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Supplementary Material

Crystal structures of new silver ion conductors $Ag_7Fe_3(X_2O_7)_4$ (X = P, As)

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Table 1. Crystal data, data collection and structure refinement parameters for $Ag_7Fe_3(P_2O_7)_4$ and $Ag_7Fe_3(As_2O_7)_4$ at 100 and 298 K.

	$Ag_7Fe_3(P_2O_7)_4$		$Ag_7Fe_3(As_2O_7)_4$	
Temperature (K)	100	298	100	298
Crystal symmetry	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$ (n^o14)	C2/c (n^o15)	$P2_1/c$ (n^o14)	C2/c (n^o15)
a (Å)	9.532(3)	9.5561(5)	9.914(1)	9.9285(3)
b (Å)	8.421(2)	8.4417(4)	8.607(1)	8.6101(2)
c (Å)	28.021(7)	28.226(1)	28.904(4)	29.0390(8)
β (^{o})	93.225(5)	93.465(2)	93.317(2)	93.523(1)
V (Å^3)	2245(1)	2272.8(3)	2462.2(7)	2477.7(2)
Z	4	4	4	4
Calculated density (g/cm^3)	4.785	4.731	5.316	5.283
Equipment	Bruker SMART CCD 1K	Bruker X8	Bruker SMART CCD 1K	Bruker X8
Radiation MoKα (Å)	0.71073	0.71073	0.71073	0.71073
Scan mode	ω - scan	ω - scan	ω - scan	ω - scan
Recording angular range 2θ (°)	5.04-58.12	2.90-73.70	4.86-57.30	2.82-86.72
Recording reciprocal space	$-12 \le h \le 12$	$-16 \le h \le 16$	$-13 \le h \le 13$	$-15 \le h \le 19$
	$0 \le k \le 11$	$0 \le k \le 14$	$-11 \le k \le 11$	$-12 \le k \le 16$
	$0 \le l \le 37$	$0 \le l \le 47$	$-38 \le l \le 38$	$-56 \le l \le 44$
Number of measured reflections	5399	5703	19136	31808
Number of independent reflections [I>3σ(I)]	3803	5254	4377	7562
R merging factor	5.08	3.44	4.76	4.12
μ (mm^{-1}) for MoKα	8.546	8.444	17.945	17.833
Twin matrix	$\begin{pmatrix} -1 & 0 & 0.33 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0.3571 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	/	/
Twin ratio (%)	0.886(1)/0.114	0.893(1)/0.107	/	/
Number of refined parameters / equations	402 / none	257 / (2)	380 / (1)	276 / (3)
Refinement method	Least squares on F	Least squares on F	Least squares on F	Least squares on F
R_1 (F) [I>3σ(I)] (%)[a]	3.83	4.22	4.09	3.16
wR_2 (F^2) [I>3σ(I)] (%)[b]	4.14	4.69	4.10	3.32
Weighting scheme	unit	unit	unit	unit
Goodness of fit	1.92	1.61	1.82	1.24
Isotropic secondary extinction (type I)	0.023(2)	0.029(2)	0.084(2)	0.195(2)
Min / Max Δρ e/Å^3	-1.06/1.86	-1.13/1.61	-0.90/1.87	-1.44/1.93

(1) ai[Ag2b] = 5 - ai[Ag2a] - ai[Ag3a] - ai[Ag3b] - ai[Ag4a] - ai[Ag4b]
(2) ai[Ag1] = 1 - ai[Ag1'] ; ai[Ag2] = 2.5 - ai[Ag3] - ai[Ag3'] - ai[Ag3''] - ai[Ag4] - ai[Ag4']
(3) ai[Ag1] = 1 - ai[Ag1'] ; ai[Ag2] = 2.5 - ai[Ag2'] - ai[Ag3] - ai[Ag3'] - ai[Ag3''] - ai[Ag4] - ai[Ag4'] - ai[Ag4'']

[a] $R_1(F) = \sum \left| |F_O| - |F_C| \right| / \sum |F_O|$. [b] $wR_2(F^2) = \left[\sum w\left(F_O^2 - F_C^2\right)^2 / \sum w\left(F_O^2\right) \right]^{1/2}$.

