# Supporting Information

# Identifying the Liquid and Glassy States of Coordination Polymers and Metal–Organic Frameworks

# Alice M. Bumstead, <sup>a</sup> Michael F. Thorne <sup>a</sup> and Thomas D. Bennett<sup>\*a</sup>

<sup>a</sup> Department of Materials Science and Metallurgy, University of Cambridge, CB3 0FS

# Email: tdb35@cam.ac.uk

- 1. Cobalt and Cadmium Pyrazinamide Dithiocyanate Coordination Polymers.
- 2. Zinc Dicyanamide.
- 3. Nicotinate MOFs.
- 4. Zeolitic Imidazolate Frameworks.

#### **1.** Cobalt and Cadmium Pyrazinamide Dithiocyanate Coordination Polymers



**Figure S1.** Pawley refinement of cobalt pyrazinamide dithiocyanate. Unit cell details were provided but no CIF could be found for this material so we cannot guarantee its purity. Several low angle peaks were missing from the diffraction pattern as well as the presence of some additional peaks of low intensity that did not fit the proposed structure. These were ascribed to a structural transition caused by grinding the crystals for powder diffraction. This was accompanied by a colour change from burgundy to yellow (**Fig. S3**).  $R_{wp} = 12.261$ . As such, all further analysis was performed on the crystals directly as opposed to the powder.

Table S1.	Data from	Pawley refine	ement of cobalt p	yrazinamide	dithiocyanate.
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R <sub>wp</sub>	Space Group	Lattice Parameters	Lattice Parameters Reported <sup>1</sup>
12.261	P-1	<i>a</i> = 6.887(4) Å	<i>a</i> = 6.8711(4) Å
		<i>b</i> = 11.052(6) Å	<i>b</i> = 11.0487(6) Å
		<i>c</i> = 14.734(5) Å	<i>c</i> = 14.6891(8) Å
		α = 95.35(6) °	α = 94.949(2) °
		$\beta = 103.523(19)$ °	β = 103.144(2) °
		γ = 95.34(4) °	γ = 93.867(2) °



Figure S2. Optical image of cobalt pyrazinamide dithiocyanate.



**Figure S3.** Image of burgundy cobalt pyrazinamide dithiocyanate (left) and resulting yellow powder obtained upon grinding. As such, all further analysis was performed on the as synthesised crystals directly as opposed to the powder.



Figure S4. Thermogravimetric analysis data for cobalt pyrazinamide dithiocyanate.



**Figure S5.** Microscope image of cobalt pyrazinamide dithiocyanate glass within an aluminium pan after heating in the DSC to 220 °C. Evidence of liquid flow is visible.



**Figure S6.** Experimental room temperature X-ray diffraction pattern of cobalt pyrazinamide dithiocyanate (b), and after heating above 200 °C (a).



**Figure S7.** Pawley refinement of cadmium pyrazinamide dithiocyanate. Unit cell details were provided but no CIF could be found for this material so we cannot guarantee its purity. Some additional peaks of low intensity that did not fit the proposed structure were observed. These may also be ascribed to a structural change caused by grinding as was observed for the cobalt analogue. However, as no colour change was observed, we cannot discern if this is the case.  $R_{wp} = 15.661$ . As such, all further analysis was performed on the crystals directly as opposed to the powder.

R <sub>wp</sub>	Space Group	Lattice Parameters	Lattice Parameters Reported <sup>1</sup>
15.661	P-1	<i>a</i> = 5.961(3) Å	<i>a</i> = 5.8871(6) Å
		<i>b</i> = 6.3920(9) Å	<i>b</i> = 6.3004(7) Å
		<i>c</i> = 11.935(2) Å	<i>c</i> = 11.8296(13) Å
		α = 95.605(7) °	α = 96.219(4) °

β = 102.848(4) °

γ = 96.821(4) °

β = 101.46(5) °

γ = 98.25(4) °

Table S2. Data from Pawley refinement of cadmium pyrazinamide dithiocyanate.



Figure S8. Microscope image of cadmium pyrazinamide dithiocyanate.



Figure S9. Thermogravimetric analysis data for cadmium pyrazinamide dithiocyanate.



**Figure S10.** Microscope image of cadmium pyrazinamide dithiocyanate after heating in the SDT to 230 °C. Evidence of liquid flow is visible. Additionally, the liquid is a darker colour than the original single crystals. This may be due to linker decomposition as mass loss for this material began above 200 °C.



