Atomic Oxygen in the Comae of Comets

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Abstract

We report on the detection of atomic oxygen lines in the spectra of 8 comets. These forbidden lines are a result of the photodissociation of the parent oxygen-bearing species directly into an excited state. We used high resolution spectra obtained at the McDonald Observatory 2.7m telescope to resolve the cometary oxygen lines from the telluric oxygen lines and from other cometary emissions. We find that the relative intensities of the two red lines (6300.304 and 6363.776 Å) are consistent with theory. The green line (5577.339 Å) has an intensity which is about 10% of the sum of the intensities of the two red lines. We show that collisional quenching may be important in the inner coma. If we assume the relative excitation rates of potential parents which have appeared in the literature, then H$_2$O would be the parent of the cometary green oxygen line. However, those rates have been questioned. We measured the width of the three oxygen lines and find that the green line is wider than either of the two red lines. The finding of a wider line could imply a different parent for the green and red lines. However, the constancy of the green to red line flux ratio suggests the parent is the same for these lines but that the exciting photons have different energies.

Keywords: Comets, coma; photochemistry; spectroscopy
Oxygen is important for the chemistry of many of the current Solar System bodies since it readily bonds with many other atoms. There are three prominent atomic oxygen lines in the optical region of the spectrum. The transition from the first excited state of the singlet branch, \(^1\text{D}\), to the ground state, \(^3\text{P}\), produces a doublet in the red at 6300.304 Å and 6363.776 Å. The second excited singlet state, \(^1\text{S}\), decays to the \(^1\text{D}\) state 90–95% of the time with a transition at 5577.339 Å; the remaining 5–10% of the time, the \(^1\text{S}\) state decays directly to the ground state (\(^1\text{S} \rightarrow ^3\text{P}\)) through two UV lines at 2958.365 and 2972.288 Å (Slanger et al. 2006a). These are all forbidden lines. The green line and the red doublet are observed in the Earth’s atmosphere and are affected by auroral activity. The green line has been observed in spectra of Venus and appears to be quite variable there (Slanger et al. 2006b). It is assumed that these lines will also be present in Mars’ atmosphere, but only the UV line at 2972.288 Å has been detected definitively (Barth et al. 1971; Leblanc et al. 2006).

The three forbidden lines are also seen in the spectra of comets. Photodissociation of oxygen-bearing parent species produces oxygen atoms in the ground \(^3\text{P}\) state or directly into the excited \(^1\text{D}\) or \(^1\text{S}\) states, depending on the parent molecule and the nature of the solar photodissociation. The red doublet is substantially stronger than the green line and the red lines are generally much stronger than the telluric red lines. The cometary green line is generally a small fraction of the intensity of the telluric green line.

To observe the oxygen in the spectra of comets, it is desirable to observe with moderately high spectral resolution in order to resolve the Doppler-shifted cometary lines from the telluric lines. The red doublet occurs in a part of the cometary spectrum which is relatively uncrowded, so contamination from other cometary species is not an issue at high spectral resolution. The spectral resolution allows for the separation of the cometary and telluric lines. The situation for the green line is quite different. In addition to the telluric green line which must be separated, the cometary green line sits in the middle of the \(^1\text{S}\) \((1,2)\) P-branch; the \(P_1(27)\) and \(P_2(26)\) lines flank the oxygen line. The \(C_2\) spectrum is quite dense. Thus, for many cometary spectra, it is impossible to derive the intensity of the green line. However, for some comets, the oxygen line is stronger than the \(C_2\) bands and can be successfully deblended from the cometary \(C_2\) and the telluric oxygen if the spectral resolution is sufficient. Some comets have been observed to have almost no \(C_2\), making detection of the green line simple (Cochran and Cochran 2001).

The green line and the red doublet are not produced by fluorescence or dissociative recombination (Festou and Feldman 1981) but instead arise from atoms produced directly in the \(^1\text{S}\) or \(^1\text{D}\) states (i.e. prompt emissions). The lifetimes of the upper states of the oxygen lines are short, with the \(^1\text{D}\) state lasting about \(\sim 110\) s and the \(^1\text{S}\) state lasting \(\sim 1\) s. Indeed, the lifetime of the \(^1\text{S}\) state is so short that its spatial distribution traces
the parent’s distribution directly, since the oxygen atom will not have time to travel far from its direct parent prior to its decay to the ground state.

