

A Detailed Model for the Decomposition of Nitramines: RDX and HMX

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Abstract:

A unified decomposition scheme for two very important cyclic nitramines, namely, RDX and HMX has been described using Ab initio Density Functional Theory (DFT) calculations. The unified decomposition scheme can successfully account for the key reactive species identified in the initiation stage of combustion of RDX and HMX experimentally or by theoretical model. Molecular parameters correspond to the computed potential energy profile of unimolecular decomposition of these nitramines were then used to obtain the thermochemistry of all identified species and reaction rate constants of each individual channel. Inclusion of these improved theoretical rate constants (as shown in Figure 1 for RDX and HMX) for all the important primary decomposition reactions give a better description for the initiation of decomposition of these nitramines. These primary decomposition reactions were then combined with

- i) Important secondary reactions of the key reactive radical intermediates, such as, CH_2NNO_2 (MN), CH_2N , NO , NO_2 , OH *etc.*
- ii) Existing nitramine reaction networks.

Figure 2 shows a flow diagram of the approach we have taken to develop our improved nitramine mechanism. The overall mechanism with 89 species and 468 reactions is general enough to describe the chemistry of similar [C, H, N, O] molecules such as nitromethane, ADN *etc.* which could be applied to understand the combustion or detonation of this class of compounds.

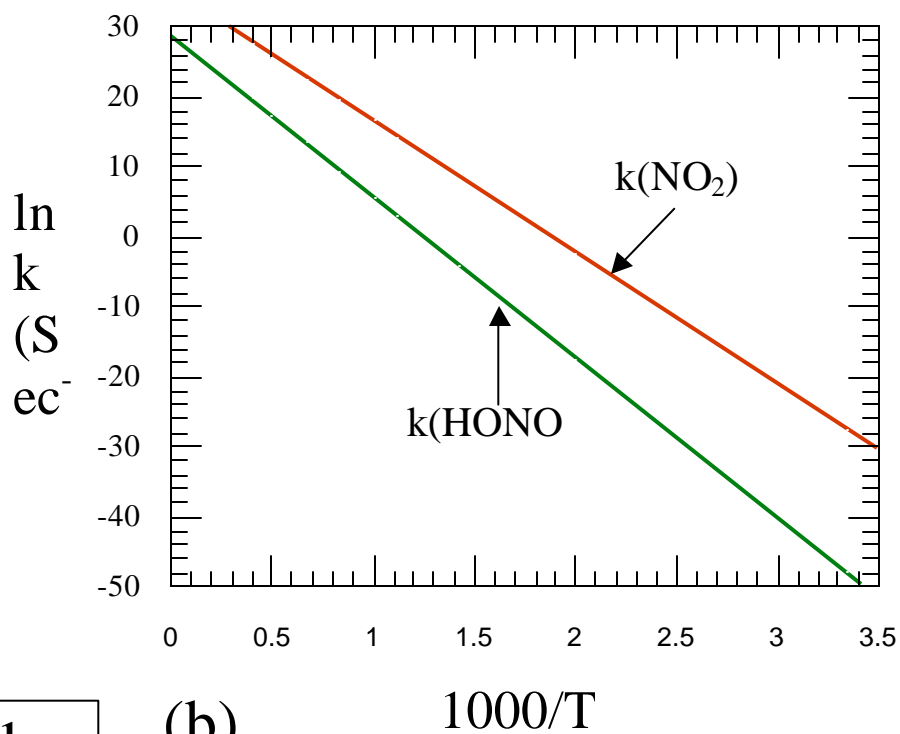
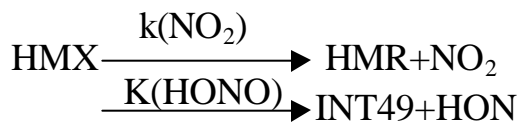
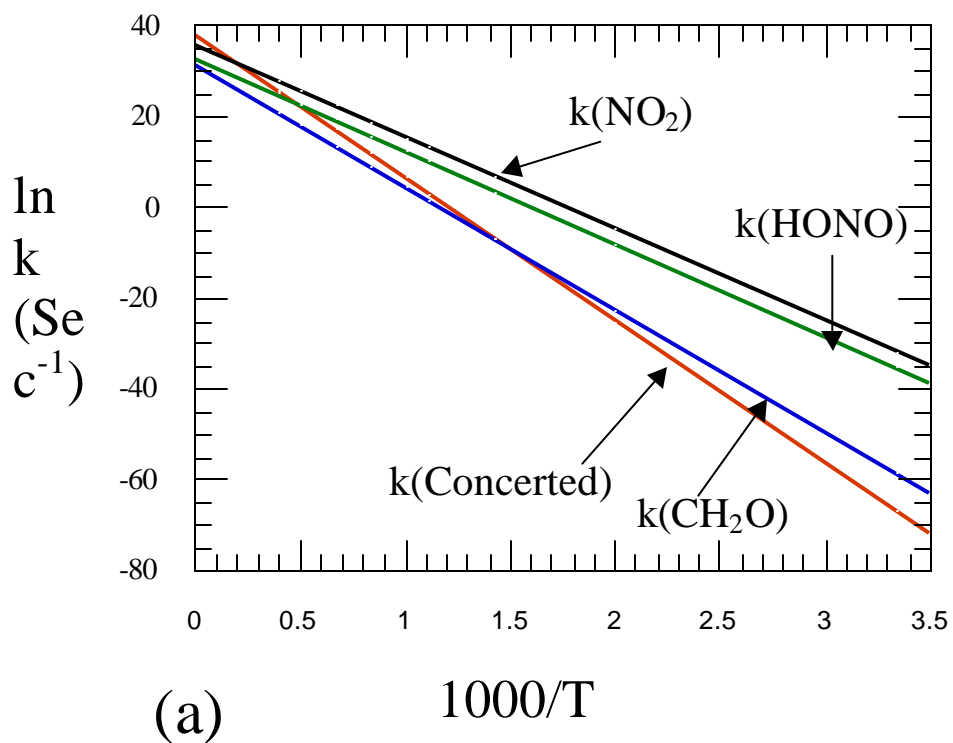
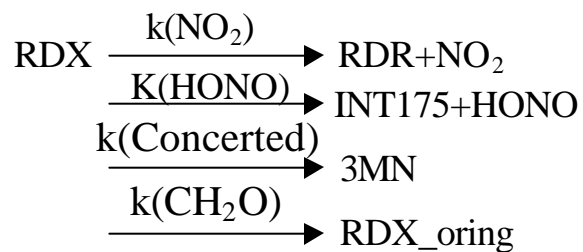


