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DIVISION B
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DONNÉES ATOMIQUES ET MOLÉCULAIRES

WORKING GROUP **MOLECULAR DATA**
DONNÉES MOLÉCULAIRES

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TRIENNIAL REPORT 2012-2014

1. Introduction

The current report covers the period from the second half of 2011 to late 2014. It is divided into three areas covering rotational, vibrational, and electronic spectroscopy. A signifcant amount of experimental and theoretical work has been accomplished over the past three years, leading to the development and expansion of a number of databases whose links are provided below. Two notable publications have appeared recently: An issue of The Journal of Physical Chemistry A in 2013 honoring the many contributions of Takeshi Oka (J. Phys. Chem. A, 117, pp. 9305-10143); and IAU Symposium 297 on Diffuse Interstellar Bands (Cami & Cox 2014). A number of the relevant papers from these volumes are cited in what follows. 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 molecules already observed in space, and on molecules related to these species. A few observational papers are mentioned to highlight some recent findings. The grouping of the molecules has been modified with respect to the previous report. Complex organic molecules are very important for ALMA, and they have attracted considerable attention in the last three years. They form the first group and include most of the so-called weed molecules. Molecules which (may) occur in circumstellar envelopes of late type stars form the second group. Additional groups deal with hydride molecules, with cations, or with other molecules. For completeness, we also include determinations of transition frequencies from radio astronomical observations, provided these are of sufficient importance.

Several databases provide rotational spectra of (mostly) molecular species of astrophysical and astrochemical relevance. The two most important sources for predictions generated from experimental data by employing appropriate Hamiltonian models are

the Cologne Database for Molecular Spectroscopy, CDMS† (Müller *et al.* 2001, 2005) with its catalog‡ and the JPL catalog¶ (Pickett *et al.* 1998). Both 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‖. 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††, aims at combining several spectroscopic, collisional, and kinetic databases. The CDMS is the rotational spectroscopy database taking part‡‡; recently, the JPL catalog has joined; several infrared databases are also involved. The project has been described by Dubernet *et al.* (2010).

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.

2.1. *Complex molecules*

An overview of molecular complexity achievable with single dish radio telescopes is provided by Belloche *et al.* (2013). They carried out molecular line surveys of the giant molecular clouds Sagittarius B2(N) and (M) close to the Galactic Center with the IRAM 30 m telescope at 3 mm with additional observations at 2 and 1.3 mm. The detections include several new molecules, isotopologues, and excited vibrational states. Follow-up ALMA Cycle-0 observations resulted in the detection of the first branched alkyl compound, *iso*-C_3H_7CN (Belloche *et al.* 2014).

Zaleski *et al.* (2013) extended the rotational specroscopy of cyanomethanimine and described the detection of the E conformer, which is presumably higher in energy than the Z conformer, but has a much larger dipole moment. Kolesniková *et al.* (2014) extended the ethyl mercaptan data sets considerably and concluded that the molecule would be present in Orion. We also emphasize investigations and astronomical detections of dimethyl ether with one D (Richard *et al.* 2013) or with one or two ^{13}C (Koerber *et al.* 2013), as well as methyl formate in its doubly torsionally excited state (Kobayashi *et al.* 2013) or several of its isotopologues (Coudert *et al.* 2013; Haykal *et al.* 2014; Tercero *et al.* 2012). There was also an account on the rotational spectroscopy of the very high lying *anti*-conformer and its tentative detection in space (Neill *et al.* 2012).

Other reports include THz frequency (Pearson *et al.* 2011) and intensity studies (Fortman *et al.* 2014; McMillan *et al.* 2014) of CH_3OH, extensive studies of $^{13}CH_3OH$ (Xu *et al.* 2014), CH_2DOH (Pearson *et al.* 2012; Coudert *et al.* 2014a), CH_3SH (Xu *et al.* 2012), and ethyl cyanide (Daly *et al.* 2013; Richard *et al.* 2012), as well as vinyl cyanide (Kisiel *et al.* 2012; Kraśnicki *et al.* 2011b; López *et al.* 2014), including redetermination of their dipole moment components (Kraśnicki & Kisiel 2011) with a considerable change in μ_b for vinyl cyanide.

