

DIVISION B / COMMISSION 5 / WORKING GROUP SPECTROSCOPIC AND RADIATIVE DATA FOR MOLECULES

| | |
|-------------------|----------------------------|
| CHAIR | Steven R. Federman |
| VICE-CHAIR | Peter F. Bernath |
| VICE-CHAIR | Holger S. P. Müller |

TRIENNIAL REPORT 2015-2017

1. Introduction

The current report covers the period from 2015 to 2017. As in our previous reports, it is divided into three areas covering rotational, vibrational, and electronic spectroscopy. A significant amount of experimental and theoretical work has been accomplished during this period, leading to the expansion of a number of databases whose links are provided below. Rather than being exhaustive, space limitations only allow us to highlight a representative sample of work on molecular spectra. Related research on collisions, reactions on grain surfaces, and astrochemistry are not included here.

2. Rotational Spectra

A large number of reports have appeared dealing with rotational spectra of molecules potentially relevant to radio-astronomical observations. Therefore, emphasis will be put on investigations dealing with molecular species already observed in space, and on molecules related to these molecules. A few observational papers are mentioned to highlight some recent findings. The grouping of the molecules has been modified slightly with respect to the previous report. Neutral organic molecules form the first group. In particular, complex organic molecules are very important for ALMA, and they have attracted considerable attention in the last three years. But we include here some unsaturated molecules which are more common in dark clouds and also smaller ones. Molecules which (may) occur in circumstellar envelopes of late type stars form the second group. Additional groups deal with hydrides, with radicals or cations with more than one heavy atom, or with other molecules. For completeness, we also include determinations of transition frequencies from radio astronomical observations, provided these are of sufficient importance as well as some rovibrational studies if their impact may have been significant enough for rotational data.

Several databases provide rotational spectra of (mostly) molecular species of astrophysical and astrochemical relevance. The most important source for predictions generated from experimental data by employing appropriate Hamiltonian models is the Cologne Database for Molecular Spectroscopy, CDMS (<http://www.astro.uni-koeln.de/cdms/>) (Müller et al. 2001, 2005) with its catalog (<http://www.astro.uni-koeln.de/cdms/catalog>). The JPL catalog (<http://spec.jpl.nasa.gov/>) (Pickett et al. 1998) continues to have some importance even if only very few new or updated entries have been created in recent years. Both web sites also provide primary information, i.e., laboratory data with uncertainties, mostly in special archive sections. Additional primary data are available in the Toyama

Microwave Atlas (<http://www.sci.u-toyama.ac.jp/phys/4ken/atlas/>). A useful resource on the detection of certain molecular transitions in space is the NIST Recommended Rest Frequencies for Observed Interstellar Molecular Microwave Transitions, which has been updated some years ago (Lovas 2004).

The European FP7 project Virtual Atomic and Molecular Data Centre, VAMDC, (<http://www.vamdc.org/>) aims at combining several spectroscopic, collisional, and kinetic databases. The CDMS is the rotational spectroscopy database taking part (<http://cdms.ph1.uni-koeln.de/cdms/portal/>); a recent report (Endres et al. 2016) provides information on the implementation. In addition, considerations involving experimental data and their uncertainties, spectroscopic parameters, and other issues related to creating CDMS catalog entries have been discussed. Recently, the JPL catalog has joined the VAMDC consortium; several infrared databases are also involved. The project has been described recently by Dubernet et al. (2016).

Other tertiary sources combining data from various databases are, e.g., Cassis (<http://cassis.cesr.fr/>), which provides tools to analyze astronomical spectra, lamda (<http://www.strw.leidenuniv.nl/~moldata/>) which also contains collisional data, or splatalogue (<http://www.splatalogue.net/>). These databases rely heavily on the CDMS and JPL catalogs for their rotational data. This applies in part also to the infrared databases HITRAN and GEISA for selected rotational or rovibrational data.

We also point out articles on using the spectroscopy programs SPFIT (Novick 2016; Drouin 2017) and PGOPHER (Western 2017).

2.1. Neutral organic molecules

Roughly half of the publications relevant for rotational spectroscopy belong to this class of molecules despite a somewhat stricter criterion for studies to be included in this section. Saturated molecules dominate in the warm and dense parts of star-forming regions, the so-called hot cores and hot corinos, and only few molecules with CC double or triple bonds have been found in these environments. Highly unsaturated molecules dominate, in contrast, in the cold and dense parts of star-forming regions, especially in dark clouds. The less dense envelopes of star-forming regions may harbor saturated as well as unsaturated molecules, and UV radiation may alter the chemistry even further.

Many exciting results have been obtained with ALMA and sometimes with other interferometers, but we want to point out that actually quite a few of the newly detected molecules were found with single dish instruments such as the 100 m Green Bank Telescope in the USA or the IRAM 30 m dish in Spain.

One of the observational highlights mentioned in our previous report, not only among the complex organic molecules, was the detection of the first branched alkyl compound in space, *iso*-propyl cyanide, in the course of an unbiased molecular line-survey of Sagittarius (Sgr) B2(N) at 3 mm which was called EMOCA, Exploring Molecular Complexity with ALMA. A very remarkable recent finding concerns propylene oxide, also known as methyloxirane, the first chiral molecule detected in space with the 100 m GBT toward the Galactic Center. But it was found in the envelope of Sgr B2, not in any of its hot cores (McGuire et al. 2016a). Its rotational spectrum was extended subsequently well into the submillimeter region (Mesko et al. 2017).

The line strengths of ethyl cyanide in the EMOCA survey were so strong that the detectability of isotopologues with two ^{13}C appeared plausible. Margulès et al. (2016a) investigated the rotational spectra of all three isotopomers of $\text{C}_2\text{H}_5\text{CN}$ with two ^{13}C and reported on their detection in the EMOCA data set. The line intensities were also used

to estimate which vibrationally excited states of C_2H_5CN isotopologues without, with one ^{13}C , and even two ^{13}C may be observable in that data set provided laboratory data become available. Müller et al. (2016c) studied the rotational spectra of the four lowest excited vibrational states of each of the two conformers of *n*-propyl cyanide and reported the detection of lines of all of these states in the EMOCA data set.

Other investigations of alkyl cyanides include rotational and rovibrational spectra of CH_3CN (Müller et al. 2015b), rotational spectra of CH_3CN isotopic species with one ^{13}C or one ^{15}N (Müller et al. 2016a), the rotational spectrum of $^{13}C_2H_5^{13}CN$ (Pienkina et al. 2017), rotational spectra of isotopic species of *iso*-propyl cyanide or in excited vibrational states (Arenas et al. 2017a; Kolesníková et al. 2017b), and the rotational spectrum of the lowest energy conformer of 2-cyanobutane (Müller et al. 2017).

Additional studies of cyanides deal with rotational and rovibrational spectra of HC_3N (Bizzocchi et al. 2017b), the far-infrared (FIR) spectrum of vinyl cyanide (Kisiel et al. 2015), and the rotational spectra of hydroxyacetonitrile (Margulès et al. 2017), vibrationally excited states of aminoacetonitrile (Kolesníková et al. 2017a; Degli Esposti et al. 2017) (also with isotopic species), and carbonyl dicyanide (Bteich et al. 2016).

Halfen et al. (2015b) extended the assignments for methyl isocyanate somewhat and found the molecules to be abundant in the Sgr B2(N) hot core. Cernicharo et al. (2016) corrected some of those assignments and presented a greatly extended line list for this molecule. However, the characterization of its rotational spectrum is not complete because it is very complicated due to two large amplitude motions. They found this molecule to be also abundant in Orion KL. Interestingly, it turned out that the molecule is by far not as abundant in comet 67P/Churyumov-Gerasimenko as initial reports suggested. A study on methyl cyanate by Kolesníková et al. (2016) is mentioned in this context.

Studies of alkanols include CH_3OH excited to its CO stretching and energetically close lying states (Pearson et al. 2015), hyperfine studies on CH_3OH (Coudert et al. 2015; Belov et al. 2016), and investigations of CHD_2OH (Ndao et al. 2016) and mono-deuterated ethanol (Walters et al. 2015). Müller et al. (2016b) demonstrated how important proper intensities are in a rotational spectrum with complex torsion-rotation interaction, here in the case of ethanol. They also pointed out the disadvantages of the commonly used set-up of the two-state Hamiltonian of tunneling spectra, here ethanethiol, and the advantages of an alternative approach. Finally, they also reported the detection of ethanol isotopomers with one ^{13}C . Zakharenko et al. (2017) and Arenas et al. (2017) studied 1,2-propanediol.

Zakharenko et al. (2015) investigated numerous formaldehyde isotopologues with one or two D, while Müller & Lewen (2017) studied $H_2C^{17}O$ along with $H_2C^{18}O$ and $H_2C^{16}O$. The ^{13}C isotopomers of ethanal (acetaldehyde) were studied by Margulès et al. (2015), and Zingsheim et al. (2017) investigated conformers and vibrational states of propanal. An extensive report on the rotational spectrum of propenal in several vibrational states was also reported (Daly et al. 2015). Studies of highly unsaturated aldehydes involve the FIR spectrum of propynal (Barros et al. 2015) and the microwave spectra of pentadiynal and heptatriynal (McCarthy et al. 2017).

