Electronic Supplementary Information (ESI)

Zn(II) Metal-Organic-Frameworks (MOFs) Derived from a Bis-pyridyl-bis-urea ligand: Effects of Crystallization Solvents on the Structures and Anion Binding Properties

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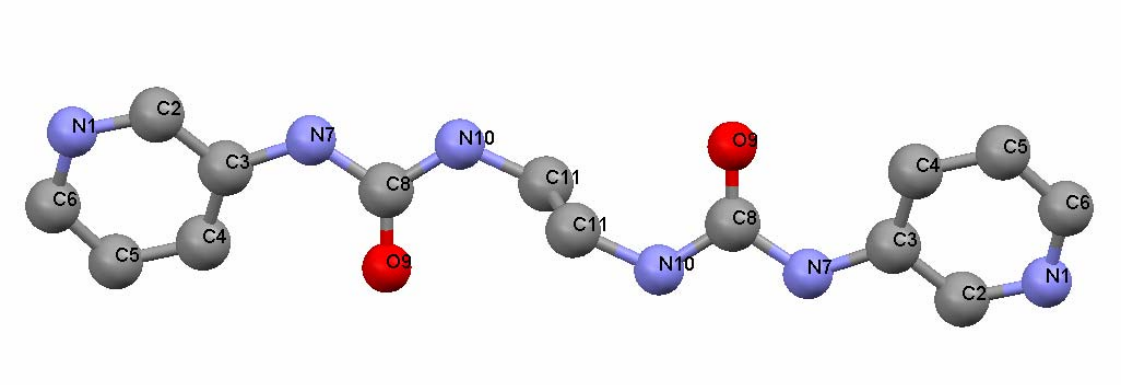
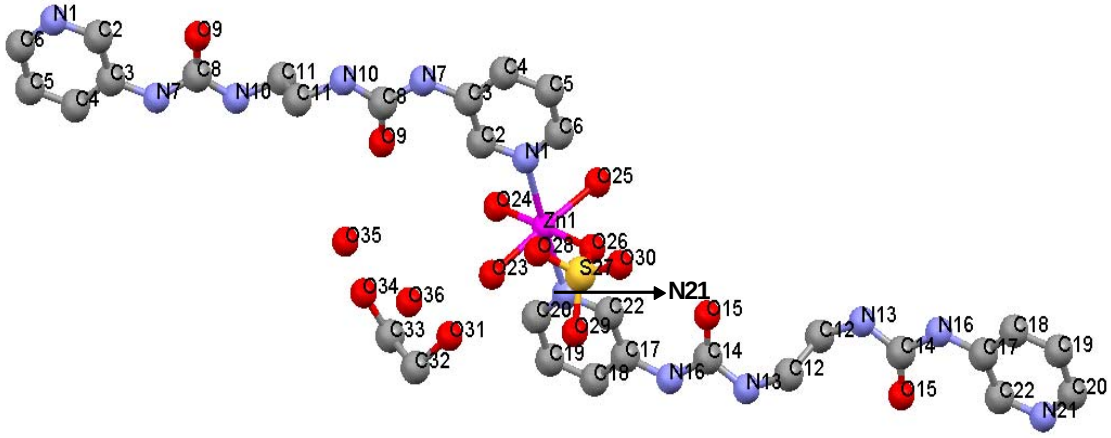
Molecular Plots and Hydrogen Bonding Parameters for 1, 2, 3, 4 and 5

Molecular Plot of 1



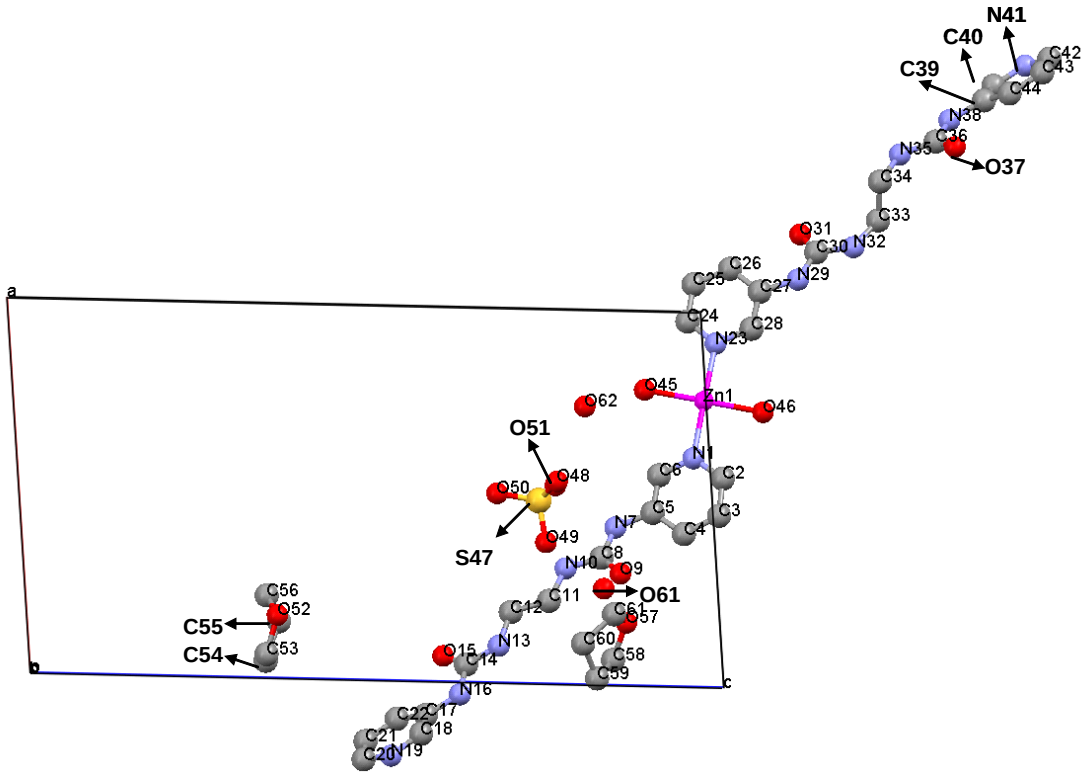
Hydrogen bonding parameters of 1					
D-H…A	D-H (Å)	H…A (Å)	D…A (Å)	D-H…A (^{0})	Symmetry operation for A
N(7)-H(7)···N(1)	0.868(18)	2.186(19)	3.0138(18)	159.2(16)	2-x, 1/2+y, 3/2-z
N(10)-H(10)···O(9)	0.816(18)	2.284(18)	3.011(2)	148.7(17)	x, 1/2-y, 1/2+z

