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

ZENG Tian, HAN Xue, CHEN Xiang, ZHANG Cong, GUO Zhao-qi, MA Hai-xia

(*School of Chemical Engineering, Northwest University, Xi'an* 710069, *China*)

Abstract: To seek forasymmetric 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-dintrobenzyl methylene)-6-(3, 5-dimethylpyrazol-1-yl) hydrazone-s-tetrazine (DMHT) were synthesized, and their single crystals were cultrivate and their structures were characterized by EA, IR and X-ray single crystal diffraction. The thermal decomposition behaviorand 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 kJ·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℃ and 213.78 ℃ for DPHX, respectively, and T_{sADT}=203.91 ℃, T_{be}=212.24 ℃, T_{bp}=218.34 ℃ 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

CLC number: TJ 55; TQ560.1; O64 **Document code:** A **DOI:** 10.11943/CJEM2018128

读者·作者·编者

《含能材料》"观点"征稿

为了丰富学术交流形式,及时传递含能材料领域同行们的学术观点和思想,《含能材料》开设了"观点"栏目。"观点"栏目的来稿应观点鲜明、内容新颖、形式上短小精悍。欢迎含能材料各领域的专家积极来稿。来稿时请附个人简介及主要研究工作介绍。

《含能材料》编辑部