Table 2. Atomic parameters, equivalent isotropic displacement parameters for α-$Ag_7Fe_3(P_2O_7)_4$ (100 K) and bond valence sums (BVS) for the cations.

Atom	Wyck.	sof	x	y	z	U_{eq}[a] (Å^2)	BVS
Ag1a	4e	1	0.49290(9)	0.1364(1)	0.05432(3)	0.0096(2)	1.196
Ag1b	4e	1	0.99959(9)	-0.6461(1)	-0.06121(3)	0.0112(2)	1.179
Ag2a	4e	1	0.24036(9)	0.0957(1)	0.35397(3)	0.0102(2)	0.982
Ag2b	4e	1	0.22920(9)	0.0703(1)	0.14246(3)	0.0102(2)	0.926
Ag3a	4e	1	0.7486(1)	0.1544(1)	0.17181(4)	0.0195(2)	0.844
Ag3b	4e	1	-0.21506(9)	0.1877(1)	0.31134(4)	0.0163(2)	0.873
Ag4a	4e	1	0.4588(1)	0.3580(1)	0.14723(3)	0.0172(2)	0.955
Fe1	4e	1	0.2484(2)	0.3262(2)	0.25142(5)	0.0061(4)	3.027
Fe2a	4e	1	0.4328(2)	-0.2784(2)	0.06431(5)	0.0053(4)	3.083
Fe2b	4e	1	0.9329(2)	0.2215(2)	0.06349(5)	0.0053(4)	3.085
P1a	4e	1	0.5464(3)	0.5094(3)	0.2443(1)	0.0056(7)	4.894
P1b	4e	1	-0.0493(3)	0.5049(3)	0.2545(1)	0.0070(7)	4.909
P2a	4e	1	0.4791(3)	0.3878(3)	0.33519(9)	0.0062(7)	4.855
P2b	4e	1	0.0290(3)	0.3823(3)	0.16526(9)	0.0058(7)	4.822
P3a	4e	1	0.7428(3)	-0.0919(3)	0.0580(1)	0.0057(7)	4.896
P3b	4e	1	0.7603(3)	-0.4111(3)	-0.05548(9)	0.0052(7)	4.962
P4a	4e	1	0.1683(3)	-0.0386(3)	0.0332(1)	0.0061(7)	4.984
P4b	4e	1	0.6669(3)	-0.5404(3)	0.03479(9)	0.0051(7)	4.917
O1a	4e	1	0.6213(8)	0.4406(9)	0.2027(3)	0.008(2)	
O1b	4e	1	-0.1259(8)	0.439(1)	0.2954(3)	0.010(2)	
O2a	4e	1	0.6056(7)	0.6660(9)	0.2622(3)	0.005(1)[b]	
O2b	4e	1	-0.1077(8)	0.6615(9)	0.2348(3)	0.008(2)	
O3a	4e	1	0.3862(8)	0.5115(9)	0.2362(3)	0.010(2)	
O3b	4e	1	0.1106(8)	0.5097(9)	0.2636(3)	0.007(2)	
O4a	4e	1	0.5729(8)	0.3882(9)	0.2889(3)	0.008(2)	
O4b	4e	1	-0.0700(7)	0.3798(9)	0.2107(3)	0.008(2)	
O5a	4e	1	0.1779(7)	0.330(1)	0.1838(3)	0.010(2)	
O5b	4e	1	0.3283(7)	0.345(1)	0.3178(3)	0.010(2)	
O6a	4e	1	0.4859(8)	0.5538(9)	0.3568(3)	0.010(2)	
O6b	4e	1	0.0265(8)	0.5478(9)	0.1450(3)	0.008(2)	
O7a	4e	1	0.5467(7)	0.2568(9)	0.3656(3)	0.008(2)	
O7b	4e	1	-0.0393(8)	0.2531(9)	0.1338(3)	0.009(2)	
O8a	4e	1	0.7291(8)	-0.5773(9)	-0.0746(3)	0.007(2)	
O8b	4e	1	0.7707(8)	0.0775(9)	0.0763(3)	0.008(2)	
O9a	4e	1	0.5846(8)	-0.1235(9)	0.0503(3)	0.009(2)	
O9b	4e	1	0.9174(7)	-0.3802(9)	-0.0487(3)	0.006(1)[b]	
O10a	4e	1	0.6854(8)	-0.2832(9)	-0.0849(2)	0.005(2)	
O10b	4e	1	0.8177(8)	-0.2191(9)	0.0867(3)	0.009(2)	
O11a	4e	1	0.2000(7)	0.0942(9)	-0.0048(3)	0.005(2)	
O11b	4e	1	0.7039(8)	-0.406(1)	-0.0027(3)	0.009(2)	
O12a	4e	1	0.0981(7)	-0.1777(9)	0.0059(3)	0.007(1)[b]	
O12b	4e	1	0.5967(7)	-0.6770(9)	0.0060(3)	0.007(2)	
O13a	4e	1	0.8019(8)	-0.592(1)	0.0607(3)	0.011(2)	
O13b	4e	1	0.3054(7)	-0.0876(9)	0.0590(3)	0.009(2)	
O14a	4e	1	0.5698(7)	-0.4616(9)	0.0693(3)	0.006(2)	
O14b	4e	1	0.0721(8)	0.0400(9)	0.0673(3)	0.009(2)	