† http://www.astro.uni-koeln.de/cdms/
‡ http://www.astro.uni-koeln.de/cdms/catalog
¶ http://spec.jpl.nasa.gov/
‖ http://www.sci.u-toyama.ac.jp/phys/4ken/atlas/
†† http://www.vamdc.org/
‡‡ http://cdms.ph1.uni-koeln.de/cdms/portal/

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Ilyushin & Hougen (2013) presented a somewhat restricted reanalysis of the rotational spectrum of acetone in its ground and its two singly excited torsional states employing a new BELGI variant. This program may be very useful for a variety of two-top internal rotor problems.

Several promising molecules can be searched for in space because of greatly extended laboratory data, such as butanone (Kroll *et al.* 2013), *n*-butyl cyanide (Ordu *et al.* 2012), 1,2- (Bossa *et al.* 2014) and 1,3-propanediol (Smirnov *et al.* 2013), urea (Remijan *et al.* 2014), and 2-aminopropanitrile (Møllendal *et al.* 2012); data on 3-aminopropanitrile are still very limited.

In addition, there are now several minor isotopologues for which searches are now viable: e.g. several isotopologues of methanimine (Motoki *et al.* 2014) and cyanamide (Kraśnicki *et al.* 2011a), deuterated formamide (Kutsenko *et al.* 2013), ^{13}C-containing ethanol (Bouchez *et al.* 2012b), and deuterated (Bouchez *et al.* 2012a) and ^{13}C-containing glycolaldehyde (Haykal *et al.* 2013).

Other studies involve H_2CNH (Dore *et al.* 2012), H_2CCNH (Degli Esposti *et al.* 2014), *n*-butanal (Hotopp *et al.* 2012), acetic acid (Ilyushin *et al.* 2013), aminoacetonitrile (Motoki *et al.* 2013) and methyleneaminoacetonitrile (Motiyenko *et al.* 2013), methylamine (Motiyenko *et al.* 2014), methyl acetate (Nguyen *et al.* 2014), acetaldehyde (Smirnov *et al.* 2014), and deuterated methyl cyanide (Nguyen *et al.* 2013).

2.2. *Circumstellar molecules*

In recent years, several molecular species were detected first in O-rich circumstellar envelopes (CSEs) of late-type stars. One recent prominent example is TiO_2, a dust-forming molecule, detected in the CSE of VY CMa (Kamiński *et al.* 2013). Initially, detections of molecules in CSEs were commonly made toward C-rich stars, in particular CW Leonis, also known as IRC +10216. Remarkable examples are the laboratory spectroscopy and detection of HMgNC (Cabezas *et al.* 2013) and the rotational spectroscopy of FeCN and FeNC (Flory & Ziurys 2011); the detection of FeCN was reported earlier, though.

Investigations of detected species involve $^{29}SiC_2$ and $^{30}SiC_2$ (Kokkin *et al.* 2011) and SiO (Müller *et al.* 2013) along with an analysis of recent NaCN data (Müller *et al.* 2012b). SiC_2 spectroscopic parameters were improved once more through radio astronomical observations (Müller *et al.* 2012a).

Further investigations include ScS and YS (Adande *et al.* 2012), ^{25}MgH and ^{67}ZnH (Bucchino & Ziurys 2013), KSH (Bucchino *et al.* 2013), AlC_3N (Cabezas *et al.* 2014), PCN (Halfen *et al.* 2012), PH_2CN (Halfen *et al.* 2014), SiC_3H (Kokkin *et al.* 2014), SiC_2N and SiC_3N (Umeki *et al.* 2014), alkali metal acetylides (Sheridan *et al.* 2011), and AlCCH (Sun *et al.* 2012). Halfen & Ziurys (2014) reported a transition frequency for the AlH $J = 2 - 1$ transition which is not compatible with numerous IR and optical studies. Therefore, we recommend to avoid using this datum until further clarification.

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; for instance, quite recently the detection of ArH^+ was reported (Barlow *et al.* 2013; Schilke *et al.* 2014). 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

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top hydrides, such as H_2O, can be observed from the ground and may be of particular importance for ALMA.

