

Generation of Chiral Cavity from Achiral Heterocyclophane Host
and Achiral Guest.

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Direct estimation of the weak nonpolar host-guest interaction is usually not easy due to the presence of other competing force fields. We here propose the heterocyclophane inclusion crystal as an appropriate system for the direct estimation.

A heterocyclophane, N, N', N'', N'''-tetramethyl-2, 11, 20, 29-tetraaza [3. 3. 3. 3] paracyclophane 1 formed a new type of host-guest inclusion complex with CHCl_3 , CH_2BrCl , CH_3CN , CH_2Cl_2 , etc., but such guest molecule of inappropriate size as n-hexane, 2-bromobutane or α -pinene was not included by 1. It was found by the X-ray analysis that these inclusion crystals were the (1:1) guest-in-host molecular inclusion complexes, in which at least three entirely different lattice structures were found depending on shapes of the guests. The crystalline complex of $1 \cdot \text{CHCl}_3$ (type I, $(R)_n$ or $(S)_n$), was chiral inclusion complex only in a crystalline state, but entirely achiral in a corresponding solution state. On the other hand, $1 \cdot \text{CH}_3\text{CN}$ (Type II $(RS)_n$), $1 \cdot \text{CH}_2\text{Cl}_2$ (Type III $(RRSS)_n$?) were racemic inclusion crystals. The difference in mode of lattice formation of the host is mainly induced by the conformation of the host which is determined by stronger host-guest interaction. So we were able to estimate the host-guest interaction by means of replacing the included guest molecule with another guest molecule in crystalline state, when the lattice energy is the same (within the same lattice structure). In the $1 \cdot \text{CHCl}_3$ crystal, for example, CHCl_3 was replaced completely with CH_2BrCl by crystalline-gaseous phase contact. Therefore, measurement of the exchange equilibrium allows estimation of weak nonpolar host-guest interaction.