[a] $U_{eq} = 1/3 \left(\sum_{ij} U_{ij} a_i^* b_j^* a_i a_j \right)$

[b] U_{iso}

Table 3. Atomic parameters and equivalent isotropic displacement parameters for α-$Ag_7Fe_3(As_2O_7)_4$ (100 K) and bond valence sums (BVS) for the cations.

Atom	Wyck.	sof	x	y	z	U_{eq}[a] ($Å^2$)	BVS
Ag1a	4e	1	0.48612(8)	0.1323(1)	0.05239(3)	0.0090(2)	1.033
Ag1b	4e	1	1.00671(9)	-0.6392(1)	-0.05821(3)	0.0119(2)	1.081
Ag2a	4e	0.993(4)	0.2403(1)	0.1022(1)	0.35093(3)	0.0144(3)	0.951
Ag2b	4e	0.95(1)	0.2284(1)	0.0833(1)	0.14210(3)	0.0135(3)	0.915
Ag3a	4e	0.902(4)	0.7581(1)	0.1525(1)	0.16910(4)	0.0226(3)	0.769
Ag3b	4e	0.948(4)	-0.2200(1)	0.1934(1)	0.31273(4)	0.0238(3)	0.806
Ag4a	4e	0.963(4)	0.4580(1)	0.3548(1)	0.14929(3)	0.0220(3)	0.945
Ag4b	4e	0.239(6)	0.0398(8)	0.130(1)	0.8529(2)	0.070(3)	0.831
As1a	4e	1	0.5459(1)	0.5285(1)	0.24359(4)	0.0052(3)	4.839
As1b	4e	1	-0.0524(1)	0.5166(1)	0.25641(4)	0.0054(3)	4.839
As2a	4e	1	0.4748(1)	0.3976(1)	0.33689(4)	0.0045(3)	4.939
As2b	4e	1	0.0297(1)	0.3921(1)	0.16408(4)	0.0052(3)	4.903
As3a	4e	1	0.7414(1)	-0.0962(1)	0.05887(4)	0.0043(3)	4.997
As3b	4e	1	0.7604(1)	-0.4070(1)	-0.05713(4)	0.0039(3)	4.904
As4a	4e	1	0.1647(1)	-0.0449(1)	0.03494(4)	0.0036(3)	4.957
As4b	4e	1	0.6636(1)	-0.5459(1)	0.03621(4)	0.0039(3)	4.992
Fe1	4e	1	0.2492(2)	0.3451(2)	0.25059(5)	0.0046(3)	3.041
Fe2a	4e	1	0.4302(1)	-0.2798(2)	0.06539(5)	0.0044(4)	3.012
Fe2b	4e	1	0.9303(1)	0.2205(2)	0.06444(5)	0.0041(4)	3.045
O1a	4e	1	0.6205(7)	0.4593(9)	0.1979(3)	0.007(2)	
O1b	4e	1	-0.1279(8)	0.4451(9)	0.3011(3)	0.008(2)	
O2a	4e	1	0.6060(7)	0.6980(9)	0.2645(3)	0.007(2)	
O2b	4e	1	-0.1162(8)	0.6840(9)	0.2349(3)	0.009(2)	
