Poster Presentation

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Thermosalient crystals – new materials for clean energy conversion

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Thermosalient compounds, colloquially known as "jumping crystals", are promising materials for fabrication of actuators that are also being considered as materials for clean energy conversion because they are capable of direct conversion of thermal energy into mechanical motion. During heating and/or cooling, these materials undergo rapid phase transitions accompanied by large and anisotropic change in their unit-cell dimensions at relatively small volume change, causing the crystals to jump up to height of several centimeters. Although the list of about a dozen reported thermosalient materials has been expanded recently, this extraordinary phenomenon remains poorly understood. The main practical burden with the analysis of these crystals is their propensity to disintegrate during the transition. By using a combination of structural, microscopic, spectroscopic, and thermoanalytical techniques, we have investigated the thermosalient effect in a prototypal example of a thermosalient solid, the anticholinergic agent oxitropium bromide, and we proposed the mechanism responsible for the effect. We found that heating/cooling over the phase transition causes conformational changes in the oxitropium cation, which are related to increased separation between the ion pairs in the lattice. On heating, this change triggers rapid anisotropic expansion by 4% of the unit cell, whereby the b axis increases by 11% and the c axis decreases by 7%. The phase transition is reversible, and shows a thermal hysteresis of approximately 20 K. Additional interesting observations were that the high-temperature phase of this material can also be obtained by short exposure of the room temperature phase to UV light or with grinding.

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