SHORT COMMUNICATION

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On the structure of $KAsSe_2$.

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Abstract

The structure of the title compound was described [Sheldrick & Häusler (1988), *Z. Anorg. Allg. Chem.* **561**, 139–148] as triclinic, space group $P\bar{1}$. It should be described as monoclinic, space group Cc.

The structure of $KAsSe_2$ has been reported (Sheldrick & Häusler, 1988) as triclinic, space group $P\bar{1}$ [$a = 6{\cdot}558$ (1), $b = 12{\cdot}628$ (2), $c = 6{\cdot}554$ (2) Å, $\alpha = 100{\cdot}43$ (2), $\beta = 107{\cdot}53$ (2), $\gamma = 100{\cdot}48$ (2)°, $Z = 4$] and refined to $R_F = 0{\cdot}075$ ($wR = 0{\cdot}081$) on the basis of 1951 reflections with $F_o^2 > 2{\cdot}0\sigma(F_o^2)$. It should be described in space group Cc. The lattice vectors [101], [10$\bar{1}$] and [010] define a C-centred monoclinic cell with $a' = 7{\cdot}750$, $b' = 10{\cdot}576$, $c' = 12{\cdot}628$ Å, $\alpha = 90{\cdot}03$, $\beta = 107{\cdot}88$, $\gamma = 89{\cdot}96$°, $Z = 8$.* The corresponding coordinate transformations are: $x' = \frac{1}{2}(x + z)$, $y' = \frac{1}{2}(x - z) + 0{\cdot}2806$, $z' = y$.

If the x coordinate of atom K(3) is decremented by 1·0 and the above transformations are then applied, pairs of atoms are closely related as x, y, z and $x, \bar{y}, \frac{1}{2} + z$. When these transformed coordinates are symmetrized and averaged, the values in Table 1 result. Since the original structure factors could not be retrieved (Sheldrick, 1989), we were unable either to carry out refinement in space group Cc or to confirm the systematic absences due to the c-glide plane (hkh with k odd in the triclinic description).

Table 1. *Coordinates* ($\times 10^4$), *space group* Cc

Numbers in square brackets are the shifts necessary to achieve the Cc symmetry.

	x'	y'	z'
K(1,3)	0·2183 [9]	0·2736 [2]	0·2591 [8]
K(2,4)	0·1527 [5]	0·0188 [3]	0·4976 [2]
As(1,3)	0·7222 [5]	0·1528 [1]	0·1768 [2]
As(2,4)	0·6668 [3]	0·0695 [2]	0·4425 [1]
Se(11,31)	0·9578 [6]	0·0094 [0]	0·2076 [4]
Se(12,32)	0·5390 [5]	0·1286 [5]	−0·0184 [2]
Se(21,41)	0·5002 [2]	0·2196 [2]	0·4999 [1]
Se(22,42)	0·4997 [4]	0·0428 [1]	0·2448 [0]

* The lattice vectors [$\bar{1}$01], [121] and [$\bar{1}$0$\bar{1}$] describe an F-centred orthorhombic cell ($a' = 10{\cdot}576$, $b' = 24{\cdot}036$, $c' = 7{\cdot}750$ Å, $\alpha = 89{\cdot}99$, $\beta = 89{\cdot}96$, $\gamma = 89{\cdot}98$°, $Z = 16$). However, no symmetry appropriate to an orthorhombic space group is present.

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