MILLIMETER WAVE SPECTRUM OF THE $^{13}C^{16}O$ DIMER

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The millimeter wave spectrum of the isotopically substituted CO dimer, $(^{13}C^{16}O)_2$ has been studied for the first time, confirming and extending a recent infrared study [1]. A total of 87 transitions in the 77 - 180 GHz region have been assigned and analyzed with a model-independent term value scheme involving 57 rotational levels with J = 0 to 8. The levels can be classified into 7 "stacks" which have symmetry classifications of either A^+/B^- or A^-/B^+, and K-values of either 0 or 1. For the normal isotope, symmetry and nuclear spin statistics cause alternate rotational levels to be missing, but for $(^{13}C^{16}O)_2$, all levels are present with an intensity alternation of 1:3 between the A and B symmetries. The four A^+/B^- stacks have not previously been observed, and the lowest of them establishes the tunneling splitting of $(^{13}C^{16}O)_2$ to be 3.769 cm^{-1}, slightly larger than the $(^{12}C^{16}O)_2$ value [2] of 3.731 cm^{-1}. Even though a considerable amount of precise experimental data is now available for the CO dimer, we still have little theoretical insight into its structure and tunneling dynamics.

References

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[2] J. Tang, A.R.W. McKellar, L.A. Surin, D.N. Fourzikov, B.S. Dumesh, and G. Winnewisser, *J. Mol. Spectrosc.* **214**, 87 (2002).