Invited Lecture

Chiral substitutions for promoting polar materials discovery

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Ferroelectric materials have many applications in the electronics industry from capacitors to data-storage. These require a polar point group which can be preferentially selected by using chiral substituents. Ferroelectrics undergo a phase transition upon heating to a paraelectric phase which can be of the order-disorder type, whereby the molecular substituents become disordered at high temperature. If the disorder is extreme enough, in the case of plastic crystals for instance, then the nature of the molecular dynamics at this high temperature is often not decipherable solely from X-ray diffraction data. Solid-state NMR experiments can be used to provide evidence to interpret fast molecular motions which are averaged out in an X-ray experiment [1].

Herein, we present the results of NMR and PXRD experiments for a potentially ferroelectric material with a high temperature paraelectric plastic phase, $(S\text{-}CTA)_2CdCl_4$ (CTA = 3-chloro-2-hydroxypropyltrimethylammonium). The unit cell and basic structural model were solved from high temperature PXRD data however the systematic absences could not provide an exact space group. Static 1H NMR spectra were measured through the phase transition temperature. The peak shape was used to rationalise the expected molecular dynamics which in turn supported our chosen space group. Investigations to model the molecular dynamics more accurately are ongoing.

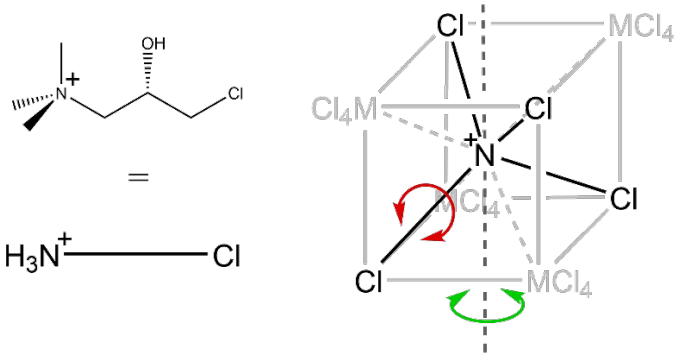

Figure 1. Tetrahedral site symmetry of the CTA molecule in $(S\text{-}CTA)_2CdCl_4$ at high temperature. Static ^1H NMR experiments determined which axis the rotational disorder occurs about.

[1] 1. S. Sturniolo, H. M. Wickins and P. Hodgkinson, J. Chem. Phys., 158, 244502 (2023)

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