Observations of O (\(^1S\)) and O (\(^1D\)) in Spectra of C/1999 S4 (LINEAR)

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ABSTRACT

We report on high spectral resolution observations of comet C/1999 S4 (LINEAR) obtained at McDonald Observatory in June and July 2000. We report unequivocal detections of the O (\(^1S\)) and O (\(^1D\)) metastable lines in emission in the cometary spectrum. These lines are well separated from any telluric or cometary emission features. We have derived the ratio of the two red doublet lines and show they are consistent with the predictions of the branching ratio. We also derived a ratio of 0.06 ± 0.01 for the green line flux to the sum of the red line fluxes. This ratio is consistent with H\(_2\)O as the dominant parent for atomic oxygen. We have measured the widths of the lines and show that the widths imply that there must be some parent of atomic oxygen in addition to the H\(_2\)O.

Keywords: Comets, composition; Spectroscopy; Photochemistry
1 Introduction

Oxygen was one of the most common elements in the solar nebula and therefore oxygen should be a major constituent of cometary ices. Much of the cometary oxygen is incorporated into H$_2$O ice with additional oxygen in CO, CO$_2$, H$_2$CO, HCOOH, CH$_3$OH, etc. As a comet is heated during its approach to the Sun, the sublimated parent gases undergo two-body and photodissociation reactions, producing the myriad of radicals and atoms observed in the cometary spectrum. One of the species commonly detected is atomic oxygen.

Figure 1 shows an energy level diagram for atomic oxygen. The strong triplet at $\sim$1304Å has been observed from above the Earth’s atmosphere with facilities such as IUE and HST (e.g. Weaver et al. 1981). This resonance fluorescence line is useful for determining the total amount of atomic oxygen in the coma, but gives no clue to the O parent species since it requires merely that O atoms in the ground 2p$^4$ 3P state be excited to the 3s 3S$^0$ state by solar photons.

In the optical region of the spectrum, three important atomic oxygen transitions exist. These are the forbidden oxygen red doublet at 6300.304 and 6363.776Å (1D – 3P) and the green line at 5577.339Å (1S – 1D). Festou and Feldman (1981) argued effectively against solar resonance fluorescence or dissociative recombination of CO$_2^+$ as excitation processes for the green and red lines. Instead, these transitions must arise from atoms produced directly in the excited 1S or 1D states by photodissociation of a parent molecule (i.e. these lines represent “prompt” emission). In addition, the lifetimes of these states are short. The lifetime at 1 au of the 1D state is about 150 sec, while the 1S state lifetime is less than 1 sec. As a result, O atoms produced in the 1S or 1D levels will decay quickly to the ground state before the atom has had a chance to travel very far from the location at which it was produced. Thus, the red and green lines represent detailed tracers of their parent’s outflow.

Photodissociation of an oxygen-bearing parent species can produce oxygen atoms in the ground 3P state or in the excited 1S or 1D states, depending on the parent molecule and the nature of the solar photodissociation. If the green line (1S – 1D) is observed then, provided that collisional deexcitition is negligible, the red doublet must also be present since every such transition produces an oxygen atom in the 1D level and the red doublet is then the only decay pathway available. For O atoms in the 1S level, 95% decay via the green line and then the red doublet and 5% decay in the near UV 2977 and 2958Å doublet. However, the red doublet can exist without the green line since oxygen atoms can be created directly in the 1D state and decay to the 3P state.

While studies of the green and red transitions offer much valuable information about the comae of comets, this information has not been utilized much in the past because of difficulty in observing these lines. All three lines are also present in telluric spectra and so observations of comets must be obtained at high spectral resolving power to separate the telluric and cometary lines (Magee-Sauer et al. 1988; Combi and
McCrosky 1991; Schultz et al. 1992; Schultz et al. 1993). Alternatively, some attempts have been made to model the distribution of the telluric lines (mostly the red doublet) and remove their signal from the cometary lines (Spinrad 1982; Delsemme and Combi 1979, 1983). In addition to contamination from the telluric lines, the 6300 Å red line is also near the Q branch of one of the NH$_2$ bands. However, moderately high spectral resolution is sufficient for differentiating the oxygen and the NH$_2$.

Unambiguous detection of the green line is much harder than the red doublet. In addition to the coincidence with the telluric green line, the cometary green line is coincident with the cometary C$_2$ (1,2) P-branch. The C$_2$ band is generally very strong and dense, making unambiguous detection of the green oxygen line very difficult. High spectral and/or spatial resolution has been used to detect the green line in comets with varying degrees of success (W. Cochran 1984; Smith and Schempp 1989; Morrison et al. 1997).

Figure 2 shows observations we have obtained of the spectral region around the green line for other comets. These data are of high spectral resolving power. A typical spectrum for comet deVico is shown in the top panel. The strong C$_2$ (1,2) band head is marked. All of the rest of the lines are attributable to C$_2$. The cometary and telluric O ($^1$S) lines are resolved from one another in this spectrum, but the contamination from C$_2$ is substantial.

