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Formation of Molecular Crystals of 1,1,2,2-Tetrakis(4-Hydroxyphenyl)Ethane with Sulfoxides

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1,1,2,2-Tetrakis(4-hydroxyphenyl)ethane (TEP), having four divergent hydroxy groups in the molecule, forms new molecular crystals to include various sulfoxides. A selective inclusion from mixture of dimethyl sulfoxide or diphenyl sulfoxide is discussed.

Keywords: 1,1,2,2-tetrakis(4-hydroxyphenyl)ethane; molecular crystal

Recently much attention has been centered on the chemistry of aggregation of molecular in the viewpoint of biological and structural chemistry.¹ We have also started a development concerning with the formation of molecular crystals with TEP to include various organic substance.^{2,3} Here, we wish to report the formation of new molecular crystals of TEP with various sulfoxides.

New molecular crystals with TEP to include various sulfoxides such as dimethyl sulfoxide (DMSO) and diphenyl sulfoxide (DPSO), was formed easily by mixing in appropriate solvent. The crystallography (Fig. 1, 2) and spectroscopy showed clearly the formation of the molecular crystals to include sulfoxide in 1:2 ratio (TEP:sulfoxide) and revealed that there is a difference in the formation of hydrogen bonding hydroxy group with sulfoxy group. Thus, in the molecular crystals

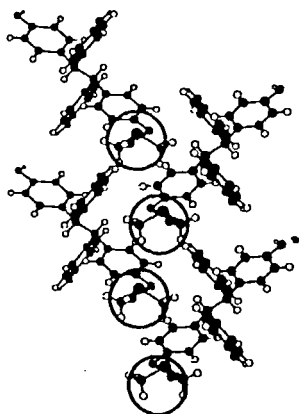


Fig. 1 Crystal Structure of TEP-2DMSO
Molecular Crystal

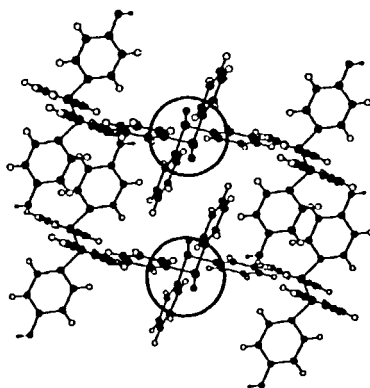


Fig. 2 Crystal Structure of TEP-2DPSO
Molecular Crystal

including DMSO, we can observe the hydrogen bonding between a sulfoxy oxygen and two hydroxy hydrogen of TEP, and another hand, in the case of DPSO, two kind of hydrogen bonding are observed, i.e. the first one is between hydrogen of hydroxy group and oxygen of sulfoxide and another one is the interaction between hydrogen of hydroxy group and π electron of benzene in DPSO. These results lead us to success of the selective inclusion from the mixture of DMSO and DPSO with TEP in variety of protic or aprotic solvents. In aprotic solvent such as benzene, ether, chloroform, and carbon tetrachloride, DMSO was preferentially included with TEP to form DMSO-TEP molecular crystals, whereas, in protic solvent, TEP predominantly included DPSO to form DPSO-TEP molecular crystals. This selectivity was interpreted in the light of polarity of DMSO and DPSO.

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