The decomposition of hydrazine in the gas phase and over an Iridium catalyst

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Hydrazine (N_2H_4) is a common rocket thruster monopropellant. Its decomposition in the gas phase was the subject of numerous experimental studies in the 1960s and 1970s, prior to the era of accurate quantum chemistry. The presently accepted kinetics model for gas phase decomposition invokes numerous radical reactions, including ~50 rate constants. Quantum chemistry calculations in the present work suggest molecular reactions occur at about the same energy requirements as free radical reactions. There are many fewer elementary radical reactions than is suggested by the accepted kinetics model. The availability of accurate reaction barriers and thermochemistry from theory suggests a revision of the kinetics models would be welcome. Radical reactions, particularly for NN cleavage, are stabilized compared to molecular reactions on a model of the thruster Ir-particle catalyst, explaining both high and low temperature decomposition products.