Electronic Supplementary Data

The supramolecular assembly of cyanurate cobalt(II) complexes: Crystal structure, TD-DFT approach and thermal study

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Table S1 - Selected IR bands (cm^{-1}) and their assignments for complex **1**

	Experimental, in solid state as KBr pellet (cm^{-1})	Theoretical [§] (cm^{-1})
(O-H) stretching (H-bonded)	3380(br)	3594 (non H-bonded)
(sp^3N-H) stretching	3380(br)	3237
(amide C=O)	1740 (s)	1781
(N-H)	1628 (vs)	1627
$_r(H_2O)$	776 (s)	794
$_w(H_2O)$	554 (s)	563

br = broad, vs = very strong, s = strong, w = weak.

[§] Basis set, LanL2MB; using conductor-like polarizable continuum model (CPCM) in water.

Table S2 - H bond parameters for complex **1**

D-H	d(D-H)	d(H..A)	d(D..A)	<DHA	A
O1--H1A	0.67(3)	2.26(3)	2.795(2)	138(3)	O6
O1--H1B	0.82(3)	1.95(3)	2.767(2)	174(2)	O12
N2--H2	0.82(3)	1.97(3)	2.787(2)	174(2)	O9
O2--H2A	0.81(3)	1.97(3)	2.778(2)	175(3)	O9
O2--H2B	0.84(2)	1.92(2)	2.731(2)	164(2)	O12
N3--H3	0.83(3)	2.04(3)	2.868(2)	176(2)	O10
O3--H3A	0.82(3)	1.94(3)	2.754(2)	173(3)	O7
O3--H3B	0.72(3)	2.19(3)	2.851(2)	153(3)	O10
O4--H4A	0.81(3)	1.93(3)	2.717(2)	162(3)	O13
O4--H4B	0.79(3)	2.09(3)	2.879(2)	178(3)	N4
N5--H5	0.94(3)	1.88(3)	2.823(2)	179(2)	O8
O5--H5A	0.74(3)	2.13(3)	2.866(2)	173(3)	N4
O5--H5B	0.78(3)	1.96(3)	2.724(2)	164(3)	O13
N6--H6	0.92(2)	1.91(2)	2.818(2)	171(2)	O6
O12--H12A	0.75(3)	2.00(3)	2.734(2)	167(3)	O11
O12--H12B	0.73(4)	2.18(4)	2.894(2)	168(3)	O2
O13--H13A	0.81(3)	1.93(3)	2.717(2)	165(3)	O11
O13--H13B	0.84(3)	2.22(3)	2.907(2)	140(2)	O4
O13--H13B	0.84(3)	2.45(3)	3.045(2)	129(2)	O5
O13--H13B	0.84(3)	2.49(3)	3.110(2)	132(3)	O8

Table S3 - Selected MOs along with their energies and compositions of complex

	Energy (ev)	(%) Composition									
		Cacid	Co(II)	Aq1	Aq2	Aq3	Aq4	Aq5	Lattice acid	Lattice aq1	Lattice aq2
α-MO											
HOMO-5	-4.29	61	11	12	1	0	1	5	7	0	0
HOMO-4	-4.23	21	12	1	2	1	6	3	37	14	3
HOMO-3	-4.17	14	3	1	0	1	1	2	71	7	0
HOMO-2	-4.06	16	24	10	2	0	7	19	21	0	0
HOMO-1	-3.95	1	1	48	48	0	0	1	0	0	0
HOMO	-2.59	0	1	88	11	0	0	0	0	0	0
LUMO	0.80	12	59	7	0	0	11	11	0	0	0
LUMO+1	1.31	6	1	0	0	1	0	1	91	0	0
LUMO+2	1.37	84	4	1	0	0	1	1	9	0	0
LUMO+3	1.88	50	36	2	5	1	1	2	2	0	0
LUMO+4	2.33	4	1	0	0	0	0	1	93	0	0
LUMO+5	2.57	45	37	2	8	1	1	2	4	0	0
β-MO											
HOMO-5	-4.23	50	18	8	1	2	5	5	11	0	0
HOMO-4	-4.17	18	3	0	0	1	0	4	67	7	0
HOMO-3	-4.16	42	29	3	0	2	10	2	8	2	0
HOMO-2	-4.03	8	30	9	1	0	3	20	28	0	1
HOMO-1	-3.94	1	5	2	0	0	0	86	4	0	0
HOMO	-2.59	0	10	40	50	0	0	0	0	0	0
LUMO	0.54	2	86	3	8	1	0	0	0	0	0
LUMO+1	1.29	52	5	0	0	41	1	1	1	0	0
LUMO+2	1.32	34	4	0	0	1	0	1	58	0	0
LUMO+3	1.64	16	60	5	1	0	9	8	1	0	0
LUMO+4	2.02	58	29	2	6	1	1	2	2	0	0
LUMO+5	2.33	5	1	0	0	0	0	1	92	0	0

