

Short Communications

The Crystal Structure of Barium Selenopentathionate Trihydrate

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In barium telluropentathionate hydrates, the S-S-Te-S-S chain of the telluropentathionate ion occurs in the *cis* form or the *trans* form depending on the hydrate. The *cis* form, with the terminal sulphur atoms on the same side of the plane through the three middle atoms, occurs in two dihydrates,^{1,2} whereas the *trans* form, with the terminal sulphur atoms on opposite sides of the plane, was recently found in a trihydrate.³ In barium selenopentathionate dihydrate, BaSe(S₂O₅)₂·2H₂O, obtained by crystallization from aqueous methanol, the selenopentathionate ion has the *cis* form.⁴

Barium selenopentathionate trihydrate, BaSe(S₂O₅)₂·3H₂O, is obtained by crystallization from water.¹ The space group is *P*2₁/*c* (No. 14) with four formula units per unit cell, and the cell dimensions are, *a* = 10.502(3) Å, *b* = 4.992(2) Å, *c* = 23.987(6) Å, β = 110.85(4)°. The space group is the same as that of barium telluropentathionate trihydrate,^{1,3} and the cell dimensions differ only slightly.

The intensity data of 2519 non-zero reflections were collected by means of a Siemens AED 1 single-crystal diffractometer using MoKα radiation. The intensities were corrected for absorption and eventually for secondary extinction. The crystal structure was solved by three-dimensional Patterson and Fourier syntheses and refined by a full-matrix least squares program. The resulting reliability index, *R*, is 0.034.

The selenopentathionate ion has the same form in this salt as in the dihydrate,⁴ namely the *cis* form. This trihydrate is thus different from barium telluropentathionate trihydrate, where the *trans* form occurs.³

The dihedral angles, SSeS/SeSS, are 106.7° and 105.9°. A view of the ion as seen along the *b* axis is shown in Fig. 1. The calculated standard deviations of the

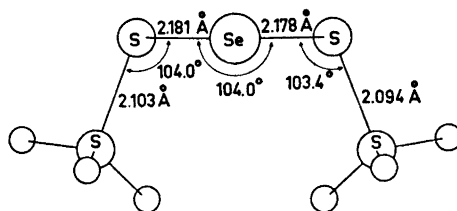


Fig. 1. A view of the selenopentathionate ion in BaSe(S₂O₅)₂·3H₂O as seen along the *b* axis.

bond lengths and angles given are 0.002 Å and 0.1°, respectively. The length of the sulphur-oxygen bonds of the sulphonate groups are in the range 1.436(4)–1.456(5) Å.

Further details of the structure will be published later.

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3. Gjerrestad, K. and Marøy, K. *Acta Chem. Scand.* **24** (1970) 3402.
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