

SPECTRA OF BENZENE AND ITS ISOTOPOMERS,  
AND THE EQUILIBRIUM STRUCTURE OF BENZENE

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High resolution spectra of benzene and of its symmetrically substituted isotopomers have been the subject of intensive investigations over the past several years. One of the results of these studies was the determination of accurate values for the ground state rotational and centrifugal distortion constants for these molecules. Isotopic scaling relations have been used to obtain approximate corrections for the zero-point vibrations to extrapolate the ground state  $B_0$  values for  $^{12}\text{C}_6\text{H}_6$ ,  $^{13}\text{C}_6\text{H}_6$ ,  $^{12}\text{C}_6\text{D}_6$ ,  $^{13}\text{C}_6\text{D}_6$ , and  $s\text{-}^{12}\text{C}_6\text{H}_3\text{D}_3$  to equilibrium values,  $B_e$ . This has made it possible to find estimates for equilibrium values of the internuclear distances of the benzene molecule,  $r_{\text{C-C}} = 1.3902 \pm 0.0002 \text{ \AA}$ ,  $r_{\text{C-H}} = 1.0862 \pm 0.0015 \text{ \AA}$ .

## Ab initio calculations as a tool in the analysis of perturbations in the vibration-rotation spectra of polyatomic molecules

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Quite often, the analysis of perturbations apparent in high-resolution vibration-rotation spectra of polyatomic molecules is a difficult task for the experimentalist. This holds in particular for less stable molecules for which only a selected set of bands can be observed. Ab initio calculations may be of considerable help in solving such problems. The following topics will be dealt with in detail: analysis of the perturbations observed in the  $\nu_3$  band of  $C_5^1$ , comparison of theoretical and experimental results for various interacting states of  $HC_3N$  and  $HC_2NC$  and prediction of a perturbation in the  $\nu_1$  band of  $HNSi$ . Accurate equilibrium geometries for  $HC_3N^2$  and  $HC_2NC^3$  will also be reported.

<sup>1</sup>N. Moazzen-Ahmadi, A. R. W. McKellar, and T. Amano, *J. Chem. Phys.* **91**, 3140 (1989)

<sup>2</sup>P. Botschwina, M. Horn, S. Seeger, and J. Flügge, *Mol. Phys.*, to be published

<sup>3</sup>P. Botschwina, M. Horn, S. Seeger, and J. Flügge, *Chem. Phys. Lett.*, to be published

### **Diode Laser Spectroscopy of Several Diatomic Metal Hydrides**

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The results of accurate measurement of the infrared spectra of several further diatomic metal hydrides will be presented.

Mass independent molecular parameters have been determined for aluminium, ytterbium and copper monohydride through measurement of the spectra of the relevant deuteride.

We have also obtained, for the first time, extensive data over SbH and SbD. (The LMR-spectrum of SbH has also recently been observed in Bonn).

Datails will be given in the poster.

**Highly Sensitive Infrared Spectroscopy: IR-REMPI Double Resonance Experiments**

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**Abstract**

The first double resonance signals involving the use of a c.w. infrared laser and multiphoton ionization spectroscopy using a pulsed UV laser has been observed in  $^{15}\text{NH}_3$ . Despite the low duty-cycle of such a combination, very strong double resonance signals were observed using a low power  $\text{CO}_2$  laser as infrared source. The observations indicate that such measurements should be possible with the extremely low power levels available from tunable diode lasers. Such a combination would allow high resolution infrared spectroscopy to be carried out with the sensitivity of ionization spectroscopy and allow application to molecular species such as clusters. Term values of  $^{15}\text{NH}_3$  have been calculated from the data.

Further double resonance experiments on  $\text{CF}_3\text{I}$  and  $\text{CF}_2\text{Cl}_2$  will be described together with the results of investigations using diode lasers.

# Anomalous Rotation-Vibration Coupling in Some Molecules

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## Abstract

It has been shown that for some molecules the dependence of the rotation constant  $B_v$  and the centrifugal distortion constant  $D_v$ , on vibration quantum number is different than that of the Pekeris-Herzberg. For these cases the Dunham method is unable to describe rovibrational bands of molecules, and the Watson approach should be applied. A few examples will be presented and tentative explanation based on the soft body or deformable body model will be suggested.

Air Broadened Spectrum of Water Vapor: the  $\nu_2$  band

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Pressure broadening and shifts of H<sub>2</sub>O rovibrational line due to air were measured precisely for 271 transitions in the  $\nu_2$  band by using the high resolution FTIR spectrometer, Bruker IFS-120 HR, at the Universität Giessen. Water vapor was introduced into the 3 m long glass cell sealed by KBr windows. Air of 1 bar was added to the cell and the broadened spectrum was recorded with a resolution of 0.0039 cm<sup>-1</sup> which allows to safely the instrumental effects on broadened line profiles.

Rotational dependences of these effects were clearly observed in the present study which includes high  $J$  transitions up to  $J = 18 \leftarrow 17$ . The observed rotational dependence is drastic. Very small pressure broadening coefficients were obtained for high  $J$  transitions, e.g. 0.011 cm<sup>-1</sup>/bar for the unresolved  $K$ -doublet,  $18_{0,18} \leftarrow 17_{1,17}$  and  $18_{1,18} \leftarrow 17_{0,17}$ , whereas medium  $J$  transitions exhibit larger broadening, i.e.  $7_{4,4} \leftarrow 6_{3,3}$  yields 0.087 cm<sup>-1</sup>/bar.

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**MOGADOC - A Bibliographic Numerical Resource for Molecular Spectroscopy and Structure**

**J. VOGT**