06-Crystallography of Organic Compounds

As small, synthetic molecules are generally used as selector, frequently bonded to silica micro particles. We have recently developed a family of new chiral stationary phases (CSPs) for HPLC applications, based on different derivatives of (R,R)-1,2-diaminocyclohexane (DACH). One of these CSPs containing the N,N-3,5-dichlorobenzyl derivative of (R,R)-1,2-DACH, is particularly effective in the separation of the enantiomers of a large number of 1,2-aminoalcohols (pharmacologically active as R-blockers) in the form of azaxolidin-2-ones. It has been shown that the knowledge of the recognition mechanism underlying such separations can lead to the design of improved CSPs. In this respect we are now investigating the origin of the stereo selective interactions between a soluble model of CSP and the enantiomers of a given chiral compound through a new model of recognition.

The selector was crystallized from chloroform. The space group is P2_12_12_1, the cell is ax = 20.71A, b = 21.08A, c = 11.40A and V = 4970.68A^3 with Z = 4. The data were collected at room temperature by a rotating anode Rigaku AFC5S equipped with a four circle diffractometer from Molecular Structure Corporation. The structure was solved by direct methods with the program SIR92 and anisotropically refined to a final R of 4.8% for 2637 reflections with 13.0°(θ).

The figure shows one of the two molecules of the selector contained in the unit cell. The latter is held together by two intermolecular hydrogen bonds.

**PS-06.03.14** HIERARCHICAL AND SPECTROSCOPIC STUDIES OF THE DIFFERENT CRYSTALLINE FORMS OF BIS(1,2,3,4-DISOPROPYLDIDEOXOGALACETOXYLACTONE)-6-O-2,6-DIISOPROPYLPHENYL) DISULFIDE. J. M. Kowalchuk, J. W. Hildebrandt, P. Knapik, Technical University of Gda, Institute of Technical Chemistry, Stefanowskiego 4/10, 80-952 Gdansk, Poland. The crystal and molecular structures of three different crystalline forms of bis(1,2,3,4-disopropyldideoxogalactono-7-0,6,0-6,0-diisopropylphenyl) disulfide (1a, 1b, and 1c) have been determined - Figure 1.

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