Book of Abstracts 27th Colloquium on High-Resolution Molecular Spectroscopy (HRMS Cologne 2021)

The 27th Colloquium on High-Resolution Molecular Spectroscopy (HRMS) was initially planned on-site. Due to the Covid-19 pandemic, the event is held for the first time as an online conference to fulfill the regulations of the government and to facilitate safe exchange of scientific information.

There are 11 invited lectures and 3 mini-symposia. Parallel sessions feature 54 contributed lectures given by PhD students and postdocs. 4 poster sessions are planned. The scientific fields covered are:

- High resolution rotational, vibrational, and electronic spectroscopy of molecules (radicals, ions, complexes, clusters, ...)
- Molecular dynamics
- Theory assisting the prediction, simulation, and interpretation of spectra
- New techniques for high-resolution spectroscopy
- Applications to atmospheric sciences, astrophysics, planetology, combustion, gas-phase biomolecules, metrology and fundamental physics, cold molecules, etc.

Program Overview

Japan (JST)	Europe (CEST)	US EST (EDT)	US West (PDT)	Sunday 29 Aug 2021	Monday 30 Aug 2021	Tuesday 31 Aug 2021	Wednesday 1 Sep 2021	Thursday 2 Sep 2021	Friday 3 Sep 2021
18.00 h	11.00 h	5.00 h	2.00 h						
						D Mini-Symposium: Precision Spectroscopy (4x 30min)			
19.00 h	12.00 h	6.00 h	3.00 h		A Poster Session 1		G Contributed Talks (3 parallel sessions à 6x 15min)	K Contributed Talks (3 parallel sessions à 6x 15min)	F/N Poster Session 2
20.00 h	13.00 h	7.00 h	4.00 h						
21.00 h	14.00 h	8.00 h	5.00 h	Welcome and Opening Lecture	B Invited Lectures (2x 45min)	E Invited Lectures (2x 45min)	H Invited Lectures (2x 45min)	L Invited Lectures (2x 45min)	O Invited Lectures (2x 45min)
22.00 h	15.00 h	9.00 h	6.00 h						
23.00 h	16.00 h	10.00 h	7.00 h		C Contributed Talks (3 parallel sessions à 6x 15min)	F Poster Session 2	I Mini-Symposium: Laboratory Astrophysics and Spectroscopy (4x 30min)	A/M Poster Session 1	P Mini-Symposium: Environmental and Atmospheric Spectroscopy (4x 30min)
24.00 h	17.00 h	11.00 h	8.00 h						
1.00 h	18.00 h	12.00 h	9.00 h						

Program, Sunday, August 29, 2021

14.00	**Welcome Address by the organizers** ***Prof. Stephan Schlemmer***, I. Institute of Physics, University of Cologne, Germany Chair of HRMS 2021 ***Prof. Frédéric Merkt***, Laboratory Physical Chemistry, ETH Zürich, Switzerland Member of the HRMS Executive Committee
14.10	**HRMS 2021 Opening Lecture** ***Pascale Ehrenfreund***, Space Policy Institute, George Washington University, U.S.A. «The search for life in our Solar System»
15.00	**International Dr. Barbara Mez-Starck Prize 2021** ***Dr. Jürgen Vogt,*** Member of the presiding board of the Dr. Barbara Mez-Starck-Foundation, Announcement of two laureates of the international Dr. Barbara Mez-Starck Prize for structural chemistry and molecular physics
15:20	End of day 1

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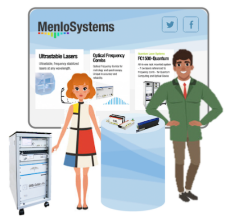

Beyond the horizon: HITRAN2020 and HITEMP data for planetary atmospheres

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The recently-released 2020 edition of the HITRAN database has continued efforts to include and improve appropriate spectroscopic data for studying a variety of planetary atmospheres. In particular, line lists for key atmospheric species (e.g., SO_2, NH_3, C_2H_2, PH_3) have received substantial updates, compared to HITRAN2016 [1], which include extending spectral coverage and improving line positions, intensities, and broadening coefficients. There are currently 55 molecules with line-by-line parameters in HITRAN, with new species being included for HITRAN2020 that have particular relevance to planetary atmospheres (e.g., GeH_4, CS_2, SO). Furthermore, additional planetary-relevant absorption cross-sections and collision-induced absorption data are now included. Pressure-broadening parameters (and their temperature dependencies) for H_2, He, CO_2 and H_2O are also provided for numerous species, allowing opacities to be calculated using HITRAN data for a variety of planetary atmospheres, including Venus, Mars, and Jupiter.

The temperature range of planetary atmospheres can substantially exceed those found on Earth, therefore it is necessary to account for significantly more transitions when modelling high-temperatures environments. In addition, high-resolution observations require accurate spectroscopic parameters to enable characterization of these atmospheres. The HITEMP database [2] provides line-by-line parameters for use at high temperature and has recently been undergoing a significant upgrade. HITEMP line lists are now available for N_2O, NO_2 [3] and CH_4 [4], while the CO, NO and OH line lists have been updated [3,5]. For CH_4, an intensity compression technique has been introduced that is capable of being accurate at modelling high-temperature spectra, and also practical to use [4].

