

Supporting information

**Thermal Stability of Emerging N6-type Energetic
Materials: Kinetic Modeling of Simultaneous
Thermal Analysis Data to Explain Sensitivity Trends**

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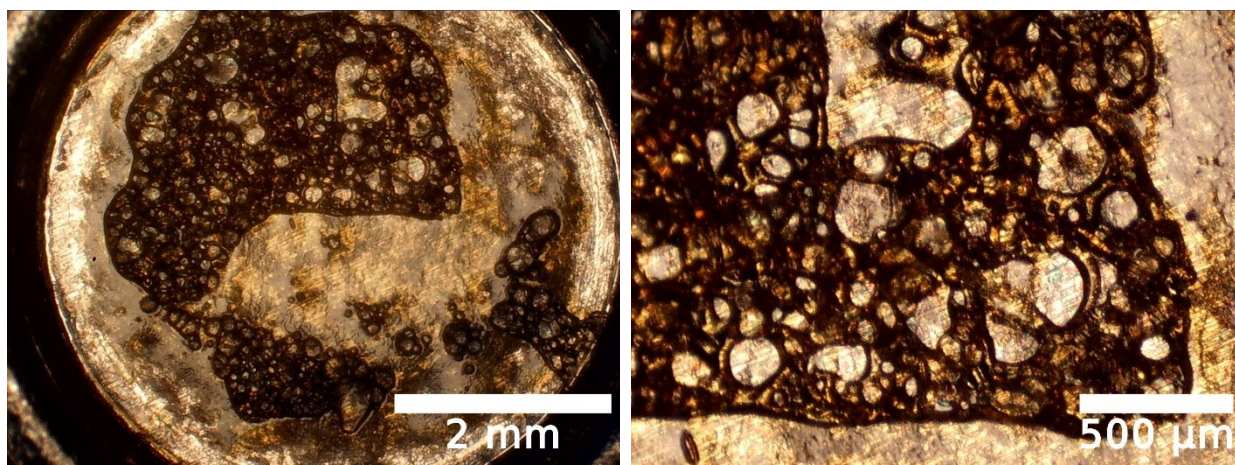


Figure S1. Optical image of the sample **1** heated at 5 K min^{-1} rate up to an endothermic peak and quenched to room temperature: photo of the whole crucible and magnified view.

