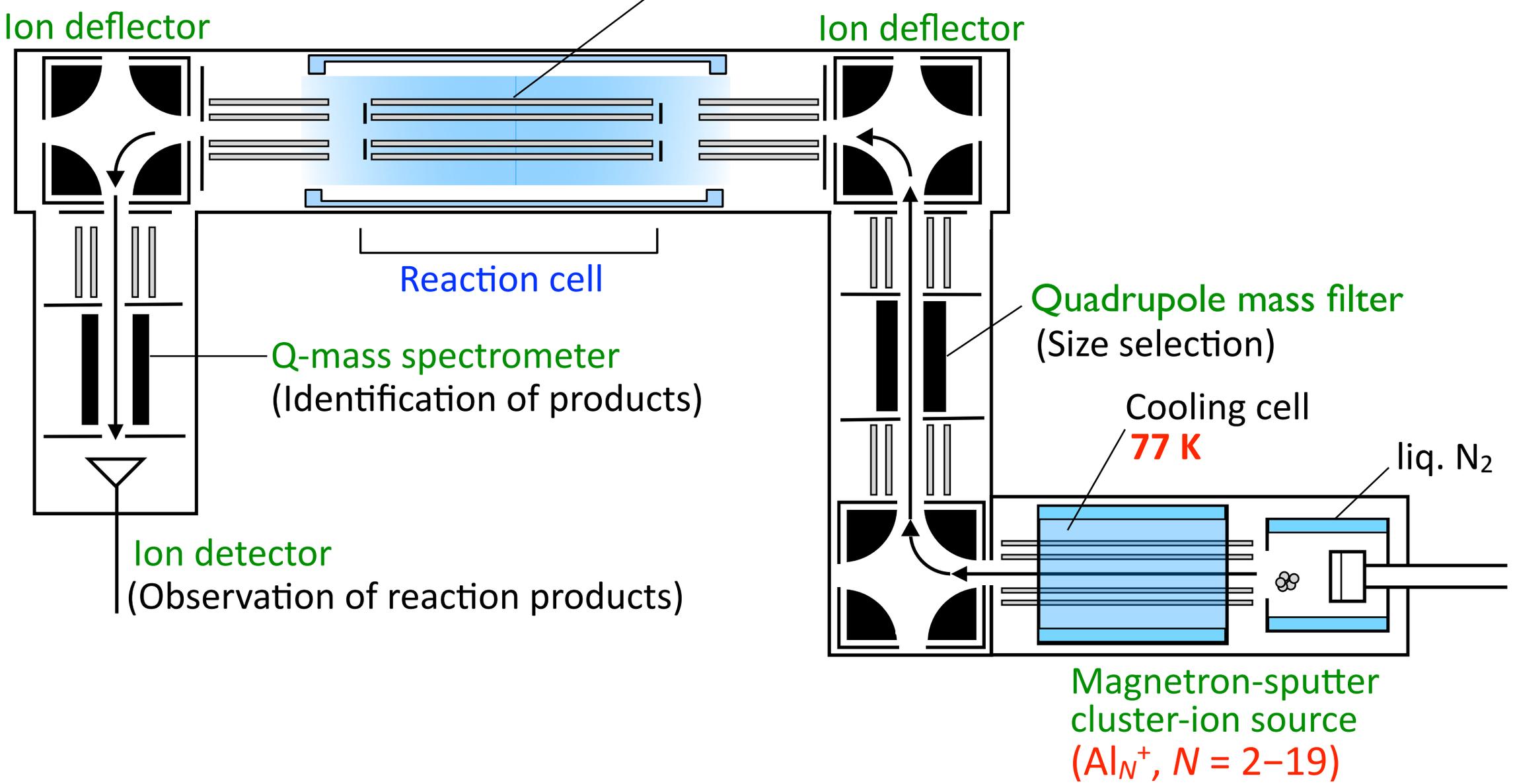
