INFRARED SPECTRUM AND ENERGY LEVELS OF THE $^{13}C^{16}O$ DIMER

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Studies of the $^{12}C^{16}O$ dimer in the infrared and millimeter wave regions [1-3] have characterized six stacks of rotational levels in the ground state, v(CO) = 0, and eight stacks in the excited state, v(CO) = 1. The symmetry of $(^{12}C^{16}O)_2$ means that the relative energies of all observed levels can be experimentally determined without model depedendence. For 28 ground state levels, energies are known with 'microwave accuracy' (<0.1 MHz), while the remaining levels are known with 'infrared accuracy' (<10 MHz). The results suggest the presence of two overlapping isomers: a C-bonded ground state (R = 4.4 Å), and an O-bonded state (R = 4.0 Å) lying only 0.877 cm^{-1} above the ground state.

The present work concerns the infrared spectrum of the 13-C substituted carbon monoxide dimer. Over 120 transitions were assigned in terms of 49 rotational levels in the excited state and 23 in the ground state. The relative energies of these levels were accurately determined without model dependence except for the interval between levels of *A* and *B* symmetry. The levels were similar to those of $(^{12}C^{16}O)_2$, and could be identified with the same labelling scheme. Differences between the two isotopes constitute a subtle probe of the intermolecular forces. Two isomers are also evident for $(^{13}C^{16}O)_2$, but their ground state energy difference increases to 1.285 cm^{-1} in $(^{13}C^{16}O)_2$. The observed isotope effects can be explained by a simple anharmonic interaction model.

References

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