

Structure, Thermal Behavior and Thermal Safety of Asymmetric 1,2,4,5-Tetrazine Compounds DPHX and DMHT

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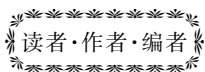
Abstract: To seek for asymmetric 1,2,4,5-tetrazine energetic compounds with good properties, 3-(*p*-nitrobenzyl methylene)-6-(3,5-dimethylpyrazol-1-yl) hydrazone-*s*-tetrazine (DPHX) and 3-(*m*-dinitrobenzyl methylene)-6-(3,5-dimethylpyrazol-1-yl) hydrazone-*s*-tetrazine (DMHT) were synthesized, and their single crystals were cultivated and their structures were characterized by EA, IR and X-ray single crystal diffraction. The thermal decomposition behavior and thermal decomposition kinetics of DPHX and DMHT were studied by differential scanning calorimeter (DSC). Their apparent activation energies were calculated by Kissinger's method. The thermal safety of DPHX and DMHT was studied by the results of thermal decomposition kinetics. Results show that both of them are monoclinic with space group $P2_1/c$. The apparent activation energies of the two compounds are 176.20 and 229.29 $\text{kJ}\cdot\text{mol}^{-1}$, respectively. The self-accelerating decomposition temperature (T_{SADT}), thermal ignition temperature (T_{be}) and critical temperature of thermal explosion (T_{bp}) are 191.83, 206.20 °C and 213.78 °C for DPHX, respectively, and $T_{\text{SADT}}=203.91$ °C, $T_{\text{be}}=212.24$ °C, $T_{\text{bp}}=218.34$ °C for DMHT, respectively. Therefore, DMHT is more stable than DPHX and has higher thermal safety.

Key words: 1,2,4,5-tetrazine derivatives; crystal structure; thermal behavior; thermal safety

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