**Figure S11.** Experimental room temperature X-ray diffraction pattern of cadmium pyrazinamide dithiocyanate (b), and after heating to 220-230 °C (a).



**Figure S12.** SDT data for pyrazinamide ligand heating to 600 °C. Green – thermogravimetric trace. Blue – heat flow trace. Exo – down.



**Figure S13.** DSC data on heating only the pyrazinamide ligand to above  $T_m$ , cooling back to room temperature and then reheating. The sample was heated to 175 °C at a rate of 10 °C min<sup>-1</sup>. This was followed by cooling back to 30 °C at 10 °C min<sup>-1</sup>. A second up scan to 175 °C at 10 °C min<sup>-1</sup> was then performed. As its thermal response was significantly different to that of the Co and Cd coordination polymers, this suggests that the features observed for those materials were not due to the presence of uncoordinated ligand and were instead due to the materials themselves.

## 2. Zinc Dicyanamide Framework.



Figure S14. Pawley refinement of zinc dicyanamide. R<sub>wp</sub> = 10.475.

R <sub>wp</sub>	Space Group	Lattice Parameters	Lattice Parameters from CIF <sup>2</sup>
10.475	Pnma	<i>a</i> = 7.5863(12) Å	<i>a</i> = 7.6209(4) Å
		<i>b</i> = 7.5566(14) Å	<i>b</i> = 7.5985(4) Å
		<i>c</i> = 12.231(2) Å	<i>c</i> = 12.0477(7) Å
		α = 90 °	α = 90 °
		β = 90 °	β = 90 °
		γ = 90 °	γ = 90 °

 Table S3. Data from Pawley refinement of zinc dicyanamide



**Figure S15.** Experimental room temperature X-ray diffraction of  $[Zn(N(CN)_2)_2]$  (b), after heating to 455 °C (a) alongside the simulated X-ray diffraction pattern of  $[Zn(N(CN)_2)_2]$  (c).



**Figure S16.** Image of white zinc dicyanamide (left) and resulting yellow powder obtained after heating to 455 °C (right).



**Figure S17.** IR spectrum of as synthesised zinc dicyanamide.  $v_{max}/cm^{-1}$  3697w ( $v_sC\equiv N + v_{as}N-C$ ), 3147w ( $v_{as}C\equiv N + v_{as}N-C$ ), 2379s ( $v_sC\equiv N$ ), 2186vs ( $v_{as}C\equiv N$ ) and 1406s ( $v_{as}N-C$ ) and 962 ( $v_sN-C$ ). Assignments based on similar studies on metal dicyanamides.<sup>3,4</sup>



**Figure S18.** IR spectrum of zinc dicyanamide after heating to 455 °C.  $v_{max}/cm^{-1}$  2361w (C=N), 2172w (N=C=N), 2065w (N=C=N), 1640w (C=N), 1288br, 1157w and 797w. Only provisional assignments given. These were based on previous work on lead dicyanamide.<sup>4</sup>

#### 3. Nicotinate Frameworks



**Figure S19.** Image of  $M(NA)_2(H_2O)_4$  complexes prior to activation. From left to right: Zn complex (white), Co complex (pink) and Cu complex (blue).



**Figure S20.** Image of  $M(NA)_2$  MOFs after activation. From left to right: Zn MOF (white), Co MOF (purple) and Cu MOF (blue).



Figure S21. Pawley refinement of  $[Zn(NA)_2(H_2O)_4]$ .  $R_{wp} = 8.878$ 

R <sub>wp</sub>	Space Group	Lattice Parameters	Lattice Parameters from CIF <sup>5</sup>
8.878	C2/m	<i>a</i> = 14.182(1) Å	<i>a</i> = 14.22(3) Å
		<i>b</i> = 6.8902(4) Å	<i>b</i> = 6.890(12) Å
		<i>c</i> = 8.4695(6) Å	<i>c</i> = 8.437(15) Å
		α = 90 °	α = 90 °
		β = 118.196(2) °	β = 117.93(3) °
		γ = 90 °	γ = 90 °

**Table S4.** Data from Pawley refinement of  $[Zn(NA)_2(H_2O)_4]$ .



**Figure S22.** Pawley refinement of  $[Zn(NA)_2]$ .  $R_{wp} = 10.426$ . The abnormal peaks shapes observed here were also seen in previous work.<sup>6</sup>

Table S5. Data from Pawley refinement of [Zn(NA)<sub>2</sub>].