The atomic oxygen observed in the spectra of cometary comae did not sublime from pure oxygen ice. Instead, oxygen is stored in the nucleus as an oxygen-bearing ice. Jackson and Cochran (2007) observed the green line in the spectrum of comet Tempel 1 following the impact of the Deep Impact spacecraft with the comet. They saw the line increase in brightness quickly after the impact and then decay. Figure 1 shows the intensity of the green line after the impact as a function of the cometocentric distance. The initial increase shows the impulsive nature of the impact. The decay started at ~2000s after the impact. After that time, the green line flux decayed as $1/\rho$, where $\rho$ is the projected cometocentric distance. This behavior is characteristic of prompt emission produced by a single-step dissociation. Since, with its short lifetime, the emission is tracing the direct parent, the behavior shown in Fig. 1 is indicative that the $^1S$ state is a daughter, and not a granddaughter, product of some species. But what is this parent? Complex oxygen-bearing species (e.g. H$_2$CO or HCOOH) can not be the parent, as they can only produce oxygen via a two-step process. In addition, Jackson and Cochran showed that the green line flux decayed much faster than the OH flux, indicating that the oxygen line did not come primarily from OH. Thus, the green line is likely to be directly produced from H$_2$O, CO$_2$, or CO. It is generally assumed that the red lines come from the dissociation of H$_2$O as this is consistent with the distribution of O ($^1D$) in the inner coma of a comet (Combi and McCrosky 1991; Fink and Johnson 1984; Magee-Sauer et al. 1988). We have used high spectral resolution observations of 8 comets to detect the green line and the red doublet of oxygen in order to try to understand the production of the atomic oxygen in cometary spectra.

2 Observations

The spectra of the comets were obtained with the 2DCoude instrument at the 2.7m Harlan J. Smith telescope of McDonald Observatory. This is a cross dispersed echelle spectrograph (Tull et al. 1995) which can be operated in two resolution modes. The lower resolving power has $R=\lambda/\Delta\lambda = 60,000$. In this mode, we obtain complete wavelength coverage from 3700 Å to 5700 Å and continued coverage from 5700 Å to 10,200 Å with increasing inter-order gaps. Thus, the green and the red lines are observed simultaneously. The other mode of this instrument has $R=200,000$. In this mode, the wavelength coverage is much smaller (1/16th of the $R=60,000$ mode) but individual lines may be more easily resolved.

We observed 8 comets for which we were able to detect cleanly both the green and red lines using the $R=60,000$ mode. The circumstances of the observations are listed in Table I. The slit was 1.2 x 8.2 arcsec for all of these observations. On some nights, multiple spectra were obtained. The number of spectra for each night is listed in the
Figure 1: The intensity of the green oxygen line at 5577.339 Å was measured immediately after the impact of comet 9P/Tempel 1 and the Deep Impact spacecraft using the HIRES instrument at Keck I. The green line initially increased in intensity and then decayed as it flowed outwards. This figure shows the intensity of the line as a function of cometocentric distance, $\rho$. The line decayed as $1/\rho$, the signature of a parent. Since the lifetime of the $^1S$ state is $\sim 1$ s at 1 au, this points to a single-step process from parent to O ($^1S$) state.

We measured the intensity and the full width half maximum (FWHM) of a Gaussian fit to the three oxygen lines for each of the spectra described in Table I. When the telluric line was not cleanly separated by the Doppler shift of the cometary lines, we would simultaneously fit Gaussians to both the cometary and telluric lines in order to deblend the two features. Each spectrum was measured independently and an average was computed from all the observations for each comet for each line.
Figure 2: The spectral regions around the three atomic oxygen lines for comet 122P/de Vico. These spectra are typical of comets with moderately strong $C_2$ bands, showing the potential $C_2$ contamination of the cometary green line. Note also the telluric oxygen line is Doppler-shifted from the cometary line. The cometary oxygen line can be deblended from the contaminating cometary $C_2$ and the telluric oxygen. In contrast, the spectral regions of the red lines are quite clean and only the telluric line needs to be deblended.
Figure 3: These spectra of comet C/1999 H1 (Lee) show a case of a comet with relatively weak C₂. It is easy to see the cometary green line and the only contaminant is the telluric line. As with de Vico, the red lines are in regions that are not busy. Again, the telluric and cometary lines can be easily deblended.
Table I: Observational Circumstances