Noteworthy is especially the investigation of HCl^+ (Gupta *et al.* 2012), which was important to establish its detection in the ISM. We point out also extensive studies of H_2O (Yu *et al.* 2012b, 2013; Coudert *et al.* 2014). Drouin *et al.* (2011) reported not only transition frequencies of H_2O around 2.6 THz, but also of HD and NH_3. Noteworthy are also the extensive investigations on sulfur isotopologues of H_2S (Azzam *et al.* 2013; Cazzoli & Puzzarini 2014; Cazzoli *et al.* 2014) and those of H_2F^+ (Amano *et al.* 2012). Although H_2F^+ is predicted to have small column densities in space, it is necessary to know selected transitions, in particular those involving the ground states, well enough.

Other studies include investigations of H_3O^+ (Yu & Pearson 2014), NH_2 (Martin-Drumel *et al.* 2014), ^{15}NH (Bailleux *et al.* 2012), several OH isotopologues (Drouin 2013), OH^- (Jusko *et al.* 2014), CH (Martin-Drumel *et al.* 2011; Truppe *et al.* 2014), and an analysis of PH_3 rotational data (Müller 2013). Müller *et al.* (2014) determined improved spectroscopic parameters for SH^+ based on radio astronomical observations of the lowest frequency transitions.

2.4. *Cations*

Cationic light hydrides were mentioned in subsection 2.3. With regard to heavier cations, the laboratory spectroscopy of C_3H^+ (Brünken *et al.* 2014) is particularly worth mentioning as it confirmed the earlier assigment of a long series of U-lines detected in the Horsehead Nebula mentioned in our last report. Gupta *et al.* (2013) reported on the rotational spectrum of H_2NCO^+ and its tentative detection in Sgr B2(N).

Other studies involve CO^+ (Spezzano *et al.* 2013), $HNNO^+$ (McCarthy *et al.* 2013), $HOSO^+$ (Lattanzi *et al.* 2011), $C_2H_3CNH^+$ (Martinez *et al.* 2013), and Terahertz spectra of N_2H^+, HCO^+, and CF^+ (Cazzoli *et al.* 2012).

2.5. *Other molecules*

We emphasize a study of several isotopologues of *c*-C_3H_2 (Spezzano *et al.* 2012), which led to the detection of *c*-C_3D_2. Other investigations, which may be worthwhile mentioning, include HCOOD and DCOOH (Cazzoli *et al.* 2011), the vinoxy radical (Endo & Nakajima 2014), HOOD (however with no tranistion frequencies) (Herberth *et al.* 2012), phenol (Kolesniková *et al.* 2013), HOSO (McCarthy *et al.* 2013), and an analysis of several O_2 isotopologues in several electronic states (Yu *et al.* 2012a).

3. Vibrational Spectra

The vibration-rotation spectra of molecules of astronomical or of potential astronomical interest are reviewed for the period 2011-2014 starting from the end of our previous report (Federman *et al.* 2012). 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 and so forth, found primarily in the Earth's atmosphere. A new edition has appeared (HITRAN 2012, Rothman *et al.* 2013); further information including updates and corrections is available†. The molecular coverage is slowly being expanded to cover planetary atmospheres other than Earth and HITRAN 2012 contains line parameters for PH_3, H_2, and CS. HITRAN is widely used for astronomical applications although it is not always suitable because of missing lines

† http://www.cfa.harvard.edu/hitran/

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and bands, particularly in the near infrared region. For high temperature applications, the HITEMP database (Rothman *et al.* 2010) for H_2O, CO_2, CO, NO, and OH is more suitable and a new edition is being prepared.

For larger molecules, individual vibration-rotation lines are no longer clearly resolved and it becomes necessary to replace line-by-line calculations by absorption cross sections. The main drawback to using cross sections is that a considerable number of laboratory measurements are needed to match the temperature and pressure conditions of the objects under observation. HITRAN also includes a number of high resolution infrared absorption cross sections for organic molecules such as methanol, ethane, and acetone, but the broadening gas is air rather than H_2, N_2, or CO_2. While the GEISA database has significant overlap with HITRAN, it contains additional molecules of interest for studies of planetary atmospheres (Jacquinet-Husson *et al.* 2011).

