Electronic Supplementary Material (ESI) for *CrystEngComm*

Electronic Supplementary Information (ESI)

Metal-organic frameworks derived from bis-pyridyl-bis-amide ligands: Effect of positional isomerism of the ligands, hydrogen bonding backbone, counter anions on the supramolecular structures and selective crystallization of sulfate anion

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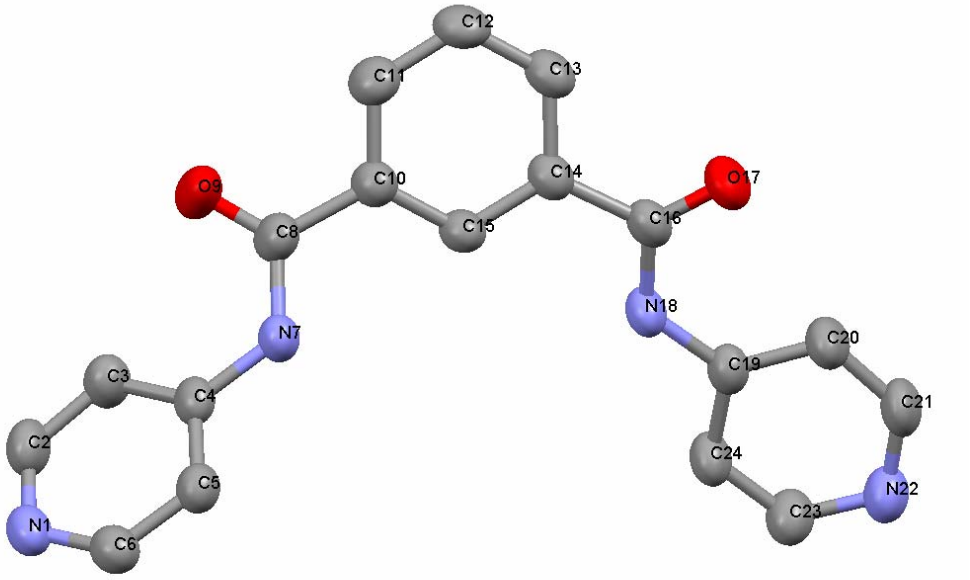
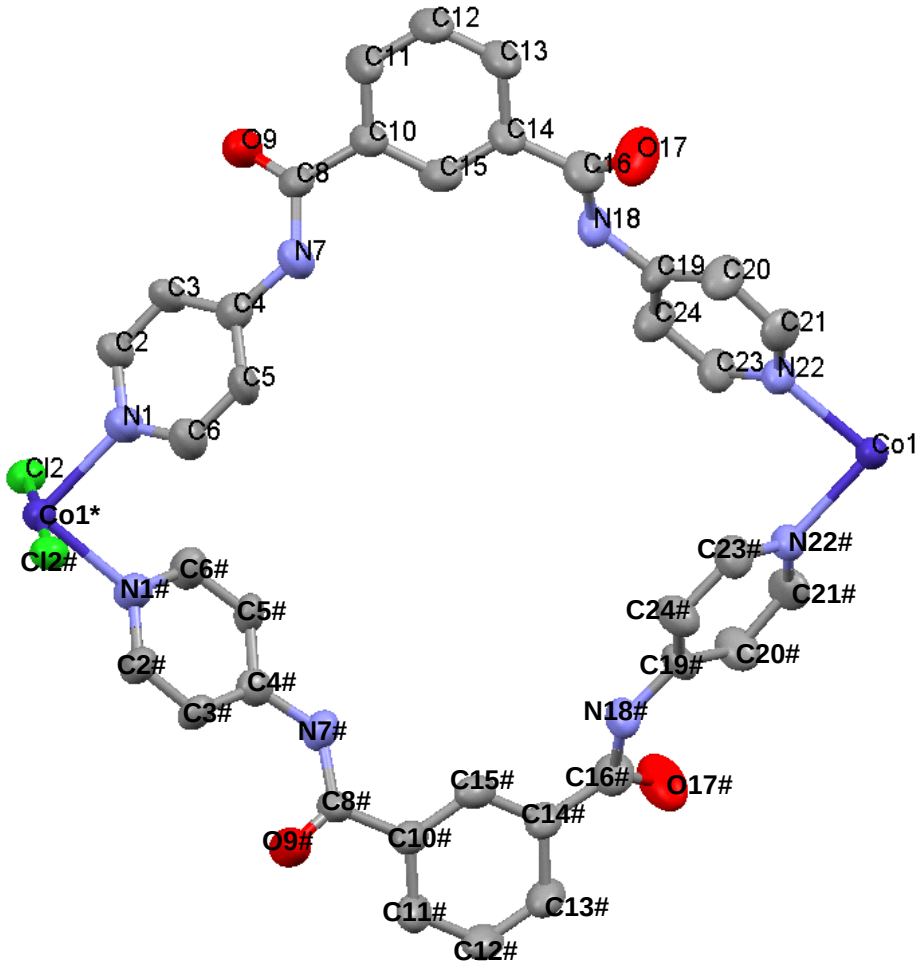
Molecular Plots and Hydrogen Bonding Parameters for L1, MOF-1, MOF-2 and MOF-3

