

*Thermomechanical effect of molecular crystals and role of halogen bonding*Sudhir Mittapalli¹, D. Sravanakumar Perumalla², Ashwini Nangia¹¹University Of Hyderabad, Hyderabad, India, ²Department of Inorganic and Physical Chemistry, Indian Institute of Science., Bengaluru, India

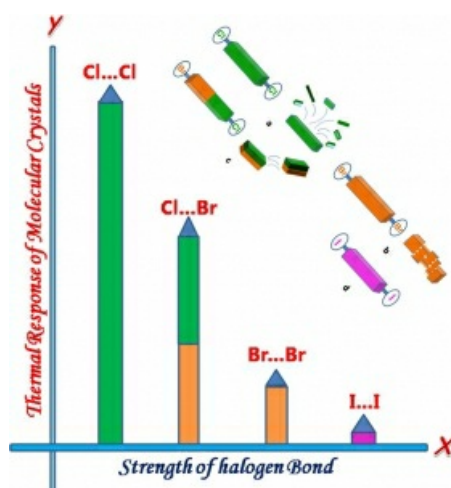
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The design and synthesis of mechanically responsive materials are fascinating and these types of materials are potential candidates for developing materials which will convert thermal energy to mechanical work. In the present investigation for the first time, we reported the thermosalient effect in a series of halo derivatives, the halo derivative with higher electronegativity and poor halogen bond strength (Cl...Cl) shown good thermal response and the decrease in effect were observed with decrease in electronegativity and increase in halogen bond strength (I...I).¹ We observed the different thermal events (jumping/explosion, and cracking) in halogen derivatives such as Compound-A (3,5-di Chloro Salicylidene), B (3-Bromo-5-Chloro Salicylidene), C (3,5-di Bromo Salicylidene) and D (3,5-di Iodo Salicylidene) in a decreasing order even they all are isomorphous, 3D isostructural and having the same type of hydrogen/halogen bonding interactions and similar packing, except the change in halogen atom. The Compound-A exists in three polymorphic Forms, two room temperature (Form I and II) and one high-temperature Form (Form III) where Form I to III is a reversible thermosalient transition and From II to III is irreversible and non-thermosalient. Compound-B and C also exist in two polymorphic Forms; Compound-B Form I to II is irreversible whereas Compound-C is reversible with thermosalient effect. The thermosalient behavior of molecular crystals is mainly due to anisotropy in the cell parameters (increase in a-axis and decrease in b, c-axes) and sudden release of accumulated strain during phase transition.² This study demonstrates the utility of halogen and hydrogen bonded molecular crystals in exhibiting thermosalient effect under thermal stress and also presents a rationale for the design of thermo-responsive crystals and energy converting materials.

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**Keywords:** [Halogen Bonding](#), [Crystal Engineering](#), [Thermosalient Effect](#)