“Jumping Crystals” – New Materials For Clean Conversion of Light and Thermal Energy Into Mechanical Motion

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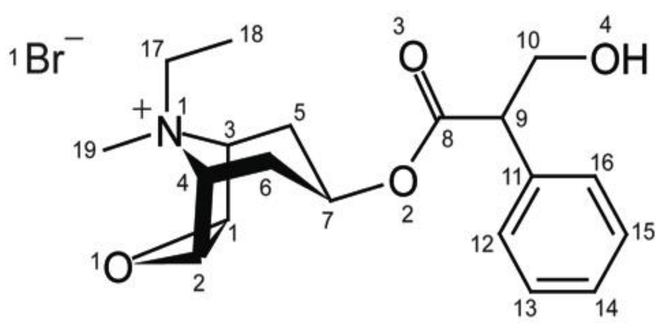
Thermosalient solids, which are occasionally colloquially referred to as “**jumping crystals**” are a prospective material basis for fabrication of efficient **actuators -** devices capable of conversion of thermal (kinetic) energy into mechanical work. When heated or cooled, these materials usually undergo sharp phase transitions, which are accompanied by sudden, large and anisotropic change in their cell volume, causing crystals to jump to heights of several times their size. Despite of their importance, the mechanism of only a couple of these transitions has been understood. Here we report and explain the mechanism underlying the jumping effect of single crystals of **oxitropium bromide,** an anticholinergic drug used in the treatment of respiratoy disorders (e.g. asthma and chronic bronchitis).

Oxitropium bromide



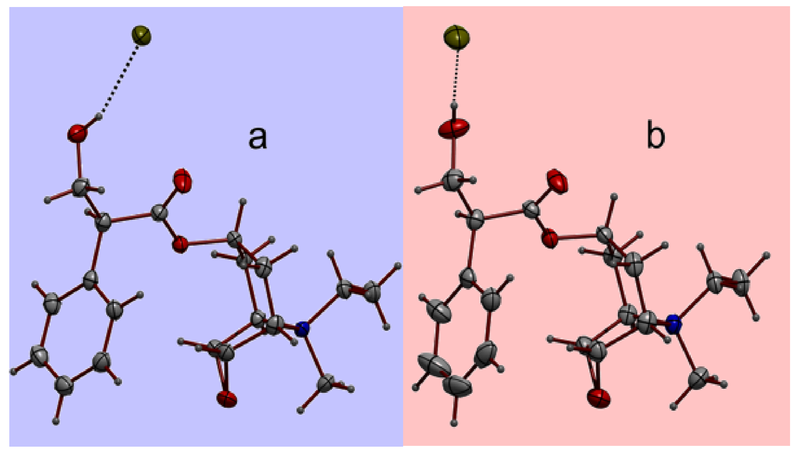
Zamir, S.; Bernstein, J.; Greenwood, D. J. *Mol. Cryst. Liq. Cryst*. **1994**, *242*, 193-200.

Three different crystal habits

Phase A	Phase A	Phase B
blocky crystals	prismatic crystals	prismatic crystals
DCM, ACN/DCM	MeOH/DCM	acetone, $CHCl_3$

Molecular structures of the forms A and B

Phase A **Phase B**



(the blocky and prismatic crystals of phase A have identical structures)

Orthorhombic, space group $P2_12_12_1$

PXRD pattern of the HT phase (form II)