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 has an extensive collection of calculated line lists designed "as input to atmospheric models of exoplanets, brown dwarfs and cool stars." G. Villanueva's site‡ provides line lists for the simulation of infrared emission spectra of comets for species such as ethane, methanol, ammonia, and water excited by solar radiation. A very useful set of infrared absorption cross sections for several hundred molecules are available from 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.

Other interesting sources of infrared data are the ACE high resolution spectral atlases of the Sun (Hase *et al.* 2010) and of the Earth's atmosphere (Hughes *et al.* 2014) recorded using a high resolution Fourier transform spectrometer in low Earth orbit. The ACE atmospheric spectra are recorded by solar occultation (i.e., using the Sun as a light source during sunrise and sunset). This geometry matches that used for exoplanet transit spectroscopy (Bernath 2014) so these spectra are a template for infrared absorption spectra of Earth-like planets.

3.1. *Diatomic molecules*

Hydrogen is the most abundant element in the Universe so it is no surprise that small diatomic hydrides are also abundant. One of the major successes of the *Herschel Space Observatory* was the detection of many diatomic hydrides, often for the first time, by rotational spectroscopy (Benz *et al.* 2013). Diatomic hydrides have large rotational constants so their pure rotational spectra fall in the Terahertz region where absorption by the Earth's atmosphere is a problem. With *Hershel* no longer operational, infrared observations from the ground with instruments such as Phoenix, CRIRES, and TEXES are attractive. The new EXES instrument on the SOFIA (Stratospheric Observatory for Infrared Astronomy) aircraft is particularly promising because it flies in the stratosphere above most of the Earth's atmosphere.

The argonium ion ($^{36}ArH^+$) was detected in the Crab Nebula by Barlow *et al.* (2013) using *Herschel*. On Earth the major isotope is ^{40}Ar from radioactive decay of ^{40}K in rocks while ^{36}Ar is the main isotope in stars because of nucleosynthetic production in supernova explosions. Improved vibration-rotation spectra of the 1-0 band of $^{36}ArH^+$

† http://www.exomol.com/
‡ http://astrobiology.gsfc.nasa.gov/Villanueva/spec.html
¶ http://nwir.pnl.gov

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and $^{38}ArH^+$ were reported by Cueto *et al.* (2014). Improved line positions have also been measured for HeH^+ by Perry *et al.* (2014).

The vibration-rotation line parameters of the hydrogen halide molecules (HF, HCl, HBr, and HI) have been revised in HITRAN 2012. Of particular interest in astronomy are the extensive lists of new line positions and intensities for HF and HCl that are used to obtain fluorine (Jönsson *et al.* 2014) and chlorine abundances. A similar extensive revision of the CH, NH, and OH line parameters has been carried out. These new line lists were created using reliable dipole moment functions and inclusion of the Herman-Wallis effect using LeRoy's LEVEL computer program†. The CH line list of Masseron *et al.* (2014) primarily focuses on electronic transitions but also includes vibration-rotation bands. The NH (Brooke *et al.* 2014a) and OH (Brooke *et al.* 2015) work adds line intensities to our previous analyses of line positions based partly on the ACE solar spectrum.

The ExoMol line lists include BeH, MgH, CaH (Yadin *et al.* 2012), SiO (Barton *et al.* 2013), NaCl, KCl (Barton et a. 2014), and PN (Yorke *et al.* 2014). These new line lists combine experimental measurements and *ab initio* calculations. Salt vapors such as NaCl and KCl are predicted to be present in hot super-Earth exoplanets (Schaefer *et al.* 2012). The infrared bands of SiO are readily observed in K-M giant and supergiant stars (Ohnaka 2014).

The vibration-rotation bands of H_2 are forbidden by electric dipole selection rules, but are observable by weak electric quadrupole transitions. The line intensities and line positions of the vibration-rotation bands of H_2 were recalculated for HITRAN 2012 based on *ab initio* results (Rothman *et al.* 2013). The line positions are estimated to have an accuracy of about 0.001 cm^{-1} and more recent results from calculations (Pachucki & Komasa 2014) and experiments (Cheng *et al.* 2012) have even higher accuracy. The HD molecule is polar and so has dipole-allowed transitions, which are also reported in HITRAN 2012.

