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Ab initio calculations of nitramine dimers[1] SHARON KOH-FALLET[2], ASEE Postdoctoral Fellow, U.S. Naval Research Laboratory, IGOR SCHWEIGERT, Code 6189, Theoretical Chemistry Section, U.S. Naval Research Laboratory — Elevated temperatures and pressures are typically thought to have opposing effects on the reaction channels of nitramine decomposition. These high temperatures promote reactions with loose transition structures (positive activation entropies and volumes), such as N-N bond homolysis. Elevated pressures promote reactions with tight transition structures (negative activation entropies and volumes), such as intramolecular and intermolecular H transfer. However, no quantitative data exists regarding the range of temperatures and pressures at which these effects become pronounced. We are pursuing ab initio calculations of the corresponding unimolecular and bimolecular transition structures with the objective of estimating the relevant thermochemical parameters and quantifying the effects of elevated temperature and pressures on the corresponding rate constants. Here, we present density functional theory and complete active space calculations of gas-phase molecular dimers of nitramines as an intermediate step toward modeling transition structures directly in the condensed phase.

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[2] secondary email: sharonekoh@gmail.com

Sharon Koh-Fallet
Naval Research Laboratory

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