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COMMISSION B5 WORKING GROUPS

Div. B / Commission B5 WG2 **Spectroscopic and Radiative Data for Molecules**

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TRIENNIAL REPORT 2018-2021

1. Introduction

The current report covers the period from 2018 to March 2021. As with previous reports, the current one 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. 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. The grouping of the molecules was modified again with respect to the previous report. Numerous detections have been reported in the course of unbiased molecular line surveys of the prototypical dark cloud TMC-1 carried out with the Yebes 40 m and IRAM 30 m dishes on one side and with the GBT 100 m telecope on the other. Several of these reports involved laboratory spectroscopic results. These form the basis of section 2.1. Purely laboratory spectroscopic studies of other molecules observed or potentially observable in dark clouds are also included. In recent years, quantum-chemical calculations of collisional processes have attracted considerable attention. These frequently use spectroscopic information on van-der-Waals complexes of the respective molecule with one H, H_2, or He. We provide information on experimental studies of such van-der-Waals complexes in section 2.2, including some studies dating further back than 2018. Small molecules, up to tetratomic species, occur in section 2.3, essentially saturated organic molecules not in section 2.1 are in section 2.4.

Several databases provide rotational spectra of (mostly) molecular species of astrophysical and astrochemical relevance. The most important source for calculations generated from experimental data by employing appropriate Hamiltonian models is the Cologne Database for Molecular Spectroscopy, CDMS (https://cdms.astro.uni-koeln.de/) (Müller et al. 2001, 2005) with its catalog in the classical incarnation (https://cdms.astro.uni-koeln.de/classic/entries/). Please note that the links have changed since the last report. 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 was 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. The JPL catalog as well as several infrared databases are part of the VAMDC consortium; the project was described recently by Albert et al. (2020).

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. *Dark cloud molecules*

One rather ubiquitous molecule found early in this period employing the IRAM 30 m radio telescope is thionitrosylium, NS^+, (Cernicharo et al. 2018). Its identity, and that of most other molecules, was confirmed through laboratory spectroscopy. More recently, HC_3O^+ (Cernicharo et al. 2020) and HC_3S^+ (Cernicharo et al. 2021b) were detected in TMC-1 and in the lab. Further reports from this consortium deal with HDCCN (Cabezas et al. 2021b), CH_3CO^+ (Cernicharo et al. 2021a), and, thus far without confirmation from laboratory measurements, HC_5NH^+ (Marcelino et al. 2020). We also mention a microwave spectroscopic study on HC_5N and HC_7N (Giesen et al. 2020), one on D_2CCN (Cabezas et al. 2021a), and a study in which unpublished transition frequencies of HNC_3 were provided (Vastel et al. 2018).

Some detection papers associated with GBT observations also report auxiliary laboratory data. These include benzonitrile, *c*-C_6H_5CN, (McGuire et al. 2018a) and 3-butynenitrile, $HCCCH_2CN$, (McGuire et al. 2020). Other studies on molecules related to the former molecule, i.e., aromatic molecules with one or few fused benzene rings, include two di- and tricyclic cyanides each (McNaughton et al. 2018), benzonitrile (Zdanovskaia et al. 2018), 4-cyanopyridine (Vogt et al. 2018; Dorman et al. 2020), phenyl isocyanate and isothiocyanate (Sun et al. 2019), benzoisonitrile (Zdanovskaia et al. 2019), acenaphthene (Gruet et al. 2020), and phenylpropiolonitrile (Buchanan et al. 2021). Noteworthy in the context of both former mentioned molecules is the extensive study of discharge products of benzene, benzene and O_2, and benzene and N_2 (McCarthy et al. 2020). Further studies of molecules loosely related to 3-butynenitrile include ethynyl isothiocyanate, HCCNCS, (Sun et al. 2018), aminopropyne, $HCCCH_2NH_2$, (Degli Esposti et al. 2018), iminopropyne, HCCCHNH, (Bizzocchi et al. 2020b), and thiopropynal, HCCCHS, (Margulès et al. 2020b).