R <sub>wp</sub>	Space Group	Lattice Parameters	Lattice Parameters from CIF <sup>7</sup>
10.426	P4 <sub>3</sub> 2 <sub>1</sub> 2	a = 7.7442(12) Å	<i>a</i> = 7.7094(2) Å
		b = 7.7442(12) Å	<i>b</i> = 7.7094(2) Å
		<i>c</i> = 20.676(9) Å	<i>c</i> = 20.3266(7) Å
		α = 90 °	α = 90 °
		β = 90 °	β = 90 °
		γ = 90 °	γ = 90 °



Figure S23. Pawley refinement of  $[Co(NA)_2(H_2O)_4]$ .  $R_{wp} = 3.086$ 

R <sub>wp</sub>	Space Group	Lattice Parameters	Lattice Parameters from CIF <sup>8</sup>
3.086	C2/m	<i>a</i> = 14.160(6) Å	<i>a</i> = 14.140(3) Å
		<i>b</i> = 6.8821(16) Å	<i>b</i> = 6.8287(14) Å
		<i>c</i> = 8.488(3) Å	<i>c</i> = 8.4776(17) Å
		α = 90 °	α = 90 °
		β = 118.308(11) °	β = 118.08(3) °
		γ = 90 °	γ = 90 °

Table S6. Data from Pawley refinement of  $[Co(NA)_2(H_2O)_4]$ .



**Figure S24.** Pawley refinement of  $[Co(NA)_2]$ .  $R_{wp} = 16.720$ . The same impurity peaks as those present, though not discussed, in Ref.<sup>6</sup> are also present in the sample here.

Table S7. Data from Pawley refinement of [Co(NA)<sub>2</sub>].

R <sub>wp</sub>	Space Group	Lattice Parameters	Lattice Parameters from CIF <sup>9</sup>
16.720	P41212	<i>a</i> = 7.690(3) Å	<i>a</i> = 7.861(13) Å
		<i>b</i> = 7.690(3) Å	<i>b</i> = 7.861(13) Å
		<i>c</i> = 20.586(13) Å	<i>c</i> = 20.92(5) Å
		α = 90 °	α = 90 °
		β = 90 °	β = 90 °
		γ = 90 °	γ = 90 °



Figure S25. Pawley refinement of  $[Cu(NA)_2(H_2O)_4]$ . R<sub>wp</sub> = 10.987

R <sub>wp</sub>	Space Group	Lattice Parameters	Lattice Parameters from CIF <sup>10</sup>
10.987	P-1	<i>a</i> = 7.0350(15) Å	<i>a</i> = 7.0300(11) Å
		<i>b</i> = 7.1944(10) Å	<i>b</i> = 7.1743(12) Å
		<i>c</i> = 8.7340(13) Å	<i>c</i> = 8.6829(12) Å
		α = 68.218(18) °	α = 68.157(2) °
		β = 68.633(16) °	β = 68.576(2) °
		γ = 62.598(10) °	γ = 62.586(2) °

**Table S8.** Data from Pawley refinement of  $[Cu(NA)_2(H_2O)_4]$ .



Figure S26. Pawley refinement of  $[Cu(NA)_2]$ .  $R_{wp} = 8.911$ .

R <sub>wp</sub>	Space Group	Lattice Parameters	Lattice Parameters from CIF <sup>11</sup>
8.911	P21/c	<i>a</i> = 10.42(2) Å	<i>a</i> = 10.693(2) Å
		<i>b</i> = 9.83(2) Å	<i>b</i> = 9.5894(19) Å
		<i>c</i> = 12.39(3) Å	<i>c</i> = 12.535(3) Å
		α = 90 °	α = 90 °
		β = 113.37(12) °	β = 112.09(3) °
		γ = 90 °	γ = 90 °

Table S9. Data from Pawley refinement of  $[Cu(NA)_2]$ .



Figure S27. SDT data for Zn(NA)<sub>2.</sub> Green – thermogravimetric trace. Blue – heat flow trace. Exo – down.



Figure S28. SDT data for Co(NA)<sub>2.</sub> Green – thermogravimetric trace. Blue – heat flow trace. Exo – down.