Molecular Plot of 2



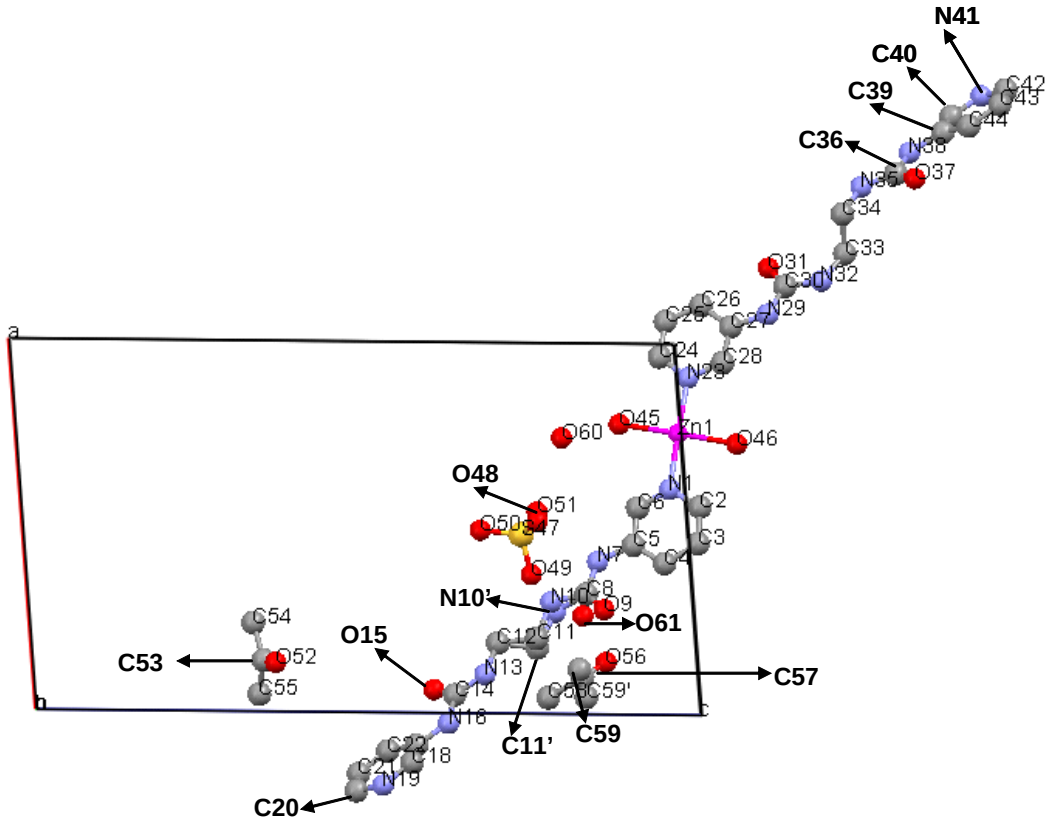
Hydrogen bonding parameters of 2					
D-H…A	D-H (Å)	H…A (Å)	D…A (Å)	D-H…A (^{0})	Symmetry operation for A
N(7)-H(7)…O(28)	0.88	2.03	2.854(3)	155	1-x, 1-y, -z
N(10)-H(10)…O(30)	0.88	1.97	2.823(3)	163	1-x, 1-y, -z
N(13)-H(13)…O(29)	0.88	2.28	3.036(3)	144	1-x, -y, 1-z
N(16)-H(16)…O(29)	0.88	1.94	2.776(3)	159	1-x, -y, 1-z
O(23)-H(23B)…O(36)	0.89(4)	1.77(4)	2.657(3)	178(3)	x, y, z
O(24)-H(24A)…O(29)	0.76(3)	1.96(4)	2.713(3)	172(3)	-1+x, y, z
O(24)-H(24B)…O(31)	0.81(4)	1.88(4)	2.677(3)	171(4)	-1+x, y, z
O(25)-H(25A)…O(35)	0.79(4)	1.92(4)	2.708(3)	175(4)	x, -1+y, z
O(25)-H(25B)…O(30)	0.76(4)	2.02(4)	2.777(3)	173(4)	-1+x, y, z
O(31)-H(31)…O(9)	0.84	1.88	2.703(3)	168	1+x, y, z
O(34)-H(34)…O(30)	0.84	1.93	2.739(3)	163	x, 1+y, z
O(35)-H(35A)…O(9)	0.88(4)	1.85(4)	2.711(3)	167(4)	x, y, z
O(35)-H(35B)…O(34)	0.80(4)	1.93(4)	2.715(3)	165(3)	x, y, z
O(36)-H(36A)...O(15)	0.83(4)	1.91(4)	2.740(3)	176(4)	x, 1+y, z
O(36)-H(36B)...O(35)	0.84(4)	2.00(4)	2.841(3)	173(3)	x, y, z