2.2. *van-der-Waals molecules involving H_2 and He*

Experimentally determined collisional data of astrochemically relevant molecules with H, H_2, and He are somewhat limited. Therefore, quantum-chemically calculated data have been used increasingly in recent years. Besides the limited experimentally determined collisional data, there are other pieces of information which can be used to evaluate the quality of the quantum-chemical calculations. These may be, e.g., pressure-broadening rotational or rovibrational measurements of transitions of an astrochemically relevant molecule by H_2 or He or rotational or rovibrational spectroscopy of van der Waals complexes of an astrochemically relevant molecule with one H_2 molecule or one He atom. We present in the following studies of the rotational spectra of such van der Waals complexes which often may include data on minor isotopic species, not only of the astrochemically relevant molecule, but also of the H_2 molecule or He atom. While we try to provide a comprehensive overview of studies in the past ∼25 years, we refrain from guaranteeing completeness.

One of the earliest studies may have been that of the van der Waals complex between He and HCN by Drucker et al. (1995). Additional investigations of this sytem were reported (Harada et al. 2002; Dempster et al. 2012). Further studies of van der Waals molecules with one He atom include those with OCS (Higgins & Klemperer 1999; Xu & Jäger 2008), with CO (McKellar et al. 1999; Surin et al. 2000b; Potapov et al. 2009b), with N_2O (Song et al. 2004), with HC_3N (Topic & Jäger 2005), with CH_3F (Higgins & Klemperer 2005), with CH_3^+ (Töpfer et al. 2018), and with HCO^+ (Salomon et al. 2019).

Among the van der Waals complexes between an astrochemically relevant molecule and one H_2 molecule, the one with CO is probably the most thoroughly studied one (Pak et al. 1999; Surin et al. 2000a; Potapov et al. 2009a,c; Jankowski et al. 2013; Potapov et al. 2015; Raston & Jäger 2015). Other complexes involve those with HCN (Ishiguro et al. 2001, 2012), with OCS (Yu et al. 2005, 2007; Michaud et al. 2008), with HC_3N (Michaud et al. 2011), with H_2O (Harada et al. 2014), with O_2 (Bunn et al. 2015), and with NH_3 (Surin et al. 2017; Tarabukin et al. 2021).

2.3. *Small molecules*

Investigations of light hydrides include CH^+ and its isotopologues (Doménech et al. 2018a; Yu et al. 2018), isotopologues of NH (Bizzocchi et al. 2018; Melosso et al. 2019), NHD (Bizzocchi et al. 2020a), deuterated ammonia (Melosso et al. 2021), and deuterated ammonium (Doménech et al. 2018b).

Reports on isotopic AlO and AlS (Breier et al. 2018), TiO (Breier et al. 2019), and FeO (Waßmuth et al. 2020) appeared. Other investigations include CN^+ (Thorwirth et al. 2019), KO (Burton et al. 2019), SO_2 with one and two ^{18}O (Margulès et al. 2020d), AlC_2 (Halfen & Ziurys 2018), and H_2CS with a plethora of isotopic species (Müller et al. 2019). Additional investigations of tetratomic molecules involved HCCO (Chantzos et al. 2019) and $HSCO^+$ (Lattanzi et al. 2018) along with their deuterated variants and HOOD (Herberth et al. 2019). We also mention a study of vibrational satellites of C_2S, C_3S, and C_4S (McGuire et al. 2018b) even though these molecules have only been found in colder environments thus far. Finally, we point out the detection of the radioactive molecule ^{26}AlF (Kamiński et al. 2018).

2.4. *Larger, mostly saturated organic molecules*

Complex organic molecules have been studied to very great extent. We list results on detected molecules first with minor isotopic species, including those not yet found in

space. This is followed by molecules closely related to such molecules which we consider as good candidates to be found. Finally, we list some studies on molecules that we currently consider to be less likely found or that are not as close to detected molecules.

