Supplementary materials

Effect of non-covalent interactions on the 2,4- and 3,5-dinitrobenzoate Eu-Cd complex structures

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I. Supplementary PXRD data

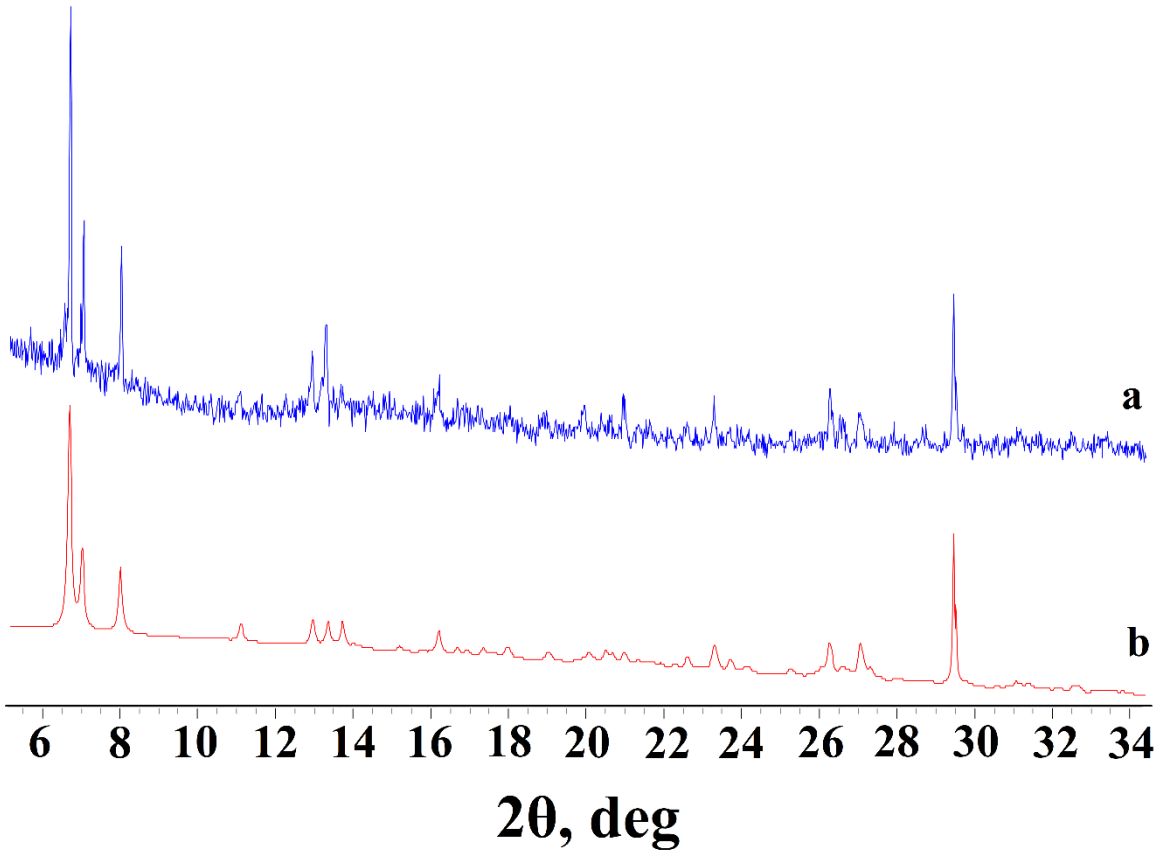

Figure S1 - Experimental (a) and calculated (b) diffractograms for compound **I**.

