

Supplementary Information

**Synthesis, crystal structure and properties of tris(benzene-1,2-diamine-N,N')-
cadmium naphthalene-1,5-disulfonate trihydrate complex compound**

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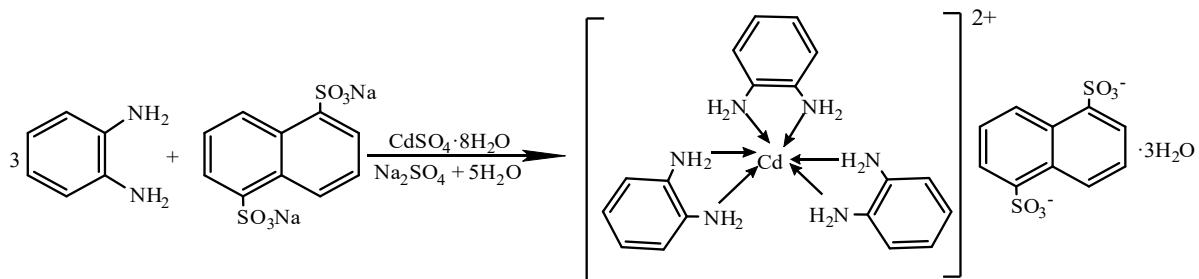
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Scheme.1. Synthesis reaction of complex compound $[Cd(OPD)_3]1,5-NDS \cdot 3H_2O$.

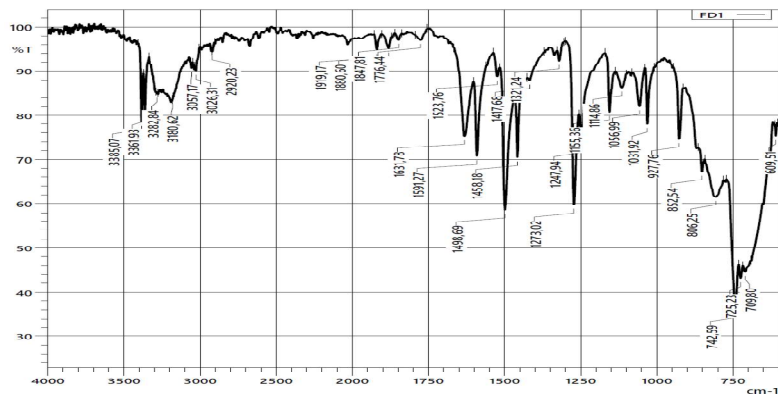


Fig. 1. IR spectrum of OPD ligand

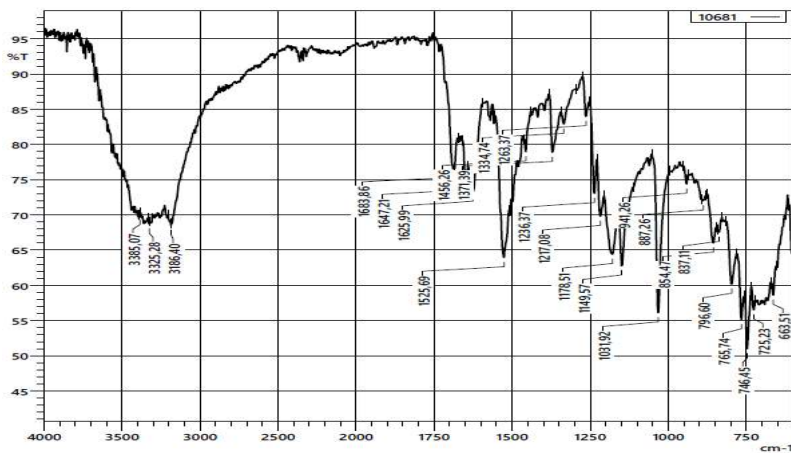


Fig 2. IR spectrum of the complex compound $[Cd(OPD)_3]1,5-NDS \cdot 3H_2O$.

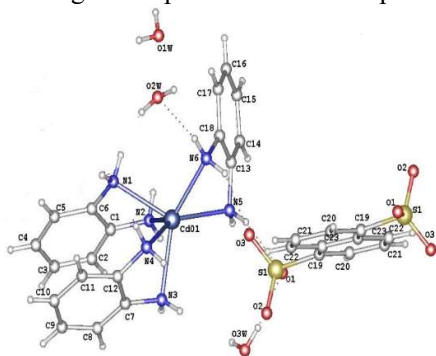


Fig. 3a. Molecular structure of the complex $[Cd(OPD)_3]1,5-NDS \cdot 3H_2O$.