In the bottom panel we show observations of comet Hyakutake. These were obtained with still higher spectral resolving power. In addition, since the comet was very close to the Earth at the time of the observations, the slit covered only the inner coma. Since C$_2$ has a longer scale length than O ($^1$S), the cometary oxygen line is much more cleanly defined than for deVico. However, it is still apparent that there must be some amount of C$_2$ contamination.

In this paper, we report the unequivocal detection of all three optical atomic oxygen lines in spectra of comet C/1999 S4 (LINEAR). Our observations of these three lines suffer from virtually no contamination from any cometary or telluric line. We use these data to study the ratio of the various transitions and to determine the widths of the cometary lines.

2 Observations and Reductions

Comet C/1999 S4 (LINEAR) was observed on 10 nights from 25 June through 17 July 2000 using the 2DCoudé spectrograph (Tull et al. 1995) on the 2.7-m Harlan J. Smith telescope at McDonald Observatory. This cross-dispersed echelle spectrograph, situated at the f/33 coudé focus of the telescope, was utilized at a resolving power R=60,000. In this mode, spectral coverage is complete from $\sim$ 3700 – 5700 Å with continued coverage with increasing interorder gaps to 1 µm. The detector is a Tektronix 2048x2048 pixel CCD with 24 µm pixels. Table 2 lists details of the observations. In all cases, the slit
projected to 1.2 × 8.2 arcsec on the sky and we summed the data along the slit. At the coudé focus, the position angle of the slit on the sky is variable with declination and hour angle. During 3 hours of observations it will rotate 45°.

In addition to the cometary spectra, observations were obtained of a ThAr hollow-cathode lamp for calibration of the wavelengths. By fitting thorium line positions from all orders, we achieved a dispersion solution with rms errors of ∼ 2.5 mÅ. An incandescent lamp was observed for flat fielding. The solar spectrum was observed with an identical instrumental setup to that used for the comets by imaging the Sun through a diffuser on the roof of the spectrograph slit room and projecting this image through the slit in the same manner as objects are observed through the telescope. Thus, we were able to use an observed solar spectrum in our reductions. At least once per observing run, we also observed α Lyr for relative flux calibration of the orders. Details of our normal reduction procedure can be found in Cochran et al. (2000).

Figure 3 shows a representative spectrum of comet LINEAR in the region of the green oxygen line. This spectrum was obtained on 17 July 2000. In the upper panel, the spectrum is shown allowing for the full strength of the telluric oxygen line. The cometary and telluric oxygen lines are separated by almost 0.8 Å and are clearly resolved. In the bottom panel, the Y axis is expanded by a factor of 8 to show better the other, weaker features in the spectrum. The C₂ (1,2) bandhead is marked. The cometary O (¹S) line is considerably stronger than the C₂ bandhead, unlike the situation with the spectra of other comets shown in figure 2. Indeed, it is reasonable to assume there is virtually no contamination of the cometary oxygen green line by weak C₂ lines. Also, it is apparent that the C₂ band in comet LINEAR is much less well developed than for the other comets. Indeed, we find the spectrum of this comet to be depleted in C₂ and C₃ relative to CN. This was confirmed by Farnham et al. (2001).

Figure 4 shows representative spectra of comet LINEAR for the regions of the red oxygen doublet lines, again from 17 July 2000. Clearly, we have resolved both of these cometary lines from the telluric lines. All of the other lines in these spectra are attributable to other species, generally NH₂. In the case of the red doublet, the cometary line is substantially stronger than the telluric line.

In order to understand the nature of the atomic oxygen in this comet’s coma, we measured the intensity ratio of the green line to the red lines. To compute this ratio, we first had to remove the underlying solar continuum spectrum from each observed spectrum. In addition, the telluric spectrum has O₂ absorption features in the spectral orders of both lines of the red doublet.

First, we needed to remove the telluric features from the two red spectra. We used the observations of α Lyr, a mostly featureless spectrum, to define the telluric spectrum. This spectrum was shifted to the rest frame of the observed solar spectrum, matched in telluric line depth and the solar spectrum was divided by the telluric spectrum to provide a “pure” solar spectrum with no telluric features. The telluric features were similarly removed from the cometary spectra, leaving a cometary emission plus
reflected solar continuum spectrum.

Then, the cometary telluric-corrected red spectra and the green spectrum (which has no telluric absorptions present) were corrected for the solar continuum. The observed green solar spectrum and the telluric-corrected red solar spectra were shifted to the cometary rest frame, the continuum of the solar spectrum was matched to the cometary continuum and the solar spectrum was subtracted.

Finally, the resultant spectra were Doppler-shifted to the laboratory rest frame. During all of these processes, we were careful to preserve the relative flux levels of the different spectra. At this point, we had spectra similar to those shown in Figures 3 and 4 for each of the observations listed in Table I.

The intensities and FWHM of all the cometary and telluric atomic oxygen lines were computed by fitting the observed lines with Gaussian profiles. We tested Lorentzian and Voigt profiles but found that a Gaussian profile was more suitable.

