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Reversible Control of Crystalline Rotors by Squeezing Their Hydrogen Bond Cloud Across a Halogen Bond-Mediated Phase Transition

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Résumé en anglais

We report on a crystalline rotor that undergoes a reversible phase transition at 145 K. Variable-temperature X-ray and 1H spin −lattice relaxation experiments, and calculations of rotational
barriers, provide a description (i) of the way in which the rotators' dynamics changes back and forth at the onset of the phase transition and (ii) of the mechanism responsible for the abrupt switching of the
crystalline rotors from a very low-energy 4-fold degenerate equilibrium state, in which the rotation is ultrafast (9.6 GHz at 145 K), to a single higher-energy state associated with a slower motion (2.3 GHz at 145 K). Our results provide evidence that the reversible change observed in the rotational barriers at the transition is due to a cooperative modulation of the C −Hrotator···Istator hydrogen bond cloud across a C −I stator···Istator−C halogen bond-mediated phase transition. In addition, we report evidence for second-harmonic generation from this material, thereby confirming with a second example the benefit of using polarized light to probe the torsional degree of freedom of chiral helix blades, as well as symmetry and dimensionality of large collections of chiral rotors in the solid state.

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