VIBRATIONALLY EXCITED C_6H

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Following the detection of the linear carbon chain radical C_6H in space, many rotational lines in the $X^2\Pi$ electronic ground state have been observed in a low pressure discharge at millimeter wavelengths[a] and in a supersonic molecular beam at centimeter wavelengths[b]. In the course of a laboratory search for new reactive hydrocarbon molecules with 6 carbon atoms, several series of harmonically related lines with rotational constants near that of C_6H in the ground vibrational state were observed in the millimeter-wave band. On the basis of the close agreement in rotational constants and intensities, two of the series were assigned to $^2\Sigma$ and $^2\Delta$ states of a low-lying excited bending vibrational level of C_6H. The standard Hamiltonian with five spectroscopic constants reproduces the observed rotational spectrum of the $^2\Delta$ state, but several high-order distortion terms in the spin-rotation interaction are needed to reproduce the spectrum of the $^2\Sigma$ state of C_6H and C_6D. From the measured intensities of the rotational lines it appears that the $^2\Sigma$ state lies very close to ground but the $^2\Delta$ state lies much higher in energy. A brief summary of the laboratory spectrum and applications to the astronomical observations will be presented.

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[a] H. Linnartz, T. Motylewski, O. Vaizert, J. P. Maier, A. J. Apponi, M. C. McCarthy, C. A. Gottlieb, and P. Thaddeus, *J. Mol. Spectrosc.* **197**, 1 (1999).
[b] M. C. McCarthy and P. Thaddeus, *J. Chem. Phys.* **122**, 174308 (2005).