It is not sufficient to compare the observed counts in the green line with those in the red line since the blaze function of the instrument is not perfectly flat. However, coudé spectra cannot be calibrated in a spectrophotometric manner since the entrance aperture is so small and it is impossible to ensure all of a standard star’s flux enters the instrument. However, since all of the spectral orders are observed simultaneously, we can use observations of a flux standard to determine the relative sensitivity of two orders. This is true as long as the focal plane is reasonably flat. We confirmed this by measuring the stellar spatial FWHM of various orders and found a variation of < 2% in the FWHM across the wavelength range of interest. To compute the sensitivity correction, we utilized our observations of α Lyr. We measured the mean continuum counts around the wavelengths of the three oxygen lines of interest. The ratios of these counts were then compared with the known flux of α Lyr (Tüg et al. 1977). The difference between the observed ratios and the real flux ratios represent the needed correction factor. We found that we did not need to correct the 6300/6364 ratio from the measured value, but the measured 5577/6300 ratio needed to be increased by 30%. This correction factor was applied to all of the flux ratios which we discuss in the next section.

3 Results

The intensity \( I \) of an emission line is dependent on the dissociative lifetime of the parent \( \tau_p \), the yield of photodissociation \( \alpha \), the branching ratio for the transition \( \beta \) and the column density of the parent \( N \) in the following manner:

\[
I = 10^{-6} \tau_p^{-1} \alpha \beta N
\]  

(1)

We observed and measured both lines of the red doublet of oxygen. Since these are both transitions from the \((2p^4)^1D\) state to the \((2p^4)^3P\) ground state, the dissociative
lifetime of the parent, the column density of the parent and the yield of photodissociation should be the same for these two transitions, so the ratio of the two line strengths should be the same as the ratio of the branching ratios.

Table 2 of Festou and Feldman (1981) gives branching ratios for the O ($^1S$) and O ($^1D$) metastable states of oxygen. From this table, we can see that the two red lines should be produced with a ratio of $\sim 3.15$ (6300/6364 Å line). Figure 5 shows the ratios which we measured for the red doublet from our comet observations. The dotted line marks the theoretical ratio calculated from the branching ratios. As can be seen from inspection of this figure, most of our observations are consistent with the branching ratio. The error bars shown are the 1-σ photon statistic errors. However, the data of 14 July 2001 (JD=2451739) are in marked disagreement with the theoretical prediction. Inspection of these data showed that a telluric O$_2$ absorption line was exactly coincident with the cometary O ($^1D – ^3P$) 6300 Å emission line on this date due to the geocentric radial velocity of the comet. This strong line was impossible to remove accurately so the measured flux for this line was underestimated and the ratio of the two red doublet lines is not the theoretical ratio. Because of this problem with the 6300 Å line, for subsequent analysis, we adopted a value for the 6300 Å line for 14 July which was $3.15 \times$ the flux of the 6364 Å line. In other words, we assumed the theoretical ratio. Excluding the data from 14 July, we derive a mean value for the red doublet ratio of $3.03 \pm 0.14$ (1σ error), in good agreement with the somewhat uncertain branching ratio.

In comparing the green line to the red doublet, we are no longer observing transitions from the same upper state, so the situation is not as simple as the intensity ratio of the red doublet. Figure 6 shows the ratio of the intensity of the green line to the sum of the intensities of the two lines of the red doublet (with the “corrected” value of the 6300 Å line flux for 14 July as mentioned above). The error bars are just the 1-σ photon counting uncertainties propagated through the calculation. In general, the ratio is approximately constant. However, two data points appear much higher. These are the data from 50 and 100 arcsec tailward on 14 July (JD=2451739). The discrepancy for these two ratios is due to the substantial error associated with the very small flux in the emission lines. Neglecting these two data points, we find the ratio of the green line to the red doublet intensity is $0.06 \pm 0.01$. This assumes that there is no collisional quenching to alter this ratio.

Our derived green line-to-red doublet lines ratio is not the first such measurement, but it is the first where the O ($^1S$) line is relatively uncontaminated by C$_2$. Previous observations have found ratios of 0.22–0.34 for comet IRAS-Araki-Alcock (W. Cochran 1984) and 0.12–0.15 for comet C/1996 B2 Hyakutake (Morrison et al. 1997). Smith and Schempp observed the O ($^1S$) and the 6300 Å O ($^1D$) lines in comet Halley and derive a ratio of these two lines (without trying to correct for the contribution of the 6364 Å line) of 0.05–0.1. Thus, except for the lowest of these limits, our derived line ratio is the lowest value of any comet. While it is possible that the line ratio is different for different comets, we note that all other cometary observations of the O ($^1S$) line have suffered from some significant C$_2$ contamination.
The ratio of the O (\(^1S\)) intensity to the sum of the O (\(^1D\)) intensities can be expressed in a similar form to equation 1.

\[
\frac{I_{5577}}{(I_{6300} + I_{6364})} = \frac{\tau_{p-green}^{-1} \alpha_{green} N_{green} \beta_{5577}}{\tau_{p-red}^{-1} \alpha_{red} N_{red} (\beta_{6300} + \beta_{6364})}
\] (2)

Recall that oxygen can be produced by the photodissociation of any number of parent molecules, either as a daughter species or a granddaughter species. Thus, evaluation of equation 2 requires knowledge of the parent(s) of the oxygen. Conversely, knowledge of the intensity ratio can lend clues to the parent species which give rise to these transitions.