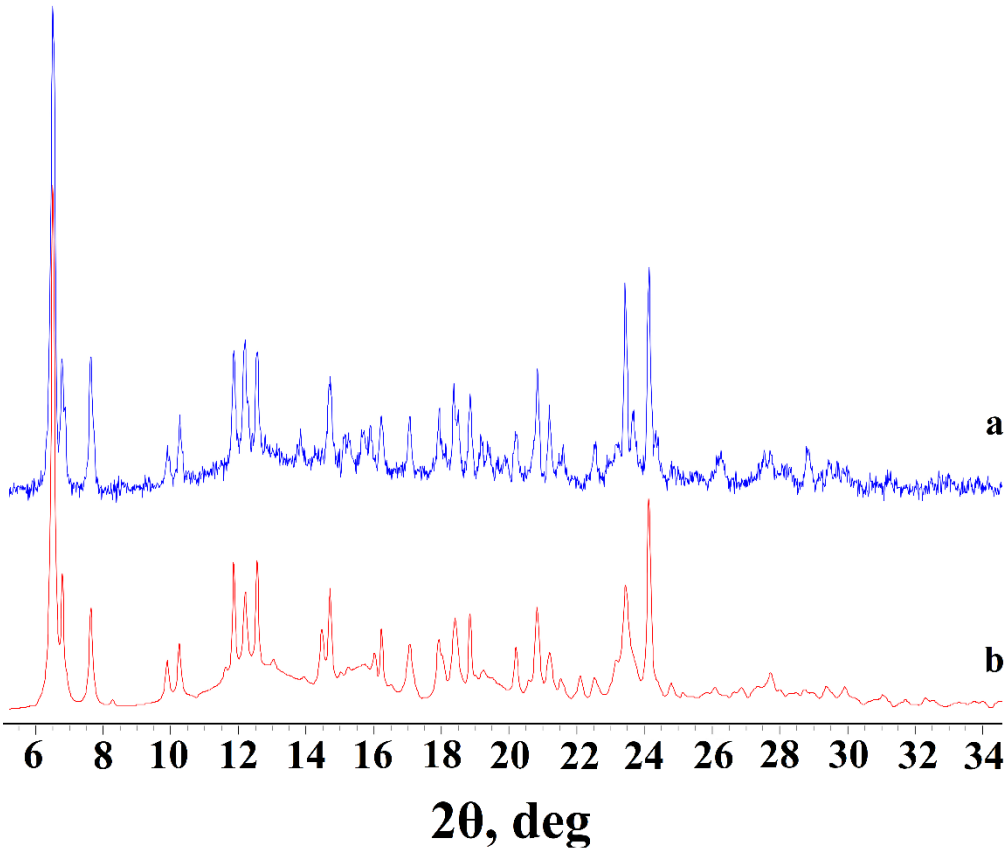

Figure S2 - Experimental (a) and calculated (b) diffractograms for compound **II**.

II. Supplementary structural data

Table S1 - Crystallographic parameters and structure refinement statistics for I, II

Compound	**I**	**II**
M	2784.17	3082.37
T (K)	100.0	100.0
Crystal system	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$
a (Å)	13.491(2)	13.6414(7)
b (Å)	13.608(2)	15.4400(8)
c (Å)	14.501(4)	16.1394(8)
α (°)	104.798(9)	67.702(2)
β (°)	103.449(9)	89.380(2)
γ (°)	101.844(7)	72.122(2)
V (Å^3)	2402.1(8)	2971.6(3)
Z	1	1
$D_{calc.}$ (g cm^{-3})	1.925	1.722
μ (mm^{-1})	1.848	1.507
θ_{max} (°)	26.000	26.000
T_{min}/T_{max}	0.6476/0.7460	0.4831/ 0.7464
Reflections collected	13148	21944
Independent reflections collected	9131	11572

Reflections with $I > 2\sigma(I)$	7397	9106
R_{int}	0.0274	0.0692
GOOF	1.093	1.050
R_1 ($I > 2\sigma(I)$)	0.0365	0.0929
wR_2 ($I > 2\sigma(I)$)	0.0814	0.2531
$\Delta\rho_{min}/\Delta\rho_{max}$ (e/Å^3)	-1.091/0.847	-3.889/ 3.117

Table S2. Continuous Shape Measures (CShM) values for the potential coordination polyhedron of Eu and Cd in **I** and **II**.

	Cd	Eu
I	Octahedron, Oh (2.859)	Capped square antiprism, C4v (1.950) Tricapped trigonal prism, D3h (2.753) Muffin, Cs (1.473)
II	Pentagonal bipyramid, D5h (9.252) Capped octahedron, C3v (8.778) Capped trigonal prism, C2v (8.320)	Square antiprism, D4d (0.440) Triangular dodecahedron, D2d (2.207) Biaugmented trigonal prism, C2v (1.393)

Table S3. N-O… π interactions in the crystal packing of I-II.

