

OSCILLATOR STRENGTHS FOR VISIBLE AND ULTRAVIOLET OBSERVATIONS OF INTERSTELLAR MOLECULES

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ABSTRACT. The accuracy of the information obtained from observations of optical-wavelength, molecular absorption features in interstellar clouds is directly limited by the accuracy of the rotational-line oscillator strengths used in the analysis of data. This paper briefly discusses optical observations of molecules in interstellar clouds; surveys molecular lifetime and oscillator strengths; and reviews laboratory techniques for obtaining these data.

1. OBSERVATIONS OF MOLECULES IN DIFFUSE INTERSTELLAR CLOUDS

The study of the structure and composition of interstellar clouds is an important step towards an understanding of the interstellar medium. Although most interstellar molecules have been discovered by radio astronomy, optical wavelength observations have several advantages (Black 1985) and, thus, can provide valuable data. For diffuse clouds (see Black 1986), absorption lines provide the only measurable information. The accuracy of the data obtained is directly limited by the accuracy of the oscillator strengths (f -values) used in the analysis.

Absorption lines of interstellar molecules can be observed where a molecule-containing volume of interstellar gas lies along the line of sight to a suitable background star. Such observations could be made throughout the entire electromagnetic spectrum, but practical absorption studies have been limited, by lack of instrumentation or of suitable background sources, to ultraviolet (including vacuum ultraviolet), visible, and infrared wavelength observations of diffuse interstellar clouds. Following Snow (1980a), we will refer to these wavelengths as 'optical'.

Early studies identified OH, CH, CN, and CH⁺ in absorption spectra of interstellar clouds obtained by ground-based telescopes. Since then, H₂, HD, C₂, and CO have also been detected through optical observations. Somerville (1987) reports tentative detection of MgH⁺ and HCl in IUE spectra. Upper limits, which impart important constraints to models of interstellar clouds, have been established for about 20 other molecules (see Snow 1979, 1980a,b).

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2.2. Compilations of Molecular Oscillator Strengths

Dumont and Remy (1982), Kuz'menko et al. (1979), Nicholls (1977) and Hsu and Smith (1977) have compiled radiative lifetime and/or transition probability data for diatomic molecules, and some data are included as footnotes in Huber and Herzberg (1979). Astronomers who require the most recent information on molecular spectra and transition probabilities, should refer to the Berkeley Newsletter (Phillips, Davis, and Eakin). These compilations are, for the most part, not critically evaluated and, except for the Newsletter, are, by their very nature, always somewhat out of date because of continuing improvements in methods for measuring (see §3) and calculating data.

Van Dishoeck and Black (1986) have prepared a critically reviewed, consistent set of molecular band oscillator strengths for 22 optical bands of 15 molecules that have been detected in interstellar clouds or that have been searched for so that upper limits to the column densities can be established. These oscillator strengths are reproduced in Table II. This table does not include oscillator strengths for all molecules that have been observed (see Snow 1979, 1980a,b) or for molecules that will be observed for the first time with ST (see Table I).

None of the compilations referred to above includes uncertainties for the oscillator strength values listed. This is unfortunate, because few astronomers have the time or the knowledge required to determine the accuracies of these fundamental data, accuracies that directly effect the measured column densities and, thus, other derived properties of the interstellar clouds.

High spectral resolution observations of the cold, absorbing material in interstellar clouds produces relatively simple, rotational-line spectra because only a few, at most, of the molecular rotational levels are populated. Consequently, determination of accurate molecular column densities from the absorption profiles, or from the equivalent widths, requires rotational line oscillator strengths. However, because of the complexity of molecular spectra, only band oscillator strengths are usually available (some exceptions for a few astronomical molecules are pointed out in §3.3). Derivation of line f -values, which are needed for analysis of the observed line profiles, from band f -values, which are tabulated, requires molecular rotational line intensity factors, also known as Hönl-London factors. The adoption of a single convention for the normalization of these (Whiting et al. 1980) has reduced, but not eliminated, troublesome errors of factors of two in the determination of line oscillator strengths. Schadee (1975) gives expressions for the Hönl-London factors for the astrophysically-important special case of the lowest rotational levels of diatomic molecules.

The neglect of vibration-rotation interaction, which is implicit in the relations given by Whiting et al. (1980) and Schadee (1975), and non-adiabatic effects can lead to subtle errors when the routine procedures are used to derive line f -values from band f -values. Morton and Dinerstein (1976) dealt with the impact of these factors on the line f -values of H_2 . Such errors are avoided if very high resolution laboratory techniques are used to measure individual rotational-line f -values.

