

Supporting Information for

Dehydrogenation of Diborane on Small Nb_n⁺ Clusters

Wen Gan,^a Lijun Geng,^a Benben Huang,^a Klavs Hansen,^b and Zhixun Luo^{a,b,}*

^a Beijing National Laboratory for Molecular Science, State Key Laboratory for Structural Chemistry of Unstable and Stable Species, Institute of Chemistry, Chinese Academy of Sciences, Beijing, 100190, China;

^b Center for Joint Quantum Studies and Department of Physics, School of Science, Tianjin University, 92 Weijin Road, Tianjin 300072, China;

^c School of Chemical Science, University of Chinese Academy of Sciences, Beijing 100049, China.

*Corresponding author. E-mail: zxlue@iccas.ac.cn (Z.L).

S1 Mass Spectrometry Experiments

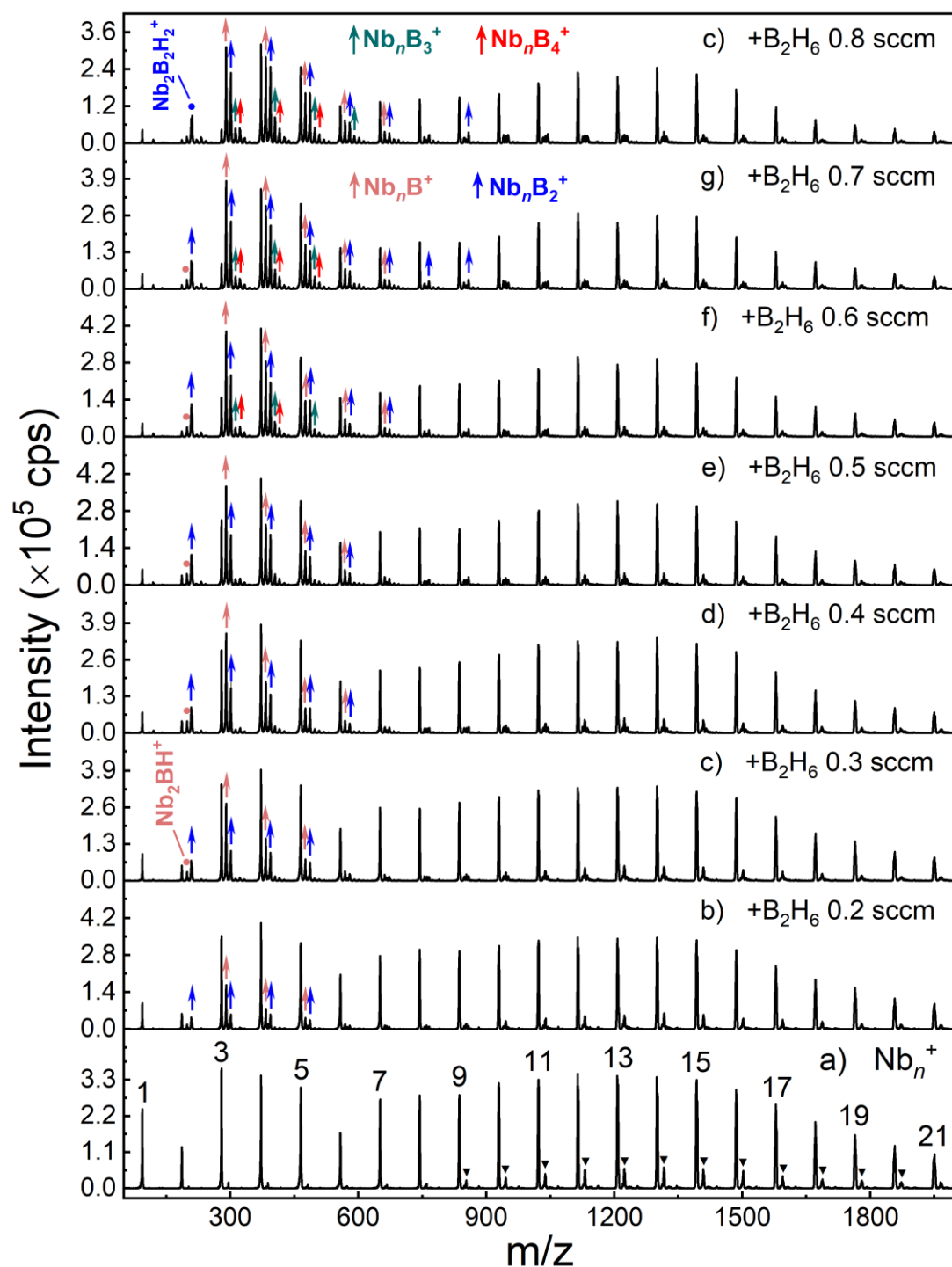


Figure S1. Reactant concentration dependence. Mass spectra of pure Nb_n^+ clusters (a) and after reacting with B_2H_6 (b-g) in the laminar flow tube at different gas concentrations corresponding to different flow rates of the reactant gas (0.3% B_2H_6 in He). The weak peaks in the nascent Nb_n^+ cluster, marked with triangles, are due to minor niobium oxide contamination.

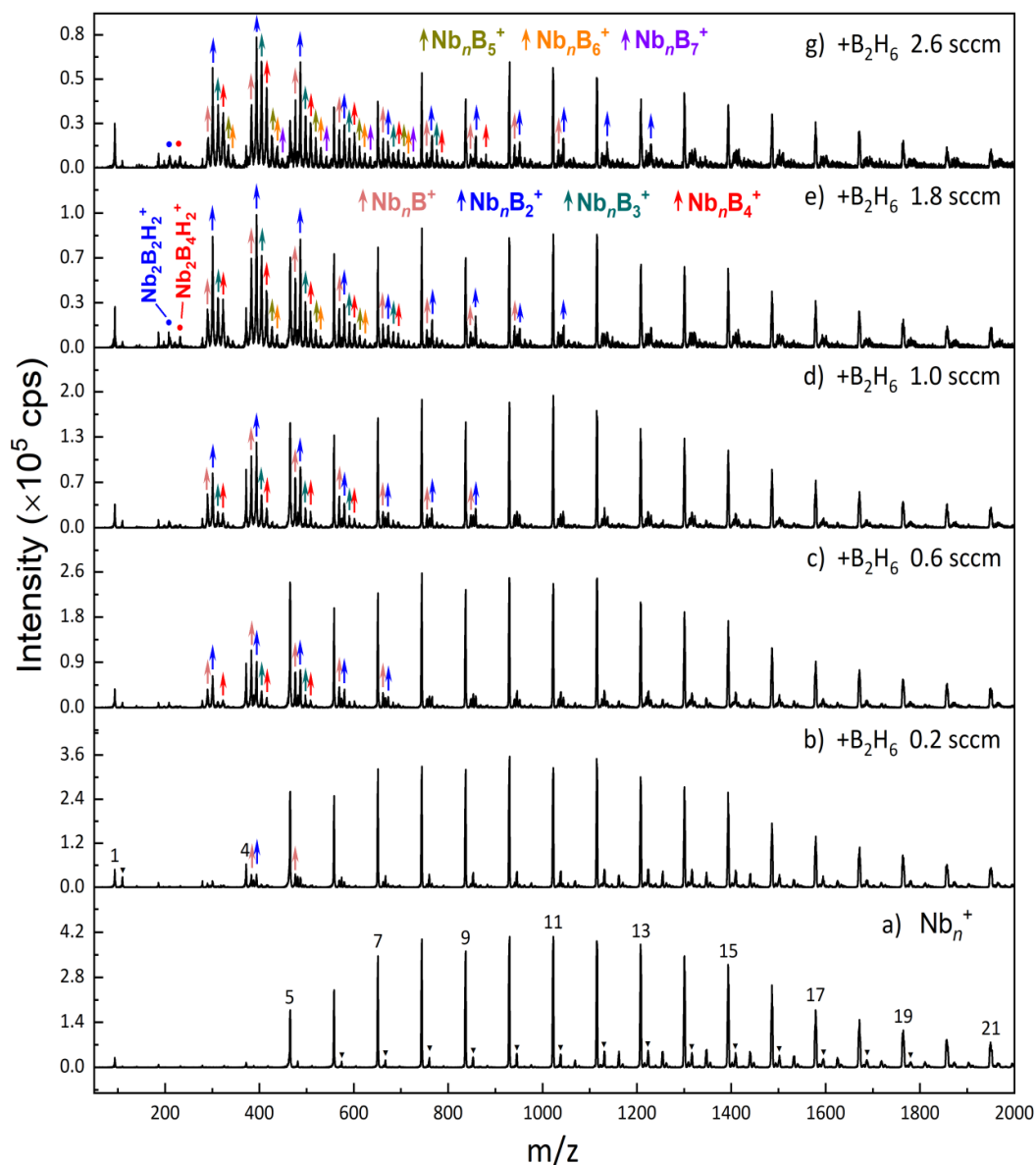


Figure S2. Concentration-dependent reactions of Nb_n^+ at a different distribution. Mass spectra of the Nb_n^+ clusters (a) and after reacting with B_2H_6 (b-g) in the laminar flow tube at different gas concentrations corresponding to different flow rates of the reactant gas (0.3% B_2H_6 in He). The weak peaks in the nascent Nb_n^+ cluster, marked with triangles, are due to minor niobium oxide contamination.

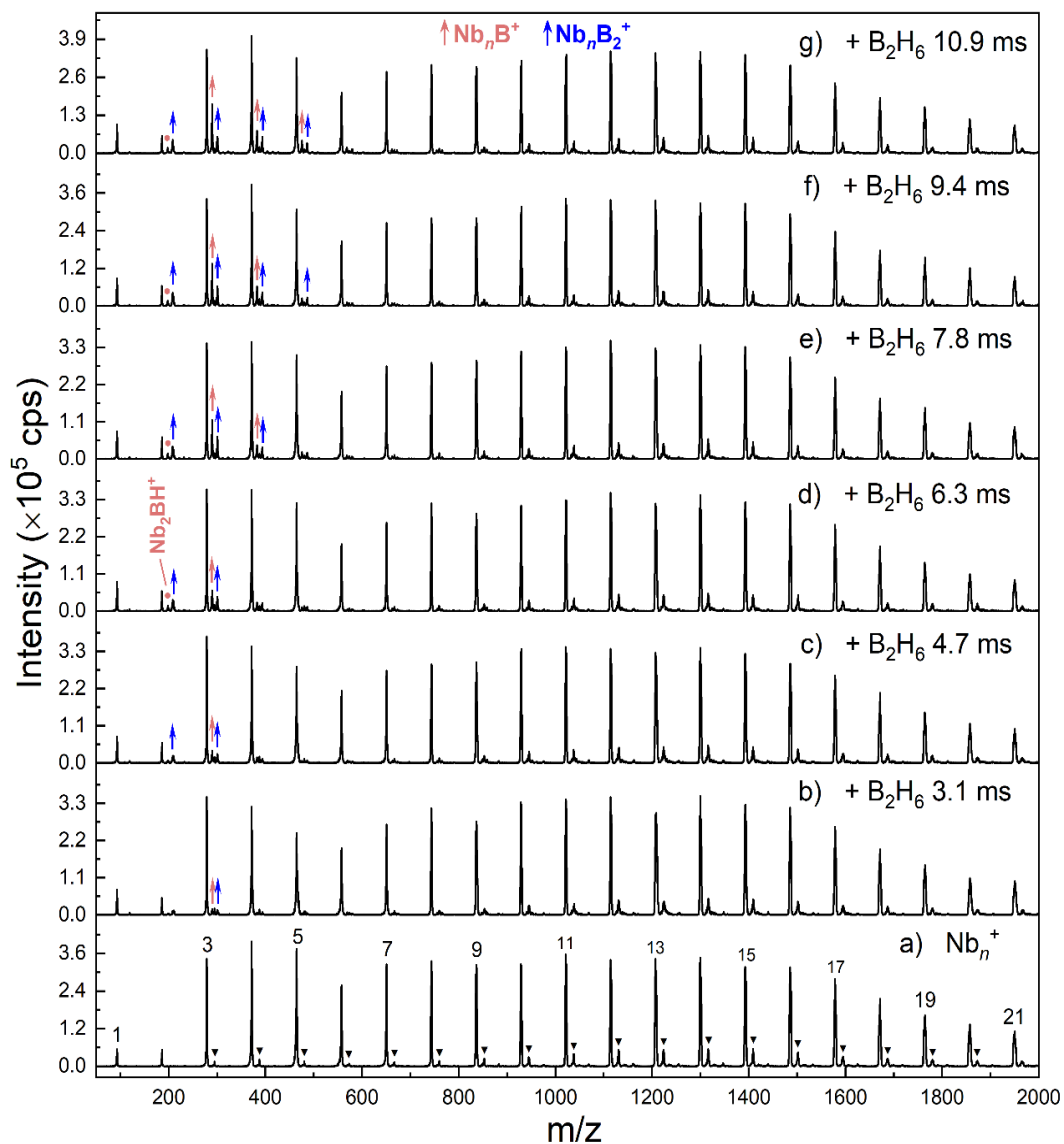


Figure S3. Reaction time dependence of 0.2 sccm B_2H_6 . Mass spectra of the nascent Nb_n^+ clusters (a), and after reacting with 0.2 sccm B_2H_6 (0.3% in He) in the laminar flow tube with controlled reaction time corresponding to 3.1, 4.7, 6.3, 7.8, 9.4, and 10.9 ms respectively (b-g). The weak peaks in the nascent Nb_n^+ cluster, marked with triangles, are due to minor niobium oxide contamination.

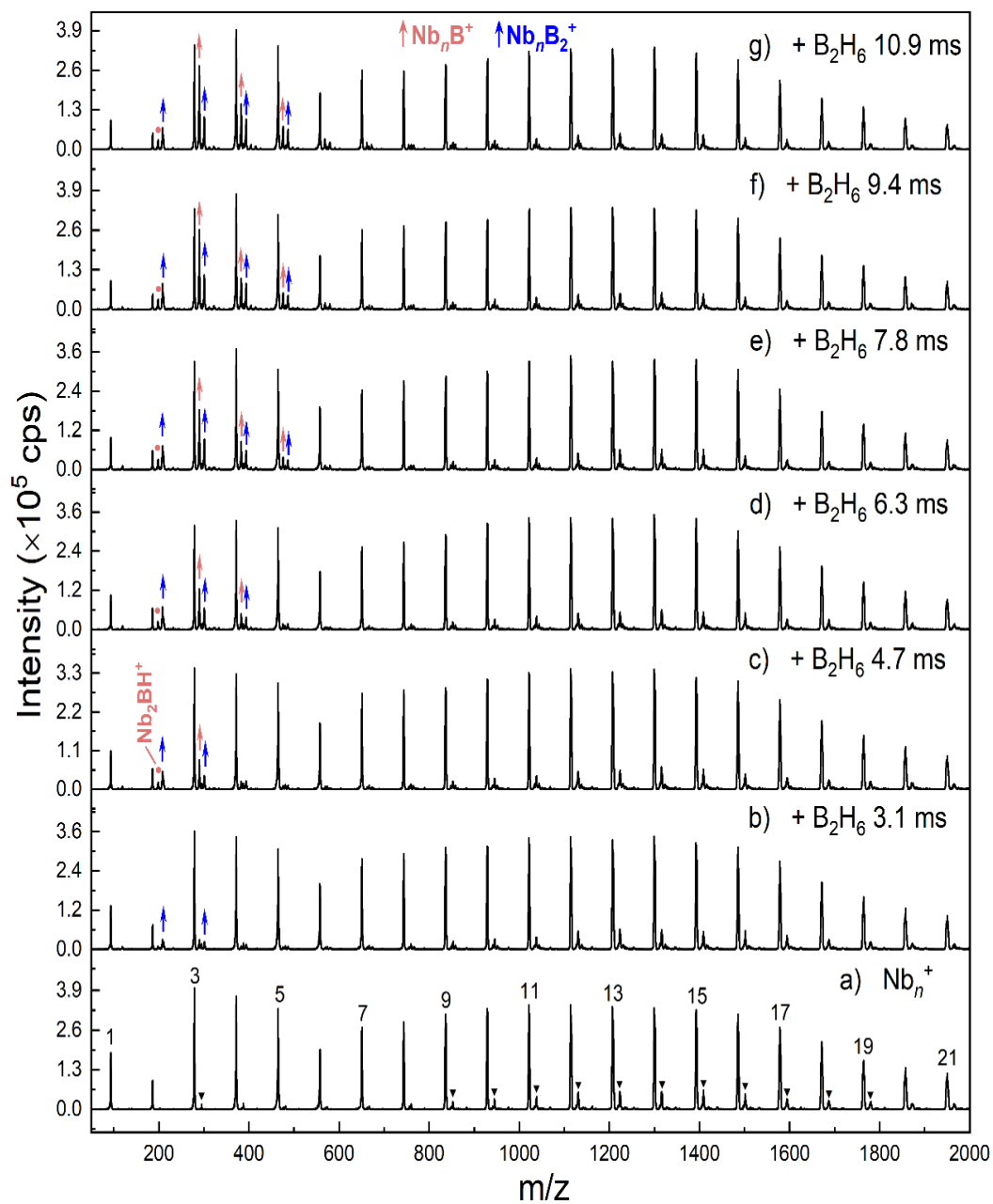


Figure S4. Reaction time dependence of 0.3 sccm B₂H₆. Mass spectra of the nascent Nb_{*n*}⁺ clusters (a), and after reacting with 0.3 sccm B₂H₆ (0.3% in He) in the laminar flow tube with controlled reaction time corresponding to 3.1, 4.7, 6.3, 7.8, 9.4, and 10.9 ms respectively (b-g). The weak peaks in the nascent Nb_{*n*}⁺ cluster, marked with triangles, are due to trace amount of niobium oxide contamination.

