

## THE GEISA97 SPECTROSCOPIC DATABANK IN THE CONTEXT OF HIGH SPECTRAL RESOLUTION RADIANCE SIMULATION

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The performances of the second generation vertical sounders like AIRS (Atmospheric Infrared Sounder) in USA, and IASI (Infrared Atmospheric Sounding Interferometer) in Europe will be highly dependent on the accuracy to which the spectroscopic parameters of the optically active atmospheric gases are known. Since 1974, the ARA (Atmospheric Radiation Analysis) group at LMD (Laboratoire de Météorologie Dynamique du CNRS, France) has developed the GEISA (Gestion et Etude des Informations Spectroscopiques Atmosphériques: Management and Study of Atmospheric Spectroscopic Information) computer accessible database system<sup>1,2</sup> to perform reliable radiative transfer calculations. The GEISA database in its 1997 version<sup>3</sup> involves 42 molecules (96 isotopic species) and contains 1,346,266 entries, between 0 and 22,656 cm<sup>-1</sup>. The included molecules are of interest for the Earth and other planet atmospheres (especially the Giant Planets). GEISA97 includes a second catalog providing, at various temperatures and pressures, the cross-sections of species exhibiting dense spectra, not suitable for a discrete parameterized format. A specific spectroscopic database has been issued, from GEISA97, for high resolution radiative transfer simulation, restricted to eleven major atmospheric molecular species : H<sub>2</sub>O, CO<sub>2</sub>, O<sub>3</sub>, N<sub>2</sub>O, CO, CH<sub>4</sub>, O<sub>2</sub>, NO, SO<sub>2</sub>, NO<sub>2</sub>, CH<sub>3</sub>D, N<sub>2</sub>, in the IASI sounding spectral range: 649 - 2800 cm<sup>-1</sup>, with an associated cross-sections database for CFC11 and CFC12, as well. The GEISA97 contents and related files will be presented.

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ELECTRONIC SPECTROSCOPY OF Rg.NO AND N<sub>2</sub>.NO MOLECULAR COMPLEXES

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The  $\bar{A} \leftarrow \bar{X}$ ,  $\bar{C} \leftarrow \bar{X}$ , and  $\bar{E} \leftarrow \bar{X}$  transitions in the Rg.NO and N<sub>2</sub>.NO molecular complexes are studied by REMPI spectroscopy. These transitions are localized on the NO moiety and correspond to Rydberg  $\leftarrow \pi^*$  electronic excitations. Of interest is the fact that the expectation value for the Rydberg radii is comparable to that of the diameter of the Rg atom. Thus there is some competition as to whether the Rydberg electron a bit encompasses the Rg atom or not. In principle, if the excited states of Rg.NO are based on an Rg.NO<sup>+</sup> core, then they should have geometries and vibrational frequencies similar to those of the corresponding cation. This is not the case, indicating that the Rydberg electron is primarily associated with NO<sup>+</sup>, and the Rg atom is interacting with the resulting NO Rydberg state. A progress report on the high resolution LIF study of the  $\bar{A} \leftarrow \bar{X}$  transitions in Rg.NO and N<sub>2</sub>.NO complexes will also be presented.

## MICROWAVE SPECTRUM OF 1-CHLORO-1,2-DIFLUOROETHANE

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The microwave spectrum of 1-chloro-1,2-difluoroethane for normal  $^{35,37}\text{ClCHF-CH}_2\text{F}$  and deuterated species  $^{35,37}\text{ClCHF-CHDF}$  has been studied by a Stark modulation spectrometer. The sample was synthesized by the photochemical reaction of  $\text{CHF}=\text{CHF}$  and  $\text{HCl(DCl)}$  and was separated by gas chromatography.

The spectrum consists of strong *b*-type and weak *a*- and *c*-type transitions. The rotational and nuclear quadrupole coupling constants of chlorine were determined by the least squares fits to the observed transition frequencies. The molecule was found to have a *trans* configuration for the Cl and F atoms. The structural parameters have been determined by the observed rotational constants and were compared with those of *ab initio* calculation and other related molecules. The nuclear quadrupole coupling constants and the C-Cl bond character derived from them are also compared with those of other related molecules.

## The linear HCN trimer: a theoretical investigation including anharmonicity effects

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Large-scale CCSD(T) and CEPA-1 calculations have been carried out for the linear HCN trimer. On the basis of the latter, a 8-dimensional anharmonic potential energy function has been constructed for the stretching vibrations which was used in variational calculations of vibrational term energies, wavefunctions and transition moments. The recommended value for the equilibrium dissociation energy into 3 monomers is  $D_e = 44$  kJ/mol. An accurate equilibrium structure for the trimer is reported. The pseudo-symmetric CH stretching vibration is the strongest stretching vibration and has a transition moment of 0.32 D, 3.9 times larger than that of the unbound CH stretching vibration. The CN stretching vibrations, with transition moments between 0.05 and 0.09 D, are all much stronger than in free HCN ( $|\mu_3| = 0.001$  D). Various predictions are made for overtones and combination tones as well as the deuterated species.

ROTATIONALLY RESOLVED  $A^2\Pi_g \leftarrow X^2\Pi_u$  ELECTRONIC ABSORPTION SPECTRUM OF THE TRIACETYLENE CATION

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We have obtained the high resolution, rotationally resolved absorption spectrum of the  $A^2\Pi_g \leftarrow X^2\Pi_u$  electronic transition of the triacetylene cation ( $H(C\equiv C)_3H^+$ ) and its dideuterated analogue. The cation was produced by discharging a mixture of  $C_2H_2$  or  $C_2D_2$  in He in a hollow cathode geometry that is incorporated in a White Cell. The spectrum was obtained at Doppler-limited resolution using a double modulation technique, that is based on a simultaneous modulation of the output of a dye/Ti:S ringlaser and the ion concentration in the cell. Both technique and details of the rotational analysis of the bands will be presented, yielding for the first time precise rotational and structural parameters and spin-orbit splittings for both electronic states.

HIGH RESOLUTION INFRARED SPECTRA OF OZONE IN THE  
5500 - 5800  $\text{cm}^{-1}$  SPECTRAL RANGE.

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The infrared spectra of  $^{16}\text{O}_3$  have been recorded using a Fourier Transform Spectrometer, operating at  $0.008 \text{ cm}^{-1}$  resolution, with a large pathlength x pressure product ( $3216 \text{ cm} \times 28.3 \text{ Torr}$ ).

Three sets of bands corresponding to  $\Delta v = 6$  have been observed :

-  $\nu_2 + 5\nu_3$  at  $5518 \text{ cm}^{-1}$  and  $\nu_1 + \nu_2 + 4\nu_3$  at  $5540 \text{ cm}^{-1}$ ;

-  $2\nu_1 + \nu_2 + 3\nu_3$  at  $5697 \text{ cm}^{-1}$ ;

-  $\nu_1 + 5\nu_3$  at  $5783 \text{ cm}^{-1}$ .

To correctly reproduce these three sets of observed ro-vibrational transitions using an effective Hamiltonian, it has been necessary to take into account numerous resonance interactions with other highly excited states : (080), (321), (420), (006) and (312).

The agreement between calculated and observed line positions and intensities is very satisfactory, the r.m.s. is near the experimental accuracy.

The parameters for all 9 states, transition moment operators, range of observed transitions and their statistics will be reported.