Optical spectroscopy of comet C/2000 WM1 (LINEAR) at the Guillermo Harro Astrophysical Observatory in Mexico

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Abstract. Preliminary analysis of middle resolution optical spectra of comet C/2000 WM1 (LINEAR) obtained on November 22, 2001 is given. The emission lines of the molecules C_2, C_3, CN, NH_2, H_2O^+ and presumably CO (Asundi and triplet bands), C_2^- were identified in these spectra. By analysing brightness distributions of C_2, C_3, 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 by using a Morse potential model.

Keywords: Comet C/2000 WM1 (LINEAR), Franck-Condon factors, gas species C_2, C_3, CN negative ions, optical spectroscopy, profile,expansion velocity, physical parameters

1. Introduction

Comets have spectra with many emission bands of small molecules. 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. The 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 P. et al., 1991). The concentration of negative ions with 22-65 amu was estimated as 0.05 cm^{-3}. The C_2^- negative ion was detected in the optical spectrum of comet Scorichenko-George (1990 VI) (Churyumov K.I. et al., 1993) where the column density was estimated to be 10^{12} cm^{-2}.

In this work we will present middle-resolution optical spectra of comet C/2000 WM1 (LINEAR) obtained with a long slit spectrograph. Such spectra can allow to calculate some physical parameters of cometary neutral atmospheres (escaping velocities of gas in the coma, lifetime of molecules and others), search for new cometary emission lines, to estimate parameters of gas and dust productivity of the comet nucleus, to detect the cometary luminescence continuum of the non-solar nature. We will also present Franck-Condon factors calculations for some of the identified molecules.

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 CCD) with the reciprocal dispersion of 3.5 $\AA$ per pixel and spectral resolution of 15 $\AA$ were used Nov. 22, and the diffraction grating with dispersion of 1.4 $\AA$ per pixel and spectral resolution of 5.4 $\AA$ was used Nov. 24. The 2.5 arcsec wide long slit was oriented along the comet tail. The length of the slit is 2.5 arcmin. Gratings with 150 l/mm and 300 l/mm were used, respectively. Four comet spectra in the spectral range of 4000-7000 $\AA$ (S/N $\sim$ 40) on Nov. 22 and five comet spectra in the spectral range of 4000-5700 $\AA$ (S/N $\sim$ 50) on Nov. 24, 2001 were obtained. The exposure time was equal to 30 min for all of the obtained spectra. A helium-argon lamp was utilized 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 of the CCD bias level, cosmic ray particles, flat fielding, and night sky contribution.

3. Determination of gas velocity and lifetime of molecules

Spectrophotometry of comet C/2000 WM1 at the distance from the Sun equal to 2.79 AU was conducted in August 2001 (Czabo Gy.M. et al., 2002), from these observations C_2, CN and CO^+ production rates were estimated. From our spectroscopic observations conducted at the distance between the comet and the Sun equal only to 1.35 AU detailed information about physical parameters of gaseous components of the neutral cometary atmosphere can be received. In order to determine the gas component expansion and the lifetime of the particles τ we built photometric profiles for the C_2, C_3 and CN emission lines along the slit (Fig. 1). The obtained monochromatic profiles then were analyzed according to Shulman's model (Shulman L.M., 1970). From this model

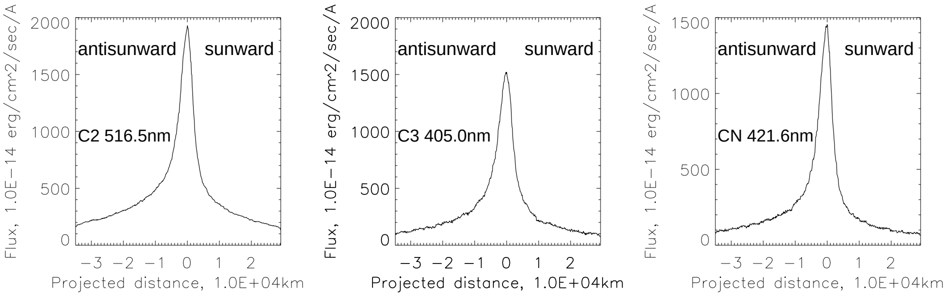

Figure 1. Distribution of surface brightness along the slit for three emission lines C_2, C_3 and CN

the surface brightness can be determined by the following formula

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

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

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

$$\lg\frac{I(\rho,\phi+\pi)}{I(\rho,\phi)} = 1.72\frac{\rho}{L_s}\sin\Theta_0\cos\phi,$$

$$\lg I(\rho,\phi+\pi)I(\rho,\phi) = const + \lg\frac{L_d}{\rho}\int_{\frac{\rho}{L_d}}^{\infty} K_0(y)dy.$$