Among the sulfur-containing species studied were dimethyl sulfide (Jabri et al. 2016), propynethial (Crabtree et al. 2016), pentadiynethial (Crabtree et al. 2016; McCarthy et al. 2017), and numerous isotopologues of HNCs isomers (McGuire et al. 2016b).

Other investigations dealt with the temperature dependent spectrum of methyl formate between 215 and 265 GHz (McMillan et al. 2016), the terahertz spectrum of methyl formate deuterated at the acid group (Duan et al. 2015), the rotational spectra of vinyl formate (Alonso et al. 2016), the ^{13}C isotopomers of methylamine (Motiyenko et al.

2016), N-methyl formamide with a tentative detection (Belloche et al. 2017), isotopic species of propene (Craig et al. 2016), and glycolic acid (Kisiel et al. 2016).

Particularly noteworthy are studies of the low-lying (near 2 THz) bending modes of all stable isotopologues of C_3 by Breier et al. (2016) and of the rotational spectrum of HDC_3 in order to verify its detection in space (Spezzano et al. 2016).

The detection of $CH_3^{35}Cl$ and $CH_3^{37}Cl$ and the tentative detection of CH_3F in the Protostellar Interferometric Line Survey (PILS) of IRAS 16293–2422 with ALMA in band 7 (Fayolle et al. 2017) came as a considerable surprise. In this context we mention the study of the CH_3F rotational spectrum by Cazzoli & Puzzarini (2015).

2.2. Circumstellar molecules

Initially, detections of molecules in CSEs were commonly made toward C-rich stars, in particular CW Leonis, also known as IRC +10216. Among the molecules detected in space, fairly specific ones for this type of environment are most Si- and several P-containing molecules, metal cyanides and isocyanides as well as metal halides; some metal halides have also been found in the envelopes of O-rich late-type stars. Carbon chain molecules, including some anionic ones, are found toward C-rich stars, but also in dark clouds.

One remarkable success example is the laboratory spectroscopy of Si_2C (McCarthy et al. 2015b) which immediately led to its detection (Cernicharo et al. 2015). In addition, the wealth of astronomical lines improved the spectroscopic parameters considerably. A very important contribution was the study of the millimeter wave spectroscopy of CCN (Anderson et al. 2015) which led to its earlier reported detection.

Other investigations include vibrationally excited C_3H (McCarthy et al. 2015a) and C_4H (Cooksy et al. 2015), the metal hydrides AlH and CrH (Halfen & Ziurys 2016), the molecules CrC and $CrCCH$ (Min & Ziurys 2016), $NaCl$ (Cabezas et al. 2016), $HNSi$ (McCarthy et al. 2015c), and $ZnSH$ (Bucchino et al. 2017).

We mention furthermore publications on molecules which may appear quite exotic from our present knowledge, but which may turn out to be not that far-fetched eventually. The molecules include silaisocyanides $XNSi$ with X being HC_2 , HC_4 , and NC (Thorwirth et al. 2015a), the heavier $HNCO$ homologs $HPCO$ and $HNSiO$ (Thorwirth et al. 2015b), and ScN , YN , and $BaNH$ (Zack et al. 2015).

Among the molecules specific for O-rich circumstellar envelopes (CSEs) of late-type stars are monoxides, including the metal-containing AlO and TiO , the hydroxide $AlOH$, and the dioxide TiO_2 . Some metal halides, e.g., $AlCl$ and $NaCl$ were found in O-rich as well as C-rich AGB stars. The investigations of isotopic TiO (Lincowski et al. 2016) and of ScO (Halfen et al. 2017) are particularly noteworthy, and that on YOH (Halfen et al. 2015a) may be mentioned.

2.3. Hydrides

Hydrides are here all molecules consisting of one non-metal atom and one or more H atoms. They may be neutral or charged. Metal hydrides have been dealt with in subsection 2.2. Even though the *Herschel* mission was terminated late in April 2013, data are still being analyzed. Moreover, the German REceiver At Terahertz frequencies (GREAT) on board of the Stratospheric Observatory For Infrared Astronomy (SOFIA) has opened new observing capabilities above 1 THz. In addition, transitions of heavier hydrides or higher rotationally excited transitions of lighter asymmetric top hydrides, such as H_2O , can be observed from the ground and may be of particular importance for ALMA.

Rovibrational studies on H_3^+ (Jusko et al. 2016) and rotational studies on HD_2^+ (Yu et al. 2017) and on H_2D^+ as well as HD_2^+ (Jusko et al. 2017a) were performed. Investigations of carbon hydrides include rotational spectroscopy of CH_2D^+ (Töpfer et al. 2016), rovibrational and rotational spectroscopy of CHD_2^+ (Jusko et al. 2017b), terahertz spectroscopy of CH_3D (Bray et al. 2017), and the determination of ground state combination differences (GSCDs) of CH_5^+ by Asvany et al. (2015), a first step in the high-resolution characterization of this very fluxional cation. $^{15}\text{NH}_2$ (Margulès et al. 2016b), ND_2 (Melosso et al. 2017), NH_3 (Sung et al. 2016; Pearson et al. 2016), $^{15}\text{NH}_3$ (Fusina et al. 2017), and NH_3D^+ (Stoffels et al. 2016) were among the nitrogen hydrides studied. Oxygen hydride studies include a very accurate IR study on OH^+ (Markus et al. 2016), terahertz spectroscopy of HD^{18}O (Yu et al. 2016), submillimeter spectroscopy of HDO (Cazzoli et al. 2015), HD^{17}O and D_2^{17}O (Puzzarini et al. 2015), and the refinement of spectroscopic parameters of H_2O^+ based on ALMA observations of a foreground galaxy in the direction of PKS 1830–211 by Muller et al. (2016).

Investigations of heavier hydrides include a rotational and rovibrational study of SiH^+ (Doménech et al. 2017), reinvestigation of the $N = 1 - 0$ transitions of SH^+ (Halfen & Ziurys 2015), an IR study of HCl^+ (Doménech et al. 2016), and a study of the ArH^+ $J = 1 - 0$ transitions (Bizzocchi et al. 2016). Muller et al. (2017) identified one misassignment in the $N = 1 - 0$ transitions of SH^+ reported by Halfen & Ziurys (2015), used the corrected data with additional rest frequencies to refine the SH^+ spectroscopic parameters, determined approximate rest frequencies for $^{34}\text{SH}^+$ (neglecting the breakdown of the Born-Oppenheimer approximation, which causes errors of order of 1 MHz), and detected extragalactic SH^+ and $^{34}\text{SH}^+$.

2.4. Radicals and cations

Neutral and cationic hydrides were mentioned in subsection 2.3. With regard to heavier radicals or cations, the laboratory spectroscopy of hydroxymethyl (Bermudez et al. 2017) and HOCO^+ and DOCO^+ (Bizzocchi et al. 2017a) are particularly noteworthy. Other species studied were methoxy (Laas & Widicus Weaver 2017), HSO (Cazzoli et al. 2016), $^{15}\text{N}_2\text{H}^+$ and $^{15}\text{N}_2\text{D}^+$ (Dore et al. 2017), N_2H^+ and N_2D^+ (Yu et al. 2015), as well as C_3H^+ (McCarthy et al. 2015a) and CF^+ (Stoffels et al. 2016).

2.5. Other molecules

We mention measurements of N^{18}O and the combined analysis with all other data of (nearly) microwave accuracy (Müller et al. 2015a), similar studies on SO isotopologs (Martin-Drumel et al. 2015b; Lattanzi et al. 2015) along with a study of the SO dimer (Martin-Drumel et al. 2015a) and high-precision measurements of OCS in its ground vibrational state (Golubiatnikov et al. 2017).

3. Vibrational Spectra

The vibration-rotation spectra of molecules of astronomical or of potential astronomical interest are reviewed for the period 2015-2017 (with a few papers from early 2018) starting from the end of our previous report (Federman et al. 2016). In addition to the references to particular molecules given below, there are a number of spectral database compilations that are useful. Perhaps the most helpful is the HITRAN database that contains vibration-rotation line parameters for a large number of species such as H_2O , CO_2 , CO , HF , HCl and so forth, found primarily in the Earth's atmosphere. A new edition has appeared, HITRAN 2016, Gordon et al. (2017); additional information is

available†. The new distribution method (HITRAN*online*‡) uses an SQL database rather than fixed character records for the line parameters that more easily allows the compilation of non-Voigt lineshape parameters and pressure-broadening data for broadeners such as H₂, He, and CO₂ (Wilzewski et al. 2016) of interest in astronomy. The molecular coverage is slowly being expanded to include planetary atmospheres other than Earth and HITRAN 2016 contains line parameters for C₂N₂ and COCl₂. HITRAN is intended for applications near room temperature so care is needed for applications at higher temperatures because of potential missing lines and bands.

