Decomposition Mechanisms of Dinitrotoluene

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ABSTRACT

In order to develop a method for effectively identifying dinitrotoluene (DNT) in the atmosphere, it is necessary to know the DNT fragmentation energies. For this purpose, its unimolecular decomposition mechanisms were studied by using density functional theory (B3LYP). For the most abundant 2,4 DNT, from among the possible homolytic cleavage pathways, it was found that the NO_2 group at C2 broke off first (see below), followed by the same group at C4, and that the decomposition of atomic O from DNT required 24 kcal/mol more energy than the NO_2 at C2. Another pathway was also investigated, which is the release of an NO group with migration of an oxygen atom to a neighboring C atom, as is observed in nitrobenzene.

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