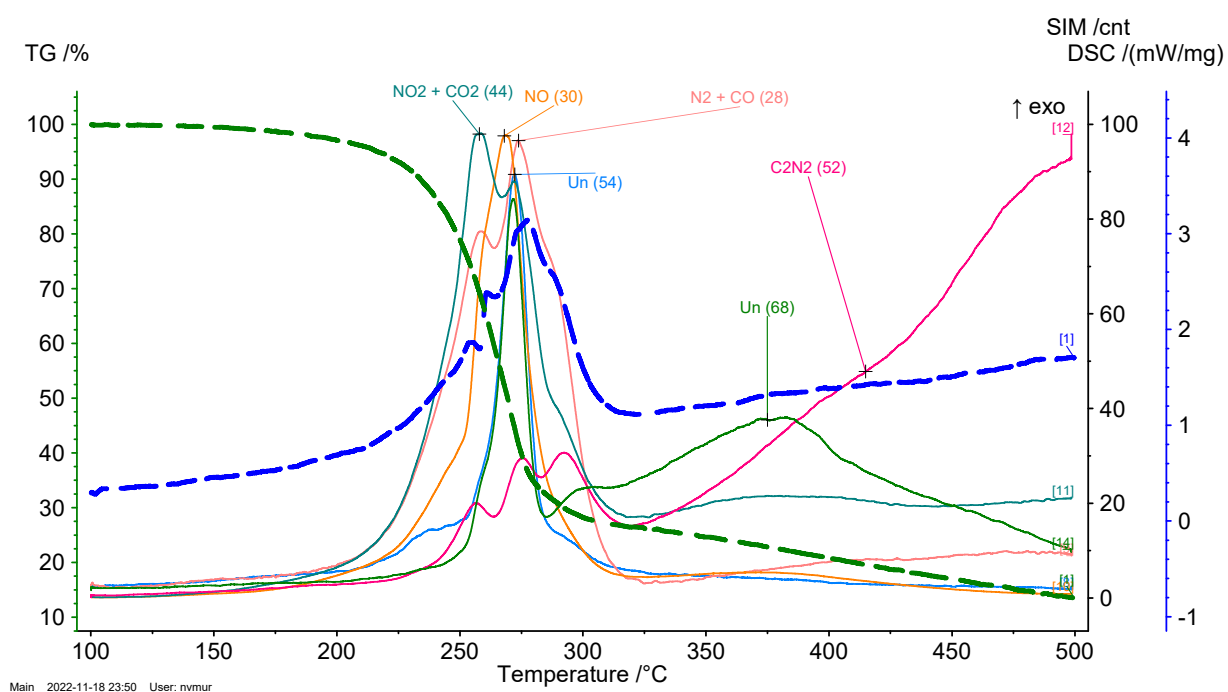


Figure S2. Thermal analysis of **2** heated at 5 K min^{-1} rate: mass loss (TG, green dashed curve), heat flow (DSC, blue dashed curve), and traces of the selected mass numbers via the mass spectrometric analysis of the evolved gases. Traces of the characteristic lines are given for main products (N_2 , NO , N_2O , NO_2 , C_2N_2 , CO_2 , and unidentified species with $m/z = 68$ and 54). Traces are plotted not in scale to allow observing their temporal behavior.

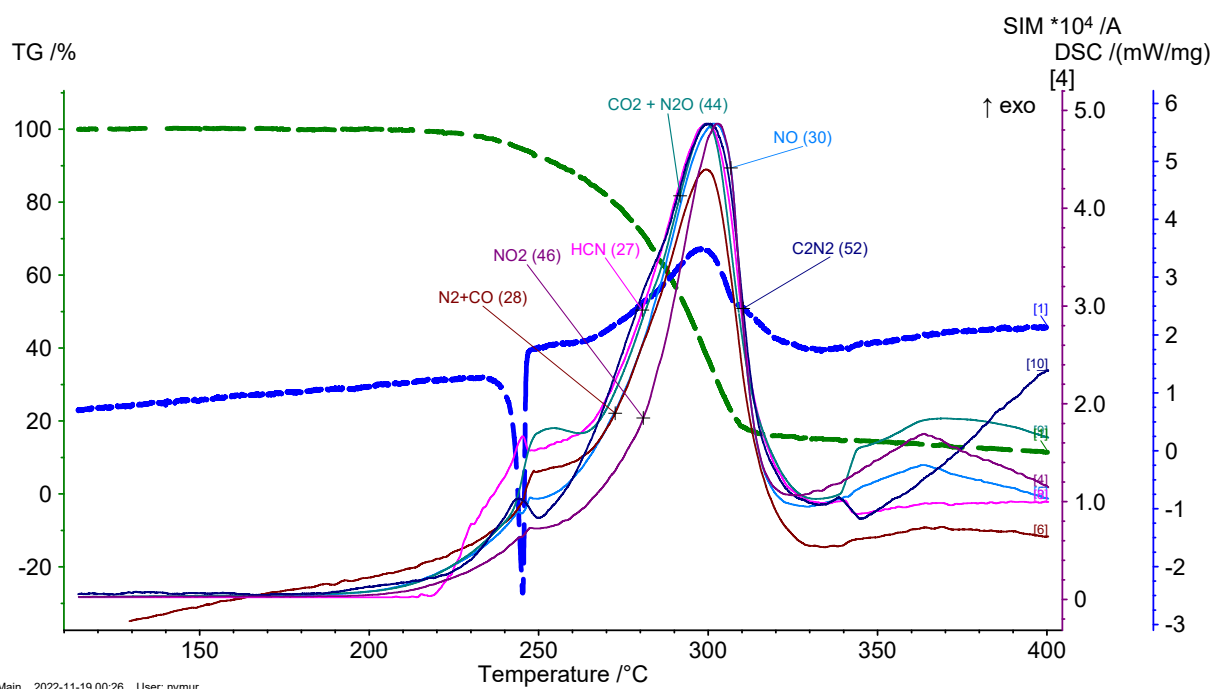


Figure S3. Thermal analysis of **3** heated at 5 K min^{-1} rate: mass loss (TG, green dashed curve), heat flow (DSC, blue dashed curve), and traces of the selected mass numbers via the mass spectrometric analysis of the evolved gases. Traces of the characteristic lines are given for main products (N_2 , NO , N_2O , NO_2 , C_2N_2 , CO_2). Traces are plotted not in scale to allow observing their temporal behavior.

