Supporting information of

Prediction of Stable Energetic Beryllium Pentazolate Salt under Ambient Conditions

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Supporting information consists of 4 figures (Figure S1-S4).

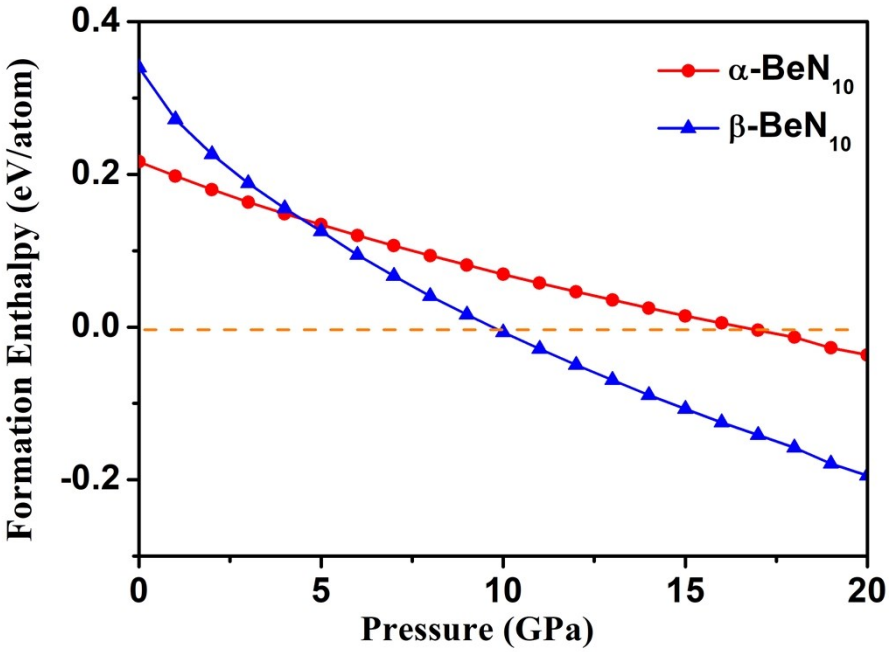

Figure S1 Formation enthalpies of α-BeN_{10} and β-BeN_{10} under the range of 0−20 GPa. The formation enthalpy was calculated by the formula: $\Delta H = H_{BeN_{10}} - H_{Be} - 5 \times H_{N_2}$, where referring the energy of most stable bulk Be and N_2 at certain pressures.

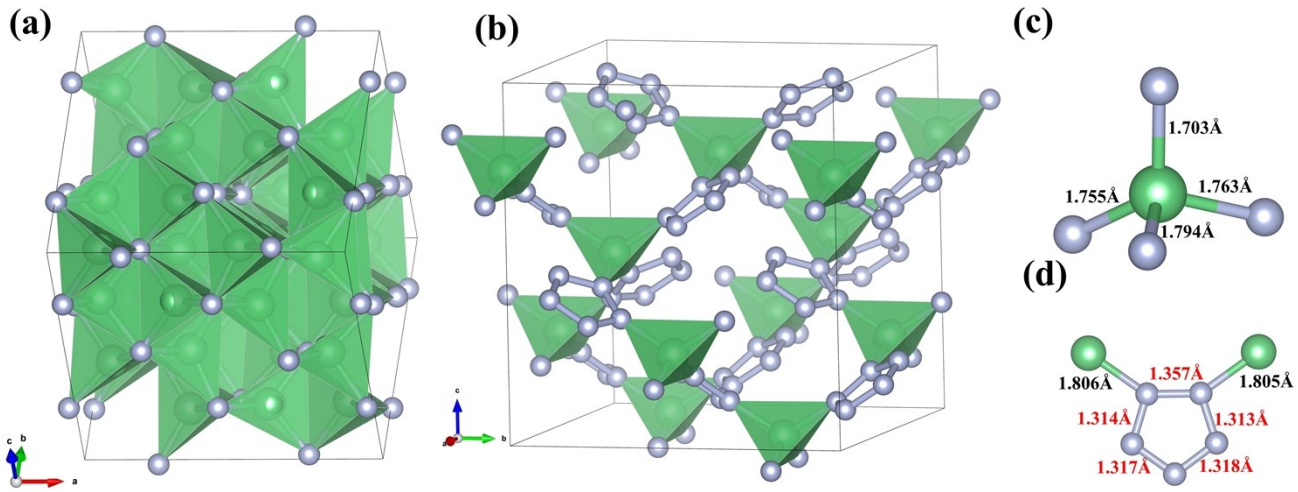

Figure S2 The bonding configuration of Be tetrahedron is presented in (a) Be_3N_2 and (b) α-BeN_{10}, the bond length in (c) Be_3N_2 and (d) α-BeN_{10}.