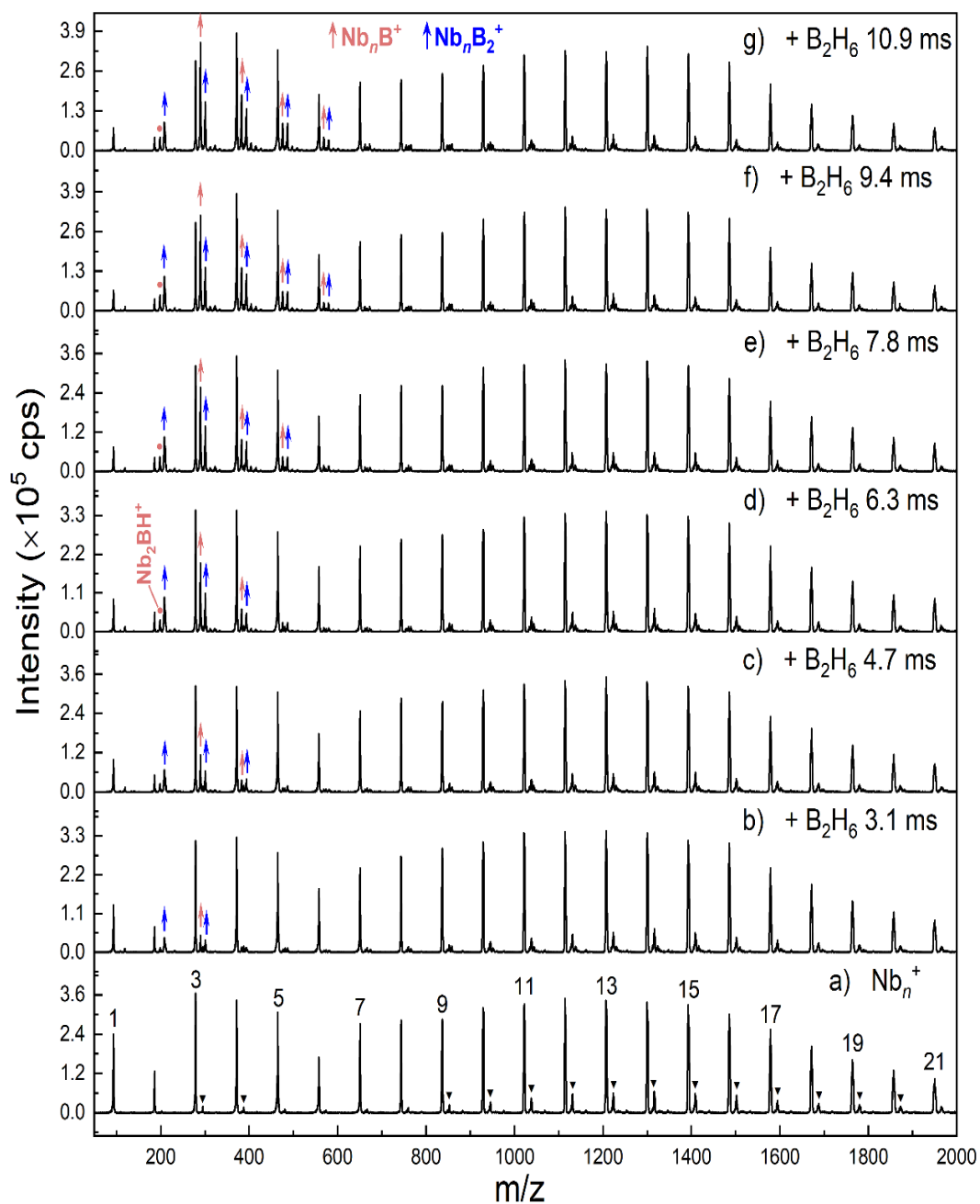


Figure S5. Reaction time dependence of 0.4 sccm B₂H₆. Mass spectra of the nascent Nb_{*n*}⁺ clusters (a), and after reacting with 0.4 sccm B₂H₆ (0.3% in He) in the laminar flow tube with controlled reaction time corresponding to 3.1, 4.7, 6.3, 7.8, 9.4, and 10.9 ms respectively (b-g). The weak peaks in the nascent Nb_{*n*}⁺ cluster, marked with triangles, are due to minor niobium oxide contamination.

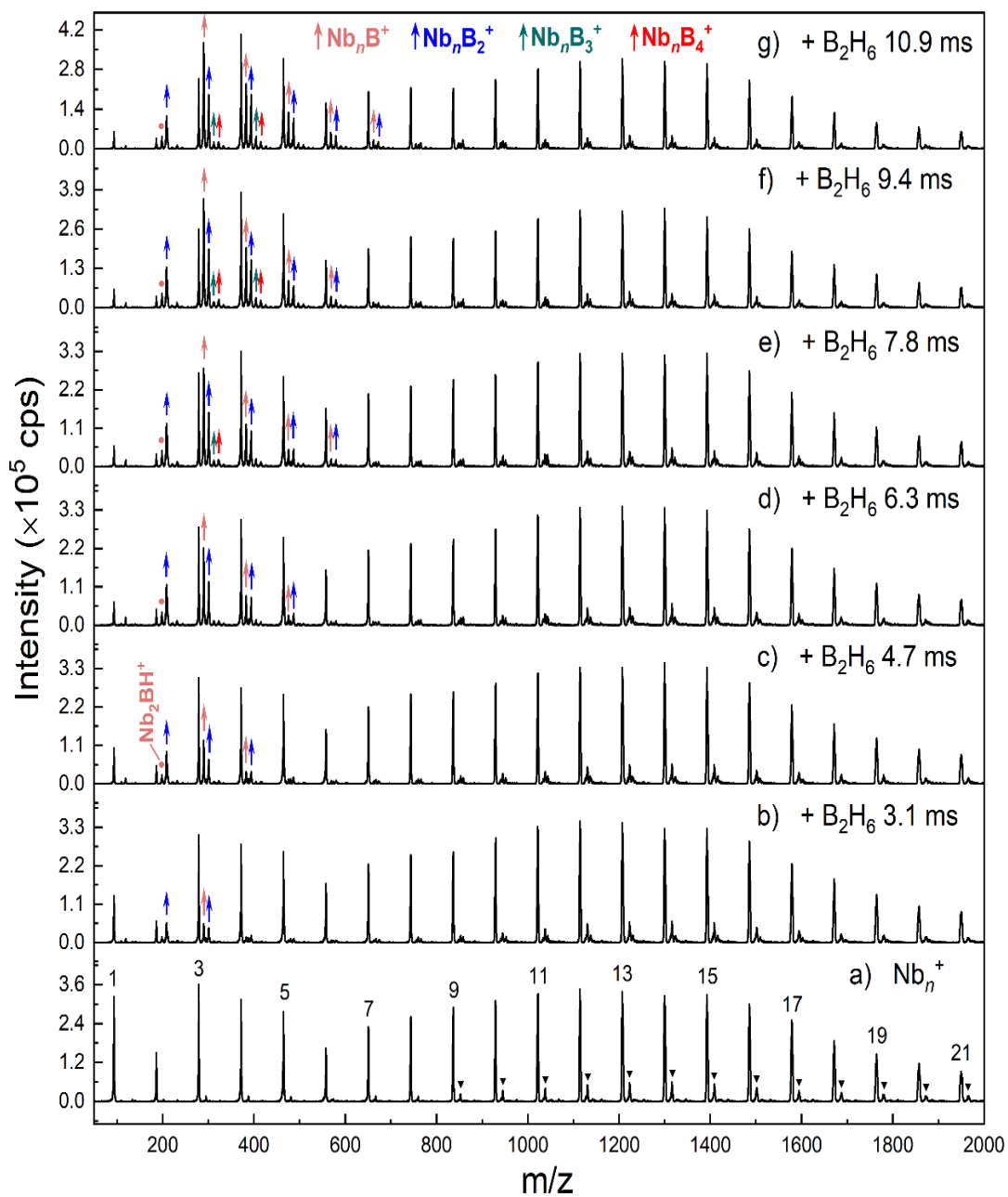


Figure S6. Reaction time dependence of 0.5 sccm B_2H_6 . Mass spectra of the nascent Nb_n^+ clusters (a), and after reacting with 0.5 sccm B_2H_6 (0.3% in He) in the laminar flow tube with controlled reaction time corresponding to 3.1, 4.7, 6.3, 7.8, 9.4, and 10.9 ms respectively (b-g). The weak peaks in the nascent Nb_n^+ cluster, marked with triangles, are due to minor niobium oxide contamination.

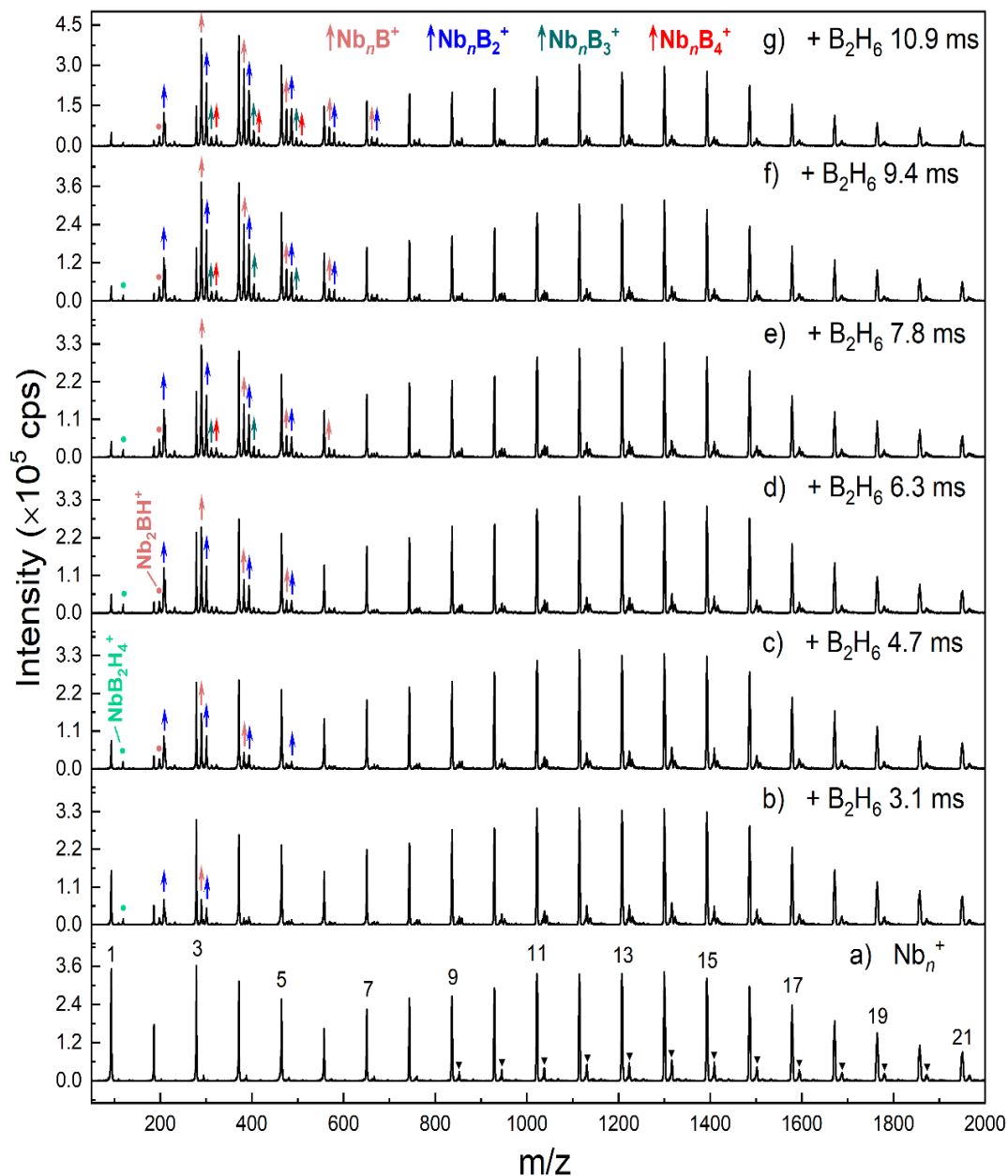


Figure S7. Reaction time dependence of 0.6 sccm B₂H₆. Mass spectra of the nascent Nb_{*n*}⁺ clusters (**a**), and after reacting with 0.6 sccm B₂H₆ (0.3% in He) in the laminar flow tube with controlled reaction time corresponding to 3.1, 4.7, 6.3, 7.8, 9.4, and 10.9 ms respectively (**b-g**). The weak peaks in the nascent Nb_{*n*}⁺ cluster, marked with triangles, are due to minor niobium oxide contamination.

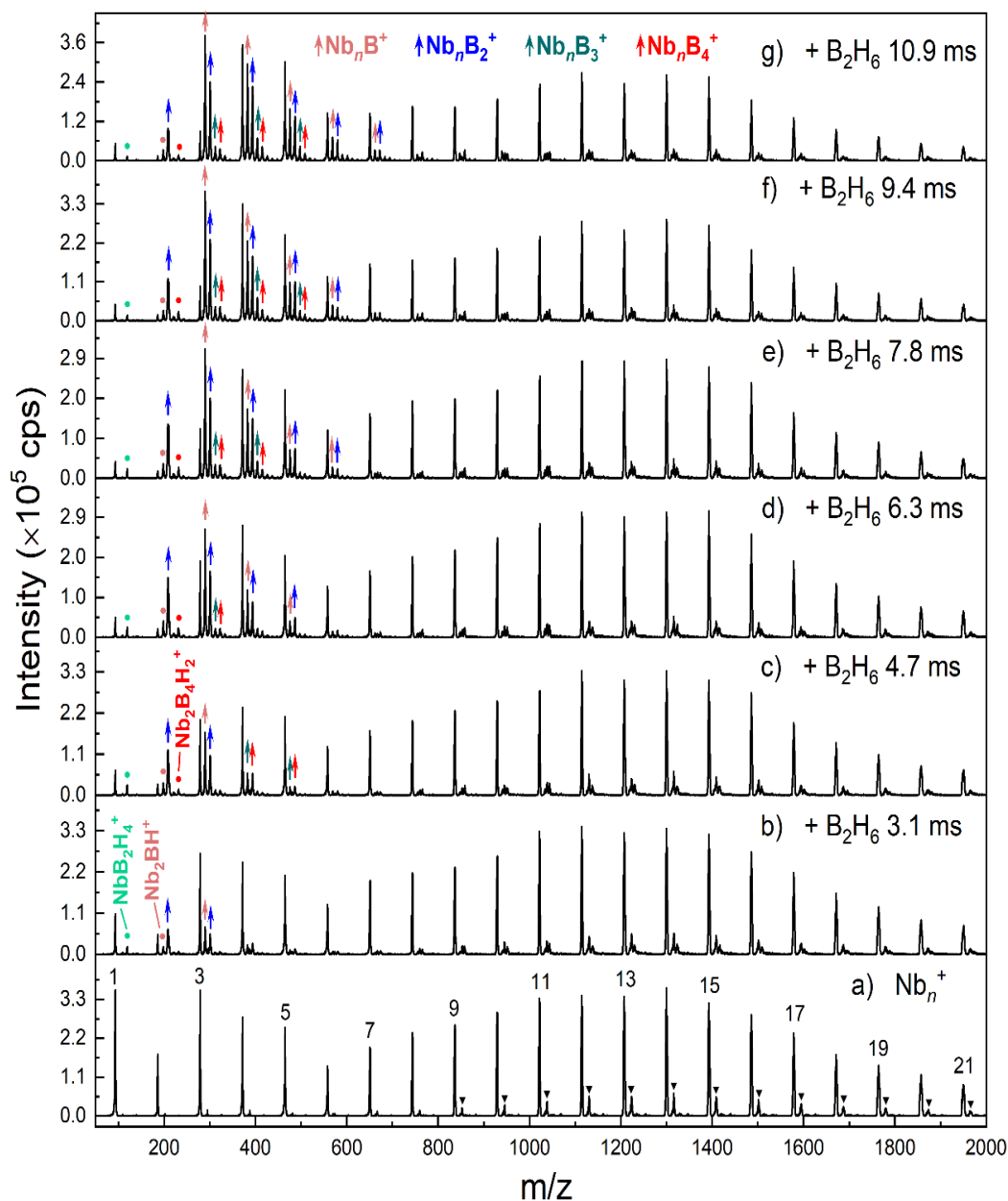


Figure S8. Reaction time dependence of 0.7 sccm B_2H_6 . Mass spectra of the nascent Nb_n^+ clusters (a), and after reacting with 0.7 sccm B_2H_6 (0.3% in He) in the laminar flow tube with controlled reaction time corresponding to 3.1, 4.7, 6.3, 7.8, 9.4, and 10.9 ms respectively (b-g). The weak peaks in the nascent Nb_n^+ cluster, marked with triangles, are due to minor niobium oxide contamination.