| Comet            | Date  | No. Spectra | Heliocentric Distance (AU) | Heliocentric Radial Velocity (km s\(^{-1}\)) | Geocentric Distance (AU) | Geocentric Radial Velocity (km s\(^{-1}\)) |
|------------------|-------|-------------|----------------------------|---------------------------------------------|--------------------------|---------------------------------------------|
| 122P/de Vico     | 3 Oct | 2           | 0.66                       | -3.41                                       | 1.00                     | -14.25                                      |
|                  | 4 Oct | 1           | 0.66                       | -2.29                                       | 0.99                     | -12.87                                      |
| C/1996 B2 (Hyakutake) | 9 Mar | 2           | 1.37                       | -32.80                                      | 0.55                     | -57.30                                      |
| C/1999 H1 (Lee)  | 30 May| 1           | 1.09                       | -23.85                                      | 1.03                     | 34.37                                       |
|                  | 21 Sep| 2           | 1.51                       | 24.97                                       | 0.87                     | -16.48                                      |
|                  | 23 Sep| 11          | 1.54                       | 24.94                                       | 0.86                     | -13.39                                      |
| D/1999 S4 (LINEAR) | 25 Jun | 4           | 0.97                       | -19.70                                      | 1.21                     | -61.21                                      |
|                  | 26 Jun| 5           | 0.96                       | -19.38                                      | 1.17                     | -61.61                                      |
|                  | 6 Jul | 4           | 0.86                       | -15.08                                      | 0.81                     | -62.84                                      |
|                  | 7 Jul | 4           | 0.85                       | -14.53                                      | 0.77                     | -62.46                                      |
|                  | 8 Jul | 2           | 0.84                       | -13.96                                      | 0.74                     | -61.92                                      |
|                  | 9 Jul | 1           | 0.84                       | -13.36                                      | 0.70                     | -61.19                                      |
|                  | 15 Jul| 1           | 0.80                       | -9.28                                       | 0.50                     | -50.11                                      |
|                  | 16 Jul| 2           | 0.79                       | -8.52                                       | 0.45                     | -46.46                                      |
|                  | 17 Jul| 5           | 0.79                       | -7.74                                       | 0.45                     | -42.03                                      |
| C/2001 A2 (LINEAR) | 24 Jul | 1           | 1.35                       | 23.58                                       | 0.42                     | 21.45                                       |
| C/2002 V1 (NEAT) | 19 Jan| 1           | 0.98                       | -40.30                                      | 0.89                     | 8.20                                        |
| C/2001 Q4 (NEAT) | 25 May| 5           | 0.98                       | 4.92                                        | 0.66                     | 45.87                                       |
|                  | 26 May| 4           | 0.98                       | 5.45                                        | 0.68                     | 46.13                                       |
|                  | 27 May| 3           | 0.98                       | 5.96                                        | 0.71                     | 46.32                                       |
| C/2006 M4 (Swan) | 31 Oct| 2           | 1.00                       | 19.48                                       | 1.02                     | 13.08                                       |

The measured spectral line width is a convolution of the intrinsic width of the line (which is dominated by the velocity dispersion of the atoms from their production) and the instrumental slit profile. In order to define the instrumental line width, we used our observations of a ThAr hollow cathode lamp. The Th lines are intrinsically quite narrow and are unresolved by our spectrograph. We measured the FWHM of 15 – 30 isolated Th lines per spectral order of interest for each night to define the instrumental line profile for that order. As would be expected, the instrumental profile is slightly wider for the redder wavelengths under study. We found very consistent instrumental line widths over the many years of observations and the slight differences are probably the result of differences in focus. Typically, we could measure the FWHM of the instrumental profiles to 0.003 Å. The intrinsic cometary line width is then just the measured line width with the instrumental width removed in quadrature. The resultant intrinsic line widths can then be converted to a velocity width.