The CN radical is found in a very wide range of sources mainly by radio and optical/IR astronomy. However, vibration-rotation lines can also be detected (Wiedemann *et al.* 1991) and new line lists for CN that include the vibration-rotation bands for CN (Brooke *et al.* 2014b), ^{13}CN, and $C^{15}N$ (Sneden *et al.* 2014) have been generated with an *ab initio* dipole moment function calculated by D. Schwenke (NASA-Ames). These extensive line lists are based on recent laboratory observations of the $B^2\Sigma^+ - X^2\Sigma^+$ and $A^2\Pi - X^2\Sigma^+$ Violet System and Red System, which extends into the near IR spectral region. A new line list has been completed for the corresponding infrared $A^2\Pi - X^2\Sigma^+$ electronic transition of the isovalent CP radical (Ram *et al.* 2014a). The Ballik-Ramsay and Phillips Systems of C_2 are also 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 C_2 in comets by solar radiation.

An important application of molecular line parameters is to extract elemental abundances from the near infrared spectra of large numbers of cool stars observed in surveys such as APOGEE (Apache Point Observatory Galactic Evolution Experiment). APOGEE is recording H-band (1.51-1.69 μm) spectra of thousands of evolved, late-type stars with a focus on red giants with a surface temperature of 3400-5000 K (Cottaar *et al.* 2014). CNO abundances are derived from CO and OH overtone spectra, and the Red System of CN. The improved line parameters for OH and CN, along with HITEMP values for CO cited above, are recommended for abundance analyses. Stellar models also

† http://leroy.uwaterloo.ca/programs/

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require dissociation energies and significant improvements have been made using the method of Active Thermochemical Tables‡. For example, the latest values for the dissociation energies D_0 for C_2, CH, CO, CN, and OH are (in eV) 6.24475, 3.57154, 11.11092, 7.72400, and 4.41129, respectively (Ruscic *et al.* 2014).

3.2. *Small polyatomic molecules*

The line parameters of ammonia (Down *et al.* 2013) and methane as given in the HITRAN 2012 database are satisfactory for most astronomical purposes at low temperatures, except for overtone and combination bands in the near infrared and visible regions. In the near infrared, Sung *et al.* (2012) have generated an empirical line list for NH_3 covering the 6300 to 7000 cm^{-1} region. By using spectra recorded over a range of sample temperatures (185-296 K), empirical lower state energies were obtained, although most of the lines still lack detailed quantum number assignments. Similar work in Grenoble (Campargue *et al.* 2013) on CH_4 has provided the WKLMC empirical line lists (5852-7919 cm^{-1}) using two temperatures (80 K and 296 K). The WKLMC methane line list is a major improvement on the band models typically used by planetary astronomers. New measurements for methane spectra in the 4800-5300 cm^{-1} region have been reported by Nikitin *et al.* (2014). For PH_3 (long detected in Jupiter and Saturn) a new analysis for the 5 bands that comprise the pentad region between 1950 and 2450 cm^{-1} has appeared (Devi *et al.* 2014). Work on high overtone and combination bands of CO_2 continues (Petrova *et al.* 2013; Lu *et al.* 2013) for applications for Venus and Mars.

