SHORT COMMUNICATION

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.


On the structure of KAsSe₂. 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

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Abstract

The structure of the title compound was described [Sheldrick & Hüsler (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 KAsSe₂ has been reported (Sheldrick & Hüsler, 1988) as triclinic, space group P1 [a = 6.558 (1), b = 12.628 (2), c = 6.554 (2) Å, α = 100.43 (2), β = 107.53 (2), γ = 100.48 (2)°, Z = 4] and refined to RF = 0.075 (wR = 0.081) on the basis of 1951 reflections with Fo² > 2.0σ(Fo²). It should be described in space group Cc.

The lattice vectors [101], [011] and [101] define a C-centred monoclinic cell with a' = 7.750, b' = 10.576, c' = 12.628 Å, α = 90°03', β = 107.88, γ = 89.96°, Z = 8.* The corresponding coordinate transformations are: x' = ½(x + z), y' = ½(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, y, y - 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 (hkk with k odd in the triclinic description).

Table 1. Coordinates (×10⁴), space group Cc

<table>
<thead>
<tr>
<th></th>
<th>x'</th>
<th>y'</th>
<th>z'</th>
</tr>
</thead>
<tbody>
<tr>
<td>K(1,3)</td>
<td>0.2183 [9]</td>
<td>0.2736 [2]</td>
<td>0.2591 [8]</td>
</tr>
<tr>
<td>K(2,4)</td>
<td>0.1527 [5]</td>
<td>0.0188 [3]</td>
<td>0.4976 [2]</td>
</tr>
<tr>
<td>As(1,3)</td>
<td>0.7222 [5]</td>
<td>0.1528 [1]</td>
<td>0.1528 [1]</td>
</tr>
<tr>
<td>As(2,4)</td>
<td>0.6668 [3]</td>
<td>0.0695 [2]</td>
<td>0.4425 [1]</td>
</tr>
<tr>
<td>Se(11,31)</td>
<td>0.9378 [6]</td>
<td>0.0094 [0]</td>
<td>0.2076 [4]</td>
</tr>
<tr>
<td>Se(12,32)</td>
<td>0.5390 [5]</td>
<td>0.1266 [5]</td>
<td>-0.0184 [2]</td>
</tr>
<tr>
<td>Se(21,41)</td>
<td>0.5002 [2]</td>
<td>0.2196 [2]</td>
<td>0.4999 [1]</td>
</tr>
<tr>
<td>Se(22,42)</td>
<td>0.4997 [4]</td>
<td>0.0428 [1]</td>
<td>0.2448 [0]</td>
</tr>
</tbody>
</table>

* The lattice vectors [101], [121] and [101] describe an F-centred orthorhombic cell (a' = 10.576, b' = 24.036, c' = 7.750 Å, α = 89.99, β = 89.96, γ = 89.98°, Z = 16). However, no symmetry appropriate to an orthorhombic space group is present.

References

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