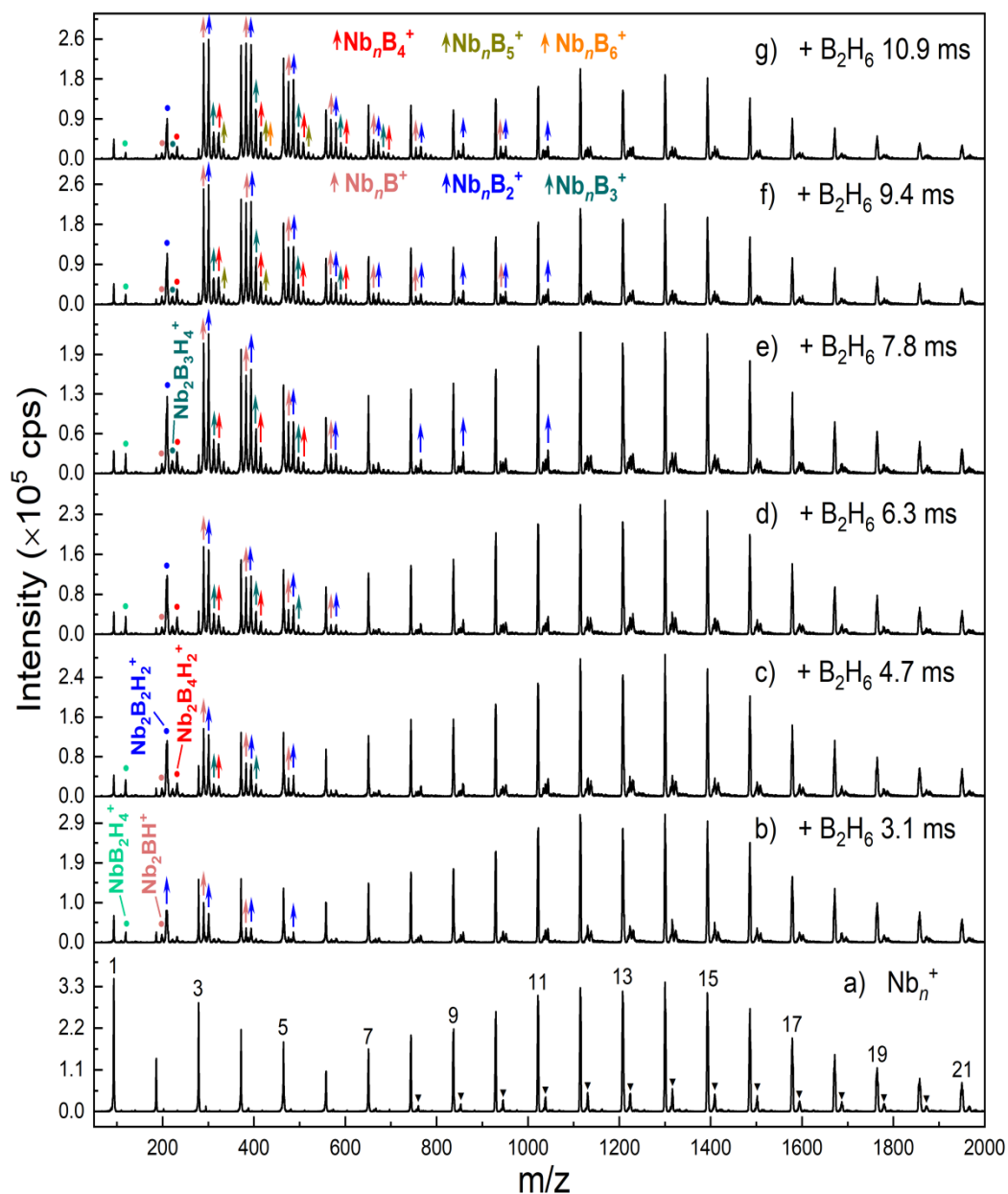


Figure S9. Reaction time dependence of 1.0 sccm B_2H_6 . Mass spectra of the nascent Nb_n^+ clusters (a), and after reacting with 1.0 sccm B_2H_6 (0.3% in He) in the laminar flow tube with controlled reaction time corresponding to 3.1, 4.7, 6.3, 7.8, 9.4, and 10.9 ms respectively (b-g). The weak peaks in the nascent Nb_n^+ cluster, marked with triangles, are due to minor niobium oxide contamination.

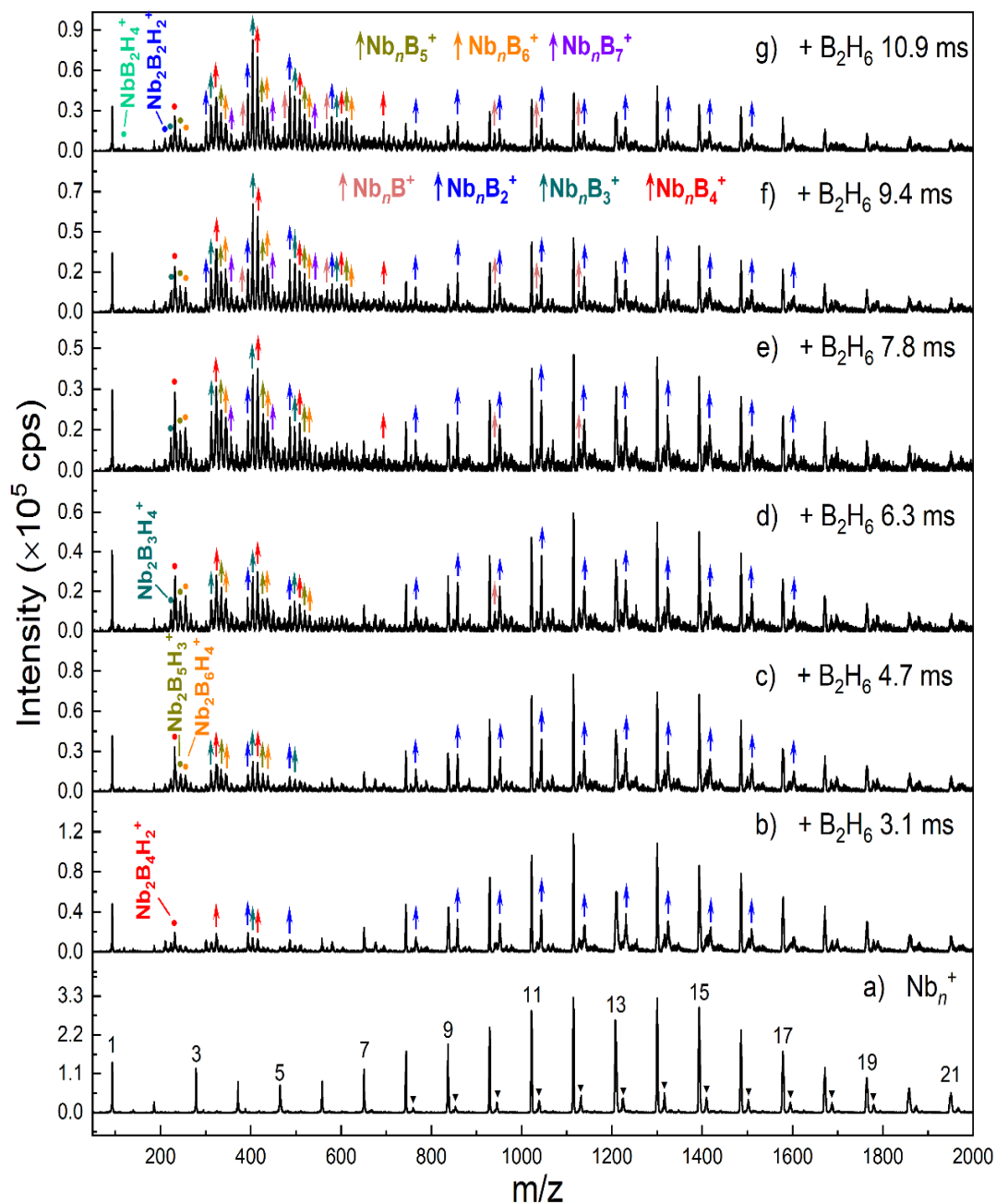


Figure S10. Reaction time dependence of 3.0 sccm B_2H_6 . Mass spectra of the nascent Nb_n^+ clusters (a), and after reacting with 3.0 sccm B_2H_6 (0.3% in He) in the laminar flow tube with controlled reaction time corresponding to 3.1, 4.7, 6.3, 7.8, 9.4, and 10.9 ms respectively (b-g). The weak peaks in the nascent Nb_n^+ cluster, marked with triangles, are due to minor niobium oxide contamination.

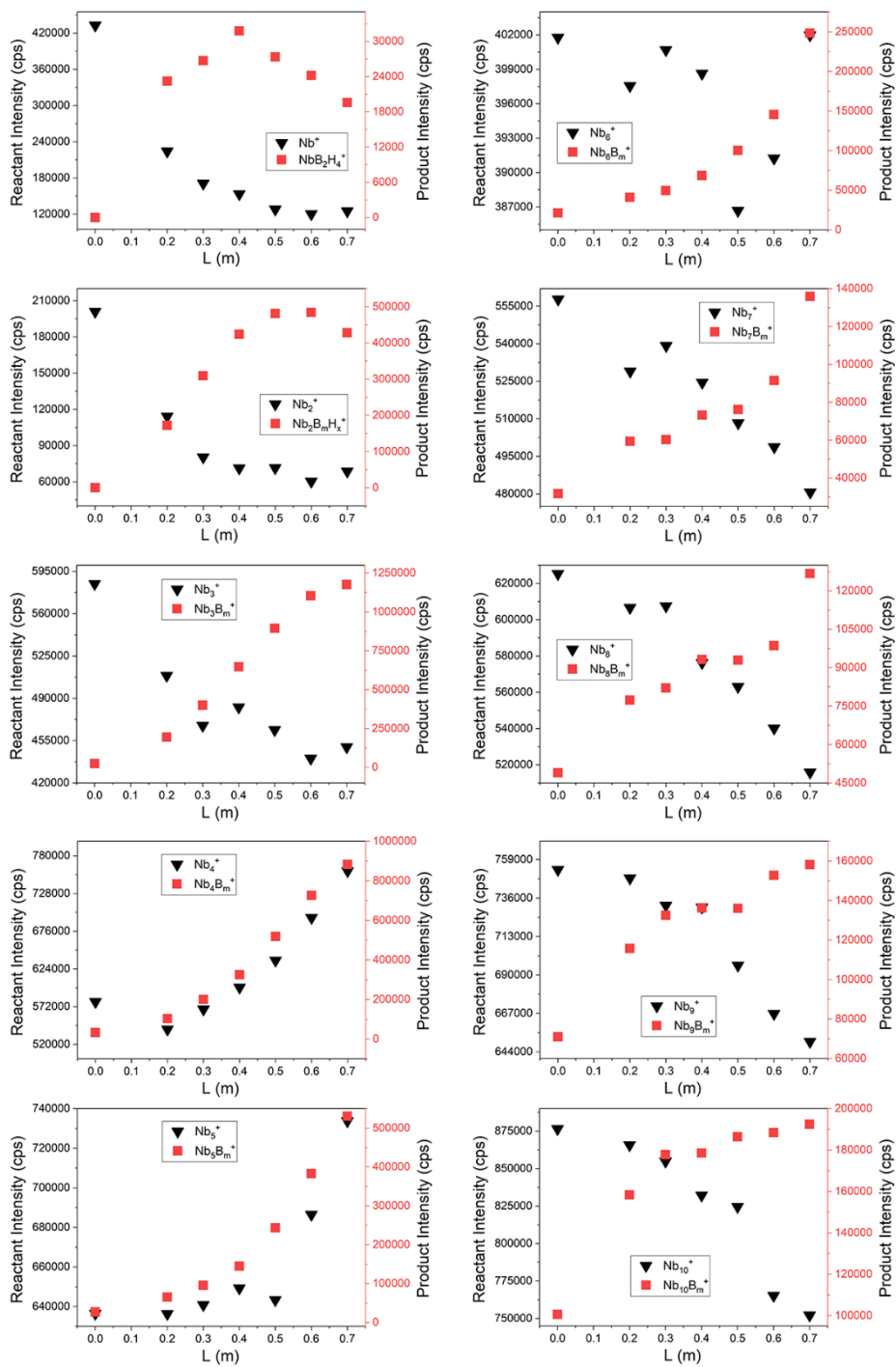


Figure S11. Absolute intensity of the Nb_n^+ ($n = 1-10$) clusters and their reaction products with $0.4 \text{ sccm B}_2\text{H}_6$ (0.3% in He) at different reaction time determined by the inlet distance.

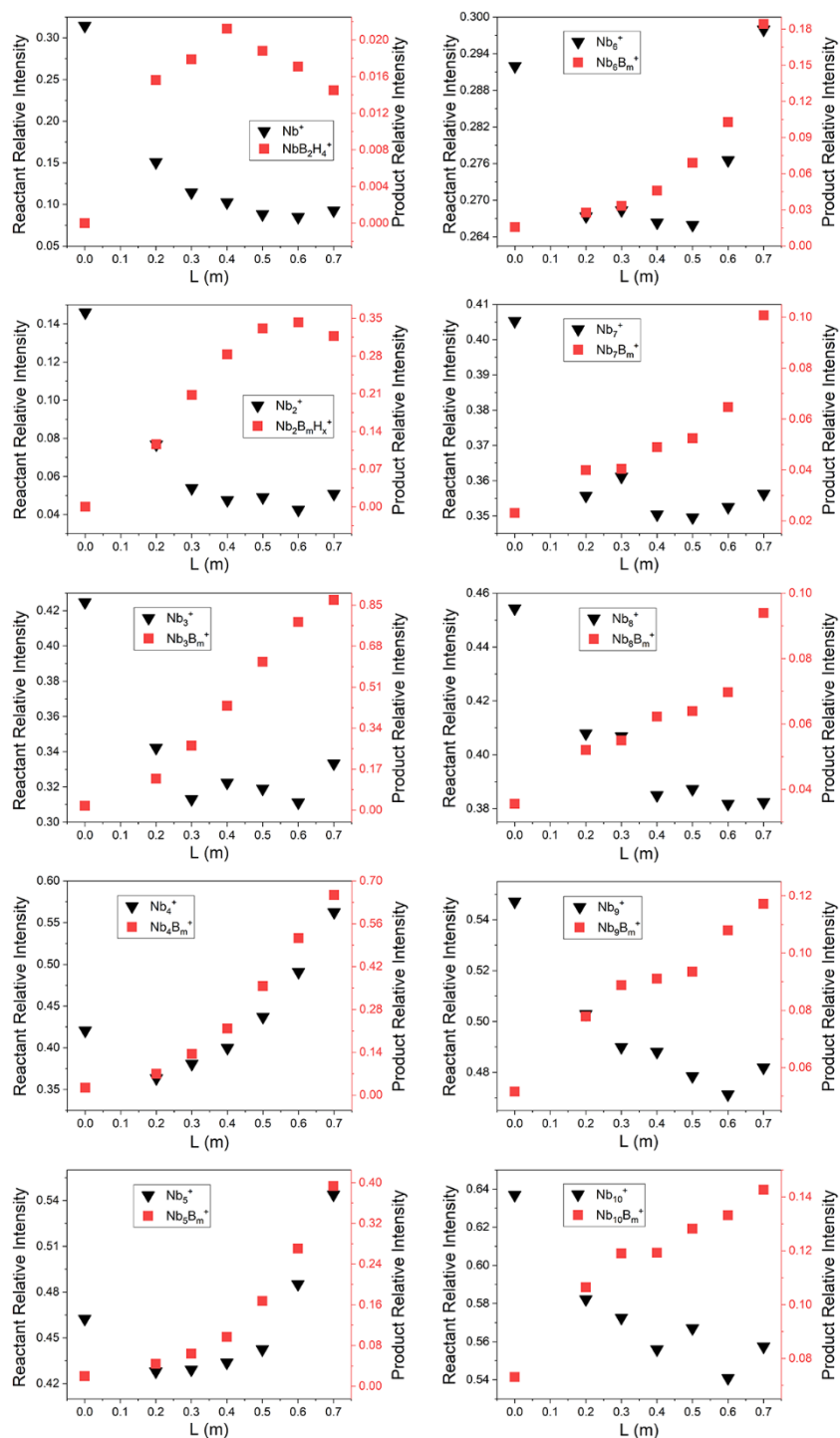


Figure S12. Relative intensity $I(\text{Nb}_n^+)/I(\text{Nb}_{13}^+)$ of the Nb_n^+ ($n = 1-10$) clusters and the products after reacting with $0.4 \text{ sccm B}_2\text{H}_6$ (0.3% in He) at different reaction time determined by the inlet distance.

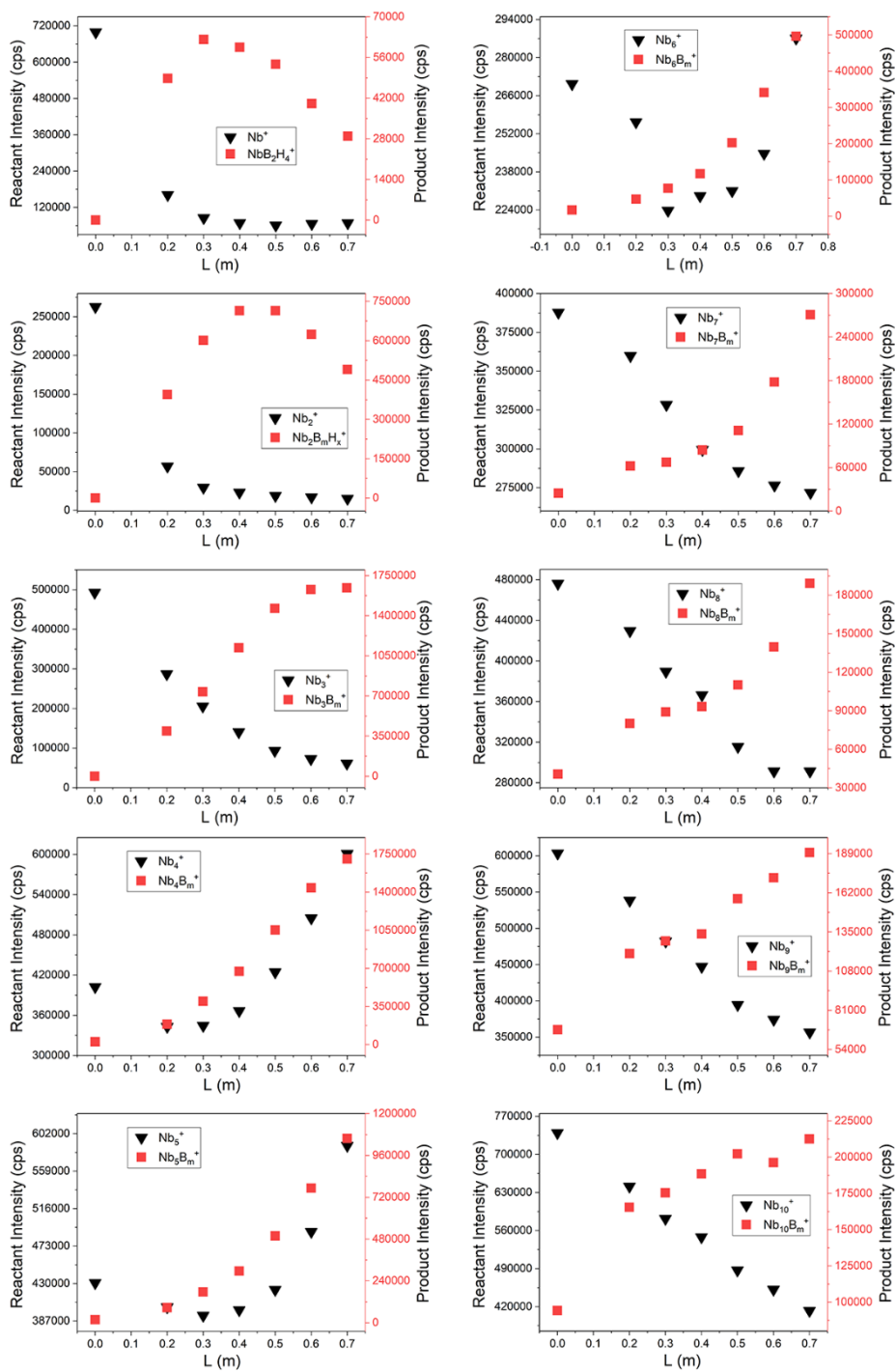


Figure S13. Absolute intensity of the Nb_n⁺ (*n* = 1-10) clusters and the products after reacting with **0.8 sccm** B₂H₆ (0.3% in He) at different reaction time determined by the inlet distance.