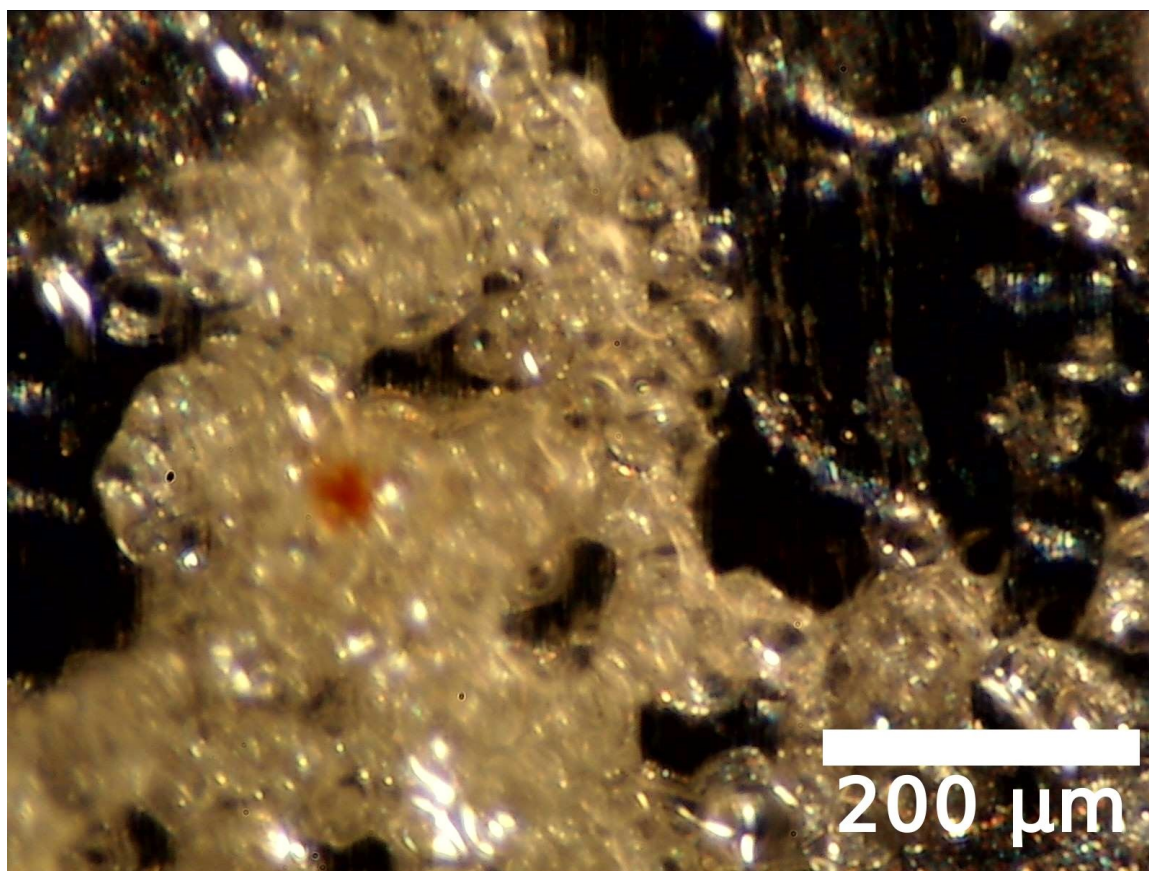


Figure S4. Optical image of the sample **5** heated at 5 K min^{-1} rate up to an endothermic peak and quenched to room temperature.