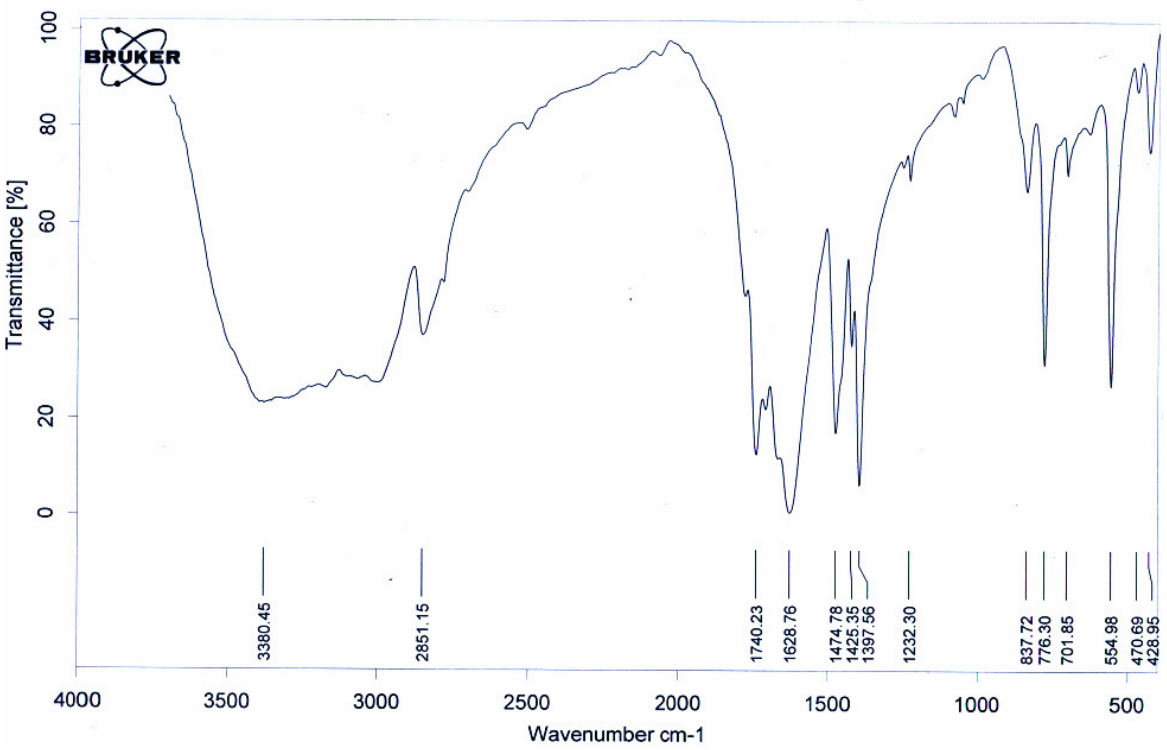


Fig. S1 - IR spectrum of complex **1**.