There are a number of web sites that have collections of spectroscopic line lists or infrared absorption cross sections that are updated regularly. The ExoMol site¶ of J. Tennyson and co-workers (Tennyson et al. 2016) has an extensive collection of calculated line lists designed “as input to atmospheric models of exoplanets, brown dwarfs and cool stars.” The GEISA database (Jacquinet-Husson et al. 2016) has vibration-rotation parameters. A very useful set of infrared absorption cross sections for several hundred molecules are available from the Pacific Northwest National Laboratory||, PNNL, for the 600-6500 cm⁻¹ (1.54-16.7 μm) range (Sharpe et al. 2004). While the PNNL spectra are not always suitable for astronomical applications because they are recorded with 1 atm of nitrogen as a broadening gas at sample temperatures of 278, 293, and 323 K, they can be very useful. A large subset of the PNNL data are now included in HITRAN 2016.

3.1. Diatomic molecules

Infrared observations from the ground are increasingly important with instruments such as Phoenix, CRILES+, and TEXES in spite of strong telluric interference. The EXES instrument on the SOFIA aircraft is particularly promising because it flies in the stratosphere above most of the Earth’s atmosphere.

Hydrogen is the most abundant element in the Universe‡ so it is no surprise that small diatomic hydrides are also abundant. For the simplest hydrides, H₂, HD (Vasilchenko et al. 2016), and D₂ (Mondelain et al. 2016), new near infrared laboratory measurements have been made by the ultrasensitive technique of cavity ring-down spectroscopy.

The vibration-rotation transitions of SiH⁺ (Doménech et al. 2017) and HCl⁺ (Doménech et al. 2016) have been detected by difference frequency laser spectroscopy of a hollow cathode discharge. The A³Π-X³Σ⁺ transition OH⁺ was re-analyzed from a Fourier transform emission spectrum (Hodges & Bernath 2017) and new fundamental vibration-rotation lines were included (Markus et al. 2016). The line parameters were much improved and a high level *ab initio* calculation of the A-X transition dipole moment function and the ground state dipole moment function were carried out. The end results were line lists with line intensities for the A-X transition and the vibration-rotation lines (Hodges et al. 2018). The OH⁺ radical is a key molecule for the formation of water in dark interstellar clouds and has also been detected in diffuse clouds (Porras et al. 2014). The new vibration-rotation line list will facilitate detection in the infrared region.

An extensive revision of the NH and OH line parameters has been carried out. These new infrared line lists were created using reliable dipole moment functions and inclusion of the Herman-Wallis effect using Le Roy’s LEVEL computer program (Le Roy 2017) and Western’s PGOPHER program (Western 2017). The NH (Brooke et al. 2015) and OH (Brooke et al. 2016) work adds line intensities to our previous analyses of line positions

† <http://www.cfa.harvard.edu/hitran/>

‡ <http://hitran.org/>

¶ <http://www.exomol.com/>

|| <http://nwir.pnl.gov>

based partly on the solar spectrum, and are recommended for stellar abundance analyses.

The ExoMol line lists now include AlO (Patrascu et al. 2015), NaH (Rivlin et al. 2015), CS (Paulose et al. 2015), CaO (Yurchenko et al. 2016), VO (McKemmish et al. 2016), NO (Wong et al. 2017a), PO (Prajapat et al. 2017), PS (Prajapat et al. 2017), and SiH (Yurchenko et al. 2017a). These new line lists combine experimental measurements and *ab initio* calculations. For AlO, NaH, CaO, VO, PS, and SiH, the line lists include electronic transitions as well as vibration-rotation bands. All of the TiO experimental data has been collected and a consistent set of rovibronic energy levels derived by least-squares fitting of the line positions (McKemmish et al. 2017).

Salt vapors such as LiF and LiCl are predicted to be present in hot super-Earth exoplanets (Schaefer et al. 2012). New vibration-rotation line lists have been created for LiF, LiCl (Bittner & Bernath 2018), NaF, KF (Frohman et al. 2016), MgF (Hou & Bernath 2017), and CaF (Hou & Bernath 2018) by combining line positions from infrared emission spectra with line strengths obtained using *ab initio* dipole moment functions.

CO is arguably the most important molecule in observational astronomy. The line lists for CO and its isotopologues have been completely revised (Li et al. 2015) and the line intensities for the overtone transitions are substantially improved. Although not vibration-rotation transitions, the Ballik-Ramsay and Phillips Systems of C₂ are prominent in the near infrared and a new perturbation analysis has demonstrated that the singlet-triplet splitting was in error by 3 cm⁻¹ (Chen et al. 2015). This analysis has astronomical implications for example in the excitation of C₂ in comets by solar radiation. The C₂ B¹Δ_g-A¹Π_u and B¹Σ_g⁺-A¹Π_u infrared electronic transitions have been extended to higher vibrational levels (Chen et al. 2016). All existing transitions of C₂ have been collected in a consistent set of rovibronic energy levels derived in a MARVEL (Measured Active Rotational-Vibrational Energy Levels) analysis (Furtenbacher et al. 2016).

3.2. Small polyatomic molecules

The line parameters of water, ammonia, and methane (as well as PH₃, SO₂, H₂S, CO₂, H₂CO, HCN, C₂H₂, C₄H₂, etc.) as given in the HITRAN 2016 database (Gordon et al. 2017) are generally satisfactory for most astronomical purposes at low temperatures, except for overtone and combination bands in the near infrared and visible regions. New partition functions for 51 molecules important in planetary atmospheres have been calculated by Gamache et al. (2017). For H₂O, new sensitive absorption measurements in the near infrared have been made in transparency windows by cavity ring-down spectroscopy (Campargue et al. 2017, 2015) and a new database compiled (Mikhailenko, et al. 2016). For NH₃, near infrared (Barton et al. 2017) and visible (Zobov et al. 2018) archival spectra recorded at Kitt Peak have been analyzed with the help of a new theoretical line list (Polyansky et al. 2016). For CH₄, additional empirical line lists have been made based on cavity ring-down spectroscopy for ¹³CH₄ (Campargue et al. 2016) and near 1 μm by Fourier transform spectroscopy (Béguier et al. 2015), and analyses of previous line lists carried out with new calculations (Rey et al. 2016; Nikitin et al. 2016). For C₂H₂, three new spectral databases have been compiled (Lyulin & Perevalov 2017; Amyay et al. 2016a; Lyulin & Campargue 2017) and a MARVEL analysis of all spectroscopic data carried out by Chubb et al. (2018). For CO₂, work continues with calculated line lists (Zak et al. 2016, 2017) and a database (Tashkun et al. 2015) for applications for Venus and Mars.

The spectroscopy of small ions benefits from new techniques such as ion traps and

frequency comb spectroscopy; at the University of Cologne new high precision spectra of H_3^+ and isotopologues (Jusko et al. 2016), CD_2H^+ (Jusko et al. 2017b), and CH_5^+ (Asvany et al. 2015) have been recorded. IR spectra of the carbon-chain molecules triacetylene (C_6H_2) (Chang et al. 2016) and C_5S (Thorwirth et al. 2017) have been recorded in a jet expansion source. New vibration-rotation line lists for PH_3 (Sousa-Silva et al. 2015), H_2CO (Al Derzi et al. 2015b), HNO_3 (Pavlyuchko et al. 2015), SO_2 (Underwood et al. 2016a), H_2O_2 (Al-Refaie et al. 2016), H_2S (Azzam et al. 2016), SO_3 (Underwood et al. 2016b), H_2^{17}O , H_2^{18}O (Polyansky et al. 2017), H_3^+ (Mizus et al. 2017), and SiH_4 (Owens et al. 2017) are available as part of ExoMol.

The spectra of hot molecules needed to simulate the spectra of cool stars, brown dwarfs, and exoplanets remain a challenge. The HITEMP database (Rothman et al. 2010) is still recommended for hot H_2O because the calculated line positions are replaced by experimental lines if they are available. For hot ammonia, laboratory spectra recorded in absorption are available (Beale et al. 2017) with some quantum number assignments obtained with the help of theoretical predictions, a MARVEL analysis of rovibrational energy levels (Al Derzi et al. 2015a), and empirical lower state energies.

There is considerable progress on the spectroscopy of hot methane with the experimental line lists of Hargreaves et al. (2015a) from absorption spectra and the analysis of emission spectra by Amyay et al. (2016b). Hargreaves et al. (2015a) describe the first experimental observations of a quasi-continuum that was predicted theoretically, but not previously observed. The basic idea is that high resolution spectra of small hot molecules can be represented by a relatively small number of strong lines and the rest of the lines (many billions) form a quasi-continuum. Two new high temperature calculated line lists for hot methane have been published. Rey et al. (2017) calculated more than 150 billion vibration-rotation transitions to model the spectrum of methane up to 3000 K; data are available on their web site†. Yurchenko et al. (2017b) have also calculated a very extensive new methane line list. Both of these new line lists have adopted the idea of using a few million “strong” lines and a quasi-continuum typically represented as “super-lines” that can be used to generate hot methane spectra. As demonstrated by Hargreaves et al. (2015a), this quasi-continuum is required to model the observed spectral energy distributions of brown dwarfs.

