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The Synchronous Thermal Decomposition Mechanism of Azoisopropane

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Abstract

The mechanism for the thermal decomposition of *trans*-azoisopropane has been studied using *ab initio* quantum mechanical approaches. The structural optimization methods include self-consistent field (SCF) and two-configuration SCF (TCSCF). Contrary to some current thought, azoisopropane decomposes through a 'synchronous' pathway, forming N_2 and two isopropyl radicals: i.e., two C-N bonds break simultaneously. The stability of the isopropyldiazenyl radical has also been studied. The barrier E_a for 2-$C_3H_7N_2$ decomposition predicted at the DZP CCSD(T) level of theory is 1·8 kcal mol^{-1}, slightly smaller than the E_a for methyldiazenyl radical CH_3N_2 predicted at the same level of theory.