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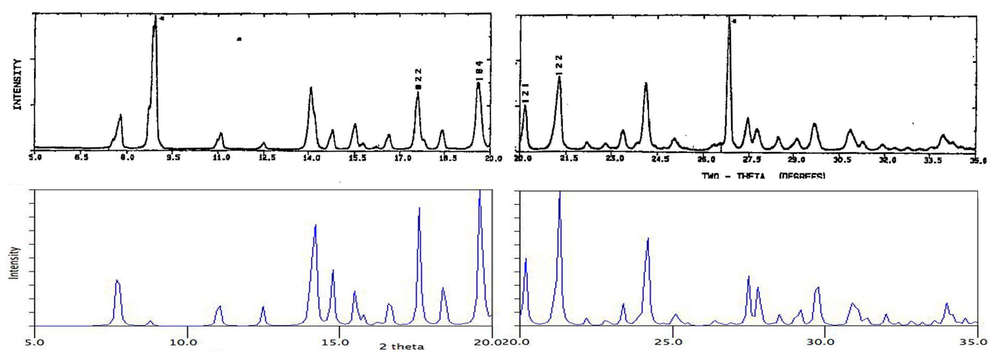
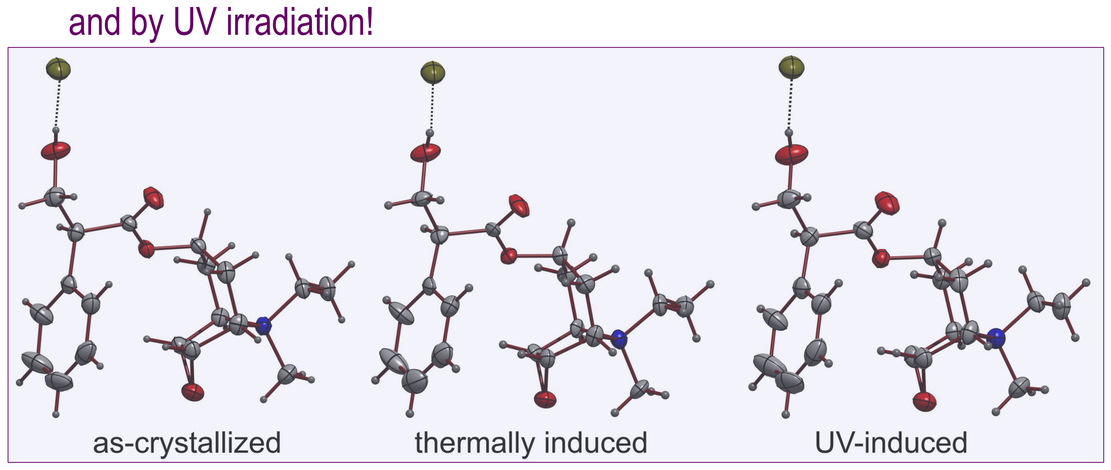


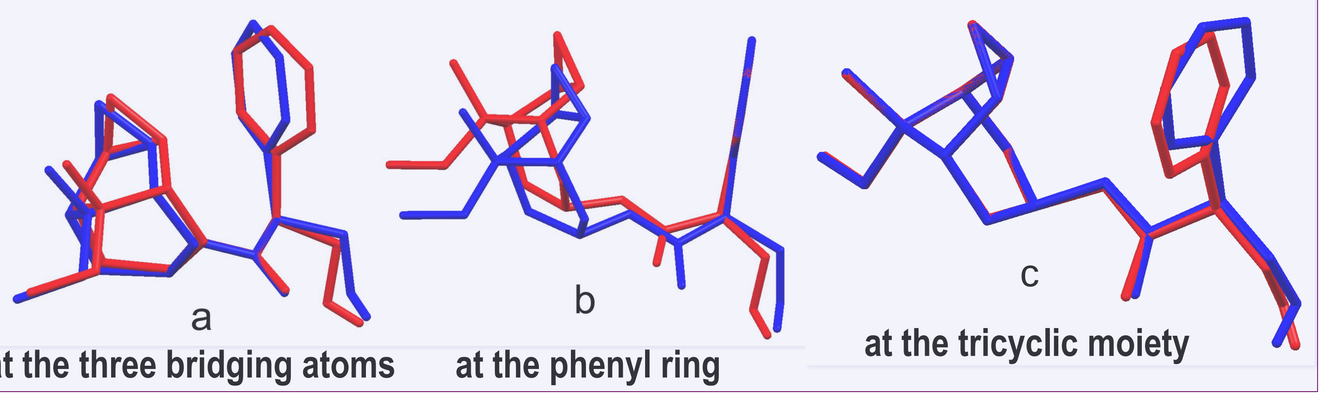
PXRD pattern of form B calculated from our sigle-crystal data, obtained by recrystallization (form B)

Perfect match!

Single crystal to single crystal phase transition, induced by heating and by UV irradiation!

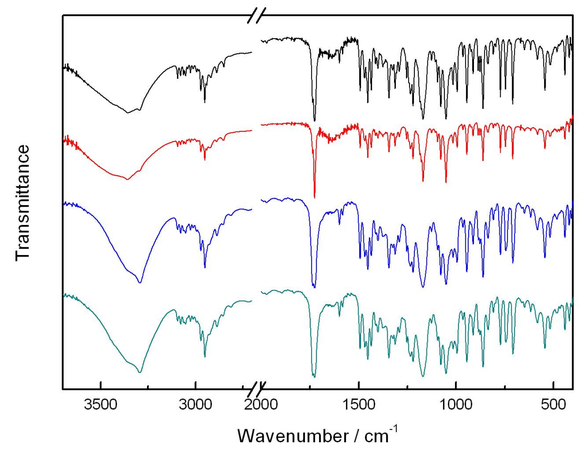


Overlapped representation of the molecular structures of phases A and B



at the three bridging atoms at the phenyl ring at the tricyclic moiety

Identical to the B phase obtained by recrystallization at RT!



