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Laboratory spectroscopy for astrophysics: Festschrift for Stephan Schlemmer

1. Introduction

The present Virtual Special Issue (VSI), "Laboratory Spectroscopy for Astrophysics", celebrates Stephan Schlemmer's remarkable contributions to the field of molecular spectroscopy, molecular collisions, and laboratory astrophysics over the last three decades, on the occasion of his 60th birthday on September 7, 2020. This VSI, guest edited by three of the authors (P. J., J. O. and H.S.P.M.), contains contributions covering all relevant forms of molecular spectroscopy, in particular involving laboratory astrophysics in the microwave, infrared or XUV part of the spectrum, at high or low resolution.

2. Curriculum vitae and scientific work

Stephan was born on September 7th, 1960, in Wuppertal, Germany. He studied physics first in his home town, and later in one of the most renowned academic centers in Germany, at the Max-Planck-Institut für Strömungsforschung in Göttingen (now known as the Max-Planck-Institut für Dynamik und Selbstorganisation). One of his notable experiences was to see Friedrich H. Hund, the "inventor" of the various Hund's cases, while being already in his 90s, giving a three-semester series of lectures about the history of quantum theory. In his Göttingen time, Stephan performed crossed molecular beam experiments, in particular on the famous prototype reaction $F + H_2$ [1–3], and finished his PhD studies with a thesis entitled "High-resolution investigations of inelastic and reactive scattering of small molecules". By the end of 1991, he continued research as a postdoctoral fellow first at the Universitá degli Studi di Perugia (Italy) with Piergiorgio Casavecchia, and in 1992 in the group of Richard J. Saykally at the University of California at Berkeley, where he used a cryogenic single-photon infrared spectrometer to obtain emission spectra of candidate interstellar aromatic molecules [4,5]. In 1994 he joined the laboratory of Dieter Gerlich at the Technische Universität Chemnitz (Germany). Gerlich (who sadly passed away in October 2020) was a recognized expert for low-temperature ion trapping techniques. According to Stephan, it was an interesting experience to arrive in an East-German town just four years after the German reunification. Together, Stephan and Dieter pioneered the development of the powerful action-spectroscopy technique of 'Laser Induced Reactions' (LIR), featuring an extremely high sensitivity that makes it possible to record high-resolution spectra of only a few hundred mass-selected ions stored in a cold ion trap. This novel method was first tested on cations of fundamental interest, such as $C_2H_2^+$ [6] and N_2^+ [7], but has since then been applied to many ions, both positively and negatively charged [8–16]. Stephan has been continuously developing novel ion trap machinery subsequently while further extending the toolbox of action spectroscopic methods, first at the Sterrewacht Leiden (2003–2004) in the Netherlands, and since October 2004 at the I. Physikalisches Institut of the Universität zu Köln in Germany. Working in this stimulating "astrophysical environment", it was his particular aim to develop action spectroscopic schemes for the measurement of purely rotational fingerprints of cold ions ([17,12,18–20], see also the 2017 special issue volume 332 "Spectroscopy in Ion Traps" of this journal). These novel methods have led to fundamental discoveries in astrochemistry, e.g., the laboratory and astronomical detection of the fundamental rotational transition of para-