Molecular Plot of L1



Hydrogen bonding parameters of L1					
D-H…A	D-H (Å)	H…A (Å)	D…A (Å)	D-H…A (^{0})	Symmetry operation for A
N(7)-H(7)…N(22)	0.875(18)	2.217(18)	3.070(2)	165.0(16)	1-x,-1/2+y,1/2-z
N(18)-H(18)…N(1)	0.894(17)	2.274(18)	3.148(2)	165.6(14)	-x,2-y,-z

Molecular Plot of MOF-1

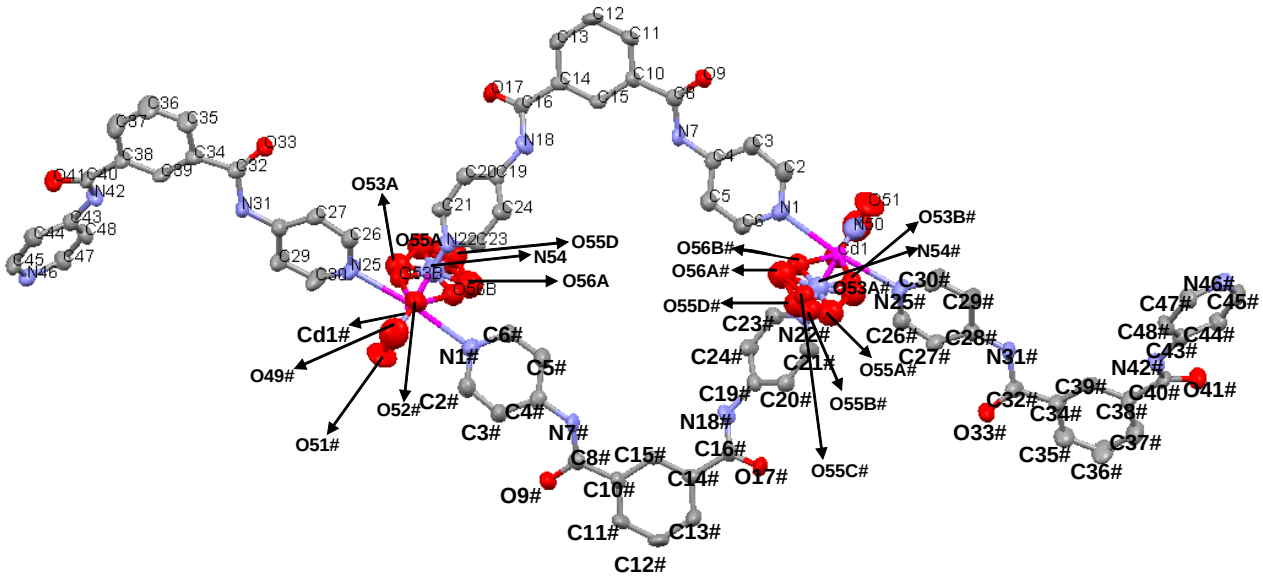


Symmetry codes of atoms

\# x-y, -y, 1/3-z
* 1+x, y, z

Hydrogen bonding parameters of MOF-1					
