ANALYSIS OF ROTATION-VIBRATION SPECTRA OF SMALL MOLECULES EMBEDDED IN PARAHYDROGEN CRYSTALS

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We have been using solid parahydrogen (p-H_2) as a matrix for high-resolution infrared spectroscopy. Small molecules embedded in solid p-H_2 are found to exhibit completely free quantized rotational motion. In previous works, we have fully analyzed the high-resolution rotation-vibration spectra of spherical top molecules (CH_4 and CD_4) in solid p-H_2.[a,b] We found that the rotational constants of these molecules decreases 10%∼20% from the gas phase values due to the interaction between the guest molecules and surrounding hydrogen molecules. This paper will focus on the analysis of the spectra of symmetric top molecules such as CD_3 and CD_3H. The ν_3 rotation-vibration transition of CD_3 shows complic! ated spectral structure due to the quantized rotational motion and the crystal field splittings. The analysis of the spectrum reveals that the reduction of the rotational constant C is three times larger than that of B. The origin of the reduction will be discussed.

[a] T. Momose, M. Miki, T. Wakabayashi, T. Shida, M.-C. Chan, S. S. Lee, T. Oka J. Chem. Phys. **107** 7707 (1997)
[b] H. Hoshina, T. Wakabayashi, T. Momose, and T. Shida, J. Chem. Phys. **110** 5728 (1999)