Methanol is the most important complex organic molecule in the sense of astrochemistry, i.e. molecules with six or more atoms containing at least one C atom. Very recently, its Zeeman effect has been studied in the laboratory (Takagi et al. 2021). Methanethiol is its sulfur homologue, which is much less abundant, but has attracted increasing interest in radio-astronomy lately. Results of investigation were published on the main isotopic species (Zakharenko et al. 2019a), on CH_3SD (Zakharenko et al. 2019b), $CH_3^{34}SH$ (Zakharenko et al. 2019c), and $^{13}CH_3SH$ (Ilyushin et al. 2020b). Further reports involve cyanomethanimine (Melosso et al. 2018), ^{13}C-containing isotopomers of propyne (Müller et al. 2020), methyl isocyanate with its ^{13}C-containing isotopomers (Kolesniková et al. 2019), singly deuterated acetaldehyde (Coudert et al. 2019), vibrationally excited methyl formate (Kobayashi et al. 2020) and its methyl-^{13}C species (Kobayashi et al. 2018), ethyl cyanide in excited vibrational states (Kisiel et al. 2020; Endres et al. 2021), methoxymethanol (Motiyenko et al. 2018), an extensive study of acetone in its ground vibrational state and the two torsional fundamentals (Ilyushin et al. 2019), an extension of the rotational spectrum of the lowest ethanediol conformer into the submillimeter (Melosso et al. 2020b), and a study of the ground and several excited vibrational states of *n*-propyl cyanide (Liu et al. 2019). We also point out a very extensive analysis of the methylamine spectrum using a hybrid tunneling-torsion Hamiltonian (Kleiner & Hougen 2020). Other studies of isotopic species of molecules detected in space include the ^{15}N isotopomers of cyanamide with additional work on the ^{13}C species (Coutens et al. 2019), CH_2DCl (Melosso et al. 2020a), ethanimine (Melli et al. 2018), several propenal isotopologues (Evangelisti et al. 2020), and a study on the ^{13}C isotopomers of acetone, focusing mainly on the symmetrically substituted one (Ordu et al. 2019).

Investigations of molecules considered to be likely candidates for detection in space comprise the hydroxymethyl radical (Chitarra et al. 2020), thioformamide (Margulès et al. 2020a), cyanoketene (Margulès et al. 2020c), methylketene (Bermúdez et al. 2018), ethyl isocyanide (Margulès et al. 2018), dimethyl sulfide (Ilyushin et al. 2020a), 3-aminopropionitrile (Richard et al. 2018), ethyl isocyanate (Kolesniková et al. 2018a), 3-methylbutyronitrile (Wehres et al. 2018), and two higher-lying conformers of 2-cyanobutane (Hermanns et al. 2019).

Finally, among the molecules currently considered by us less likely to be found in space are alkaline and alkaline-earth cyanoacetylides (Cabezas et al. 2019), dithioformic acid (Prudenzano et al. 2018), ethynethiol (Lee et al. 2019), aminomethylium (Markus et al. 2019), which is isoelectronic to C_2H_4, vinyl mercaptan (Martin-Drumel et al. 2019), methoxyamine (Kolesniková et al. 2018c), S-methyl thioformate (Jabri et al. 2020), acetylacetylene (Lengsfeld et al. 2021(@), methoxyacetaldehyde (Kolesniková et al. 2018b), ethylmethylamine (Koziol et al. 2020), and methyl cyanoacetate (Gregory et al. 2021).

3. Vibrational Spectra

The vibration spectra of molecules of astronomical or of potential astronomical interest are reviewed for the period 2018-2020 (including a few papers in early 2021) starting from the end of our previous report (`https://www.iau.org/science/scientific_bodies/working_groups/309/`). In addition to the citations for particular molecules, there are a number of spectral database compilations that are useful. Perhaps the most helpful is the HITRAN database that contains mainly 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, HITRAN2020 (Gordon et al. 2021), has been submitted for publication, but many updates to HITRAN2016, Gordon et al. (2017) have already appeared such as for OH; additional information is available at HITRAN*online* (`https://hitran.org/`).

The HITRAN molecular coverage is being expanded to include planetary atmospheres other than Earth and already contains line parameters for molecules such as C_2N_2, PH_3 and CS that are primarily for planetary applications. HITRAN2020 will add SO and GeH_4 to this list. In addition, HITRAN now includes line parameters and cross sections for pressure broadening by H_2, He, H_2O and CO_2 for selected species, not just air. While the GEISA database has significant overlap with HITRAN, it contains additional molecules of interest for studies of planetary atmospheres (Jacquinet-Husson et al. 2016).

