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COMMISSION 14: ATOMIC AND MOLECULAR DATA[1]

(DONNEES ATOMIQUES ET MOLECULAIRES)

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In recognition of its special interdisciplinary character, IAU Commission 14 is linked directly to the Executive Committee. The Commission's role is to inform the astronomical community of new developments in the diverse fields of research which involve atoms and molecules. Conversely it endeavours to sensitize the research community active in those fields to the specific needs of astronomy, especially concerning basic data and modeling tools. More generally, Commision 14 tries to foster long term relations and collaborations between the two communities and, when necessary, to alert funding authorities to the specific needs of ground and space based astronomy for specific atomic and molecular data.

This report is one of the main contributions of Commission 14 to the information of the astronomical community. Several meetings concerned, at least in part, with the need and availability of atomic and molecular data for astrophysics were also sponsored or co-sponsored. In the last triennium, Commission 14 cosponsored IAU Symposium 194 "Astrochemistry: From Molecular Cloud to Planetary Systems" held in Sogwipo (Korea) from Aug. 23 to 27, 1999 and organized by Commission 34. A Joint Discussion: JD1 on "Atomic and Molecular Data for Astrophysics, New Developments, Case Studies and Future Needs" has been planned for the XXIVth IAU General Assembly in Manchester (Aug. 7-19, 2000) and cosponsored by Commissions 15, 16, 29, 34, 36, 40 and 44. Several other Joint Discussions to be held at the Manchester General Assembly are co-sponsored by this commission.

The present report comprises six sections established by the specialized Working Groups of Commission 14. It is made available on the Commission 14 Website:
`http://ww.obspm.fr/IAU14`
and its mirror `http://cfa-www.harvard.edu/amp/iau14`.

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[1]Committee of the Executive Committee.

5. WORKING GROUP 5: MOLECULAR STRUCTURE AND TRANSITION DATA

PRESIDENT: E. F. VAN DISHOECK
VICE-PRESIDENT: J. H. BLACK

The following summary has been prepared by E.F. van Dishoeck and J.H. Black, with contributions sent by S. Leach, T. Oka, F. Rostas, L. Rothman, P.L. Smith and K. Yoshino in the summer of 1999. Other topics have been added through a search of the (vast) literature. Because of space limitations, a complete overview or list of references is not possible and only a few highlights limited to gas-phase molecules of actual or potential astrophysical interest are given. With the advent of electronic versions of the astrophysical and chemical physics journals, other related references can readily be found by searching on the appropriate keywords or authors.

5.1. Fundamental Data and Databases

The recommended values of fundamental physical constants have been officially revised by CODATA for the first time since 1986. The new 1998 recommended values are based on all data available through 1998 December 31 and will be published in detail soon (Mohr & Taylor 2000). The new values of constants are available electronically through the US National Institute of Standards and Technology (NIST) at `http://physics.nist.gov/constants`. Uncertainties in several fundamental constants have been greatly reduced by means of precise atomic spectroscopic measurements. For example, an absolute measurement of the H I 1s–2s two-photon transition frequency yielded improved values of both the Rydberg constant and the hydrogen ground-state Lamb shift (Udem et al. 1997).

The WWW is rapidly growing into the primary tool to access and search molecular data bases. For example, the GEISA databank of infrared transitions of molecules of atmospheric interest, 1997 edition, is available at `http://www.ara.polytechnique.fr/alexei_index.html`. The HITRAN database is available through `http://www.hitran.com/` and the 1996 Edition has been presented by Rothman et al. (1998). The JPL database of microwave transitions can be found through `http://spec.jpl.nasa.gov`, whereas the Lovas database is accessible through `http://physics.nist.gov/PhysRefData/`.

The UMIST data file of rate coefficients for interstellar chemical reactions can be found at `http://saturn.phy.umist.ac.uk` (Millar et al. 1997). Tables with recently measured neutral-neutral reactions at low temperature are given by Rowe et al. (2000). A table with 2000 reactions appropriate for the modeling of the photochemistry of planetary atmospheres is contained in Yung & DeMore (1998).

Optical constants of solid materials of interest in astronomy are available through `http://aragorn.astro.uni-jena.de/Group/Subgroups/Labor/Labor/odata.html` (Henning et al. 1999), whereas a summary of laboratory spectra of interstellar ices can be found at `http://www.strw.leidenuniv.nl/~lab`. Recent reviews of laboratory experiments on solid state material and PAHs compared with ISO and other space-based data are given in d'Hendecourt, Joblin & Jones (1999) and Ehrenfreund et al. (1999).