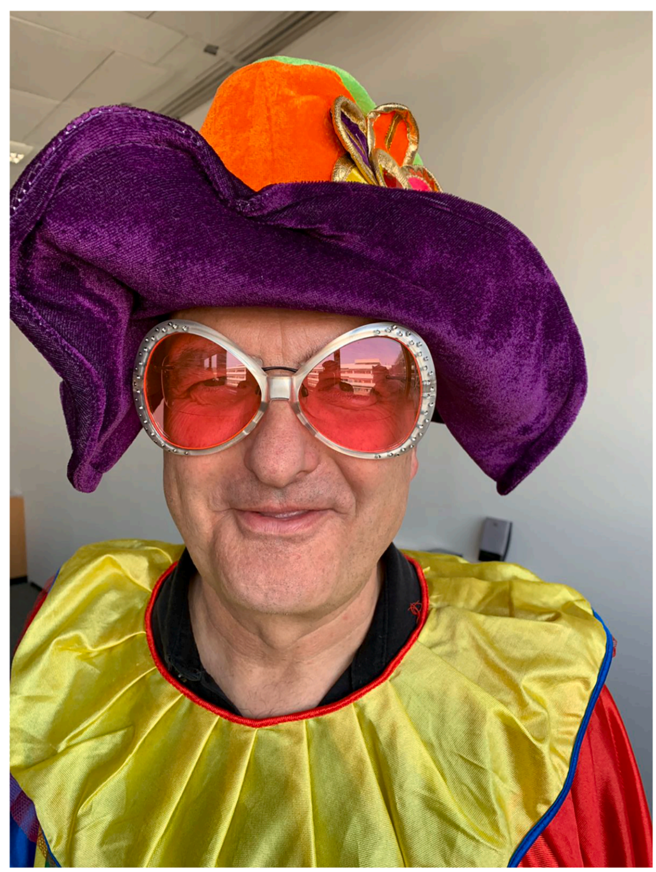

Fig. 1. Stephan Schlemmer at the institute's carnival party 2019 in Köln featuring his most favorite lab coat.

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H_2D^+ and ortho-D_2H^+ [17,21,22].

But the molecule that captivated Stephan's interest most thoroughly is the one referred to as the 'enfant terrible of molecular spectroscopy' by Takeshi Oka [23]: protonated methane, CH_5^+. Seeing that conventional spectroscopic methods struggle to provide an understanding of the dynamics of this floppy molecule (for instance, spectra recorded early on by Oka and coworkers [24] were too crowded to allow interpretation) was one of the reasons why Stephan joined Dieter Gerlich's group and developed the low-temperature LIR approach. This work led first to the recording of a low-resolution overview spectrum [25,26] of CH_5^+, and later to a spectrum [27,28,23] containing 2897 highly resolved lines, which enabled the determination of combination differences in the ground vibrational state [29]. With these energy level patterns in the ground state established, a first zeroth-order superrotor model of CH_5^+ has been developed by Stephan, Hanno Schmiedt and Per Jensen [30]. The same authors also showed in a seminal paper [31] that for molecules belonging to the $\boldsymbol{G}_{240}$ nuclear permutation-inversion group (i.e., the molecular symmetry group of CH_5^+), a separate symmetry classification of vibrational and rotational wavefunctions is impossible. Therefore CH_5^+ has no purely rotational spectrum; the low-energy spectrum is rovibrational.

In the course of these studies, Stephan pushed the development of new ion trapping machines operating at the lowest possible temperatures, at the moment 4 K, and the combination of these apparatuses with different radiation sources. Two new machines have been constructed in the Köln laboratories [32] with the help of some of the authors of this Editorial and with Sandra Brünken. Based on Stephan's long-standing collaboration with researchers at the Free Electron Laser for Infrared eXperiments (FELIX) Laboratory [33] at Radboud University in Nijmegen, The Netherlands, one of these machines, called FELion [34], is now permanently coupled to the IR beamline and available as user facility. The combination of a cryogenic ion trap with the widely tunable IR radiation of FELIX enabled Stephan and his coworkers to obtain the first cryogenic vibrational fingerprints of hitherto undetected cationic molecules. Many of his (young) group members travel regularly to Nijmegen to run FELIX beam-shifts day and night and to enjoy Dutch language and lifestyle. Six papers in this VSI are based on experiments performed at FELIX, three of which employ FELion.