Взаимодействие	O–Cg, Å	Symmetry code	O–Perp, Å	O-C_{min}	N-O...Cg,^{O}
Complex I					
N(3)–O(3)… π(2,4-Nbz)	3.525(5)	1-X,1-Y,1-Z	3.251	3.305(6)	127.7(3)
N(6)–O(6)… π(MeCN)	3.213(5)			3.187(8)	81.5(3)
N(7)–O(15)… π(2,4-Nbz)	3.373(5)		3.150	3.173(7)	83.7(3)
N(8)–O(18)… π(2,4-Nbz)	2.962(5)	-X,1-Y,1-Z	2.920	3.061(6)	112.8(3)
N(10)–O(24)… π(2,4-Nbz)	3.219(5)	-X,1-Y,1-Z	3.096	3.141(7)	90.9(3)
N(11)–O(26)… π(2,4-Nbz)	3.455(6)	X,1+Y,Z	3.204	3.214(7)	143.8(5)
Complex II					
N(4)–O(6)… π(Phen)	3.567(8)	1-X,-Y,2-Z	3.129	3.231(13)	161.4(6)
N(5)–O(10)… π(Phen)	3.694(10)	1+X,Y,Z	3.517	3.621(13)	147.2(8)
N(10)–O(23)… π(3,5-Nbz)	3.508(10)	2-X,-Y,1-Z	3.334	3.343(12)	94.2(6)
N(6)–O(11)… π(3,5-Nbz)	3.443(7)		3.193	3.208(10)	156.8(6)
N(12)-O(30) … π(3,5-Nbz)	3.343(9)		3.048	3.049(10)	120.3(7)
N(9)-O(21)… π(MeCN)	3.261(20)		3.260		

Note. Cg is the centroid of aromatic rings, Perp is the perpendicular to the ring plane, α is the angle between the planes of aromatic moieties.

Table S4. C-H…O interactions in the crystal packing of I-II.

Interaction	Distance, Å				D – H…A, °
	D–H	Symmetry code	H...A	D...A	
	Complex I				
C(3S)–H(3SA)…O(14)	0.98		2.51	3.074(8)	117
C(4)–H(4)…O(4)	0.95	1-x,2-y,1-z	2.39	3.096(7)	131
C(14)–H(14)…O(3)	0.95		2.56	3.312(7)	136
C(18)–H(18)…N(1S)	0.95	-x,1-y,2-z	2.51	3.388(10)	153
C(20)–H(20)…O(10)	0.95	1-x,1-y,2-z	2.39	3.327(7)	167
C(28)–H(28)…O(21)	0.95	-x,1-y,2-z	2.58	3.313(8)	134
C(30)–H(30)…O(20)	0.95	x,y,-1+z	2.52	3.148(8)	124
C(36)–H(36)…O(15)	0.95	x,-1+y,z	2.35	3.223(8)	152
C(37)–H(37)…O(12)	0.95	1-x,1-y,2-z	2.45	3.359(7)	159
C(38)–H(38)…O(9)	0.95		2.47	3.420(7)	173
	Complex II				
C(12)–H(12)…O(25)	0.95	-1+x,y,z	2.60	3.497(11)	158
C(19)–H(19)…O(29)	0.95	x,-1+y,z	2.42	3.235(13)	144
C(26)–H(26)…O(28)	0.95	2-x,1-y,1-z	2.47	3.178(16)	131
C(41)–H(41)…O(24)	0.95	2-x,-y,2-z	2.58	3.438(13)	150
C(35)–H(35)…O(14)	0.95	1-x,-y,2-z	2.53	2.998(13)	111

Table S5. N-O…N interactions in the crystal packing of I-II.

Interaction	Distance, Å		Symmetry code	O – N…O, °
	N…O	O…O		
Complex I				
N(6)...O(6)	2.964(8)	3.169(6)	x,y,1+z	88.1(4)
N(11)...O(12)	2.944(8)	3.008(7)	1-x,2-y,2-z	81.4(4)
Complex II				
N(5)...O(27)	2.897(15)	2.964(11)	2-x,-y,1-z	80.9(6)
N(7)...O(23)	2.986(12)	3.143(10)	1-x,2-y,2-z	85.9(5)

Table S6. Stacking interactions in the crystal packing of **I-II**.