In addition to our R=60,000 resolution spectra listed in Table I, we also observed comet Hyakutake with the R=200,000 mode on 30 Mar 1996 (\(R_h=0.94\) AU, \(\Delta=0.19\) AU). With these observations we only detected the green line and the 6300 Å line, while the 6364 Å line fell in an interorder gap. In the R=200,000 mode, the intrinsic cometary
Table II: Measured Line Ratios

| Comet                  | 6300/6364 flux ratio | 5577/(6300+6364) flux ratio |
|------------------------|----------------------|----------------------------|
| 122P/de Vico           | 3.22 ± 0.02          | 0.08 ± 0.003               |
| C/1996 B2 (Hyakutake)  | 2.98 ± 0.04          | 0.09 ± 0.001               |
| C/1999 H1 (Lee)        | 3.19 ± 0.16          | 0.08 ± 0.01                |
| D/1999 S4 (LINEAR)     | 3.04 ± 0.14          | 0.06 ± 0.01                |
| C/2001 A2 (LINEAR)     | 2.92                 | 0.11                       |
| C/2002 V1 (NEAT)       | 3.08                 | 0.09                       |
| C/2001 Q4 (NEAT)       | 3.23 ± 0.18          | 0.09 ± 0.02                |
| C/2006 M4 (Swan)       | 3.07 ± 0.04          | 0.09 ± 0.01                |
| **Average**            | **3.09 ± 0.12**      | **0.09 ± 0.014**           |

The intensity \( I \) of an emission line is dependent on the photodissociative 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 \( N \) as

\[
I = 10^{-6}\tau_p^{-1}\alpha\beta N \quad \text{photons cm}^{-2}\text{s}^{-1}
\]

The red lines are both transitions from the \( (2p^4)^1D \) to the \( (2p^4)^3P \) ground state so their lifetimes, column density and yields should be the same. Thus, the ratio of their fluxes should be the same as the ratio of their branching ratios. Storey and Zeippen (2000) have derived a theoretical value of 2.997 for the red doublet ratio based on the Einstein A values. Sharpee and Slanger (2006) measured this ratio in terrestrial nightglow spectra and found a ratio of \( 2.997 \pm 0.016 \). The average value for each observed comet is listed in Table II and plotted in Fig. 4. We find an average value of \( 3.09 \pm 0.12 \) for these eight comets, which is in agreement within the error bars with the theoretical and nightglow values.

In the absence of collisional quenching, the ratio of the O \( ^1S - ^1D \) intensity to the sum of the O \( ^1D - ^3P \) intensities can be expressed as

\[
\frac{I_{5577}}{(I_{6300} + I_{6364})} = \frac{\tau_p^{-1}(^1S)\alpha(^1S)\beta_{5577}N(^1S)}{\tau_p^{-1}(^1D)\alpha(^1D)(\beta_{6300} + \beta_{6364})N(^1D)}
\]

In order to evaluate this equation, one needs to know the parent(s) of the oxygen to know what values of lifetimes, yields and branching ratios to use. Festou and Feldman
Figure 4: The average ratio of the two lines of the red oxygen doublet for each of the eight comets is shown. The average value of the eight comets is shown as a solid line and the 1σ error range is denoted with dashed lines.

(1981) listed in their Table 3 some effective excitation rates for the dissociation. These are reproduced in Table III. Festou and Feldman estimate that these values are only accurate to ±50% because of variations in the solar EUV flux. Inspection of this table shows that we expect a very different value for the green-to-red line ratio for H$_2$O than for CO and CO$_2$. Thus, the observed values for this line ratio may shed light on the potential parent. The ratios we find are listed in Table II. These ratios have been corrected for the relative response of the red and green orders of the spectrograph by use of observations of α Lyr (the green-to-red flux ratio needed to be increased by 30%, as per Cochran and Cochran 2001). Figure 5 shows our measured values for the ratio of the green line flux to the sum of the line fluxes from the two red lines. We find an average value of $I_{5577}/(I_{6300} + I_{6364}) = 0.09 ± 0.01$. Using the values of Festou and Feldman, this is consistent with water as the parent of the oxygen.

The slit covered from ~1200 to ~3500 km from the optocenter and thus included the highest density regions of the coma. It is only in this very inner coma that collisional quenching would have any effect. The collisional quenching coefficients of O ($^1$S) and O ($^1$D) by H$_2$O are comparable but the O ($^1$D) lifetime is ~150 times longer than the
Table III: Festou and Feldman (1981) Effective Excitation Rates

| Parent | Excitation Rate (s\(^{-1}\) at 1AU) | Ratio O\(^{(1S)}\)/O\(^{(1D)}\) |
|--------|----------------------------------|-----------------------------|
| H\(_2\)O | 7.12\(\times\)10\(^{-8}\) | 8.12\(\times\)10\(^{-7}\) | \(\sim 0.1\) |
| CO     | <4\(\times\)10\(^{-8}\) | <4\(\times\)10\(^{-8}\) | \(\sim 1\) |
| CO\(_2\) | 4.4\(\times\)10\(^{-7}\) | 5\(\times\)10\(^{-7}\) | \(\sim 1\) |

O\(^{(1S)}\) lifetime. Festou and Feldman (1981) showed that this will result in a flatter column density profile for the red lines than for the green line. In addition, the red line intensities might be lower than they would be in the absence of quenching.

