

FD01 15:00 – 15:17

**PRECISION SATURATED ABSORPTION SPECTROSCOPY OF $^{130}\text{Te}_2$
FROM 22100 – 22600 cm^{-1}**

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Atomic and molecular transitions provide useful frequency references. From 18500 – 23800 cm^{-1} $^{130}\text{Te}_2$ has many absorptions which have been previously tabulated [1]. The precision of this tabulation is limited by Doppler broadening. We have measured Doppler-free saturated absorption spectra from 22100 – 22600 cm^{-1} with a precision and absolute accuracy of 0.0003 cm^{-1} . We were able to obtain this level of precision and accuracy by using a Fabry-Perot Cavity locked to a stabilized HeNe laser and 2 electro-optic modulators to produce frequency markers spaced by 25 MHz. The frequencies for these markers were generated by synthesizers using a GPS disciplined temperature controlled quartz crystal oscillator as their reference. The absolute optical frequency accuracy was calibrated using the D_1 hyperfine transitions in Cs. This level of precision has allowed us to measure individual rotationally resolved lines predominated by transitions from the ground state, XO_g^+ ($v = 0 - 8$), to the excited state BO_u^+ ($v = 0 - 14$). We have compiled a precise list of over 5000 lines and assigned most of them. Using the previously determined parameters of the XO_g^+ state [2], we have determined parameters of the BO_u^+ state with improved accuracy and precision.

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[2] J. Vergès, *et al.*, *Physica Scripta*, **25**, 338 (1982).

**SPECTROSCOPIC OBSERVATION AND DEPERTURBATION TREATMENT OF
THE $A^1\Sigma^+$ AND $b^3\Pi_0$ STATES IN LiCs MOLECULE**

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The first excited singlet states in alkali dimers, $A^1\Sigma^+$ in heteronuclear molecules as well as their $A^1\Sigma^+_u$ counterparts in homonuclears, become increasingly difficult to characterize when the mass of constituent atoms is growing. The reason is in close proximity of the $b^3\Pi$ ($b^3\Pi_u$) states which interact with the A states via the spin-orbit coupling, whose strength in general increases with the atomic mass [1]. But a presence of singlet-triplet mixed levels may be taken to advantage as they open access to usually 'dark' triplet states of alkali molecules, inaccessible from the singlet ground state.

In our work polarization labelling spectroscopy technique [2] was used to investigate the $A^1\Sigma^+ \leftarrow X^1\Sigma^+$ band system of the $^7\text{LiCs}$ molecule in a heat-pipe oven. All 27 observed vibrational levels of the A state were found to be subject to strong perturbations assigned to interaction with the $b^3\Pi_0$ state. The deperturbation analysis provided molecular constants of the A and b states and a value of the electronic part of the spin-orbit interaction matrix element $\langle b^3\Pi_0 | H_{so} | A^1\Sigma^+ \rangle$. The molecular constants were compared with theoretical calculations [3].

[1] O. Docenko, M. Tamanis, R. Ferber, T. Bergeman, S. Kotochigova, A.V. Stolyarov, A. de Faria Nogueira, C.E. Fellows, *Phys. Rev. A* **81**, 042511 (2010)

[2] W. Jastrzebski and P. Kowalczyk, *Phys. Rev. A* **51**, 1046 (1995)

[3] M. Elkork, D. Houalla, M. Korek, *Can. J. Phys.* **87**, 1079 (2009)

**OPTICAL POPULATION OF IODINE MOLECULE UNGERADE STATES
CORRELATING WITH $I(^2P_{1/2}) + I(^2P_{1/2})$ DISSOCIATING LIMIT FROM
UNGERADE $B0_u^+$ STATE**

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We successfully utilize three-step scheme of population of selected rovibronic levels of *gerade* $\beta 1_g$ and $D'2_g$ iodine ion-pair (IP) states via the $B0_u^+$ and $1_u(bb)$ states correlating with the 2-nd, $I_2(ab)$, and 3-rd, $I_2(bb)$, dissociation limits of the iodine valence states (see [1] and references).

$$I_2(\beta 1_g, \nu_\beta, J_\beta \xleftarrow{h\nu_2} 1_u(bb), \nu_{1u}, J_{1u} \xleftarrow{h\nu_f} B0_u^+, \nu_B, J_B \xleftarrow{h\nu_1} X0_g^+, \nu_X, J_X), (1)$$

for example ($h\nu_f$ is Nd:YAG laser generation).

There some intriguing features in this scheme:

- the $1_u(bb) \leftarrow B0_u^+$ transition is electric dipole forbidden.
- the $\Delta J = \pm 2$ lines present at this and the $I_2(\beta 1_g \leftarrow 1_u(bb))$ electric dipole allowed transitions.

In this report, we communicate on results of studies mechanism of optical transitions involved in scheme (1).