The spectra of hot molecules needed to simulate the spectra of cool stars, brown dwarfs, and exoplanets remains a challenge. For hot water, calculations continue to improve (Polyansky *et al.* 2013), but the BT2 line list (Barber *et al.* 2006) remains the standard for astronomical applications. A new extensive compilation of the vibration-rotation energy levels of water has appeared (Tennyson *et al.* 2013). For hot ammonia, laboratory spectra recorded in emission are available (Hargreaves *et al.* 2011, 2012a) and with at least two groups providing rather good calculated spectra (Huang *et al.* 2011a,b; Yurchenko *et al.* 2011). There is much recent progress on the spectroscopy of hot methane with the experimental line lists of Hargreaves *et al.* (2012b) and two comprehensive calculated line lists (Yurchenko & Tennyson 2014; Rey *et al.* 2014a); a calculation for CH_3D has also been carried out (Rey *et al.* 2014b). For CO_2, HITRAN 2012 for cold molecules and HITEMP, CDSD-4000 (Tashkun & Perevalov 2011) and calculations for 13 isotopologues for hot molecules (Huang *et al.* 2014) are recommended. New internal partition functions for NH_3 and PH_3 (Sousa-Silva *et al.* 2014) have been published. A new line list for HCN and HNC has been prepared by Barber *et al.* (2014) combining both experimental and theoretical work.

The pure rotational spectrum of NH_3D^+ has been tentatively identified in Orion (Cernicharo *et al.* 2013), based on a new infrared laboratory spectrum (Doménech *et al.* 2013). H_2Cl^+ has been detected by *Herschel*, but not H_2F^+; new infrared spectra of H_2F^+ have been measured with a Fourier transform spectrometer (Fujimori *et al.* 2013).

The carbon chain molecules C_3 and C_5 can be detected in the circumstellar envelopes of carbon stars by infrared observations (Hargreaves *et al.* 2014). Improved laboratory spectra of C_3 have been reported in the 3 μm region (Krieg *et al.* 2013) and high resolution photoelectron spectroscopy has been used to refine the vibrational frequencies of C_5 (Weichman *et al.* 2013).

‡ http://atct.anl.gov/

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3.3. *Large molecules*

There is continuing strong interest in large carbon-containing molecules such as C_{60} (e.g., Berné & Tielens 2012) and polycyclic aromatic hydrocarbons (PAHs). For PAH molecules the NASA-Ames database has been updated and new features added (Boersma *et al.* 2014). Extensive calculations by the NASA-Ames group have continued, for example, on dehydrogenated PAHs (Mackie *et al.* 2014) and PAH clusters (Ricca *et al.* 2013). High resolution infrared absorption spectra of the ν_{68} mode of pyrene near 1184 cm^{-1} were recorded by Brumfield *et al.* (2012). ZEKE photoelectron spectroscopy was used to measure the frequencies of the benzoperylene cation (Zhang *et al.* 2012). There is continuing discussion on the nature of these 'PAH' bands in astronomical sources, for example with the suggestion that mixed aromatic/aliphatic organic nanoparticles, MAONs, rather than free flying PAHs are the carrier (Kwok & Zhang 2013). Improved infrared absorption spectra of C_{60}^+ and C_{60}^- in neon matrices have been measured by Kern *et al.* (2013) and C_{60}^+ has been identified in emission in the interstellar medium (Berné *et al.* 2013).

4. Electronic Spectra

Recent work on electronic spectra, such as line identification, energy levels, and related data needed for photochemical models, are described. These data include 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. Both empirical (experimental and astronomical) and theoretical results are presented. The section is divided into four topics: 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. Although some of the work is noted in the sections on rotational and vibrational spectra, electronic spectroscopy is stressed here.

4.1. *Interstellar matter*

Because observations and analyses of CO and its photochemistry is central to astrophysical studies, a large body of new work has appeared since the last report. Oscillator strengths and predissociation rates with improved precision are now available for a number of transitions in CO isotopologues (Eidelsberg *et al.* 2012, 2014; Heays *et al.* 2014a; Stark *et al.* 2014); another study focused on self shielding among the isotopologues (Chakraborty *et al.* 2012). Since CO photodissociation involves line absorption, self shielding, which arises when dissociating transitions become optically thick, allows molecules in the cloud interior to be protected. A theoretical study on predissociation in the E state (Majumder *et al.* 2014) obtained a line width consistent with earlier measurements. Using a newly developed technique, Ng and colleagues (Gao *et al.* 2011a, 2012, 2013a,b) measured branching fractions for the atomic products arising from dissociation for specific rotational levels. Branching fractions were also obtained for other systems, including CO_2 and N_2 (Gao *et al.* 2011b; Pan *et al.* 2011; Lu *et al.* 2014) as well as O_2 (Holland & Shaw 2012; Zhou *et al.* 2014a). Similar studies involve N_2 photoionization (Holland & Shaw 2012; O'Keeffe *et al.* 2012) and CO_2 photoionization (Furch *et al.* 2013).