3.3. Large molecules

With the identification of interstellar C_{60}^+ in the near IR, there is continuing strong interest in large carbon-containing molecules such as C_{60} and polycyclic aromatic hydrocarbons (PAHs). For PAH molecules, the NASA-Ames database (now version 3.0) has been updated in 2018 and new features added (Bauschlicher et al. 2018). Extensive calculations by the NASA-Ames group and others have continued, for example, on dehydrogenated PAHs (Mackie et al. 2015), nitrogen-containing PAHs (Mattioda et al. 2017), and the effect of aliphatic groups on PAH spectra (Sadjadi et al. 2015). Spectra of several jet-cooled PAHs in the C-H stretching region were recorded by Maltseva et al. (2016). The IR spectra of $\text{C}_{42}\text{H}_{18}^+$ were recorded by infrared multiphoton dissociation of ions stored a trap using radiation from a free electron laser (Zhen et al. 2017).

For larger molecules, line-by-line spectroscopic data is typically not available or is not very useful because of missing hot bands and/or minor isotopologues. Infrared absorption cross sections are then needed to model astronomical observations. Although not often the case, these cross sections should be based on spectra recorded under similar conditions

† <http://theorets.univ-reims.fr/>

of pressure, temperature, and composition as found in the astronomical object. Such high resolution cross sections are becoming available for example for benzene (C_6H_6) with N_2 , H_2 -He broadeners at low temperatures for the atmospheres of Titan and Jupiter (Sung et al. 2016). Infrared absorption cross sections for cold propane broadened by hydrogen (Wong et al. 2017b) and helium (Wong et al. 2017c) have also been recently been published. For hot Jupiter exoplanets, cross sections for high temperature hydrocarbons are needed and data in the 3 μm region have been recorded for ethane (Hargreaves et al. 2015b), propane (Beale et al. 2016), and propene (Buzan et al. 2016). The quasi-continuum found for hot methane is even more prominent for other small hot hydrocarbons.

4. Electronic Spectra

This section focuses on electronic spectra, including line identification, energy levels, and related data needed for photochemical models. Absorption cross sections (or equivalently lifetimes, transition probabilities, and oscillator strengths), predissociation widths and rates, and analyses of anomalies in line strength and width caused by perturbations between energy levels are presented. Results from both experimental and theoretical efforts are given. The four topics discussed here are interstellar matter (including diffuse molecular clouds, disks around newly formed stars, and comets whose chemistry is similar), metal hydrides and oxides in the atmospheres of late-type stars, the atmospheres of planets and their satellites, and larger molecules. Of particular note are a topical review on theoretical calculations of open shell molecules (Tennyson et al. 2016) and three comprehensive studies where a significant body of results are compiled. Furtenbacher et al. (2016) describe an analysis for six singlet, six triplet, and two quintet states in $^{12}C_2$. The same group performed a similar analysis on eleven low-lying electronic states in $^{48}Ti^{16}O$ (McKemmish et al. 2017). Moreover, Dapra et al. (2016) present an updated database of wavelengths, oscillator strengths, and damping parameters for CO transitions from the $X^1\Sigma^+$ ground state to the $A^1\Pi$, $B^1\Sigma^+$, $C^1\Sigma^+$, $E^1\Pi$, and $d^3\Delta$ electronic states. We also note that Heays et al. (2017) assembled photodissociation and photoionization cross sections for molecules of astrochemical interest.

4.1. Interstellar matter

A significant body of new results on CO, N_2 , and C_2 appeared in the past three years. Analysis of perturbations was a main focus of the work on CO. Spectroscopic studies revealed perturbations of the $A^1\Pi$ state for $^{12}C^{16}O$ (Ostrowska-Kopeć et al. 2015; Niu et al. 2015b, 2016b), for $^{13}C^{16}O$ (Niu et al. 2016a), $^{12}C^{18}O$ (Trivikram et al. 2017), $^{12}C^{17}O$ (Hakalla 2015; Hakalla et al. 2016), and $^{13}C^{17}O$ (Hakalla et al. 2017). Niu et al. (2015a) studied perturbations in the main isotopologues of CO and N_2 at high temperature (900 K). Experimental oscillator strengths were a focus of the work by Lemaire et al. (2016) on $A^1\Pi-X^1\Sigma^+$ bands in $^{13}C^{18}O$, by Kang et al. (2015) on transitions from the ground electronic state involving the $A^1\Pi$, $C^1\Sigma^+$, and $E^1\Pi$ states in the main isotopologue, and by Eidelsberg et al. (2017) on $W^1\Pi-X^1\Sigma^+$ bands and the Rydberg complexes between 92.9 and 93.5 nm in $^{13}C^{18}O$. Eidelsberg et al. (2017) also determined predissociation rates from their spectra. Theoretical efforts examined the isotopic dependence of predissociation in the $E^1\Pi$ state (Lefebvre-Brion & Majumder 2015), as well as predissociation (Lefebvre-Brion & Kalemos 2016a) and associated branching ratios (Lefebvre-Brion & Kalemos 2016b) for the $W^1\Pi$ state in $^{12}C^{16}O$.

A number of contributions on N_2 appeared during the past three years. Oscillator

strengths were obtained for valence shell excitations experimentally (Liu et al. 2016) and theoretically (Lavín & Velasco 2016, 2017). An *ab initio* calculation (Ni et al. 2017) provided line intensities for bands in the $A^3\Sigma_u^+-B^3\Pi_g$ system. Branching ratios for channels leading to N_2 photodissociation were measured by Song et al. (2016). Lefebvre (2015) studied perturbations involving the valence $b^1\Sigma_u^+$ and $c^1\Sigma_u^+$ states. Last, Hollenstein et al. (2017) demonstrated a new experimental technique by obtaining data on N_2 .

Results on singlet, triplet, and quintet states of C_2 were reported. Chen et al. (2015) recorded spectra of the Phillips system ($A^1\Pi_u-X^1\Sigma_g^+$), while Chen et al. (2016) studied bands in the $B^1\Delta_g-A^1\Pi_u$ and $B^1\Sigma_g^+-A^1\Pi_u$ systems. Chen et al. (2015) also examined the Ballik-Ramsay system ($b^3\Sigma_g^- - a^3\Pi_u$). Other efforts on transitions involving triplet states included the lowest thirteen vibrational levels in the $e^3\Pi_g$ state (Welsh et al. 2017) and observations of bands associated with the $3^3\Pi_g$ (Krechivska et al. 2017) and $4^3\Pi_g$ (Krechivska et al. 2015) states. The measurements also yielded a pathway to C_2 dissociation (Welsh et al. 2017) and new determinations of the ionization energies for the $a^3\Pi_u$ and $X^1\Sigma_g^+$ states (Krechivska et al. 2016). Bornhauser et al. (2015) and Bornhauser et al. (2017) analyzed spectra of $1^5\Pi_u-1^5\Pi_g$ bands and described the presence of predissociation in the high-lying quintet state and perturbations involving vibrational levels in the $d^3\Pi_g$ state. A theoretical study (Sharma 2015) yielded excitation energies for the eight lowest lying excited states.

Results for simple hydrides, their ions, and their isotopologues appeared in print. For carbon-bearing molecules, CH photoionization (Gans et al. 2016), CH^+ photoionization (O'Connor et al. 2016), spectra of the $B^2\Sigma^- - X^2\Pi$ system in CD (Szajna et al. 2017), and the Renner-Teller levels of the \tilde{A} state in CCH (Tokaryk et al. 2015) were studied. Zhao et al. (2015a) detected new transitions of $A^3\Pi - X^3\Sigma^-$ bands for OH^+ in interstellar spectra from which they obtained improved line positions and oscillator strengths, and Hodges & Bernath (2017) derived molecular constants for this system from laboratory spectra. Zhao et al. (2015b) detected absorption from the $A^2\Sigma^+ - X^2\Pi$ (0,0) band of SH in diffuse clouds and compiled line positions and oscillator strengths for future studies. SH^+ photodissociation cross sections were determined theoretically by McMillan et al. (2016). For completeness, we note that the transition dipole moment between the $X^1\Sigma_g^+$ and $B^1\Sigma_u^+$ states of H_2 (Simmen et al. 2014) and the photodissociation cross sections of H_2^+ (Babb 2015; Zammit et al. 2017) were obtained from theoretical calculations.

Other relevant molecules were studied in the recent past. Electronic spectra of CS_2 were acquired by Sunanda et al. (2015), and cross sections for photoabsorption, photoionization, and photodissociation of CS_2 were measured by Holland & Shaw (2016). Additional work on photodissociation included theoretical studies on NH_3 (Xie et al. 2015), HCN and HNC (Chenel et al. 2016; Aguado et al. 2017), and H_2CO (Tanaka et al. 2017). Tanaka et al. (2017) also calculated photoionization cross sections. A new set of potential energy surfaces (Ndengué et al. 2016) were obtained in a study of Renner-Teller coupling in HCO.