TABLE II

Critically-Compiled Band Oscillator Strengths for Some Interstellar Molecules (from van Dishoeck and Black 1986)

Species	Transition	band	λ (Å)	f^a	Reference
CO	$A^1\Pi-X^1\Sigma^+$	(0,0)	1545	1.6(-2)	Field et al. (1983); Albritton (1976) idem idem idem
		(1,0)	1510	3.4(-2)	
		(11,0)	1264	2.4(-4)	
		(12,0)	1246	1.1(-4)	
		(13,0)	1230	4.8(-5)	
	$B^1\Sigma-X^1\Sigma^+$	(0,0)	1151	1.0(-2)	Cooper & Langhoff (1981); W. Smith (1978) idem
$C^1\Sigma-X^1\Sigma^+$	(0,0)	1088	8.9(-2)		
		(1,0)	1063	1.8(-3)	idem
	$E^1\Pi-X^1\Sigma^+$	(0,0)	1078	1.0(-1)	W. Smith (1978)
CH	$A^2\Delta-X^2\Pi$	(0,0)	4300	5.1(-3)	Larsson & Siegbahn (1983a)
		(1,0)	3850	1.6(-3)	idem
	$B^2\Sigma-X^2\Pi$	(0,0)	3880	3.1(-3)	Brzozowski et al. (1976)
CH ⁺	$A^4\Pi-X^1\Sigma^+$	(0,0)	4233	5.5(-3)	Larsson & Siegbahn (1983b)
		(1,0)	3958	3.3(-3)	idem
C ₂	$A^1\Pi_u-X^1\Sigma_g^+$	(2,0)	8750	1.7(-3)	van Dishoeck (1983)
		(3,0)	7720	7.5(-4)	idem
CN	$B^2\Sigma^+-X^2\Sigma^+$	(0,0)	3874	3.4(-2)	Larsson et al. (1983)
OH	$A^2\Sigma^+-X^2\Pi$	(0,0)	3080	1.1(-3)	Wang & Huang (1980); G. Smith & Crosley (1981)
		(0,0)	1222	1.2(-2)	van Dishoeck et al. (1983)
HCl	$C^2\Pi-X^1\Sigma^+$	(0,0)	1290	1.5(-1)	van Dishoeck et al. (1983); P. Smith et al. (1980)
		(0,0)	3350	7.5(-3)	Fairchild et al. (1984); Hofzumahaus & Stuhl (1985)
CO ⁺	$A^2\Pi-X^2\Sigma^+$	(2,0)	4260	8.6(-4)	Mahan & O'Keefe (1981); Holland & Maier (1972)
MgH	$A^2\Pi-X^2\Sigma^+$	(0,0)	5180	1.6(-1)	Kirby et al. (1979)
MgO	$B^1\Sigma^+-X^1\Sigma^+$	(0,0)	4998	1.5(-1)	Diffenderfer et al. (1983)
NaH	$A^1\Sigma^+-X^1\Sigma^+$	(8,0)	3991	2.3(-2)	Kirby & Dalgarno (1978)
H ₂ O	$\tilde{C}^1B_1-\tilde{X}^1A_1$	b	1240	1.0(-2)	P. Smith et al. (1981)
		b	1114	3.0(-2)	idem
H ₂ O ⁺	$\tilde{E}^1B_1-\tilde{X}^1A_1$	c	6147	7.8(-5)	Möhlmann et al. (1978); W. Smith et al. (1984)
		c	6147	7.8(-5)	idem
C ₃	$\tilde{A}^1\Pi_u-\tilde{X}^1\Sigma_g^+$	b	4050	1.8(-2)	Clegg & Lambert (1982)

a. notation $x(z) \equiv x \times 10^z$

b. (0,0,0) - (0,0,0)

c. (0,8,0) - (0,0,0)

3. LABORATORY MEASUREMENTS OF MOLECULAR OSCILLATOR STRENGTHS

3.1. Introduction

Molecular oscillator strengths can be determined by a variety of techniques; the main ones can be referred to as 'emission', 'lifetime', and 'absorption'. Emission techniques require that absolute intensities be measured and that the thermodynamic state of the emitting gas or plasma be known. Difficulties in accurately obtaining such information have meant that most molecular transition probabilities have been measured by the other two techniques, which are discussed in the next sections.

