

Hydrogen bonded rings are a common structural feature of many host lattices. A reorientational process has been reported in the six-membered ring of O-H...O hydrogen bonds in the clathrate of Dianin's compound (DC) with ethanol [1]. Hydroxyl groups were found to exhibit concerted rotational jumps involving approximate rotations around C-O bonds, thus changing the direction of hydrogen bonding in the ring. Although an analogous six-membered hydrogen bonded ring is present in host structure of hydroquinone, a similar reorientational process has not been reported in any of its clathrates.

We have performed molecular dynamics simulations of the ethanol clathrates of DC and the methanol clathrate of hydroquinone. The simulations reproduce the observed reorientational process in the clathrate of DC but not in the clathrate of hydroquinone. We attribute this difference in behaviour to the larger ring size in the clathrate of DC as well as its greater flexibility.

We have also investigated the role of the guest molecules in the reorientational process. In the case of DC, ethanol appears to serve as a mediator, lowering the activation energy of reorientation through hydrogen bonding to oxygen atoms in the ring. The flexibility of the six-membered ring in DC enables hydroxyl groups of the ring to participate in hydrogen bonds with the guest.

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Keywords: host-guest systems, dynamics, simulations

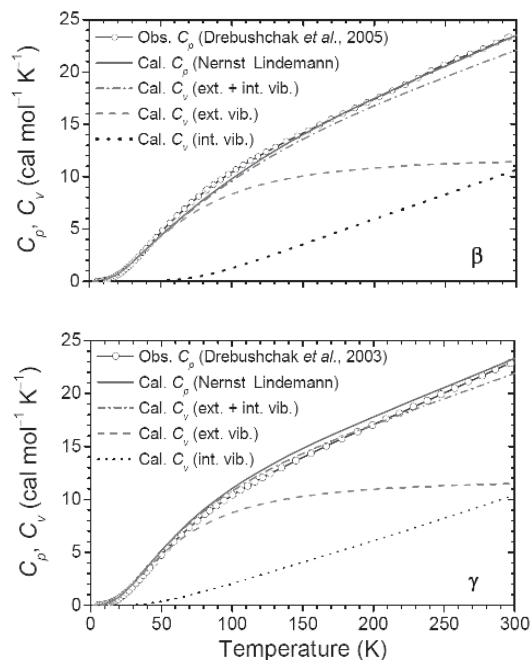
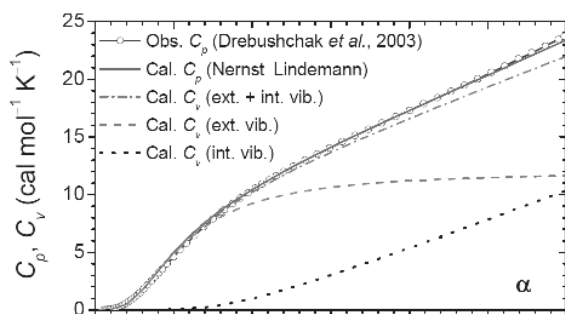
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Dynamic and thermodynamic properties of glycine polymorphs from diffraction data

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Synchrotron data to 0.5 Å resolution of the α -, β - and γ -polymorphs of glycine were collected between 10 and 298 K at KEK, SPring-8 and the ESRF. Data were processed with RAPID AUTO, DENZO/SCALEPACK or SAINT+ and structures were refined with SHELXL-97, yielding $R_{\text{int}} \approx R_1 \leq 5\%$. Simultaneous analyses of the multi-temperature atomic displacement parameters were performed to obtain librational and translational frequencies [1]. The external vibration frequencies from a normal mode analysis and the internal vibration frequencies from a two-layer ONIOM(B3LYP/6-311+G(2d,p):PM3) method and a glycine cluster model were used together with the Einstein, Debye, and Nernst-Lindemann molecular models to determine heat capacities C_V , C_p that are in agreement with C_p from calorimetry [2-3].



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Observation of the photo-excited state of $[\text{Co}^{\text{III}}(\text{en})_3]^{3+}$ by picosecond time-resolved XAFS

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Studying photochemical reaction in liquid with subnanosecond time-resolution gives information for understanding fundamental chemistry, biology and also for developing new materials and devices. [1]-[4] Monitoring the dynamic phenomenon requires a sensitive tool to investigate the electronic state and the structure with atomic resolution. However, studies of the excited state of tris(ethylenediamine)cobalt(III) ($[\text{Co}^{\text{III}}(\text{en})_3]^{3+}$) have been performed only using optical spectroscopic methods, [5] from which it is difficult to estimate the molecular structure with atomic resolution. Here, we have performed time-resolved X-ray absorption fine structure (TR-XAFS) on the $[\text{Co}^{\text{III}}(\text{en})_3]^{3+}$ dissolved in aqueous.

All measurements were performed in fluorescence method at the cobalt *K*-edge on the undulator beamline NW14A at the Photon Factory Advanced Ring. [6] X-ray pulses at 794 kHz were monochromatized by a Si(111) monochromator and used for the probe. A third harmonic of Ti:Sapphire laser operating at a frequency of 945 Hz was used for the pump source. The pump and probe measurements were performed