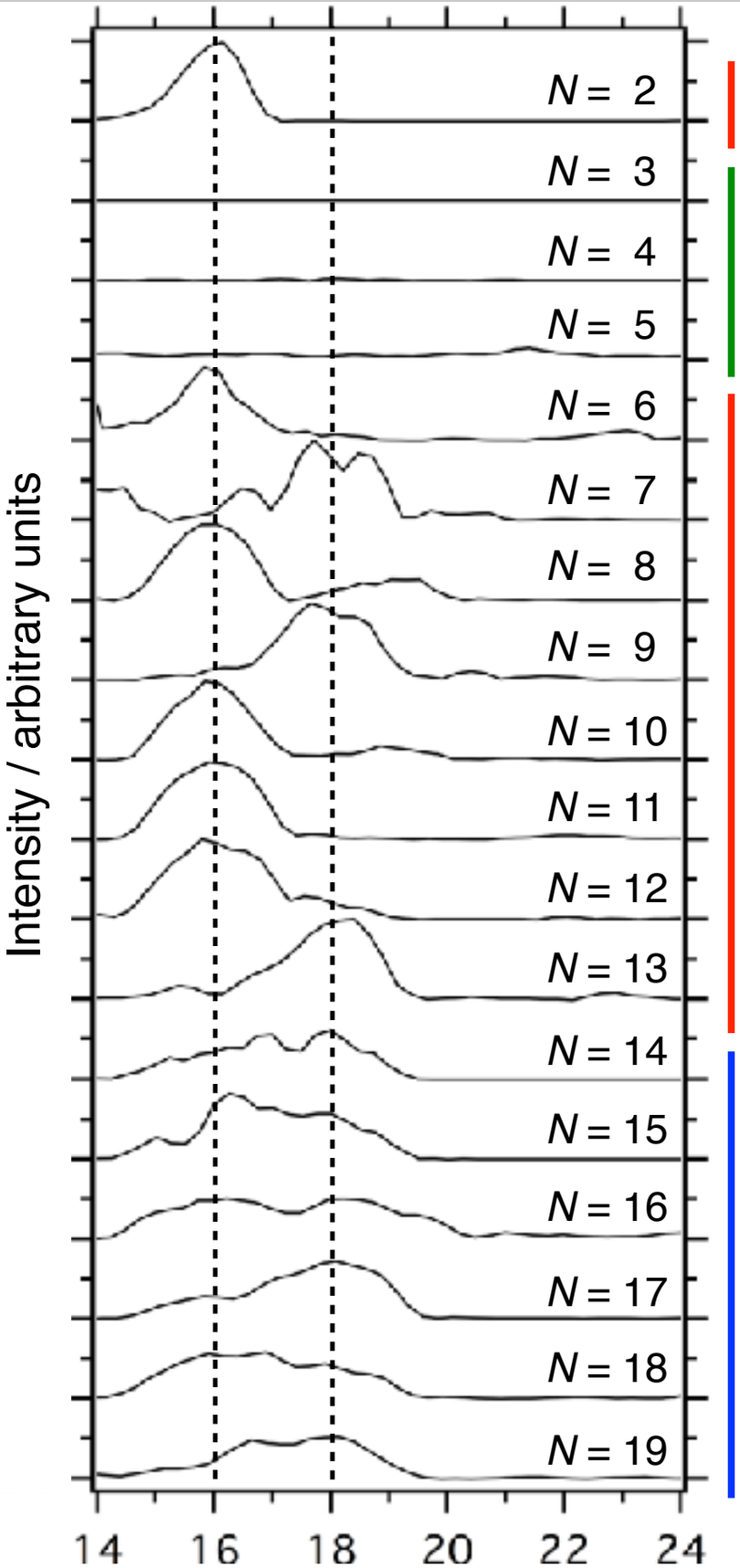
Reaction of Al_N^+ with H_2O