4.2. Late-type stars

During the reporting period a number of studies on hydrides, carbides, and oxides, including charged species, appeared. Experiments on the $b^3\Sigma^- - a^3\Pi$ system of AlH were performed by Szajna et al. (2017). Steglich & Maier (2015) examined electronic transitions in silicon carbide compounds and SiC_6H_4 through a combination of measurements and theoretical calculations. Three papers described new results on CaH, its ions, and isotopologues. Watanabe et al. (2016) analyzed the first two excited $^2\Sigma^+$ states of CaH,

Velasco et al. (2017) calculated oscillator strengths and photoionization cross sections for Rydberg series in CaH, and Condoluci et al. (2017) reassigned vibronic transitions in the $1^1\Sigma$ and $2^1\Sigma$ states in CaH⁺ from observations of spectra for CaD⁺. A study of the $C^1\Sigma^+-X^1\Sigma^+$ and $F^1\Pi-X^1\Sigma^+$ transitions in CaO (Stewart et al. 2016) also appeared. Spectra of the $D^2\Sigma^+-X^2\Sigma^+$ transitions in YO were obtained by Zhang et al. (2017). Computations of spectroscopic constants were reported for the $X^1\Sigma^+$ and $1^3\Pi$ states of AlO⁺ (Sghaier et al. 2016). Spectroscopic constants and lifetimes were calculated for low-lying singlet and triplet states in MgO (Bauschlicher & Schwenke 2017) and for singlet states in SiO (Bauschlicher 2016).

4.3. Planetary atmospheres

SO₂ continues to draw attention. Spectral studies of the \tilde{C}^1B_2 state include the experimental efforts of Park et al. (2015), Park et al. (2016a), Jiang et al. (2016), and Park et al. (2016b) and theoretical calculations by Klos et al. (2016), Jiang et al. (2017), and Zak & Tennyson (2017). Furthermore, L ev eque et al. (2015) provide theoretical assignments of the Clements bands.

Other studies focused on S₂ and O₂. Zhang et al. (2015) computed a potential energy curve and spectroscopic constants for the $b^1\Sigma_g^+$ state of S₂, while Sarka et al. (2017) examined the electronic properties and isotope effects theoretically for triplet states in this molecule. As for O₂, a comprehensive analysis yielded energy levels, band constants, and potentials for the $X^3\Sigma^-$, $a^1\Delta_g$, and $b^1\Sigma_g^+$ states for six isotopologues (Yu et al. 2014), and Lefebvre-Brion et al. (2016) reported an *ab initio* study of quintet states. Germann & Willitsch (2016) developed a theory to treat fine- and hyper-fine structure in O₂ photoionization.

4.4. Larger molecules

Work continued on taking spectra of large carbon-bearing species in order to reveal the species responsible for absorption seen as Diffuse Interstellar Bands. Maier and his group acquired data from matrix and gas-phase experiments on HC₅H and H₂C₅ (Steglich et al. 2015), oxygen-containing polycyclic hydrocarbon cations and protonated analogues (Chakraborty et al. 2015), C₇H₃⁺ (Rice et al. 2015), oxygenated carbon chain cations (Hardy et al. 2016), C₅H and its cation (Fulara et al. 2016), coronene and corannulene cations (Hardy et al. 2017), and C₄₂H₁₈⁺ (Campbell & Maier 2017b). Other efforts include the measurements on protonated nitrogen-based PAHs (Noble et al. 2015), photoionization and photodissociation of toluene (Monfredini et al. 2016), and the photo-stability of hydrogenated PAHs (Wolf et al. 2016). Fullerene cations were also studied (Strelnikov et al. 2015; Campbell et al. 2016a,b; Campbell & Maier 2017a; Spieler et al. 2017).

Steven R. Federman
Chair of Working Group

References

- Aguado, A., Roncero, O., Zanchet, A., Ag undez, M., & Cernicharo, J. 2017, *ApJ*, 838, 33
 Al Derzi, A. R., Furtenbacher, T., Tennyson, J. Yurchenko, S. N., & Cs asz ar, A. G. 2015a, *JQSRT*, 161, 117
 Al Derzi, A. R., Yachmenev, A., Tennyson, J., & Yurchenko, S. N. 2015b, *MNRAS*, 448, 1704
 Al-Refaeie, A. F., Polyansky, O. L., Ovsyannikov, R. I., Tennyson, J., & Yurchenko, S. N. 2016, *MNRAS*, 461, 1012
 Alonso, E. R., Kolesnikov a, L., Tercero, B., et al. 2016, *ApJ*, 832, 42

- Amyay, B., Fayt, A., Herman, M., & Vander Auwera, J. 2016a, *JPhChRD*, 45, 023103
- Amyay, B., Louviot, M., Pirali, O., et al. 2016b, *JChPh*, 144, 024312
- Anderson, J. K., Halfen, D. T., & Ziurys, L. M. 2015, *JMoSp*, 307, 1
- Arenas, B. E., Gruet, S., Steber, A. L., Giuliano, B. M., & Schnell, M. 2017a, *PCCP*, 19, 1751
- Arenas, B. E., Gruet, S., Steber, A. L., & Schnell, M. 2017, *JMoSp*, 337, 9
- Asvany, O., Yamada, K. M. T., Brünken, S., Potapov, A., & Schlemmer, S. 2015, *Sci*, 347, 1346
- Azzam, A. A. A., Tennyson, J., Yurchenko, S. N., & Naumenko, O. V. 2016, *MNRAS*, 460, 4063
- Babb, J. F. 2015, *ApJS*, 216, 21
- Barros, J., Appadoo, D., McNaughton, D., et al. 2015, *JMoSp*, 307, 44
- Barton, E. J., Polyansky, O. L., Yurchenko, S. N., et al. 2017, *JQSRT*, 203, 392
- Bauschlicher, C. W. 2016, *CPL*, 658, 76
- Bauschlicher, C. W., Ricca, A., Boersma, C., & Allamandola, L. J. 2018, *ApJS*, 234, 32
- Bauschlicher, C. W., & Schwenke, D. W. 2017, *CPL*, 683, 62
- Beale, C. A., Hargreaves, R. J., & Bernath, P. F. 2016, *JQSRT*, 182, 219
- Beale, C. A., Hargreaves, R. J., Coles, P., Tennyson, J., & Bernath, P. F. 2017, *JQSRT*, 203, 410
- Béguier, S., Liu, A. W., & Campargue, A. 2015, *JQSRT*, 166, 6
- Belloche, A., Meshcheryakov, A. A., Garrod, R. T., et al. 2017, *A&A*, 601, A49
- Belov, S. P., Golubiatnikov, G. Y., Lapinov, A. V., et al. 2016, *JChPh*, 145, 024307
- Bermudez, C., Bailleux, S., & Cernicharo, J. 2017, *A&A*, 598, A9
- Bittner, D. M., & Bernath, P. F. 2018, *ApJS*, 235, 8
- Bizzocchi, L., Dore, L., Degli Esposti, C., & Tamassia, F. 2016, *ApJ*, 820, L26
- Bizzocchi, L., Lattanzi, V., Laas, J., et al. 2017a, *A&A*, 602, A34
- Bizzocchi, L., Tamassia, F., Laas, J., et al. 2017b, *ApJS*, 233, 11
- Bornhauser, P., Marquardt, R., Gourlaouen, C., et al. 2015, *JChPh*, 142, 094313
- Bornhauser, P., Visser, B., Beck, M., et al. 2017, *JChPh*, 146, 114309
- Bray, C., Cuisset, A., Hindle, F., et al. 2017, *JQSRT*, 189, 198
- Breier, A. A., Büchling, T., Schnierer, R., et al. 2016, *JChPh*, 145, 234302
- Brooke, J. S. A., Bernath, P. F., & Western, C. M. 2015, *JChPh*, 143, 026101
- Brooke, J. S. A., Bernath, P. F., Western, C. M., et al. 2016, *JQSRT*, 168, 142
- Bteich, S. B., Tercero, B., Cernicharo, J., et al. 2016, *A&A*, 592, A43
- Bucchino, M. P., Adande, G. R., Halfen, D. T., & Ziurys, L. M. 2017, *JChPh*, 147, 154313
- Buzan, E. M., Hargreaves, R. J., & Bernath, P. F. 2016, *MolAs*, 3-4, 16
- Cabezas, C., Cernicharo, J., Quintana-Lacaci, G., et al. 2016, *ApJ*, 825, 150
- Campargue, A., Béguier, S., Zbiri, Y., et al. 2016, *JMoSp*, 326, 115
- Campargue, A., Mikhailenko, S. N., Lohan, B. G., et al. 2015, *JQSRT*, 157, 135
- Campargue, A., Mikhailenko, S. N., Vasilchenko, S., et al. 2017, *JQSRT*, 189, 407
- Campbell, E. K., Holz, M., & Maier, J. P. 2016, *ApJ*, 826, L4
- Campbell, E. K., Holz, M., Maier, J. P., et al. 2016, *ApJ*, 822, 17
- Campbell, E. K., & Maier, J. P. 2017a, *ApJ*, 835, 221
- Campbell, E. K., & Maier, J. P. 2017b, *ApJ*, 850, 69
- Cazzoli, G., Lattanzi, V., Alonso, J. L., Gauss, J., & Puzzarini, C. 2015, *ApJ*, 806, 100
- Cazzoli, G., Lattanzi, V., Kirsch, T., et al. 2016, *A&A*, 591, A126
- Cazzoli, G., & Puzzarini, C. 2015, *JPCA*, 119, 1765
- Cernicharo, J., Kisiel, Z., Tercero, B., et al. 2016, *A&A*, 587, L4
- Cernicharo, J., McCarthy, M. C., Gottlieb, C. A., et al. 2015, *ApJ*, 806, L3
- Chakraborty, A., Fulara, J., & Maier, J. P. 2015, *JChPh*, 143, 084312
- Chang, C.-H., Agarwal, J., Allen, W. D., & Nesbitt, D. J. 2016, *JChPh*, 144, 074301
- Chen, W., Kawaguchi, K., Bernath, P. F., & Tang, J. 2015, *JChPh*, 142, 064317
- Chen, W., Kawaguchi, K., Bernath, P. F., & Tang, J. 2016, *JChPh*, 144, 064301
- Chenel, A., Roncero, O., Aguado, A., Agúndez, M., & Cernicharo, J. 2016, *JChPh*, 144, 144306
- Chubb, K. L., Joseph, M., Franklin, J., et al. 2018, *JQSRT*, 204, 42
- Condoluci, J., Janardan, S., Calvin, A. T., et al. 2017, *JChPh*, 147, 214309
- Cooksy, A. L., Gottlieb, C. A., Killian, T. C., et al. 2015, *ApJS*, 216, 30

