INTERMOLECULAR BENDING LEVELS AND INFRARED SPECTROSCOPY OF OPEN-SHELL DIATOM-DIATOM COMPLEXES

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A theoretical framework has been developed to describe the bending levels associated with an intermolecular potential of moderate anisotropy between an open-shell diatom and a diatomic partner, such as OH–CO or OH–N_2. The model explicitly allows for coupling between the electronic and spin angular momenta of the open-shell OH radical and the vibrational angular momentum arising from the intermolecular bending motions of the complex. Using a dipole-quadrupole interaction potential, energies, wave functions, and transition moments are calculated to reveal the intermolecular energy pattern and expected bending vibrational spectrum for a moderately anisotropic system. The predicted spectrum is compared to that experimentally observed for the OH–N_2 complex in the OH overtone region. Explicit consideration of the OH radical spin-orbit ($\hat{l} \cdot \hat{s}$) and spin-decoupling ($\hat{j} \cdot \hat{s}$) interactions indicates that the spin-orbit splitting in the complex can differ significantly from that of the OH monomer.

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