5. Arnett, M. A. and McKelvey, D. R. In Coetzee, J. F. and Ritchie, C. D. *Solute-Solvent Interactions*, Marcel Dekker, New York 1969, Chapter 6.
6. Kirshenbaum, I. *Physical Properties and Analysis of Heavy Water*, McGraw, New York 1951, Chapter 1.
7. Vidulich, G. A., Evans, D. F. and Kay, R. L. *J. Phys. Chem.* **71** (1967) 656.
8. Kielland, J. *J. Am. Chem. Soc.* **59** (1937) 1675.
9. Salomaa, P. and Mattsén, M. *Acta Chem. Scand.* **25** (1971) 361.
10. D'Aprano, A. *J. Phys. Chem.* **75** (1971) 3290.

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The Structure of 2,5-Diphenyl-6a-selenathiophthene

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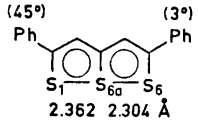
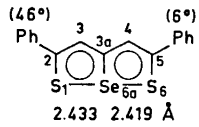
The structure study of 2,5-diphenyl-6a-thiathiophthene (I) showed that although the molecule is symmetrically substituted, the S–S bonds there are



(I)



(II)

unequal,[1] *i.e.* S(1)–S(6a) = 2.362(3) Å and S(6a)–S(6) = 2.304(3) Å. The difference in S–S bond lengths in I may, according to the results from *CNDO/2* calculations on phenyl substituted 6a-thiathiophthenes,[2] be due to the different twist of the phenyl-groups.

A structure investigation of crystals of 2,5-diphenyl-6a-selenathiophthene (II) isomorphous with those of I, have been carried out in order to find to which extent the phenyl substituents affect the sulphur-selenium bonding in II. Preliminary results are given here.

Due to the isomorphism the twist of the phenyl groups is almost the same in II as in I, and the sulphur-selenium distances in II are S(1)–Se(6a) = 2.433(3) Å and Se(6a)–S(6) = 2.419(3) Å. Thus, the sulphur-selenium bonding in II is less affected by the phenyl substituents than is the S–S bonding in I.

Other bond lengths in the 6a-selenathiophthene system of II are: S(1)–C(2) = 1.71(1) Å, Se(6a)–C(3a) = 1.87(1) Å, S(6)–C(5) = 1.72(1) Å, C(2)–C(3) = 1.38(2) Å, C(3)–C(3a) = 1.41(2) Å, C(3a)–C(4) = 1.36(2) Å, and C(4)–C(5) = 1.43(2) Å.

A sample of 2,5-diphenyl-6a-selenathiophthene was generously supplied by Reid.[3] The crystals are red and belong to the orthorhombic space group $P2_12_12_1$. The cell dimensions are $a = 12.040(4)$ Å, $b = 15.195(5)$ Å, and $c = 8.086(3)$ Å. There are four molecules per unit cell; $D_c = 1.613$ g cm^{-3}, $D_m = 1.61$ g cm^{-3}.

The structure analysis is based on X-ray data collected on a paper-tape controlled Siemens AED diffractometer using Mo$K\alpha$ radiation. 1262 reflections were observed within $\theta = 27°$.

The structure was solved by the heavy atom method and refined by full matrix least squares. The present R factor is 0.05.

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1. Hordvik, A. *Acta Chem. Scand.* **22** (1968) 2398; **25** (1971) 1583.
2. Hansen, L. K., Hordvik, A. and Sæthre, L. J. *Chem. Commun.* **1972** 222.
3. Reid, D. H. *J. Chem. Soc.* **C 1971** 3187.

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