INTERMOLECULAR FREQUENCIES OF N_2O–KR AND SYMMETRY BREAKING OF THE N_2O BENDING MODE IN THE PRESENCE OF A RARE GAS

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Rotationally-resolved infrared spectra of N_2O–Ar and N_2O-Kr van der Waals clusters are studied in the region of the N_2O ν_1 vibration ($\approx 2224\ \mathrm{cm}^{-1}$) using a tunable Quantum Cascade laser source to probe a pulsed supersonic jet. The N_2O-Kr ν_1 fundamental band is re-analyzed, together with previous ν_3 band data, using a unified scheme to fit the (small) observed Kr isotope splittings. This scheme is then transferred to analyze the bending combination band of N_2O-Kr near 2257 $\mathrm{cm}^{-1}$where isotope effects are much larger due to stretch-bend Coriolis interactions. As a result, N_2O–Kr intermolecular bend (33.29 cm^{-1}) and stretch (34.48 cm^{-1}) frequencies are directly determined for the first time.

We also report observation of weak spectra for both N_2O-Ar and -Kr corresponding to the (ν_1, ${\nu_2}^{l_2}$, ν_3) = (1,1^1,0) ← (0,1^1,0) hot band of N_2O, located around 2209.8cm^{-1}. In the presence of Argon/Krypton atom, the doubly-degenerate ν_2 bending mode of the N_2O monomer splits into an in-plane and an out-of-plane mode. These two infrared bands are heavily linked by Coriolis interactions and their analysis yields the magnitude of the splitting of the bending modes which are significantly smaller than those observed in the analogous CO_2-containing dimers [a]. The experimental results obtained here are valuable for testing the accuracy of theoretical calculation toward a better understanding of intermolecular interactions.

[a] T.A. Gartner, A.J. Barclay, A.R.W. McKellar, and N. Moazzen-Ahmadi, Phys. Chem. Chem. Phys. 22, 21488-21493 (2020).