Solution of these equations gives values for v and τ (Table 1). From this table we can see that real expansion velocities of 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 formula (Delsemme A.H., 1982) which gives values in the range $500 - 600$ ms^{-1}.

Table I. Physical parameters of gaseous cometary components of C_2, C_3 and CN

Species	Velocity, ms^{-1}	$Lifetime$, $10^6 s$
C_2 (5165 Å)	482.3	1.45
C_3 (4050 Å)	239.8	0.2
CN (4200 Å)	88.3	1.0

4. Possible detection of C_2^- and CO in comet C/2000 WM1

The catalogs of the spectral lines in comet Brorsen-Metcalf (Brown M.E. et al., 1996) and in comet Bradfield 1980 Y1 (Cosmovici C.V. et al., 1982) were used for identification of the emission lines in the comet C/2000 WM1 (LINEAR) spectra. Fig. 2 shows distribution of energy in the spectrum obtained in the coma region at the distance $\sim$ 500 km from the nucleus (position angle of the prolonged radius vector in the sunward direction). On four spectra we found emission lines of the following neutral molecules: 110 were of C_2, 55 of NH_2, 8 of CN, 4 of C_3, 10 of CO (Asundi and triplet bands), 3 of CH. We observed the following ionic species also: H_2O^+ (5 emission lines) and C_2^- (presumably two lines). Comparison of the relative intensities of the identified emission lines of 6-0 (7229.12 $\AA$), 7-0 (6726.47 $\AA$) Asundi and 5-0 (5670.76 $\AA$) triplet bands of the CO molecule (see Fig. 3) with corresponding values of Franck-Condon factors yield a good agreement (Table 3 and (Kuzmenko N.E. et al., 1984)). But for 11-1 (5761.05 $\AA$), 8-0 (6244.56 $\AA$, 6257.85 $\AA$, 6267.80 $\AA$), 8-1 (7007.06 $\AA$) Asundi and 15-3 (4445.47 $\AA$), 11-2 (4935.93 $\AA$) triplet bands Franck-Condon factors (see section 5) are very low. Possibly another molecules are responsible for the origin of these emission lines. Unfortunately, the atmospheric conditions during observations were not favorable 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