HITRAN is intended for applications near room temperature so care is needed for applications at higher temperatures because of potential missing lines and bands. For sources with elevated temperature, the HITEMP database is being updated and extended (https://hitran.org/hitemp/). So far new line parameters are available for hot NO, NO_2, N_2O (Hargreaves et al. 2019), CO (Li et al. 2015), OH and CH_4 (Hargeaves et al. 2020).

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 and ethane, but the broadening gas is usually air. HITRAN2020 is adding infrared absorption cross sections for molecules with broadening gases such as H_2, He, N_2 and CO_2. In addition, some cross sections of hot hydrocarbons such as ethane and propane are being added for exoplanet applications. HITRAN also contains a very extensive set of collision induced absorption data (Karman et al. 2019) for important astronomical systems such as H_2-H_2.

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 (`http://www.exomol.com/`) of J. Tennyson, S. Yurchenko and co-workers (Tennyson et al. 2020) has an extensive collection of calculated line lists designed "as input to atmospheric models of exoplanets, brown dwarfs and cool stars." A very useful set of infrared absorption cross sections for several hundred molecules is 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 was included in HITRAN2016.

The cross sections and line lists created by the Bernath group are available on the MoLLIST site (`http://bernath.uwaterloo.ca/molecularlists.php`); the MoLLIST paper is a review article (Bernath 2020). The TheoReTS site (Theoretical Reims–Tomsk Spectral data, `http://theorets.tsu.ru`) has collected the calculated line lists for molecules such as CH_4, SiH_4 and GeH_4 from the Tyuterev, Rey and Nikitin collaboration.

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. For the simplest hydrides, H_2, D_2 (Józwiak et al. 2020a) and HD (Józwiak et al. 2020b), new vibration-rotation line positions and intensities were calculated including hyperfine structure. New calculations of vibration-rotation line positions and Einstein A values for the primordial molecules HD, HD^+ and HeH^+ were published (Amaral et al. 2019). The vibration-rotation lines of CH^+ and $^{13}CH^+$ fundamental bands were measured with 80 kHz precision in a cryogenic ion trap experiment by Doménech et al. (2018a). Similar measurements were made for the fundamental bands of CN^+ and $C^{15}N^+$ (Doménech et al. 2020).

The ExoMol vibration-rotation line lists now include SiS (Upadhyay et al. 2018), SH (Yurchenko, et al. 2018; Gorman et al. 2019), NS (Yurchenko, et al. 2018), AlH (Yurchenko, et al. 2018a), MgO (Li et al. 2019), TiO (McKemmish et al. 2019), and PH (Langleben et al. 2019). These new line lists combine experimental measurements and *ab initio* calculations. For SH (Gorman et al. 2019), AlH, MgO and TiO, the line lists include electronic transitions as well as vibration-rotation bands. A new vibration-rotation line list for CS and various isotopologues was prepared by Hou & Wei (2020). Line lists and radiative cooling functions were computed for the ground states of LiH isotopologues by Diniz et al. (2018).

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 AlF and AlCl (Yousefi & Bernath 2018) by combining line positions from infrared emission spectra with line strengths obtained using *ab initio* dipole moment functions. TiO has been detected in the stratosphere of hot Jupiter exoplanets (Nugroho et al. 2017). A vibration-rotation spectrum of TiO and its isotopologues has been recorded with a diode laser using a laser ablation jet expansion source (Witsch et al. 2021).

3.2. *Small polyatomic molecules*

The line parameters of water, ammonia, and methane (as well as PH_3, SO_2, H_2S, CO_2, H_2CO, HCN, C_2H_2, C_4H_2, etc.) as given in the HITRAN 2020 database (Gordon et al. 2021) are generally satisfactory for most astronomical purposes at low temperatures, except for overtone and combination bands in the near infrared and visible regions. For H_2O, a new line list was calculated for rotation–vibration levels up to 41000 cm^{-1} by the ExoMol team (Polyansky et al. 2018). This line list was validated and used to assign lines for hot water at 1950 K in the 6250–6670 cm^{-1} region (Rutkowski et al. 2018). A set of energy levels for H_2O (Furtenbacher et al. 2020) and O-isotopologues (Furtenbacher et al. 2020) derived from experimental observations were published.