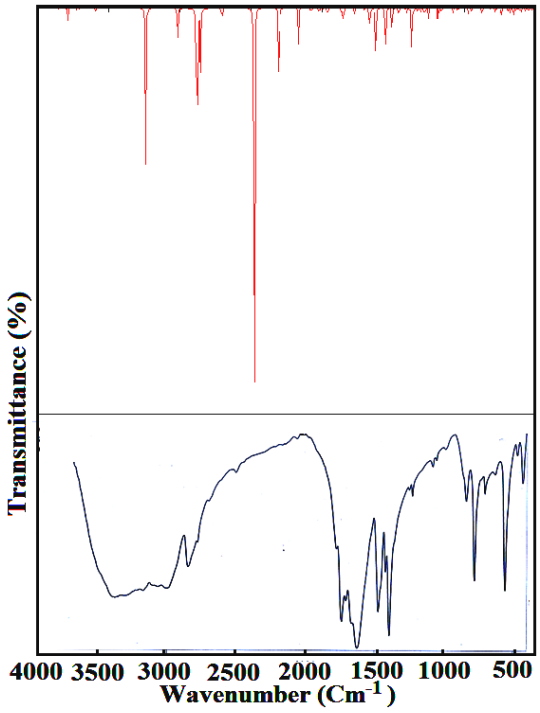


Fig. S2 - Theoretical [red line, using basis set LanL2MB; using conductor-like polarizable continuum model (CPCM) in water] and experimental [black line, as KBr pellet] IR spectra of complex **1**.