- Coudert, L. H., Gutlé, C., Huet, T. R., Grabow, J.-U., & Levshakov, S. A. 2015, *JChPh*, 143, 044304
- Crabtree, K. N., Martin-Drumel, M.-A., Brown, G. G., et al. 2016, *JChPh*, 144, 124201
- Craig, N. C., Groner, P., Conrad, A. R., Gurusinghe, R., & Tubergen, M. J. 2016, *JMoSp*, 328, 1
- Daly, A. M., Bermúdez, C., Kolesníková, L., & Alonso, J. L. 2015, *ApJS*, 218, 30
- Dapra, M., Niu, M. L., Salumbides, E. J., Murphy, M. T., & Ubachs, W. 2016, *ApJ*, 826, 192
- Degli Esposti, C., Dore, L., Melosso, M., et al. 2017, *ApJS*, 230, 26
- Doménech, J. L., Drouin, B. J., Cernicharo, J., Herrero, V. J., & Tanarro, I. 2016, *ApJ*, 833, L32
- Doménech, J. L., Schlemmer, S., & Asvany, O. 2017, *ApJ*, 849, 60
- Dore, L., Bizzocchi, L., Wirström, E. S., et al. 2017, *A&A*, 604, A26
- Drouin, B. J. 2017, *JMoSp*, 340, 1
- Duan, C., Carvajal, M., Yu, S., et al. 2015, *A&A*, 576, A39
- Dubernet, M. L., Antony, B. K., Ba, Y. A., et al. 2016, *JPhysB*, 49, 074003
- Eidelsberg, M., Lemaire, J. L., Federman, S. R., et al. 2017, *A&A*, 602, A76
- Endres, C. P., Schlemmer, S., Schilke, P., Stutzki, J., & Müller, H. S. P. 2016, *JMoSp*, 327, 95
- Fayolle, E. C., Öberg, K. I., Jørgensen, J. K., et al. 2017, *NatA*, 1, 703
- Federman, S. R., Bernath, P. F., & Müller, H. S. P. 2016, *Trans. IAU*, 29A, 137
- Frohman, D. J., Bernath, P. F., & Brooke, J. S. A. 2016, *JQSRT*, 169, 104
- Fulara, J., Nagy, A., Chakraborty, A., & Maier, J. P. 2016, *JChPh*, 144, 244309
- Furtenbacher, T., Szabo, I., Császár, A. G., et al. 2016, *ApJS*, 224, 44
- Fusina, L., Di Leonardo, G., Canè, E., et al. 2017, *JQSRT*, 203, 417
- Gamache, R. R., Roller, C., Lopes, E., et al. 2017, *JQSRT*, 203, 70
- Gans, B., Holzmeier, F., Krüger, J., et al. 2016, *JChPh*, 144, 204307
- Germann, M., & Willitsch, S. 2016, *JChPh*, 145, 044314
- Golubiatnikov, G. Y., Belov, S. P., & Lapinov, A. V. 2017, *R&QE*, 59, 715
- Gordon, I. E., Rothman, L. S., Hill, C., et al. 2017, *JQSRT*, 203, 3
- Hakalla, R. 2015, *JQSRT*, 164, 231
- Hakalla, R., Niu, M. L., Field, R. W., et al. 2016, *RSC Adv.*, 6, 31588
- Hakalla, R., Niu, M. L., Field, R. W., et al. 2017, *JQSRT*, 189, 312
- Halfen, D. T., Keogh, J. P., & Ziurys, L. M. 2015a, *JMoSp*, 314, 79
- Halfen, D. T., Ilyushin, V. V., & Ziurys, L. M. 2015, *ApJ*, 812, L5
- Halfen, D. T., Min, J., & Ziurys, L. M. 2017, *JMoSp*, 331, 1
- Halfen, D. T., & Ziurys, L. M. 2015, *ApJ*, 814, 119
- Halfen, D. T., & Ziurys, L. M. 2016, *ApJ*, 833, 89
- Hardy, F.-X., Rice, C. A., Chakraborty, A., Fulara, J., & Maier, J. P. 2016, *ApJ*, 824, 9
- Hardy, F.-X., Rice, C. A., & Maier, J. P. 2017, *ApJ*, 836, 37
- Hargreaves, R. J., Bernath, P. F., Bailey, J., & Dulick, M. 2015a, *ApJ*, 813, 12
- Hargreaves, R. J., Buzan, E., Dulick, M., & Bernath, P. F. 2015b, *MolAs*, 1, 20
- Heays, A. N., Bosman, A. D., & van Dishoeck, E. F. 2017, *A&A*, 602, A105
- Hodges, J. N., & Bernath, P. F. 2017, *ApJ*, 840, 81
- Hodges, J. N., Bittner, D. M., & Bernath, P. F. 2018, *ApJ*, 855, 21
- Holland, D. M. P., & Shaw, D. A. 2016, *CP*, 479, 151
- Hollenstein, U., Schmutz, H., Agner, J. A., Somavilla, M., & Merkt, F. 2017, *JChPh*, 146, 014201
- Hou, S., & Bernath, P. F. 2017, *JQSRT*, 203, 511
- Hou, S., & Bernath, P. F. 2018, *JQSRT*, in press
- Jabri, A., Van, V., Nguyen, H. V. L., et al. 2016, *A&A*, 589, A127
- Jacquinet-Husson, N., Armante, R., Scott, N. A., et al. 2016, *JMoSp*, 327, 31
- Jiang, B., Kumar, P., Klos, J., et al. 2017, *JChPh*, 146, 154305
- Jiang, J., Park, G. B., & Field, R. W. 2016, *JChPh*, 144, 144312
- Jusko, P., Konietzko, C., Schlemmer, S., & Asvany, O. 2016, *JMoSp*, 319, 55
- Jusko, P., Stoffels, A., Thorwirth, S., et al. 2017b, *JMoSp*, 332, 59

