

Table 3: Ordered moments from refining the low-temperature data from D10 and D23 using Irep(4). Two refinements were performed: one constraining the moments to lie only along \mathbf{a} ; and a second with the moments free in the (a, c) plane. The residuals for each refinement are also shown. All moment values are given in μ_B . Note that both nuclear and magnetic Bragg peaks were measured and that the refinements included both nuclear and magnetic structures.

	D10		D23	
Scanned reflections:	421		269	
Independent reflections:	417		121	
Irep(4)	$(M_x, 0, M_z)$	$(M_x, 0, 0)$	$(M_x, 0, M_z)$	$(M_x, 0, 0)$
Moment along a	3.13 (8)	3.33 (7)	3.3 (1)	3.62 (6)
Moment along c	-0.6 (1)	—	-0.6 (1)	—
Total moment	3.36 (9)	3.33 (7)	3.5 (1)	3.62 (6)
R_{F^2}	8.759	9.14	10.50	11.51
R_{wF^2}	46.47	47.30	22.77	25.06
R_F	11.32	11.71	9.714	10.56
χ^2	4.198	4.359	0.8128	0.9853

most likely present.

A schematic of the magnetic structure for CoPS_3 is shown in figure 7. The originally published structure is shown in figure 7(b), while the results for the current refinement are shown in figure 7(c). The current refinement results in a structure that is qualitatively identical to that for NiPS_3 [8].

The temperature dependence of the (010) Bragg peak was followed as a function of temperature to quantify the critical behaviour of the sublattice magnetization in CoPS_3 . The results are shown in figure 8. The Bragg peak intensity decreases as a power law with an exponent of $2\beta = 0.60 \pm 0.01$ close to T_N , which was established to be 119.1 ± 0.1 K in the analysis. The exponent was determined from fitting data in the temperature range $109 \leq T < T_N$, or from a reduced temperature $(1 - T/T_N) \leq 0.085$. The exponent is roughly similar to that expected for a phase transitions in a three-dimensional material, suggesting that CoPS_3 may be less two-dimensional than some of the other members of the MPS_3 family. The temperature dependence is remarkably similar to that observed for NiPS_3 , with the same exponent within approximately the same reduced temperature range.