

Energetics of RDX and HMX using Natural Linear Scaling Coupled Cluster

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We present the results of a recently developed linear scaling coupled cluster method study on RDX and HMX. This work is a continuation of previous regular coupled cluster study for ground state geometries and energetics on the same systems. Understanding the structures of these compounds is of great interest to design better explosives, and a daunting task due to the presence of numerous conformers. This work attempts to reproduce the regular coupled cluster results, with significant computation time savings, and allows for a benchmarking of the Natural Linear Scaling Coupled Cluster (NLSCC) on an uncommon family of compounds.