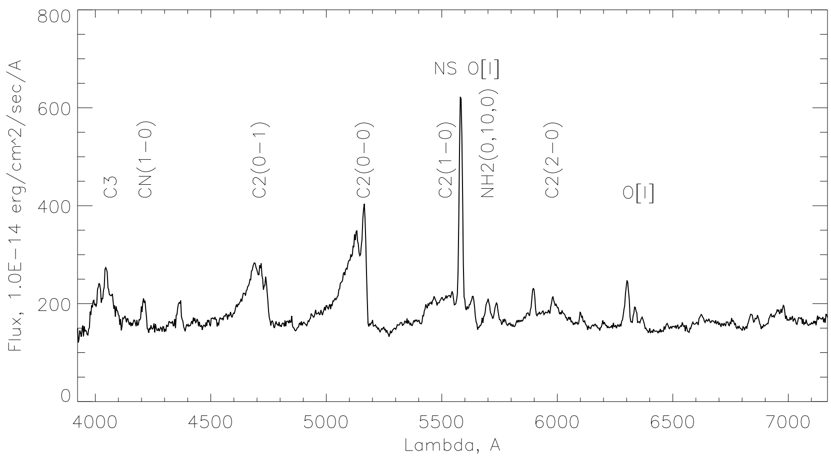

Figure 2. The spectrum of comet C/2000 WM1 (LINEAR) on Nov. 22, 2001

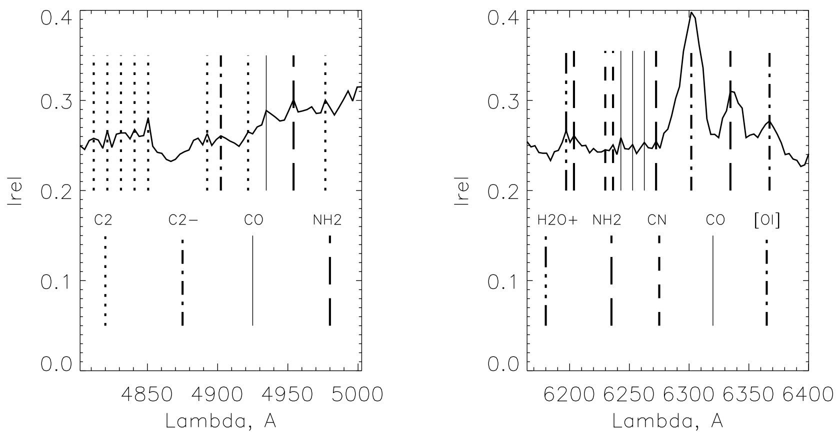

Figure 3. Two spectral regions of comet C/2000 WM1 spectrum obtained on Nov. 22, 2001 (with spectral lines of the CO molecule for λ = 4935.93 $\AA$, 6244.56 $\AA$, 6257.85 $\AA$, 6267.80 $\AA$ and with the spectral line of the C_2^- negative ion for λ = 4902.02 $\AA$)

C_2^- $B^2\Sigma_u^+ - X^2\Sigma_g^+$ bands (see Fig. 3 for vibrational transition 1-0). This correspond to wavelengths 4902.0 $\AA$ (λ_{teor}= 4902.10 $\AA$, vibrational transition 1-0) and 5363.3 $\AA$ (λ_{teor}= 5363.37 $\AA$, vibrational transition 1-1). The emission relative intensities (for 4902.0$\AA$ - I_{rel}= 0.26 and for 5363.3 $\AA$ - I_{rel}= 0.3) are in good agreement with the the Franck-Condon factors values for these transitions (see Table 2 and (Kuzmenko N.E. et al., 1984)). But there are no other C_2^- transitions with high Franck-Condon factors in the comet spectrum (for example λ_{teor}= 5415.87 $\AA$, vibrational transition 0-0, λ_{teor}= 5912.69 $\AA$, vibrational transition 1-2, λ_{teor}= 5987.82 $\AA$, vibrational transition 0-1). So C_2^- detection is very tentative.

Let us consider a 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 P. et al., 1991). This value is on 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 electron densities in the inner coma (Wekhof A., 1981). Such theoretical predictions, though agree with the experimental results of investigations on comet Halley, also and disagree with those of high C_2^- abundance in comet Scorichenko-George. Special conditions are required for high density of C_2^- in comets. First, we need regions with high electron densities because C_2^- formation proceeds most likely via electron attachment to C_2. Second, due to a short C_2^- photodissociation lifetime this ion can be destructed slowly only in the inner coma. Third, the rate constant for C_2^- reaction with atomic hydrogen is much higher than that for reaction with molecular hydrogen (Barckholtz C. et al., 2001). All these considerations led us to conclude that C_2^- abundance is largest in inner comae of comets. It is more likely to detect this ion in water-depleted comets because the atomic hydrogen concentration may be low in such comets. In outer coma C_2^- abundance may be higher than that of other negative ions like CN^- and OH^- because the C_2 scale length is about ten times higher than that of CN (Combi M.R. and Fink U., 1997).

Another feature of the comet WM1 optical spectrum is a 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 C.V. et al., 1982). These authors considered dissociative recombination of CO_2^+ or HCO^+ as a possible mechanism for explaning origin of 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 K.I. et al., 1993). For C_2^- formation high electron densities are also required.

