MONDAY June 21 8:30 AM	TUESDAY June 22 8:30 AM	WEDNESDAY June 23 8:30 AM	THURSDAY June 24 8:30 AM	FRIDAY June 25 8:30 AM
	TA. Mini-symposium: Large Amplitude Motions	WA. Mini-symposium: Large Amplitude Motions	RA. Rotational structure/frequencies	FA. Mini-symposium: Spectroscopy with Undergraduates
	TB. Instrument/Technique Demonstration	WB. Instrument/Technique Demonstration	RB. Mini-symposium: Precision Spectroscopy for Fundamental Physics	FB. Clusters/Complexes
	TC. Dynamics and kinetics	WC. Dynamics and kinetics	RC. Astronomy	FC. Astronomy
	TD. Fundamental interest	WD. Non-covalent interactions	RD. Non-covalent interactions	FD. Small molecules
	TE. Comparing theory and experiment	WE. Theory and Computation	RE. Atmospheric science	FE. Atmospheric science
	TF. Linelists	WF. Linelists	RF. Spectroscopy as an analytical tool	FF. Spectroscopy as an analytical tool
MA. Plenary	TG. Plenary	WG. Plenary	RG. Plenary	FG. Plenary
	TH. Mini-symposium: Large Amplitude Motions	WH. Mini-symposium: Large Amplitude Motions	RH. Mini-symposium: Large Amplitude Motions	FH. Mini-symposium: Spectroscopy with Undergraduates
	TI. Instrument/Technique Demonstration	WI. Mini-symposium: Precision Spectroscopy for Fundamental Physics	RI. Mini-symposium: Precision Spectroscopy for Fundamental Physics	FI. Clusters/Complexes
	TJ. Astronomy	WJ. Astronomy	RJ. Dynamics and kinetics	FJ. Photodissociation and photochemistry
	TK. Comparing theory and experiment	WK. Theory and Computation	RK. Structure determination	FK. Structure determination
	TL. Ions	WL. Large molecules	RL. Electronic structure, potential energy surfaces	FL. Small molecules
	TM. Lineshapes, collisional effects	WM. Radicals	RM. Action spectroscopy (incl. PE, PD, PI, LIR)	FM. Chirality and stereochemistry

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2021

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TE13 **8:48 – 8:49**

TRAJECTORY-BASED SIMULATION OF FAR-INFRARED CIA PROFILES OF CH_4-N_2 FOR MODELING TITAN'S ATMOSPHERE

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Far-infrared opacity of tropospheric and lower stratospheric layers in Titan's atmosphere is dominated by collision-induced absorption (CIA) in various molecular pairs containing N_2, CH_4, and H_2. The presently available spectra of these pairs are often insufficiently accurate for reliably analyzing observed Titan spectra. Analysis of emission spectra from Titan's atmosphere recorded with the Cassini Composite Infrared Spectrometer (CIRS)[a] suggests that the Borysow et al. model[b] for CH_4-N_2 CIA coefficients underestimates absorption by about 50%.

We present the trajectory-based study of the rototranslational CIA band in CH_4-N_2. Assuming rigid monomers, potential energy and induced dipole are characterized quantum-chemically at the CCSD(T)/CCSD(T)-F12b levels of theory. The Monte Carlo strategy is adopted to obtain the dipole autocorrelation function. The original procedure is employed to sample initial conditions throughout the phase space of a molecular pair. The autocorrelation function is derived from an ensemble of 5 to 10 million classical trajectories obtained through the solution of Hamilton equations in the space-fixed reference frame. The Fourier transform of the autocorrelation function yields the CIA band profile. We propose a new semiempirical model for CH_4-N_2 CIA that allows us to reproduce CIRS spectra recorded at low and high emission angles in the equatorial region[a]. This work is partially supported by RFBR-CNRS grant 18-55-16006 and NASA HITRAN grant.

[a]Bézard et al. (2020). Icarus. 344, 113261.
[b]Borysow, et al. (1993). Icarus. 105, 175.