H_2 is attracting much attention as an innovative energy carrier alternative to conventional fuels. One of the methods to produce hydrogen is a use of Al or its alloys to reduce H_2O to H_2 because of its efficiency, safety, and environmental friendliness.

Al_N^+ + H_2O → ?



Size dependence of reaction products

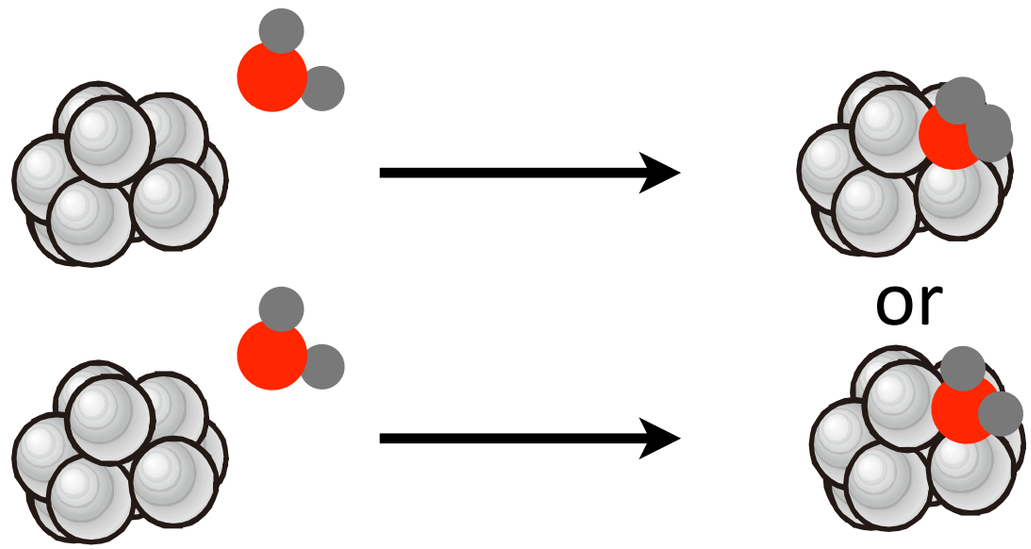


E_{col}: about 0.2 eV in the center of mass frame

N = 3–5: No reaction products

N = 2, 6–13: Al_NO^+ or $Al_N(H_2O)^+$

selective formation



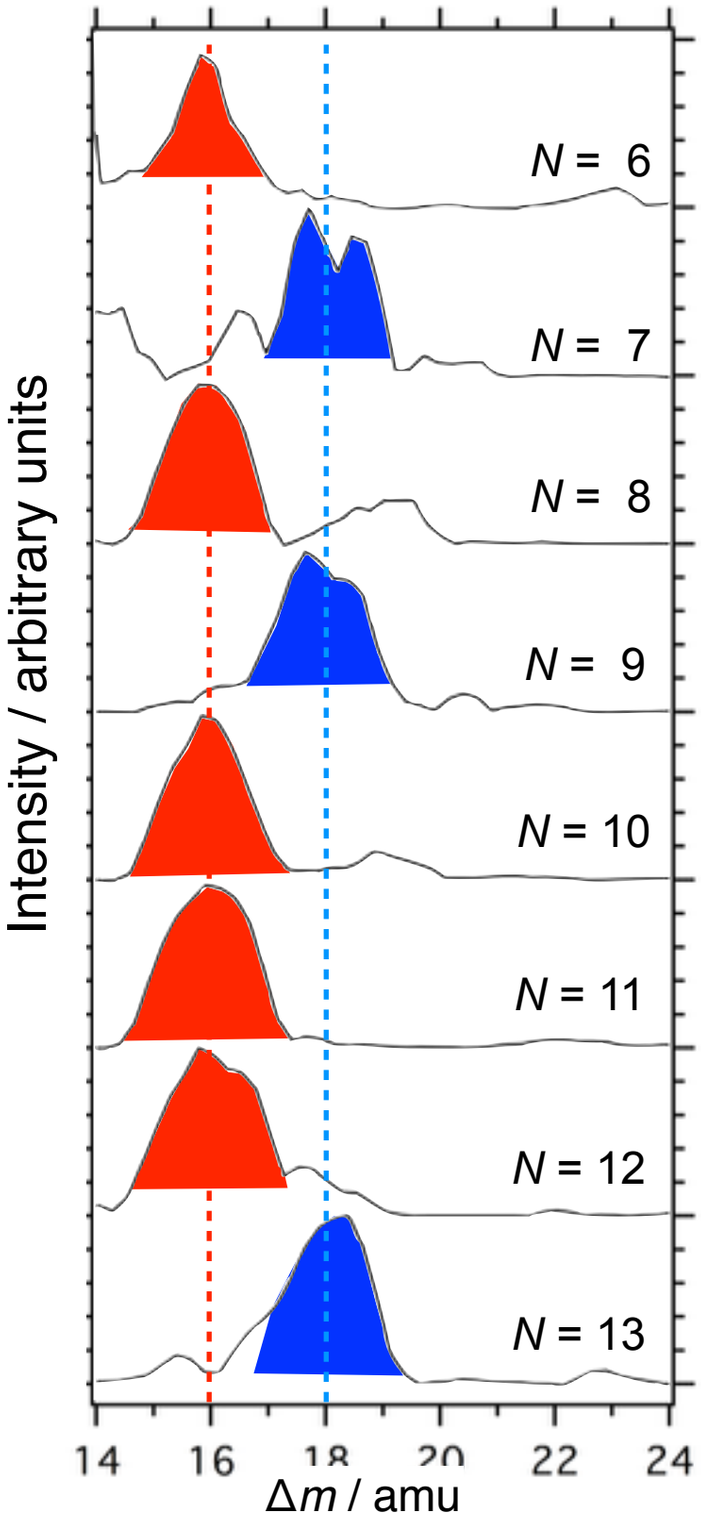
N = 14–19: both Al_NO^+ and $Al_N(H_2O)^+$