D-H…A	D-H (Å)	H…A (Å)	D…A (Å)	D-H…A (^{0})	Symmetry operation for A
N(18)-H(18)…Cl(2)	0.86	2.44	3.251(4)	156.5	1+y, x, -z

Molecular Plot of MOF-2

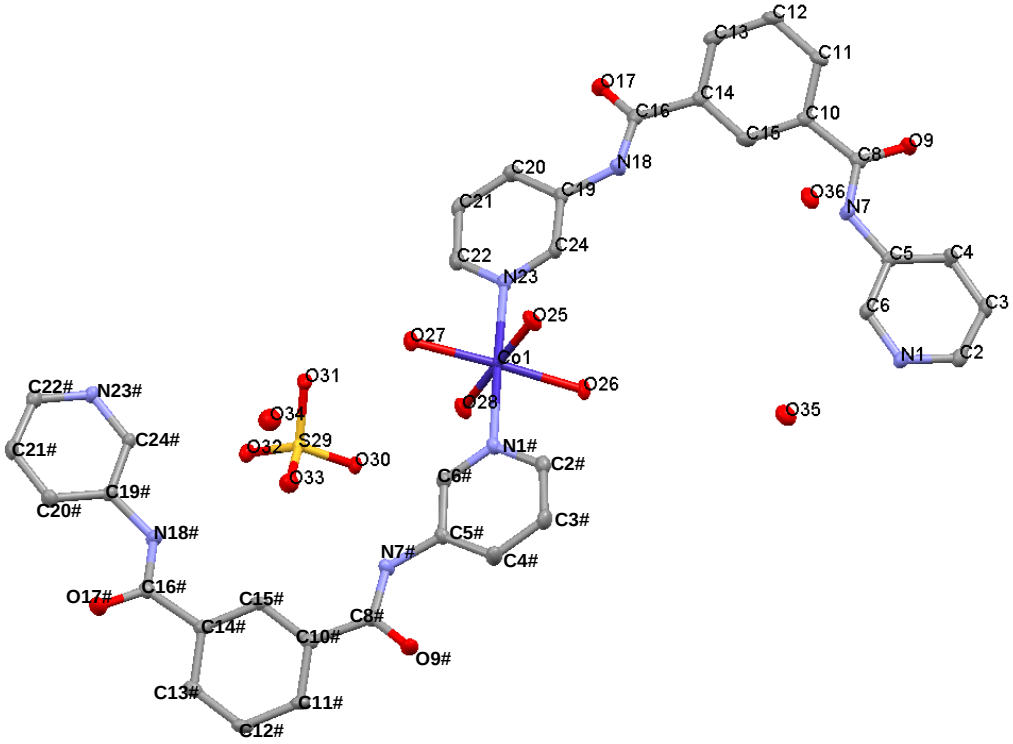


Symmetry codes of atoms

-x, 1-y, -z

Hydrogen bonding parameters of MOF-2					
D-H…A	D-H (Å)	H…A (Å)	D…A (Å)	D-H…A (^{0})	Symmetry operation for A
N(7)-H(7)…O(52)	0.86	2.24	3.024(9)	150.7	1-x, 1-y, -z
N(18)-H(18)…O(9)	0.86	2.19	2.949(9)	146.4	-x, 2-y, -z
N(42)-H(42)…O(33)	0.86	2.12	2.962(9)	165.1	2-x, -y, 1-z