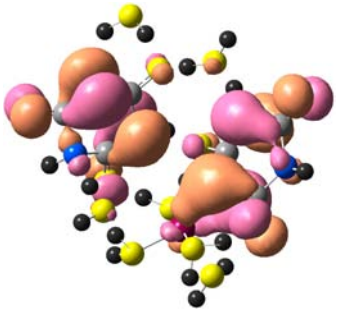
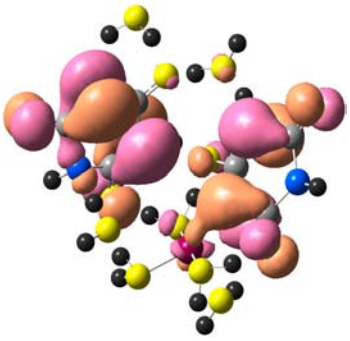
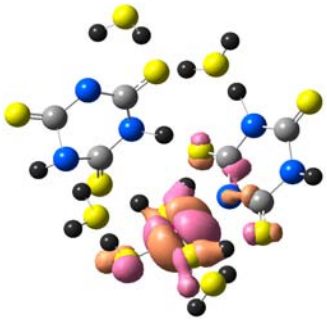
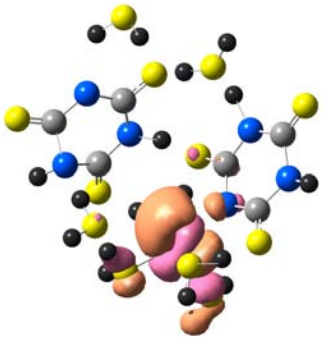
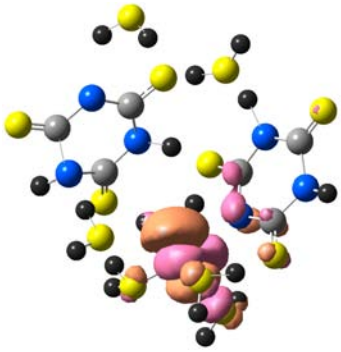
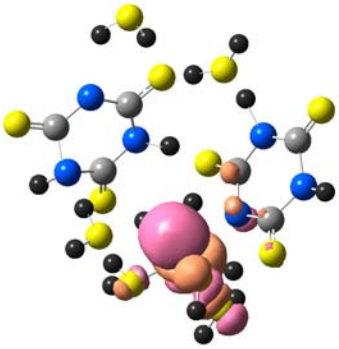
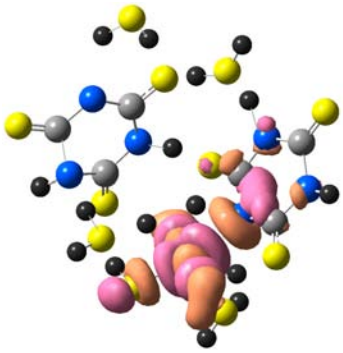
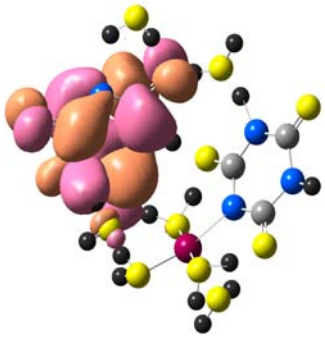
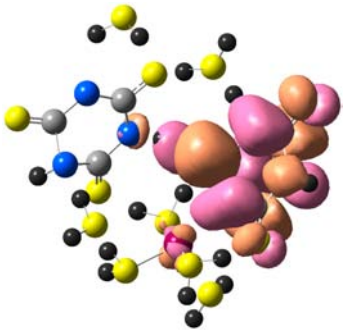
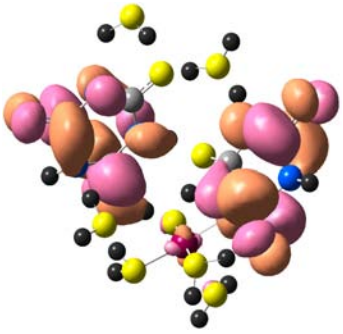
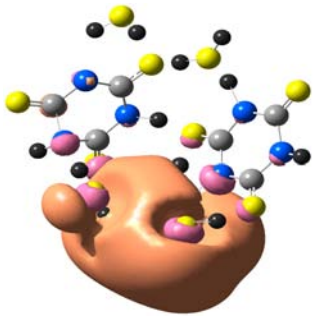
α-MOs			
 HOMO-5, -4.29eV cacid; 61%, Co(II); 11%, aq1; 12%, aq2; 1%, aq3; 0, aq4; 1%, aq5; 5%, lattice acid; 7%, lattice aq1; 0, lattice aq2; 0	 HOMO-4, -4.23eV cacid; 21%, Co(II); 12%, aq1; 1%, aq2; 2%, aq3; 1%, aq4; 6%, aq5; 3%, lattice acid; 37%, lattice aq1; 14%, lattice aq2; 3%	 HOMO-3, -4.17eV cacid; 14%, Co(II); 3%, aq1; 1%, aq2; 0, aq3; 1%, aq4; 1%, aq5; 2%, lattice acid; 71%, lattice aq1; 7%, lattice aq2; 0	 HOMO-2, -4.06eV cacid; 16%, Co(II); 24%, aq1; 10%, aq2; 2%, aq3; 0, aq4; 7%, aq5; 19%, lattice acid; 21%, lattice aq1; 0, lattice aq2; 0
 HOMO-1, -3.95eV cacid; 1%, Co(II); 1%, aq1; 48%, aq2; 48%, aq3; 0, aq4; 0, aq5; 1%, lattice acid; 0, lattice aq1; 0, lattice aq2; 0	 HOMO, -2.59eV cacid; 0, Co(II); 1%, aq1; 88%, aq2; 11%, aq3; 0, aq4; 0, aq5; 0, lattice acid; 0, lattice aq1; 0, lattice aq2; 0	 LUMO, -0.80eV cacid; 12%, Co(II); 59%, aq1; 7%, aq2; 0, aq3; 0, aq4; 11%, aq5; 11%, lattice acid; 0, lattice aq1; 0, lattice aq2; 0	 LUMO+1, 1.31eV cacid; 6%, Co(II); 1%, aq1; 0, aq2; 0, aq3; 1%, aq4; 0, aq5; 1%, lattice acid; 91%, lattice aq1; 0, lattice aq2; 0
 LUMO+2,1.37eV cacid; 84%, Co(II); 4%, aq1; 1%, aq2; 0, aq3; 0, aq4; 1%, aq5; 1%, lattice acid; 9%, lattice aq1; 0, lattice aq2; 0	 LUMO+3,1.88eV cacid; 50%, Co(II); 36%, aq1; 2%, aq2; 5%, aq3; 1%, aq4; 1%, aq5; 2%, lattice acid; 2%, lattice aq1; 0, lattice aq2; 0	 LUMO+4,2.33eV cacid; 4%, Co(II); 1%, aq1; 0, aq2; 0, aq3; 0, aq4; 0, aq5; 1%, lattice acid; 93%, lattice aq1; 0, lattice aq2; 0	 LUMO+5,2.57eV cacid; 45%, Co(II); 37%, aq1; 2%, aq2; 8%, aq3; 1%, aq4; 1%, aq5; 2%, lattice acid; 4%, lattice aq1; 0, lattice aq2; 0

