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Synthesis and Properties of *N*-alkyltriazole-cyanoborane Propellant Fuels

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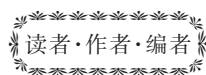
Abstract: To develop novel hypergolic propellant fuels with high density, low viscosity, wide liquid temperature range, high specific impulse, and high decomposition temperature, a series of *N*-alkyltriazole cyanoborane complexes were prepared in a straight forward way by treating *N*-substituted triazoles hydrogen chloride salts and NaBH₃CN. The synthesized compounds were characterized by IR, NMR and HRMS for their structures, and measured by differential scanning calorimetry (DSC), densimeter and viscometer for their thermostability, density, viscosity and ID. On the other hand, Gaussian 09 was used to optimize the crystal structure and calculate the formation enthalpy, based on which Explo5 v6.02 was employed to predict the theoretical specific impulse. Four out of five compounds were found to be liquid at room temperature and proved to be hypergolic with white fuming nitric acid (WFNA) by the droplet test. Especially, *N*-Propyl-1,2,3-triazole cyanoborane complex (**3**) demonstrated attractive properties such as short ID time (12 ms), high density (1.024 g·cm⁻³), good thermostability ($T_d=233$ °C, onset), good I_{sp} (201.7 s) and ρI_{sp} (357 s·g·cm⁻³), super low viscosity (16 mPa·s) and wide liquid range ($T_m < -70$ °C), showing the promising application potential as a propellant fuel candidate.

Key words: synthesis; *N*-alkyltriazole cyanoborane; liquid propellant; borane fuels

CLC number: V511; O62

Document code: A

DOI: 10.11943/CJEM2018164



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