Fig. 1

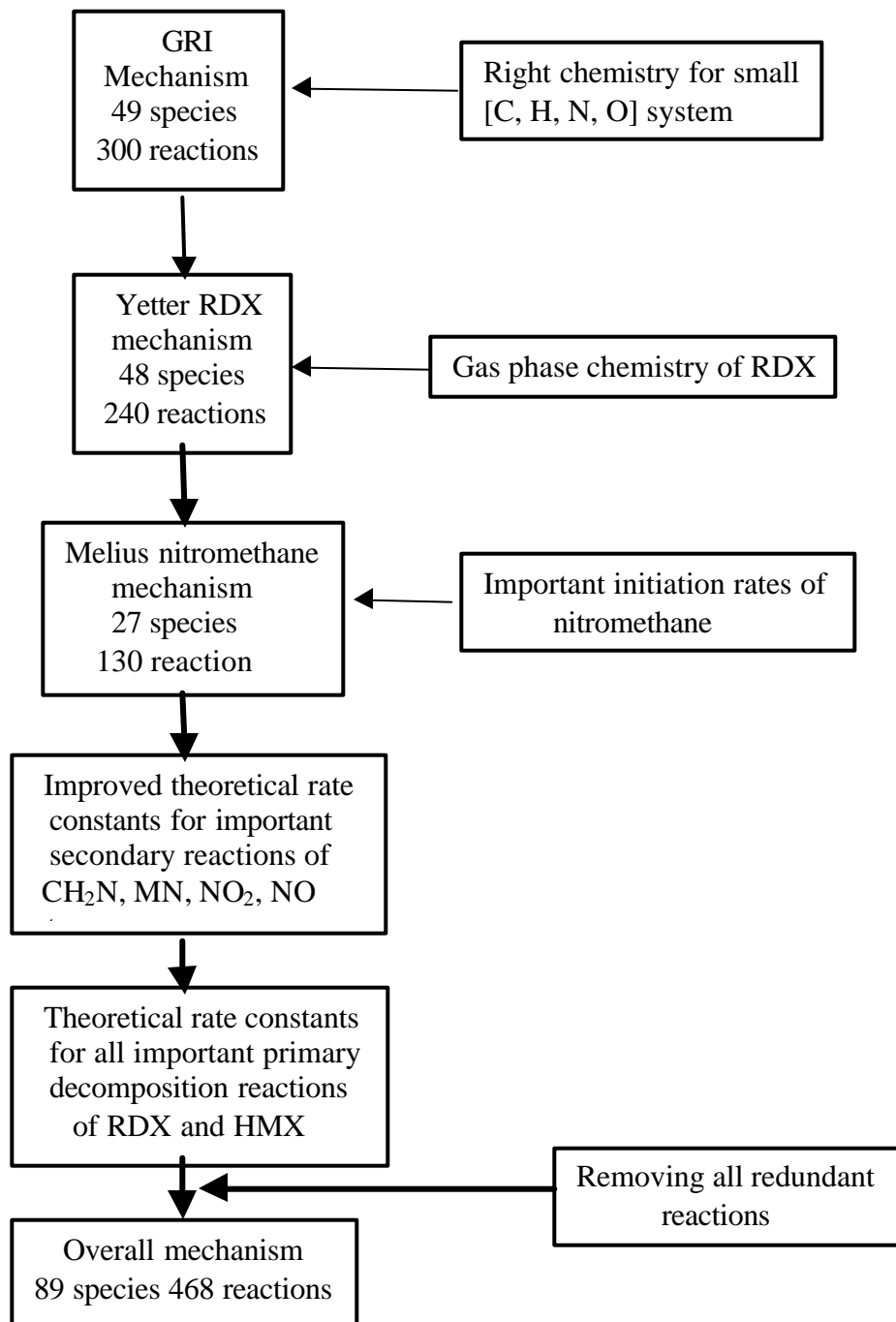


Fig. 2