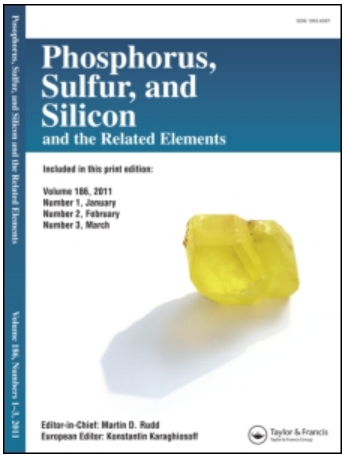

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Stereochemical Studies on Four Diastereoisomers of 1-Phenyl-2-Phenylthio-2-(2-Tetrahydropyran-2-Ylthio)Ethanol, $C_{19}H_{22}O_2S_2$

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Stereochemistry of the diastereoisomers of the title compound and comparison to its propanol derivative are discussed.

Keywords: hemithiodithioacetal; diastereoisomer; crystal structure

INTRODUCTION

In connection with the study of dithio- and hemithioacetals, compounds which are hemithiodithioacetals have been synthesized and characterized[1]. Separation and crystallization of the diastereomers and their X-ray structure determinations make it possible to study their configurations and conformations in crystalline state.

Molecular Structures

The isomers **1**, **2** and **4** crystallize in acentric space groups $P2_12_12_1$, $P2_12_12_1$ and $Pna2_1$, respectively, as a conglomerate of enantiomeric

crystals and isomer **3** in a centric spacegroup $P2_1/c$ as a racemate. Structures of **2** and **4** are presented in Figs. 1 and 2, respectively.

Configurations and Conformations

The configurations at the atoms C1, C2 and C15 found in structure determinations are *SSR*, *RSS*, *SRS* (and *RSR*) and *SSS* for **1-4**, respectively. The tetrahydropyranyl group has a similar chair conformation in each isomer, but bonding to S is equatorial in **1** and **2** and axial in **3** and **4**.

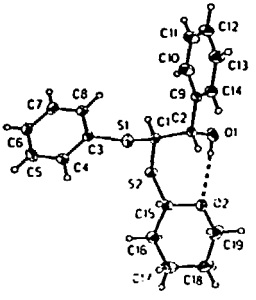

FIGURE 1. Structure of **2** with configurations *RSS*.

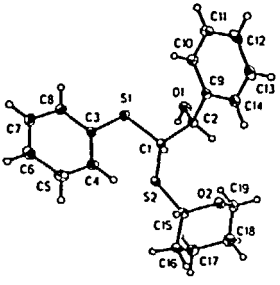

FIGURE 2. Structure of **4** with configurations *SSS*.

Geometry

Some torsion angles around S-atoms are listed in Table 1.

TABLE 1. Selected torsion angles of the isomers **1-4** (°).

	1	**2**	**3**	**4**
S1-C1-C2-O1	-62.93	171.55	66.30	-45.80
S1-C1-S2-C15	-52.91	-65.68	-96.26	-154.53

References

[1] J. Kansikas, K. Sipilä and T. Hase, *Acta Chem. Scand.*, **50**, 1147 (1996).