Interaction	Cg–Cg, Å	Symmetry code	Cg–Perp, Å	C-C$_{min}$	α, deg	β, deg	γ, deg
Complex I							
Phen –2,4-Nbz	3.688(3)	1-X,1-Y,1-Z	3.420(2)	3.460(7)	13.2(3)	21.6	8.4
Phen –2,4-Nbz	3.648(3)	-X,1-Y,1-Z	3.470(2)	3.432(7)	1.0(3)	18.0	18.1
Complex II							
Phen – Phen	3.574(6)	2-X,-Y,2-Z	3.349(4)	3.382(14)	0.0(5)	20.5	20.5

Note. Cg is the centroid of aromatic rings, Perp is the perpendicular to the ring plane, α is the angle between the planes of aromatic moieties.

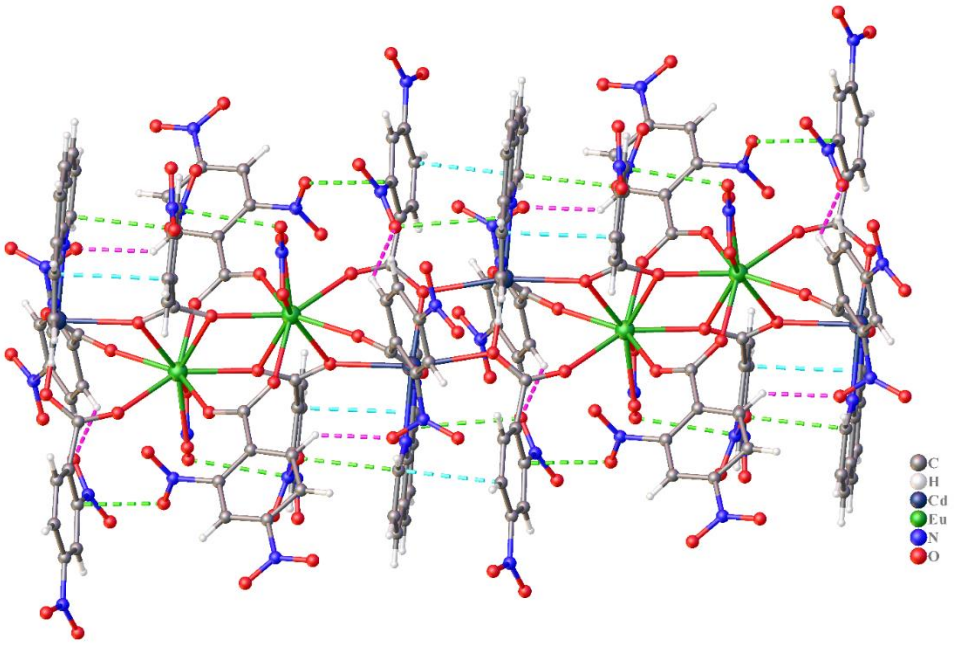

Figure S3 – Non-covalent interactions in the structure of the complex **I**. Green dashed line - N-O…π interactions, purple line - C-H…O, light blue line - stacking interactions.