Under the const. collision energy condition, whether the oxidation reaction proceeds depends on the size.

Size dependence of the reaction products

$$Al_N^+ + H_2 \rightarrow Al_N(H_2O)^+ \longrightarrow Al_NO^+ + H_2$$

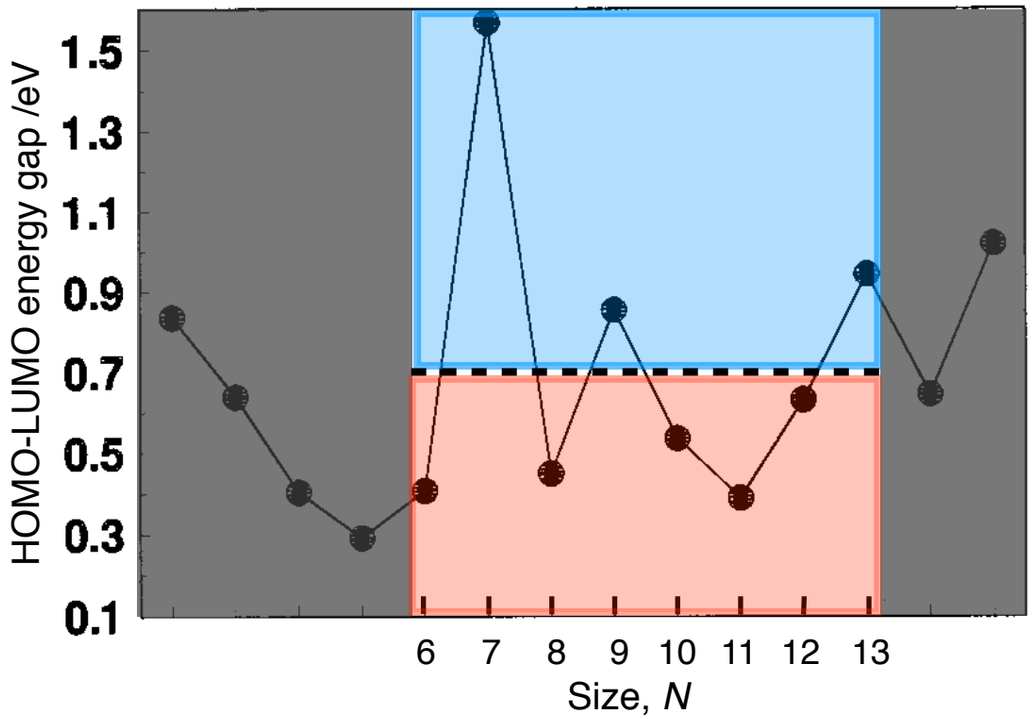
The barrier of the oxidation reaction depends on size.



N = **6, 8, 10, 11, 12**: **Low** barrier

N = **7, 9, 13**: **High** barrier

A possible explanation is by HOMO-LUMO energy gaps.