Stephan inherited the millimeter to terahertz equipment from his predecessor Gisbert Winnewisser, which has been updated and modified considerably over the years. His group continued to investigate in particular molecules of radio-astronomical interest usually with high sensitivity and high accuracy. Early works include a study on HSOD and the determination of the structure of HSOH [35], and an extensive study on SiS [36], a heavy homolog of the CO molecule. Among later investigations are those of *iso*-propyl cyanide [37], which was detected later in space as the first molecule with a branched backbone, acetic acid [38], propanal [39], and of isotopic thioformaldehyde with determination of structural parameters [40]. Among the more recent publications is a series of papers on methanethiol isotopologs, the latest one on $^{13}CH_3SH$ [41]. Three contributions in this VSI are based on millimeter to terahertz measurements in Cologne.

In addition, the arsenal of mm-wave spectrometers has been enriched with state-of-the art modern equipment over the years, driven by Stephan and Nadine Wehres. One route were emission spectrometers that use radio astronomical heterodyne receiver technology to capture the instantaneous room-temperature emission of molecules, and operate in the range 270–390 GHz (coincident with Band 7 of the ALMA telescope) [42,43] and 75–110 GHz (Band 3 of ALMA) [44]. Another route were the construction of several chirped pulse spectrometers [45], the highest frequency one now operating in the range 70–110 GHz. Noteworthy is also the intracavity millimeter jet spectrometer OROTRON, which was already employed by Gisbert Winnewisser, Leonid Surin, and Igor Pak [46]. Stephan and Leonid with students and colleagues produced many interesting results, for example on the CO dimer [47], clusters of few He atoms with CO [48], rotational and rovibrational spectra of the H_2-CO van der Waals complex [49], and rotational spectra of the H_2-NH_3 complex [50]. One contribution in this VSI is based on measurements with both the Köln OROTRON and chirped pulse spectrometers.

One project particularly close to Stephan's heart is the Cologne Database for Molecular Spectroscopy[1] [51–53]. Despite its importance for astronomers, in particular those involved in radio-astronomical observations, it was frequently affected by funding problems as it was often deemed being not scientific enough for one funding agency, but too scientific for another one.

3. Prizes and international collaborations

Stephan has published more than 220 papers in international peer-reviewed journals, as well as book articles, representing important contributions in the field of high resolution molecular spectroscopy and astrochemistry. He has been awarded several prizes, including the Otto-Hahn Medal for his PhD thesis in 1992 (awarded by the Max-Planck-Society), the Morino lectureship for chemical physics (Morino foundation, Japan) in 2009, and the Gay-Lussac-Humboldt Prize in 2015 (awarded by the French Ministry for Education and Research). Very recently, he has been awarded an ERC Advanced Grant, which will enable him to investigate his favourite molecules in even more detail in the future. Over the years, he supervised dozens of PhD, master and bachelor students.

Along with his scientific endeavours, Stephan has fostered with great enthusiasm exchange with many groups in the world for many years. As a result, the Cologne Astrophysics Laboratory has been the part-time home of many national and international visitors. Frequent or longer staying visitors include Adam Walters from Toulouse, France, Li-Hong Xu and Ron M. Lees from Saint John, NB, Canada, Jean-Baptiste Bossa from Leiden, The Netherlands at that time, Patrice Theulé from Marseille, France, Marie-Aline Martin-Drumel from Paris, France, José L. Doménech from Madrid, Spain, Charles R. Markus, who is now at Caltech, USA, John B. Dudek from Hartwick College, Oneonta, USA, Igor Savić from Novi Sad, Serbia, Hiroshi Kohguchi and some of his students from Hiroshima, Japan, Kaori Kobayashi from Toyama, Japan, Jean-Claude Guillemin from Rennes, France, Vadim Ilyushin from Kharkiv, Ukraine, and Sven Herbers, now in Nijmegen, The Netherlands. One especially notable visitor over the years (since 1998!) has been Koichi Yamada. His visits were initially hosted by Gisbert Winnewisser and later by Stephan and Thomas Giesen, who is now professor in Kassel, Germany. The prolific scientific exchange as well as spending time with old friends were obvious reasons for his many visits. Another one was to visit a particular winery at the Ahr river, sample selected wines, and get a few bottles shipped to his home in Japan. We may point out that (red) wine from the Ahr is also appreciated by Stephan and by some of the authors of this Editorial.

