CLIMBING UP THE POTENTIAL WELL: LONG-PATH IR DIODE LASER SPECTRA OF THE CO-Ne COMPLEX

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For weakly-bound complexes like CO-Ne, we are interested in the whole of the potential energy surface, not just the part near the minimum. To obtain this information, we need to 'climb up the well' to observe and assign transitions involving excited rotational and vibrational levels.

Previously, the IR spectrum of CO-Ne in the 2140 cm^{-1} region of the C-O stretch was studied using a combination of the diode laser / pulsed jet and the FTIR / long-path cell techniques,[a] and the K_a = 0 and 1 levels in the v_{CO} = 0 and 1 vibrational states were observed, as well as the $v_2 = 1$ excited bending level for $v_{CO} = 1$.

In the present work, we use an IR diode laser to probe a 200 m path through a mixture of CO and Ne at 47 K. The high resolution and sensitivity of the laser enable us to use a low sample pressure (1.4 Torr), which means that many more details can be resolved, compared to the earlier FTIR work. At the same time, since the sample temperature is higher than in a jet source, many excited rotational and vibrational states are accessible. The new spectrum enables us to assign the K_a = 2 and 3 states of CO-Ne, as well as $v_2 = 1$ for $v_{CO} = 0$ and also one component of the $v_2 = 1$, $K_a = 1$ state.

But even for a relatively simple and light system like CO-Ne, we remain far from the goal of assigning most of the observed lines: the sides of the potential are still too slippery to climb! Precise theoretical modelling will be necessary to rescue us from the well. For the rescuer, the reward will be a complete characterization of intermolecular forces in the attractive region of the potential.

[a] R.W. Randall, A.J. Cliffe, B.J. Howard, and A.R.W. McKellar, Mol. Phys. 79, 1113 (1993).