The Crystal Structure of Cesium Triselenocyanate

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The crystal structures of potassium triselenocyanate hemihydrate, $K(SeCN)_3 \cdot \frac{1}{2}H_2O$, and rubidium triselenocyanate hemihydrate, $Rb(SeCN)_3 \cdot \frac{1}{2}H_2O$, have been determined.[1,2] This note briefly reports the results of a crystal structure determination of cesium triselenocyanate, $Cs(SeCN)_3$. In the potassium salt, no molecular symmetry is required. In the rubidium salt, the triselenocyanate ion lies across a crystallographic mirror plane, with the middle selenocyanate group in the plane. In the cesium salt, the middle selenocyanate group is located on a crystallographic twofold axis.

The triselenocyanate ion in the cesium salt is shown in Fig. 1. The Se–Se bond length is 2.650(3) Å, and the Se–Se–Se bond angle 178.3(1)°. The middle selenocyanate group, located on a twofold axis, is exactly linear, and the terminal selenocyanate groups are linear within the error.

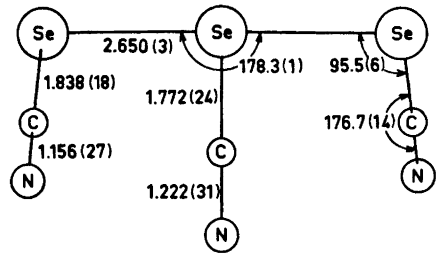

Fig. 1. The triselenocyanate ion in $Cs(SeCN)_3$, as seen normal to the plane through the middle selenocyanate group and the terminal selenium atoms.

Table 1. Se-Se bond lengths and Se-Se-Se bond angles in linear three-selenium systems.

	Se_1-Se_2	Se_2-Se_3	$\angle Se_1-Se_2-Se_3$
$K(SeCN)_3 \cdot \frac{1}{2}H_2O$	2.689(4) Å	2.648(4) Å	176.0(3)°
$Rb(SeCN)_3 \cdot \frac{1}{2}H_2O$	2.656(3)	2.656(3)	176.9(3)
$Cs(SeCN)_3$	2.650(3)	2.650(3)	178.3(1)
$[SeC(NH_2)_2]_3Cl_2 \cdot H_2O$	2.597(2)	2.717(2)	173.8(1)
$[SeC(NH_2)_2]_3Br_2 \cdot H_2O$	2.623(2)	2.711(2)	173.9(1)

Cesium triselenocyanate forms brown monoclinic prisms extended along the c axis, with $a = 7.969(4)$ Å, $b = 21.156(10)$ Å, $c = 5.593(4)$ Å, and $\beta = 98.84(6)°$. The space group, from systematic absences and subsequent structure analysis, is $C2/c$ (No. 15). and there are four formula units per unit cell; density, calc. 3.18, found 3.18 g/cm³.

Intensities were estimated visually from integrated Weissenberg photographs around the a and c axes, taken with Cu$K\alpha$ radiation using the multi-film technique. 637 independent reflections were observed with measurable intensities, from seven layers $0kl - 2kl$ and $hk0 - hk3$. The intensities were at later stages corrected for absorption and for secondary extinction.

The structure was solved by three-dimentional Patterson and Fourier methods using the heavy-atom technique. Full-matrix least squares refinement, with anisotropic temperature factors on all atoms, brought the reliability index, R, down to 0.062.

The least squares plane through a terminal selenocyanate group and the middle selenium atom makes an angle of 43.9° with the plane through the middle selenocyanate group and the terminal selenium atoms.

Table 1 gives Se–Se bond lengths and Se–Se–Se bond angles in the triselenocyanate ion in the potassium, rubidium, and cesium salts, and in the triselenourea ion in the dichloride and dibromide salts.[3]

Details of the structure will be published later.

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2. Hauge, S. *Acta Chem. Scand.* **25** (1971). *In press.*
3. Hauge, S., Opedal, D. and Aarskog, J. *Acta Chem. Scand.* **24** (1970) 1107.

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