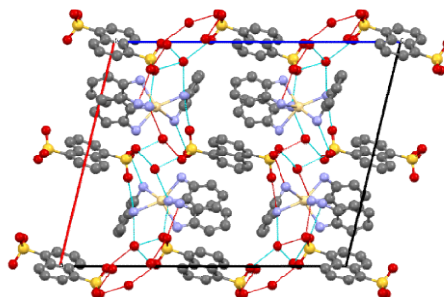


Fig. 3b. Plotting of the complex compound $[Cd(OPD)_3]1,5-NDS \cdot 3H_2O$ along the c axis (blue lines depict hydrogen bonds).

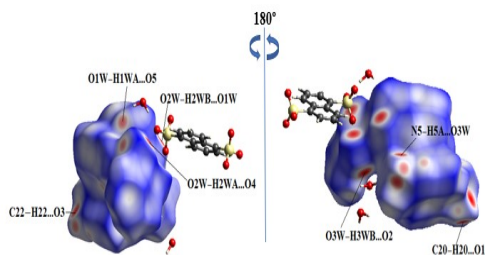
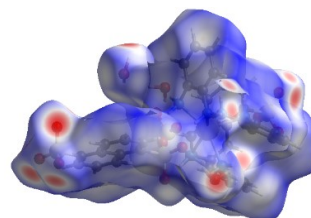
Table 1. Geometry of hydrogen bonds of complex compound $[\text{Cd}(\text{OPD})_3]1,5\text{-NDS}\cdot 3\text{H}_2\text{O}$

$D-H\cdots A$	$D-H, \text{\AA}$	$H\cdots A, \text{\AA}$	$D\cdots A, \text{\AA}$	DHA, angle
O3W-H3WA...O1	0.8500	1.9700	2.812(4)	172.00
N1-H1B...O5	0.89(3)	2.23(3)	3.010(4)	147(3)
O3W-H3WB...O2	0.8500	2.0100	2.849(4)	168.00
N2-H2A...O5	0.89(3)	2.39(3)	3.129(3)	141(3)
N2-H2B...O4	0.89(2)	2.58(2)	3.363(4)	147(3)
O2W-H2WA...O4	0.8500	2.0600	2.852(4)	155.00
N3-H3A...O2	0.89(3)	2.34(3)	3.083(4)	141(3)
O2W-H2WB...O1W	0.8500	2.5600	3.042(6)	117.00
N4-H4A...O4	0.89(2)	2.07(2)	2.914(3)	160(2)
N4-H4B...O3W	0.88(3)	2.17(3)	3.047(4)	173(3)
O1W-H1WA...O5	0.8500	2.2100	3.005(5)	157.00
N5-H5A...O3W	0.89(3)	2.40(3)	3.265(4)	166(3)
N5-H5B...O1	0.89(3)	2.16(3)	3.000(4)	159(2)
O1W-H1WB...O2W	0.8500	2.1400	2.963(5)	163.00
N6-H6A...O3	0.89(3)	2.14(3)	2.940(4)	150(2)
N6-H6B...O2W	0.89(3)	2.04(3)	2.913(4)	165(3)
C20-H20...O1	0.9300	2.4100	2.835(4)	108.00
C22-H22...O3	0.9300	2.4600	3.081(4)	124.00

Symmetry codes: 1-x, 1-y, -z; 2-x, 1-y, 1-z; x, 1+y, z; 1-x, 1/2+y, 1/2-z; 1-x, -1/2+y, 1/2-z; x, -1+y, z; x, 5/2-y, -1/2+z; 2-x, 1/2+y, 1/2-z; x, 5/2-y, 1/2+z; x, 3/2-y, 1/2+z; 1-x, 2-y, -z; 2-x, 1/2+y, 1/2-z; x, 3/2-y, -1/2+z; 1-x, 2-y, -z; 2-x, -1/2+y, 1/2-z; 2-x, -1/2+y, 1/2-z; x, 1/2-y, 1/2+z; x, 1/2-y, -1/2+z.

Table 2. Crystal data of the complex $[\text{Cd}(\text{OPD})_3]1,5\text{-NDS}\cdot 3\text{H}_2\text{O}$

Parameters	Values	Parameters	Values
Formula	$[\text{Cd}(\text{OPD})_3]1,5\text{-NDS}\cdot 3\text{H}_2\text{O}$	Crystal size, mm	0.20 x 0.28 x 0.30
Molecular mass	777.15	Temperature T, ok	566
Syngonia	monoclinic	Scan interval θ , o	$\theta = 2.6\text{--}71.4^\circ$
Spatial group	P21/c	Interval h,k,l	-21: 21; -8: 10; -26: 27
a, \AA	17.6185(2)	Total reflexes	33725
b, \AA	8.3960(1)	The number of independent reflexes	6140
c, \AA	22.0916(2)	R_{int}	0.059
α°	90	$F^2 \geq 2\sigma(F^2)$	5302
β°	103.787(1)	No. of reflections	6140
γ°	90	No. of parameters	473
V, \AA^3	3173.75(6)	RI, wR2(1>2 σ (I))	0.0333, 0.0886, 1.08
Z	4	$\Delta_{\text{pmin/max}} \text{e}\text{\AA}^{-3}$	-0.54, 0.53
$D_x \text{g}/\text{cm}^3$	1.627	CCDC-number	2268254
$\mu(\text{CuK}\alpha)$, mm^{-1}	7.279		

