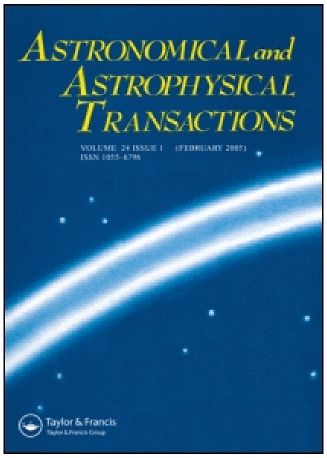

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SPECTRAL OBSERVATIONS OF COMET C/2000 WM1 (LINEAR) IN MEXICO

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Preliminary analysis of intermediate-resolution optical spectra of comet C/2000 WM1 (LINEAR) obtained on November 22–24, 2001, and April 5, 2002, is given. The emission lines of the C_2, C_3, CN, NH_2 and presumably CO (Asundi and triplet bands) molecules and H_2O^+ and C_2^- ions were identified in these spectra. By analysing the brightness distributions of the C_2, C_3 and CN emission lines along the spectrograph slit we determined some physical parameters of these neutral molecules:, the velocity of expansion of molecules within the coma and their lifetimes. The Franck–Condon factors for the CO Asundi bands and C_2^- bands were calculated using a Morse potential model.

Keywords: Comet C/2000 WM1 (LINEAR); Franck–Condon factors; Gas species C_2, C_3 and CN; Negative ions; Optical spectroscopy; Profile; Expansion velocity; Physical parameters

1 INTRODUCTION

The study of cometary spectra can give information about the chemical composition of comet nuclei. The negative ions play an important role in cometary chemistry. Negatively charged molecular radicals were identified in the inner coma (2300 km from the nucleus) of comet Halley on the basis of mass spectra obtained on board the Giotto spacecraft on March 14, 1986 (Chaizy et al., 1991). The concentration of negative ions with 22–65 amu was estimated as $0.05\,\mathrm{cm}^{-3}$. The C_2^- negative ion was detected in the optical spectrum of comet Scorichenko–George (1990 VI) (Churyumov et al., 1993) where the column density was estimated to be $10^{12}\,\mathrm{cm}^{-2}$.

In this work we shall present intermediate-resolution optical spectra of comet C/2000 WM1 (LINEAR) obtained with a long-slit spectrograph. Such spectra can allow us to calcu-

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late some physical parameters of cometary neutral atmospheres (escaping velocities of gas in the coma, lifetime of molecules and others), to search for new cometary emission lines and to estimate parameters of gas and dust productivity of the comet nucleus.

2 OBSERVATIONS AND DATA REDUCTION

Spectroscopic observations of comet C/2000 WM1 have been carried out with the 2.12 m telescope of the Guillermo Haro Observatory in Cananea, Sonora, Mexico, operated by the National Institute of Astrophysics, Optics and Electronics. The diffraction gratings of the Boller and Chivens spectrographs (long slit and charge-coupled device (CCD)) with a reciprocal dispersion of 3.5 Å pixel^{-1} and a spectral resolution of 15 Å were used on November 22, 2001, and April 5, 2002. A diffraction grating with a dispersion of 1.4 Å pixel^{-1} and a spectral resolution of 5.4 Å was used on November 24, 2001. The long slit 2.5″ wide was oriented along the comet tail. The length of the slit is 2.5′. Gratings with 150 lines mm^{-1} and 300 lines mm^{-1}, respectively, were used. Four comet spectra in the spectral range 4000–7000 Å (S/N $\approx$ 40) on November 22, 2001, and five comet spectra in the spectral range 4000–5700 Å (S/N $\approx$ 50) on November 24, 2001, were obtained. The exposure time was equal to 30 min for all the obtained spectra. A helium–argon lamp was utilised in order to calibrate the spectra for wavelengths. All spectra were processed with the help of the 'LONG' ESO-MIDAS and the Research System IDL computer programs allowing for reductions in the CCD bias level, cosmic-ray particles, flat fielding and night sky contribution.

