	149
C(20)-H(20)...O(1W)#2	0.93	2.53	3.404(5)	157
C(24)-H(24)...O(3)#3	0.93	2.60	3.300(3)	133
C(28)-H(28)...O(8)#4	0.93	2.46	3.279(4)	147
C(37)-H(37)...O(1)#5	0.93	2.59	3.390(3)	144

Symmetry transformations used to generate equivalent atoms:
#1 x+1,y,z+1 #2 x+1,y,z #3 -x,-y,-z+1 #4 x,y,z+1 #5 -x,-y+1,-z+2