# Hot stuff: A new thermal pathway for a high explosive

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TATB (1,3,5-triamino-2,4,6-trinitrobenzene) is an important explosive compound because of its extensive use in munitions and worldwide weapons systems. Despite its importance, researchers have been trying to understand its response to temperature extremes for the past 50 years.

A Lawrence Livermore National Laboratory (LLNL) team has uncovered a new thermal decomposition pathway for TATB that has a significant bearing on computational models that predict the energy release and thermal behavior of TATB and possibly other insensitive high explosives (IHEs). The research appears in *Propellants, Explosives, Pyrotechnics*.

TATB is widely viewed as the most stable IHE, as it is not easily detonated by external stimuli. It does not undergo the thermal sequence of deflagration-to-detonation (DDT), which is unique among explosives. It requires a proper detonation chain to initiate, so handling the material is relatively free from accidental initiation if proper safety methods are followed.

One aspect of this safety envelope is how the material responds to temperature extremes; whether this material becomes more sensitive and is no longer safe to handle when subjected to abnormal thermal environments.

"Our goal with this project was to understand the behavior experimentally to construct computational models predicting behavior for any thermal exposure conditions," said LLNL scientist Keith Morrison, a co-author of the work.

The study has established a new understanding of IHE decomposition and lays the foundations for linking complex molecular processes to kinetic and thermodynamic measurements of IHE.

"This new decomposition reaction of TATB has traditionally been overlooked in the literature, and our study highlights novel molecular pathways occurring as IHE is heated above its stability limit," said LLNL scientist John Reynolds, also a co-author. "These pathways can help constrain the physiochemical properties of current and future IHE compounds, allowing for predicting behavior and safe handling of energetic materials."

**More information:** Keith D. Morrison et al, TATB thermal decomposition: Expanding the molecular profile with cryo-focused pyrolysis GC-MS, *Propellants, Explosives, Pyrotechnics* (2024). DOI: 10.1002/prep.202300268

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