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Authors: Qi-Long Yan, Lin-Lin Liu, Wei He, Chunjia Luo, Avital Shlomovich, Pei-Jin Liu, Jie Kong, Michael Gozin

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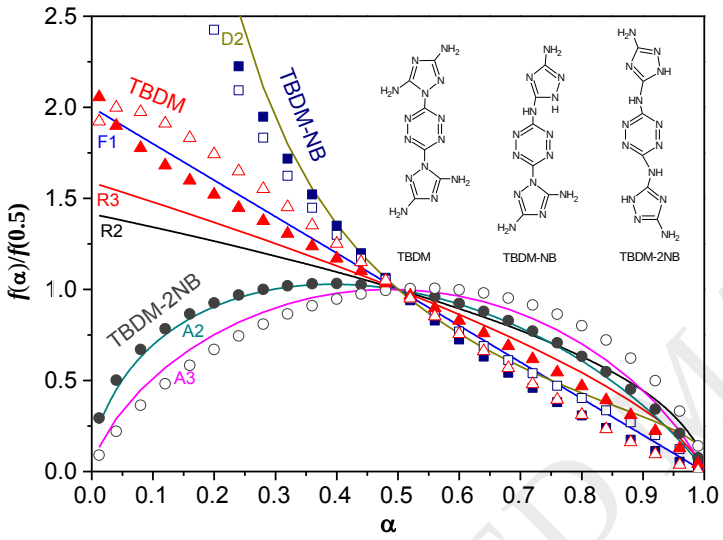
Decomposition Kinetics and Thermolysis Products Analyses of Energetic Diaminotriazole-substituted Tetrazine Structures

Qi-Long Yan[1,*], Lin-Lin Liu[1], Wei He[1], Chunjia Luo[2], Avital Shlomovich[3], Pei-Jin Liu[1], Jie Kong[2,*], Michael Gozin[3,*]

[1]*Sci Techn Combust, Thermo-struct, Internal Flow Lab, Northwestern Polytechnical University, Xian 710072, China*
[2]*School of Science, Northwestern Polytechnical University, Xian 710072, China*
[3]*School of Chemistry, Faculty of Exact Science, Tel Aviv University, Tel Aviv, 69978, Israel*

*Corresponding authors: qilongyan@nwupu.edu.cn (Q.L. Yan); kongjie@nwpu.edu.cn (J. Kong); cogozin@gmail.com (M. Gozin).

Graphical Abstract



The Diaminotriazole group has great effect on the physical models and activation energies of the initial decomposition of tetrazine derivatives.

Highlights

- The heat flow behavior of three insensitive and thermostable *s*-tetrazine derivatives was evaluated.
- The mass loss properties of these compounds were compared with DSC results.
- Their decomposition kinetic parameters and physical models were determined.
- The gaseous products were analyzed with proposed initial thermolysis mechanisms.

Abstract

The thermal behaviour, decomposition kinetics and mechanisms of three diaminotriazole-substituted tetrazine compounds have been investigated using simultaneous DSC-TG and TG/MS techniques. It has been found that TBDM-2NB is much more stable than TBDM-NB and TBDM, where the latter decomposes in two steps with different kinetic parameters. The TBDM decomposes with peak temperature of 379.0 °C, while it is 355.6 °C and 386.5 °C for TBDM-NB and TBDM-2NB, respectively. The activation energy of the first step of TBDM is much higher (176.2 kJ.mol^{-1}) than the second step (102.3 kJ.mol^{-1}). The decomposition of TBDM-NB follows 2-d diffusion model, while it is a first order reaction model for TBDM and nucleation growth model for TBDM-2NB. The rearrangement of *s*-tetrazine ring is typical for thermal decomposition of the title compounds, which may undergo a homo-scission to produce N_2 and followed by production of NH_3.

Keywords: Thermal decomposition; Kinetics; Tetrazine; Stability; Gas products.