If the parent is H\(_2\)O then the reactions which might apply are

\[
\begin{align*}
\text{H}_2\text{O} + h\nu & \rightarrow \text{H} + \text{OH} \\
\text{H}_2\text{O} + h\nu & \rightarrow \text{H}_2 + \text{O} \(^{(1S)}\) \\
\text{H}_2\text{O} + h\nu & \rightarrow \text{H}_2 + \text{O} \(^{(1D)}\) \\
\text{H}_2\text{O} + h\nu & \rightarrow 2\text{H} + \text{O} \(^{(3P)}\)
\end{align*}
\]

Huestis (2006) points out that production of O\(^{(1S)}\) by photodissociation of H\(_2\)O has never been reported in the laboratory literature. He goes on to claim that no experiment has been attempted so that there is no experimental basis for the estimate of its yield.

As noted in the introduction, the further decay of OH into some form of oxygen was shown not to be an important source of O\(^{(1S)}\) because the decay of OH flux after the impact of the Deep Impact spacecraft with Tempel 1 was much slower than that for the green line flux.

If the parent is CO\(_2\) then the relevant reactions are

\[
\begin{align*}
\text{CO}_2 + h\nu & \rightarrow \text{CO} + \text{O} \(^{(1D)}\) \\
\text{CO}_2 + h\nu & \rightarrow \text{CO} + \text{O} \(^{(1S)}\) \\
\text{CO}_2 + h\nu & \rightarrow \text{CO} + \text{O} \(^{(3P)}\)
\end{align*}
\]

Huestis (2006) points out that for these equations the yield of O\(^{(1S)}\) has been measured in a number of studies and it approaches unity in a narrow window around 112.5 nm. However, for CO\(_2\), the yield of O\(^{(1D)}\) has never been measured. This experiment is difficult because of the rapid quenching, but it is believed that O\(^{(1D)}\) is the primary product over much of the absorption spectrum.

The production of oxygen from the dissociation of CO is possible, but it is slower than the production from H\(_2\)O and CO\(_2\) by up to an order of magnitude because of the
bond strength of the CO molecule (Bhardwaj and Haider 2002). In addition, Cochran and Cochran (2001) showed that the production of the oxygen from CO in comet 1999 S4 (LINEAR) was inconsistent with UV observations showing a depletion of CO in its coma. Thus, we dismiss CO as a parent.

In addition to measuring the line intensities for the three oxygen lines, we also measured the line widths listed in Table IV. The derived intrinsic line widths, after removal of the instrumental profile, in both Å and km s\(^{-1}\), are tabulated.

The red lines can be formed without forming the green line. Since both transitions are from the same upper state to the ground state, they should have the same line width. Figure 6 shows the 6300 Å line velocity plotted against the 6364 Å line velocity for the individual spectra on each comet. In a few cases, the uncertainties in the line widths made it impossible to discern any width greater than the instrumental width. These points are plotted with a width of 0 km s\(^{-1}\) in this figure. With the exception of these few spectra with lines which could not be measured, the two lines of the red doublet have the same width.
Table IV: Measured Oxygen Line Widths

| Comet                  | 5577 Intrinsic | 6300 Intrinsic | 6364 Intrinsic |
|------------------------|----------------|----------------|----------------|
|                        | FWHM velocity | FWHM velocity | FWHM velocity |
|                        | Å              | Å              | Å              |
|                        | km s\(^{-1}\)  | km s\(^{-1}\)  | km s\(^{-1}\)  |
| 122P/de Vico           | 0.073±0.031    | 2.4            | 0.034±0.016    | 1.0            | 0.025±0.018    | 0.7            |
| C/1996 B2 (Hyakutake)  | 0.080±0.011    | 2.6            | 0.073±0.009    | 2.1            | 0.043±0.015    | 1.2            |
| C/1999 H1 (Lee)        | 0.085±0.038    | 2.7            | 0.036±0.028    | 0.6            | 0.049±0.026    | 0.8            |
| D/1999 S4 (LINEAR)     | 0.067±0.011    | 2.2            | 0.050±0.008    | 1.4            | 0.058±0.012    | 1.6            |
| C/2001 A2 (LINEAR)     | 0.058±0.011    | 1.9            | 0.009±0.009    | 0.3            | 0.040±0.044    | 1.1            |
| C/2002 V1 (NEAT)       | 0.095±0.011    | 3.1            | 0.046±0.038    | 1.3            | 0.052±0.042    | 1.5            |
| C/2001 Q4 (NEAT)       | 0.079±0.007    | 2.5            | 0.031±0.017    | 0.9            | 0.033±0.018    | 0.9            |
| C/2006 M4 (Swan)       | 0.080±0.038    | 2.6            | 0.049±0.014    | 1.4            | 0.057±0.011    | 1.6            |