3.2. Lifetime Measurements

Wiese (1968), Corney (1970), Imhof and Read (1977), and Erman (1979a) have reviewed methods and techniques for direct measurements of atomic and molecular lifetimes. A number of measured lifetimes are tabulated by Erman (1979a,b).

The principal advantage of lifetime measurements, as a way of determining oscillator strengths, is that absolute radiometry and number density determinations are not necessary. There are, however, experimental situations that can lead to systematic error in lifetime measurements: blends, cascades, collisional de-excitation and mixing, radiation trapping, and escape of excited molecules from the detection region (see Erman 1979a).

Lifetime data must be converted to oscillator strengths in order to be of use in the extraction of molecular column densities from observed spectra. If the electronic transition moment, R_e , does not vary strongly with the internuclear distance, \bar{r} , the conversion formulae given by Larsson (1983) can be applied in the case of diatomic molecules. However, if R_e varies strongly with \bar{r} , additional data are required in order to avoid introducing uncertainties into the results. Measured relative branching ratios from a common upper level to various lower vibrational levels, or calculated values of the \bar{r} -dependence of R_e , can be used. Absorption techniques (§3.3) avoid the uncertainties associated with conversion of lifetimes to oscillator strengths.

Electron excitation techniques were first applied to comprehensive measurements of molecular lifetimes of astrophysical interest by Hesser (1968), who used electron-excitation, phase-shift apparatus. Erman and his colleagues developed the more efficient high-frequency deflection technique (Erman 1975), which has been used to measure a number of lifetimes for molecules seen in astronomical spectra (Erman 1979a,b).

In laser fluorescence lifetime measurements, excited levels of molecules are selectively populated by short, intense pulses of laser radiation. Because only the excited level of interest is populated, there are no cascades and no requirements for high resolution spectrometers to resolve emission from the decay of a number of upper levels.

For neutral species, laser fluorescence measurements are limited to lifetimes that are shorter than about 10 μ sec, in order to keep the excited molecules within the field of view of the apparatus while they

decay. Trapping techniques (Wineland et al. 1983) have been used to extend laser fluorescence lifetime measurements to ions. Because the emitting species are confined, longer lifetimes can be measured. Mahan and O'Keefe (1981) obtained lifetimes for N_2^+ , CO^+ , CH^+ , and CD^+ in this manner.

3.3. Absorption Measurements

Laboratory absorption measurements with high resolution, photoelectric spectrometers come closest to measuring directly the oscillator strengths for single rotational lines that are needed for analysis of astronomical spectra. No radiometric calibration of the spectrometer is required, but the difficulties in obtaining the necessary large column densities have limited such work to stable molecules that are gases or that have high vapor pressures at room temperature.

The author and his colleagues have used the scanning photoelectric spectrometer (Yoshino et al. 1980) at the Harvard-Smithsonian Center for Astrophysics (CfA) to measure f -values for some individual rotational lines of molecules that are seen, or expected, in interstellar clouds. Oscillator strengths for some rotational lines in the Schumann-Runge bands of O_2 have been published (P. Smith et al. 1984) and some preliminary values for ultraviolet lines of H_2CO have been presented (Connor et al. 1982). Earlier work, which employed photographic detection and, thus, required calibration of the D - $\log(E)$ characteristics of the emulsion, provided f -values for interstellar lines of two bands of H_2O (P. Smith et al. 1981) and of HCl (P. Smith et al. 1980).

Laboratory absorption measurements have usually been made on molecules that are warmer than those in the interstellar medium. At the higher temperatures, several molecular rotational levels are populated and, therefore, the laboratory spectra are significantly more complex than the interstellar ones. As a consequence, the lines seen in the interstellar spectra cannot always be resolved in the laboratory, despite, for example, a resolving power of 2×10^5 in the case of the CfA spectrometer.

Supersonic molecular jet techniques (Levy 1984) are now being used to produce cold molecules for laboratory spectroscopy, and Erman et al. (1983) have found that collisional effects are substantially reduced when the static gas target used in the high-frequency deflection technique is replaced by a jet. Supersonic jets have not yet been applied to absorption spectroscopy of molecules seen in interstellar clouds but such a jet is being developed, in part for this purpose, at the CfA. The simple absorption spectra produced by supersonic-jet-cooled molecules will be very similar to the absorption spectra of molecules in diffuse interstellar clouds. Thus, the application of high-resolution laboratory spectroscopic techniques will be able, in most cases, to provide unambiguously the accurate oscillator strengths needed for detailed interpretation of astronomical observations and increased understanding of the properties of these clouds.

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