3 DETERMINATION OF THE GAS VELOCITY AND LIFETIME OF MOLECULES

Spectrophotometry of comet C/2000 WM1 at a distance from the Sun equal to 2.79 AU was conducted in August 2001 (Czabo et al., 2002); from these observations the C_2, CN and CO^+ production rates were estimated. From our spectroscopic observations conducted at a distance between the comet and the Sun equal to only 1.35 AU, detailed information about the physical parameters of gaseous components of the neutral cometary atmosphere can be obtained. In order to determine the gas component expansion and the lifetime τ of the particles we built photometric profiles for the C_2, C_3 and CN emission lines along the slit. The obtained mono-

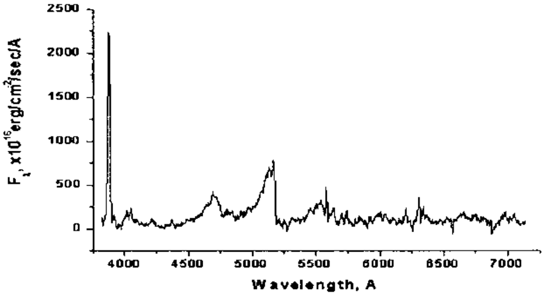

FIGURE 1 Energy distribution in the spectrum of comet C/2000 WM1 (LINEAR) on April 5, 2002 (10:35 universal time (UT)).

TABLE I Values of the velocity v and lifetime τ.

Species	v (m s^{-1})	τ (10^6 s)
C_2 (5165 Å)	482.3	1.45
C_3 (4050 Å)	239.8	0.2
CN (4200 Å)	88.3	1.0

chromatic profiles were then analysed according to Shulman's (1970) model. From this model the surface brightness can be determined by the following formula:

$$\mathrm{I}(\rho,\phi)=\frac{\mathrm{A}}{\rho}\left(1-\frac{2\rho}{\mathrm{L_s}}\sin\Theta\cos\phi\right)\int_{\rho/\mathrm{L_d}}^{\infty}\mathrm{K_0(y)\,dy}-\frac{2\mathrm{A}}{\mathrm{L_s}}\cos\Theta\mathrm{E_i}\left(-\frac{\rho}{\mathrm{L_d}}\right), \tag{1}$$

where A is a proportional coefficient, Θ is the phase angle of the comet, $\mathrm{L_d}=\mathrm{v}\tau$ is the characteristic scale of the molecule path, τ is the molecular lifetime, $\mathrm{L_s}=2\mathrm{v}^2/\mathrm{a}$ is a characteristic scale of the region of the spherical symmetry, a is the radiation acceleration of molecules and $\mathrm{E_i}$ is the exponential integral function.

The logarithm of the asymmetry of the line's brightness profile is

$$\log\left(\frac{\mathrm{I}(\rho,\phi+\pi)}{\mathrm{I}(\rho,\phi)}\right)=1.72\,\frac{\rho}{\mathrm{L_s}}\sin\Theta_0\cos\phi, \tag{2}$$

$$\log\left[\mathrm{I}(\rho,\phi+\pi)\mathrm{I}(\rho,\phi)\right]=\mathrm{constant}+\log\left(\frac{\mathrm{L_d}}{\rho}\right)\int_{\rho/\mathrm{L_d}}^{\infty}\mathrm{K_0(y)\,dy}. \tag{3}$$

Solution of these equations gives values for v and τ (Table I). From this table we can see that real expansion velocities of the C_2, C_3 and CN molecules in the coma of comet C/2000 WM1 differ noticeably from expansion velocities for gas, determined by Delsemme's (1982) formula, which gives values in the range 500–600 m s^{-1}.