Molecular Plot of 3



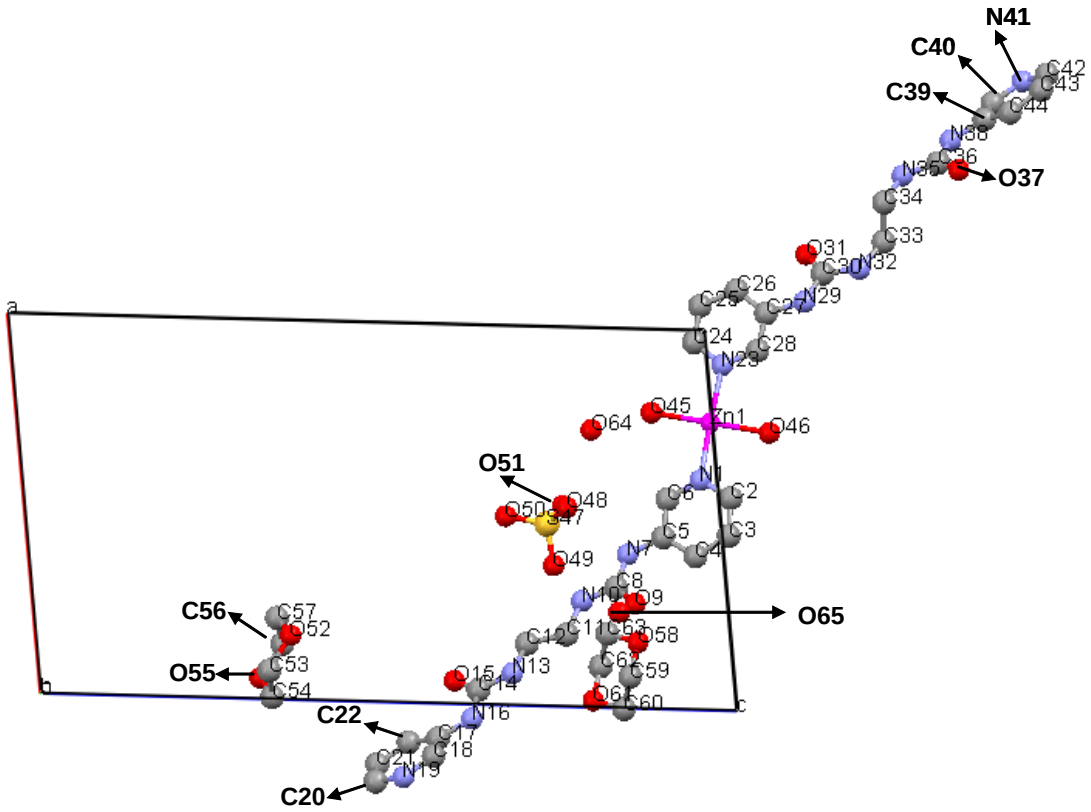
Hydrogen bonding parameters of 3					
D-H…A	D-H (Å)	H…A (Å)	D…A (Å)	D-H…A (^{0})	Symmetry operation for A
N(7)-H(7)…O(48)	0.86	2.05	2.864(4)	158	x, y, z
N(10)-H(10)…O(49)	0.86	2.19	2.950(5)	147	x, y, z
N(13)-H(13)…O(51)	0.86	2.08	2.886(5)	156	1/2-x, 1/2+y, 3/2-z
N(16)-H(16)…O(51)	0.86	2.12	2.919(4)	155	1/2-x, 1/2+y, 3/2-z
N(29)-H(29)…O(50)	0.86	2.03	2.872(4)	168	1/2+x, 1/2-y, 1/2+z
N(32)-H(32)…O(48)	0.86	2.01	2.832(4)	159	1/2+x, 1/2-y, 1/2+z
N(35)-H(35)…O(51)	0.86	2.03	2.856(5)	161	2-x,-y,2-z
N(38)-H(38)…O(50)	0.86	2.10	2.938(4)	165	2-x,-y,2-z
O…O	O…O (Å)				Symmetry operation for O
O(9)…O(63)	2.689(4)				x, y, z
O(15)...O(46)	2.621(4)				-1/2+x,1/2-y,-1/2+z
O(31)...O(62)	2.742(4)				2-x,-y,2-z
O(37)...O(45)	2.643(4)				1/2+x,1/2-y,1/2+z
O(45)…O(62)	2.673(4)				x, y, z
O(45)…O(37)	2.643(4)				-1/2+x,1/2-y,-1/2+z
O(46)…O(63)	2.629(4)				1-x,1-y,2-z
O(46)…O(15)	2.621(4)				1/2+x,1/2-y,1/2+z
O(49)…O(63)	2.752(4)				1/2-x, -1/2+y, 3/2-z

Molecular Plot of 4



Hydrogen bonding parameters of 4					
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(48)	0.86	1.97	2.786(6)	159	x, y, z
N(13)-H(13)…O(51)	0.86	2.36	3.099(6)	144	1/2-x, 1/2+y, 3/2-z
N(16)-H(16)…O(51)	0.86	2.05	2.882(6)	163	1/2-x, 1/2+y, 3/2-z
N(29)-H(29)…O(50)	0.86	2.08	2.912(5)	162	1/2+x, 1/2-y, 1/2+z
N(32)-H(32)…O(48)	0.86	2.02	2.828(5)	156	1/2+x, 1/2-y, 1/2+z
N(35)-H(35)…O(51)	0.86	2.05	2.876(5)	160	2-x, -y, 2-z
N(38)-H(38)…O(50)	0.86	2.05	2.903(5)	170	2-x, -y, 2-z
O…O	O…O (Å)				Symmetry operation for O
O(9)…O(61)	2.720(6)				x, y, z
O(15)…O(46)	2.652(5)				-1/2+x,1/2-y,-1/2+z
O(31)…O(60)	2.732(4)				2-x,-y,2-z
O(37)…O(45)	2.656(4)				1/2+x,1/2-y,1/2+z
O(45)…O(60)	2.691(4)				x, y, z
O(45)…O(37)	2.656(4)				-1/2+x,1/2-y,-1/2+z
O(46)…O(61)	2.671(5)				1-x,1-y,2-z