O3a	4e	1	0.3752(7)	0.5290(9)	0.2363(3)	0.009(2)	
O3b	4e	1	0.1187(8)	0.5239(9)	0.2626(3)	0.008(2)	
O4a	4e	1	0.5797(7)	0.3977(9)	0.2899(3)	0.009(2)	
O4b	4e	1	-0.0791(7)	0.3829(9)	0.2100(2)	0.007(2)	
O5a	4e	1	0.1867(7)	0.3423(9)	0.1836(3)	0.008(2)	
O5b	4e	1	0.3151(7)	0.3531(9)	0.3170(2)	0.005(2)	
O6a	4e	1	0.4765(8)	0.574(1)	0.3597(3)	0.012(2)[b]	
O6b	4e	1	0.0258(8)	0.571(1)	0.1432(3)	0.012(2)[b]	
O7a	4e	1	0.5429(8)	0.2492(9)	0.3665(2)	0.008(2)	
O7b	4e	1	-0.0380(8)	0.2445(9)	0.1324(3)	0.009(2)	
O8a	4e	1	0.7304(7)	-0.5882(9)	-0.0758(2)	0.007(1)[b]	
O8b	4e	1	0.7712(7)	0.0858(9)	0.0767(3)	0.007(1)[b]	
O9a	4e	1	0.5745(7)	-0.1253(9)	0.0513(3)	0.007(2)	
O9b	4e	1	0.9277(7)	-0.3793(9)	-0.0503(3)	0.007(2)	
O10a	4e	1	0.6813(8)	-0.2696(9)	-0.0890(3)	0.007(2)	
O10b	4e	1	0.8182(7)	-0.2343(9)	0.0895(2)	0.007(2)	
O11a	4e	1	0.1998(8)	0.1057(9)	-0.0026(3)	0.008(2)	
O11b	4e	1	0.6992(7)	-0.3946(9)	-0.0013(2)	0.006(1)[b]	
O12a	4e	1	0.0974(7)	-0.1939(9)	0.0042(3)	0.007(2)	
O12b	4e	1	0.5955(7)	-0.6905(9)	0.0041(2)	0.006(1)[b]	
O13a	4e	1	0.8069(8)	-0.5928(9)	0.0659(3)	0.009(1)[b]	
O13b	4e	1	0.3080(7)	-0.0904(9)	0.0647(2)	0.006(1)[b]	
O14a	4e	1	0.5544(7)	-0.4686(9)	0.0713(3)	0.007(1)[b]	
O14b	4e	1	0.0562(7)	0.0349(9)	0.0705(3)	0.007(1)[b]	

[a] $U_{eq} = 1/3 \left(\sum_{ij} U_{ij} a_i^* b_j^* a_i a_j \right)$

[b] U_{iso}

Table 4. Atomic parameters and equivalent isotropic displacement parameters for β-$Ag_7Fe_3(P_2O_7)_4$ (298 K) and bond valence sums (BVS) for the cations.

Atom	Wyck.	sof	x	y	z	U_{eq}[a] ($Å^2$)	BVS
Ag1	8f	0.7(2)	0.2567(9)	0.387(1)	0.4433(3)	0.0196(9)	1.115
Ag1'	8f	0.3(2)	0.244(9)	0.402(11)	0.438(4)	0.028(4)	1.138

