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Supporting information for article:

Spin resolved charge density and wave function refinements using Mollynx: a review

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Chemical Formulae	MnCu(pba)(H2O)3,2H2O		Cu2L2(N3)2 / C9H14CuF3N5O2		
Space group	Pnma		$P2_1/n$		
Cell parameters: a,b,c (Å)	12.7858(5), 21.2972(8), 5.1864(2)		10.5618(5), 9.4465(6), 13.6214(7) β = 108.379 (7)		
Experiment	XRD	PND	XRD	UND	PND
Unique reflections	6 880 (I>3σ(I))	228 (hkl; h-kl)	15731 7 208 (I>3 σ (I) and sinθ/λ < 1Å^{-1})	5049 2303 (I>3 σ (I))	474 212 (F_N>5.10^{-12}cm)
Temperature (K)	10	10	10	30	2
Wavelength (Å)	0.71073	0.83	0.71073	0.832	0.84
Maximum resolution (Å^{-1})	1.13	0.49	1.0	0.78	0.5
Refinement program	Mollynx-mult		Mollynx-mult		
R (%)	2.17	6.47	2.30		1.94
R_w (%)	1.62	2.20	1.52	5.5	7.83
GoF	1.54	1.85	1.07	1.67	1.37
Parameters	413	37	626	298	29

Chemical Formulae	SO_2 N_2 C_{14} H_{19}		$YTiO_3$	
Space group	$P2_1/a$		Pnma	
Cell parameters: a,b,c (Å)	9.340(2)/19.482(4)/8.634(1) β = 115.13(1)/		5.6900(4) / 7.5830(5) / 5.3180(3)	
Experiment	XRD	PND	XRD	PND
Unique reflections	8800 (I>0) 6744 (I>3σ)	352	4584	148
Temperature (K)	114	5.3	20	5
Wavelength (Å)	0.71073	1.173	0.35302	0.84/1.4
Maximum resolution ($Å^{-1}$)	0.91	0.55	1.67	
R_{int} (%)	1.8		3.66	
Refinement program	Mollynx-mult		Mollynx-mult	
R (%)	1.85	7.03	1.40	17.21
R_w (%)	2.39	0.61	1.12	8.84
GoF	0.85	1.72	1.18	4.14
Parameters	405	70	207	27
Refinement program			Mollynx-orb	
R (%)			1.39	19.47
R_w (%)			1.12	9.21
GoF			1.18	4.31
Parameters			73	9