We have:

- shown that the $1_u(bb) \leftarrow B0_u^+$ transition cannot have magnetic dipole or electric quadrupole character and do not occur due to Stark effect;

- analyzed wavenumbers of the transitions involved in optical population of the $I_2(D0_g^+$ and $\beta 1_g)$ states via the $0_g^+, 1_u(bb)$ states and shown that both upper states are populated via *the same* rovibronic levels of the lower states mixed by hyperfine interaction:

$$I_2(D0_g^+, \nu_D, J_D \xleftarrow{h\nu_2} 0_g^+(bb), \nu_0, J_0/1_u(bb), \nu_{1u}, J_{1u} \xleftarrow{h\nu_f} B0_u^+, \nu_B, J_B) (2)$$

$$I_2(\beta 1_g, \nu_\beta, J_\beta \xleftarrow{h\nu_2} 0_g^+(bb), \nu_0, J_0/1_u(bb), \nu_{1u}, J_{1u} \xleftarrow{h\nu_f} B0_u^+, \nu_B, J_B) (3)$$

- analyzed dichroism of the $\Delta J = 0, \pm 2$ lines of the $I_2(\beta 1_g \leftarrow 1_u(bb))$ transitions and shown that they are due to hyperfine interactions between 0_u^- and $1_u(bb)$ states.

Hyperfine interaction we have found is very interesting feature. All three, 0_g^+ , 0_u^- and $1_u(bb)$ states correlating with the $I(^2P_{1/2}) + I(^2P_{1/2})$ dissociation limit are coupling by hyperfine interaction, and energy gaps between rovibronic states which may be coupled by the interaction according to selection rule $\Delta J \leq 2$ are large, $\Delta E \geq 0.7 \text{ cm}^{-1}$.

**TWO-COLOUR POLARISATION SPECTROSCOPY IN Rb₂:
THE 5¹Σ_u⁺ AND 5¹Π_u STATES**

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Two-colour polarisation labelling experiments have been used to explore the excitation spectrum of the rubidium dimer in the region 25500 - 27000 cm⁻¹, probing two mutually interacting states. They were identified from *ab initio* calculations as the 5¹Σ_u⁺ and 5¹Π_u states, both correlated with the atomic asymptote Rb(5s) + Rb(5d). Products of two or more excitation spectra had to be taken to allow common features in the exceptionally congested spectra to emerge, finally revealing rather irregular vibrational progressions. Treating these as related to single states with (numerous) local perturbations, we propose spectroscopic parameters and potential energy curves to describe the levels observed. Observations cover some 20 vibrational levels in both the 5¹Σ_u⁺ and 5¹Π_u states.

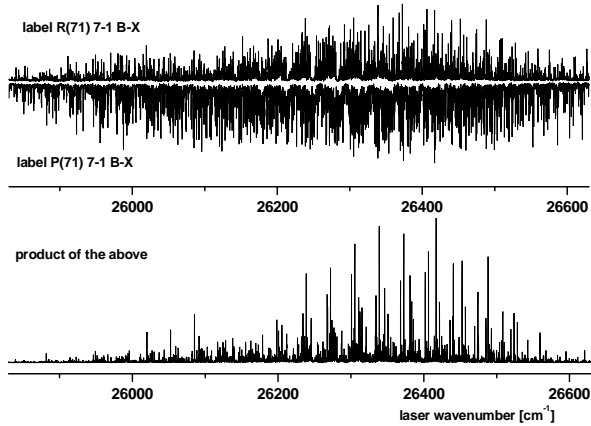


Figure. Upper trace: crowded and irregular Rb₂ polarisation spectra, recorded when labelling the ground state level ($v''=1, J''=71$) via R(71) and P(71) transitions of the (7-1) band in the B¹Π_u←X¹Σ_g⁺ system with a pulsed dye laser (linewidth ~0.3 cm⁻¹). Lower trace: the product of these two spectra enhances the common features above the still-congested background. Strong Q lines are Q(71) 5¹Π_u←X, and the strong P,R doublets are transitions to 5¹Σ_u⁺.

**THE USE OF LASER EXCITED RO-VIBRATIONAL SPECTRA OF OH
RADICALS AS A PROBE OF A GAS PHASE COMPOSITION**

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Atmospheric pressure plasmas characterized by high concentration of radicals and low gas temperatures are found to be suitable for many applications [1]. Often the gas composition in the discharge is unknown because of the air diffusion in to the stream of the feed gas. Correspondingly, methods to probe the gas composition in the discharge zone with high spatial resolution are strongly desirable. In the present work the high resolved laser-induced fluorescence (LIF) ro-vibrational spectroscopy is used to probe the gas composition through the excitation of OH radicals generated in the discharge region and measurement of the fluorescence signal decay time accompanied by rotational/vibrational energy transfer. Two types of discharge are investigated: glow discharge above water surface [2] and so called Ar “plasma jet” working in ambient air [3].