Ag2	8f	0.90(6)	0.50562(7)	0.33123(7)	0.35626(2)	0.0334(2)	0.838
Ag3	8f	0.13(3)	0.547(4)	0.944(3)	0.319(2)	0.060(4)	0.864
Ag3'	8f	0.52(3)	0.5238(6)	0.9297(5)	0.3117(4)	0.039(1)	0.865
Ag3''	8f	0.32(2)	0.500(1)	0.906(2)	0.3271(3)	0.046(1)	0.839
Ag4	8f	0.33(2)	0.2988(7)	0.589(1)	0.3484(3)	0.049(1)	0.937
Ag4'	8f	0.30(2)	0.2841(8)	0.635(2)	0.3561(3)	0.066(2)	0.821
Fe1	4e	1	0	0.0716(1)	1/4	0.0080(2)	2.976
Fe2	8f	1	0.31632(6)	0.97198(7)	0.43654(2)	0.0064(1)	3.062
P1	8f	1	0.2977(1)	0.2529(1)	0.24590(4)	0.0082(2)	4.880
P2	8f	1	0.2226(1)	0.1325(1)	0.33540(4)	0.0081(2)	4.893
P3	8f	1	0.5077(1)	0.6602(1)	0.44364(4)	0.0072(2)	4.919
P4	8f	1	0.4180(1)	0.7894(1)	0.53368(3)	0.0062(2)	4.946
O1	8f	1	0.3731(4)	0.1840(4)	0.2054(1)	0.0151(8)	
O2	8f	1	0.3565(3)	0.4097(4)	0.2642(1)	0.0124(7)	
O3	8f	1	0.1377(3)	0.2565(4)	0.2370(1)	0.0125(7)	
O4	8f	1	0.3212(3)	0.1310(4)	0.2904(1)	0.0102(6)	
O5	8f	1	0.0752(3)	0.0816(4)	0.3170(1)	0.0138(7)	
O6	8f	1	0.2246(4)	0.2969(4)	0.3553(1)	0.0162(8)	
O7	8f	1	0.2914(4)	0.0036(4)	0.3666(1)	0.0126(7)	
O8	8f	1	0.4781(3)	0.8285(4)	0.4254(1)	0.0106(6)	
O9	8f	1	0.6650(3)	0.6283(4)	0.4504(1)	0.0109(7)	
O10	8f	1	0.4318(4)	0.5347(4)	0.4148(1)	0.0139(7)	
O11	8f	1	0.4515(3)	0.6548(4)	0.4965(1)	0.0104(6)	
O12	8f	1	0.3465(3)	0.9252(4)	0.5057(1)	0.0092(6)	
O13	8f	1	0.5536(3)	0.8409(4)	0.5597(1)	0.0121(7)	
O14	8f	1	0.3229(3)	0.7106(4)	0.5681(1)	0.0095(6)	

[a] $U_{eq} = 1/3 \left(\sum_{ij} U_{ij} a_i^* b_j^* a_i a_j \right)$

Table 5. Atomic parameters and equivalent isotropic displacement parameters for β-$Ag_7Fe_3(As_2O_7)_4$ (298 K) and bond valence sums (BVS) for the cations.

