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Acta Cryst. (1989). **C45**, 2029

On the structure of KAsSe_2 . By MOSHE KAPON AND GEORGE M. REISNER, *Department of Chemistry, Technion – Israel Institute of Technology, 32000 Haifa, Israel* and RICHARD E. MARSH, *Arthur Amos Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, California 91125, USA*

(Received 20 June 1989; accepted 19 July 1989)

Abstract

The structure of the title compound was described [Sheldrick & Häusler (1988), *Z. Anorg. Allg. Chem.* **561**, 139–148] as triclinic, space group $P1$. It should be described as monoclinic, space group Cc .

The structure of KAsSe_2 has been reported (Sheldrick & Häusler, 1988) as triclinic, space group $P1$ [$a = 6.558$ (1), $b = 12.628$ (2), $c = 6.554$ (2) Å, $\alpha = 100.43$ (2), $\beta = 107.53$ (2), $\gamma = 100.48$ (2)°, $Z = 4$] and refined to $R_F = 0.075$ ($wR = 0.081$) on the basis of 1951 reflections with $F_o^2 > 2.0\sigma(F_o^2)$. It should be described in space group Cc . The lattice vectors $[101]$, $[10\bar{1}]$ and $[010]$ define a C -centred monoclinic cell with $a' = 7.750$, $b' = 10.576$, $c' = 12.628$ Å, $\alpha = 90.03$, $\beta = 107.88$, $\gamma = 89.96$ °, $Z = 8$.* The corresponding coordinate transformations are: $x' = \frac{1}{2}(x + z)$, $y' = \frac{1}{2}(x - z) + 0.2806$, $z' = y$.

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

* The lattice vectors $[\bar{1}01]$, $[121]$ and $[\bar{1}0\bar{1}]$ describe an F -centred orthorhombic cell ($a' = 10.576$, $b' = 24.036$, $c' = 7.750$ Å, $\alpha = 89.99$, $\beta = 89.96$, $\gamma = 89.98$ °, $Z = 16$). However, no symmetry appropriate to an orthorhombic space group is present.

0108-2701/89/122029-01\$03.00

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]

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).

References

- SHELDRICK, W. S. (1989). Personal communication.
SHELDRICK, W. S. & HÄUSLER, H.-J. (1988). *Z. Anorg. Allg. Chem.* **561**, 139–148.

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Acta Cryst. (1989). **C45**, 2029–2030

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