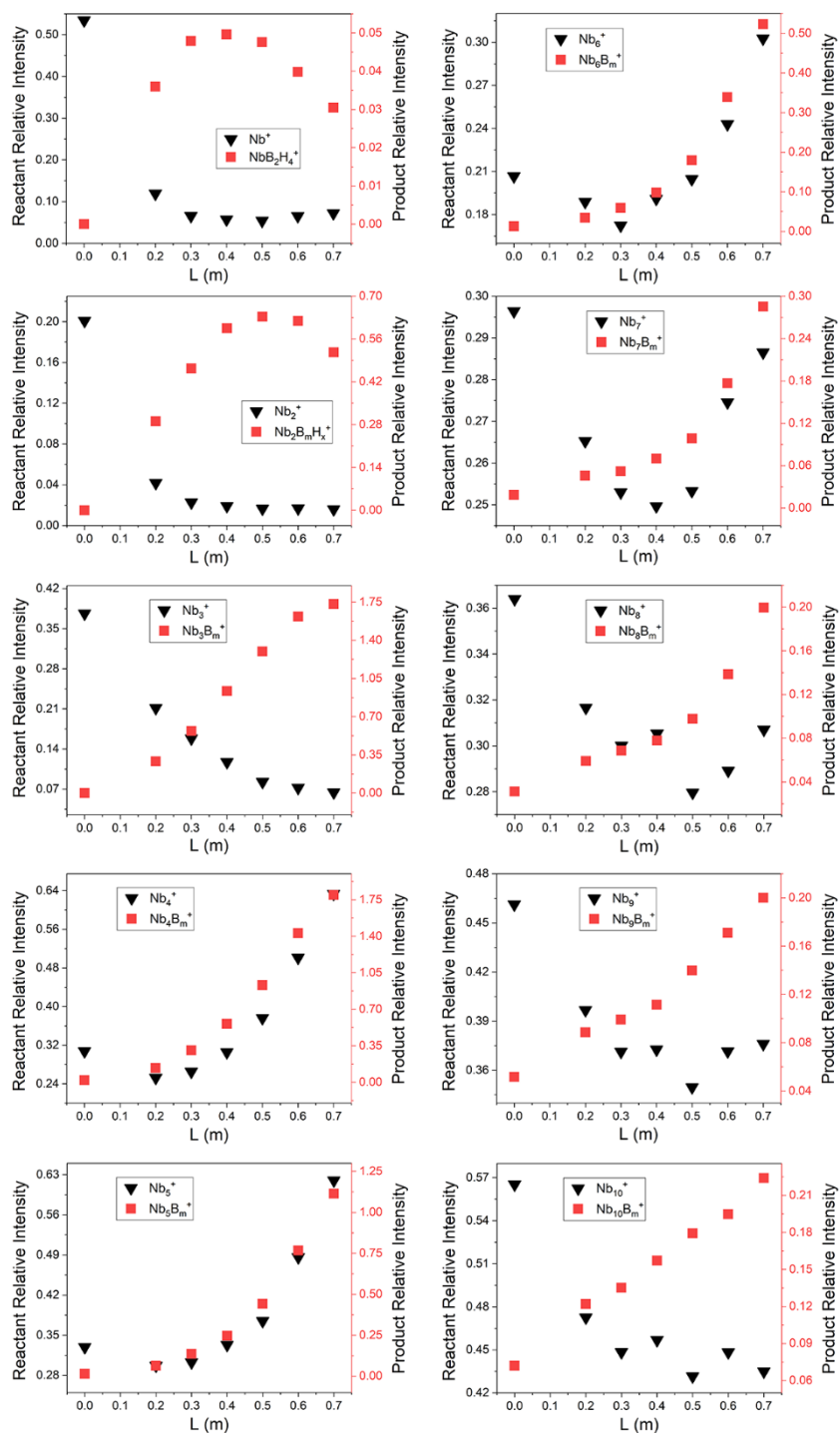


Figure S14. Relative intensity $I(\text{Nb}_n^+)/I(\text{Nb}_{13}^+)$ of the Nb_n^+ ($n = 1-10$) clusters and the products after reacting with **0.8 sccm** B_2H_6 (0.3% in He) at different reaction time determined by the inlet distance.

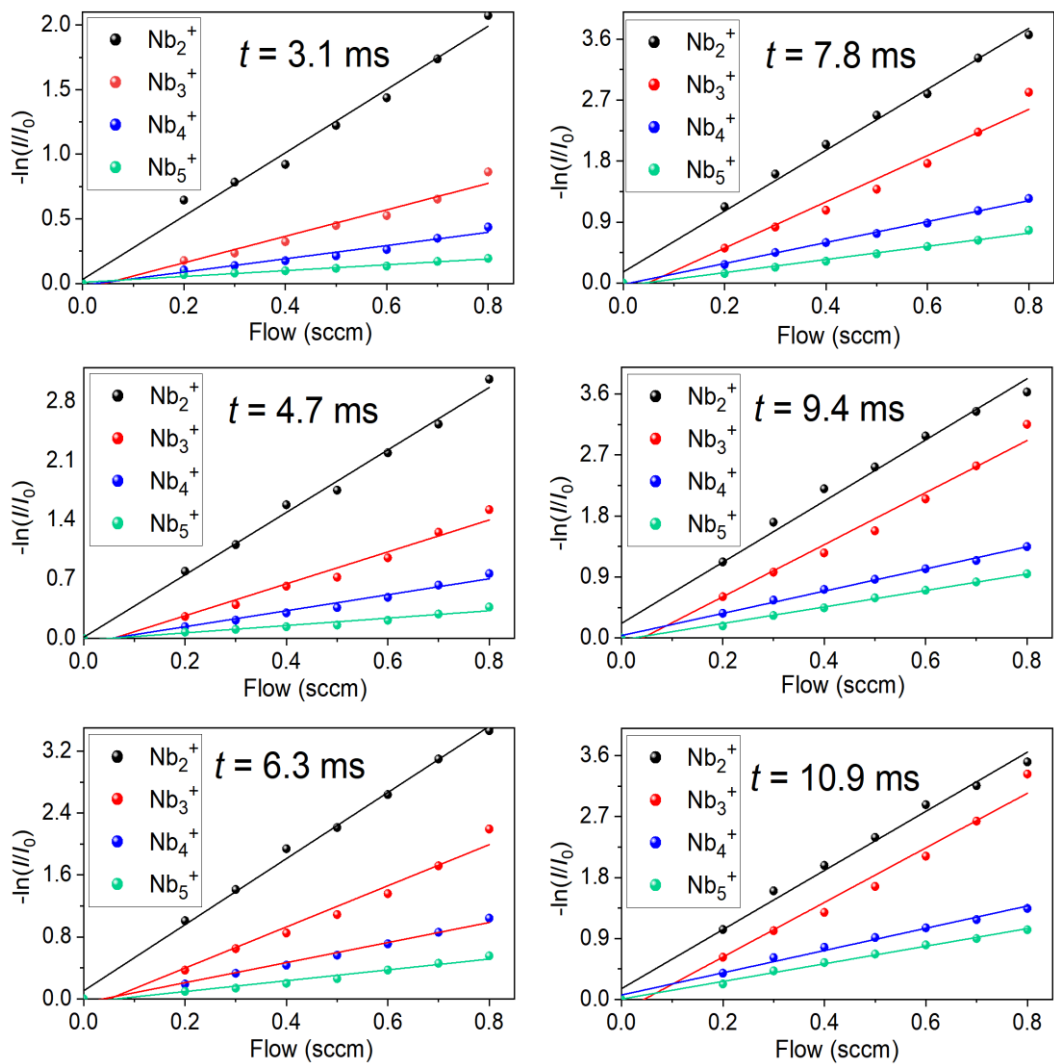


Figure S15. Linear fitting of $-\ln(I/I_0)$ of Nb_n^+ ($n=2-5$) vs. the flow (0-0.8 sccm) of the B_2H_6 reactant (0.3% in He), under the varied conditions of different reaction time ($t = 3.1, 4.7, 6.3, 7.8, 9.4, 10.9$ ms, respectively).

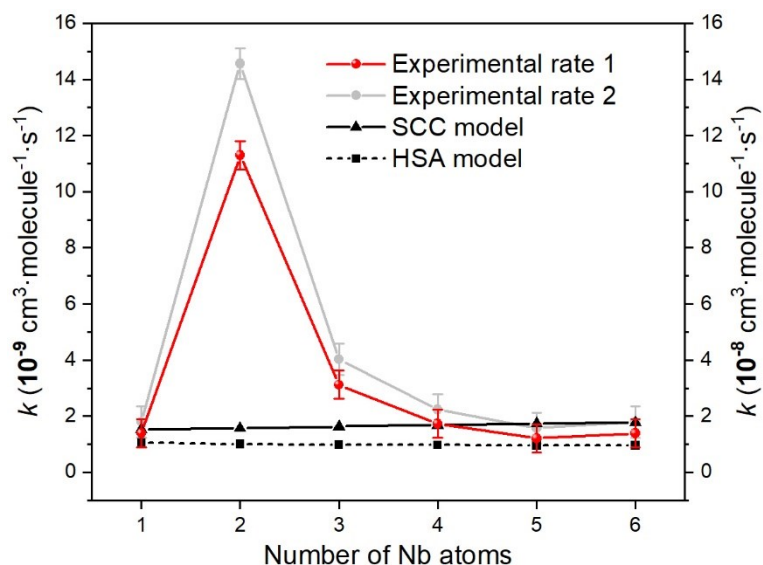


Figure S16. The experimentally determined reaction rates of Nb_n^+ ($n = 1-6$) reacting with B_2H_6 using two methods (rate 1 and 2), in a comparison with the theoretically simulated rate constants based on the SCC model and HSA model. The scale and tick labels for experimental rate 2 is displayed on the right axis. The systemic errors are considered through error propagation based on the equations, including the measure of the mass peak intensities, the measure of vacuum, and the estimation of the molecular beam density.

S2 Optimized Structures and Thermodynamics

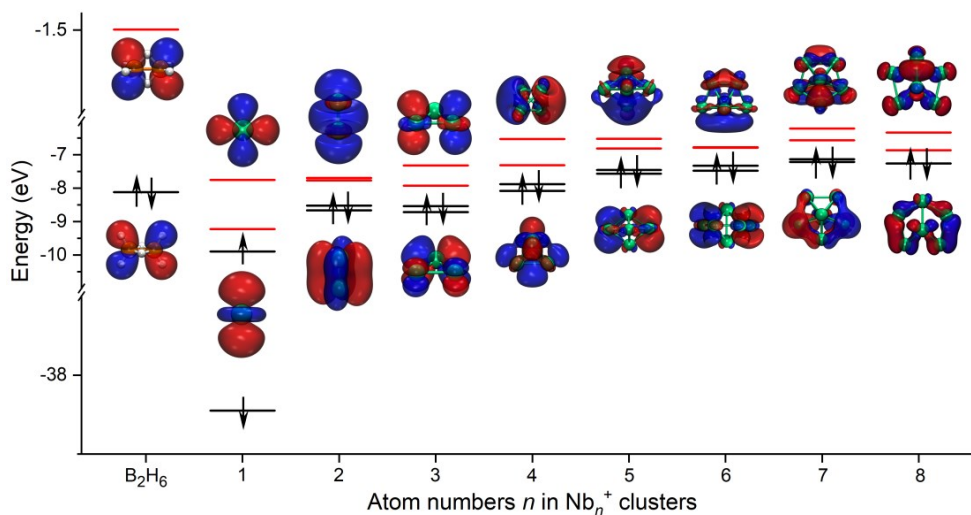


Figure S17. Frontier orbital analysis. The highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbitals (LUMO) of the Nb_n^+ clusters in a comparison with that of B_2H_6 .

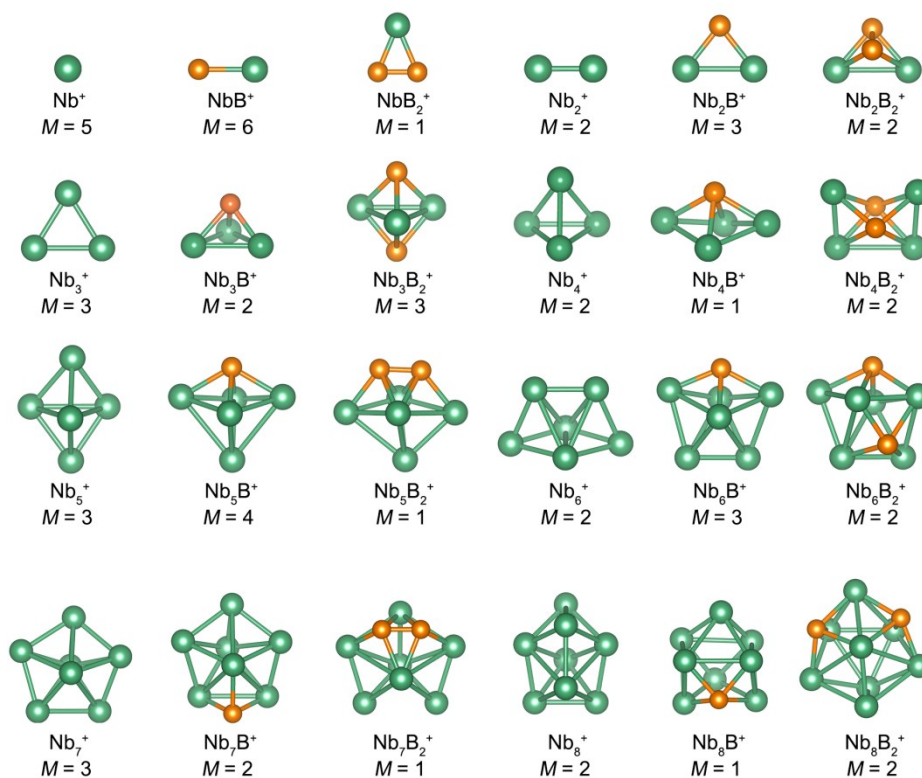


Figure S18. The optimized structures of Nb_nB_m^+ clusters ($n = 1-9$, $m = 0-2$). Spin multiplicities (M) are shown below each isomer.

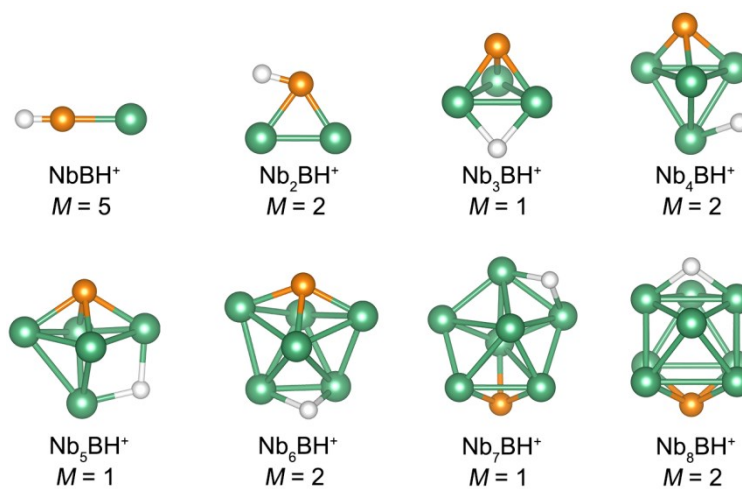


Figure S19. The optimized structures of Nb_nBH^+ clusters ($n = 1-8$). Spin multiplicities (M) are shown below each isomer.