**Figure S29.** SDT data for Cu(NA)<sub>2.</sub> Green – thermogravimetric trace. Blue – heat flow trace. Exo – down.

## 4. Zeolitic Imidazolate Frameworks



Figure S30. Pawley refinement of  $Zn(Im)_{1.95}(bIm)_{0.05}$ .  $R_{wp}$  = 4.805

Table S10. Data from	Pawley refinement	of Zn(Im) <sub>1.95</sub> (blm) <sub>0.05</sub> .
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R <sub>wp</sub>	Space Group	Lattice Parameters	Lattice Parameters from CIF <sup>12</sup>
4.805	Pbca	<i>a</i> = 15.473(2) Å	<i>a</i> = 15.6620(14) Å
		<i>b</i> = 15.500(2) Å	<i>b</i> = 15.6621(13) Å
		<i>c</i> = 18.035(2) Å	<i>c</i> = 18.2073(19) Å
		α = 90 °	α = 90 °
		β = 90 °	β = 90 °
		γ = 90 °	γ = 90 °



Figure S31. <sup>1</sup>H nuclear magnetic resonance spectra of  $Zn(Im)_{1.95}(bIm)_{0.05}$ .  $\delta$ H (500 MHz; DCI

(35%)/D<sub>2</sub>O:DMSO-d6 (1:5); Me<sub>4</sub>Si) 9.61 (1H, s, Hb), 9.09 (1H, s , Ha), 7.99 (2H, m, aromatic) 7.66 (4H, m, aromatic), 2.69 (DMSO), 0.00 (TMS).



Figure S32. Thermogravimetric analysis data for  $Zn(Im)_{1.95}(bIm)_{0.05}$ .



**Figure S33.** DSC data on heating the crystalline  $Zn(Im)_{1.95}(bIm)_{0.05}$  to above  $T_m$ , cooling back to room temperature and reheating above  $T_g$ . The sample was heated to an initial temperature of 40 °C. Then the sample was heated to 450 °C at a rate of 10 °C min<sup>-1</sup>. This was followed by cooling back to 40 °C at 10 °C min<sup>-1</sup>. A second up scan to 450 °C at 10 °C min<sup>-1</sup> was then performed to determine  $T_g$ .



**Figure S34.** <sup>1</sup>H nuclear magnetic resonance spectra of  $a_g Zn(Im)_{1.95}(bIm)_{0.05}$ .  $\delta H$  (500 MHz; DCl (35%)/D<sub>2</sub>O:DMSO-d6 (1:5); Me<sub>4</sub>Si) 9.61 (1H, s, Hb), 9.06 (1H, s, Ha), 8.05 (2H, m, aromatic) 7.67 (4H, m, aromatic), 2.69 (DMSO), 0.00 (TMS).



Figure S35. Pawley refinement of  $Zn(Im)_{1.95}(ClbIm)_{0.05}$ .  $R_{wp} = 5.175$ 

Table S11. Data from	Pawley refinement o	f Zn(Im) <sub>1.95</sub> (ClbIm) <sub>0.05</sub>
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R <sub>wp</sub>	Space Group	Lattice Parameters	Lattice Parameters from CIF <sup>12</sup>
5.175	Pbca	<i>a</i> = 15.497(2) Å	<i>a</i> = 15.6620(14) Å
		<i>b</i> = 15.553(2) Å	<i>b</i> = 15.6621(13) Å
		<i>c</i> = 18.012(2) Å	<i>c</i> = 18.2073(19) Å
		α = 90 °	α = 90 °
		β = 90 °	β = 90 °
		γ = 90 °	γ = 90 °



**Figure S36.** <sup>1</sup>H nuclear magnetic resonance spectra of  $Zn(Im)_{1.95}(ClbIm)_{0.05}$ .  $\delta$ H (500 MHz; DCl (35%)/D<sub>2</sub>O:DMSO-d6 (1:5); Me<sub>4</sub>Si) 9.67 (1H, s, Hc), 9.09 (1H, s, Ha), 8.02 (2H, m, aromatic) 7.67 (3H, m, aromatic), 2.70 (DMSO), 0.00 (TMS).



Figure S37. Thermogravimetric analysis data for Zn(Im)<sub>1.95</sub>(ClbIm)<sub>0.05</sub>.