Infrared spectral atlases of the Sun have been published (Wallace et al. 1996), which are of value for spectroscopic studies of highly excited states of some molecules.

Links to many of the electronic molecular databases can be found through the IAU Astrochemistry working group at `http://www.strw.leidenuniv.nl/~iau34`. The proceedings of IAU Symposium 197 on Astrochemistry include several reviews on basic molecular processes and data needs (Minh & van Dishoeck 2000).

5.2. Electronic Spectra

Small molecules: The hydrogen molecule is still intensively studied. Photoionization cross sections of He and H_2 have been computed (Yan, Sadegpour & Dalgarno 1998). The UV emission continuum in H_2 excited by electron impact has been investigated (Abgrall et al. 1997). Laser spectroscopy has been used to probe the 86–90 nm spectrum of H_2 at high resolution (Reinhold, Hogervorst & Ubachs 1996) and to study some of its inter-Rydberg transitions (Ubachs, Hinnen & Reinhold 1997). The ground state of the hydrogen molecule changes character in strong magnetic fields (Kravchenko & Liberman 1998), which might affect the spectrum of a magnetic white dwarf (see also Detmer et al. 1997, 1998).

Work has continued on the UV spectrum and oscillator strengths of CO. New oscillator strengths have been measured for the B–X (0,0) and (1,0) bands (Stark et al. 1999a) and in the A–X system (Federman et al. 1997). Measurements in this system have been extended from $v' = 9 - 17$ (Jolly et al. 1997) to $v' = 13 - 21$ for $v'' = 0$ (Stark et al. 1998), and $v' = 11 - 23$ (Eidelsberg et al. 1999). There are also new *ab initio* calculations of the A–X transition dipole moment (Spielfiedel et al. 1999), which agree well with these and other experiments. Laboratory data and improved calculations of the intersystem transition oscillator strengths have been obtained (Rostas et al. 1999), which resolve earlier discrepancies. Tunable picosecond lasers have been used to measure lifetimes in the $E^1\Pi$ $v = 0$ and $v = 1$ states of three isotopic varieties of CO (Cacciani et al. 1998). High-resolution spectroscopy has been performed on the A–X system in $^{12}C^{18}O$ (Beaty et al. 1997). The EUV spectrum of CO excited by electron impact has been studied at high resolution (Ciocca, Kanik & Ajello 1997), as well as the A–X system (Beegle et al. 1999). The *nd* triplet Rydberg series of CO has been studied by laser-induced fluorescence; the resulting analysis led to rotational term values and an improved value of the ionization limit (Mellinger, Vidal & Jungen 1996).

High-resolution vacuum UV spectroscopy has been performed on N_2 (Roncin, Subtil & Launay 1998) and an atlas of the spectrum has been published in the astrophysical literature (Roncin & Launay 1998). An on-line atlas of the spectrum of N_2 has been introduced at the CfA at `http://cfa-www.harvard.edu/amdata/ampdata/cfamols.html`; this searchable database contains linelists for the region 84 nm to 100 nm, a compilation of f-value measurements and calculations, and a list of references.

Laboratory measurements of the UV absorption of O_2 have continued. The Schumann-Runge bands have been measured in absorption at 670 K and new spectroscopic constants have been derived for the ground state $X^3\Sigma_g^-$ (Cheung et al. 1996). A comparative high-resolution study of predissociation linewidths in the Schumann-Runge bands has been carried out (Dooley et al. 1998). Oscillator strengths in the Herzberg I system (Yoshino, Huestis & Nicholls 1998) and in the Herzberg II system (Yoshino et al. 1999) have been presented.

Absorption cross sections of H_2O at 120 to 188 nm have been measured by Yoshino et al. (1996, 1997), and the product distribution after photodissociation at 130 nm by Zanganeh et al. (1999). Calculations have been performed by van Harrevelt & van Hemert (1999). Nitrogen oxides have been investigated: absorption cross sections of NO_2 in the visible and UV have been recorded (Yoshino, Esmond & Parkinson 1997), the $\beta(9, 0)$ band of NO has been investigated in the vacuum UV (Yoshino et al. 1998), and the γ-band system of NO has been studied (Danielak et al. 1997).

