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Reaction initiation and chemical energy release in nitramines[1]

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Available kinetic data for condensed-phase reactions responsible for reaction initiation and chemical energy release in reacting explosives is extremely limited, even for widely used classes of molecular explosives such as nitramines. Transient temperatures and stresses generated in different initiation scenarios can vary by several orders of magnitude making it difficult to interpret kinetic data from initiation measurements. In this presentation, I will describe an ongoing theoretical effort aimed at identifying the dominant reaction mechanisms under different thermodynamic conditions, estimating the corresponding rate constants, and developing reduced-order rate models suitable for mesoscale simulations of detonation initiation.

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