**Figure S38.** DSC data on heating the crystalline  $Zn(Im)_{1.95}(ClbIm)_{0.05}$  to above  $T_m$ , cooling back to room temperature and reheating above  $T_g$ . The sample was heated to an initial temperature of 40 °C. Then the sample was heated to 450 °C at a rate of 10 °C min<sup>-1</sup>. This was followed by cooling back to 40 °C at 10 °C min<sup>-1</sup>. A second up scan to 450 °C at 10 °C min<sup>-1</sup> was then performed to determine  $T_g$ .



**Figure S39.** <sup>1</sup>H nuclear magnetic resonance spectra of  $a_g$ Zn(Im)<sub>1.95</sub>(ClbIm)<sub>0.05</sub>.  $\delta$ H (500 MHz; DCl (35%)/D<sub>2</sub>O:DMSO-d6 (1:5); Me<sub>4</sub>Si) 9.68 (1H, s, Hc), 9.10 (1H, s, Ha), ), 8.02 (2H, m, aromatic) 7.67 (3H, m, aromatic), 2.69 (DMSO), 0.00 (TMS).



Figure S40. Pawley refinement of  $Zn(Im)_{1.95}(bIm)_{0.025}(ClbIm)_{0.025}$ .  $R_{wp} = 5.059$ 

R <sub>wp</sub>	Space Group	Lattice Parameters	Lattice Parameters fi	rom CIF <sup>12</sup>
5.059	Pbca	<i>a</i> = 15.486(3) Å	<i>a</i> = 15.6620(14) Å	
		<i>b</i> = 15.528(2) Å	<i>b</i> = 15.6621(13) Å	
		<i>c</i> = 18.028(3) Å	<i>c</i> = 18.2073(19) Å	
		α = 90 °	α = 90 °	
		β = 90 °	β = 90 °	
		γ = 90 °	γ = 90 °	
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Table S12. Data from Pawley refinement of Zn(Im)<sub>1.95</sub>(bIm)<sub>0.025</sub>(ClbIm)<sub>0.025</sub>

Figure S41. <sup>1</sup>H nuclear magnetic resonance spectra of Zn(Im)<sub>1.95</sub>(bIm)<sub>0.025</sub>(ClbIm)<sub>0.025</sub>. δH (500 MHz; DCl (35%)/D2O:DMSO-d6 (1:5); Me4Si) 9.68 (1H, s, Hc), 9.62 (1H, s, Hb), 9.08 (1H, s, Ha), 8.04 (2H, m, aromatic) 7.66 (7H, m, aromatic), 2.69 (DMSO), 0.00 (TMS).



Figure S42. Thermogravimetric analysis data for Zn(Im)<sub>1.95</sub>(bIm)<sub>0.025</sub>(ClbIm)<sub>0.025</sub>.



**Figure S43.** DSC data on heating the crystalline  $Zn(Im)_{1.95}(bIm)_{0.025}(ClbIm)_{0.025}$  to above  $T_m$ , cooling back to room temperature and reheating above  $T_g$ . The sample was heated to an initial temperature of 40 °C. Then the sample was heated to 450 °C at a rate of 10 °C min<sup>-1</sup>. This was followed by cooling back to 40 °C at 10 °C min<sup>-1</sup>. A second up scan to 450 °C at 10 °C min<sup>-1</sup> was then performed to determine  $T_g$ .



**Figure S44.** <sup>1</sup>H nuclear magnetic resonance spectra of  $a_g Zn(Im)_{1.95}(bIm)_{0.025}(ClbIm)_{0.025}$ .  $\delta H$  (500 MHz; DCl (35%)/D2O:DMSO-d6 (1:5); Me4Si) 9.65 (1H, s, Hc), 9.60 (1H, s, Hb), 9.09 (1H, s, Ha), 8.02 (2H, m, aromatic) 7.67 (7H, m, aromatic), 2.70 (DMSO), 0.00 (TMS).