The $A^3\Phi$ –$X^3\Delta$ system (γ bands) of TiO has been measured in the laboratory and sunspots, providing improved molecular constants, RKR potential energy curves, and Franck-Condon factors (Ram et al. 1999). Several new electronic states of TiO have been identified (Barnes, Merer & Metha 1997). Theoretical transition moments in all the low-lying singlet and triplet systems of TiO have been computed (Langhoff 1997). The absorption spectrum of supersonically cooled CH_3OH has been observed (Sominska & Gedanken 1996). The $X^2\Sigma^+$ and $A^2\Pi$ states of SiO^+ have been investigated through fast-ion-beam laser spectroscopy (Rosner et al. 1998). The emission spectrum of the A-X system of SiH and SiD

has been recorded (Ram, Engleman & Bernath 1998). Although He_2 has a repulsive ground electronic state, it does possess bound excited states and discrete transitions between them: Focsa, Bernath, & Colin (1998) have obtained new spectra and carried out a global analysis of the six lowest excited states of He_2.

Recent studies of photodissociation processes include SiH^+ (Stancil et al. 1997), SiO (Jolicard et al. 1997, Drira et al. 1998), CO (Andic et al. 1999), and CH_2 (Kroes et al. 1997).

The upper state of the 141.5 nm transition of CH_2 has been characterized through *ab initio* calculations by Yamaguchi & Schaefer (1997). Several bands of CH, CH^+ and their isotopomers have been analyzed (Bembenek 1997a,b; Bembenek, Kępa, & Rytel 1997, Zachwieja 1997, Kępa et al. 1996).

Mahon et al. (1997) have determined transition probabilities in the $A^1\Pi$–$X^1\Sigma^+$ system of CS. The CS_2 spectrum has been studied by Cossard-Magos et al. (1996, 1997, 1998). New bands in the $A^1\Pi_u$–$X^1\Sigma_g^+$ system of C_3 have been observed through laser induced fluorescence (Baker et al. 1997). A 630 nm band system of FeH has been identified with the $e^6\Pi$–$c^6\Sigma^+$ transition (Goodridge, Hullah & Brown 1998) and the 532 nm green bands with $e^6\Pi$–$^6\Delta$ (Goodridge et al. 1997). Laser-induced fluorescence has been measured in $^{13}CO_2^+$ $\tilde{A}^2\Pi_u$–$\tilde{X}^2\Pi_g$ (Varfalvy, Lafleur & Larzillière 1996).

Absorption by SO_2 is important in the atmospheres of Io and Venus; the UV photoabsorption cross sections of SO_2 at 198–220 nm have been recorded with a vacuum ultraviolet Fourier transform spectrometer (Stark et al. 1999b).

Large molecules, PAHs, carbon chains and fullerenes: Considerable progress has been made recently in the investigation of large molecules in the gas phase. Only a small sample of such work can be cited. An exciting development has been the possible identification of some diffuse interstellar bands (DIBs) with an electronic transition in C_7^- based upon laboratory spectra of gas-phase carbon-chain molecules (Tulej et al. 1998, Kirkwood et al. 1998). Extensive studies of the electronic spectra of carbon-chain molecules, radicals and ions have been conducted by Maier (1997) and co-workers (e.g., Wyss, Grutter & Maier 1999, Grutter, Wyss & Maier 1999), using mass selected matrix spectroscopy, supersonic slit jet plasma spectroscopy, hollow cathode spectroscopy and two color photodetachment spectroscopy. More observational data on DIBs are needed to confirm or refute the possible assigment of C_7^-; see, e.g., Cami et al. (1997) and McCall et al. (1999) for recent data.

A summary of the laboratory results on the photophysics of PAHs and the astrophysical implications was given by Leach (1996a). A data base of spectra of neutral and ionized PAHs has been prepared by the NASA-Ames group (e.g., Allamandola, Hudgins & Sandford 1999, Hudgins & Allamandola 1999). The photoionization quantum yield of PAHs is an important parameter in astrophysical modeling of their formation and destruction, and has been measured for a series of PAHs in the 5–25 eV range by Jochims, Baumgärtel & Leach (1996), who also established 'rules of thump' for other species. Another important parameter is the structure-dependent photostability of PAH cations, studied by Allain et al. (1996a,b), Allain & Leach (1997) and Jochims, Baumgärtel & Leach (1999). Work has also been carried out on the dissociative ionization of PAHs in the 8–35 eV photon energy range (Jochims et al. 1997). Ultraviolet pumping of PAHs has been investigated (Robinson, Beegle & Wdowiak 1997), and electronic spectra of cold gas-phase PAH cations have been recorded (Bréchignac & Pino 1999). Theoretical modeling of the formation and photodestruction of PAHs was performed using the new laboratory data (e.g., Allain et al. 1996a,b; 1997).