Festou and Feldman (1981) argued convincingly that the parent of cometary O must be \(\text{H}_2\text{O}, \text{CO}, \text{or CO}_2\) since any other more complex oxygen-bearing ice (e.g. HCOOH or \(\text{H}_2\text{CO}\)) does not produce oxygen as a first product of photodissociation but only as part of subsequent decay of radicals. The production of oxygen by these other ices would produce oxygen with a radial extent in the coma which is inconsistent with observations.

The nature of the parent(s) of these three lines is not just of academic interest. Direct observations of \(\text{H}_2\text{O}\) in cometary comae through the Earth’s atmosphere are difficult, although for some very bright comets water has been detected with the KAO (e.g., Mumma et al. 1986; Larson et al. 1991) or via the “hot” bands (Mumma et al. 1996; Dello Russo et al. 2000). We can use the primary daughter, OH, as a proxy for studying water. However, observations of OH are difficult because the (0,0) band of OH is at 3080 Å where atmospheric transmission is low. Observations of OH are best done with a UV telescope such as IUE or HST (e.g. Weaver et al. 1981; Feldman et al. 1987), but OH can be detected with some ground-based instruments (e.g. Cochran and Schleicher 1993; A’Hearn et al. 1995). Radio observations can also be used to study OH and are excellent for velocity resolution but generally are lacking in spatial resolution because of the very long wavelength and, hence, large beam size (e.g. Bockelée-Morvan et al. 1990; Crovisier 1989; Gérard 1990). Sometimes, however, observations of O (\(^1D\)) are used as a tracer of water and the column densities of oxygen are converted to \(\text{H}_2\text{O}\) production rates under the assumption that all of the oxygen comes from \(\text{H}_2\text{O}\) (e.g. Spinrad, 1982; Fink and DiSanti, 1990; Magee-Sauer et al. 1990; Schultz et al. 1992).

Our observations of both the green oxygen line and the red doublet can verify the validity of the assumption that all of the \(^1D\) state comes from photodissociation of \(\text{H}_2\text{O}\). If we assume that there is only one dominant parent of oxygen, then the column densities of the parent in the numerator and denominator of equation 2 are identical. Then, the effective excitation rate for photodissociation of a parent molecule is proportional to \(\tau^{-1} \alpha \beta\). These excitation rates for \(\text{H}_2\text{O}, \text{CO}, \text{and CO}_2\) are given in Table 1. Examination of the effective excitation rates in Table 1 in comparison with our derived ratio of 0.06 indicates that the likely parent of the forbidden oxygen lines in the coma of comet LINEAR is \(\text{H}_2\text{O}\). For \(\text{CO}_2\), Festou and Feldman (1981) and Delsemme (1980) derive very different values from one another for the green to red line ratio. However, neither value is consistent with our observed value of 0.06.
In addition to measuring the ratio of the line intensities, we measured the widths of the cometary O lines. An observed line has a width which is the convolution of the instrumental line width and the velocity line width in the coma. In order to determine the actual cometary line width, therefore, the measured line width must be corrected for the instrumental line widths.

We measured the instrumental line widths for each echelle order by using our observations of the ThAr hollow-cathode lamp. The intrinsic widths of the Th lines are very narrow. The lines are only just resolved with the coudé spectrograph at R=500,000, so they can be used to measure accurately the instrumental profile at R=60,000. The hollow-cathode lamp optics were designed to give a pupil matching that of the telescope and to illuminate the slit similarly to an object. Thus, the observed Th line widths are excellent measures of the spectrograph instrumental profile width. The instrumental widths are a function of wavelength, so for each spectral order we measured many thorium line widths. This procedure was completed for at least one arc lamp spectrum per night. Next, we measured the line widths for all three oxygen lines in each cometary spectrum. From these measurements, we could compute the average values for the instrumental width and the convolved widths and could determine a deconvolved oxygen width for each line by subtracting the instrumental from the measured line widths in quadrature.

Table III lists our results. Examination of this table shows that all three oxygen lines are wider than the instrumental resolution. This added line width is a measure of the velocity dispersion of the gas in the coma. Our width for the 6300Å line is consistent with the width of the same line in Kohoutek (1973 XII; Huppler et al. 1975) though our error bars are much smaller. Smyth et al. (1995) used observations with R=190,000 and found OI 6300 Å line widths of 2.07-3.22 km/sec, also in good agreement. Their data were obtained at heliocentric distances of 0.8 and 1.6 au.