A new vibration-rotation line list for hot NH_3 was computed by Coles et al. (2019); then N quadrupole hyperfine structure was added to make a second NH_3 line list (Coles et al. 2019). Experimental line lists for NH_3 at 293–900 K for the 4800–9000 cm^{-1} region were prepared by Beale et al. (2020). Spectra of NH_3 at room temperature were also analyzed in the 5650-6350 cm^{-1} (Cacciani et al. 2021) and 7400-8600 cm^{-1} (Vander Auwera & Vanfleteren 2018) regions. High resolution $^{15}NH_3$ spectra were measured in the 350 to 2000 cm^{-1} region (Canè et al. 2019).

There has been considerable progress on the analysis of CH_4 spectra. New spectra of hot CH_4 (620-1715 K) emission in the 3 μm region were analyzed by Amyay et al. (2018). Diode laser absorption spectra of $^{13}CH_4$ were recorded in the tetradecad (5695-5850 cm^{-1}) at 296 K and 80 K (Konefal et al. 2018). Wong et al. (2019) measured infrared

absorption cross sections of hot CH_4 (295-1000 K) in the near infrared (5200-9200 cm^{-1}), which were then used to validate the new HITEMP CH_4 line list (Hargeaves et al. 2020). Very recently, line broadening of hot CH_4 by H_2 for the ν_3 mode was measured (Yousefi et al. 2021).

For C_2H_2 (Chubb et al. 2020), C_2H_4 (Mant et al. 2018), CO_2 (Yurchenko et al. 2020), SiO_2 (Owens et al. 2020), and NaOH (Owens et al. 2021), ExoMol vibration-rotation databases were calculated. New cavity ringdown measurements of CO_2 in the 8311-8679 cm^{-1} interval were carried out (Karlovets et al. 2020). Frequency combs are used to improve the measurement accuracy of line positions for near infrared bands, e.g., by Wu et al. (2020). The CDSD-296 database of experimental line positions and intensities for room temperature CO_2 was updated (Tashkun, et al. 2019). Infrared spectra of Si_2C (Witsch et al. 2019) were recorded by diode laser absorption in a supersonic jet spectrometer, and spectra for C_3 (Schröder et al. 2018) were measured by cavity ring-down spectroscopy in the 3 μm region.

The infrared spectra in the CH stretching region of CH_3D^+ (Scrape et al. 2019) and $CD_2H_2^+$ (Chang & Nesbitt 2018) were measured by slit-jet absorption spectroscopy. A new vibration-rotation line list was calculated for H_3O^+ (Yurchenko et al. 2020).

3.3. *Large molecules*

There is continuing strong interest in large carbon-containing molecules such as polycyclic aromatic hydrocarbons (PAHs) and related molecules. For PAH molecules, the NASA-Ames database (now version 3.2) has been updated in 2020 with a description of the experimental spectra that are included (Mattioda et al. 2020). Extensive calculations by the several groups have continued, for example, on deuterated PAHs (Yang et al. 2020), hydrogenated PAH isomers (Pla et al. 2020), PAH ions (Maragkoudakis et al. 2020), the effect of aliphatic side groups on PAH spectra (Buragohain et al. 2020), PAH overtones (Chen et al. 2019), and so forth. Spectra of several jet-cooled PAHs were recorded by Lemmens et al. (2019).

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 of pressure, temperature, and composition as found on the astronomical object. Such high resolution cross sections are becoming available for example propene, C_3H_6, (Sung et al. 2018) and n-butane, C_4H_{10}, (Sung et al. 2020) with N_2 as a broadener at low temperatures for the atmosphere of Titan. Infrared absorption cross sections for cold propane (Wong et al. 2019) in the 3.3 μm region, cold isobutane (Hewett et al. 2020a), ethane (Hewett et al. 2020b; Dodangodage et al. 2020), and neopentane (Bernath et al. 2020) were recently published.