5. C_2^- and CO Franck-Condon factors calculations

Franck-Condon factors (FCF) play a fundamental role for determination of column density of cometary diatomic molecules (Churyumov K.I. 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 wave functions. Algebraic and numerical techniques have been devised to perform such calculations, one of the most accurate methods is the one based on the Morse potential and 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 normalization constants and Laguerre polynomials. The numerical evaluation was done in the closed interval [0.4 $\mathring{A}$; 2.5 $\mathring{A}$] with a step size of h = 0.01 $\mathring{A}$. Although there are many ways to calculate Franck-Condon factors using a Morse oscillator, a special software was written following the technique (Halmann and

Laulicht, 1965). The spectroscopic data for this ion, obtained by photodetachment spectroscopy, were used. (Jones P.L. et al., 1980) report the following spectroscopic constants for C_2^- ion: ω_e= 1969.076(0.165), $\omega_e x_e$ = 14.902(0.098) for $B^2\Sigma_u^+$ state; ω_e= 1781.329(0.066), $\omega_e x_e$ = 11.719(0.018) for $X^2\Sigma_g^+$ electronic state. In this paper the Franck-Condon factors were calculated for v_1 =0 - 7 and v_2 = 0 - 10 with low accuracy, only with one significant number. (Mead R.D. et al., 1985), by using ultrahigh resolution spectroscopy, report more accurate values: ω_e= 1969.542(0.084), $\omega_e x_e$ = 15.100(0.057), μ= 6.0, r_e = 1.2234 Å for $B^2\Sigma_u^+$ state; ω_e= 1781.202(0.020), $\omega_e x_e$ = 11.6716(0.0048), μ = 6.0, r_e = 1.2684 Å for $X^2\Sigma_g^+$ electronic state. The standard deviation between the Franck-Condon factors based on the spectroscopic constants of (Jones P.L. et al., 1980) and (Mead R.D. et al., 1985) is 0.002. By taking into account standard deviation of harmonic and anharmonic frequency with spectroscopic data of (Mead R.D. et al., 1985), we obtain a standard deviation of Morse Franck-Condon factors as 5×10^{-4}. These results can be used for detecting the presence of C_2^- in comets, atmospheres of cold carbon stars, and in diffuse molecular clouds.

Additionally, the values of Franck-Condon factors were calculated for some vibrational transitions of the triplet and Asundi bands which emission bands we presumably identified in the spectrum of comet C/2000 WM1 (LINEAR): for the triplet bands - 5-0, FCF = 0.135; 11-2, FCF = 0.019; 15-3, FCF = 0.00012 and for the Asundi bands - 8-0, FCF = 0.0012, 8-1, FCF = 0.0291; 11-1, FCF = 0.000092. For Asundi FCF values calculations we used the following spectroscopic

Table II. Franck-Condon factors for C_2^- $B^2\Sigma_u^+ - X^2\Sigma_g^+$ transitions. Spectroscopic constants ω_e and $\omega_e x_e$, μ and r_e were taken from (Mead R.D. et al., 1985).

$v_2 \backslash v_1$	0	1	2	3	4	5	8
0	0.7179	0.2494	0.0311	0.0015	$< 10^{-4}$	$< 10^{-4}$	$< 10^{-4}$
1	0.2265	0.3268	0.3648	0.0766	0.0052	0.0001	$< 10^{-4}$
2	0.0465	0.2943	0.1224	0.3994	0.1264	0.0109	0.0002
3	0.0078	0.1005	0.2804	0.0299	0.3881	0.1748	0.0183
4	0.0011	0.0236	0.1437	0.2309	0.0011	0.3531	0.2188
5	0.0002	0.0045	0.0446	0.1699	0.1721	0.0057	0.3084
6	$< 10^{-4}$	0.0007	0.0105	0.0671	0.1792	0.1176	0.0253
7	$< 10^{-4}$	0.0001	0.0021	0.0192	0.0879	0.1747	0.0732
8	$< 10^{-4}$	$< 10^{-4}$	0.0004	0.0044	0.0298	0.1048	0.1605

Table III. Morse Franck-Condon factors of CO for the transition $a'^3\Sigma^+ - a^3\Pi$. Spectroscopic data were taken from (Huber K.P. and Herzberg G., 1976).

