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

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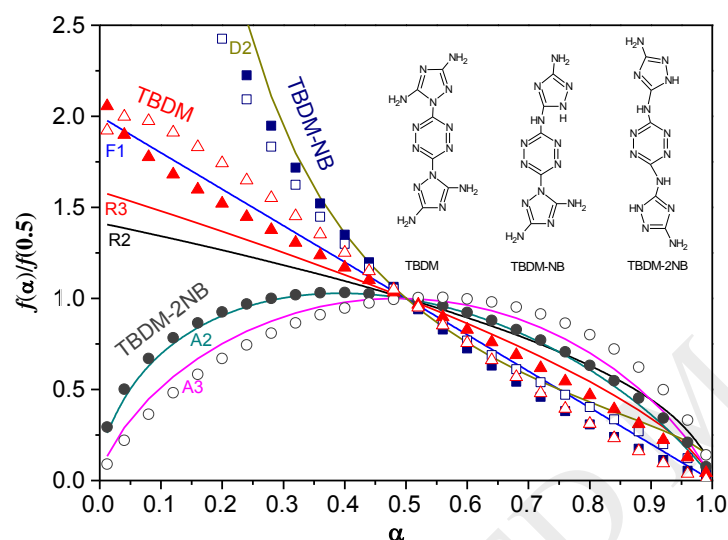
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## Graphical Abstract



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<sup>-1</sup>) than the second step (102.3 kJ.mol<sup>-1</sup>). 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<sub>2</sub> and followed by production of NH<sub>3</sub>.

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

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