4 POSSIBLE DETECTION OF C_2^- AND CO IN COMET C/2000 WM1

The catalogues of the spectral lines in comet Brorsen–Metcalf (Brown et al., 1996) and in comet Bradfield 1980 Y1 (Cosmovici et al., 1982) were used for identification of the emission lines in comet C/2000 WM1 (LINEAR) spectra. Figure 1 shows the distribution of energy in the spectrum obtained in the coma region at a distance of about 5000 km from the nucleus (the position angle of the prolonged radius vector in the sunward direction). On seven spectra we found emission lines of the following neutral molecules: C_2, NH_2, CN, C_3, CO (Asundi and triplet bands) and CH. We observed the following ionic species also: H_2O^+ and C_2^-. The relative intensities of the possible identified emission lines of 6–0 (7229.12 Å) and 7–0 (6726.47 Å) Asundi and 5–0 (5670.76 Å) triplet bands of the CO molecule are in good agreement with the values of the Franck–Condon factors (Kuzmenko et al., 1984) and those calculated by us. However, for 11–1 (5761.05 Å), 8–0 (6244.56, 6257.85 and 6267.80 Å) and 8–1 (7007.06 Å) Asundi and 15–3 (4445.47 Å) and 11–2 (4935.93 Å) triplet bands the Franck–Condon factors are very low. Possibly other molecules are responsible for the origin of these emission lines. Unfortunately, the atmospheric conditions during observations were not favourable to ensure reliable photometric measurements of absolute fluxes of emission lines. So our identification of CO in the spectrum of comet C/2000 WM1 is tentative.

In the spectrum we also found two emission lines, whose wavelengths are close to the theoretical wavelengths of the spectral lines of the C_2^- B $^2\Sigma_u^+ - X\ ^2\Sigma_g^+$ bands. This corresponds to wavelengths of 4902.0 Å ($\lambda_{theor} = 4902.10$ Å for vibrational transition 1–0) and 5363.3 Å ($\lambda_{theor} = 5363.37$ Å for vibrational transition 1–1). The emission relative intensities (for 4902.0 Å, $I_{rel} = 0.26$ and, for 5363.3 Å, $I_{rel} = 0.3$) are in good agreement with the values of the Franck–Condon factors for these transitions (Kuzmenko et al. (1984)) and those calculated by us (Churyumov et al., 2002). However, there are no other C_2^- transitions with high Franck–Condon factors in the comet spectrum (e.g. $\lambda_{theor} = 5415.87$ Å for vibrational transition 0–0, $\lambda_{theor} = 5912.69$ Å for vibrational transition 1–2 and $\lambda_{theor} = 5987.82$ Å for vibrational transition 0–1). So C_2^- detection is very tentative.

Let us consider possible C_2^- detection in comet C/2000 WM1. The column density of negative ions with 22–65 amu in comet Halley can be estimated as $10^7\,cm^{-2}$ (Chaizy et al., 1991). This value is five orders of the magnitude smaller than that of the column density of C_2^- ions in comet Scorichenko–George. Theoretical calculations predict for comet Halley a negative ion abundance as low as 10^{-6}–10^{-10} of the electron densities in the inner coma (Wekhof, 1981). Although such theoretical predictions agree with the experimental results of investigations on comet Halley, they also disagree with those of high C_2^- abundance in comet Scorichenko–George. Special conditions are required for a high density of C_2^- in comets. Firstly, we need regions with high electron densities because C_2^- formation proceeds most probably via electron attachment to C_2. Secondly, owing to a short C_2^- photodissociation lifetime this ion can be destructed slowly only in the inner coma. Thirdly, the rate constant for C_2^- reaction with atomic hydrogen is much higher than that for reaction with molecular hydrogen (Barckholtz et al., 2001). All these considerations led us to conclude that C_2^- abundance is largest in the inner comae of comets. It is more probable that this ion can be detected in water-depleted comets because the atomic hydrogen concentration may be low in such comets. In the outer coma, C_2^- abundance may be higher than that of other negative ions such as CN^- and OH^- because the C_2 scale length is about ten times that of CN (Combi and Fink, 1997).

