

Table 1. Crystal data, data collection and structure refinement parameters for $\text{Ag}_2\text{Na}_5\text{Fe}_3(\text{As}_2\text{O}_7)_4$ and $\text{Ag}_5\text{Na}_2\text{Fe}_3(\text{P}_2\text{O}_7)_4$ at 100 and 298 K.

	$\text{Ag}_2\text{Na}_5\text{Fe}_3(\text{As}_2\text{O}_7)_4$		$\text{Ag}_5\text{Na}_2\text{Fe}_3(\text{P}_2\text{O}_7)_4$	
Temperature (K)	100	298	100	298
$M_r/\text{g mol}^{-1}$	1545.58	1545.58	1448.63	1448.63
Crystal symmetry	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	C2/c (n ^o 15)	C2/c (n ^o 15)	C2/c (n ^o 15)	C2/c (n ^o 15)
$a/\text{Å}$	9.973(2)	9.9512(3)	28.551(5)	9.5375(3)
$b/\text{Å}$	8.549(2)	8.5741(2)	8.363(1)	8.3886(3)
$c/\text{Å}$	28.664(6)	28.8231(8)	30.064(6)	28.0971(9)
β°	94.152(3)	93.910(1)	111.890(3)	93.623(2)
$V/\text{Å}^3$	2437.6(8)	2453.5(1)	6661(2)	2243.4(3)
Z	4	4	12	4
Calculated density (g.cm^{-3})	4.2104	4.1828	4.3322	4.2876
Equipment	Bruker SMART CCD 1K	Bruker X8	Bruker SMART CCD 1K	Bruker X8
Radiation MoK α (Å)	0.71073	0.71073	0.71073	0.71073
Scan mode	ω - scan	ω - scan	ω - scan	ω - scan
Recording angular range 2θ (°)	5.70 – 57.32	5.66 – 89.14	4.96 – 57.5	2.90 – 73.1
Recording reciprocal space	$-12 \leq h \leq 13$ $-10 \leq k \leq 11$ $-38 \leq l \leq 38$	$-19 \leq h \leq 17$ $-15 \leq k \leq 15$ $-54 \leq l \leq 52$	$-36 \leq h \leq 38$ $-11 \leq k \leq 11$ $-40 \leq l \leq 39$	$-15 \leq h \leq 15$ $-14 \leq k \leq 14$ $-46 \leq l \leq 46$
Number of measured reflections	9766	54142	21371	54056
Number of independent reflections [$I > 3\sigma(I)$]	2522	7600	2803	4784
R merging factor (%)	3.58	3.40	7.10	3.32
μ (mm^{-1}) for MoK α	14.317	14.223	6.970	6.899
Number of refined parameters / restrictions	212 / 2	242 / 2	358 / 6	255 / 2
Refinement method	Least squares on F	Least squares on F	Least squares on F	Least squares on F
R_1 (F) [$I > 3\sigma(I)$] (%) ^a	2.64	3.11	5.45	2.62
wR_2 (F^2) [$I > 3\sigma(I)$] (%) ^b	2.73	3.20	5.66	2.64
Weighting scheme	unit	unit	unit	unit
Goodness of fit	1.36	0.95	2.71	0.93
Isotropic secondary extinction (type I)	0.049(2)	0.028(1)	0.016(4)	0.023(2)
Min / Max $\Delta\rho$ $e/\text{Å}^3$	-0.71 / 1.61	-1.84 / 1.85	-1.74 / 1.64	-1.80 / 1.37

$$^a R_1(F) = \frac{\sum \left| |F_o| - |F_c| \right|}{\sum |F_o|} \cdot \quad ^b wR_2(F^2) = \left[\frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)} \right]^{1/2}$$