Fig. 4. Hirschfeld surface of the complex compound $[\text{Cd}(\text{OPD})_3]1,5\text{-NDS}\cdot 3\text{H}_2\text{O}$ by cation.Fig. 4. Total Hirschfeld surface area of the complex compound $[\text{Cd}(\text{OPD})_3]1,5\text{-NDS}\cdot 3\text{H}_2\text{O}$.

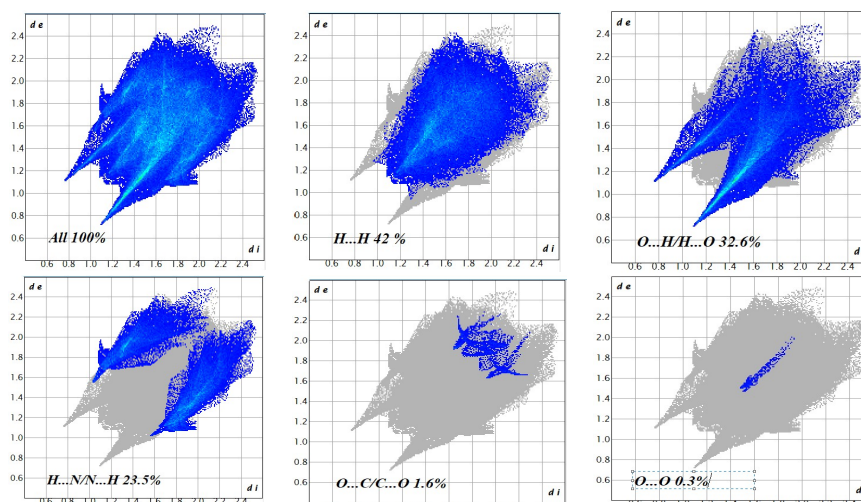


Fig 5. 2D fingerprint view of the Hirschfeld surface of the $[Cd(OPD)_3]1,5-NDS \cdot 3H_2O$ complex.

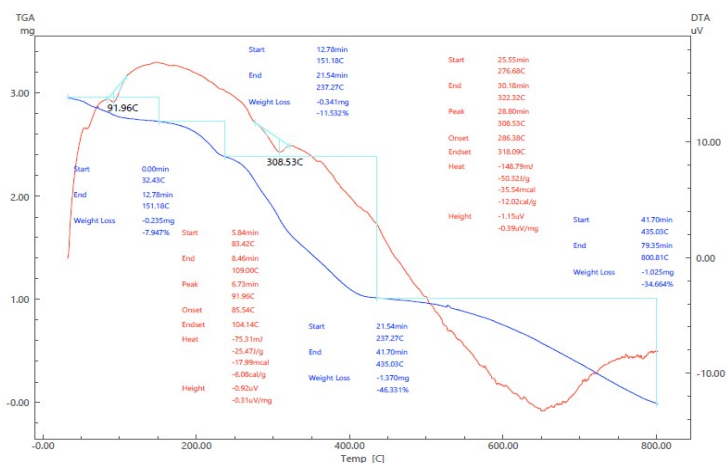


Fig.6. Derivatogram of the complex compound $[Cd(OPD)_3]1,5-NDS \cdot 3H_2O$

Table 3. Thermal analysis of the complex compound $[Cd(OPD)_3]1,5-NDS \cdot 3H_2O$

No	Temperature, °C	Lost mass, mg.	Mass loss, %	The amount of energy consumed ($\mu V \cdot s / mg$)	Time spent (min)
1	32-151°C	0.235	7.947	16.84	12.78
2	151-237°C	0.341	11.532	14.41	8.76
3	237-435°C	1.37	46.331	2.915	20.16
4	435-800°C	1.025	34.664	8.58	37.65

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Datablock: exp_1063

Space Group: P21/c, **Cell:** *a* 17.618Å *b* 8.396Å *c* 22.092Å, α 90° β 103.7870(10)° γ 90°

Formula: C₁₈ H₂₄ Cd₁ N₆ 2+, C₁₀ H₆ O₆ S₂ 2-, 3(H₂ O₁), Temperature: 566.15 K

▼ User Details

Reliability Score

2

2D Diagram

True

2D/3D Match

Full

2D/3D Last Edited

User Compound Name

[tris\(benzene-1,2-diamine\)-cadmium naphthalene-1,5-disulfonate hydrate](#)

User Identifier

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▼ Additional Details

Deposition Number

2268254

Refcode

Compound Name

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