The additions of planetary-relevant molecules and spectroscopic parameters for HITRAN2020 will be discussed, along with recent updates to the HITEMP database. Note that a companion poster by I. Gordon will discuss the improvements in HITRAN2020 that are relevant to the remote sensing of terrestrial atmosphere.

[1] I. E. Gordon, et al., *J. Quant. Spectrosc. Radiat. Transfer*, **2016**, 203, 3-67.

[2] L. S. Rothman, et al., *J. Quant. Spectrosc. Radiat. Transfer*, **2010**, 111, 2139-2150.

[3] R. J. Hargreaves, et al., *J. Quant. Spectrosc. Radiat. Transfer*, **2019**, 232, 35-53.

[4] R. J. Hargreaves, et al., *Astrophys. J. Supp. Ser.*, **2020**, 247, A55.

[5] G. Li, et al., *Astrophys. J. Supp. Ser.*, **2015**, 216, A15.

Continuum absorption by pure CO_2 and CO_2-Ar mixture at millimeter waves: Meticulous measurements and classical trajectory-based simulation

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We acknowledge full co-authorship of A. A. Balashov, M. A. Koshelev and A. O. Koroleva from Institute of Applied Physics RAS, Nizhny Novgorod, Russia.

This study of the millimeter wave continuum absorption in the CO_2-X (X=Ar, CO_2) mixtures was, in particular, inspired by the success of the classical trajectory-based formalism recently developed to simulate collision-induced absorption (CIA) spectra [1-3]. On the one hand, the agreement, once achieved, between experimental data and the calculated results promotes a better understanding of the nature of the continuum on a much broader scale. On the other hand, the knowledge of the CO_2 continuum is required to model the radiative processes in the CO_2-rich planetary atmospheres, such as those of Venus and Mars.

Experimental spectra of continuum absorption in pure CO_2 and a mixture of CO_2 with Ar were recorded at room temperature and pressures up to 2 atm using a resonator spectrometer [4]. Measurements covered 105-240 GHz range allowing determining frequency dependence of the continuum absorption.

The agreement between the measured and trajectory-based data supports the reliability of both our experimental and theoretical methods. Previously available experimental data on the CO_2-X millimeter wave continuum were obtained on a rare frequency grid and, in general, are characterized by unsatisfactory accuracy. Classical trajectory-based formalism made it possible to examine the variation of the far-infrared/mw spectral profile of CO_2-Ar dimer as a function of temperature. The structureless pedestal of the CIA profile corresponding to free/quasibound pairs states is supplemented by the weak signatures of intermolecular vibrational bands of true dimers. Conspicuous fingerprints of intermolecular vibrational bands are seen at extremely low temperatures, which transform to the CIA-like, virtually structureless envelope as the temperature of the simulation increases.

This work was partially supported by RFBR projects No. 18-55-16006.

[1] Daniil Oparin et al, J Quant Spectrosc Radiat Transfer, **2017**, 196, 87-93.

[2] Daniil Chistikov et al, J Chem Physics, **2019**, 151(19), 194106.

[3] Tatyana Odintsova et al, J Quant Spectrosc Radiat Transfer, **2021**, 258, 107400.

[4] Maksim Koshelev et al, IEEE Transactions on Terahertz Science and Technology, **2018**, 8(6), 773.

HITRAN2020 and remote sensing of the terrestrial atmosphere

I. E. Gordon[1], R. J. Hargreaves[1], L. S. Rothman[1], R. Hashemi[1], E. V. Karlovets[1], F. S. Skinner[1], E. K. Conway[1], A. A. Finenko[2,1], R. V. Kochanov[3,1]

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The HITRAN database is essential to the remote sensing of the terrestrial atmosphere. The new 2020 edition of the database will be presented. It is a coordinated effort that includes dozens of international experimentalists, theoreticians, atmospheric and planetary scientists who measure, calculate and validate the HITRAN data.

The lists for almost all of the HITRAN molecules in the line-by-line section were updated (and several additional molecules have been added) in comparison with the previous compilation HITRAN2016 [1]. The extent of these improvements range from updating a few lines of certain molecules to complete replacements of the lists and introducing additional isotopologues. Many new vibrational bands were added to the database, extending the spectral coverage and completeness of the line lists. Six new molecules were also added to HITRAN, including CH_3F, CS_2, CH_3I, and NF_3 that are all important for remote sensing. 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 [2,3]; broadening by water vapor [4]; update of collision-induced absorption sets [5],to name a few.

The HITRAN2020 edition continues to take advantage of the new database structure and interface available at www.hitran.org [6] and through the HITRAN Application Programming Interface (HAPI) [7].The functionality of both tools has been extended for the new edition.

Some of the validation efforts will be demonstrated. Note, a parallel poster by R. Hargreaves regarding improvements concerning planetary atmospheres.

This work is supported by NASA

[1] Gordon et al., *JQSRT,* **2017,** 203, 3–69.
[2] Hashemi et al., *JQSRT*, **2020,** 256, 107283.
[3] Hashemi et al., *JQSRT*, **2021,** 271, 107735.
[4] Tan et al., *J. Geophys. Res. Atmos.,* **2019,** 2019JD030929
[5] Karman et al., *Icarus.,***2019,** 328, 160–175.
[6] Hill et al., *JQSRT*, **2016,** 177, 4–14.
[7] Kochanov et al., *JQSRT*, **2016,** 177, 15–30.