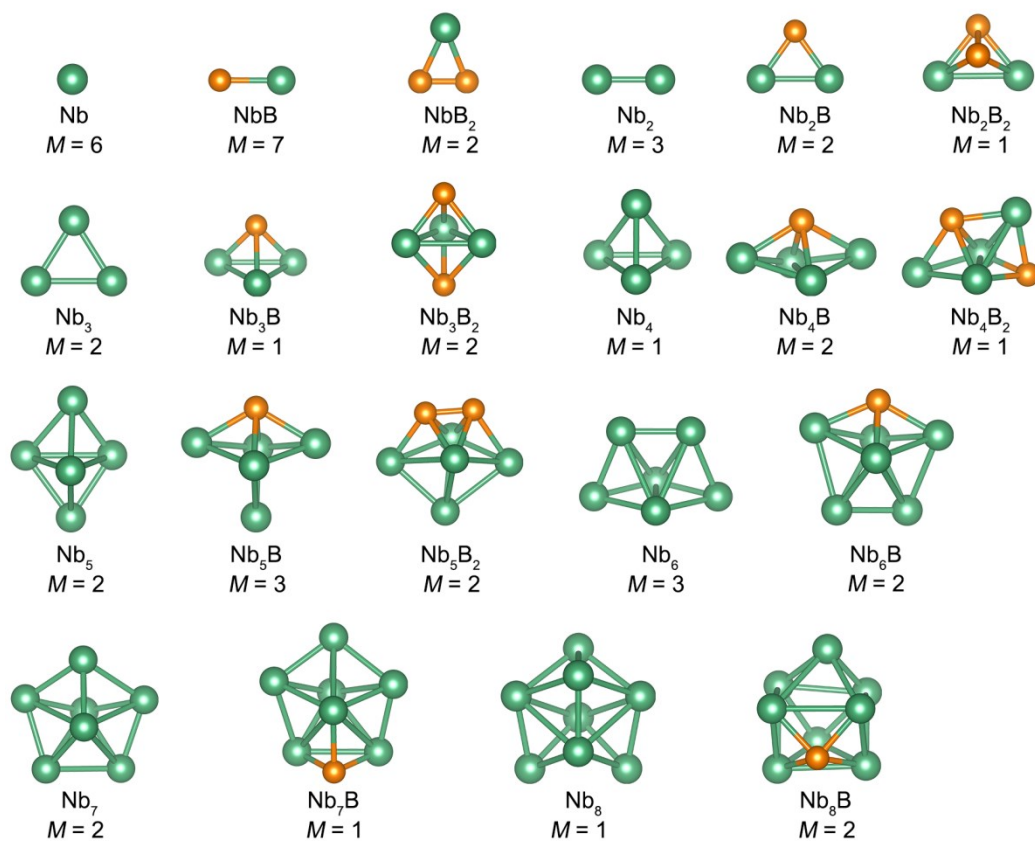


Figure S20. The optimized structures of neutral Nb_nB_m clusters ($n = 1-8$, $m = 0-2$). Spin multiplicities (M) are shown below each isomer.

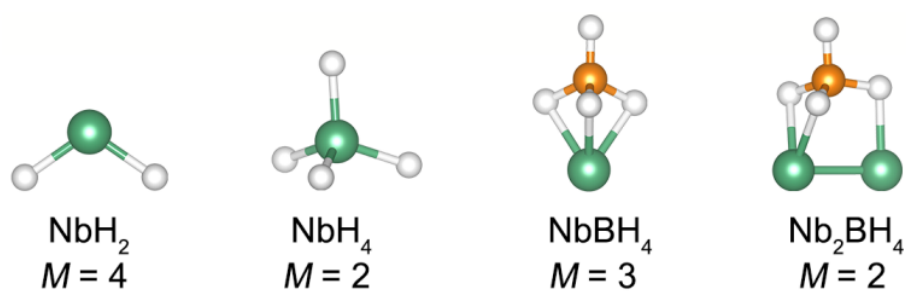


Figure S21. The optimized structures of neutral $\text{Nb}_n\text{B}_x\text{H}_y$ clusters. Spin multiplicities (M) are shown below each isomer.

Table S1. Thermodynamics energy changes (ΔG) for $\text{Nb}_n^+ + \text{B}_2\text{H}_6 \rightarrow \text{Nb}_n\text{B}_2^+ + 3\text{H}_2$. The pre-superscripts refer to spin multiplicities. Energies are given in eV.

Thermodynamics energy changes (eV)	
${}^5\text{Nb}^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{NbB}_2^+ + 3\text{H}_2$	$\Delta G = 2.95$
${}^2\text{Nb}_2^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_2\text{B}_2^+ + 3\text{H}_2$	$\Delta G = 1.65$
${}^3\text{Nb}_3^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_3\text{B}_2^+ + 3\text{H}_2$	$\Delta G = -0.20$
${}^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_4\text{B}_2^+ + 3\text{H}_2$	$\Delta G = -0.60$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_5\text{B}_2^+ + 3\text{H}_2$	$\Delta G = -1.47$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_6\text{B}_2^+ + 3\text{H}_2$	$\Delta G = -1.52$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_7\text{B}_2^+ + 3\text{H}_2$	$\Delta G = -0.61$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_8\text{B}_2^+ + 3\text{H}_2$	$\Delta G = -0.72$

Table S2. Thermodynamics energy changes (ΔG) for $\text{Nb}_n^+ + \text{B}_2\text{H}_6 \rightarrow \text{Nb}_n\text{BH}_x^+ + \frac{6-x-y}{2} \text{H}_2 + \text{BH}_y$. The pre-superscripts refer to spin multiplicities. Energies are given in eV.

Thermodynamics energy changes (eV)	
${}^5\text{Nb}^+ + \text{B}_2\text{H}_6 \rightarrow {}^5\text{NbBH}^+ + \text{BH} + 2\text{H}_2$	$\Delta G = 5.24$
${}^2\text{Nb}_2^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_2\text{BH}^+ + \text{BH} + 2\text{H}_2$	$\Delta G = 4.74$
${}^3\text{Nb}_3^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_3\text{BH}^+ + \text{BH} + 2\text{H}_2$	$\Delta G = 3.22$
${}^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_4\text{BH}^+ + \text{BH} + 2\text{H}_2$	$\Delta G = 3.47$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_5\text{BH}^+ + \text{BH} + 2\text{H}_2$	$\Delta G = 3.05$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_6\text{BH}^+ + \text{BH} + 2\text{H}_2$	$\Delta G = 1.93$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_7\text{BH}^+ + \text{BH} + 2\text{H}_2$	$\Delta G = 3.47$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_8\text{BH}^+ + \text{BH} + 2\text{H}_2$	$\Delta G = 3.03$
${}^5\text{Nb}^+ + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + \text{BH}_2 + 2\text{H}_2$	$\Delta G = 5.61$
${}^2\text{Nb}_2^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + \text{BH}_2 + 2\text{H}_2$	$\Delta G = 4.69$
${}^3\text{Nb}_3^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + \text{BH}_2 + 2\text{H}_2$	$\Delta G = 3.09$
${}^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + \text{BH}_2 + 2\text{H}_2$	$\Delta G = 2.90$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + \text{BH}_2 + 2\text{H}_2$	$\Delta G = 2.85$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_6\text{B}^+ + \text{BH}_2 + 2\text{H}_2$	$\Delta G = 1.58$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_7\text{B}^+ + \text{BH}_2 + 2\text{H}_2$	$\Delta G = 3.23$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_8\text{B}^+ + \text{BH}_2 + 2\text{H}_2$	$\Delta G = 2.95$
${}^5\text{Nb}^+ + \text{B}_2\text{H}_6 \rightarrow {}^5\text{NbBH}^+ + \text{BH}_3 + \text{H}_2$	$\Delta G = 1.57$
${}^2\text{Nb}_2^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_2\text{BH}^+ + \text{BH}_3 + \text{H}_2$	$\Delta G = 1.08$
${}^3\text{Nb}_3^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_3\text{BH}^+ + \text{BH}_3 + \text{H}_2$	$\Delta G = -0.44$
${}^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_4\text{BH}^+ + \text{BH}_3 + \text{H}_2$	$\Delta G = -0.19$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_5\text{BH}^+ + \text{BH}_3 + \text{H}_2$	$\Delta G = -0.61$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_6\text{BH}^+ + \text{BH}_3 + \text{H}_2$	$\Delta G = -1.73$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_7\text{BH}^+ + \text{BH}_3 + \text{H}_2$	$\Delta G = -0.19$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_8\text{BH}^+ + \text{BH}_3 + \text{H}_2$	$\Delta G = -0.64$
${}^5\text{Nb}^+ + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + \text{BH}_4 + \text{H}_2$	$\Delta G = 4.57$
${}^2\text{Nb}_2^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + \text{BH}_4 + \text{H}_2$	$\Delta G = 3.65$
${}^3\text{Nb}_3^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + \text{BH}_4 + \text{H}_2$	$\Delta G = 2.05$
${}^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + \text{BH}_4 + \text{H}_2$	$\Delta G = 1.86$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + \text{BH}_4 + \text{H}_2$	$\Delta G = 1.81$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_6\text{B}^+ + \text{BH}_4 + \text{H}_2$	$\Delta G = 0.54$

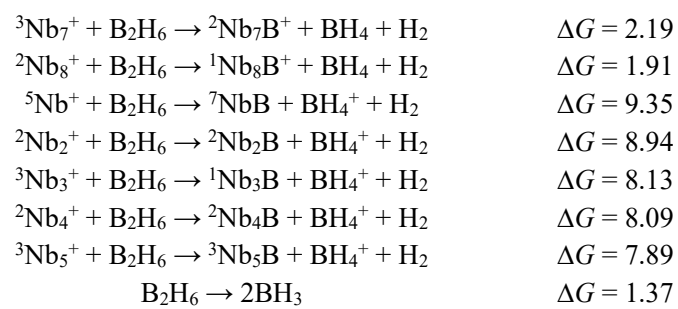


Table S3. Thermodynamics energy changes (ΔG) for $\text{Nb}_n^+ + \text{B}_2\text{H}_6 \rightarrow \text{Nb}_{n-x}\text{B}^+ + \text{Nb}_x\text{BH}_4 + \text{H}_2$. The pre-superscripts refer to spin multiplicities. Energies are given in eV.

Thermodynamics energy changes (eV)	
${}^2\text{Nb}_2^+ + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^3\text{NbBH}_4 + \text{H}_2$	$\Delta G = 5.48$
${}^3\text{Nb}_3^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^3\text{NbBH}_4 + \text{H}_2$	$\Delta G = 3.70$
${}^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^3\text{NbBH}_4 + \text{H}_2$	$\Delta G = 3.29$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^3\text{NbBH}_4 + \text{H}_2$	$\Delta G = 2.78$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^3\text{NbBH}_4 + \text{H}_2$	$\Delta G = 2.71$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_6\text{B}^+ + {}^3\text{NbBH}_4 + \text{H}_2$	$\Delta G = 2.40$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_7\text{B}^+ + {}^3\text{NbBH}_4 + \text{H}_2$	$\Delta G = 3.51$
${}^1\text{Nb}_9^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_8\text{B}^+ + {}^3\text{NbBH}_4 + \text{H}_2$	$\Delta G = 3.01$
${}^3\text{Nb}_3^+ + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^2\text{Nb}_2\text{BH}_4 + \text{H}_2$	$\Delta G = 5.62$
${}^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^2\text{Nb}_2\text{BH}_4 + \text{H}_2$	$\Delta G = 5.04$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^2\text{Nb}_2\text{BH}_4 + \text{H}_2$	$\Delta G = 4.31$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^2\text{Nb}_2\text{BH}_4 + \text{H}_2$	$\Delta G = 3.78$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^2\text{Nb}_2\text{BH}_4 + \text{H}_2$	$\Delta G = 4.67$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_6\text{B}^+ + {}^2\text{Nb}_2\text{BH}_4 + \text{H}_2$	$\Delta G = 3.83$
${}^1\text{Nb}_9^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_7\text{B}^+ + {}^2\text{Nb}_2\text{BH}_4 + \text{H}_2$	$\Delta G = 4.71$
${}^2\text{Nb}_{10}^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_8\text{B}^+ + {}^2\text{Nb}_2\text{BH}_4 + \text{H}_2$	$\Delta G = 4.49$

Table S4. Thermodynamics energy changes (ΔG) for $\text{Nb}_n^+ + \text{B}_2\text{H}_6 \rightarrow \text{Nb}_{n-1}\text{B}_2^+ + \text{NbH}_{2x} + (3-x)\text{H}_2$. The pre-superscripts refer to spin multiplicities. Energies are given in eV.

Thermodynamics energy changes (eV)	
${}^2\text{Nb}_2^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{NbB}_2^+ + {}^4\text{NbH}_2 + 2\text{H}_2$	$\Delta G = 7.14$
${}^2\text{Nb}_2^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{NbB}_2^+ + {}^2\text{NbH}_4 + \text{H}_2$	$\Delta G = 5.81$
${}^3\text{Nb}_3^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_2\text{B}_2^+ + {}^4\text{NbH}_2 + 2\text{H}_2$	$\Delta G = 4.98$
${}^3\text{Nb}_3^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_2\text{B}_2^+ + {}^2\text{NbH}_4 + \text{H}_2$	$\Delta G = 3.64$
${}^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_3\text{B}_2^+ + {}^4\text{NbH}_2 + 2\text{H}_2$	$\Delta G = 4.32$
${}^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_3\text{B}_2^+ + {}^2\text{NbH}_4 + \text{H}_2$	$\Delta G = 2.99$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_4\text{B}_2^+ + {}^4\text{NbH}_2 + 2\text{H}_2$	$\Delta G = 3.61$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_4\text{B}_2^+ + {}^2\text{NbH}_4 + \text{H}_2$	$\Delta G = 2.27$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_5\text{B}_2^+ + {}^4\text{NbH}_2 + 2\text{H}_2$	$\Delta G = 2.72$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_5\text{B}_2^+ + {}^2\text{NbH}_4 + \text{H}_2$	$\Delta G = 1.39$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_6\text{B}_2^+ + {}^4\text{NbH}_2 + 2\text{H}_2$	$\Delta G = 3.62$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_6\text{B}_2^+ + {}^2\text{NbH}_4 + \text{H}_2$	$\Delta G = 2.29$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_7\text{B}_2^+ + {}^4\text{NbH}_2 + 2\text{H}_2$	$\Delta G = 4.01$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_7\text{B}_2^+ + {}^2\text{NbH}_4 + \text{H}_2$	$\Delta G = 2.67$
${}^1\text{Nb}_9^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_8\text{B}_2^+ + {}^4\text{NbH}_2 + 2\text{H}_2$	$\Delta G = 3.67$
${}^1\text{Nb}_9^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_8\text{B}_2^+ + {}^2\text{NbH}_4 + \text{H}_2$	$\Delta G = 2.34$

Table S5. Thermodynamics energy changes (ΔG) for $\text{Nb}_n^+ + \text{B}_2\text{H}_6 \rightarrow \text{Nb}_x\text{B}_2^+ + \text{Nb}_{n-x} + 3\text{H}_2$. The pre-superscripts refer to spin multiplicities. Energies are given in eV.

Thermodynamics energy changes (eV)	
${}^2\text{Nb}_2^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{NbB}_2^+ + {}^6\text{Nb} + 3\text{H}_2$	$\Delta G = 8.33$
${}^3\text{Nb}_3^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{NbB}_2^+ + {}^3\text{Nb}_2 + 3\text{H}_2$	$\Delta G = 7.90$
${}^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{NbB}_2^+ + {}^2\text{Nb}_3 + 3\text{H}_2$	$\Delta G = 9.46$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{NbB}_2^+ + {}^1\text{Nb}_4 + 3\text{H}_2$	$\Delta G = 9.44$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{NbB}_2^+ + {}^2\text{Nb}_5 + 3\text{H}_2$	$\Delta G = 9.71$
${}^3\text{Nb}_3^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_2\text{B}_2^+ + {}^6\text{Nb} + 3\text{H}_2$	$\Delta G = 6.16$
${}^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_2\text{B}_2^+ + {}^3\text{Nb}_2 + 3\text{H}_2$	$\Delta G = 6.93$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_2\text{B}_2^+ + {}^2\text{Nb}_3 + 3\text{H}_2$	$\Delta G = 8.16$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_2\text{B}_2^+ + {}^1\text{Nb}_4 + 3\text{H}_2$	$\Delta G = 8.13$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_2\text{B}_2^+ + {}^2\text{Nb}_5 + 3\text{H}_2$	$\Delta G = 9.35$
${}^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_3\text{B}_2^+ + {}^6\text{Nb} + 3\text{H}_2$	$\Delta G = 5.51$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_3\text{B}_2^+ + {}^3\text{Nb}_2 + 3\text{H}_2$	$\Delta G = 5.96$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_3\text{B}_2^+ + {}^2\text{Nb}_3 + 3\text{H}_2$	$\Delta G = 7.17$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_3\text{B}_2^+ + {}^1\text{Nb}_4 + 3\text{H}_2$	$\Delta G = 8.10$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_3\text{B}_2^+ + {}^2\text{Nb}_5 + 3\text{H}_2$	$\Delta G = 8.79$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_4\text{B}_2^+ + {}^6\text{Nb} + 3\text{H}_2$	$\Delta G = 4.79$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_4\text{B}_2^+ + {}^3\text{Nb}_2 + 3\text{H}_2$	$\Delta G = 5.22$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_4\text{B}_2^+ + {}^2\text{Nb}_3 + 3\text{H}_2$	$\Delta G = 7.39$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_4\text{B}_2^+ + {}^1\text{Nb}_4 + 3\text{H}_2$	$\Delta G = 7.79$
${}^1\text{Nb}_9^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_4\text{B}_2^+ + {}^2\text{Nb}_5 + 3\text{H}_2$	$\Delta G = 8.25$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_5\text{B}_2^+ + {}^6\text{Nb} + 3\text{H}_2$	$\Delta G = 3.90$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_5\text{B}_2^+ + {}^3\text{Nb}_2 + 3\text{H}_2$	$\Delta G = 5.29$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_5\text{B}_2^+ + {}^2\text{Nb}_3 + 3\text{H}_2$	$\Delta G = 6.93$
${}^1\text{Nb}_9^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_5\text{B}_2^+ + {}^1\text{Nb}_4 + 3\text{H}_2$	$\Delta G = 7.10$
${}^2\text{Nb}_{10}^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_5\text{B}_2^+ + {}^2\text{Nb}_5 + 3\text{H}_2$	$\Delta G = 7.84$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_6\text{B}_2^+ + {}^6\text{Nb} + 3\text{H}_2$	$\Delta G = 4.81$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_6\text{B}_2^+ + {}^3\text{Nb}_2 + 3\text{H}_2$	$\Delta G = 5.67$
${}^1\text{Nb}_9^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_6\text{B}_2^+ + {}^2\text{Nb}_3 + 3\text{H}_2$	$\Delta G = 7.08$
${}^2\text{Nb}_{10}^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_6\text{B}_2^+ + {}^1\text{Nb}_4 + 3\text{H}_2$	$\Delta G = 7.53$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_7\text{B}_2^+ + {}^6\text{Nb} + 3\text{H}_2$	$\Delta G = 5.19$
${}^1\text{Nb}_9^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_7\text{B}_2^+ + {}^3\text{Nb}_2 + 3\text{H}_2$	$\Delta G = 5.82$
${}^2\text{Nb}_{10}^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_7\text{B}_2^+ + {}^2\text{Nb}_3 + 3\text{H}_2$	$\Delta G = 7.51$
${}^1\text{Nb}_9^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_8\text{B}_2^+ + {}^6\text{Nb} + 3\text{H}_2$	$\Delta G = 4.85$
${}^2\text{Nb}_{10}^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_8\text{B}_2^+ + {}^3\text{Nb}_2 + 3\text{H}_2$	$\Delta G = 5.77$

Table S6. Thermodynamics energy changes (ΔG) for $\text{Nb}_n^+ + \text{B}_2\text{H}_6 \rightarrow \text{Nb}_x^+ + \text{Nb}_{n-x}\text{B}_2 + 3\text{H}_2$. The pre-superscripts refer to spin multiplicities. Energies are given in eV.