Molecular Plot of MOF-3



Symmetry codes of atoms

1-x, 1/2+y, 1/2-z

Hydrogen bonding parameters of MOF-3					
D-H…A	D-H (Å)	H…A (Å)	D…A (Å)	D-H…A (^{0})	Symmetry operation for A
N(7)-H(7)…O(33)	0.86	2.36	3.182(3)	160.8	1-x, -1/2+y, 1/2-z
N(18)-H(18)…O(33)	0.86	2.51	3.329(3)	160.0	1-x, -1/2+y, 1/2-z
O(25)-H(25A)…O(32)	0.82	1.93	2.734(3)	167.9	x, -1+y, z
O(25)-H(25B)…O(17)	0.74(4)	2.09(4)	2.832(3)	173(4)	2-x, -1/2+y, 1/2-z
O(26)-H(26A)…O(31)	0.82	1.93	2.682(3)	152.8	x, -1+y, z
O(26)-H(26B)…O(36)	0.79(4)	1.92(4)	2.702(3)	170(4)	1-x, -y, 1-z
O(27)-H(27A)…O(31)	0.82	1.96	2.719(3)	153.0	1-x, -1/2+y, 1/2-z
O(27)-H(27B)…O(35)	0.83(4)	1.80(4)	2.623(3)	174(4)	x, y, z
O(28)-H(28A)…O(30)	0.82	1.91	2.710(3)	166.1	1-x, -1/2+y, 1/2-z
O(28)-H(28B)…O(9)	0.75(4)	2.12(4)	2.864(3)	173(4)	-1+x, y, z
O(34)-H(34A)…O(36)	1.05(5)	1.79(5)	2.837(3)	177(4)	1-x, 1-y, 1-z
O(34)-H(34B)…O(33)	0.98(6)	1.86(6)	2.816(3)	165(5)	x, y, z
O(35)-H(35A)…O(32)	0.76(4)	1.97(4)	2.712(3)	166(4)	1-x, 1-y, -z
O(35)-H(35B)…O(34)	0.98(5)	1.84(5)	2.795(3)	167(4)	1-x, -1/2+y, 1/2-z
O(36)-H(36A)…O(9)	0.88(5)	1.96(5)	2.797(3)	159(4)	2-x, -y, 1-z
O(36)-H(36B)…O(30)	0.81(5)	1.84(5)	2.647(3)	175(4)	1-x, -1/2+y, 1/2-z