Figure S45. Pawley refinement of  $Zn_{0.8}Co_{0.2}(Im)_{1.95}(bIm)_{0.025}(ClbIm)_{0.025}$ .  $R_{wp} = 6.399$ 

R <sub>wp</sub>	Space Group	Lattice Parameters	Lattice Parameters from CIF <sup>12</sup>
6.399	Pbca	a = 15.28(5) Å	a = 15.6620(14) Å
		b = 15.55(5) Å	b = 15.6621(13) Å
		c = 17.98(5) Å	c = 18.2073(19) Å
		α = 90 °	$\alpha = 90$ °
		β = 90 °	β = 90 °
		γ = 90 °	γ = 90 °



**Figure S46.** <sup>1</sup>H nuclear magnetic resonance spectra of  $Zn_{0.8}Co_{0.2}(Im)_{1.95}(bIm)_{0.025}(ClbIm)_{0.025}$ .  $\delta$ H (500 MHz; DCl (35%)/D2O:DMSO-d6 (1:5); Me<sub>4</sub>Si) 9.68 (1H, s, Hc), 9.63 (1H, s, Hb), 9.09 (1H, s, Ha), 7.91 (2H, m, aromatic) 7.67 (7H, m, aromatic), 2.70 (DMSO), 0.00 (TMS).



Figure S47. TGA data for  $Zn_{0.8}Co_{0.2}(Im)_{1.95}(bIm)_{0.025}(ClbIm)_{0.025}$ 



**Figure S48.** <sup>1</sup>H nuclear magnetic resonance spectra of  $a_g Zn_{0.8}Co_{0.2}(Im)_{1.95}(bIm)_{0.025}(ClbIm)_{0.025}$ .  $\delta$ H (500 MHz; DCl (35%)/D<sub>2</sub>O:DMSO-d6 (1:5); Me<sub>4</sub>Si) 9.70 (1H, s, Hc), 9.60 (1H, s, Hb), 9.07 (1H, s, Ha), 8.02 (2H, m, aromatic) 7.67 (7H, m, aromatic), 2.70 (DMSO), 0.00 (TMS).



**Figure S49.** PXRD of glass ZIFs after heating to 450  $^{\circ}$ C under argon at 10  $^{\circ}$ C min<sup>-1</sup>, followed by cooling back to room temperature. a)  $a_g Zn(Im)_{1.95}(bIm)_{0.05}$ . b)  $a_g Zn(Im)_{1.95}(ClbIm)_{0.05}$ . c)  $a_g Zn(Im)_{1.95}(bIm)_{0.025}(ClbIm)_{0.025}$ . d)  $a_g Zn_{0.8}Co_{0.2}(Im)_{1.95}(bIm)_{0.025}(ClbIm)_{0.025}$ .



Figure S50. Optical Images of glass ZIFs a)  $a_gZn(Im)_{1.95}(bIm)_{0.05}$  b)  $a_gZn(Im)_{1.95}(ClbIm)_{0.05}$  c)  $a_gZn(Im)_{1.95}(bIm)_{0.025}(ClbIm)_{0.025}$  d)  $a_gZn_{0.8}Co_{0.2}(Im)_{1.95}(bIm)_{0.025}$ .

Sample	C (%)	H (%)	N (%)
Zn(Im) <sub>1.95</sub> (bIm) <sub>0.05</sub>	36.2	2.7	26.2
a <sub>g</sub> Zn(lm) <sub>1.95</sub> (blm) <sub>0.05</sub>	36.3	2.8	26.4
Predicted	36.9	3.0	27.8
Zn(Im) <sub>1.95</sub> (ClbIm) <sub>0.05</sub>	36.6	2.8	26.5
a <sub>g</sub> Zn(Im) <sub>1.95</sub> (ClbIm) <sub>0.05</sub>	36.2	2.8	26.4
Predicted	36.6	3.0	27.5
Zn(Im) <sub>1.95</sub> (bIm) <sub>0.025</sub> (ClbIm) <sub>0.025</sub>	36.2	2.8	26.3
a <sub>g</sub> Zn(Im) <sub>1.95</sub> (bIm) <sub>0.025</sub> (ClbIm) <sub>0.025</sub>	36.4	2.6	26.2
Predicted	36.7	3.0	27.6
Co <sub>0.2</sub> Zn <sub>0.8</sub> (Im) <sub>1.95</sub> (bIm) <sub>0.025</sub> (ClbIm) <sub>0.025</sub>	36.5	2.8	26.4
a <sub>g</sub> Co <sub>0.2</sub> Zn <sub>0.8</sub> (Im) <sub>1.95</sub> (bIm) <sub>0.025</sub> (ClbIm) <sub>0.025</sub>	36.6	2.8	26.4
Predicted	36.9	3.0	27.8

 Table S14. CHN analysis of the ZIFs produced in this body of work and the resulting glasses.

### **Supplementary References**

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