Thermodynamics energy changes (eV)	
${}^2\text{Nb}_2^+ + \text{B}_2\text{H}_6 \rightarrow {}^5\text{Nb}^+ + {}^2\text{NbB}_2 + 3\text{H}_2$	$\Delta G = 7.48$
${}^3\text{Nb}_3^+ + \text{B}_2\text{H}_6 \rightarrow {}^5\text{Nb}^+ + {}^1\text{Nb}_2\text{B}_2 + 3\text{H}_2$	$\Delta G = 6.59$
${}^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow {}^5\text{Nb}^+ + {}^2\text{Nb}_3\text{B}_2 + 3\text{H}_2$	$\Delta G = 5.95$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^5\text{Nb}^+ + {}^1\text{Nb}_4\text{B}_2 + 3\text{H}_2$	$\Delta G = 6.11$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^5\text{Nb}^+ + {}^2\text{Nb}_5\text{B}_2 + 3\text{H}_2$	$\Delta G = 5.31$
${}^3\text{Nb}_3^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_2^+ + {}^2\text{NbB}_2 + 3\text{H}_2$	$\Delta G = 6.62$
${}^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_2^+ + {}^1\text{Nb}_2\text{B}_2 + 3\text{H}_2$	$\Delta G = 6.92$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_2^+ + {}^2\text{Nb}_3\text{B}_2 + 3\text{H}_2$	$\Delta G = 5.96$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_2^+ + {}^1\text{Nb}_4\text{B}_2 + 3\text{H}_2$	$\Delta G = 6.10$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_2^+ + {}^2\text{Nb}_5\text{B}_2 + 3\text{H}_2$	$\Delta G = 6.26$
${}^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_3^+ + {}^2\text{NbB}_2 + 3\text{H}_2$	$\Delta G = 7.81$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_3^+ + {}^1\text{Nb}_2\text{B}_2 + 3\text{H}_2$	$\Delta G = 7.79$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_3^+ + {}^2\text{Nb}_3\text{B}_2 + 3\text{H}_2$	$\Delta G = 6.81$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_3^+ + {}^1\text{Nb}_4\text{B}_2 + 3\text{H}_2$	$\Delta G = 7.91$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_3^+ + {}^2\text{Nb}_5\text{B}_2 + 3\text{H}_2$	$\Delta G = 7.54$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_4^+ + {}^2\text{NbB}_2 + 3\text{H}_2$	$\Delta G = 7.49$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_4^+ + {}^1\text{Nb}_2\text{B}_2 + 3\text{H}_2$	$\Delta G = 7.45$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_4^+ + {}^2\text{Nb}_3\text{B}_2 + 3\text{H}_2$	$\Delta G = 7.43$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_4^+ + {}^1\text{Nb}_4\text{B}_2 + 3\text{H}_2$	$\Delta G = 7.99$
${}^1\text{Nb}_9^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_4^+ + {}^2\text{Nb}_5\text{B}_2 + 3\text{H}_2$	$\Delta G = 7.40$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_5^+ + {}^2\text{NbB}_2 + 3\text{H}_2$	$\Delta G = 7.47$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_5^+ + {}^1\text{Nb}_2\text{B}_2 + 3\text{H}_2$	$\Delta G = 8.39$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_5^+ + {}^2\text{Nb}_3\text{B}_2 + 3\text{H}_2$	$\Delta G = 7.84$
${}^1\text{Nb}_9^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_5^+ + {}^1\text{Nb}_4\text{B}_2 + 3\text{H}_2$	$\Delta G = 8.18$
${}^2\text{Nb}_{10}^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_5^+ + {}^2\text{Nb}_5\text{B}_2 + 3\text{H}_2$	$\Delta G = 7.86$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_6^+ + {}^2\text{NbB}_2 + 3\text{H}_2$	$\Delta G = 8.43$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_6^+ + {}^1\text{Nb}_2\text{B}_2 + 3\text{H}_2$	$\Delta G = 8.82$
${}^1\text{Nb}_9^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_6^+ + {}^2\text{Nb}_3\text{B}_2 + 3\text{H}_2$	$\Delta G = 8.04$
${}^2\text{Nb}_{10}^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_6^+ + {}^1\text{Nb}_4\text{B}_2 + 3\text{H}_2$	$\Delta G = 8.66$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_7^+ + {}^2\text{NbB}_2 + 3\text{H}_2$	$\Delta G = 7.90$
${}^1\text{Nb}_9^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_7^+ + {}^1\text{Nb}_2\text{B}_2 + 3\text{H}_2$	$\Delta G = 8.06$
${}^2\text{Nb}_{10}^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_7^+ + {}^2\text{Nb}_3\text{B}_2 + 3\text{H}_2$	$\Delta G = 7.56$
${}^1\text{Nb}_9^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_8^+ + {}^2\text{NbB}_2 + 3\text{H}_2$	$\Delta G = 7.67$
${}^2\text{Nb}_{10}^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_8^+ + {}^1\text{Nb}_2\text{B}_2 + 3\text{H}_2$	$\Delta G = 8.11$
${}^2\text{Nb}_{10}^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_9^+ + {}^2\text{NbB}_2 + 3\text{H}_2$	$\Delta G = 7.95$

Table S7. Thermodynamics energy changes (ΔG) for $\text{Nb}_n^+ + \text{B}_2\text{H}_6 \rightarrow \text{Nb}_x\text{B}^+ + \text{Nb}_{n-x}\text{B} + 3\text{H}_2$. The pre-superscripts refer to spin multiplicities. Energies are given in eV.

Thermodynamics energy changes (eV)	
${}^2\text{Nb}_2^+ + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^7\text{NbB} + 3\text{H}_2$	$\Delta G = 10.00$
${}^3\text{Nb}_3^+ + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^2\text{Nb}_2\text{B} + 3\text{H}_2$	$\Delta G = 8.73$
${}^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^1\text{Nb}_3\text{B} + 3\text{H}_2$	$\Delta G = 9.12$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^2\text{Nb}_4\text{B} + 3\text{H}_2$	$\Delta G = 8.75$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^3\text{Nb}_5\text{B} + 3\text{H}_2$	$\Delta G = 8.53$
${}^3\text{Nb}_3^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^7\text{NbB} + 3\text{H}_2$	$\Delta G = 8.22$
${}^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^2\text{Nb}_2\text{B} + 3\text{H}_2$	$\Delta G = 8.15$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^1\text{Nb}_3\text{B} + 3\text{H}_2$	$\Delta G = 8.21$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^2\text{Nb}_4\text{B} + 3\text{H}_2$	$\Delta G = 7.83$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^3\text{Nb}_5\text{B} + 3\text{H}_2$	$\Delta G = 8.56$
${}^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^7\text{NbB} + 3\text{H}_2$	$\Delta G = 7.81$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^2\text{Nb}_2\text{B} + 3\text{H}_2$	$\Delta G = 7.41$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^1\text{Nb}_3\text{B} + 3\text{H}_2$	$\Delta G = 7.46$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^2\text{Nb}_4\text{B} + 3\text{H}_2$	$\Delta G = 8.03$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^3\text{Nb}_5\text{B} + 3\text{H}_2$	$\Delta G = 8.24$
${}^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^7\text{NbB} + 3\text{H}_2$	$\Delta G = 7.30$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^2\text{Nb}_2\text{B} + 3\text{H}_2$	$\Delta G = 6.89$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^1\text{Nb}_3\text{B} + 3\text{H}_2$	$\Delta G = 7.89$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^2\text{Nb}_4\text{B} + 3\text{H}_2$	$\Delta G = 7.94$
${}^1\text{Nb}_9^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^3\text{Nb}_5\text{B} + 3\text{H}_2$	$\Delta G = 7.92$
${}^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^7\text{NbB} + 3\text{H}_2$	$\Delta G = 7.24$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^2\text{Nb}_2\text{B} + 3\text{H}_2$	$\Delta G = 7.78$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^1\text{Nb}_3\text{B} + 3\text{H}_2$	$\Delta G = 8.25$
${}^1\text{Nb}_9^+ + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^2\text{Nb}_4\text{B} + 3\text{H}_2$	$\Delta G = 8.07$
${}^2\text{Nb}_{10}^+ + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^3\text{Nb}_5\text{B} + 3\text{H}_2$	$\Delta G = 8.33$
${}^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_6\text{B}^+ + {}^7\text{NbB} + 3\text{H}_2$	$\Delta G = 6.92$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_6\text{B}^+ + {}^2\text{Nb}_2\text{B} + 3\text{H}_2$	$\Delta G = 6.93$
${}^1\text{Nb}_9^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_6\text{B}^+ + {}^1\text{Nb}_3\text{B} + 3\text{H}_2$	$\Delta G = 7.18$
${}^2\text{Nb}_{10}^+ + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_6\text{B}^+ + {}^2\text{Nb}_4\text{B} + 3\text{H}_2$	$\Delta G = 7.28$
${}^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_7\text{B}^+ + {}^7\text{NbB} + 3\text{H}_2$	$\Delta G = 8.04$
${}^1\text{Nb}_9^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_7\text{B}^+ + {}^2\text{Nb}_2\text{B} + 3\text{H}_2$	$\Delta G = 7.82$
${}^2\text{Nb}_{10}^+ + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_7\text{B}^+ + {}^1\text{Nb}_3\text{B} + 3\text{H}_2$	$\Delta G = 8.35$
${}^1\text{Nb}_9^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_8\text{B}^+ + {}^7\text{NbB} + 3\text{H}_2$	$\Delta G = 7.53$
${}^2\text{Nb}_{10}^+ + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_8\text{B}^+ + {}^2\text{Nb}_2\text{B} + 3\text{H}_2$	$\Delta G = 7.60$

Table S8. Thermodynamics energy changes (ΔG) for $\text{Nb}_n^+ + \text{Nb}_m^+ + \text{B}_2\text{H}_6 \rightarrow \text{Nb}_n\text{B}^+ + \text{Nb}_m\text{B}^+ + 3\text{H}_2$. The pre-superscripts refer to spin multiplicities. Energies are given in eV.

Thermodynamics energy changes (eV)	
$2\ ^5\text{Nb}^+ + \text{B}_2\text{H}_6 \rightarrow 2\ ^6\text{NbB}^+ + 3\text{H}_2$	$\Delta G = 4.79$
$^5\text{Nb}^+ + ^2\text{Nb}_2^+ + \text{B}_2\text{H}_6 \rightarrow ^6\text{NbB}^+ + ^3\text{Nb}_2\text{B}^+ + 3\text{H}_2$	$\Delta G = 3.87$
$^5\text{Nb}^+ + ^3\text{Nb}_3^+ + \text{B}_2\text{H}_6 \rightarrow ^6\text{NbB}^+ + ^2\text{Nb}_3\text{B}^+ + 3\text{H}_2$	$\Delta G = 2.27$
$^5\text{Nb}^+ + ^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow ^6\text{NbB}^+ + ^1\text{Nb}_4\text{B}^+ + 3\text{H}_2$	$\Delta G = 2.08$
$^5\text{Nb}^+ + ^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow ^6\text{NbB}^+ + ^4\text{Nb}_5\text{B}^+ + 3\text{H}_2$	$\Delta G = 2.03$
$^5\text{Nb}^+ + ^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow ^6\text{NbB}^+ + ^3\text{Nb}_6\text{B}^+ + 3\text{H}_2$	$\Delta G = 0.76$
$^5\text{Nb}^+ + ^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow ^6\text{NbB}^+ + ^2\text{Nb}_7\text{B}^+ + 3\text{H}_2$	$\Delta G = 2.41$
$^5\text{Nb}^+ + ^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow ^6\text{NbB}^+ + ^1\text{Nb}_8\text{B}^+ + 3\text{H}_2$	$\Delta G = 2.13$
$2\ ^2\text{Nb}_2^+ + \text{B}_2\text{H}_6 \rightarrow 2\ ^3\text{Nb}_2\text{B}^+ + 3\text{H}_2$	$\Delta G = 2.96$
$^2\text{Nb}_2^+ + ^3\text{Nb}_3^+ + \text{B}_2\text{H}_6 \rightarrow ^3\text{Nb}_2\text{B}^+ + ^2\text{Nb}_3\text{B}^+ + 3\text{H}_2$	$\Delta G = 1.35$
$^2\text{Nb}_2^+ + ^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow ^3\text{Nb}_2\text{B}^+ + ^1\text{Nb}_4\text{B}^+ + 3\text{H}_2$	$\Delta G = 1.17$
$^2\text{Nb}_2^+ + ^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow ^3\text{Nb}_2\text{B}^+ + ^4\text{Nb}_5\text{B}^+ + 3\text{H}_2$	$\Delta G = 1.12$
$^2\text{Nb}_2^+ + ^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow ^3\text{Nb}_2\text{B}^+ + ^3\text{Nb}_6\text{B}^+ + 3\text{H}_2$	$\Delta G = -0.15$
$^2\text{Nb}_2^+ + ^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow ^3\text{Nb}_2\text{B}^+ + ^2\text{Nb}_7\text{B}^+ + 3\text{H}_2$	$\Delta G = 1.49$
$^2\text{Nb}_2^+ + ^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow ^3\text{Nb}_2\text{B}^+ + ^1\text{Nb}_8\text{B}^+ + 3\text{H}_2$	$\Delta G = 1.21$
$2\ ^3\text{Nb}_3^+ + \text{B}_2\text{H}_6 \rightarrow 2\ ^2\text{Nb}_3\text{B}^+ + 3\text{H}_2$	$\Delta G = -0.25$
$^3\text{Nb}_3^+ + ^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_3\text{B}^+ + ^1\text{Nb}_4\text{B}^+ + 3\text{H}_2$	$\Delta G = -0.44$
$^3\text{Nb}_3^+ + ^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_3\text{B}^+ + ^4\text{Nb}_5\text{B}^+ + 3\text{H}_2$	$\Delta G = -0.49$
$^3\text{Nb}_3^+ + ^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_3\text{B}^+ + ^3\text{Nb}_6\text{B}^+ + 3\text{H}_2$	$\Delta G = -1.76$
$^3\text{Nb}_3^+ + ^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_3\text{B}^+ + ^2\text{Nb}_7\text{B}^+ + 3\text{H}_2$	$\Delta G = -0.11$
$^3\text{Nb}_3^+ + ^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_3\text{B}^+ + ^1\text{Nb}_8\text{B}^+ + 3\text{H}_2$	$\Delta G = -0.39$
$2\ ^2\text{Nb}_4^+ + \text{B}_2\text{H}_6 \rightarrow 2\ ^1\text{Nb}_4\text{B}^+ + 3\text{H}_2$	$\Delta G = -0.62$
$^2\text{Nb}_4^+ + ^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow ^1\text{Nb}_4\text{B}^+ + ^4\text{Nb}_5\text{B}^+ + 3\text{H}_2$	$\Delta G = -0.67$
$^2\text{Nb}_4^+ + ^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow ^1\text{Nb}_4\text{B}^+ + ^3\text{Nb}_6\text{B}^+ + 3\text{H}_2$	$\Delta G = -1.94$
$^2\text{Nb}_4^+ + ^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow ^1\text{Nb}_4\text{B}^+ + ^2\text{Nb}_7\text{B}^+ + 3\text{H}_2$	$\Delta G = -0.30$
$^2\text{Nb}_4^+ + ^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow ^1\text{Nb}_4\text{B}^+ + ^1\text{Nb}_8\text{B}^+ + 3\text{H}_2$	$\Delta G = -0.57$
$2\ ^3\text{Nb}_5^+ + \text{B}_2\text{H}_6 \rightarrow 2\ ^4\text{Nb}_5\text{B}^+ + 3\text{H}_2$	$\Delta G = -0.72$
$^3\text{Nb}_5^+ + ^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow ^4\text{Nb}_5\text{B}^+ + ^3\text{Nb}_6\text{B}^+ + 3\text{H}_2$	$\Delta G = -1.99$
$^3\text{Nb}_5^+ + ^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow ^4\text{Nb}_5\text{B}^+ + ^2\text{Nb}_7\text{B}^+ + 3\text{H}_2$	$\Delta G = -0.35$
$^3\text{Nb}_5^+ + ^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow ^4\text{Nb}_5\text{B}^+ + ^1\text{Nb}_8\text{B}^+ + 3\text{H}_2$	$\Delta G = -0.62$
$2\ ^2\text{Nb}_6^+ + \text{B}_2\text{H}_6 \rightarrow 2\ ^3\text{Nb}_6\text{B}^+ + 3\text{H}_2$	$\Delta G = -3.26$
$^2\text{Nb}_6^+ + ^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow ^3\text{Nb}_6\text{B}^+ + ^2\text{Nb}_7\text{B}^+ + 3\text{H}_2$	$\Delta G = -1.62$
$^2\text{Nb}_6^+ + ^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow ^3\text{Nb}_6\text{B}^+ + ^1\text{Nb}_8\text{B}^+ + 3\text{H}_2$	$\Delta G = -1.90$
$2\ ^3\text{Nb}_7^+ + \text{B}_2\text{H}_6 \rightarrow 2\ ^2\text{Nb}_7\text{B}^+ + 3\text{H}_2$	$\Delta G = 0.03$
$^3\text{Nb}_7^+ + ^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_7\text{B}^+ + ^1\text{Nb}_8\text{B}^+ + 3\text{H}_2$	$\Delta G = -0.25$
$2\ ^2\text{Nb}_8^+ + \text{B}_2\text{H}_6 \rightarrow 2\ ^1\text{Nb}_8\text{B}^+ + 3\text{H}_2$	$\Delta G = -0.53$

Table S9. Thermodynamics energy changes (ΔG) for $\text{Nb}_n^+ + \text{Nb}_m + \text{B}_2\text{H}_6 \rightarrow \text{Nb}_n\text{B}^+ + \text{Nb}_m\text{B} + 3\text{H}_2$. The pre-superscripts refer to spin multiplicities. Energies are given in eV.