Stephan is known for his very modest and friendly personality, creating a family-like atmosphere in the Cologne group. The group very often celebrates common parties, dinners, outings, and, perhaps most important as Fig. 1 shows, the annual carnival in Köln (which are all obviously dearly missed during the Covid pandemic). In his free time, Stephan enjoys very much riding his (steel vintage) road bike, to repair and build things at home, and to spend "quality time" with his wife Tamara and his son Paul.

4. Papers in this VSI

This Virtual Special Issue (VSI) comprises 35 contributions, which are listed in the reference section below in order of their appearance [54–88]. The contributions cover very diverse fields. One very large

[1] https://cdms.astro.uni-koeln.de/

group involves rotational, vibrational, or rovibrational spectroscopy of complex organic molecules, starting with the relatively small methanol molecule whose Zeeman effect was studied extensively at millimeter wavelengths [54]. Another contribution deals with the millimeter-wave spectrum of the $^{13}CH_3OD$ isotopic species [81]. Extensive rotation-vibration interactions in low-lying vibrational states of CH_3CN were revealed [70]. Investigations of slightly larger molecules involve vinylacetylene [79], acetylacetylene [62], propanoic acid [87], ethyl methyl ether [64], methyl cyanoacetate [65], and propylene oxide [66]. Among the mono-cyclic aromatic molecules are phenylpropiolonitrile [58] and imidazole [72]. Various contributions describe studies of larger carbonaceous compounds, such as photo-electron spectroscopy of seven oxygen-containing molecules [67], and infrared studies of 1-cyano- and 1-isocyanoadamantane [78] and polyaromatic species [77,76] up to sizes of more than 40 C-atoms [82].

An impressive number of reports deal with ions and radicals, most of them cations, whose investigations were frequently carried out employing ion traps including 22-pole traps from Cologne. The contributions deal with the diatomics NO^+ [68] and NO [83] and with the early universe molecule candidate H_2He^+ [57]. Three manuscripts address one of Stephan's favorite molecules, H_3^+: one involving recombination [71], one proposing how to access very highly excited rovibrational levels [84], and one on forbidden rotational transitions and their importance to astrophysics [88]. Rovibrational spectra of CH^+-He and CH^+-He_4 are also reported [55]. One article describes infrared spectra and structural aspects of cations consisting of the 5d metals Pt, Ir, or Ta and CH_2 [80]. The hyperfine-resolved rotational spectrum of D_2CCN was studied [69] after HDCCN was detected in space. One contribution deals with the vibrational spectrum of the iminomethylium ion [85] and one with protonated glycine [86]. Reports on optical spectra involve $Si_4C_2^+$ [59], or phenol, aniline, and cyclopentadiene radical cations [73]. Two papers deal with the vibrational spectra of cations derived from large polycyclic aromatic hydrocarbons [76,82].

Finally, molecules not belonging to these main categories include an extensive study of the rovibrational spectra of several TiO isotopologs [61], the electronic spectra of C_3 isotopologs with one ^{13}C [74], a quantum-chemical study of HAlNP [56], an extension of the hyperfine characterization of NH_2D and NHD_2 [60], the rotational spectroscopy of symmetrically deuterated isotopologs of NH_3-H_2 [63], and an infrared spectroscopic characterization of SeC_3Se [75].

Stephan's interests and collaborations are very diverse. Two important manuscripts intended to be part of the Festschrift, however, did not fit into the scope of the Journal of Molecular Spectroscopy and thus appear elsewhere. One is concerned with the vibrational spectra of $LiCl_2^-$ solvated by one to three water molecules [89], and one with the ammonia snow line in young stellar objects and the desorption of ammonium salts [92].

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