4 Discussion

We have measured the intensity ratio of the \(^1\text{S}\) to \(^1\text{D}\) lines. We can use the effective excitation rates of Table II to infer the parent. However, inspection of this table shows that these rates are not constrained well. Indeed, with the rates quoted, it can be seen that CO\(_2\) is a more efficient producer of O \(^1\text{S}\) than H\(_2\)O. Therefore, we investigated other details about this comet and about the rates which might have an affect on our conclusions.

A potential parent for the oxygen is the photodissociation of CO. Evidence of CO in cometary comae can be found with the CO Fourth Positive group in the UV, with the IR CO bands and with CO\(^+\) in the tail of comets. All three of these lines of evidence were examined for this comet and it was shown that comet LINEAR was depleted in CO relative to other comets. We used our tailwards observations to search for the CO\(^+\). We detected no CO\(^+\) in any of our spectra. However, a non-detection of this ion
is not a strong constraint on the quantity of CO since ion tails can be quite narrow or even absent and therefore we may not have sampled the ion tail.

HST observations of LINEAR using the Space Telescope Imaging Spectrograph (STIS) on 5 July 2000 were used to detect several lines of the CO Fourth Positive group and to derive a production rate of CO of $\sim 5 \times 10^{26} \text{sec}^{-1}$ (Weaver et al. 2001). This yields an upper limit of CO/H$_2$O of 0.6%. On that same date, CSHELL was used on the IRTF to detect the R1 line of the (1,0) band of CO at $\sim 2151 \text{cm}^{-1}$ and to derive a CO production rate of $7 \pm 2 \times 10^{26} \text{sec}^{-1}$ (Mumma et al. 2001a). The derived yield of CO/H$_2$O is 0.9%. These derived yields for comet LINEAR can be compared with comets Lee (1.8%; Mumma et al. 2001b), Halley (3.5%; Eberhardt 1999), Hyakutake ($\sim 10–14\%$, Mumma et al. 2001a) and Hale-Bopp (12.3%; DiSanti et al. 1999, 2001) to show that LINEAR is depleted in CO relative to H$_2$O when compared with other comets. Indeed, in comet LINEAR, the yield of CO is so low that, coupled with the low excitation rates, it would be difficult to produce much oxygen from CO relative to that which is produced from H$_2$O. Thus, we conclude from the low yield and the fact that for a CO parent the green and red lines should be in a ratio of 1:1 that CO is not an important parent of the oxygen in comet LINEAR.

Direct observational evidence for the presence of CO$_2$ in cometary comae is more difficult than for CO. CO$_2$ is a linear symmetric molecule and its ground state does not absorb photons in the visible or UV and it has no allowed radio transitions. The IR transitions cannot be detected except from above the Earth’s atmosphere. Some high-vibrational overtones of the IR fundamental bands will fall in the near-IR windows, but these overtone bands are very weak. Thus, there are no observed CO$_2$ bands in cometary spectra. However, the presence of CO$_2$ can be deduced in two ways: CO$_2^+$ emissions in the UV and visible spectrum of the tail, and the Cameron bands of CO in the UV (1990–2160 Å). Generally, the CO$_2^+$ bands are difficult to detect because they are weak and occur in the near-UV. They are not included in our bandpass so we cannot comment on if they were present.

The Cameron CO bands arise from photodissociation of CO$_2$ (Lawrence 1972; Weaver et al. 1994) and therefore represent a good proxy for the CO$_2$. HST with STIS was used to search for these bands but the Cameron bands were not detected (Weaver, personal communication, 2001). HST is 10$\times$ less sensitive at the Cameron band wavelengths than at the wavelengths of the CO Fourth Positive band, so the failure to detect the Cameron bands does not definitively mean that there are no Cameron band emissions. Still, a preliminary estimate by Weaver is that CO$_2$/H$_2$O is $\leq 5\%$ for comet LINEAR. This ratio is slightly lower than or comparable to that found for five other comets using data from the IUE (Feldman et al. 1997) and HST (Weaver et al. 1994). Feldman et al. also found that CO$_2$/CO ratios of $>1$ are common. Inspection of Table II (line 3) shows that CO$_2$ is a more efficient producer of O (1$^1S$) than H$_2$O, so even with the low CO$_2$/H$_2$O implied by the STIS observations, CO$_2$ could be a significant source of O (1$^1S$).

We have ignored the effects of solar activity in this study, even though the Sun was
active during the time of our observations. The photodissociation of most species is sensitive to the solar ultraviolet flux. Flux in discrete UV wavelength bins are responsible for the photodissociation of different branches. A rate coefficient, $k$, for a wavelength interval from $\lambda_1$ to $\lambda_2$ can be computed from

$$k(\Delta \lambda) = \int_{\lambda_1}^{\lambda_2} \sigma(\lambda)\Phi(\lambda)d\lambda$$

where $\sigma(\lambda)$ is a photo absorption cross-section and $\Phi(\lambda)$ is the photon flux at wavelength $\lambda$.