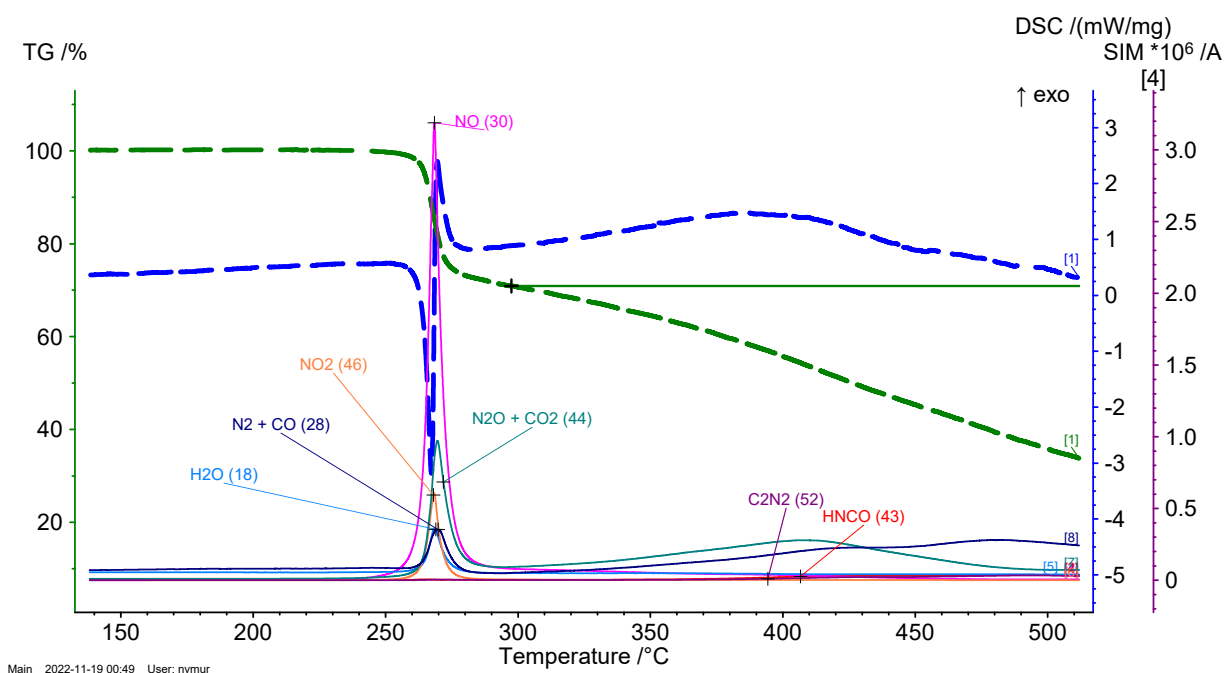


Figure S5. Thermal analysis of **5** heated at 5 K min^{-1} rate: mass loss (TG, green dashed curve), heat flow (DSC, blue dashed curve), and traces of the selected mass numbers via the mass spectrometric analysis of the evolved gases. Traces of the characteristic lines are given for main products (N_2 , NO , N_2O , NO_2 , C_2N_2 , CO_2). Traces are plotted not in scale to allow observing their temporal behavior.