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 (1) interstellar matter (including diffuse molecular clouds, disks around newly formed stars, and comets whose chemistry

is similar), (2) the atmospheres of planets and their satellites, (3) metal hydrides, oxides, and related molecules in the atmospheres of late-type stars, and (4) larger molecules. The distinction of where to place a molecule in the first three topics is based on its most likely environment, but it can be observed in others as well.

4.1. *Interstellar matter*

New results on simple hydrides, as well as their ions and isotopologues, appeared since 2017. Medcraft et al. (2019) presented a comprehensive study of the 0-0, 1-0, and 2-2 vibronic bands of the C $^2\Sigma^+$–X $^2\Pi$ transition in CH, and Coudert et al. (2019) studied the photoelectron spectrum of methylene (CH_2) experimentally and theoretically. Another theoretical study (Chakrabarti et al. 2019) calculated bound and continuum states in CH. The ExoMol group published an analysis of measured spectra for ^{14}NH (Darby-Lewis et al. 2019). Heays et al. (2018) obtained high-resolution spectra of the OH and OD D $^2\Sigma^-$–X $^2\Pi$ system, from which transition frequencies, oscillator strengths, and line widths are provided. Photoionization cross sections were measured by (Dodson et al. 2018; Harper et al. 2019), The near-threshold spectrum for OH^+ photodissociation was presented by Hechtfischer et al. (2019). Recent work on oscillator strengths for the Lyman and Werner Bands of H_2 (Xiong et al. 2019) were determined experimentally, and a line list for A $^2\Sigma^+$–X $^2\Pi$ transitions in SH was reported (Gorman et al. 2019).

A number of analyses focused on CO, N_2, C_2, and S_2. Details of predissociation in CO isotopologues were obtained by measuring branching fractions for levels in C and O products (e.g., Shi et al. 2018; Jiang et al. 2019; Chi et al. 2020a,b). Other efforts on CO include an experimental study of perturbations in the A $^1\Pi$ $v = 1$ level in $^{12}C^{18}O$ (Malicka et al. 2020) and results on CO photoionization, both experimental (Holland & Shaw 2020) and theoretical (Modak & Antony 2019). Measurements and calculations were performed on CO^+, providing results on perturbations in the $v = 0$ and 1 levels of the A $^2\Pi_i$ state (Hakalla et al. 2019), on B $^2\Sigma^+$–X $^2\Sigma^+$ transitions (Ventura et al. 2020), and on molecular constants and transition probabilities for low-lying states (Xing et al. 2018a). Efforts on transitions in N_2, which is isoelectronic with CO, involved a line list with transition probabilities for several bands (Western et al. 2018), an analysis of the C $^3\Pi_u$–B $^3\Pi_g$ system (Ventura & Fellows 2019), an absorption spectrum of $^{14}N^{15}N$ to examine spin-forbidden transitions (Heays et al. 2019), and a theoretical study of the C $^3\Pi_u$–B $^3\Pi_g$ and C$''$ $^5\Pi_u$–A$'$ $^5\Sigma_g^+$ systems (da Silva et al. 2020). Velasco & Lavín (2020) calculated oscillator strengths for bands in the c_4' $^1\Sigma_u^+$–X $^1\Sigma_g^+$ system of N_2, and a correction to branching fractions for atomic products in N_2 photodissociation was published (Song et al. 2018). Radiative and nonradiative decay rates were computed for the C $^2\Sigma_u^+$ state of N_2^+ as a function of temperature and isotopologue by Stemmle et al. (2020). Recent spectroscopic studies on C_2 include an extension of reported vibrational levels for the D $^1\Sigma_u^+$ state (Krechkivska et al. 2018), a detection of a strong perturbation in the $v = 10$ level of the b $^3\Sigma_g^-$ state from observations of the Swan band sequence in a comet (Nelson et al. 2018), and an expanded investigation of perturbations in the A $^1\Pi_u$ state (Nakajima 2019). Other efforts provided a line list for the eight lowest states with lifetimes for its isotopologues from the ExoMol team (Yurchenko et al. 2018b), an update to this line list for $^{12}C_2$ that provided data on higher lying states (McKemmish et al. 2020), and a suite of calculations yielding a value for D_0 (Karton 2019). Oscillator strengths for the B $^3\Sigma_u^-$–X $^3\Sigma_g^-$ system in S_2 were determined by Stark et al. (2018), while Lewis et al. (2018) examined perturbations associated with the upper state through computations. A combined experimental and theoretical effort on six low-lying states in S_2 yielded spectroscopic constants as well as a value for D_o (Qin et al. 2019a). Other theoretical studies

focused on the six lowest-lying triplet states (Xing et al. 2020a), yielding lifetimes, and on eleven triplet states, providing photochemical absorption sections for S_2 isotopologues (Sarka et al. 2019).

