**Polymorph Dependent Initial Thermal Decay Mechanism of 1,1-Diamino-2,2-Dinitroethylene (FOX-7)**

**Huaiyu Jiang, †,‡ Qingjie Jiao, † and Chaoyang Zhang\*‡,$**

† *State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, Beijing 100081, China.*

‡*Institute of Chemical Materials, China Academy of Engineering Physics (CAEP), P. O. Box 919-311, Mianyang, Sichuan 621900, China.*

$*Beijing Computational Science Research Center, Beijing 100048, China.*

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**S1: Evolution of some key species of α-FOX-7 heated under various temperature types (constant temperature of 2300 K, 3000K and temperature-programmed heating from 300 to 3000 K).**



**Figure S1.** Evolution of some key species of α-FOX-7 heated under various temperature types (constant temperature of 2300 K, 3000K and temperature-programmed heating from 300 to 3000 K).

**S2: Evolution of some key species of β-FOX-7 heated under various temperature types (constant temperature of 2300 K, 3000K and temperature-programmed heating from 300 to 3000 K).**



**Figure S2.** Evolution of some key species of β-FOX-7 heated under various temperature types (constant temperature of 2300 K, 3000K and temperature-programmed heating from 300 to 3000 K).

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**S4: Comparison in number of final products of three FOX-7 polymorphs heated at 2300 K.**



**Figure S4.** Comparison in number of final products of three FOX-7 polymorphs heated at 2300 K.

**S5: Comparison in number of final products of three FOX-7 polymorphs heated at 3000 K.**



**Figure S5.** Comparison in number of final products of three FOX-7 polymorphs heated at 3000 K.

**S6: Comparison in number of final products of three FOX-7 polymorphs heated from 300 to 3000 K.**



**Figure S6.** Comparison in number of final products of three FOX-7 polymorphs heated from 300 to 3000 K.