Poster

$(CN_5H_4)_2[B_{12}H_{12}] \cdot 2\ H_2O$: A Low-Carbon High-Energy Compound Based on 5-Aminotetrazolium and Dodecahydro-*closo*-Dodecaborate Ions

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In the realm of high energetic materials, 5-aminotetrazole ($H_2N–CN_4H$) is a well-established chemical [1]. In contrast, dodecahydro-*closo*-dodecaborates are renowned for their exceptional stability within the hydroborate family, owing to their *quasi*-aromatic high-symmetry structure. Simple salts of $[B_{12}H_{12}]^{2-}$ with alkali and alkaline-earth metals exhibit thermal stability up to around 700 °C. However, when the icosahedral $[B_{12}H_{12}]^{2-}$ anion is combined with energetic cations, these salts become less stable and decompose at far lower temperatures (200–300 °C), having the capability to release large amounts of energy upon their structural collapse [2, 3]. For instance, $(N_2H_5)_2[B_{12}H_{12}] \cdot 2\ N_2H_4$ sets free 435 kJ/mol of energy under inert-gas conditions.

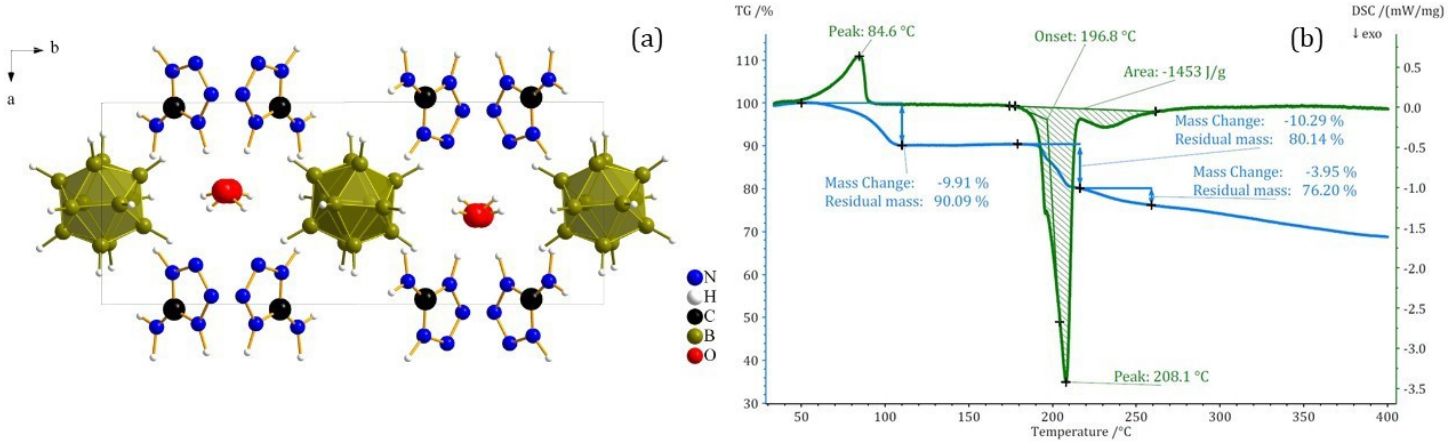

Figure 1. View at the crystal structure of $(CN_5H_4)_2[B_{12}H_{12}] \cdot 2\ H_2O$ along [001] (a)(left) and thermal decomposition of $(CN_5H_4)_2[B_{12}H_{12}] \cdot 2\ H_2O$ as screened by TG and DSC (b)(right).

The reaction between 5-aminotetrazole and the aqueous acid $(H_3O)_2[B_{12}H_{12}]$ in a molar ratio of 1 : 2 leads to the formation of bis-5- aminotetrazolium dodecahydro-*closo*-dodecaborate dihydrate $(CN_5H_3)_2[B_{12}H_{12}] \cdot 2\ H_2O$ (Figure 1, (a)). This compound crystallizes monoclinically in the space group $P2_1/c$ with lattice parameters of a = 726.23(4) pm, b = 1772.06(9) pm, c = 707.35(4) pm and β = 101.534(3)° for Z = 2. Its thermal decomposition under a nitrogen-gas atmosphere results in the release of 452 kJ/mol (Figure 1, (b)).

[1] Delalu H., Karaghiosoff K., Klapötke T. M., Miró Sabaté C. (2015). *Cent. Eur. J. Energ. Mater*. **7**, 197–209.

[2] Zimmermann L. W., Aghaei Hakkak R., Ranjbar M., Schleid Th. (2024). *Int. J. Hydrog. Energy*. **49**, 1469–1477.

[3] Aghaei Hakkak R., Schleid Th. (2024). *J. Solid State Chem*. **329**, 124416 (1-7).