Atom	Wyck.	sof	x	y	z	U_{eq} [a] ($Å^2$)	BVS
Ag1	8f	0.65(6)	0.2652(4)	0.3834(3)	0.4480(3)	0.0179(3)	1.065
Ag1'	8f	0.35(6)	0.256(1)	0.3881(10)	0.4412(6)	0.0216(8)	1.082
Ag2	8f	0.55(5)	0.515(1)	0.3368(5)	0.3570(3)	0.0259(4)	0.802
Ag2'	8f	0.28(5)	0.494(2)	0.350(2)	0.3507(5)	0.024(1)	0.878
Ag3	8f	0.41(1)	0.5205(3)	0.9403(2)	0.3128(2)	0.0477(8)	0.774
Ag3'	8f	0.13(1)	0.5276(8)	0.9656(9)	0.2954(9)	0.22(1)	0.924
Ag3''	8f	0.31(1)	0.4985(3)	0.9190(6)	0.3288(1)	0.0497(7)	0.741
Ag4	8f	0.26(2)	0.276(1)	0.6002(9)	0.3517(2)	0.051(1)	0.861
Ag4'	8f	0.30(1)	0.3129(6)	0.5872(7)	0.3453(1)	0.0374(7)	0.965
Ag4''	8f	0.26(1)	0.7883(7)	0.147(1)	0.3552(1)	0.084(2)	0.750
As1	8f	1	0.29914(3)	0.27251(4)	0.24488(1)	0.00904(5)	4.904
As2	8f	1	0.22055(3)	0.14531(3)	0.33709(1)	0.00873(5)	4.923
As3	8f	1	0.50902(3)	0.65672(3)	0.44247(1)	0.00706(5)	5.001
As4	8f	1	0.41431(3)	0.79555(3)	0.53542(1)	0.00598(5)	4.961
Fe1	4e	1	0	0.09580(6)	1/4	0.0079(1)	3.016
Fe2	8f	1	0.31887(4)	0.97096(4)	0.43530(1)	0.00658(7)	3.047
O1	8f	1	0.3741(3)	0.1995(3)	0.20022(8)	0.0182(6)	
O2	8f	1	0.3607(2)	0.4411(3)	0.26531(8)	0.0159(5)	
O3	8f	1	0.1295(2)	0.2761(3)	0.23741(8)	0.0142(5)	
O4	8f	1	0.3294(2)	0.1423(3)	0.29117(7)	0.0123(4)	
O5	8f	1	0.0644(2)	0.0974(3)	0.31632(7)	0.0157(5)	
O6	8f	1	0.2242(4)	0.3220(3)	0.3589(1)	0.0255(7)	
O7	8f	1	0.2876(3)	-0.0032(3)	0.36795(7)	0.0152(5)	
O8	8f	1	0.4785(2)	0.8387(2)	0.42463(8)	0.0126(4)	
O9	8f	1	0.6754(2)	0.6273(3)	0.44999(8)	0.0131(4)	
O10	8f	1	0.4302(2)	0.5209(3)	0.41104(8)	0.0148(5)	
O11	8f	1	0.4502(2)	0.6446(2)	0.49796(7)	0.0125(4)	
O12	8f	1	0.3452(2)	0.9418(2)	0.50413(7)	0.0108(4)	
O13	8f	1	0.5578(2)	0.8422(3)	0.56469(8)	0.0136(4)	
O14	8f	1	0.3067(2)	0.7159(3)	0.57063(7)	0.0113(4)	

[a] $U_{eq} = 1/3 \left(\sum_{ij} U_{ij} a_i^* b_j^* a_i a_j \right)$

Table 6. Second and third order displacement parameters in $Å^2$ for Ag1 (replacing Ag1 and Ag1' in the split-site models) in β-$Ag_7Fe_3(P_2O_7)_4$ and β-$Ag_7Fe_3(As_2O_7)_4$ (298 K).

	β-$Ag_7Fe_3(P_2O_7)_4$	β-$Ag_7Fe_3(As_2O_7)_4$
U_{11}	0.0191(2)	0.0214(1)
U_{22}	0.0147(1)	0.01478(9)
U_{33}	0.0401(2)	0.0335(1)
U_{12}	-0.0068(1)	-0.00564(8)
U_{13}	0.0139(2)	0.0140(1)
U_{23}	-0.0115(1)	-0.00878(9)
C111	-0.0007(1)	-0.00053(7)
C112	0.00077(7)	0.00047(4)
C113	-0.00034(3)	-0.00020(1)
C122	-0.00094(8)	-0.00040(4)
C123	0.00041(2)	0.00021(1)
C133	-0.00016(1)	-0.000081(6)
C222	0.0010(1)	0.00052(9)
C223	-0.00048(3)	-0.00019(2)
C233	0.00017(1)	0.000063(6)
C333	-0.000063(7)	-0.000023(3)

Table 7. Distances (Å) between neighbor silver sites and size (Å) of the oxygen windows connecting these sites along the diffusion paths for $Ag_7Fe_3(P_2O_7)_4$ and $Ag_7Fe_3(As_2O_7)_4$ at 100 and 298 K.