TF. Linelists

Tuesday, June 22, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Frances M Skinner, Harvard-Smithsonian Center for Astrophysics, Malden, MA, USA

TF01 **8:00 – 8:01**

HITRAN2020: ACT (ACCURACY, COMPLETENESS, TRACEABILITY)

IOULI E GORDON, LAURENCE S. ROTHMAN, ROBERT J. HARGREAVES, ROBAB HASHEMI, EKATERINA KARLOVETS, FRANCES M SKINNER, ARTEM FINENKO, EAMON K CONWAY, KYLE NELSON, TIJS KARMAN, *Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, USA*; YAN TAN, *Hefei National Laboratory for Physical Science at Microscale, University of Science and Technology of China, Hefei, China*; ROMAN KOCHANOV, *Laboratory of Quantum Molecular Mechanics and Radiation Processes, Tomsk State University, Tomsk, Russia*; CHRISTIAN HILL, *Atomic and Molecular Data Unit, International Atomic Energy Agency, Vienna, Austria*.

The HITRAN2020 database will be publicly released this year. It is a coordinated effort of experimentalists, theoreticians, atmospheric and planetary scientists who measure, calculate and validate the HITRAN data. The lists for most of the HITRAN molecules in the line-by-line section were updated in comparison with the previous compilation HITRAN2016[a]. The extent of the updates ranges from updating a few lines of certain molecules to complete replacements of the lists and introducing additional isotopologues. Six new molecules (SO, CH_3F, GeH_4, CS_2, CH_3I, and NF_3) were also added to HITRAN. In addition, the accuracy of the parameters for major atmospheric absorbers has been increased, often featuring sub-percent uncertainties. The number of parameters was also increased significantly, now incorporating, for instance, non-Voigt line profiles for many gases; broadening by water vapor[b]; update of collision-induced absorption sets[c].

The new edition will continue taking advantage of the modern structure and interface available at www.hitran.org and the HITRAN Application Programming Interface[d]. Their functionality has been extended for the new edition. This talk will provide a brief overview of HITRAN2020[e] and its main improvements with respect to the previous edition.

[a]Gordon et al., (2017). JQSRT. 203, 3–69.
[b]Tan et al., (2019) J. Geophys. Res. Atmos. 2019JD030929.
[c]Karman et al., (2019) Icarus 328, 160–175.
[d]Kochanov et al., (2016) JQSRT. 177, 15–30.
[e]This work is supported by NASA.

TF02 **8:04 – 8:05**

A URANIUM ATLAS IN ASCII FORMAT, 20000 – 27000 cm^{-1}

AMANDA J. ROSS, PATRICK CROZET, *Inst. Lumière Matière, Univ Lyon 1 & CNRS, Université de Lyon, Villeurbanne, France*; DENNIS W. TOKARYK, *Department of Physics, University of New Brunswick, Fredericton, NB, Canada*; ALLAN G. ADAM, *Department of Chemistry, University of New Brunswick, Fredericton, NB, Canada*.

This work was motivated by difficulties encountered while trying to calibrate laser excitation spectra, taken in short (1 cm^{-1}) scans around 438 nm, by matching optogalvanic transitions from a Uranium-Argon hollow cathode lamp to peaks listed in a widely-circulated 'informal report' on the Uranium spectrum (11000 –25900 cm^{-1}) from Los Alamos[a]. Short pieces of excitation spectra often fell between secure calibration lines, because many of the weaker features had been excluded from the printed linelist. To remedy this, we have re-recorded emission from a commercial Uranium hollow-cathode lamp 19800 – 27400 cm^{-1} on a Fourier transform spectrometer, at an instrumental resolution of at 0.04 cm^{-1}. The wavenumber scale was fine-tuned to match earlier reference data[abc] to within 0.003 cm^{-1}. This spectrum (together with its peak list) is proposed in ascii format[d] as a possible aid to calibration of laser excitation spectra in the blue, violet and near UV. It extends the spectrum reported by Sarmiento and co-workers[b] that focused on calibration of astronomical spectrographs in the near IR and visible.

[a]An atlas of uranium emission intensities in a hollow cathode discharge; Palmer, Keller & Engleman, Los Alamos report LA 8251-MS, (1980)
[b]Comparing the emission spectra of U and Th hollow cathode lamps, and a new U line list; Sarmiento *et al.*, A & A, 618, A118, (2018)
[c]Uranium and iodine standards measured by means of Fourier-transform spectroscopy; Gerstenkorn, *et al.*, A & A, 58, 255-66, (1977)
[d]A uranium atlas, from 365 to 505 nm; Ross *et al.* J Mol Spectrosc , 369, 111270, (2020)