Fig. S3 - Surface plot of some frontier molecular orbital of complex **1** (Contd.).

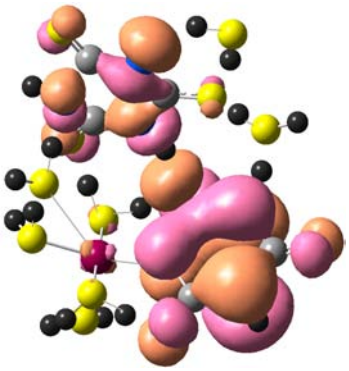
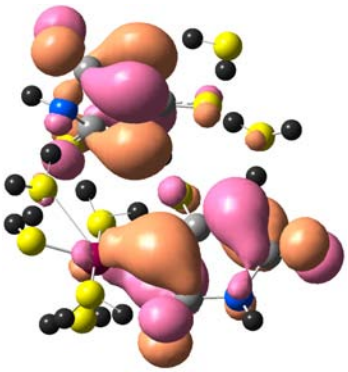
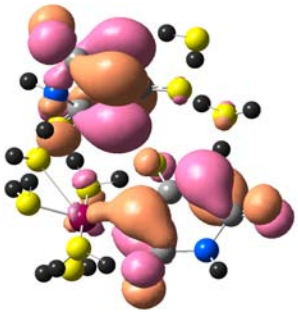
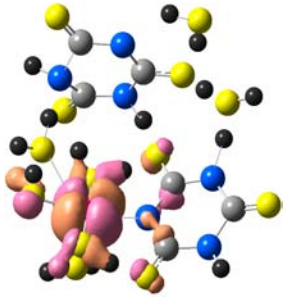
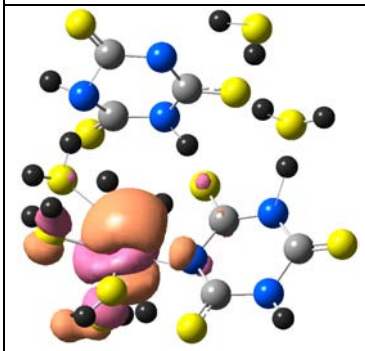
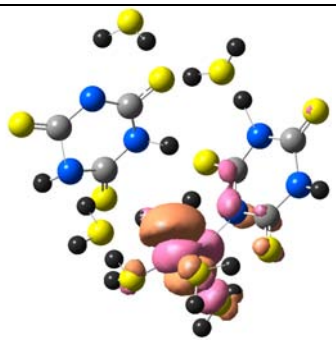
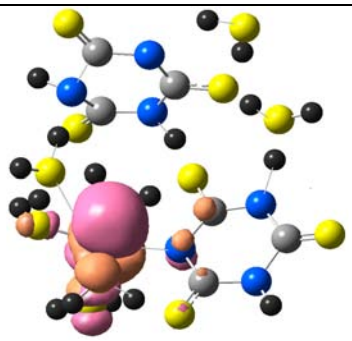
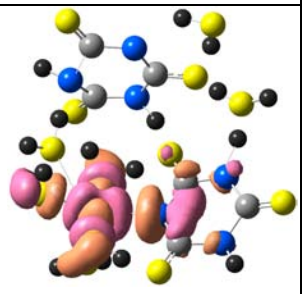
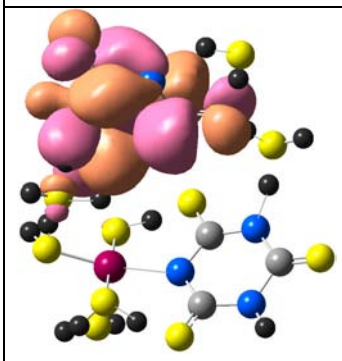
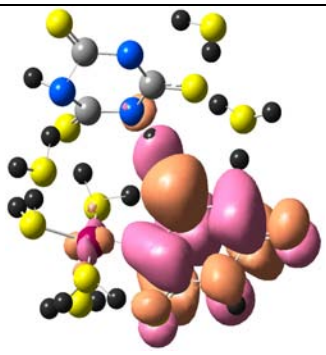
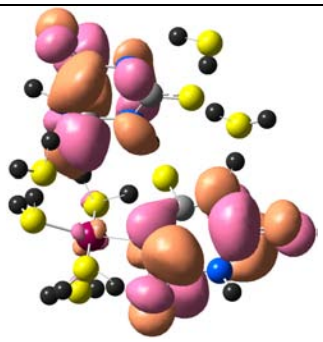
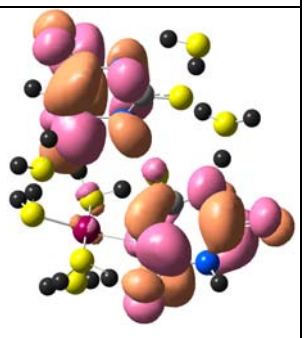
β-MOs			
 HOMO-5,-4.23eV cacid; 50%, Co(II); 18%, aq1; 8%, aq2; 1%, aq3; 2%, aq4; 5%, aq5; 5%, lattice acid; 11%, lattice aq1; 0, lattice aq2; 0	 HOMO-4,-4.17eV cacid; 18%, Co(II); 3%, aq1; 0, aq2; 0, aq3; 1%, aq4; 0, aq5; 4%, lattice acid; 67%, lattice aq1; 7%, lattice aq2; 0	 HOMO-3,-4.16eV cacid; 42%, Co(II); 29%, aq1; 3%, aq2; 0, aq3; 2%, aq4; 10%, aq5; 2%, lattice acid; 8%, lattice aq1; 2%, lattice aq2; 0	 HOMO-2,-4.03eV cacid; 8%, Co(II); 30%, aq1; 9%, aq2; 1%, aq3; 0, aq4; 3%, aq5; 20%, lattice acid; 28%, lattice aq1; 0, lattice aq2; 1%