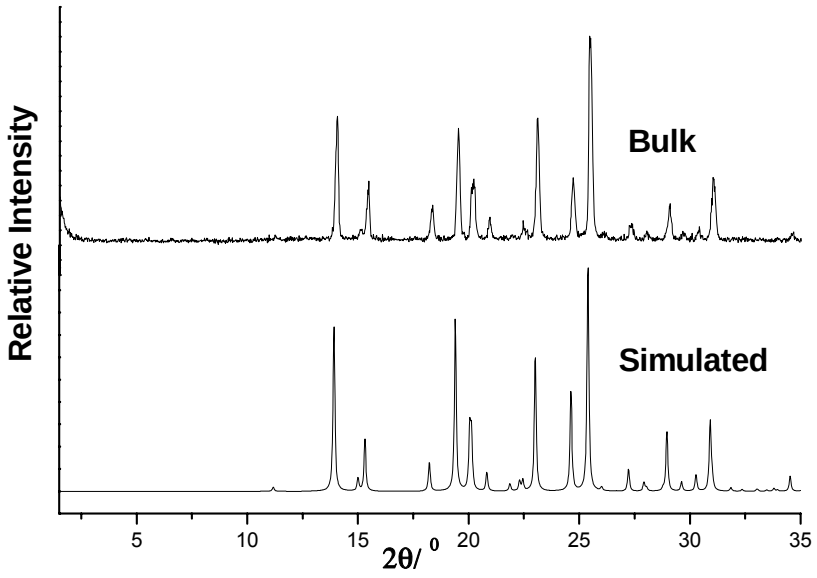
Molecular Plot of 5



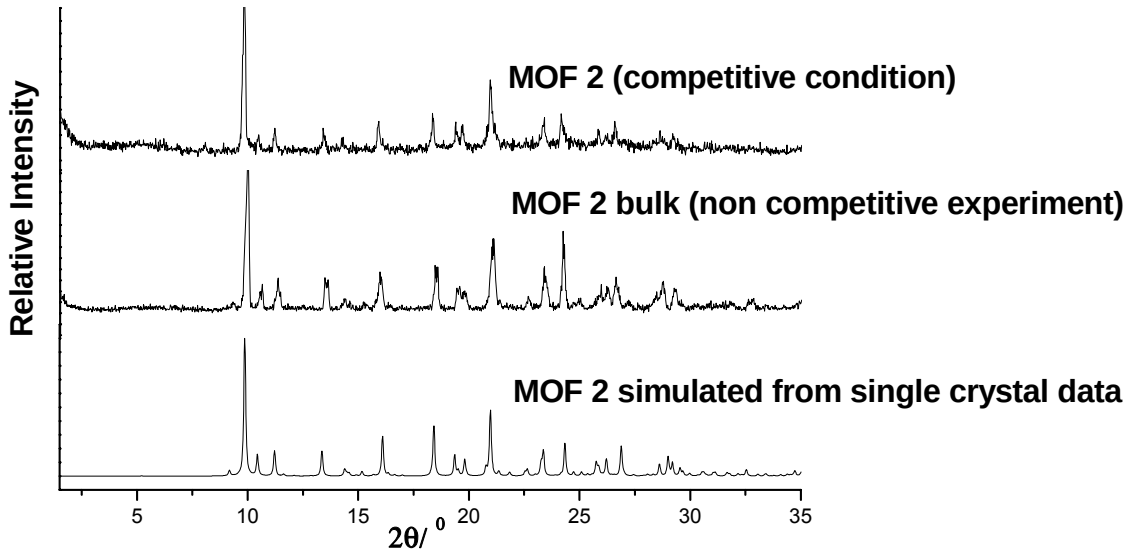
Hydrogen bonding parameters of 5					
D-H…A	D-H (Å)	H…A (Å)	D…A (Å)	D-H…A (^{0})	Symmetry operation for A
N(7)-H(7)…O(48)	0.86	2.08	2.882(3)	155	x, y, z
N(10)-H(10)…O(49)	0.86	2.08	2.913(3)	164	x, y, z
N(13)-H(13)…O(51)	0.86	2.08	2.892(3)	157	1/2-x,1/2+y,3/2-z
N(16)-H(16)…O(51)	0.86	2.17	2.971(3)	154	1/2-x,1/2+y,3/2-z
N(29)-H(29)…O(50)	0.86	2.01	2.843(3)	165	1/2+x,1/2-y,1/2+z
N(32)-H(32)…O(48)	0.86	2.08	2.893(3)	158	1/2+x,1/2-y,1/2+z
N(35)-H(35)…O(51)	0.86	2.06	2.883(3)	161	2-x,-y,2-z
N(38)-H(38)…O(50)	0.86	2.06	2.916(3)	171	2-x,-y,2-z
O(45)-H(45A).. O(64)	0.75(3)	1.93(4)	2.674(3)	170(4)	x, y, z
O(45)-H(45B)…O(37)	0.75(4)	1.91(4)	2.651(3)	176(4)	-1/2+x,1/2-y,-1/2+z
O(46)-H(46A)…O(65)	0.73(4)	1.90(4)	2.633(3)	171(4)	1-x,1-y,2-z
O(46)-H(46B)…O(15)	0.83(4)	1.82(4)	2.642(3)	176(4)	1/2+x,1/2-y,1/2+z
O(64)-H(64A)…O(31)	0.81(4)	1.93(4)	2.725(3)	169(3)	2-x,-y,2-z
O(64)-H(64B)…O(51)	0.66(4)	2.39(4)	2.998(3)	154(5)	x, y, z
O(65)-H(65A)…O(9)	0.78(3)	1.95(3)	2.734(3)	176(3)	x, y, z
O(65)-H(65B)…O(49)	0.73(4)	2.04(4)	2.764(3)	172(4)	1/2-x,1/2+y,3/2-z