- Jusko, P., Töpfer, M., Müller, H. S. P., et al. 2017a, *JMoSp*, 332, 33
- Kang, X., Liu, Y. W., Xu, L. Q., et al. 2015, *ApJ*, 807, 96
- Kisiel, Z., Martin-Drumel, M.-A., & Pirali, O. 2015, *JMoSp*, 315, 83
- Kisiel, Z., Pszczółkowski, L., Białkowska-Jaworska, E., & Charnley, S. B. 2016, *JMoSp*, 321, 13
- Kłos, J., Alexander, M. H., Kumar, P., et al. 2016, *JChPh*, 144, 174301; erratum, *JChPh*, 144, 209901
- Kolesníková, L., Alonso, E. R., Mata, S., & Alonso, J. L. 2017a, *ApJS*, 229, 26
- Kolesníková, L., Alonso, E. R., Mata, S., Cernicharo, J., & Alonso, J. L. 2017, *ApJS*, 233, 24
- Kolesníková, L., Alonso, J. L., Bermúdez, C., et al. 2016, *A&A*, 591, A75
- Krechivska, O., Bacskay, G. B., Troy, T. P., et al. 2015, *JCPA*, 119, 12102
- Krechivska, O., Bacskay, G. B., Welsh, B. A., et al. 2016, *JChPh*, 144, 144305
- Krechivska, O., Welsh, B. A., Bacskay, G. B., et al. 2017, *JChPh*, 146, 134306
- Laas, J. C., & Widicus Weaver, S. L. 2017, *ApJ*, 835, 46
- Lattanzi, V., Cazzoli, G., & Puzzarini, C. 2015, *ApJ*, 813, 4
- Lavín, C., & Velasco, A. M. 2016, *ApJ*, 816, 58
- Lavín, C., & Velasco, A. M. 2017, *ApJS*, 229, 19
- Le Roy, R. J. 2017, *JQSRT*, 186, 167
- Lefebvre, R. 2015, *JChPh*, 142, 074106
- Lefebvre-Brion, H., & Kalemoss, A. 2016a, *JChPh*, 144, 134302
- Lefebvre-Brion, H., & Kalemoss, A. 2016b, *JChPh*, 145, 166102
- Lefebvre-Brion, H., Liebermann, H. P., Amero, J. M., & Vázquez, G. J. 2016, *JChPh*, 144, 144302
- Lefebvre-Brion, H., & Majumder, M. 2015, *JChPh*, 142, 164306
- Lemaire, J. L., Eidelsberg, M., Heays, A. N., et al. 2016, *JPhB*, 49, 154001
- Lévêque, C., Taïeb, R., & Köppel, H. 2015, *CP*, 460, 135
- Li, G., Gordon, I. E., Rothman, L. S., et al. 2015, *ApJS*, 216, 15
- Lincowski, A. P., Halfen, D. T., & Ziurys, L. M. 2016, *ApJ*, 833, 9
- Liu, Y.-W., Kang, X., Xu, L.-Q., et al. 2016, *ApJ*, 819, 142
- Lovas, F. J. 2004, *JPCRD*, 33, 177
- Lyulin, O. M., & Campargue, A. 2017, *JQSRT*, 203, 461
- Lyulin, O. M., & Perevalov, V. I. 2017, *JQSRT*, 201, 94
- Mackie, C. J., Peeters, E., Bauschlicher, C. W., & Cami, J. 2015, *ApJ*, 799, 131
- Maltseva, E., Petrignani, A., Candian, A., et al. 2016, *ApJ*, 831, 58
- Margulès, L., Belloche, A., Müller, H. S. P., et al. 2016a, *A&A*, 590, A93
- Margulès, L., Martin-Drumel, M. A., Pirali, O., et al. 2016, *A&A*, 591, A110
- Margulès, L., McGuire, B. A., Senent, M. L., et al. 2017, *A&A*, 601, A50
- Margulès, L., Motiyenko, R. A., Ilyushin, V. V., & Guillemin, J. C. 2015, *A&A*, 579, A46
- Markus, C. R., Hodges, J. N., Perry, A. J., et al. 2016, *ApJ*, 817, 138
- Martin-Drumel, M. A., Hindle, F., Mouret, G., et al. 2015b, *ApJ*, 799, 115
- Martin-Drumel, M. A., van Wijngaarden, J., Zingsheim, O., et al. 2015a, *JMoSp*, 307, 33
- Mattioda, A. L., Bauschlicher, C. W., Ricca, A., et al. 2017, *AcSpA*, 181, 286
- McCarthy, M. C., Baraban, J. H., Changala, P. B., et al. 2015b, *JPhChL*, 6, 2107
- McCarthy, M. C., Crabtree, K. N., Martin-Drumel, M.-A., et al. 2015a, *ApJS*, 217, 10
- McCarthy, M. C., Tamassia, F., & Thorwirth, S. 2015c, *MolPh*, 113, 2204
- McCarthy, M. C., Zou, L., & Martin-Drumel, M.-A. 2017, *JChPh*, 146, 154301
- McGuire, B. A., Carroll, P. B., Loomis, R. A., et al. 2016a, *Sci*, 352, 1449
- McGuire, B. A., Martin-Drumel, M.-A., Thorwirth, S., et al. 2016b, *PCCP*, 18, 22693
- McKemmish, L. K., Masseron, T., Sheppard, S., et al. 2017, *ApJS*, 228, 15
- McKemmish, L. K., Yurchenko, S. N., & Tennyson, J. 2016, *MNRAS*, 463, 771
- McMillan, E. C., Shen, G., McCann, J. F., McLaughlin, B. M., & Stancil, P. C. 2016, *JPhB*, 49, 084001
- McMillan, J. P., Fortman, S. M., Neese, C. F., & De Lucia, F. C. 2016, *ApJ*, 823, 1
- Melosso, M., Degli Esposti, C., & Dore, L. 2017, *ApJS*, 233, 15
- Mesko, A. J., Zou, L., Carroll, P. B., & Widicus Weaver, S. L. 2017, *JMoSp*, 335, 49

- Mikhailenko, S. N., Kassi, S., Mondelain, D., Gamache, R. R., & Campargue, A. 2016, *JQSRT*, 179, 198
- Min, J., & Ziurys, L. M. 2016, *JChPh*, 144, 184308
- Mizus, I. I., Alijah, A., Zobov, N. F., et al. 2017, *MNRAS*, 468, 1717
- Mondelain, D., Kassi, S., Sala, T., et al. 2016, *JMoSp*, 326, 5
- Monfredini, T., Fantuzzi, F., Nascimento, M. A. C., Wolff, W., & Boechar-Roberty, H. M. 2016, *ApJ*, 821, 4
- Motiyenko, R. A., Margulès, L., Ilyushin, V. V., et al. 2016, *A&A*, 587, A152
- Muller, S., Müller, H. S. P., Black, J. H., et al. 2016, *A&A*, 595, A128
- Muller, S., Müller, H. S. P., Black, J. H., et al. 2017, *A&A*, 606, A109
- Müller, H. S. P., Belloche, A., Xu, L.-H., et al. 2016b, *A&A*, 587, A92
- Müller, H. S. P., Brown, L. R., Drouin, B. J., et al. 2015b, *JMoSp*, 312, 22
- Müller, H. S. P., Drouin, B. J., Pearson, J. C., et al. 2016a, *A&A*, 586, A17
- Müller, H. S. P., Kobayashi, K., Takahashi, K., Tomaru, K., & Matsushima, F. 2015a, *JMoSp*, 310, 92
- Müller, H. S. P., & Lewen, F. 2017, *JMoSp*, 331, 28
- Müller, H. S. P., Schlöder, F., Stutzki, J., & Winnewisser, G. 2005, *JMoSt*, 742, 215
- Müller, H. S. P., Thorwirth, S., Roth, D. A., & Winnewisser, G. 2001, *A&A*, 370, L49
- Müller, H. S. P., Walters, A., Wehres, N., et al. 2016c, *A&A*, 595, A87
- Müller, H. S. P., Zingsheim, O., Wehres, N., et al. 2017, *JPCA*, 121, 7121
- Ndao, M., Kwabia Tchana, F., Coudert, L. H., et al. 2016, *JMoSp*, 326, 136
- Ndengué, S. A., Dawes, R., & Guo, H. 2016, *JChPh*, 144, 244301
- Ni, C., Cheng, J., & Cheng, X. 2017, *JMoSp*, 331, 17
- Nikitin, A. V., Rey, M., Tashkun, S. A., et al. 2016, *JQSRT*, 168, 207
- Niu, M. L., Hakalla, R., Trivikram, M. T., et al. 2016a, *MolPh*, 114, 2857
- Niu, M. L., Heays, A. N., Jones, S., et al. 2015a, *JMoSp*, 315, 137
- Niu, M. L., Ramirez, F., Salumbides, E. J., & Ubachs, W. 2015b, *JChPh*, 142, 044302
- Niu, M. L., Salumbides, E. J., Heays, A. N., et al. 2016b, *MolPh*, 114, 627
- Noble, J. A., Dedonder, C., & Jouvét, C. 2015, *A&A*, 577, A79
- Novick, S. E. 2016, *JMoSp*, 329, 1
- O'Connor, A. P., Becker, A., Blaum, K., et al. 2016, *PhRvL*, 116, 113002
- Ostrowska-Kopeć, M., Piotrowska, I., Kępa, R., et al. 2015, *JMoSp*, 314, 63
- Owens, A., Yachmenev, A., Thiel, W., Tennyson, J., & Yurchenko, S. N. 2017, *MNRAS*, 471, 5025
- Park, G. B., Jiang, J., & Field, R. W. 2016b, *JChPh*, 144, 144313
- Park, G. B., Jiang, J., Saladrigas, C. A., & Field, R. W. 2016a, *JChPh*, 144, 144311
- Park, G. B., Womack, C. C., Whitehill, A. R., et al. 2015, *JChPh*, 142, 144201
- Patrascu, A. T., Yurchenko, S. N., & Tennyson, J. 2015, *MNRAS*, 449, 3613
- Paulose, G., Barton, E. J., Yurchenko, S. N., & Tennyson, J. 2015, *MNRAS*, 454, 1931
- Pavlyuchko, A. I., Yurchenko, S. N., & Tennyson, J. 2015, *MNRAS*, 452, 1702
- Pearson, J. C., Daly, A. M., & Lees, R. M. 2015, *JMoSp*, 318, 70
- Pearson, J. C., Yu, S., & Pirali, O. 2016, *JChPh*, 145, 124301
- Pickett, H. M., Poynter, R. L., Cohen, E. A., et al. 1998, *JQSRT*, 60, 883
- Pienkina, A. O., Margulès, L., Motiyenko, R. A., Müller, H. S. P., & Guillemin, J.-C. 2017, *A&A*, 601, A2
- Polyansky, O. L., Ovsyannikov, R. I., Kyubens, A. A., et al. 2016, *JMoSp*, 327, 21
- Polyansky, O. L., Ovsyannikov, R. I., Kyuberis, A. A., et al. 2017, *MNRAS*, 466, 1363
- Porrás, A. J., Federman, S. R., Welty, D. E., et al. 2014, *ApJ*, 781, L8
- Prajapat, L., Jagoda, P., Lodi, L., et al. 2017, *MNRAS*, 472, 3648
- Puzzarini, C., Cazzoli, G., Harding, M. E., Vázquez, J., & Gauss, J. 2015, *JChPh*, 142, 124308
- Rey, M., Nikitin, A. V., Campargue, A., et al. 2016, *PCCP*, 18, 176
- Rey, M., Nikitin, A. V., & Tyuterev, V. G. 2017, *ApJ*, 847, 105
- Rice, C. A., Hardy, F.-X., Gause, O., & Maier, J. P. 2015, *ApJ*, 812, L4
- Rivlin, T., Lodi, L., Yurchenko, S. N., Tennyson, J., Le Roy, R. J. 2015, *MNRAS*, 451, 634