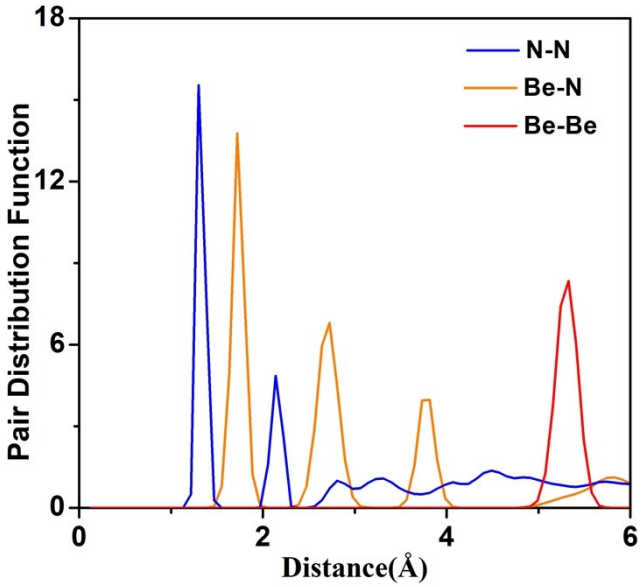

Figure S3 The pair distribution function (**g**(**r**)) for different atom pairs in β-BeN_{10} from the *AIMD* simulations at 0 GPa and 600 K.

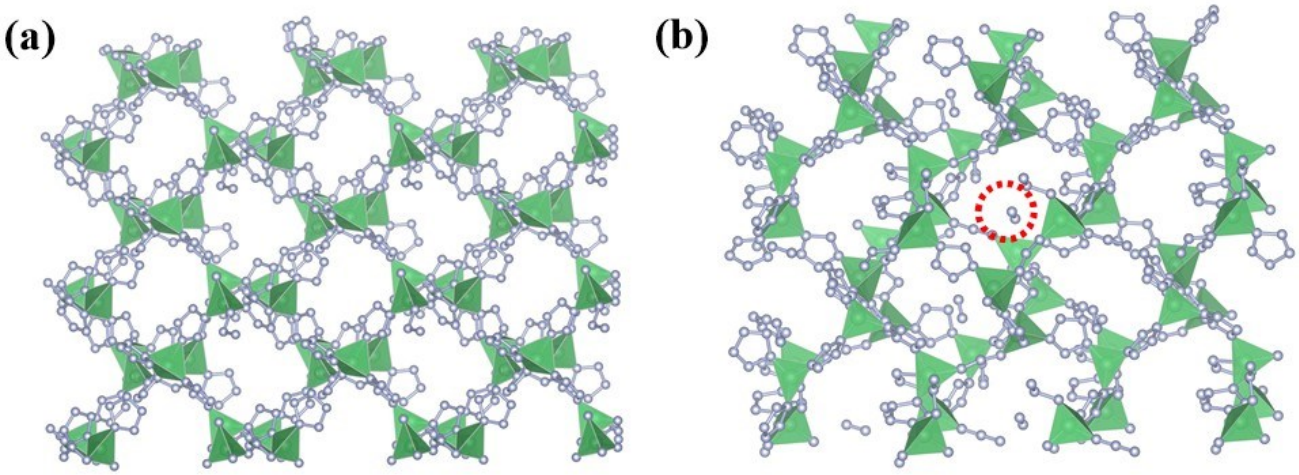

Figure S4 (a) The final structure of β-BeN_{10} in AIMD simulations at 800 K. (b) The structure at 2 ps of the β-BeN_{10} in AIMD simulations at 1000 K.

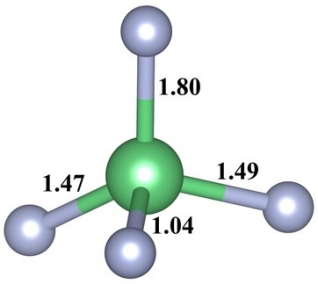

Figure S5 -ICOHP values for chemical bonds in Be_3N_2.