

PROGRESS IN UNDERSTANDING THE INFRARED SPECTRA OF He- AND Ne-C₂D₂

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Infrared spectra of He-C₂H₂ were recorded around 1990 in Roger Miller's lab, but detailed rotational assignment was apparently not possible even with the help of theoretical predictions. So there were no published experimental spectra of helium-acetylene van der Waals complexes until our recent work on He-C₂D₂ in the ν_3 region (~ 2440 cm⁻¹).^a The problem is that this complex lies close to the free rotor limit, so that most of the intensity in the spectrum piles up in tangles of closely spaced lines located close to the monomer rotational transitions, $R(0)$, $P(1)$, etc.

Our previous He-C₂D₂ assignments were limited to the $R(0)$ region, that is, the $j = 1 \leftarrow 0$ subband, where j represents C₂D₂ rotation. Here, we extend the analysis to $j = 0 \leftarrow 1$ and $2 \leftarrow 1$ transitions with the help of new spectra obtained using a tunable OPO laser probe and a cooled supersonic jet nozzle. These subbands are weaker, not only because of the Boltzmann factor, but also the 2:1 nuclear spin statistics of j = even:odd C₂D₂ levels. Moreover, the $j = 0 \leftarrow 1$ subband is overlapped by strong (C₂D₂)₂ transitions. We use a term value approach, obtaining a self-consistent set of "experimental" energy levels which can be directly compared with theory or fitted in terms of a Coriolis model. Challenges also arise with Ne-C₂D₂, which is not quite so close to the free rotor limit, but still has many overlapping lines. Insights gained here help in assigning the tricky $R(1)$ region for Ne-C₂D₂.

^aM. Rezaei, N. Moazzen-Ahmadi, A.R.W. McKellar, B. Fernández, and D. Farrelly, *Mol. Phys.* **110**, 2743 (2012).