XRPD Patterns for 1, 2, 3, 4 and 5

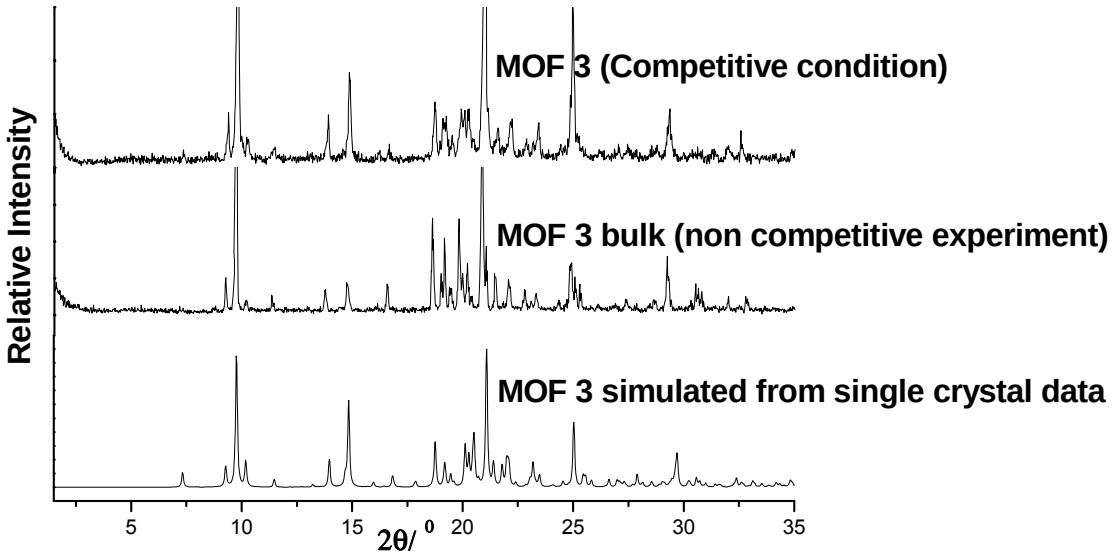
1



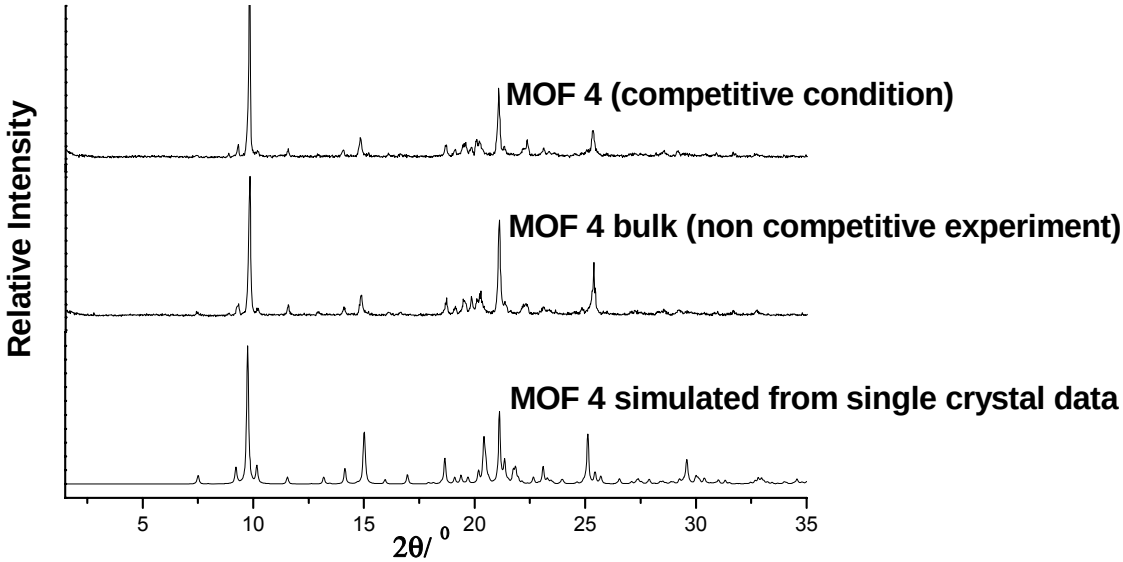
MOF 2



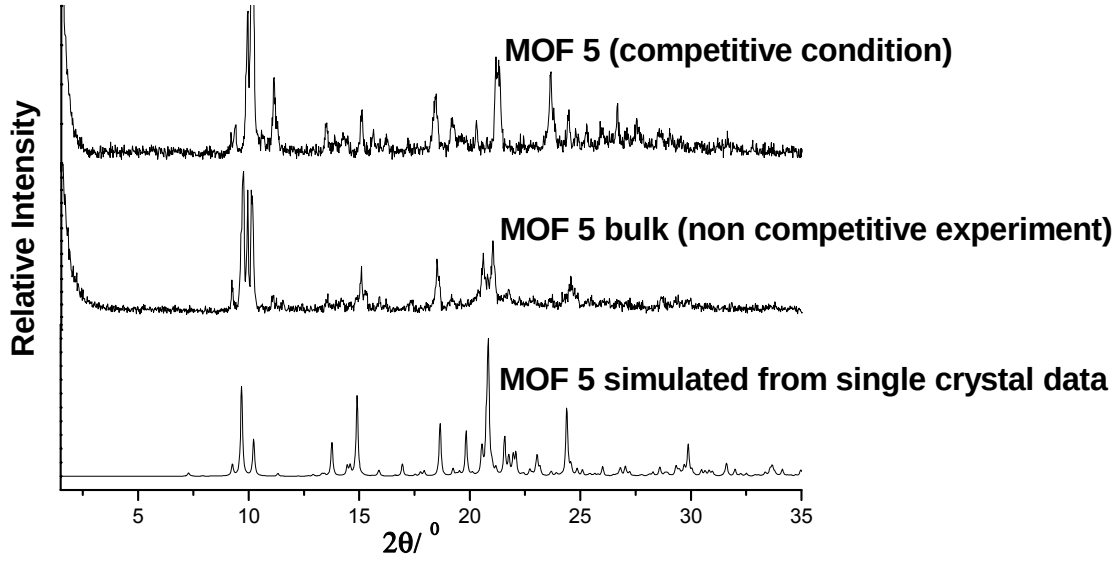
MOF 3


MOF 3 (Competitive condition)
MOF 3 bulk (non competitive experiment)
MOF 3 simulated from single crystal data
Relative Intensity
5
10
15
20
25
30
35
2θ/ 0

MOF 4

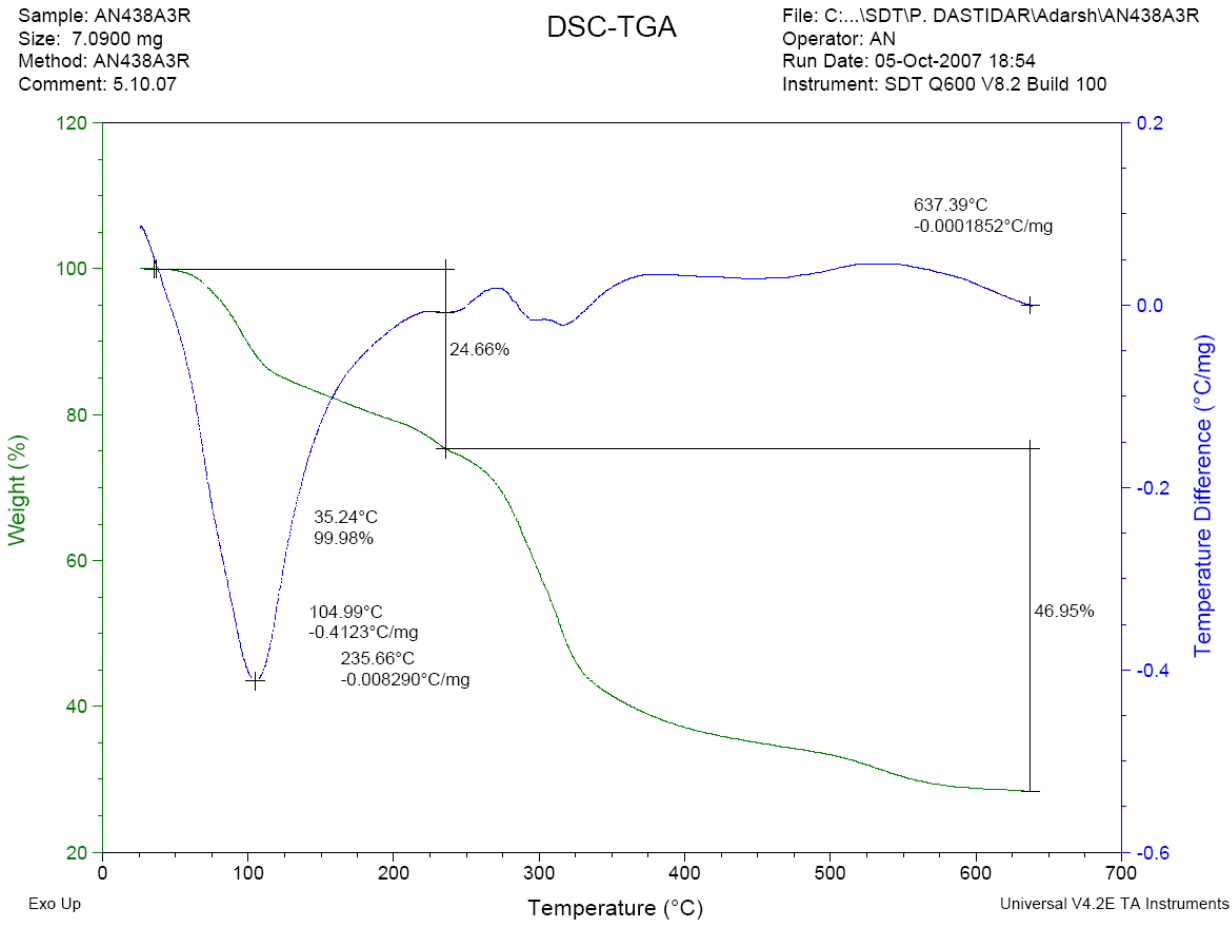

MOF 4 (competitive condition)
MOF 4 bulk (non competitive experiment)
MOF 4 simulated from single crystal data
Relative Intensity
5
10
15
20
25
30
35
2θ/ 0

