AB INITIO STUDY ON THE VIBRATIONAL SIGNATURES OF Ar_nH^+ (n=2–3)

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A progression of strong bands in the 900–2200 cm^{-1} region are observed in the infrared laser photodissociation spectrum of Ar_3H^+.[a] In this talk, computational studies were conducted to examine the structures, binding energies, and infrared spectra for Ar_nH^+ (n=2–3). We found that the minimum structure for Ar_2H^+ is linear and centrosymmetric, while Ar_3H^+ can be either T-shaped or linear.[b] A series of potential energy surfaces at the CCSD(T)/aug-cc-pVTZ level of theory and basis set was constructed and used for the calculation of anharmonic spectrum using discrete variable representation (DVR).[c] Anharmonic theory can reproduce the observed strong bands, which were associated with the core Ar_2H^+ ion. These bands are assigned as combination bands of the asymmetric Ar-H^+ stretch with multiple quanta of the symmetric Ar-H^+ stretch.

[a] D.C. McDonald II, D.T. Mauney, D. Leicht, J.H. Marks, J.A. Tan, J.-L. Kuo, and M.A. Duncan, J. Chem. Phys. 145, 231101 (2016).

[b] J.A. Tan and J.-L. Kuo, J. Phys. Chem. A 124, 7726–7734 (2020).

[c] J.C. Light, I.P. Hamilton, and J. V. Lill, J. Chem. Phys. 82, 1400 (1985).