 HOMO-1,-3.94eV cacid; 1%, Co(II); 5%, aq1; 2%, aq2; 0, aq3; 0, aq4; 0, aq5; 86%, lattice acid; 4%, lattice aq1; 0, lattice aq2; 0	 HOMO,-2.59eV cacid; 0, Co(II); 10%, aq1; 40%, aq2; 50%, aq3; 0, aq4; 0, aq5; 0, lattice acid; 0, lattice aq1; 0, lattice aq2; 0	 LUMO,0.54eV cacid; 2%, Co(II); 86%, aq1; 3%, aq2; 8%, aq3; 1%, aq4; 0, aq5; 0, lattice acid; 0, lattice aq1; 0, lattice aq2; 0	 LUMO+1,1.29eV cacid; 52%, Co(II); 5%, aq1; 0, aq2; 0, aq3; 41%, aq4; 1%, aq5; 1%, lattice acid; 1%, lattice aq1; 0, lattice aq2; 0
 LUMO+2,1.32eV cacid; 34%, Co(II); 4%, aq1; 0, aq2; 0, aq3; 1%, aq4; 0, aq5; 1%, lattice acid; 58%, lattice aq1; 0, lattice aq2; 0	 LUMO+3,1.64eV cacid; 16%, Co(II); 60%, aq1; 5%, aq2; 1%, aq3; 0, aq4; 9%, aq5; 8%, lattice acid; 1%, lattice aq1; 0, lattice aq2; 0	 LUMO+4,2.02eV cacid; 58%, Co(II); 29%, aq1; 2%, aq2; 6%, aq3; 1%, aq4; 1%, aq5; 2%, lattice acid; 2%, lattice aq1; 0, lattice aq2; 0	 LUMO+5,2.33eV cacid; 5%, Co(II); 1%, aq1; 0, aq2; 0, aq3; 0, aq4; 0, aq5; 1%, lattice acid; 92%, lattice aq1; 0, lattice aq2; 0

Fig. S3 (Contd.) - Surface plot of some frontier molecular orbital of complex **1**.