MOF 5

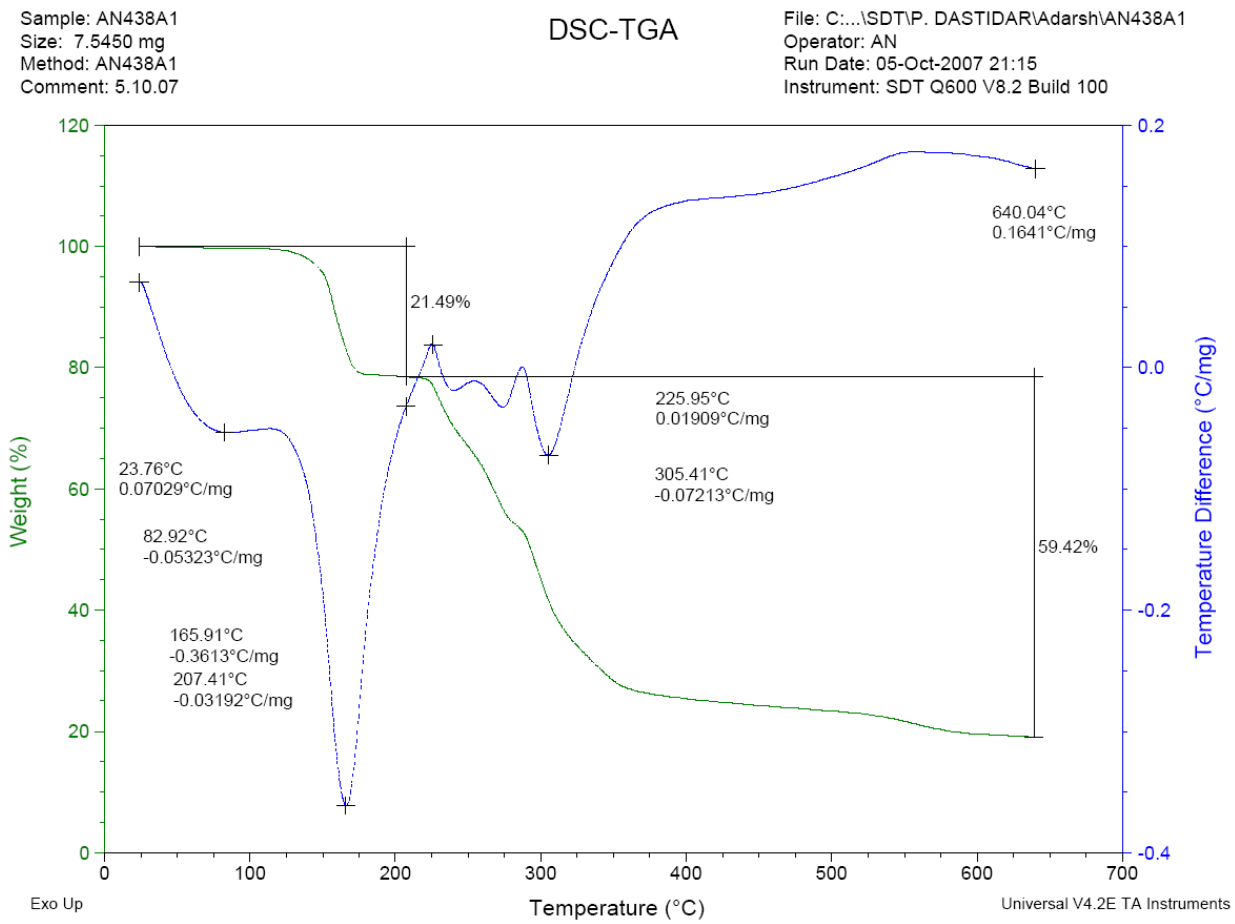

MOF 5 (competitive condition)
MOF 5 bulk (non competitive experiment)
MOF 5 simulated from single crystal data
Relative Intensity
5
10
15
20
25
30
35
2θ/ 0