New measurements of the Ångström ($B^1\Sigma^+ - A^1\Pi$) and fourth positive ($A^1\Pi - X^1\Sigma^+$) systems improved our knowledge of the perturbations affecting the A state. Hakalla & Zachwieja (2012) and Hakalla *et al.* (2013) studied Ångström system bands in the rare

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$^{13}C^{17}O$ isotopologue; Hakalla and colleagues obtained spectra for these bands in other isotopologues (Hakalla *et al.* 2012a,b; Kępa *et al.* 2014; Hakalla *et al.* 2014). As for the A–X system of bands, Kępa *et al.* (2011) and Gavilan *et al.* (2013) provided further details on the perturbations in $^{13}C^{16}O$, while Niu *et al.* (2013) analyzed $^{12}C^{16}O$ spectra. Lifetimes for the main isotopologue were obtained by Blokland *et al.* (2011). A time-dependent quantum mechanical study (Majumder *et al.* 2012) yielded oscillator strengths; the slight differences with experimental results likely arise from perturbations in the A state. Moreover, accurate line positions were measured for transitions that are sensitive to the proton-to-electron mass ratio (de Nijs *et al.* 2011; Salumbides *et al.* 2012; Niu *et al.* 2015), and de Nijs *et al.* (2013) tested mass-scaling relations among isotopologues for the $a^3\Pi$ state.

Since N_2 and CO are isoelectronic, photochemical models of interstellar environments need to take this into account (Heays *et al.* 2014b). Much like the studies on CO discussed above, new experimental results on oscillator strengths and predissociation (Heays *et al.* 2011; Wu *et al.* 2012) were reported. Cross sections for electron-impact excitation (Malone *et al.* 2012) and photoionization efficiencies for N_2 isotopologues (Randazzo *et al.* 2014) were obtained as well. Little & Tennyson (2013) studied the singlet **and** triplet states of N_2 through *ab initio* calculations. Wu *et al.* (2013) characterized far ultraviolet absorption of N_3 and N_2^+ in an N_2 matrix.

Other simple carbon-bearing molecules received attention in the past three years. Measurements on the Swan band system ($d^3\Pi - a^3\Pi$) in C_2 produced new molecular constants for several bands (Chan *et al.* 2013; Yeung *et al.* 2013; Bornhauser *et al.* 2013) and line strengths for others including the $^{12}C^{13}C$ isotopologue (Brooke *et al.* 2013; Ram *et al.* 2014b). Higher-lying vibrational levels in the X, A, a, and d states were observed by Nakajima & Endo (2013); they also analyzed perturbations seen in the $v = 8$ level of the d state. Nakajima & Endo (2014) described further studies of the $d^3\Pi_g - c^3\Sigma_u^+$ band system. Hupe *et al.* (2012) analyzed perturbations involving the F state that were seen in astronomical spectra. An *ab inito* study by Schmidt & Bacskay (2011) provided spectroscopic constants for a newly identified quintet state. The $A^2\Pi - X^2\Sigma^+$ and $B^2\Pi - X^2\Sigma^+$ band systems in CN and its isotopologues were studied by Bernath and colleagues. Spectroscopic results on $^{12}C^{15}N$ (Colin & Bernath 2012), $^{13}C^{14}N$ (Ram & Bernath 2012), and $^{13}C^{15}N$ (Colin & Bernath 2014) were published, and line strengths in the form of oscillator strengths were derived for $^{12}C^{14}N$ (Brooke *et al.* 2014b) and its isotopologues (Sneden *et al.* 2014). Hyperfine structure in spectra of the A–X band was discussed by Forthomme *et al.* (2014). Recent theoretical efforts on CN involved molecular properties of its low-lying electronic states (Shi *et al.* 2011a) and the determination of photodissociation cross sections (El-Qadi & Stancil 2013). Two studies on C_3 appeared; one provides laboratory spectra on A–X bands for C_3 and its isotopologues (Haddad *et al.* 2014) and the other gives oscillator strengths for a number of these bands based on astronomical measurements (Schmidt *et al.* 2014).