Thermodynamics energy changes (eV)	
${}^5\text{Nb}^+ + {}^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^7\text{NbB} + 3\text{H}_2$	$\Delta G = 4.62$
${}^5\text{Nb}^+ + {}^3\text{Nb}_2 + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^2\text{Nb}_2\text{B} + 3\text{H}_2$	$\Delta G = 3.77$
${}^5\text{Nb}^+ + {}^2\text{Nb}_3 + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^1\text{Nb}_3\text{B} + 3\text{H}_2$	$\Delta G = 2.61$
${}^5\text{Nb}^+ + {}^1\text{Nb}_4 + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^2\text{Nb}_4\text{B} + 3\text{H}_2$	$\Delta G = 2.26$
${}^5\text{Nb}^+ + {}^2\text{Nb}_5 + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^3\text{Nb}_5\text{B} + 3\text{H}_2$	$\Delta G = 1.77$
${}^5\text{Nb}^+ + {}^3\text{Nb}_6 + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^2\text{Nb}_6\text{B} + 3\text{H}_2$	$\Delta G = 0.86$
${}^5\text{Nb}^+ + {}^2\text{Nb}_7 + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^1\text{Nb}_7\text{B} + 3\text{H}_2$	$\Delta G = 2.37$
${}^5\text{Nb}^+ + {}^1\text{Nb}_8 + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^2\text{Nb}_8\text{B} + 3\text{H}_2$	$\Delta G = 2.35$
${}^2\text{Nb}_2^+ + {}^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^7\text{NbB} + 3\text{H}_2$	$\Delta G = 3.70$
${}^2\text{Nb}_2^+ + {}^3\text{Nb}_2 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^2\text{Nb}_2\text{B} + 3\text{H}_2$	$\Delta G = 2.86$
${}^2\text{Nb}_2^+ + {}^2\text{Nb}_3 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^1\text{Nb}_3\text{B} + 3\text{H}_2$	$\Delta G = 1.69$
${}^2\text{Nb}_2^+ + {}^1\text{Nb}_4 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^2\text{Nb}_4\text{B} + 3\text{H}_2$	$\Delta G = 1.34$
${}^2\text{Nb}_2^+ + {}^2\text{Nb}_5 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^3\text{Nb}_5\text{B} + 3\text{H}_2$	$\Delta G = 0.86$
${}^2\text{Nb}_2^+ + {}^3\text{Nb}_6 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^2\text{Nb}_6\text{B} + 3\text{H}_2$	$\Delta G = -0.05$
${}^2\text{Nb}_2^+ + {}^2\text{Nb}_7 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^1\text{Nb}_7\text{B} + 3\text{H}_2$	$\Delta G = 1.45$
${}^2\text{Nb}_2^+ + {}^1\text{Nb}_8 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^2\text{Nb}_8\text{B} + 3\text{H}_2$	$\Delta G = 1.44$
${}^3\text{Nb}_3^+ + {}^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^7\text{NbB} + 3\text{H}_2$	$\Delta G = 2.10$
${}^3\text{Nb}_3^+ + {}^3\text{Nb}_2 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^2\text{Nb}_2\text{B} + 3\text{H}_2$	$\Delta G = 1.25$
${}^3\text{Nb}_3^+ + {}^2\text{Nb}_3 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^1\text{Nb}_3\text{B} + 3\text{H}_2$	$\Delta G = 0.09$
${}^3\text{Nb}_3^+ + {}^1\text{Nb}_4 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^2\text{Nb}_4\text{B} + 3\text{H}_2$	$\Delta G = -0.26$
${}^3\text{Nb}_3^+ + {}^2\text{Nb}_5 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^3\text{Nb}_5\text{B} + 3\text{H}_2$	$\Delta G = -0.75$
${}^3\text{Nb}_3^+ + {}^3\text{Nb}_6 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^2\text{Nb}_6\text{B} + 3\text{H}_2$	$\Delta G = -1.66$
${}^3\text{Nb}_3^+ + {}^2\text{Nb}_7 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^1\text{Nb}_7\text{B} + 3\text{H}_2$	$\Delta G = -0.15$
${}^3\text{Nb}_3^+ + {}^1\text{Nb}_8 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^2\text{Nb}_8\text{B} + 3\text{H}_2$	$\Delta G = -0.17$
${}^2\text{Nb}_4^+ + {}^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^7\text{NbB} + 3\text{H}_2$	$\Delta G = 1.92$
${}^2\text{Nb}_4^+ + {}^3\text{Nb}_2 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^2\text{Nb}_2\text{B} + 3\text{H}_2$	$\Delta G = 1.07$
${}^2\text{Nb}_4^+ + {}^2\text{Nb}_3 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^1\text{Nb}_3\text{B} + 3\text{H}_2$	$\Delta G = -0.10$
${}^2\text{Nb}_4^+ + {}^1\text{Nb}_4 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^2\text{Nb}_4\text{B} + 3\text{H}_2$	$\Delta G = -0.45$
${}^2\text{Nb}_4^+ + {}^2\text{Nb}_5 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^3\text{Nb}_5\text{B} + 3\text{H}_2$	$\Delta G = -0.93$
${}^2\text{Nb}_4^+ + {}^3\text{Nb}_6 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^2\text{Nb}_6\text{B} + 3\text{H}_2$	$\Delta G = -1.84$
${}^2\text{Nb}_4^+ + {}^2\text{Nb}_7 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^1\text{Nb}_7\text{B} + 3\text{H}_2$	$\Delta G = -0.34$
${}^2\text{Nb}_4^+ + {}^1\text{Nb}_8 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^2\text{Nb}_8\text{B} + 3\text{H}_2$	$\Delta G = -0.35$
${}^3\text{Nb}_5^+ + {}^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^7\text{NbB} + 3\text{H}_2$	$\Delta G = 1.87$
${}^3\text{Nb}_5^+ + {}^3\text{Nb}_2 + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^2\text{Nb}_2\text{B} + 3\text{H}_2$	$\Delta G = 1.02$
${}^3\text{Nb}_5^+ + {}^2\text{Nb}_3 + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^1\text{Nb}_3\text{B} + 3\text{H}_2$	$\Delta G = -0.15$
${}^3\text{Nb}_5^+ + {}^1\text{Nb}_4 + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^2\text{Nb}_4\text{B} + 3\text{H}_2$	$\Delta G = -0.50$
${}^3\text{Nb}_5^+ + {}^2\text{Nb}_5 + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^3\text{Nb}_5\text{B} + 3\text{H}_2$	$\Delta G = -0.98$
${}^3\text{Nb}_5^+ + {}^3\text{Nb}_6 + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^2\text{Nb}_6\text{B} + 3\text{H}_2$	$\Delta G = -1.89$
${}^3\text{Nb}_5^+ + {}^2\text{Nb}_7 + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^1\text{Nb}_7\text{B} + 3\text{H}_2$	$\Delta G = -0.39$
${}^3\text{Nb}_5^+ + {}^1\text{Nb}_8 + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^2\text{Nb}_8\text{B} + 3\text{H}_2$	$\Delta G = -0.40$
${}^2\text{Nb}_6^+ + {}^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_6\text{B}^+ + {}^7\text{NbB} + 3\text{H}_2$	$\Delta G = 0.59$

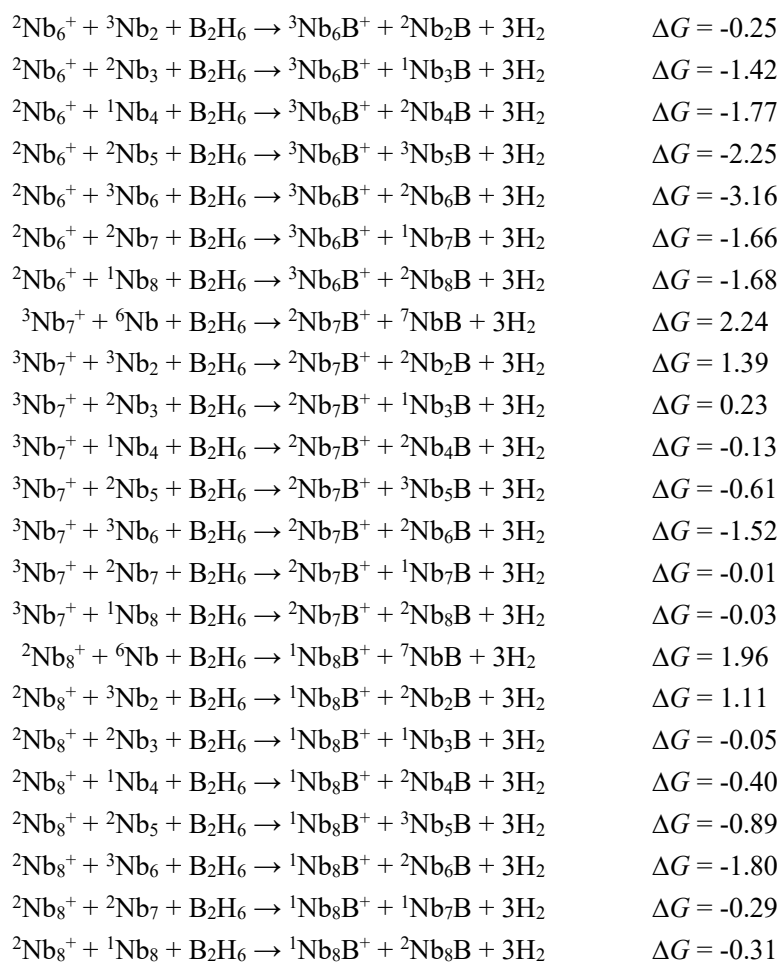


Table S11. Thermodynamics energy changes (ΔG) for $\text{Nb}_n^+ + \text{Nb}_m + \text{B}_2\text{H}_6 \rightarrow \text{Nb}_m\text{B}_2^+ + \text{Nb}_n + 3 \text{H}_2$. The pre-superscripts refer to spin multiplicities. Energies are given in eV.

Thermodynamics energy changes (eV)	
$^5\text{Nb}^+ + ^3\text{Nb}_2 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_2\text{B}_2^+ + ^6\text{Nb} + 3 \text{H}_2$	$\Delta G = 1.20$
$^5\text{Nb}^+ + ^2\text{Nb}_3 + \text{B}_2\text{H}_6 \rightarrow ^3\text{Nb}_3\text{B}_2^+ + ^6\text{Nb} + 3 \text{H}_2$	$\Delta G = -1.00$
$^5\text{Nb}^+ + ^1\text{Nb}_4 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_4\text{B}_2^+ + ^6\text{Nb} + 3 \text{H}_2$	$\Delta G = -1.71$
$^5\text{Nb}^+ + ^2\text{Nb}_5 + \text{B}_2\text{H}_6 \rightarrow ^1\text{Nb}_5\text{B}_2^+ + ^6\text{Nb} + 3 \text{H}_2$	$\Delta G = -2.86$
$^5\text{Nb}^+ + ^3\text{Nb}_6 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_6\text{B}_2^+ + ^6\text{Nb} + 3 \text{H}_2$	$\Delta G = -2.91$
$^5\text{Nb}^+ + ^2\text{Nb}_7 + \text{B}_2\text{H}_6 \rightarrow ^1\text{Nb}_7\text{B}_2^+ + ^6\text{Nb} + 3 \text{H}_2$	$\Delta G = -2.13$
$^5\text{Nb}^+ + ^1\text{Nb}_8 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_8\text{B}_2^+ + ^6\text{Nb} + 3 \text{H}_2$	$\Delta G = -2.03$
$^2\text{Nb}_2^+ + ^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow ^1\text{NbB}_2^+ + ^3\text{Nb}_2 + 3 \text{H}_2$	$\Delta G = 3.39$
$^2\text{Nb}_2^+ + ^2\text{Nb}_3 + \text{B}_2\text{H}_6 \rightarrow ^3\text{Nb}_3\text{B}_2^+ + ^3\text{Nb}_2 + 3 \text{H}_2$	$\Delta G = -0.56$
$^2\text{Nb}_2^+ + ^1\text{Nb}_4 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_4\text{B}_2^+ + ^3\text{Nb}_2 + 3 \text{H}_2$	$\Delta G = -1.27$
$^2\text{Nb}_2^+ + ^2\text{Nb}_5 + \text{B}_2\text{H}_6 \rightarrow ^1\text{Nb}_5\text{B}_2^+ + ^3\text{Nb}_2 + 3 \text{H}_2$	$\Delta G = -2.41$
$^2\text{Nb}_2^+ + ^3\text{Nb}_6 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_6\text{B}_2^+ + ^3\text{Nb}_2 + 3 \text{H}_2$	$\Delta G = -2.47$
$^2\text{Nb}_2^+ + ^2\text{Nb}_7 + \text{B}_2\text{H}_6 \rightarrow ^1\text{Nb}_7\text{B}_2^+ + ^3\text{Nb}_2 + 3 \text{H}_2$	$\Delta G = -1.69$
$^2\text{Nb}_2^+ + ^1\text{Nb}_8 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_8\text{B}_2^+ + ^3\text{Nb}_2 + 3 \text{H}_2$	$\Delta G = -1.59$
$^3\text{Nb}_3^+ + ^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow ^1\text{NbB}_2^+ + ^2\text{Nb}_3 + 3 \text{H}_2$	$\Delta G = 3.75$
$^3\text{Nb}_3^+ + ^3\text{Nb}_2 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_2\text{B}_2^+ + ^2\text{Nb}_3 + 3 \text{H}_2$	$\Delta G = 2.00$
$^3\text{Nb}_3^+ + ^1\text{Nb}_4 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_4\text{B}_2^+ + ^2\text{Nb}_3 + 3 \text{H}_2$	$\Delta G = -0.91$
$^3\text{Nb}_3^+ + ^2\text{Nb}_5 + \text{B}_2\text{H}_6 \rightarrow ^1\text{Nb}_5\text{B}_2^+ + ^2\text{Nb}_3 + 3 \text{H}_2$	$\Delta G = -2.06$
$^3\text{Nb}_3^+ + ^3\text{Nb}_6 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_6\text{B}_2^+ + ^2\text{Nb}_3 + 3 \text{H}_2$	$\Delta G = -2.11$
$^3\text{Nb}_3^+ + ^2\text{Nb}_7 + \text{B}_2\text{H}_6 \rightarrow ^1\text{Nb}_7\text{B}_2^+ + ^2\text{Nb}_3 + 3 \text{H}_2$	$\Delta G = -1.33$
$^3\text{Nb}_3^+ + ^1\text{Nb}_8 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_8\text{B}_2^+ + ^2\text{Nb}_3 + 3 \text{H}_2$	$\Delta G = -1.23$
$^2\text{Nb}_4^+ + ^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow ^1\text{NbB}_2^+ + ^1\text{Nb}_4 + 3 \text{H}_2$	$\Delta G = 4.05$
$^2\text{Nb}_4^+ + ^3\text{Nb}_2 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_2\text{B}_2^+ + ^1\text{Nb}_4 + 3 \text{H}_2$	$\Delta G = 2.31$
$^2\text{Nb}_4^+ + ^2\text{Nb}_3 + \text{B}_2\text{H}_6 \rightarrow ^3\text{Nb}_3\text{B}_2^+ + ^1\text{Nb}_4 + 3 \text{H}_2$	$\Delta G = 0.11$
$^2\text{Nb}_4^+ + ^2\text{Nb}_5 + \text{B}_2\text{H}_6 \rightarrow ^1\text{Nb}_5\text{B}_2^+ + ^1\text{Nb}_4 + 3 \text{H}_2$	$\Delta G = -1.75$
$^2\text{Nb}_4^+ + ^3\text{Nb}_6 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_6\text{B}_2^+ + ^1\text{Nb}_4 + 3 \text{H}_2$	$\Delta G = -1.80$
$^2\text{Nb}_4^+ + ^2\text{Nb}_7 + \text{B}_2\text{H}_6 \rightarrow ^1\text{Nb}_7\text{B}_2^+ + ^1\text{Nb}_4 + 3 \text{H}_2$	$\Delta G = -1.02$
$^2\text{Nb}_4^+ + ^1\text{Nb}_8 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_8\text{B}_2^+ + ^1\text{Nb}_4 + 3 \text{H}_2$	$\Delta G = -0.92$
$^3\text{Nb}_5^+ + ^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow ^1\text{NbB}_2^+ + ^2\text{Nb}_5 + 3 \text{H}_2$	$\Delta G = 4.34$
$^3\text{Nb}_5^+ + ^3\text{Nb}_2 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_2\text{B}_2^+ + ^2\text{Nb}_5 + 3 \text{H}_2$	$\Delta G = 2.59$
$^3\text{Nb}_5^+ + ^2\text{Nb}_3 + \text{B}_2\text{H}_6 \rightarrow ^3\text{Nb}_3\text{B}_2^+ + ^2\text{Nb}_5 + 3 \text{H}_2$	$\Delta G = 0.39$
$^3\text{Nb}_5^+ + ^1\text{Nb}_4 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_4\text{B}_2^+ + ^2\text{Nb}_5 + 3 \text{H}_2$	$\Delta G = -0.32$
$^3\text{Nb}_5^+ + ^3\text{Nb}_6 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_6\text{B}_2^+ + ^2\text{Nb}_5 + 3 \text{H}_2$	$\Delta G = -1.52$
$^3\text{Nb}_5^+ + ^2\text{Nb}_7 + \text{B}_2\text{H}_6 \rightarrow ^1\text{Nb}_7\text{B}_2^+ + ^2\text{Nb}_5 + 3 \text{H}_2$	$\Delta G = -0.74$
$^3\text{Nb}_5^+ + ^1\text{Nb}_8 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_8\text{B}_2^+ + ^2\text{Nb}_5 + 3 \text{H}_2$	$\Delta G = -0.64$
$^2\text{Nb}_6^+ + ^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow ^1\text{NbB}_2^+ + ^3\text{Nb}_6 + 3 \text{H}_2$	$\Delta G = 4.34$
$^2\text{Nb}_6^+ + ^3\text{Nb}_2 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_2\text{B}_2^+ + ^3\text{Nb}_6 + 3 \text{H}_2$	$\Delta G = 2.60$
$^2\text{Nb}_6^+ + ^2\text{Nb}_3 + \text{B}_2\text{H}_6 \rightarrow ^3\text{Nb}_3\text{B}_2^+ + ^3\text{Nb}_6 + 3 \text{H}_2$	$\Delta G = 0.39$
$^2\text{Nb}_6^+ + ^1\text{Nb}_4 + \text{B}_2\text{H}_6 \rightarrow ^2\text{Nb}_4\text{B}_2^+ + ^3\text{Nb}_6 + 3 \text{H}_2$	$\Delta G = -0.32$
$^2\text{Nb}_6^+ + ^2\text{Nb}_5 + \text{B}_2\text{H}_6 \rightarrow ^1\text{Nb}_5\text{B}_2^+ + ^3\text{Nb}_6 + 3 \text{H}_2$	$\Delta G = -1.46$
$^2\text{Nb}_6^+ + ^2\text{Nb}_7 + \text{B}_2\text{H}_6 \rightarrow ^1\text{Nb}_7\text{B}_2^+ + ^3\text{Nb}_6 + 3 \text{H}_2$	$\Delta G = -0.74$

