

CRYSTAL STRUCTURE ANALYSIS OF 1,1,2,2-TETRAKIS(3-METHYL-4-HYDROXYPHENYL)ETHANE INCLUSION CRYSTALS

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Enclosed in the host frameworks, physical properties of guest molecule such as solubility or guest release speed can be controlled by inclusion mode. 1,1,2,2-tetrakis(4-hydroxyphenyl)ethane, TEP, is known as a tetrapodal flexible host molecule which crystallizes with small guest molecules such as organic solvents.

In our previous study, three characteristic host frameworks were recognized in TEP inclusion crystal, which governed guest release properties. We focused on a TEP derivative, 1,1,2,2-tetrakis(3-methyl-4-hydroxyphenyl)ethane, TEOC (Fig.1), in which the methyl group next to hydroxy group deteriorates the hydrogen bonding capability. It is of interests to investigate the effect of methyl group to the framework structure and guest inclusion ability of TEOC comparing with TEP inclusion crystal.

Unexpectedly, crystal structure analysis revealed that TEOC-acetone and TEP-acetone inclusion crystals have similar structure. Also, in the case of TEOC-methanol (Fig.2) and corresponding TEP crystal, same 1D chain framework with guest joints was observed. Although the TEP-methanol has flat chain structure, the TEOC chain was zigzag shape due to steric effect of methyl group, and additional host molecules were attached to the chain. From these results, the influence of methyl substitution would be limited if the host framework has enough cavity around itself.

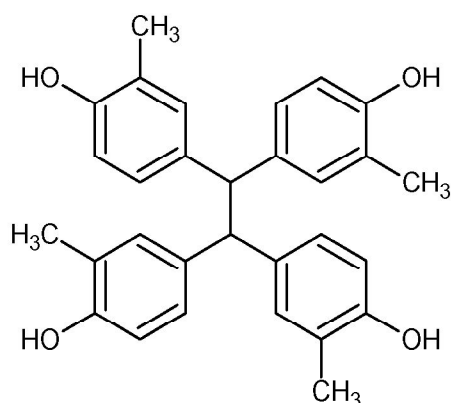


Fig. 1

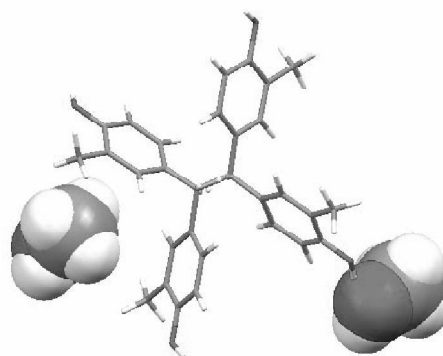


Fig. 2