COHERENT RAMAN SPECTRA OF THE ν_1 MODE OF $^{10}BF_3$ AND $^{11}BF_3$

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High resolution (0.001 cm^{-1}) coherent anti-Stokes Raman spectroscopy (CARS) was used to directly examine the ν_1 symmetric stretching mode of the D_{3h} molecules $^{10}BF_3$ and $^{11}BF_3$. Calculated spectra were constructed using rovibrational parameters deduced from published infrared hot band, combination band, and difference band studies, and the similarity to the experimental CARS spectra confirms the validity of the constants. No significant perturbations by Fermi resonance or Coriolis interactions with nearby states are observed, in marked contrast to the case of sulfur trioxide, a similar D_{3h} molecule recently studied. Since the boron nucleus is at the center of mass, the $^{10}BF_3$ and $^{11}BF_3$ ν_1 Q-branches are the same according to the harmonic oscillator model. Interestingly, the observed frequency of $^{11}BF_3$ is 0.198 cm^{-1} higher than that of $^{10}BF_3$. This result is reproduced almost exactly (0.200 cm^{-1}) using *ab initio* calculations (B3LYP/cc-pVTZ) that included evaluation of cubic and quartic force constants and x_{ij} anharmonicity constants. *Ab initio* methods also predict to within 1% the ΔB and ΔC changes in the rotational constants in going from the ground state to the v = 1 vibrational level.