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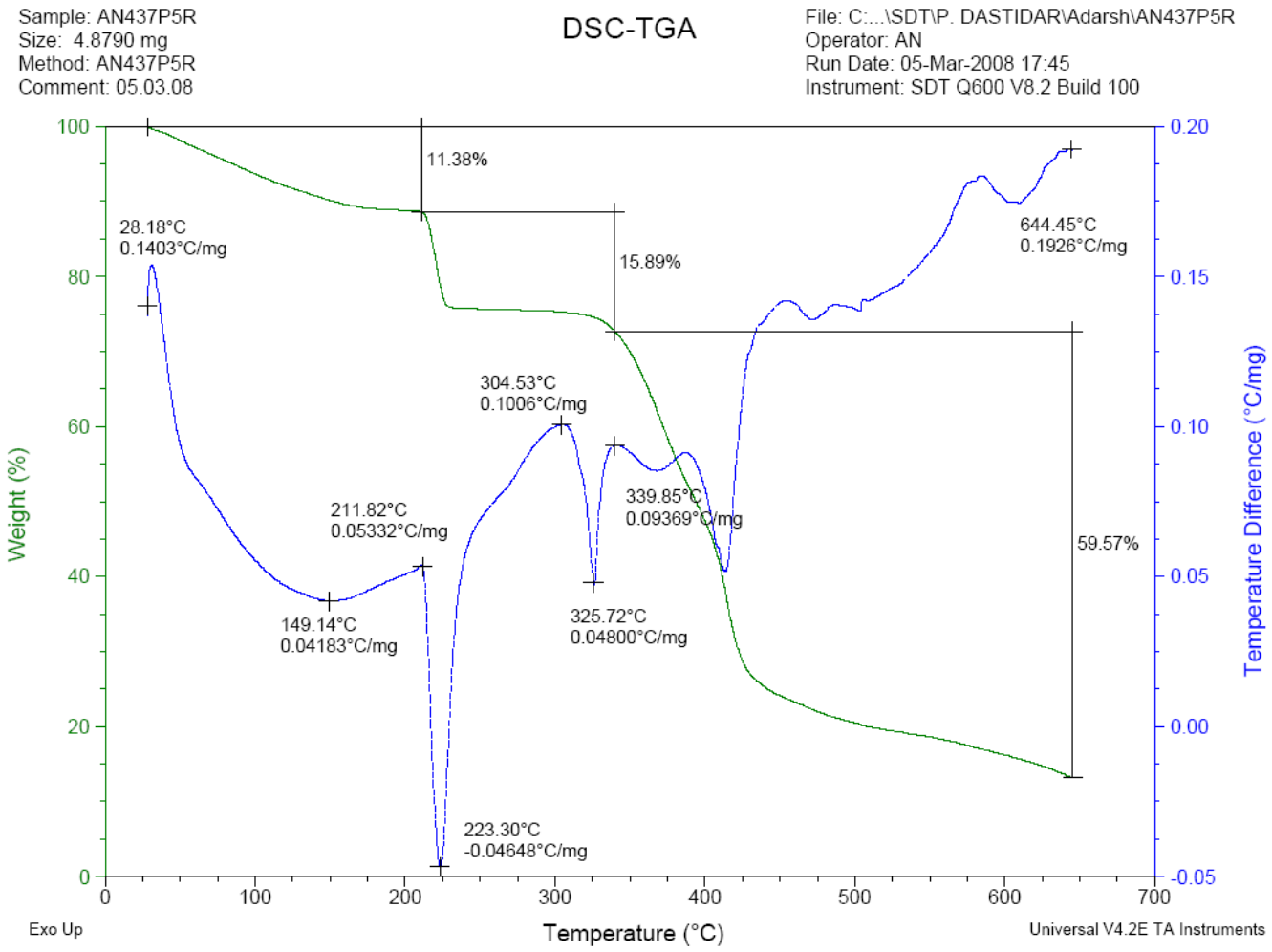