$v_2 \setminus v_1$	0	1	2	3	4	5	6
0	0.0413	0.1119	0.1666	0.1810	0.1606	0.1236	0.0858
1	0.1525	0.1945	0.0999	0.0141	0.0048	0.0429	0.0813
2	0.2563	0.0808	0.0033	0.0746	0.0957	0.0472	0.0051
3	0.2584	0.0012	0.1119	0.0667	0.0003	0.0347	0.0717
4	0.1738	0.1051	0.0794	0.0070	0.0812	0.0519	0.0015
5	0.0819	0.2056	0.0003	0.1048	0.0273	0.0147	0.0664
6	0.0277	0.1756	0.0981	0.0484	0.0329	0.0762	0.0064
7	0.0068	0.0887	0.1941	0.0100	0.0992	0.0003	0.0576

constants: ω_e= 1228.6, $\omega_e x_e$ = 10.468, μ= 6.8562, r_e = 1.3523 $\AA$ for the $a'^3\Sigma^+$ state; ω_e= 1743.41, $\omega_e x_e$ = 14.36,r_e = 1.20574 $\AA$ for the $a^3\Pi_r$ state (Huber K.P. and Herzberg G., 1976). For calculations of triplet FCF values we used the following spectroscopic constants: ω_e= 1171.94, $\omega_e x_e$ = 10.635, μ= 6.8562, r_e = 1.3696 $\AA$ for the $d^3\Delta_i$ state; ω_e= 1743.41, $\omega_e x_e$ = 14.36, r_e = 1.20574 $\AA$ for the $a^3\Pi_r$ state (Huber K.P. and Herzberg G., 1976).

6. Conclusions

We obtained middle 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^-. A 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 analysis of brightness distribution of the identified emission lines of these molecules. By analyzing brightness distribution of C_2, C_3, 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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References

Barckholtz C., Snow T.P. and Bierbaum V.M : 2001, *Astrophys. J.* 547, 171-174 pp.

Brown M.E., Bouchez A.H., Spinrad H. and Jons-Krull C.M.: 1996, *The Astronomical Journal.* 112(3), 1197-1202 pp.

Chaizy P., Reme H., Sauvaud J.A., d' Uston C., Lin R.P., Larson D.E., Mitchell D.L., Anderson K.A., Carlson C.W., Korth A. and Mendis D.A.: 1991, *Nature.* 349, 393-396 pp.

Churyumov K.I., Chernyi G.F. and Shapovalova A.I.: 1993, *Astron. Lett.* 19, 332-334 pp.

Combi M.R. and Fink U.: 1997, *Astrophys. J.* 484, 879-890 pp.

Cosmovici C.V., Barbieri C., Bonoli C., Bortoletto F. and Hamzaoglu E.: 1982, *Astron. Astrophys.* 114, 373-387 pp.

Czabo Gy.M., Kiss L.L., Sarneczky K. and Sziladi K.: 2002, *Astron. Astrophys.* 384,702-710 pp.

Delsemme A.H.: 1982. Comets. *in IAU Coll. N 61.* 85 p.

Jones P.L., Mead R.D., Kohler B.E., Rosner S.D. and Lineberger W.C.: 1980. *J. Chem. Phys.* 73, 4419-4432 pp.

Halmann M. and Laulicht I.: 1965, *J. Chem. Phys.* 43, 438-448 pp.

Huber K.P. and Herzberg G.: 1976, Constants of Diatomic Molecules. *Molecular spectra and molecular structure*, Van Nostrand Reinhold Company, New York, 716 p.

Kuzmenko N.E., Kuznetsova L.A. and Kuzyakov Yu.A.: 1984, Frank-Condon factors for diatomic molecules. *Moscow University publishing.* 342 p. (in Russian).

Mead R.D., Hefter U., Schulz P.A. and Lineberger W.C.: 1985, *J. Chem. Phys.* 82, 1723-1731 pp.

Shulman L. M.: 1970, Distribution of the neutral matter density in the cometary atmosphere. *Astrometry and Astrophysisc*, 11, 26-30 pp. (in Russian)

Wekhof A.: 1981, *Earth, Moon and Planets.* 24, 157-173 pp.