Festou and Feldman’s (1981) excitation rates for CO$_2$ utilized the quiet Sun flux of Huebner and Carpenter (1979) and the photodissociation cross-sections of Lawrence (1972a,b). The cross-sections are for wavelengths bluer than Ly $\alpha$. For Delsemme’s (1980) line ratio, the solar flux and cross-sections are illustrated in his Figure 2. The caption indicates the solar flux is for the “mean” Sun. Oppenheimer and Downey (1980) pointed out that the solar UV flux is quite variable during the solar cycle and can cause a change in the excitation rates of a factor of two or more. Budzień et al. (1994) showed that near solar maximum it is important to consider the short-term variability of the Sun since the amplitude of the 27-day variation in some solar parameters approaches that of the 11-year cycle of activity (see their Figure 3).

Since CO$_2$ is such an important constituent for the atmospheres of Mars and Venus, several newer analyses have been done of the photo absorption cross-sections (though the conditions in these atmospheres are very different than in the cometary coma so that derived photodissociation rate coefficients from these studies are not applicable to comets). Lewis and Carver (1983) have derived new absorption cross-sections from 1200 to 1970Å including measuring the effects of temperature on the cross-sections (measurements were made at 200, 300, and 370K). They found that the temperature effect is small at the shorter wavelengths, passing through a minimum at 1400Å, but that the cross-section can vary by as much as a factor of 20 at 1900Å when raising the temperature from 200 to 370K. In addition, Anbar et al. (1993) pointed out that the cross-section measurements show large variations in 10-20Å scales so that calculations of the excitation rates can be sensitive to the wavelength resolution. The extent to which these two factors (resolution and temperature) are important to comets is presently unknown. Also unknown is how important the wavelength channel of the new cross-sections, relative to the FUV channel measured by Lawrence (1972a,b), are for the photodissociations needed to produce the oxygen. Detailed calculations will be necessary to quantify this effect, though the calculation of new excitation factors is outside the scope of this paper.

For oxygen produced from the photolysis of H$_2$O, the range of effective excitation rates listed in Table II probably encompasses a range of solar activity. Festou (1981) showed that the relative importance of the different photodissociation channels varies with solar activity. Lyman $\alpha$ increases from 24% of the pathway for a quiet Sun to 39% for an active Sun, while the photodissociation branch from 1357–1860Å decreases from
72% to 58% with the increase in activity. The channel with \( \lambda < 1357 \text{Å} \) (but not including Ly \( \alpha \)) stays roughly constant at 3–4%. Within these channels, the branches that produce the oxygen lines also change relative importance so that in total, the \((1D)\) is produced 6.7% of the time for a quiet Sun and 9.8% of the time for an active Sun, while the numbers for \((1S)\) are 0.6% and 1.0%. Fortuitously, the relative ratio of these two lines is about the same for either a quiet or active Sun. Crovisier (1989) agreed on the relative branching to produce oxygen for the two non-Ly \( \alpha \) channels but found that Ly \( \alpha \) dissociated only 10% of the time to oxygen while Festou lists this branch as active 25% of the time. Budzien et al. (1994) found that the photodestruction rates can vary by 30% from solar minimum to maximum, but concluded that the quantum yield of OH and O \((1D)\) from \( \text{H}_2\text{O} \) photodissociation is relatively insensitive to solar flux variations. Since we are trying to determine the relative production of the oxygen green and red lines, it is probably reasonable to ignore the details of the solar activity for our study.

Thus, our data show a ratio of green to red intensity of 0.06 and this value is relatively constant despite the fact that the comet was quite variable and was, in fact, disintegrating. The constancy of this ratio, despite the activity, indicates that the scale lengths of the parent of each state are very similar. This, however, does not preclude separate parents for the two states.

The line intensity ratio of 0.06 is inconsistent with \( \text{CO}_2 \) as the dominant parent using the effective excitation rates of \( \text{CO}_2 \) of either Festou and Feldman (1981) or Delsemme (1980), although the predicted ratios in these two works are quite different. The intensity ratio predicted for \( \text{H}_2\text{O} \) is consistent with the observed ratio since the effective excitation rates given span a range. However, the caveats mentioned above about solar flux and cross-sections must be remembered when drawing any conclusions.

Regardless of the actual parent which gives rise to the oxygen transitions which we have detected, the determined line widths indicate something about the nature of the gas which populates these states. Recall that the oxygen atom can be formed in either the ground state or the excited state. 95% of the atoms which are in the \((1S)\) state will decay back to the ground state via the \((1D)\) state and while doing so they will produce \((1D)\) lines which are as wide as the \((1S)\) line.

We measured the \((1S)/(1D)\) flux ratio to be 0.06. Thus, most of the atoms formed in the \((1D)\) state. However, the \((1S)\) line is wider than the \((1D)\) lines and both lines of the red doublet are of a consistent width. These two facts, in combination, imply that atoms which start in the \((1D)\) state form lines with a lower velocity dispersion (narrower) than atoms which start in the \((1S)\) state.