TGA of 2, 3, 4 and 5

MOF 2



MOF 3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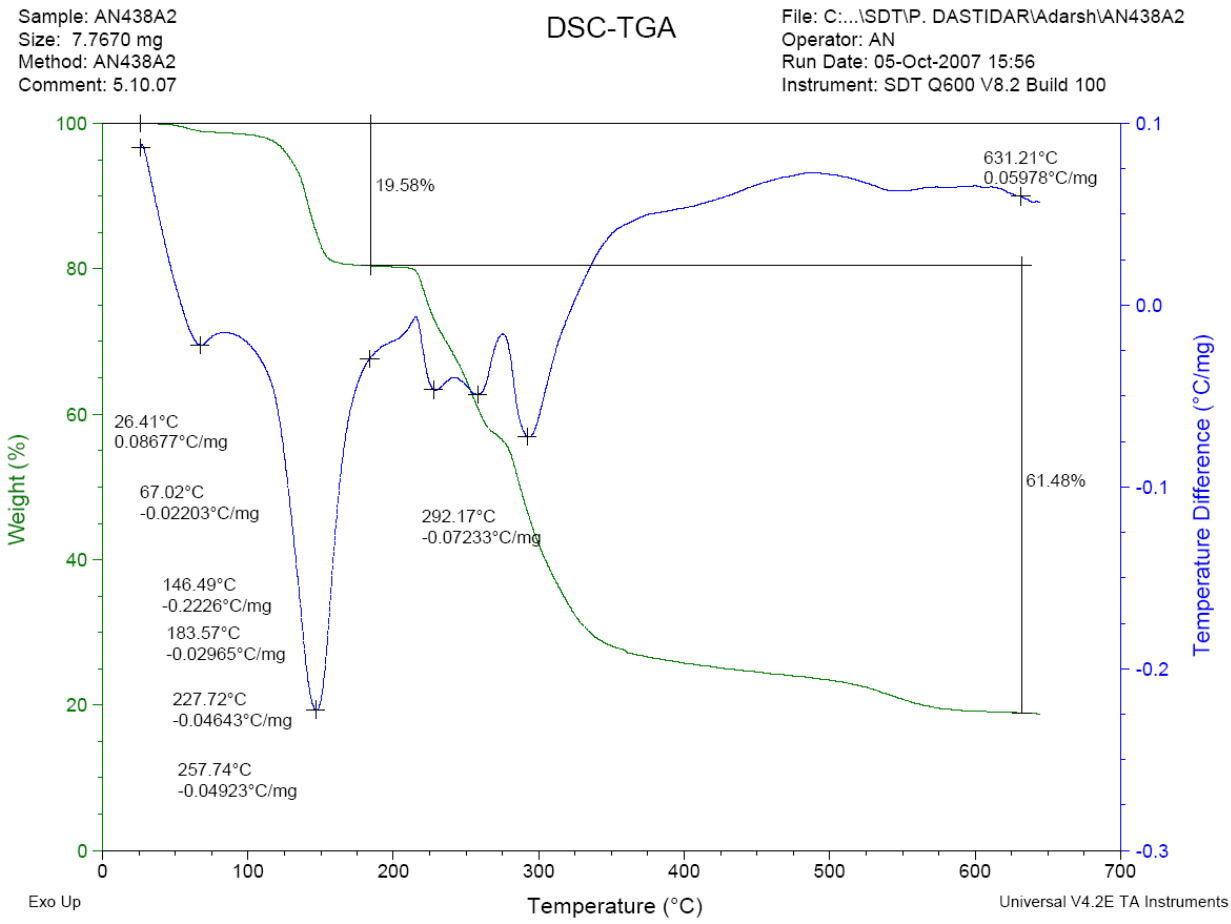
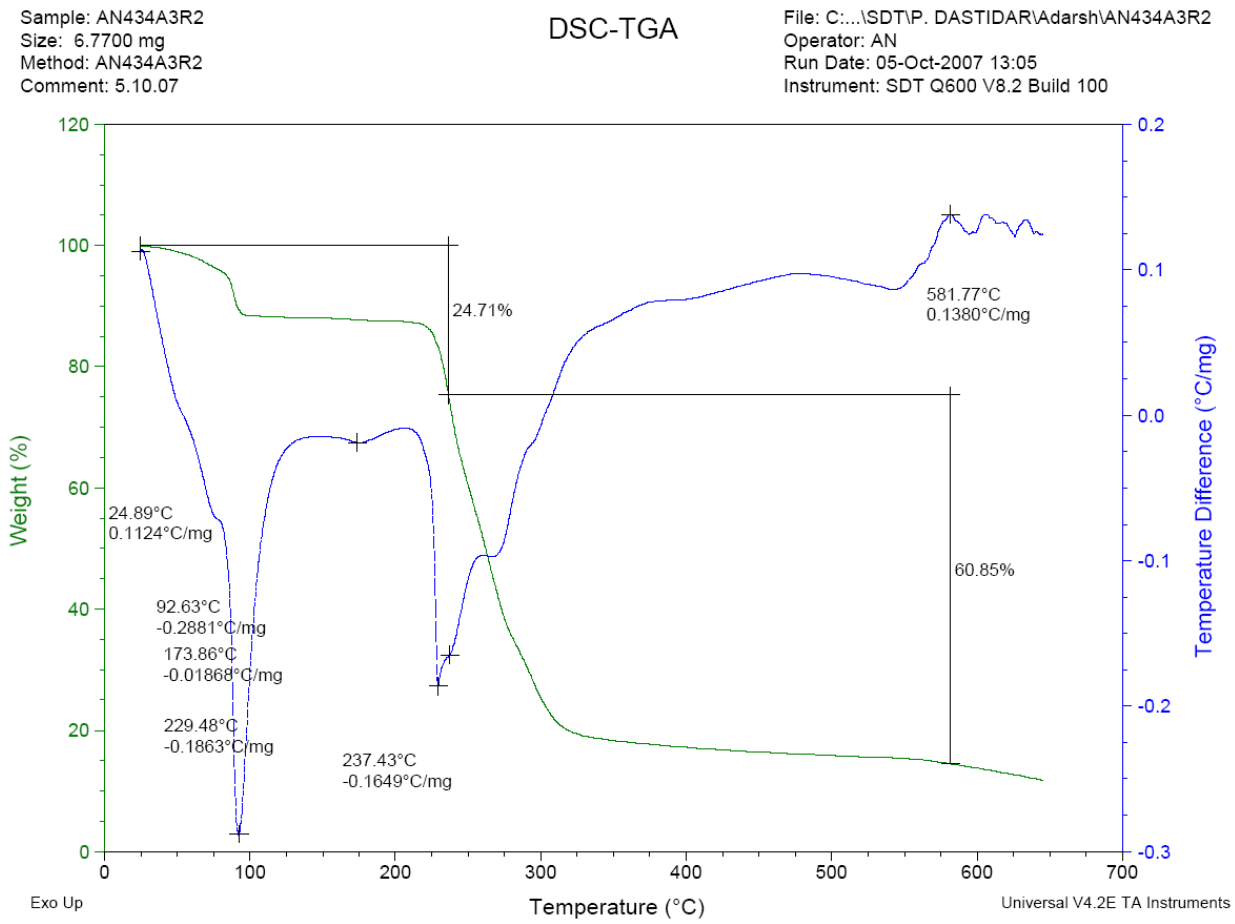
Size: 7.5450 mg
Method: AN438A1
Comment: 5.10.07
DSC-TGA
File: C:...\SDT\P. DASTIDAR\Adarsh\AN438A1
Operator: AN
Run Date: 05-Oct-2007 21:15
Instrument: SDT Q600 V8.2 Build 100
640.04°C
0.1641°C/mg
21.49%
225.95°C
0.01909°C/mg
305.41°C
-0.07213°C/mg
23.76°C
0.07029°C/mg
82.92°C
-0.05323°C/mg
59.42%
165.91°C
-0.3613°C/mg
207.41°C
-0.03192°C/mg
Weight (%)
Temperature Difference (°C/mg)
Temperature (°C)
Exo Up
Universal V4.2E TA Instruments