The laboratory work on fullerenes concerns ground state and triplet state absorption of neutral species, partially hydrogenated fullerenes and other fullerenes derivatives as well as studies on their non-linear optical properties. The spectra in the range 200–800 nm by Bensasson et al. (1997, 1998a,b) and Bini et al. (1998) provided the possibility of testing whether some of the DIBs and other aspects of interstellar extinction such as the 217 nm peak are due to these species. In particular, the spectra of $C_{60}H_{18}$ and $C_{60}H_{36}$ do not

support the suggestion that the 217 nm peak is due to partially hydrogenated fullerenes. New evidence for the presence of interstellar C_{60}^+ has been provided by Foing & Ehrenfreund (1997). A special issue of *Journal of Physics B* was devoted to Fullerenes and it includes articles on the electronic spectra of these molecules (see Leach 1996b, and other articles in that volume).

5.3. Vibrational transitions

H_3^+, long assumed to be the universal protonator and the initiator of interstellar chemistry, has been detected through its vibrational transitions in the molecular material toward the deeply embdeed young stellar objects GL 2136 and W 33A (Geballe & Oka 1996). Subsequently, it has been observed in several other dense clouds (McCall et al. 1999). The agreement between the observed and model column densities provides direct support of the ion-molecule reaction scheme for the formation of interstellar molecules. Subsequent observations of H_3^+ in the diffuse interstellar medium show surprisingly high abundances, however, which cannot readily be explained by existing diffuse cloud models if the commonly accepted values for the cosmic ray ionization rate and the H_3^+ dissociative recombination rate are used (McCall et al. 1998a,b; Geballe et al. 1999)

Infrared transition probabilities and the corresponding opacity of SiO have been calculated by Drira et al. (1997) and Aringer et al. (1997). Hot bands in the infrared spectrum of H_2O have been calculated by Viti et al. (1997).

5.4. Rotational transitions

For nearly 20 years, the cyanopolyyne HC_9N has been the largest molecule identified in interstellar space. This has changed with the radioastronomical detection of $HC_{11}N$ by Bell et al. (1997). The CfA group led by P. Thaddeus has been very productive in the last three years in finding new spectra of carbon-chain molecules both in the laboratory (e.g., McCarthy et al. 1997, 1998, 1999) and in space. New laboratory spectra include those of HC_n (n=7,8,9,11), $HC_{2n+1}N$ (n=5,6,7,8), carbon ring chains H_2C_{2n+1} (n=2,3,4) and $H_2C_{2n}N$ (n=2,3), SiC_n (n=3,5,6,7,8) and many more. The species H_2C_5, $HC_{11}N$, HC_n (n=7,8) have been detected in TMC–1 (Langer et al. 1997, Bell et al. 1999) and SiC_3 in IRC+10216 (Apponi et al. 1999). The discovery of SiC_3 is particularly noteworthy because this is the first time that the rhombic structure, theoretically predicted to be more stable than the linear structure, is observed in isolated form.

The submillimeter spectra of so-called 'hot cores' in massive star-forming reveal the presence of complex saturated organic molecules at high abundances (e.g., Nummelin et al. 1998). A fraction of the lines is still unidentified, but are likely due to highly-excited rotational lines in the ground- and/or excited vibrational states of known molecules or their isotopes. De Lucia, Herbst and co-workers have provided new laboratory measurements of $HCOOCH_3$ (Oesterling et al. 1999), CH_3SH (Bettens et al. 1999), CH_3OCH_3 (Groner et al. 1998), C_2H_5OH (Pearson et al. 1997), and c-C_2H_4O (Pan et al. 1998) to address this problem. Updated tables of CH_3OH and $^{13}CH_3OH$ are provided by Xu & Lovas (1997).

The rotational spectra of a wide variety of molecules containing metals and/or second-row elements have been measured in the group of L. Ziurys, and astronomical searches for several of these species have been pursued. Recent examples of laboratory data include those of NaCH (Xin & Ziurys 1998), NaS (Li & Ziurys 1997), AlNC (Robinson, Apponi & Ziurys 1997), FeC (Allen et al. 1996), and alkaline earth hydroxide radicals (Ziurys et al. 1996).

Terahertz spectroscopy of astrophysically relevant species in preparation of the SOFIA and FIRST missions is carried out in the Cologne group of G. Winnewisser (1997). Recent measurements include NH (Klaus, Takano & Winnewisser 1997), NH_2 (Muller et al. 1999), PH (Klisch et al. 1998) and SH (Klisch et al. 1996). Improved determinations of the CO rotational transitions have been obtained for use as secondary standards near 60 THz (Wappelhorst et al. 1997).

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