We end this section by describing recent work on small carbon-based nitrides and sulfides. Transition probabilities and the corresponding radiative lifetimes involving ten low-lying states in CN were computed by Yin et al. (2018a), and Syme & McKemmish (2020) compiled a list of transition frequencies from experimentally measured rovibronic energy levels for eight doublet states in $^{12}C^{14}N$. Spectroscopic efforts on CS included analysis of the a′ $^3\Sigma^+$–a $^3\Pi$ band at infrared wavelengths (Sunanda et al. 2019) where perturbations were found and computed lifetimes for a number of singlet and triplet states (Sun & Shi 2020; Xing et al. 2020b). Photodissociation rates were determined theoretically by Pattillo et al. (2018) and Xu et al. (2019). The reaction pathway for CS_2 dissociation was followed by femtosecond photoelectron techniques (Smith et al. 2018). Generalized oscillator strengths for transitions in CS_2 up to 6.3 eV were calculated by Oliveira et al. (2019).

4.2. *Planetary atmospheres*

We describe recent publications on molecular species often associated with atmospheres of planets and their satellites. Bernath & Bittner (2020) created a line list for the a $^1\Delta$–X $^3\Sigma^-$ transition in SO and suggested the presence of this molecule in Io's atmosphere. Theoretical lifetimes were determined for several excited triplet states (Feng & Zhu 2019a), and in a subsequent paper Feng & Zhu (2019c) provided lifetimes for excited singlet states. Similar calculations on doublet, quartet, and sextet states of SO^+ were performed by Guo & Zhu (2020). A theoretical investigation of the ã $^3B_1$ state of SO_2 (Kumar et al. 2019) yielded improvements in comparison with measured transition frequencies involving the ground state, $\tilde{X}$ $^1A_1$. Excitation energies and oscillator strengths for excited states in SO_2, as well as for H_2O, N_2, and CO, were derived theoretically (Cabral Tenorio et al. 2019). Oscillator strengths and integral cross sections involving valence-shell excitation in O_2 (Liu et al. 2018) and N_2, O_2, and C_2H_2 (Liu et al. 2019) were obtained through the use of inelastic x-ray scattering and scattering by fast electrons. New cross sections for near ultraviolet (UV) transitions in H_2O were measured by Ranjan et al. (2020) for use in photochemical models of habitable planet atmospheres. The vacuum UV cross section for CO_2 was obtained at temperatures between 150 and 800 K to aid in modeling exoplanet atmospheres (Venot et al. 2018). Other vacuum UV measurements on NH_3 provided data on the absorption spectrum between 5.4 and 10.8 eV (Limão-Vieira et al. 2019), which was used to calculate oscillator strengths from a reanalysis of the observed structures, and data on the relaxation dynamics of high-lying Rydberg states seen via photoelectron imaging (Svoboda et al. 2019).

4.3. *Late-type stars*

An extensive body or work on metal oxides and related molecules appeared in the past three years. An ExoMol line list for the five lowest-lying states in isotopologues of MgO (Li et al. 2019) was presented, and a theoretical effort (Bai et al. 2020) calculated radiative lifetimes for spin-forbidden transitions in this molecule. Measured lifetimes and branching fractions for B $^2\Sigma^+$–X $^2\Sigma^+$ vibronic bands in AlO were acquired (Bai & Steimle 2020), while Trabelsi & Francisco (2018) studied photodissociation of AlOH involving singlet and triplet states theoretically. Einstein A coefficients and radiative lifetimes were calculated for singlet (Feng & Zhu 2019b) and triplet (Feng & Zhu 2019d) states in SiO. The 1+1 REMPI spectrum of SiO yielded the ionization potential for this molecule