- Rothman, L. S., Gordon, I. E., Barber, R. J., et al. 2010, *JQSRT*, 111, 2139
- Sadjadi, S. A., Zhang, Y., & Kwok, S. 2015, *ApJ*, 801, 34
- Sarka, K., Danielache, S. O., Kondorskiy, A., & Nanbu, S. 2017, *CP*, 488, 36
- Schaefer, L., Lodders, K., & Fegley, B. 2012, *ApJ*, 755, 41
- Sghaier, O., Linguerrri, R., Mogren Al Mogren, M., Francisco, J. S., & Hochlaf, M. 2016, *ApJ*, 826, 163
- Sharma, S. 2015, *JChPh*, 142, 024107
- Sharpe, S. W., Johnson, T. J., Sams, R. L., et al. 2004, *ApSpe*, 58, 1452
- Simmen, B., Mátyus, E., & Reiher, M. 2014, *JChPh*, 141, 154105
- Song, Y., Gao, H., Chang, Y.-C., et al. 2016, *ApJ*, 819, 23
- Sousa-Silva, C., Al-Refaie, A. F., Tennyson, J., & Yurchenko, S. N. 2015, *MNRAS*, 446, 2337
- Spezzano, S., Gupta, H., Brünken, S., et al. 2016, *A&A*, 586, A110
- Spieler, S., Kuhn, M., Postler, J., et al. 2017, *ApJ*, 846, 168
- Steglich, M., Fulara, J., Maity, S., Nagy, A., & Maier, J. P. 2015, *JChPh*, 142, 244311
- Steglich, M., & Maier, J. P. 2015, *ApJ*, 801, 119
- Stewart, J. T., Sullivan, M. N., & Heaven, M. C. 2016, *JMoSp*, 322, 18
- Stoffels, A., Kluge, L., Schlemmer, S., & Brünken, S. 2016, *A&A*, 593, A56
- Strelnikov, D., Kern, B., & Kappes, M. M. 2015, *A&A*, 584, A55
- Sunanda, K., Shastri, A., Das, A. K., & Sekhar, B. N. R. 2015, *JQSRT*, 151, 76
- Sung, K., Toon, G. C., & Crawford, T. J. 2016, *Icar*, 271, 438
- Sung, K., Yu, S., Pearson, J., et al. 2016, *JMoSp*, 327, 1
- Szajna, W., Hakalla, R., Kolek, P., & Zachweija, M. 2017, *JQSRT*, 187, 167
- Szajna, W., Zachweija, M., & Hakalla, R. 2016, *JMoSp*, 324, 48
- Tanaka, H. K., Prudente, F. V., Medina, A., et al. 2017, *JChPh*, 146, 094310
- Tashkun, S. A., Perevalov, V. I., Gamache, R. R., & Lamouroux, J. 2015, *JQSRT*, 152, 45
- Tennyson, J., Lodi, L., McKemmish, L. K., & Yurchenko, S. N. 2016, *JPhB*, 49, 102001
- Tennyson, J., Yurchenko, S. N., Al-Refaie, A. F., et al. 2016, *JMoSp*, 327, 73
- Thorwirth, S., Kaiser, R. I., Crabtree, K. N., et al. 2015a, *ChCom*, 51, 11305
- Thorwirth, S., Lattanzi, V., & McCarthy, M. C. 2015b, *JMoSp*, 310, 119
- Thorwirth, S., Salomon, T., Fanghänel, S., Kozubal, J. R., & Dudek, J. B. 2017, *CPL*, 684, 262
- Tokaryk, D. W., Vervloet, M., & Phi, T.-T. 2015, *JMoSp*, 310, 113
- Töpfer, M., Jusko, P., Schlemmer, S., & Asvany, O. 2016, *A&A*, 593, L11
- Trivikram, T. M., Hakalla, R., Heays, A. N., et al. 2017, *MolPh*, 115, 3178
- Underwood, D. S., Tennyson, J., Yurchenko, S. N., et al. 2016a, *MNRAS*, 459, 3890
- Underwood, D. S., Yurchenko, S. N., Tennyson, J., et al. 2016b, *MNRAS*, 462, 4300
- Vasilchenko, S., Mondelain, D., Kassi, S., et al. 2016, *JMoSp*, 326, 9
- Velasco, A. M., Lavín, C., Díaz-Tinoco, M., & Ortiz, J. V. 2017, *JQSRT*, 187, 161
- Walters, A., Schäfer, M., Ordu, M. H., et al. 2015, *JMoSp*, 314, 6
- Watanabe, K., Yoneyama, N., Uchida, K., et al. 2016, *CPL*, 657, 1
- Welsh, B. A., Krechkivska, O., Nauta, K., et al. 2017, *JChPh*, 147, 024305
- Western, C. M. 2017, *JQSRT*, 186, 221
- Wilzewski, J. S., Gordon, I. E., Kochanov, R. V., et al. 2016, *JQSRT*, 168, 193
- Wolf, M., Kiefer, H. V., Langeland, J., et al. 2016, *ApJ*, 832, 24
- Wong, A., Billinghurst, B., & Bernath, P. F. 2017c, *MolAs*, 8, 36
- Wong, A., Hargreaves, R. J., Billinghurst, B., & Bernath, P. F. 2017b, *JQSRT*, 198, 141
- Wong, A., Yurchenko, S. N., Bernath, P., et al. 2017a, *MNRAS*, 470, 882
- Xie, C., Zhu, X., Ma, J., et al. 2015, *JChPh*, 142, 091101
- Yu, S., Drouin, B. J., & Miller, C. E. 2014, *JChPh*, 141, 174302
- Yu, S., Pearson, J. C., Amano, T., & Matsushima, F. 2017, *JMoSp*, 331, 6
- Yu, S., Pearson, J. C., Drouin, B. J., et al. 2015, *JMoSp*, 314, 19
- Yu, S., Pearson, J. C., Drouin, B. J., et al. 2016, *JMoSp*, 328, 27
- Yurchenko, S. N., Amundsen, D. S., Tennyson, J., & Waldmann, I. P. 2017b, *A&A*, 605, A95
- Yurchenko, S. N., Blissett, A., Asari, U., et al. 2016, *MNRAS*, 456, 4524
- Yurchenko, S. N., Sinden, F., Lodi, L., et al. 2017a, *MNRAS*, 473, 5324

- Zack, L. N., Burchino, M. P., Binns, M. K. L., et al. 2015, *JMoSp*, 317, 10
- Zak, E. J., & Tennyson, J. 2017, *JChPh*, 147, 094305
- Zak, E., Tennyson, J., Polyansky, O. L., et al. 2016, *JQSRT*, 177, 31
- Zak, E., Tennyson, J., Polyansky, O. L., et al. 2017, *JQSRT*, 189, 267
- Zakharenko, O., Bossa, J.-B., Lewen, F., Schlemmer, S., & Müller, H. S. P. 2017, *JMoSp*, 333, 23
- Zakharenko, O., Motiyenko, R. A., Margulès, L., & Huet, T. R. 2015, *JMoSp*, 317, 41
- Zammit, M. C., Savage, J. S., Colgan, J., et al. 2017, *ApJ*, 851, 64
- Zhang, D., Zhang, Q., Zhu, B., et al. 2017, *JChPh*, 146, 114303
- Zhang, L.-L., Zhang, J., Meng, Q.-T., & Song, Y.-Z. 2015, *PhyS*, 90, 035403
- Zhao, D., Galatzutdinov, G. A., Linnartz, H., & Krelowski, J. 2015a, *ApJ*, 805, L12
- Zhao, D., Galatzutdinov, G. A., Linnartz, H., & Krelowski, J. 2015b, *A&A*, 79, L1
- Zhen, J., Castellanos, P., Bouwman, J., Linnartz, H., & Tielens, A. G. G. M. 2017, *ApJ*, 836, 28
- Zingsheim, O., Müller, H. S. P., Lewen, F., Jørgensen, J. K., & Schlemmer, S. 2017, *JMoSp*, 342, 125
- Zobov, N. F., Coles, P. A., Ovsyannikov, R. I., et al. 2018, *JQSRT*, 209, 224