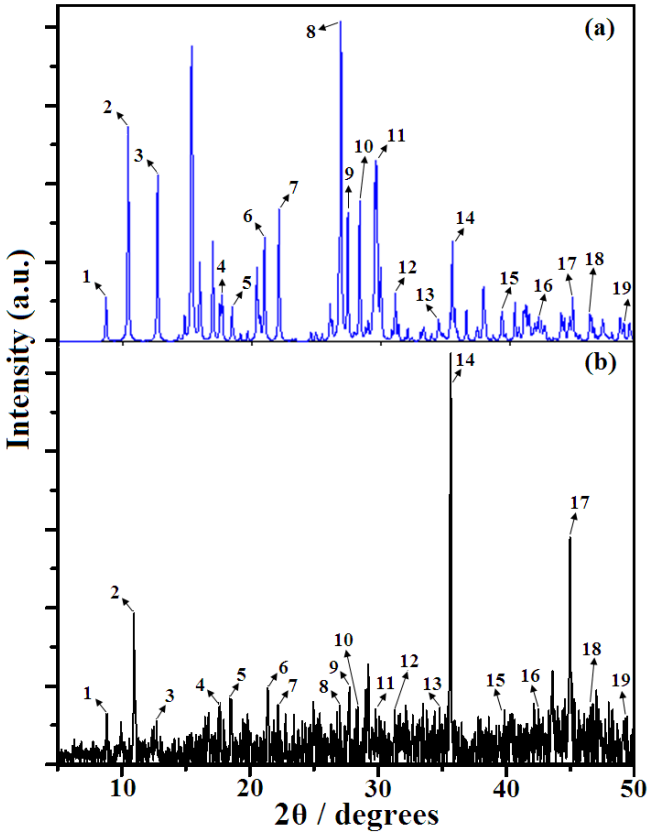


Fig. S4 - XRPD pattern of complex **1** [(a) simulated; (b) as synthesized]. Similarity in simulated and as-synthesized pattern indicates high purity of the compound. Some apparent differences can be attributed to preferred crystallite orientation.

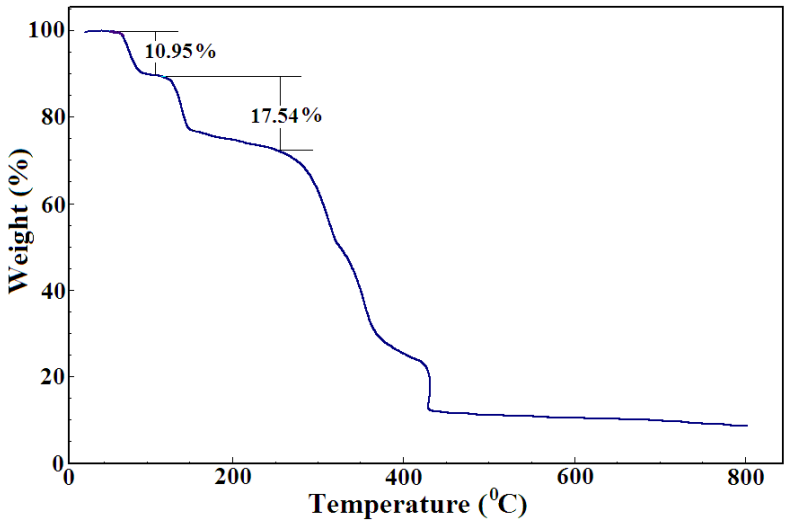


Fig. S5 - TGA of complex **1** carried out under N_2 atmosphere.