However, recall also that the lifetime of the \((1D)\) state at 1 AU is about 150 sec, while for the \((1S)\) state it is less than 1 sec. Both are extremely short and, as a result, the line widths are a measure of the velocity dispersion of the parent, not the oxygen; the wider green line implies that its parent has a higher velocity dispersion than the red doublet parent. This is suggestive that the parent of the O in the \((1S)\) state and the parent of the majority of the O in the \((1D)\) state are not the same.
5 Summary

In this paper, we have reported on high spectral resolution observations of comet C/1994 S4 (LINEAR) with which we have detected unequivocally three oxygen metastable lines.

1. We have derived the ratio of the line strengths of the two lines of the red oxygen doublet and have shown that this ratio is as predicted by the branching ratios commonly reported in the literature.

2. We have derived the ratio of the line strength of the green line to the sum of the strengths of the red lines and shown that it was approximately constant with a value of 0.06 ± 0.01. This ratio is consistent with H$_2$O as the dominant parent for the atomic oxygen. However, based on line width measurements, there may be another parent contributing to the oxygen.

3. We have measured the widths of the three oxygen lines and have shown that the green line is wider than the red lines, implying a higher velocity dispersion for the upper level than the lower level. Since 95% of the upper level (green line) atoms decay to the ground state via the red doublet, this implies that atoms which originate in the upper state have a higher velocity dispersion than those which originate in the lower excited state.

4. We discussed the implications of solar activity and of the various physical parameters for our conclusions. Solar activity is probably a secondary effect that will not change our conclusions. New rate coefficients for the photodissociation of CO$_2$ to oxygen will need to be calculated before CO$_2$ can be eliminated as a contributing parent on the basis of the line ratios.

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| Date       | UT Start | $R_h$ (AU) | $\dot{R}_h$ (km sec$^{-1}$) | $\Delta$ $R_h$ (AU) | Exposure Time (s) | PA Tail$^1$ | Position of Slit$^2$ |
|------------|----------|------------|----------------------------|----------------------|-------------------|-------------|---------------------|
| 25 Jun 2000 | 08:47    | 0.97       | -19.7                      | 1.21                 | 1800              | 270.7       | optocenter          |
|            | 09:25    |            |                            |                      | 1800              |             | optocenter          |
|            | 09:59    |            |                            |                      | 1800              |             | optocenter          |
|            | 10:33    |            |                            |                      | 1800              |             | optocenter          |
| 26 Jun 2000 | 08:26    | 0.96       | -19.4                      | 1.17                 | 1800              | 270.7       | optocenter          |
|            | 09:05    |            |                            |                      | 1800              |             | optocenter          |
|            | 09:39    |            |                            |                      | 1800              |             | optocenter          |
|            | 10:12    |            |                            |                      | 1800              |             | optocenter          |
|            | 10:46    |            |                            |                      | 1200              |             | optocenter          |
| 06 Jul 2000 | 09:03    | 0.86       | -15.1                      | 0.81                 | 1800              | 274.6       | optocenter          |
|            | 09:38    |            |                            |                      | 1800              |             | optocenter          |
|            | 10:13    |            |                            |                      | 1800              |             | optocenter          |
|            | 10:49    |            |                            |                      | 1800              |             | optocenter          |
| 07 Jul 2000 | 09:07    | 0.85       | -14.5                      | 0.77                 | 1800              | 275.7       | optocenter          |
|            | 09:41    |            |                            |                      | 1800              |             | optocenter          |
|            | 10:29    |            |                            |                      | 1800              |             | optocenter          |
|            | 10:53    |            |                            |                      | 1200              |             | optocenter          |
| 08 Jul 2000 | 08:46    | 0.84       | -14.0                      | 0.74                 | 1800              | 277.1       | optocenter          |
|            | 09:20    |            |                            |                      | 1800              |             | optocenter          |
| 09 Jul 2000 | 08:47    | 0.84       | -13.4                      | 0.70                 | 1800              | 278.7       | optocenter          |
| 14 Jul 2000 | 09:04    | 0.80       | -10.0                      | 0.53                 | 1800              | 295.8       | optocenter          |
|            | 09:41    |            |                            |                      | 1800              |             | 50 arcsec west      |
|            | 10:17    |            |                            |                      | 1800              |             | 100 arcsec west     |
|            | 10:51    |            |                            |                      | 1200              |             | optocenter          |
| 15 Jul 2000 | 09:59    | 0.80       | -9.3                       | 0.50                 | 1200              | 302.5       | optocenter          |
| 16 Jul 2000 | 10:23    | 0.79       | -0.4                       | 0.48                 | 1800              | 311.0       | optocenter          |
|            | 10:57    |            |                            |                      | 1200              |             | optocenter          |
| 17 Jul 2000 | 08:22    | 0.79       | -7.7                       | 0.45                 | 1800              | 321.8       | optocenter          |
|            | 08:59    |            |                            |                      | 1800              |             | 25 arcsec west      |
|            | 09:49    |            |                            |                      | 1800              |             | 10 arcsec west, 10 north |
|            | 10:24    |            |                            |                      | 1800              |             | 10 arcsec east, 10 south |
|            | 10:57    |            |                            |                      | 1200              |             | optocenter          |

Notes:

1. Position angle of predicted extended heliocentric radius vector (north through east)
2. Slit position relative to optocenter
Table II: Effective Excitation Rates for Dissociation

| Parent  | Excitation Rate (sec\(^{-1}\) at 1 AU) | Ratio      |
|---------|--------------------------------------|------------|
|         | O \(^1\)S                          | O \(^1\)D  | O \(^1\)S/ O \(^1\)D |
| H\(_2\)O* | \(7 - 12 \times 10^{-8}\)          | \(8 - 12 \times 10^{-7}\) | ~0.1          |
| CO*     | \(< 4 \times 10^{-8}\)             | \(< 4 \times 10^{-8}\)     | ~1            |
| CO\(_2\)* | \(4.4 \times 10^{-7}\)             | \(5 \times 10^{-7}\)      | ~1            |
| CO\(_2\)† |                                      |                 | ~0.3         |

*Source: Festou and Feldman (1981), Table 3
†Source: Delsemme (1980)
Table III: The Oxygen Line Widths

| Transition | Measured Cometary Widths (Å) | Measured Instrumental Widths (Å) | Intrinsic Cometary Widths (Å) | Derived Outflow Velocity (km sec$^{-1}$) |
|------------|-------------------------------|---------------------------------|-------------------------------|----------------------------------------|
| O ($^1 S$) 5577Å | 0.110 ± 0.006 | 0.087 ± 0.003 | 0.067 ± 0.003 | 3.60±0.16 |
| O ($^1 D$) 6300Å | 0.107 ± 0.005 | 0.094 ± 0.003 | 0.051 ± 0.003 | 2.43±0.14 |
| O ($^1 D$) 6364Å | 0.118 ± 0.004 | 0.103 ± 0.005 | 0.058 ± 0.003 | 2.73±0.14 |
6 Figure Captions

Figure 1: An energy level diagram of atomic oxygen for the lowest level transitions to the ground state. The ground state splitting has been exaggerated so the splitting is apparent. The J=1 level is really 0.02eV above the J=2 level, while the J=0 level is 0.03eV above the J=2 level. The $^1\text{D} - ^3\text{P}$ J=2-0 transition at 6391.733 Å is not shown since it is only predicted and has not been detected. The wavelengths are given in Angstroms.

Figure 2: High spectral resolution observations of other comets. Observations of 122P/1995 S1 (deVico) are shown in the upper panel with R=60,000. The slit covered 870km×5845km centered on the optocenter. The positions of the cometary and telluric lines are shown. Obviously, both the cometary and telluric O ($^1\text{S}$) are heavily contaminated by C$_2$. Observations of C/1996 B2 (Hyakutake) are shown in the bottom panel. The spectral resolution is higher than for deVico; the comet was quite close to the Earth so the spatial resolution is high. The slit covered 46km×1249km centered on the optocenter. Therefore, there is less likely to be C$_2$ in the aperture and the O ($^1\text{S}$) lines are less contaminated than for deVico.

Figure 3: The region of the O ($^1\text{S}$) oxygen line. This spectrum of the optocenter of LINEAR was obtained on 17 July 2000. The upper panel shows the spectral region scaled to the telluric line. The cometary line is clearly well separated from the telluric one. The lower panel shows an expansion of the Y axis. The C$_2$ (1,2) bandhead is marked. The cometary O ($^1\text{S}$) is much stronger even than the C$_2$ bandhead. It is clear that there is virtually no contamination of the cometary O ($^1\text{S}$) line by cometary C$_2$ or telluric O ($^1\text{S}$).

Figure 4: The regions of the O ($^1\text{D}$) oxygen lines. The 6300 Å line region is shown in the upper panel, while the 6364 Å line region is shown in the lower. Again, the cometary and telluric lines are well separated and no other species contaminates the cometary lines. The NH$_2$ band designations are in the bent notation.

Figure 5: The ratio of the observed 6300 Å red line to the 6364 Å red line. The cometary optocenter ratios are shown as solid dots and the non-optocenter ratios are shown as open squares. The theoretical ratio is denoted by a dashed line. The data uphold the theoretical prediction with the exception of the four data points from 14 July (JD=2451739). These points are discussed in the text.

Figure 6: The ratio of the observed green line to the sum of the red lines. The symbols are the same as for figure 5. The two high values of the ratio are the low signal/noise points at 50 and 100 arcsec tailward from 14 July. Except for these two data points, the green-to-red ratio is approximately constant, with a value of 0.06 ± 0.01. The mean is denoted by a solid line with the error envelope noted with dashed lines.
Figure 1: Cochran and Cochran 2001
Figure 2: Cochran and Cochran 2001
Figure 3: Cochran and Cochran 2001
Counts

LINEAR 17 July 2000
(R=60,000)

NH$_2$ (0,3,0) - (0,0,0)

Telluric O ($^1$D)

Counts

LINEAR 17 July 2000
(R=60,000)

NH$_2$ (0,3,0) - (0,0,0)

Telluric O ($^1$D)

Figure 4: Cochran and Cochran 2001
Figure 5: Cochran and Cochran 2001
Figure 6: Cochran and Cochran 2001