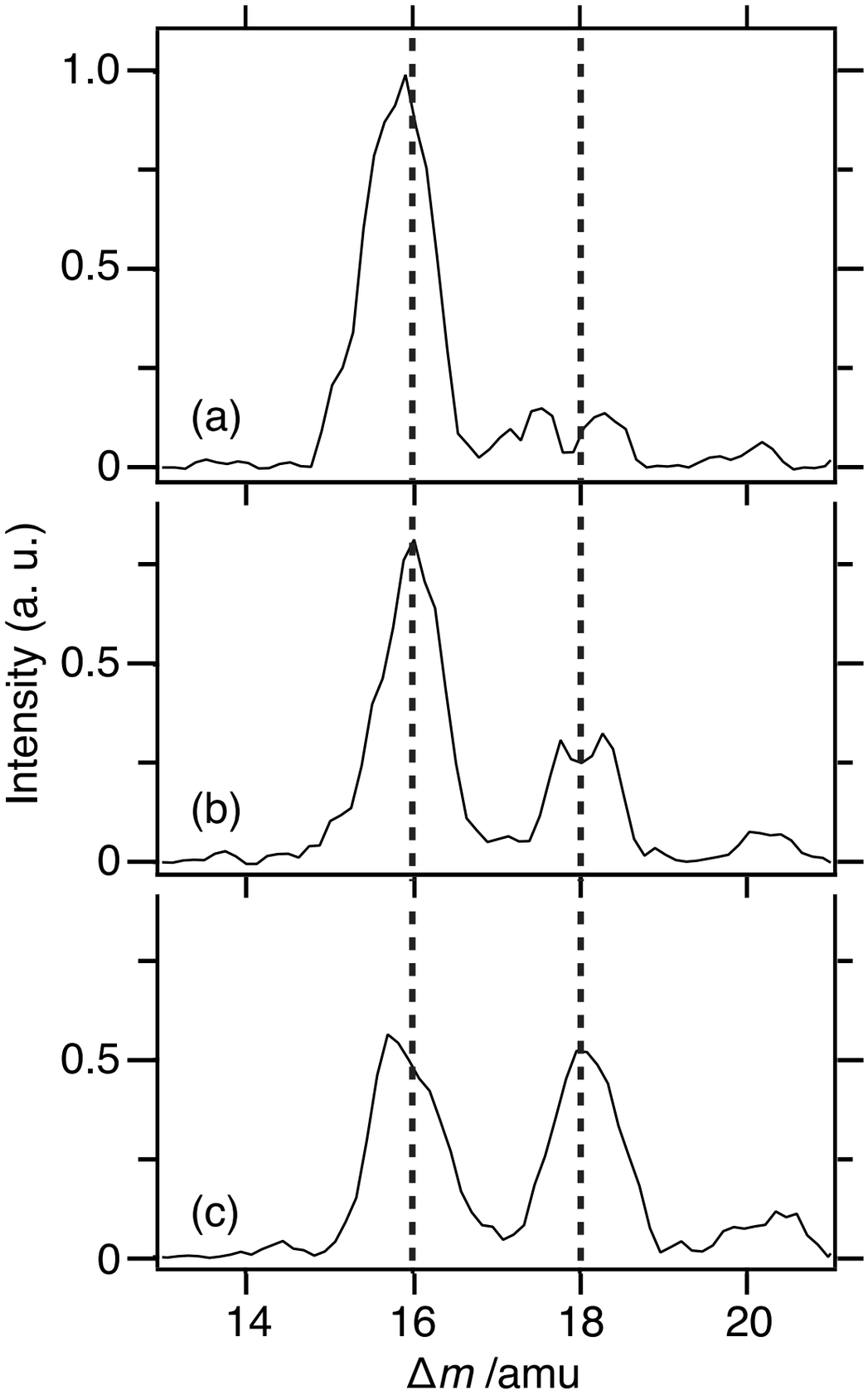
(Rao and Jena, *J. Chem. Phys.* **111**, 1890, 1999)

polarizability of Al_N^+: $\alpha_{AlN+} \approx \dfrac{2e^2R^2}{\Delta E_{HL}}$

A small ΔE_{HL} causes a large polarisability, and a large internal energy of $[Al_N(H_2O)^+]^*$.