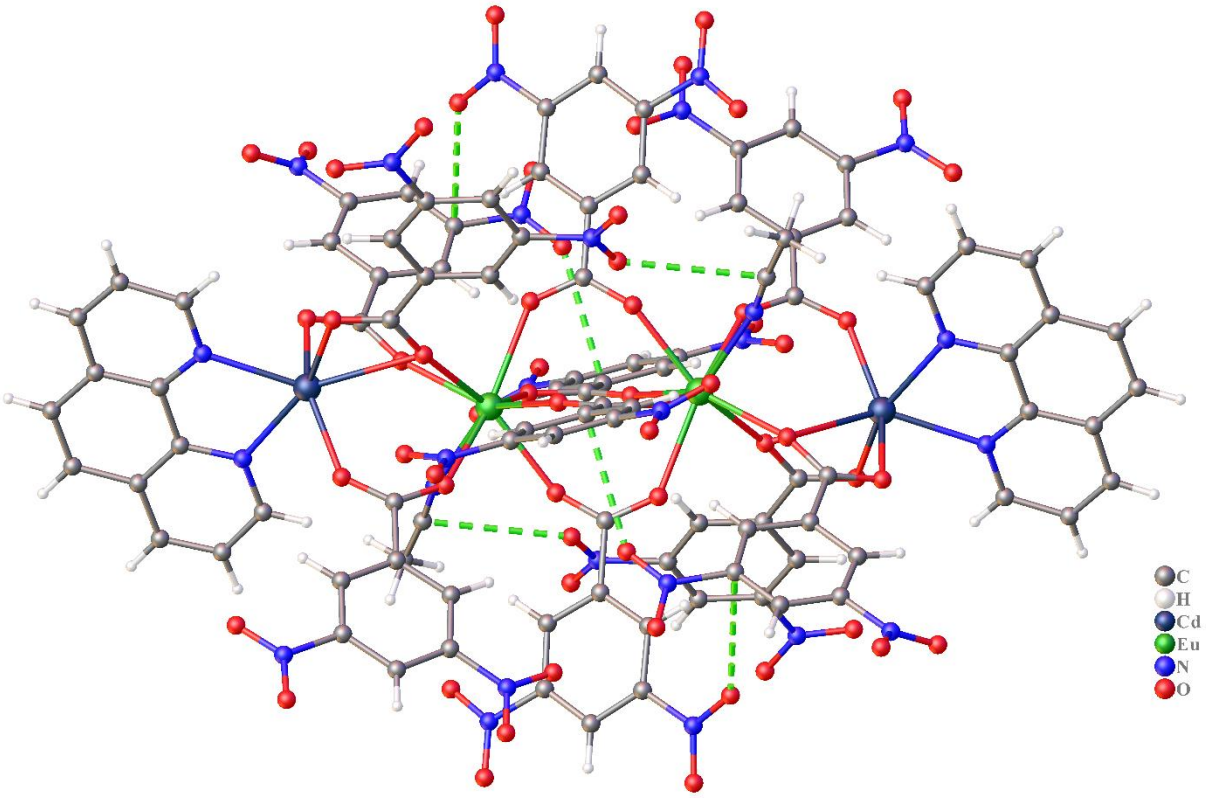

Figure S4 – Non-covalent interactions in the structure of the complex **II**. Green dashed line - N-O…π interactions.

III. Supplementary DTA data

III. Supplementary Differential thermal analysis (DTA) data

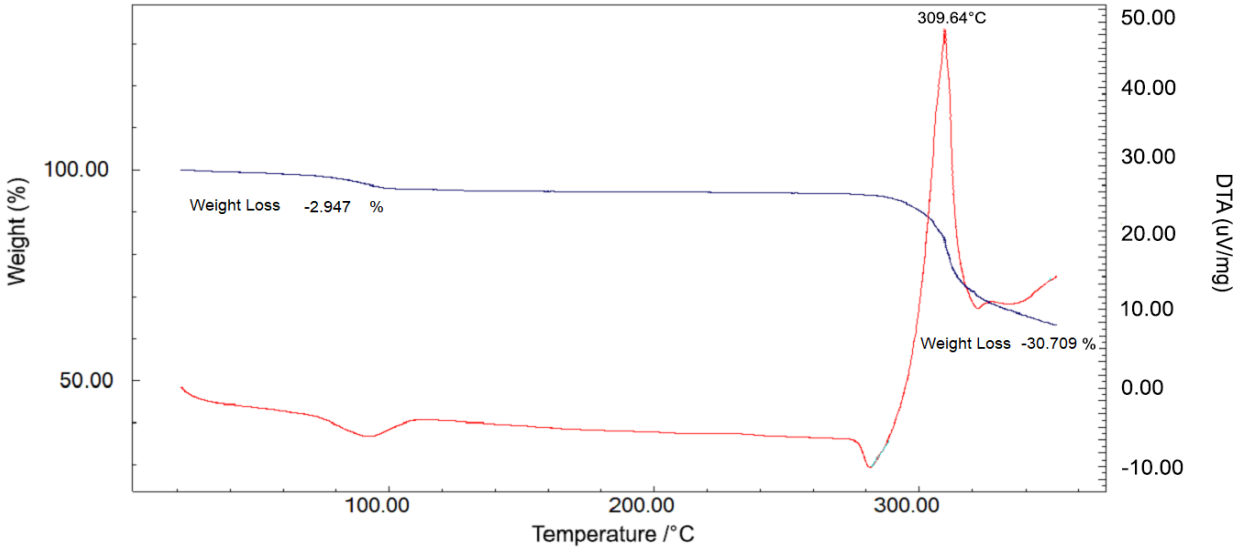

Figure S5 – Differential thermal analysis (DTA**)** data for compound **II**.