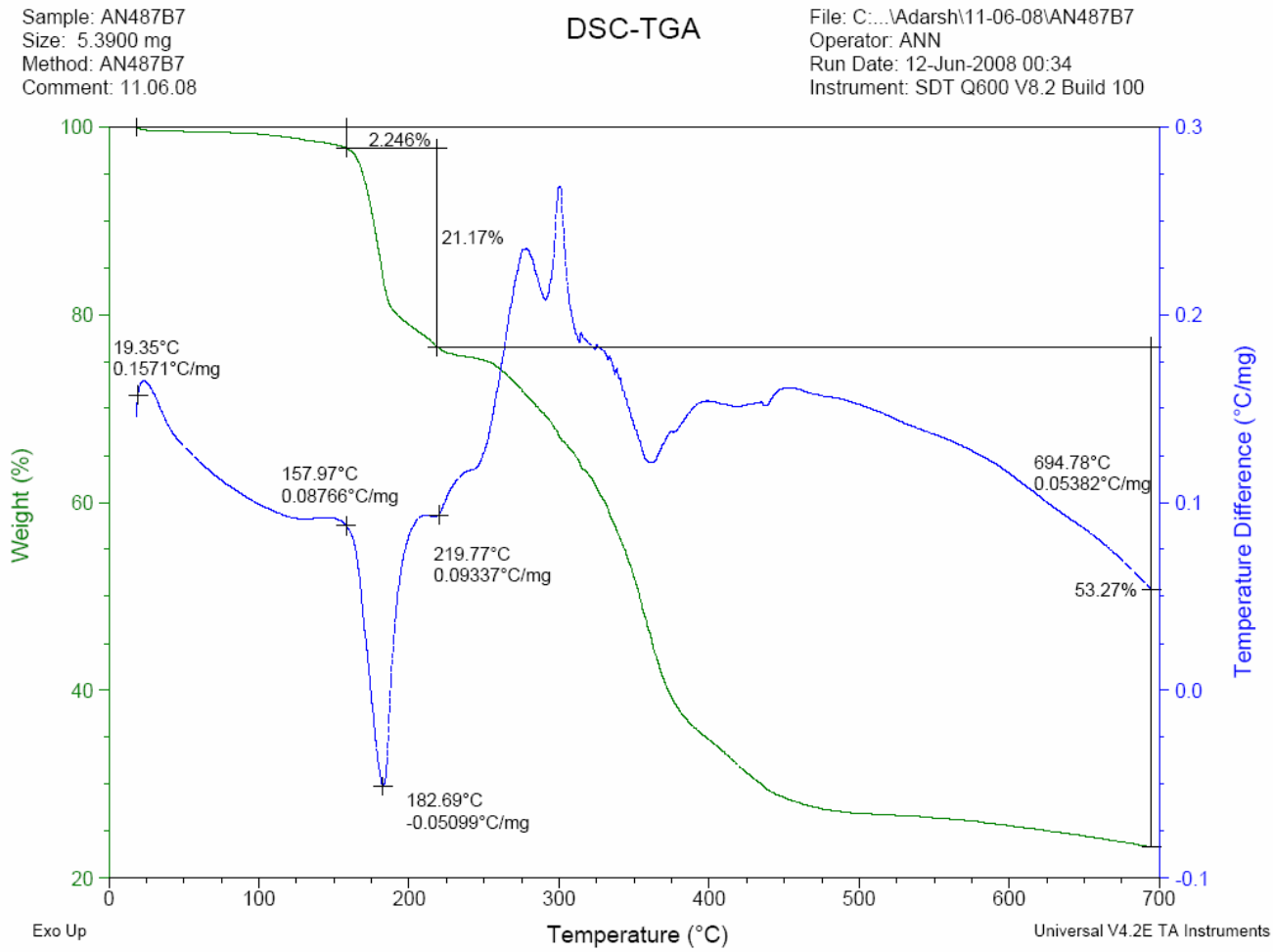
TGA of MOF-1, MOF-2 and MOF-3