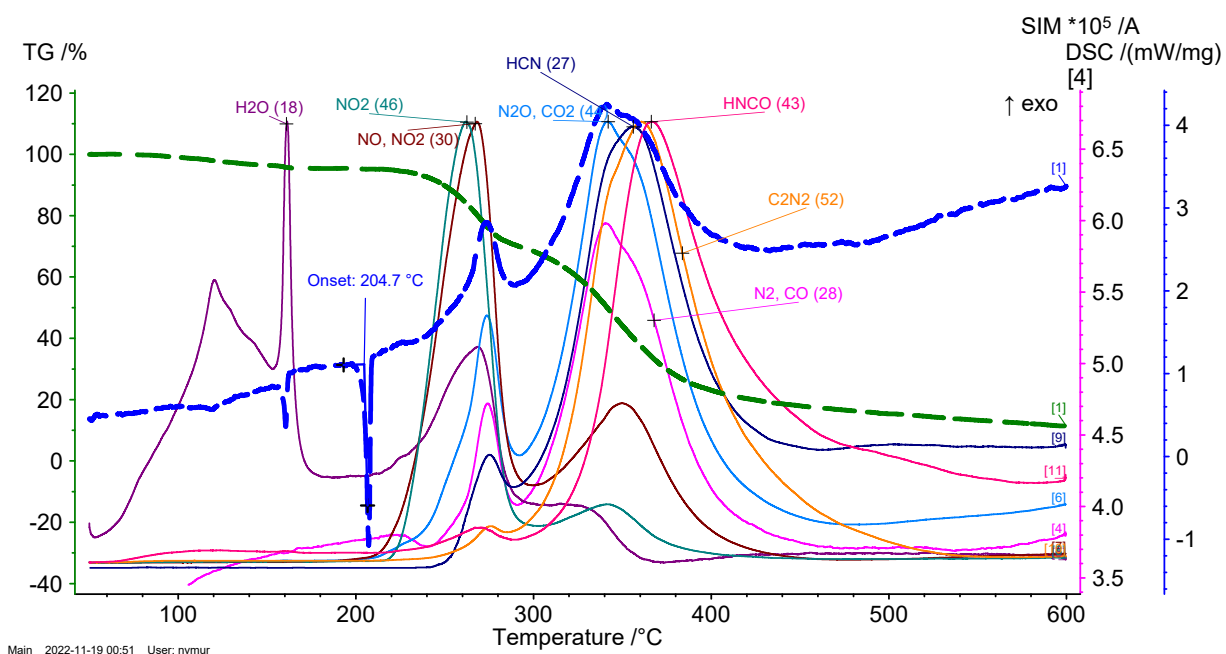


Figure S6. Thermal analysis of **4** heated at 5 K min^{-1} rate: mass loss (TG, green dashed curve), heat flow (DSC, blue dashed curve), and traces of the selected mass numbers via the mass spectrometric analysis of the evolved gases. Traces of the characteristic lines are given for main products (NO , N_2O , NO_2 , H_2O , HCN , HCNO , C_2N_2 , CO_2). Traces are plotted not in scale to allow observing their temporal behavior.

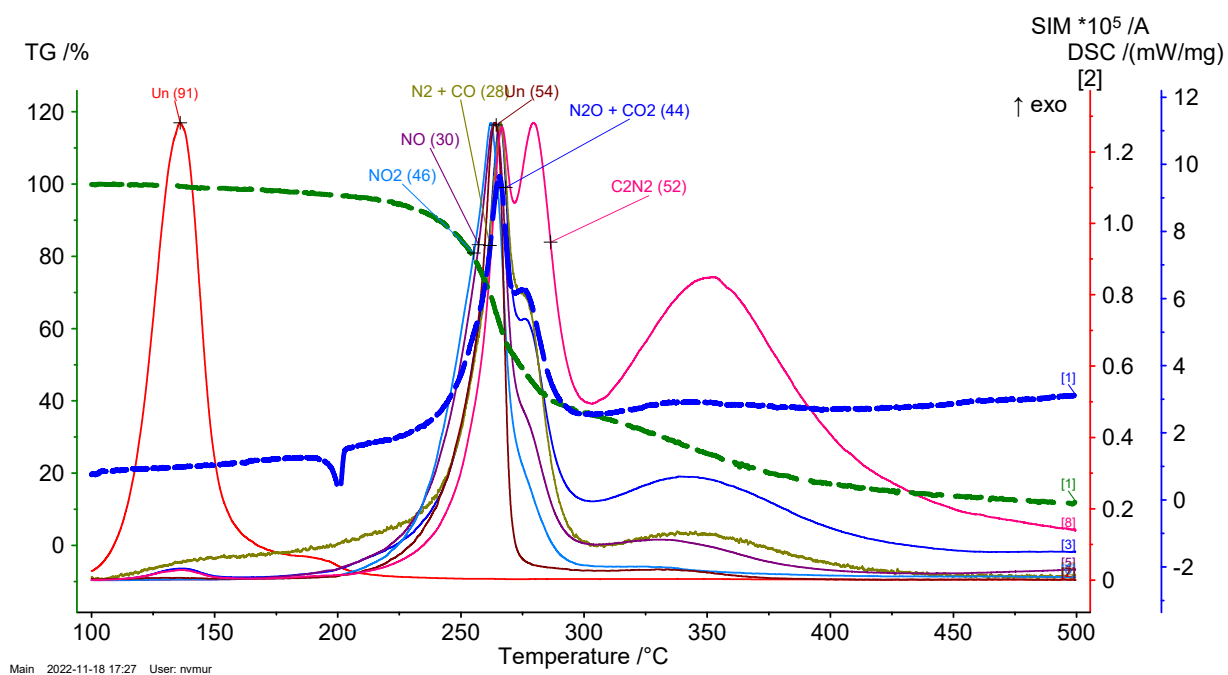


Figure S7. Thermal analysis of **1** heated at 5 K min^{-1} rate: mass loss (TG, green dashed curve), heat flow (DSC, blue dashed curve), and traces of the selected mass numbers via the mass spectrometric analysis of the evolved gases. Traces of the characteristic lines are given for main products (N_2 , NO, N_2O , NO_2 , C_2N_2 , CO_2 , and unidentified species with $m/z = 91$ and 54). Traces are plotted not in scale to allow observing their temporal behavior.