Ground $X^2\Pi$ state of OH radicals was excited by the tunable dye laser to the vibrational level $v'=1$ of $A^2\Sigma^+$ state. The effect of N_2 , O_2 and H_2O addition as OH quenchers on LIF signal intensity and decay time was measured. From LIF spectra it is found that at 20-40 ns after the laser excitation the intensity of the vibrational band (1,1) drastically decreases because of collisions with N_2 , whereas much stronger vibrational band (0,0) starts to dominate in all the spectra. Time decay of the LIF signal at band (0,0) reveals exponential decay with time constant of 39 ns in “plasma jet” and even shorter decay in the glow discharge. The radiative decay time of OH $A^2\Sigma^+$ ($v'=1$, $v'=0$) to ground state is about 0.6×10^{-5} s and hence experimentally observed much shorter decay time is related to collisional quenching of OH by N_2 , O_2 , H_2O . The high resolution LIF rotational spectra of OH ($A^2\Sigma^+ - X^2\Pi$) in the plasma at 0 ns, 50 ns and 150 ns after the laser pulse is used in order to investigate the rotational energy transfer processes. Based on experimental results the model of LIF ro-vibrational transfer has been developed in order to calculate mole fractions of N_2 , O_2 and H_2O in the plasmas with high spatial resolution. The method is used to determine the gas composition in the “plasma jet” working in ambient air with a spatial resolution of better than 1 mm and to calculate the water vapor in the center of glow discharge above water where as high as 10% of H_2O was detected which is explained by non-equilibrium evaporation and sputtering of water surface.

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FT HIGH ROTATIONAL SPECTRUM OF THE $A^3P_0-X^1S^+$ AND $B^3P_1-X^1S^+$ TRANSITIONS OF THE InBr MOLECULE

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The emission spectrum of InBr molecule has been recorded in the region 300-400 nm on BOMEM DA8 Fourier Transform Spectrometer at an apodized resolution of 0.06 cm^{-1} using microwave excitation technique. The rotational structure of (0, 0), (0, 1) and (1, 0) bands of the A-X system of InBr⁷⁹ and (0, 0) band of B-X system has been analyzed and accurate rotational constants of the A^3P_0 and B^3P_1 states are determined. In the (0, 0) band it is possible to observe rotational lines up to $J=300$ or so, which has necessitated invoking of H_0'' . The analysis is confirmed by assigning rotational lines of isotopic species, InBr⁸¹ in the (0, 1) and (1, 0) bands up to $J=195$. In the B^3P_1 state, L- doubling has been found and the coefficient q has been determined for the $v=0$ level. The rotational constants have been determined from the rotational analysis.

ELECTRONIC STRUCTURE AND SPECTROSCOPY OF O_2 AND O_2^+ G. J. Vázquez¹, H. P. Liebermann², H. Lefebvre-Brion³¹Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México (UNAM), Cuernavaca, México 62210²Fachbereich C-Mathematik und Naturwissenschaften, Universität Wuppertal, Gaußstraße 20, Wuppertal, Germany D-42119³Institut des Sciences Moleculaires d'Orsay, Orsay Cedex, France 91405

We carried out a comprehensive ab initio SCF MRD-CI study of the electronic structure of O_2 and O_2^+ . Potential energy curves (PECs) of about 120 electronic states of O_2 and about 80 of O_2^+ , as well as a number of states of O_2^{++} were computed. The cc-pVQZ basis set augmented with diffuse functions was employed. Spectroscopic parameters (T_e , T_v , ω_e , B_e , D_e , D_0 , μ , IP, etc.) are reported for several of the bound states and, generally speaking, a good agreement is found with the experimental counterparts. A preliminary sample of the results will be presented. The electronic absorption spectrum of O_2 has proved difficult to analyze/interpret due to the unusually large number of electronic states which arise from the peculiar open-shell structure of both the oxygen atomic fragments and the O_2 molecule. For instance, there are 62 valence molecular electronic states which correlate to the six lowest dissociation limits resulting from the three valence O-atom fragment states (3P , 1D , 1S). In addition, there are several $n\lambda$ Rydberg series converging to the $X^{2\Pi_g}$ ground ionic state and to the lowest two excited states $A^4\Pi_{ui}$ and $A^2\Pi_u$. Hence, the energy region below about 16 eV, is rather congested with electronic states. Furthermore, a number of interactions of various types among them result in rovibronic perturbations which manifest themselves, e.g., as irregular vibronic structure, hence severely complicating the assignment of the absorption features and the analysis and interpretation of the spectrum. An overview of the electronic states and spectroscopy of O_2 will be presented. A chief motivation of this study of O_2 was to try to provide a theoretical insight on the nature, energetic position, shape, and dissociation asymptotes, of electronic states located in the 4 eV energy region encompassed between the O_2^+ ground state $X^2\Pi_g$ (IP=12.07 eV) and the first excited state $A^4\Pi_{ui}$ (IP= 16.10 eV). This in order to aid in the interpretation of experimental data related to the mechanism(s) of the neutral dissociation of the O_2^{**} superexcited (Rydberg) states, which competes with autoionization. We are currently striving to compute PECs of relatively highly excited states of O_2 located in the 12-16 eV energy region which might help to visualize possible pathways for the neutral XUV photodissociation of the I, I' and I'' $^3\Pi_u$ superexcited states of O_2 leading to the $O(^3P) + O(^3S, ^5S)$ dissociation limits.