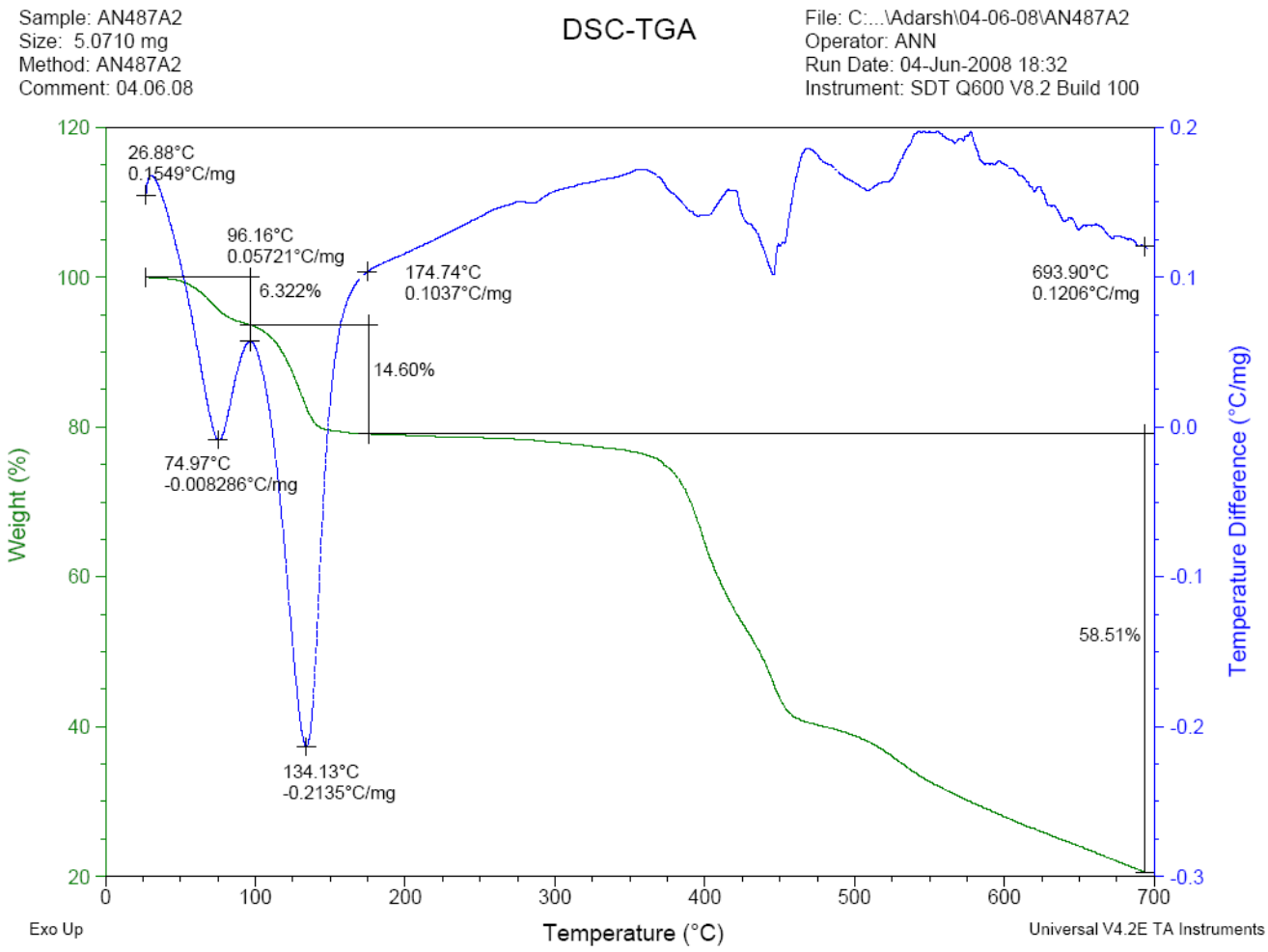
MOF 1



MOF_2



MOF 3



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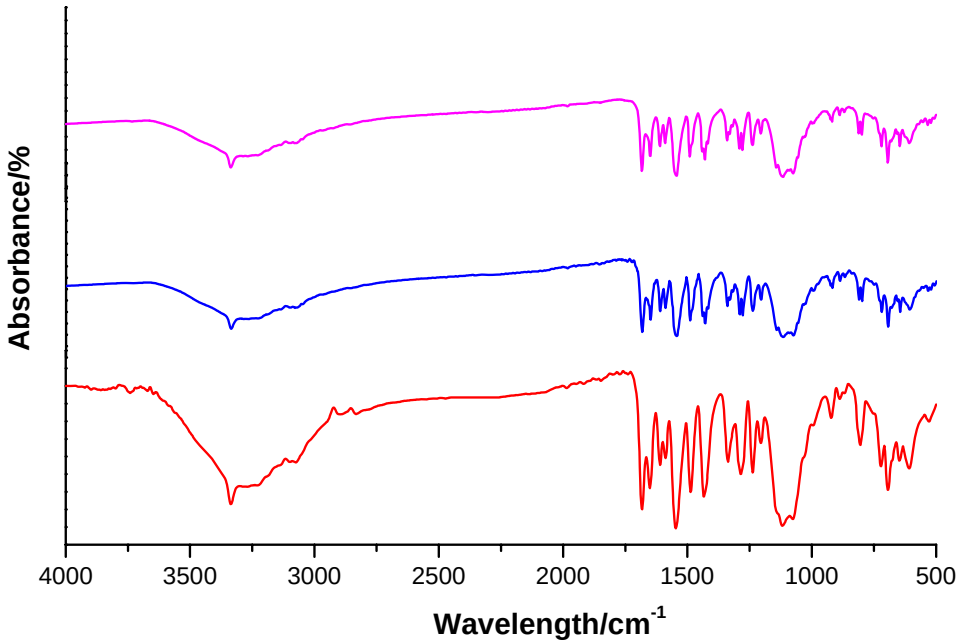
Selective crystallization of sulfate using L1′ and Cd(II) salts