MOF 4

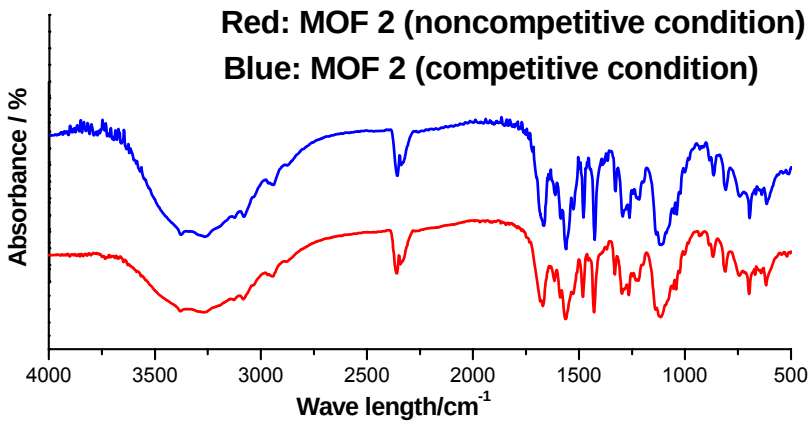

Sample: AN438A2
Size: 7.7670 mg
Method: AN438A2
Comment: 5.10.07
DSC-TGA
File: C:...\SDT\P. DASTIDAR\Adarsh\AN438A2
Operator: AN
Run Date: 05-Oct-2007 15:56
Instrument: SDT Q600 V8.2 Build 100
19.58%
631.21°C
0.05978°C/mg
61.48%
26.41°C
0.08677°C/mg
67.02°C
-0.02203°C/mg
292.17°C
-0.07233°C/mg
146.49°C
-0.2226°C/mg
183.57°C
-0.02965°C/mg
227.72°C
-0.04643°C/mg
257.74°C
-0.04923°C/mg
Weight (%)
Temperature Difference (°C/mg)
Temperature (°C)
Exo Up
Universal V4.2E TA Instruments

MOF 5

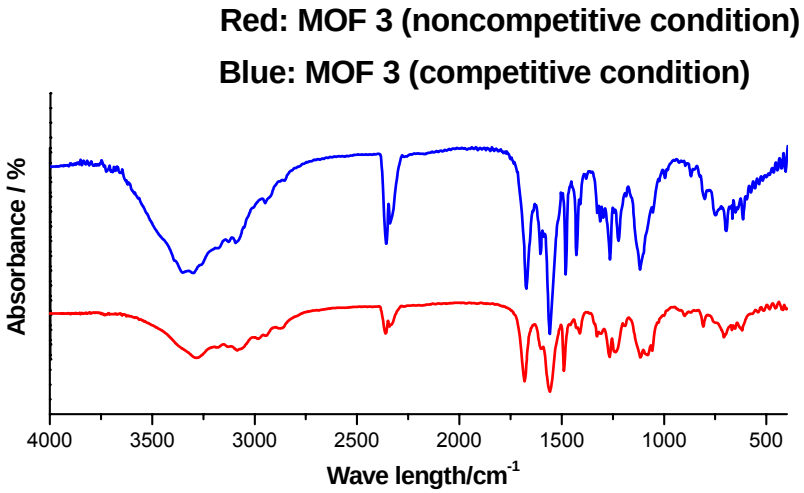

Sample: AN434A3R2
Size: 6.7700 mg
Method: AN434A3R2
Comment: 5.10.07
DSC-TGA
File: C:...\SDT\P. DASTIDAR\Adarsh\AN434A3R2
Operator: AN
Run Date: 05-Oct-2007 13:05
Instrument: SDT Q600 V8.2 Build 100
24.71%
60.85%
581.77°C
0.1380°C/mg
24.89°C
0.1124°C/mg
92.63°C
-0.2881°C/mg
173.86°C
-0.01868°C/mg
229.48°C
-0.1863°C/mg
237.43°C
-0.1649°C/mg
Weight (%)
Temperature Difference (°C/mg)
Temperature (°C)
Exo Up
Universal V4.2E TA Instruments

IR of 2, 3, 4 and 5

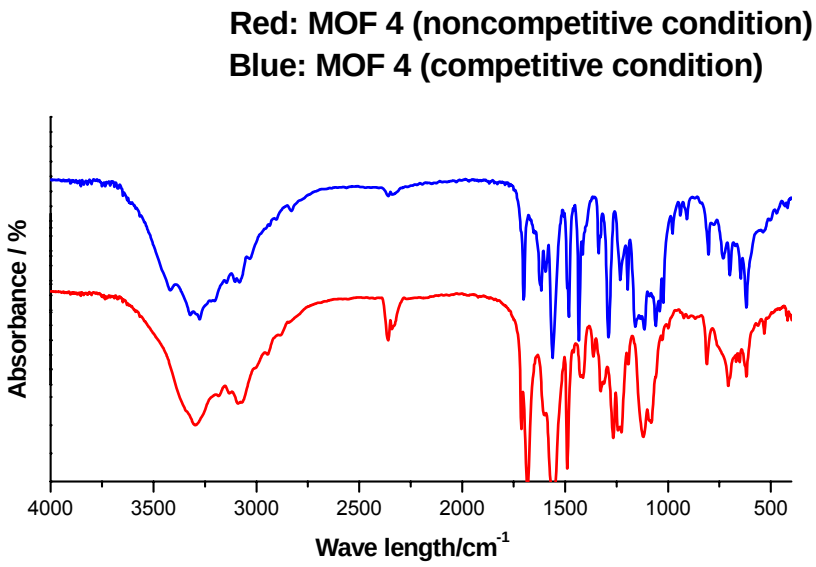
MOF 2



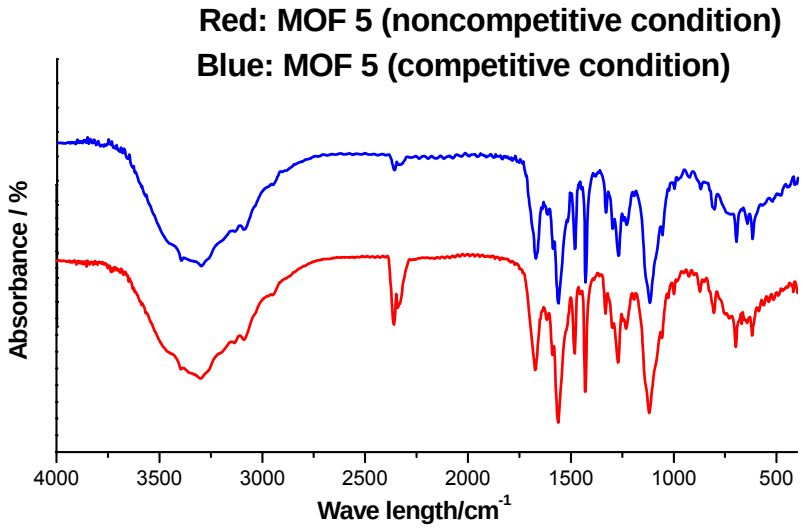
MOF 3



MOF 4


Red: MOF 4 (noncompetitive condition)
Blue: MOF 4 (competitive condition)
Absorbance / %
4000
3500
3000
2500
2000
1500
1000
500
Wave length/cm-1

MOF 5


Red: MOF 5 (noncompetitive condition)
Blue: MOF 5 (competitive condition)
Absorbance / %
4000
3500
3000
2500
2000
1500
1000
500
Wave length/cm-1