

MS12 O5**Crystal Structures of Normal Long-Chain Alkyl Dihalides**

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Normal long-chain aliphatic compounds have been studied to elucidate the principles of a crystallization of organic compounds such as calamitic liquid-crystals, because the molecular skeleton consisted of a simple *trans* zigzag straight hydrocarbon chain. The molecular shape of these compounds can be regarded as a rod-like one, and the molecules form a layered structure similar to those of the smectic liquid-crystals. Moreover, some of these long-chain compounds exhibited a high-temperature rotator phase just below their melting points, in which molecules have some degree of motional freedom, comparable with that in liquid-crystals. Thus, these long-chain compounds have been studied as model compounds for smectic liquid-crystals in addition to basic polymers.

In order to perform the investigations of phase transition mechanism, it is important to obtain detailed crystallographic data. Many researchers have been analyzed the crystal structure of many different kinds of normal long-chain aliphatic compounds. We have systematically analyzed the crystal structures of the alkane- α,ω -diols containing 10-24 carbon atoms using single-crystal X-ray diffraction method [1,2], and one of the present authors has studied the phase transition phenomena of the series of the alkane- α,ω -diols containing 13-24 carbon atoms [3].

In the present meeting, we report a result of the crystal structure analysis of 1,16-diiodohexadecane in order to clarify an effect of the terminal groups in the normal long-chain compounds on a construction of the layer structure.

The molecule, 1,16-diiodohexadecane, is centrosymmetric and all torsion angles are close to $\pm 180^\circ$, that is, the molecular structure including both terminal iodine (I) atoms has an all-*trans* conformation. The molecules form layers with a thickness of *c*. In the layers, the long axes of all molecules are inclined to the *ab* plane. The layers are arranged in parallel manner between the neighboring layers, forming a bookshelf motif. The molecular arrangement is similar to that of smectic C phase of liquid-crystals.

The results of structure analyses of 1,16-Dichlorohexadecane [4] and 1,16-Dibromohexadecane [5] have been reported. These compounds are arranged in a zigzag manner between adjacent layers, forming a herringbone motif. These molecular arrangements are similar to those of the tilted smectic C phase of liquid-crystals. Therefore, the structural feature of 1,16-diiodohexadecane is different from those of 1,16-Dichlorohexadecane and 1,16-Dibromohexadecane. It is considered that this difference is caused by the difference of the steric hindrance of atoms located in both ends of the molecular skeleton.

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