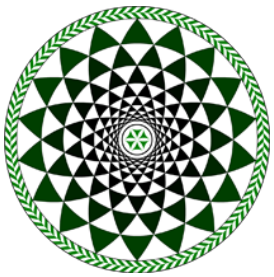

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The effect of the unconventional hydrogen bond on the CH3 group rotations in the acid/base molecular complexes

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A forecast of the strength of hydrogen bonds in the molecular complexes is important in the designing of the novel organic materials exhibiting polar or semiconducting properties. In such materials, besides the formation of relatively strong hydrogen bonds we expect either the formation of infinite chains of molecules in the crystal lattice or the stacking alignment of molecules, which favors the desired electrical or optical properties. Recently, the intriguing complexes have been obtained with derivatives of either pyrazine or bipyridil to form supramolecular architectures. The interactions between an acid and base molecule, mainly via hydrogen bonds, lead to a variety of crystal structures. The complex formation by an engagement of the lone electron pairs as the proton acceptors substantially changes the symmetry of the molecule and consequently the environment of methyl groups, which affects their dynamics.
The parameters of the methyl (-CH3) group rotational potential may be a probe of both the charge transfer phenomenon and the local contacts in the crystal. The most important technique we used to determine methyl group dynamics in molecular complexes involved neutron scattering. The parameters of the -CH3 rotational potential can be estimated on its basis. Particularly we can derive (i) the tunneling splitting at low temperature, (ii) the jump-diffusional rotation rate at moderate temperature (Quasielastic Neutron Scattering [QENS]), and (iii) the torsional energy (Inelastic Neutron Scattering [INS]). The number of the observed tunneling peaks for the particular molecular complex is related to the number of the inequivalent methyl groups in the crystal structure.
Several examples show an effect of the unconventional C-H…O or C-H…N hydrogen bonds and so called short contacts on the possible tunneling of the CH3 groups at low temperatures.

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