Identical experiments as carried out for **L1′** and Co(II) salts were repeated with Cd(II) salts and the isolated crystalline product was characterized by elemental analysis, FT-IR and X-ray powder diffraction. These data as listed below clearly indicate the formation of corresponding $CdSO_4$ MOF structure of which was published recently (ref. 12 of the manuscript).

Elemental analysis:

	%
Analytical data calc. for $C_{18}H_{18}N_4O_8CdS$	C, 38.41; H, 3.22; N, 9.95
Found in competitive experiments	
(L1′:CdSO4:$Cd(NO_3)_2$, $Cd(OAc)_2$, $Cd(ClO_4)_2$)	C, 37.83; H, 3.50; N, 9.53
L1′:$CdSO_4$: 2[$Cd(NO_3)_2$, $Cd(OAc)_2$, $Cd(ClO_4)_2$	C, 37.60; H, 3.27; N, 9.51

FT-IR



FT-IR of $CdSO_4$ MOF of **L1′** under various conditions; noncompetitive condition (red); competitive conditions - L1′:CdSO4:Cd(NO3)2, Cd(OAc)2, Cd(ClO4)2, (blue), iv) L1′:CdSO4: 2[Cd(NO3)2, Cd(OAc)2, Cd(ClO4)2] (magenta).

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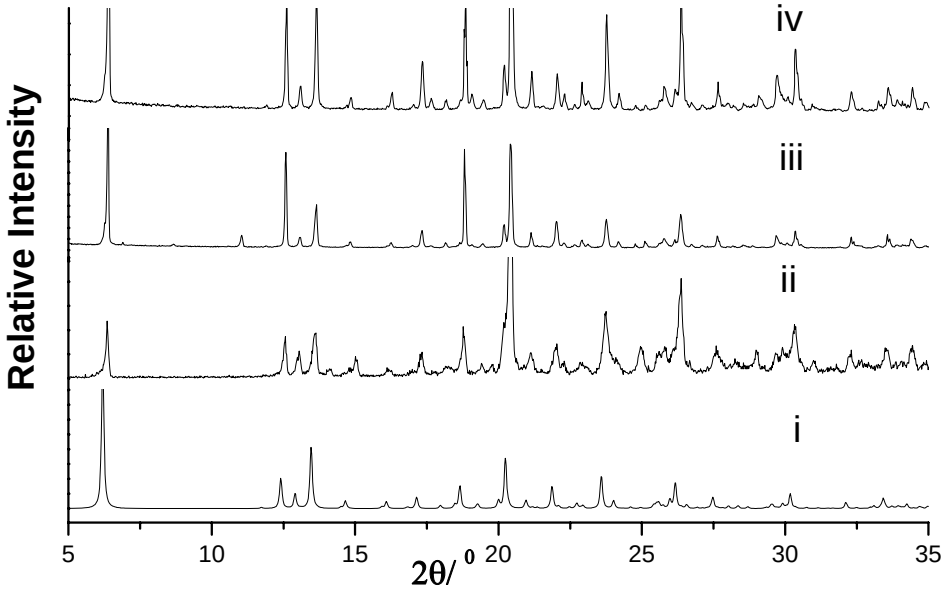
XRPD



XRPD patterns i) Simulated from the single crystal data of $CdSO_4$ MOF of **L1′;** ii) bulk solid under noncompetitive condition; under competitive conditions – iii) L1′:CdSO4:Cd(NO3)2, Cd(OAc)2, Cd(ClO4)2, iv) L1′:CdSO4: 2[Cd(NO3)2, Cd(OAc)2, Cd(ClO4)2].