

## MS22-P03 | PHASE TRANSITIONAL BEHAVIOR AND CHARGE DENSITY STUDY OF DRUG

### METHIMAZOLE

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In this study, phase transitional behavior and electron density distribution in the crystals of drug methimazole were carefully investigated. The compound presents rich polymorphic diversity, where among all the phase transitions a peculiar, previously unknown, solid-state process was discovered, which can be especially important for the dosage form and storing of the active pharmaceutical ingredient. This phase transition is characterized by the exceptional features, such as the  $\lambda$ -shaped contour of the DCS curve, practical absence of thermal hysteresis, the low integral value of configurational heat capacity and existence of "heating memory". The nature of this process was revealed and it can be considered to be the 2nd order phase transition controlled by the cooperative effect. Charge density analysis for the phase existing at low temperature was performed. For the system with two molecules in the asymmetric cell, distribution of the electron density around sulfur atoms was studied, topological characteristics of the N–H $\cdots$ S hydrogen bonds, including local source function, were described.

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