Molecular Design of Long Intra-annular Nitrogen Chains:3H-tetrazolo[1,5-d]tetrazole-Based High-Energy-Density Materials

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February 10, 2021

Abstract

Energetic compounds containing long nitrogen chain, have been a research hotspot. Fused heterocycles are stable due to their aromatic systems. The compound obtained by combining long nitrogen chain and fused ring can not only retain good energetic property, but also ensure better stability. This work designed eight fused heterocycle-based energetic compounds, 3H-tetrazolo[1,5-d]tetrazole (1) and its derivatives (2-8), containing a nitrogen chain with seven nitrogen atoms. The HOF, thermal stability, and energetic properties of these compounds were studied by using the DFT method. The results show that the introduction of -NO2, -N3, -NF2, -ONO2, -NHNO2 groups increased the density, HOF, detonation velocity, and detonation pressure greatly. The densities of 3, 5, 7, and 8 fall within the range designated for high-energy-density materials. The calculated detonation velocity of the compounds 3 and 8 are up to 9.86 km s-1 and 9.78 km s-1, which are superior to that of CL-20. The kinetic study of the thermal decomposition mechanism indicates that the N-R bonds maybe not the weakest bonds of these compounds. The tetrazole ring opening of the heterocycle-based energetic compounds, followed by N2 elimination is predicted to be the primary decomposition channel, whether or not they have substituent groups.

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