${}^2\text{Nb}_6^+ + {}^1\text{Nb}_8 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_8\text{B}_2^+ + {}^3\text{Nb}_6 + 3 \text{H}_2$	$\Delta G = -0.64$
${}^3\text{Nb}_7^+ + {}^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow {}^1\text{NbB}_2^+ + {}^2\text{Nb}_7 + 3 \text{H}_2$	$\Delta G = 4.46$
${}^3\text{Nb}_7^+ + {}^3\text{Nb}_2 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_2\text{B}_2^+ + {}^2\text{Nb}_7 + 3 \text{H}_2$	$\Delta G = 2.72$
${}^3\text{Nb}_7^+ + {}^2\text{Nb}_3 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_3\text{B}_2^+ + {}^2\text{Nb}_7 + 3 \text{H}_2$	$\Delta G = 0.52$
${}^3\text{Nb}_7^+ + {}^1\text{Nb}_4 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_4\text{B}_2^+ + {}^2\text{Nb}_7 + 3 \text{H}_2$	$\Delta G = -0.19$
${}^3\text{Nb}_7^+ + {}^2\text{Nb}_5 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_5\text{B}_2^+ + {}^2\text{Nb}_7 + 3 \text{H}_2$	$\Delta G = -1.34$
${}^3\text{Nb}_7^+ + {}^3\text{Nb}_6 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_6\text{B}_2^+ + {}^2\text{Nb}_7 + 3 \text{H}_2$	$\Delta G = -1.39$
${}^3\text{Nb}_7^+ + {}^1\text{Nb}_8 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_8\text{B}_2^+ + {}^2\text{Nb}_7 + 3 \text{H}_2$	$\Delta G = -0.51$
${}^2\text{Nb}_8^+ + {}^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow {}^1\text{NbB}_2^+ + {}^1\text{Nb}_8 + 3 \text{H}_2$	$\Delta G = 4.26$
${}^2\text{Nb}_8^+ + {}^3\text{Nb}_2 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_2\text{B}_2^+ + {}^1\text{Nb}_8 + 3 \text{H}_2$	$\Delta G = 2.52$
${}^2\text{Nb}_8^+ + {}^2\text{Nb}_3 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_3\text{B}_2^+ + {}^1\text{Nb}_8 + 3 \text{H}_2$	$\Delta G = 0.31$
${}^2\text{Nb}_8^+ + {}^1\text{Nb}_4 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_4\text{B}_2^+ + {}^1\text{Nb}_8 + 3 \text{H}_2$	$\Delta G = -0.39$
${}^2\text{Nb}_8^+ + {}^2\text{Nb}_5 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_5\text{B}_2^+ + {}^1\text{Nb}_8 + 3 \text{H}_2$	$\Delta G = -1.54$
${}^2\text{Nb}_8^+ + {}^3\text{Nb}_6 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_6\text{B}_2^+ + {}^1\text{Nb}_8 + 3 \text{H}_2$	$\Delta G = -1.59$
${}^2\text{Nb}_8^+ + {}^2\text{Nb}_7 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_7\text{B}_2^+ + {}^1\text{Nb}_8 + 3 \text{H}_2$	$\Delta G = -0.81$

Table S12. Thermodynamics energy changes (ΔG) for $\text{Nb}_n^+ + \text{Nb}_m + \text{B}_2\text{H}_6 \rightarrow \text{Nb}_m\text{B}_2^+ + \text{Nb}_n + 3 \text{H}_2$. The pre-superscripts refer to spin multiplicities. Energies are given in eV.

Thermodynamics energy changes (eV)	
${}^5\text{Nb}^+ + {}^3\text{Nb}_2 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^7\text{NbB} + 3 \text{H}_2$	$\Delta G = 3.26$
${}^5\text{Nb}^+ + {}^2\text{Nb}_3 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^7\text{NbB} + 3 \text{H}_2$	$\Delta G = 1.30$
${}^5\text{Nb}^+ + {}^1\text{Nb}_4 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^7\text{NbB} + 3 \text{H}_2$	$\Delta G = 0.81$
${}^5\text{Nb}^+ + {}^2\text{Nb}_5 + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^7\text{NbB} + 3 \text{H}_2$	$\Delta G = 0.48$
${}^5\text{Nb}^+ + {}^3\text{Nb}_6 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_6\text{B}^+ + {}^7\text{NbB} + 3 \text{H}_2$	$\Delta G = -0.80$
${}^5\text{Nb}^+ + {}^2\text{Nb}_7 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_7\text{B}^+ + {}^7\text{NbB} + 3 \text{H}_2$	$\Delta G = 0.72$
${}^5\text{Nb}^+ + {}^1\text{Nb}_8 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_8\text{B}^+ + {}^7\text{NbB} + 3 \text{H}_2$	$\Delta G = 0.65$
${}^2\text{Nb}_2^+ + {}^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^2\text{Nb}_2\text{B} + 3 \text{H}_2$	$\Delta G = 4.21$
${}^2\text{Nb}_2^+ + {}^2\text{Nb}_3 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^2\text{Nb}_2\text{B} + 3 \text{H}_2$	$\Delta G = 0.90$
${}^2\text{Nb}_2^+ + {}^1\text{Nb}_4 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^2\text{Nb}_2\text{B} + 3 \text{H}_2$	$\Delta G = 0.40$
${}^2\text{Nb}_2^+ + {}^2\text{Nb}_5 + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^2\text{Nb}_2\text{B} + 3 \text{H}_2$	$\Delta G = 0.07$
${}^2\text{Nb}_2^+ + {}^3\text{Nb}_6 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_6\text{B}^+ + {}^2\text{Nb}_2\text{B} + 3 \text{H}_2$	$\Delta G = -1.20$
${}^2\text{Nb}_2^+ + {}^2\text{Nb}_7 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_7\text{B}^+ + {}^2\text{Nb}_2\text{B} + 3 \text{H}_2$	$\Delta G = 0.31$
${}^2\text{Nb}_2^+ + {}^1\text{Nb}_8 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_8\text{B}^+ + {}^2\text{Nb}_2\text{B} + 3 \text{H}_2$	$\Delta G = 0.24$
${}^3\text{Nb}_3^+ + {}^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^1\text{Nb}_3\text{B} + 3 \text{H}_2$	$\Delta G = 3.41$
${}^3\text{Nb}_3^+ + {}^3\text{Nb}_2 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^1\text{Nb}_3\text{B} + 3 \text{H}_2$	$\Delta G = 2.05$
${}^3\text{Nb}_3^+ + {}^1\text{Nb}_4 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^1\text{Nb}_3\text{B} + 3 \text{H}_2$	$\Delta G = -0.41$
${}^3\text{Nb}_3^+ + {}^2\text{Nb}_5 + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^1\text{Nb}_3\text{B} + 3 \text{H}_2$	$\Delta G = -0.74$
${}^3\text{Nb}_3^+ + {}^3\text{Nb}_6 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_6\text{B}^+ + {}^1\text{Nb}_3\text{B} + 3 \text{H}_2$	$\Delta G = -2.01$
${}^3\text{Nb}_3^+ + {}^2\text{Nb}_7 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_7\text{B}^+ + {}^1\text{Nb}_3\text{B} + 3 \text{H}_2$	$\Delta G = -0.49$
${}^3\text{Nb}_3^+ + {}^1\text{Nb}_8 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_8\text{B}^+ + {}^1\text{Nb}_3\text{B} + 3 \text{H}_2$	$\Delta G = -0.57$
${}^2\text{Nb}_4^+ + {}^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^2\text{Nb}_4\text{B} + 3 \text{H}_2$	$\Delta G = 3.36$
${}^2\text{Nb}_4^+ + {}^3\text{Nb}_2 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^2\text{Nb}_4\text{B} + 3 \text{H}_2$	$\Delta G = 2.01$
${}^2\text{Nb}_4^+ + {}^2\text{Nb}_3 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^2\text{Nb}_4\text{B} + 3 \text{H}_2$	$\Delta G = 0.05$
${}^2\text{Nb}_4^+ + {}^2\text{Nb}_5 + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^2\text{Nb}_4\text{B} + 3 \text{H}_2$	$\Delta G = -0.78$

${}^2\text{Nb}_4^+ + {}^3\text{Nb}_6 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_6\text{B}^+ + {}^2\text{Nb}_4\text{B} + 3 \text{H}_2$	$\Delta G = -2.05$
${}^2\text{Nb}_4^+ + {}^2\text{Nb}_7 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_7\text{B}^+ + {}^2\text{Nb}_4\text{B} + 3 \text{H}_2$	$\Delta G = -0.54$
${}^2\text{Nb}_4^+ + {}^1\text{Nb}_8 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_8\text{B}^+ + {}^2\text{Nb}_4\text{B} + 3 \text{H}_2$	$\Delta G = -0.61$
${}^3\text{Nb}_5^+ + {}^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^3\text{Nb}_5\text{B} + 3 \text{H}_2$	$\Delta G = 3.16$
${}^3\text{Nb}_5^+ + {}^3\text{Nb}_2 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^3\text{Nb}_5\text{B} + 3 \text{H}_2$	$\Delta G = 1.80$
${}^3\text{Nb}_5^+ + {}^2\text{Nb}_3 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^3\text{Nb}_5\text{B} + 3 \text{H}_2$	$\Delta G = -0.16$
${}^3\text{Nb}_5^+ + {}^1\text{Nb}_4 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^3\text{Nb}_5\text{B} + 3 \text{H}_2$	$\Delta G = -0.65$
${}^3\text{Nb}_5^+ + {}^3\text{Nb}_6 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_6\text{B}^+ + {}^3\text{Nb}_5\text{B} + 3 \text{H}_2$	$\Delta G = -2.26$
${}^3\text{Nb}_5^+ + {}^2\text{Nb}_7 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_7\text{B}^+ + {}^3\text{Nb}_5\text{B} + 3 \text{H}_2$	$\Delta G = -0.74$
${}^3\text{Nb}_5^+ + {}^1\text{Nb}_8 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_8\text{B}^+ + {}^3\text{Nb}_5\text{B} + 3 \text{H}_2$	$\Delta G = -0.81$
${}^2\text{Nb}_6^+ + {}^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^2\text{Nb}_6\text{B} + 3 \text{H}_2$	$\Delta G = 2.26$
${}^2\text{Nb}_6^+ + {}^3\text{Nb}_2 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^2\text{Nb}_6\text{B} + 3 \text{H}_2$	$\Delta G = 0.90$
${}^2\text{Nb}_6^+ + {}^2\text{Nb}_3 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^2\text{Nb}_6\text{B} + 3 \text{H}_2$	$\Delta G = -1.06$
${}^2\text{Nb}_6^+ + {}^1\text{Nb}_4 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^2\text{Nb}_6\text{B} + 3 \text{H}_2$	$\Delta G = -1.56$
${}^2\text{Nb}_6^+ + {}^2\text{Nb}_5 + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^2\text{Nb}_6\text{B} + 3 \text{H}_2$	$\Delta G = -1.89$
${}^2\text{Nb}_6^+ + {}^2\text{Nb}_7 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_7\text{B}^+ + {}^2\text{Nb}_6\text{B} + 3 \text{H}_2$	$\Delta G = -1.64$
${}^2\text{Nb}_6^+ + {}^1\text{Nb}_8 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_8\text{B}^+ + {}^2\text{Nb}_6\text{B} + 3 \text{H}_2$	$\Delta G = -1.72$
${}^3\text{Nb}_7^+ + {}^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^1\text{Nb}_7\text{B} + 3 \text{H}_2$	$\Delta G = 3.89$
${}^3\text{Nb}_7^+ + {}^3\text{Nb}_2 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^1\text{Nb}_7\text{B} + 3 \text{H}_2$	$\Delta G = 2.53$
${}^3\text{Nb}_7^+ + {}^2\text{Nb}_3 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^1\text{Nb}_7\text{B} + 3 \text{H}_2$	$\Delta G = 0.57$
${}^3\text{Nb}_7^+ + {}^1\text{Nb}_4 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^1\text{Nb}_7\text{B} + 3 \text{H}_2$	$\Delta G = 0.07$
${}^3\text{Nb}_7^+ + {}^2\text{Nb}_5 + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^1\text{Nb}_7\text{B} + 3 \text{H}_2$	$\Delta G = -0.26$
${}^3\text{Nb}_7^+ + {}^3\text{Nb}_6 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_6\text{B}^+ + {}^1\text{Nb}_7\text{B} + 3 \text{H}_2$	$\Delta G = -1.53$
${}^3\text{Nb}_7^+ + {}^1\text{Nb}_8 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_8\text{B}^+ + {}^1\text{Nb}_7\text{B} + 3 \text{H}_2$	$\Delta G = -0.09$
${}^2\text{Nb}_8^+ + {}^6\text{Nb} + \text{B}_2\text{H}_6 \rightarrow {}^6\text{NbB}^+ + {}^2\text{Nb}_8\text{B} + 3 \text{H}_2$	$\Delta G = 3.67$
${}^2\text{Nb}_8^+ + {}^3\text{Nb}_2 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_2\text{B}^+ + {}^2\text{Nb}_8\text{B} + 3 \text{H}_2$	$\Delta G = 2.31$
${}^2\text{Nb}_8^+ + {}^2\text{Nb}_3 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_3\text{B}^+ + {}^2\text{Nb}_8\text{B} + 3 \text{H}_2$	$\Delta G = 0.35$
${}^2\text{Nb}_8^+ + {}^1\text{Nb}_4 + \text{B}_2\text{H}_6 \rightarrow {}^1\text{Nb}_4\text{B}^+ + {}^2\text{Nb}_8\text{B} + 3 \text{H}_2$	$\Delta G = -0.15$
${}^2\text{Nb}_8^+ + {}^2\text{Nb}_5 + \text{B}_2\text{H}_6 \rightarrow {}^4\text{Nb}_5\text{B}^+ + {}^2\text{Nb}_8\text{B} + 3 \text{H}_2$	$\Delta G = -0.48$
${}^2\text{Nb}_8^+ + {}^3\text{Nb}_6 + \text{B}_2\text{H}_6 \rightarrow {}^3\text{Nb}_6\text{B}^+ + {}^2\text{Nb}_8\text{B} + 3 \text{H}_2$	$\Delta G = -1.75$
${}^2\text{Nb}_8^+ + {}^2\text{Nb}_7 + \text{B}_2\text{H}_6 \rightarrow {}^2\text{Nb}_7\text{B}^+ + {}^2\text{Nb}_8\text{B} + 3 \text{H}_2$	$\Delta G = -0.23$

REFERENCES

- (1) Knickelbein, M. B.; Yang, S. Photoionization Studies of Niobium Clusters: Ionization Potentials for Nb₂–Nb₇₆. *J. Chem. Phys.* **1990**, *93*, 5760-5767.