Supporting Information

Decomposition Mechanism of Zinc Ammine Borohydride: A First-Principles Calculation

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Table S1 The simplified reaction pathway, energy barrier and reaction enthalpy for the decomposition of $[Zn(NH_3)_2][BH_4]_2$. E_b and E_b-ZEP are the energy barrier ignoring and including the zero-point energy, respectively. ΔH represents the enthalpy ignoring the zero-point energy. ΔH-ZPE and ΔH_{300K} are the calculated enthalpies at T=0 K and 300 K, respectively, including the vibrational energies. The units of enthalpies and entropies are in eV.

Simplified reaction pathway	E_b	E_b-ZEP	ΔH	ΔH-ZPE (0K)	ΔH_{300K} (300K)
$2BH_4^- \rightarrow B_2H_7^- + H^-$ (IS1→TS4→FS4)	1.58	1.52	0.56	0.63	0.62
$B_2H_7+NH_3 \rightarrow BH_4^-+NH_3BH_3$ (FS4→TS5→FS5)	1.15	1.30	-0.55	-0.39	-0.45
$BH_4^-+NH_3 \rightarrow NH_3BH_3+H^-$ (IS→TS6→FS6)	1.59	1.54	0.01	0.15	0.11