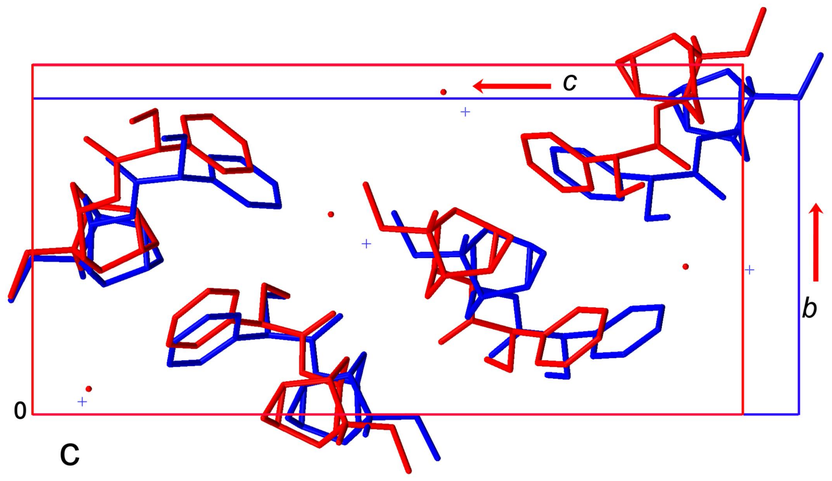
phase A (blocky)

phase A (prismatic)

heated A phase

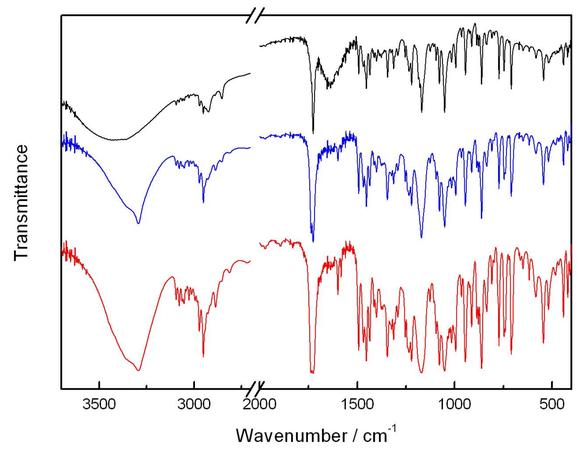
UV irradiated A phase

Crystal packing of phases A and B



Phase A
b = 10.1512 Å, c = 24.6291 Å

Phase B
b = 11.2179 Å, c = 22.8043 Å



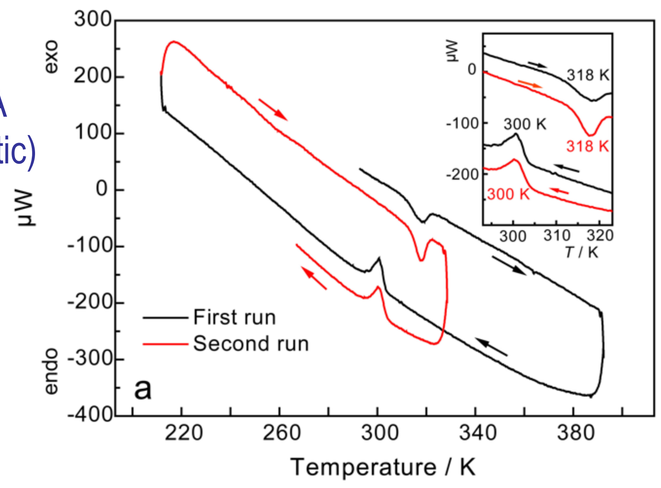
phase A (blocky)

phase A (blocky) UV irradiated

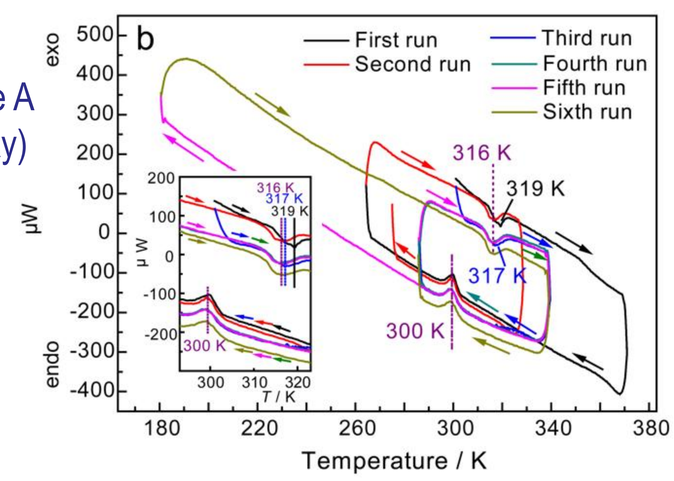
phase A (blocky)+KBr UV irradiated

DSC measurements

Phase A (prismatic)



Phase A (blocky)



Phase A (original)