Dalton Transactions

ROYAL SOCIETY OF CHEMISTRY

CORRECTION

View Article Online
View Journal | View Issue

Cite this: *Dalton Trans.*, 2023, **52**, 2898

Correction: Wide band gap thiophosphates $ASrPS_4$ (A = Li, Na, K, Rb, Cs): cation size effect induced successive structural transformation

Yi Huang,[a] Junben Huang[b] and Yong Zhang*[a,c]

DOI: 10.1039/d3dt90024j

rsc.li/dalton

Correction for 'Wide band gap thiophosphates $ASrPS_4$ (A = Li, Na, K, Rb, Cs): cation size effect induced successive structural transformation' by Yi Huang *et al.*, *Dalton Trans.*, 2022, **51**, 15067–15073, https://doi.org/10.1039/D2DT02321K.

The authors regret the inconsistences between crystal data in the cif and Table 1 as published in their original submission. The correct Table 1 is as follows:

Table 1 Crystal data and structure refinement for $ASrPS_4$ (A = Li, Na, K, Rb, Cs)

Empirical formula	$LiSrPS_4$	$NaSrPS_4$	$KSrPS_4$	$RbSrPS_4$	$CsSrPS_4$
Formula weight	253.77	269.82	285.93	332.30	379.74
Crystal system	Tetragonal	Monoclinic	Orthorhombic	Orthorhombic	Orthorhombic
Space group	$I4_1/acd$	$P2_1/c$	*Pnma*	*Pnma*	*Pnma*
Unit cell dimensions (Å)	a = 11.5042(6)	a = 9.128(2)	a = 16.8490(17)	a = 17.3427(6)	a = 18.0743(12)
	b = 11.5042(6)	b = 10.429(3)	b = 6.6365(6)	b = 6.6969(2)	b = 6.7904(5)
	c = 19.9690(18)	c = 7.0685(16)	c = 6.5607(8)	c = 6.5130(2)	c = 6.4174(4)
		β = 101.051°			
Z/V (Å^3)	16/2642.8(4)	4/660.4(3)	4/733.61(13)	4/756.43(4)	4/787.62(9)
Density (g cm^{-3})	2.551	2.714	2.589	2.918	3.202
Absorption coefficient (mm^{-1})	9.529	9.603	9.154	14.721	12.553
F (000)	1920	512	544	616	688
Completeness to theta	98%	99.7%	98.8%	99.1%	99.7%
Goodness-of-fit on F^2	1.002	1.008	1.183	1.127	1.138
Final R indices $[F_o^2 > 2\sigma(F_o^2)]$[a]	R_1 = 0.0236,	R_1 = 0.0379,	R_1 = 0.0770,	R_1 = 0.0206,	R_1 = 0.0313,
	wR_2 = 0.0636	wR_2 = 0.0817	wR_2 = 0.2129	wR_2 = 0.0458	wR_2 = 0.0750
R indices (all data)[a]	R_1 = 0.0397,	R_1 = 0.0532,	R_1 = 0.0815,	R_1 = 0.0225,	R_1 = 0.0382,
	wR_2 = 0.0710	wR_2 = 0.0885	wR_2 = 0.2158	wR_2 = 0.0464	wR_2 = 0.0797
Largest diff. peak and hole (e Å^{-3})	0.374 and −0.464	0.889 and −0.650	3.699 and −1.422	1.620 and −1.368	1.287 and −1.069

[a] $R_1 = F_o - F_c/F_o$ and $wR_2 = [w(F_o^2 - F_c^2)^2/wF_o^4]^{1/2}$ for $F_o^2 > 2\sigma(F_o^2)$.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

[a]*School of Materials Science and Engineering, Harbin Institute of Technology, Harbin 150001, China. E-mail: yongzhang@hit.edu.cn*
[b]*School of Materials Science and Engineering, Education Ministry Key Laboratory of Nonferrous Materials Science and Engineering, Central South University, Changsha 410083 Hunan, China*
[c]*School of Materials Science and Engineering, Zhengzhou University, Zhengzhou 450001, PR China*