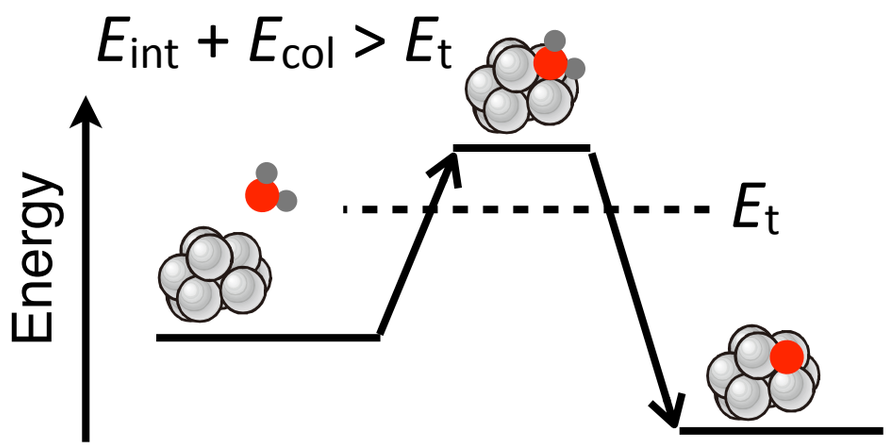
However, dipole–induced dipole interaction is in the range of 0.01–0.1 eV: this is generally comparable or lower than the ion–dipole interaction.

Collision-energy dependence （N = 11）



P_{H2O} = 1.9 × 10^{-3} Pa

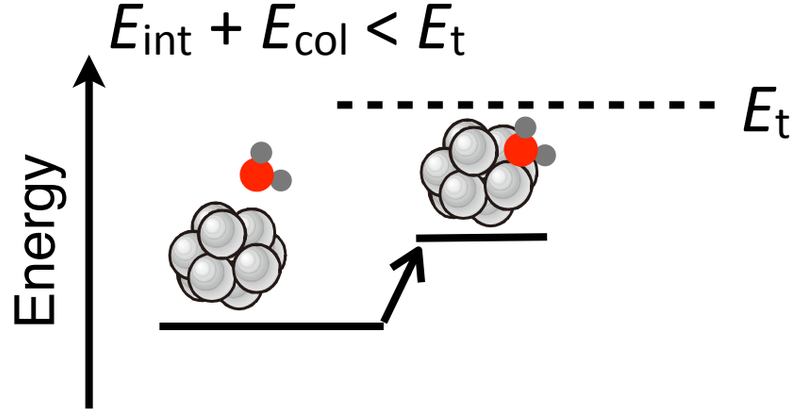
E_{col} = 0.21 eV



P_{H2O} = 1.4 × 10^{-3} Pa

E_{col} = 0.18 eV

Deceleration occurred before reacting with H_2O.



P_{H2O} = 0.9 × 10^{-3} Pa

E_{col} = 0.15 eV

The reaction proceeds favorably at a higher collision energy; the internal energy of the precursor complex $[Al_{11}(H_2O)^+]^*$ would be the driving force of the reaction.

Summary

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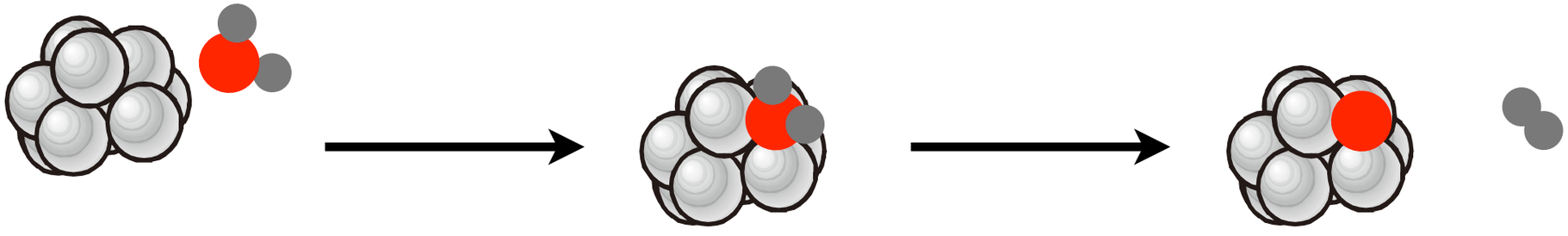

$Al_N^+ + H_2O$ $[Al_N(H_2O)^+]^*$ $Al_NO^+ + H_2$

The H_2 generation reaction occurs only if $[Al_N(H_2O)^+]^*$ has high internal energy.

(M. Arakawa, K. Kohara, T. Ito, and A. Terasaki, *Eur. Phys. J. D* **67**, 80, 2013)