Studies also focused on other species found in interstellar clouds and comets. Theoretical work appeared on photoabsorption and photodissociation for H_2 (Mezei *et al.* 2014), HeH^+ (Loreau *et al.* 2013; Miyake *et al.* 2011), ArH^+ (Roueff *et al.* 2014), LiH^+ (Bovino *et al.* 2011), NH_3 (Chatterley *et al.* 2013), and H_2O (Jiang *et al.* 2012; Zhou *et al.* 2014b). Low-lying states in CS were studied theoretically by Shi *et al.* (2011b), and Ponzi *et al.* (2014) reported theoretical calculations on CS photoionization. Calculations on low-lying states of HCl (Engin *et al.* 2012) were performed as well. Experimental lifetimes on the $\tilde{A}^2A_1$ state of NH_2 were measured by N'Doumi & Halpern (2012). Photoionization cross sections for CO, N_2, and H_2O were also determined theoretically

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(Ruberti *et al.* 2014). It is also worth noting a compilation of transition probabilities for several diatomic species (Billoux *et al.* 2014).

4.2. *Late-type stars*

During this reporting period, new results on MgH, FeH, and ZrO were published. Hinkle *et al.* (2013) identified lines from isotopologues of MgH associated with the A–X system, and GharibNezhad *et al.* (2013) provided transition probablities for lines of the A–X and B'–X systems for the main isotopologue. Furthermore, Zhang & Steimle (2014) conducted Zeeman spectroscopy on the A–X (0,0) band. An *ab initio* study of the A and B' states of MgH also yielded transition probabilities (Mostafanejad & Shayesteh 2012). Low-lying electronic states of FeH were described by theory (DeYonker & Allen 2012), as were the $e^1\Pi - X^1\Sigma^+$ and ${}^1\Sigma^+ - X^1\Sigma^+$ systems of ZrO (Shanmugavel & Sriramachandran 2011), where the latter study presented data including oscillator strengths.

4.3. *Planetary atmospheres*

The molecules CO_2 and SO_2 continue to draw attention by experimentalists and theorists. Photoabsorption cross sections for electronic transitions in CO_2 were obtained through experimental measurements (Archer *et al.* 2013; Venot *et al.* 2013) and theoretical calculations (Grebenshschikov 2012, 2013). Low-lying electronic states were also studied theoretically (Zhou *et al.* 2013). As for SO_2, excited state dynamics were studied experimentally (Wilkinson *et al.* 2014) and theoretically (Mai *et al.* 2014; Lévêque *et al.* 2014), while Xie *et al.* (2013) determined potential energy surfaces for the two lowest singlet and two lowest triplet states.

Data needs for other molecules were also addessed. Absorption cross sections for isotopologues of SO were obtained theoretically by Danielache *et al.* (2014). A global fit to transitions across the spectrum for O_2 yielded isotopically invariant data for the X, a, and b states (Yu *et al.* 2012a), from which an detailed analysis of the airglow bands was accomplished (Drouin *et al.* 2013). Measurements on absorption cross sections for C_2H_2 (Cheng *et al.* 2011) were also reported.

4.4. *Larger Molecules*

Most studies of electronic transitions in large molecules seek correspondences with wavelengths associated with diffuse interstellar bands. Here we give a sampling of the efforts in this area. PAH-related species have drawn considerable attention. Recent spectroscopic measurements included results on neutral species by Gredel *et al.* (2011) and on ionized species by Garkusha *et al.* (2011), Bonaca & Bilalbegović (2011), and Hardy *et al.* (2013). A combined experimental and theoretical study on propadienylidene (C_3H_2) was conducted by Stanton *et al.* (2012). Chakrabarty *et al.* (2013) measured the spectrum of the triacetylene cation. A theoretical computation by Majumdar *et al.* (2014) provided the spectrum of the cyanomethyl anion (CH_2CN^-). The photoionization of cyanoacetylene was also the focus of an experimental study (Leach *et al.* 2014).

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