α-$Ag_7Fe_3(P_2O_7)_4$ (100 K)			
Ag1a—Ag1a	3.822(1)	R[9a,9a]	1.89(1)
Ag1a—Ag2b	3.664(2)	R[6a,10a,13b]	1.836(8)
Ag1a—Ag4a	3.234(1)	R[6a,10a,14a]	2.110(8)
Ag1a—Ag3a	3.987(2)	R[6a,8b,14a]	2.337(8)
Ag1b—Ag1b	4.221(2)	R[9b,9b]	1.84(1)
Ag1b—Ag2a	3.422(1)	R[6b,10b,13a]	1.870(8)
Ag1b—Ag3b	4.030(2)	R[6b,8a,14b]	2.351(8)
Ag4a—Ag2b	3.263(1)	R[5a,6a]	2.08(1)
Ag4a—Ag3b	3.841(2)	R[3a,8a]	2.31(1)
Ag4a—Ag2a	3.498(2)	R[1a,7a,13a]	2.503(8)
Ag4a—Ag3a	3.291(2)	R[1a,6a]	1.88(1)
Ag3a—Ag3b	3.916(2)	R[1a,3b]	2.25(1)
		R[1b,3a]	2.21(1)
α-$Ag_7Fe_3(As_2O_7)_4$ (100 K)			
Ag1a—Ag1a	3.812(1)	R[9a,9a]	1.94(1)
Ag1a—Ag2b	3.768(1)	R[6a,10a,13b]	1.815(8)
Ag1a—Ag4a	3.417(1)	R[6a,10a,14a]	2.053(8)
Ag1a—Ag3a	4.199(1)	R[6a,8b,14a]	2.311(8)
Ag1b—Ag1b	4.139(3)	R[9b,9b]	1.89(1)
Ag1b—Ag2a	3.614(1)	R[6b,10b,13a]	1.830(8)
Ag1b—Ag4b	3.278(7)	R[6b,10b,14b]	2.092(8)
Ag1b—Ag3b	4.268(2)	R[6b,8a,14b]	2.335(8)
Ag4a—Ag2b	3.261(2)	R[2a,10a]	2.15(1)
Ag4a—Ag3b	3.946(2)	R[5a,7a]	2.34(1)
Ag4a—Ag2a	3.672(2)	R[1a,7a,13a]	2.473(8)
Ag4a—Ag3a	3.466(2)	R[1a,6a]	1.90(1)
Ag4b—Ag2a	3.045(9)	R[2b,10b]	2.13(1)
Ag4b—Ag3a	3.238(9)	R[5b,7b]	2.32(1)
Ag4b—Ag2b	3.242(8)	R[1b,7b,13b]	2.484(8)
Ag4b—Ag3b	3.153(8)	R[1b,6b]	1.85(1)
Ag3a—Ag3b	4.159(2)	R[3a,4b]	2.28(1)
		R[1b,3a]	2.22(1)
β-$Ag_7Fe_3(P_2O_7)_4$ (298 K)			
Ag1—Ag1	3.96(1)	R[9,9]	1.88(2)
Ag1—Ag2	3.553(9)	R[6,10,13]	1.883(3)
Ag1’—Ag4	3.0(1)	R[6,10,14]	2.152(3)
Ag1’—Ag3	3.8(1)	R[6,8,14]	2.357(3)
Ag4—Ag2	2.94(1)	R[5,6]	2.157(3)
Ag4’—Ag3’’	3.22(2)	R[3,8]	2.344(2)
Ag4’—Ag2	3.13(1)	R[1,7,13]	2.538(3)
Ag4—Ag3	2.78(4)	R[1,6]	1.89(3)
Ag3’—Ag3’	3.48(2)	R[1,3]	2.232(2)
β-$Ag_7Fe_3(As_2O_7)_4$ (298 K)			
Ag1—Ag1	3.82(1)	R[9,9]	1.908(2)
Ag1’—Ag2’	3.65(2)	R[6,10,13]	1.834(2)
Ag1’—Ag4	3.19(2)	R[6,10,14]	2.075(2)
Ag1’—Ag3’’	4.03(1)	R[6,8,14]	2.327(2)
Ag4’—Ag2’	2.71(2)	R[2,10]	2.151(2)
Ag4’’—Ag3’’	3.26(1)	R[5,7]	2.352(2)
Ag4’’—Ag2	3.17(1)	R[1,7,13]	2.504(2)
Ag4—Ag3	3.04(1)	R[1,6]	1.888(2)
Ag3’—Ag3’	2.66(4)	R[1,3]	2.266(2)