Another feature of the optical spectrum of comet WM1 is the possible presence of weak CO Asundi and triplet bands. The first detection of such bands in the optical spectrum of comet Bradfield 1980 Y1 was reported by Cosmovici et al. (1982). These workers considered dissociative recombination of $CO_2{}^+$ or HCO^+ as a possible mechanism for explaining the origin of the Asundi and triplet bands. It was also noted that reactions of dissociative recombination require high electron densities. Interestingly, C_2^- bands were observed simultaneously before our observations only in comet Scorichenko–George (Churyumov et al., 1993). For C_2^- formation, high electron densities are also required.

5 CALCULATIONS OF C_2^- AND CO FRANCK–CONDON FACTORS

Franck–Condon factors play a fundamental role in the determination of the column density of cometary diatomic molecules (Churyumov et al., 1993). These factors can be determined if the harmonic frequency ω_e, the anharmonic frequency $\omega_e x_e$, the reduced mass μ and the internuclear distance r_e are known. This involves the calculation of an overlap between vibrational wavefunctions. Algebraic and numerical techniques have been devised to perform such calculations; one of the most accurate methods is that based on the Morse potential and the Rydberg–Klein–Rees models. For the present case we have chosen a Morse potential model based on a Simpson composite quadrature and compare its precision with the Rydberg–Klein–Rees calculations available in the literature.

This special numerical technique avoids overflows and underflows upon evaluation of the normalisation constants and Laguerre polynomials. The numerical evaluation was made in the closed interval [0.4 Å; 2.5 Å] with a step size h = 0.01 Å. Although there are many ways to calculate Franck–Condon factors using a Morse oscillator, special software was written following the technique by Halmann and Laulicht (1965). Spectroscopic data for this ion, obtained by photodetachment spectroscopy, were used. Jones et al. (1980) reported the following spectroscopic constants for the C_2^- ion: $\omega_e = 1969.076$ (0.165) and $\omega_e x_e = 14.902$ (0.098) for the B $^2\Sigma_u^+$ state; $\omega_e = 1781.329$ (0.066) and $\omega_e x_e = 11.719$ (0.018) for the X $^2\Sigma_g^+$ electronic state. In this paper the Franck–Condon factors were calculated for $v_1 = 0$–7 and $v_2 = 0$–10 with low accuracy, with only one significant number. Mead et al. (1985), by using ultrahigh-resolution spectroscopy, reported more accurate values: $\omega_e = 1969.542$ (0.084) $\omega_e x_e = 15.100$ (0.057), $\mu = 6.0$ and $r_e = 1.2234$ Å for the B $^2\Sigma_u^+$ state; $\omega_e = 1781.202$ (0.020), $\omega_e x_e = 11.6716$ (0.0048), $\mu = 6.0$ and $r_e = 1.2684$ Å for the X $^2\Sigma_g^+$ electronic state. The standard deviation between the Franck–Condon factors based on the spectroscopic constants of Jones et al. (1980) and Mead et al. (1985) is 0.002. By taking into account the standard deviation of harmonic and anharmonic frequency with the spectroscopic data of Mead et al. (1985), we obtained the standard deviation of Morse Franck–Condon factors as 5×10^{-4}. These results can be used to detect the presence of C_2^- in comets, in the atmospheres of cold carbon stars and in diffuse molecular clouds.

6 CONCLUSIONS

We obtained intermediate-spectral-resolution observations of the bright comet C/2000 WM1 (LINEAR) at the Guillermo Haro Astrophysical Observatory in Mexico. We found emission lines of the following neutral radicals: C_2, NH_2, CN, C_3, CH and possibly CO. We also observed the following ionic species: H_2O^+ and presumably C_2^-. The possible presence in the spectra of CO and C_2^- emissions lines is discussed. Franck–Condon factors for C_2^- and CO (Asundi bands) were calculated and were used for the analysis of the brightness distribution of the identified emission lines of these molecules. By analysing the brightness distribution of C_2, C_3 and CN emission lines along the spectrograph slit the escape velocity of these molecules from the nucleus and their lifetimes were determined.

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