(Stollenwerk et al. 2019). Radiative lifetimes for low-lying states in SiO^+ were computed by Qin et al. (2020), while Yin et al. (2018b) determined theoretical radiative lifetimes for doublet states in PO. For calcium-containing molecules, perturbations in the A′ $^1\Pi$ and C $^1\Sigma^+$ states of CaO were examined (Bresler et al. 2020), the ExoMol group presented a compilation of rovibronic transitions for CaOH from published measurements, and perturbations were analyzed from a spectroscopic study of low-lying states in CaO^+ (VanGundy et al. 2018). Spectroscopic constants and line positions for several systems in the TiO molecule were provided by Bittner & Bernath (2018) and Hodges & Bernath (2018). Line lists for dipole-allowed transitions involving 13 low-lying states for TiO isotopologues were produced by McKemmish et al. (2019), and Pavlenko et al. (2020) verified the accuracy of the lists through astronomical observations. Bernath (2020) and Bernath & Cameron (2020) determined absorption cross sections for transitions in TiO, while Cheng et al. (2020) computed oscillator strengths for transitions in this molecule. Tennyson and colleagues analyzed electronic transitions in $^{89}Y^{16}O$ (Smirnov et al. 2019) and $^{90}Zr^{16}O$ (McKemmish et al. 2018).

We now consider recent efforts on metal hydrides. Corzo et al. (2018) calculated oscillator strengths for transitions involving Rydberg states in MgH, while the ExoMol team provided line lists for transitions between the A $^1\Pi$ and X $^1\Sigma^+$ states in isotopologues of AlH (Yurchenko, et al. 2018a) and Szajna et al. (2018) studied A $^2\Pi$–X $^2\Sigma^+$ bands of AlD^+ experimentally, finding the B $^2\Sigma^+$ state perturbed A $^2\Pi$. Biglari et al. (2018) calculated lifetimes for singlet, triplet, and quintet states in SiH^+. Work on calcium hydrides included a spectroscopic analysis of bands in the B/B″ $^2\Sigma^+$–X $^2\Sigma^+$ system in CaH (Watanabe et al. 2018) and line lists for B $^2\Sigma^+$–X $^2\Sigma^+$ and A $^2\Pi$–X $^2\Sigma^+$ transitions in CaH and CaD by Alavi & Shayesteh (2018). Cheng & DeYonker (2019) examined low-lying states in FeH^+ theoretically.

We conclude this section with a discussion of molecules containing carbon and nitrogen. Transition probabilities and lifetimes were computed for triplet (Xing et al. 2019b) and singlet (Zhang & Wang 2019) states in SiC and for the lowest-lying doublet states in SiN (Xing et al. 2018b). These molecular properties were determined theoretically for singlet states in AlN (Xing et al. 2019a), for singlet, triplet, and quintet states in PN (Qin et al. 2019b), and for quintet states in NS^+ (Zhou et al. 2019). Molecular constants were derived from spectroscopic measurements of the $\tilde{A}\ ^1B_2$–$\tilde{X}\ ^1A_1$ transitions in SiC_2 (Zhang et al. 2020). Jerosimić & Milovanović (2018) calculated spin-orbit and vibronic interactions in low-lying states in FeCN.

4.4. *Larger Molecules*

Large molecules are believed to be responsible for the diffuse interstellar bands seen at visible and near infrared wavelengths and to act as seeds for the aerosols seen in Titan's atmosphere. Recent experimental investigations on PAH molecules included a combined experimental and theoretical study of the bisanthenequinone cation (Chen et al. 2018), determination of the threshold energy for dissociating the 1-ethynylpyrene cation (Rouillé et al. 2019), and a spectroscopic analysis of the thiophenoxy radical (Sato et al. 2020). The electronic structure for carbon chains was studied theoretically (Reddy et al. 2019; Ghosh et al. 2019) and the vibronic structure of HC_5N^+ was examined through photoelectron spectroscopy (Gans et al. 2019a) and *ab initio* calculations (Gans et al. 2019b). The relevance of fullerences was described in a review (Linnartz et al. 2020) and examined through a spectroscopic analysis of $He@C_{60}^+$ (Campbell et al. 2020).

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