Errors are the combined standard deviations from the multiple measurements of each comet and the multiple lines of Th except for 2001 A2 and 2001 Q4. There was only a single spectrum for each of these comets so the instrumental measurement error was used as the comet error.

Figure 6: The line widths from the individual spectra of the eight comets are plotted for the two lines of the red doublet. The comets are denoted with the same symbols as in Figures [1] and [5]. The diagonal dotted line is the equality line. The large plus marks the average values for each width and their standard deviations.
Figure 7: The line widths for the green lines of the individual spectra are plotted against the widths of the 6300 Å line in the left side of the plot and for 6364 Å in the right side. The dotted line denotes equality. The average values and standard deviations are shown with the big plusses. The filled symbols are for comets, such as Lee, where the O (1S) line dominates the C2 features; the open symbols are for comets such as de Vico where we had significant C2 signal.

If the green line is present, it will decay to the red doublet 90–95% of the time. Thus, if the red and green lines are produced by the same process and the same energy photons, then they should be the same widths. Figure 7 shows the width of the green line in comparison with each of the red lines. In these observations, the green line is not the same width as the red lines. Festou (1981) listed the excess velocity for the creation of the O (1S) state from Ly α photons as 1.6 km s$^{-1}$ and of the O (1D) state as 1.8 km s$^{-1}$. Thus, there would be the expectation that the red lines were broader than the green line. However, this is not what we observe. Figure 7 shows that it is the green line which is the widest of the lines. Inspection of the data also shows that we get the same result for comets with very weak C2 as we do for those with stronger C2, so our deblending was quite successful. The difference in the line widths for the green and red lines must point to additional parent(s) for the green line or to dissociation to the 1S state by photons with higher energy than Ly α, the presumed exciter of the 1D state.
In addition to the R=60,000 observations shown in Table IV we have three spectra of comet Hyakutake from 30 March 1996 obtained with the R=200,000 mode. In this setup, we cannot observe all three lines simultaneously, but we were able to observe the 5577 Å and 6300 Å lines in one spectral image. Figure 8 is a plot of the green line and the 6300 Å line from these observations. At this resolving power, the instrumental widths are a much smaller fraction of the cometary line widths than with R=60,000. As with the R=60,000 spectra, the instrumental width of the red line is wider than that of the green line, but the intrinsic cometary line width of the green line is wider than that of the red line. Thus, our conclusions from Figure 7 are not biased by the lines being just a bit wider than the instrumental widths at the lower resolving power.

Comet Hyakutake was quite close to the Earth (∆ = 0.19 AU) when we observed it at R=200,000. Thus, each pixel in the spatial direction along our 8 arcsec slit subtended only 17.9 km at the comet. We extracted the spectra in 7 chunks along the slit to investigate whether the line width changed in the very inner coma. We found that the intrinsic FWHM was constant across the slit for both the green and red lines, with the average FWHM of the green line being 0.088 ± 0.003 Å and the red line being 0.056 ± 0.002 Å. Thus, the line widths from extraction along the whole slit, shown in Fig. 8 are not widened by outflow in the inner 400 km of the coma. In addition, the line intensity of the green line decreased more quickly with cometocentric distance than did the red line. This is shown in Figure 9. The flat distribution of the red line flux out to 400 km (and possibly the green line flux out to 100 km) is consistent with quenching in the inner coma. These profiles agree well with Case B of Festou and Feldman (1981; their figs. 2 and 3).

4 Discussion

Spectra of comets tell us about the physical and chemical processes taking place within the cometary comae. In addition, comets are excellent laboratories for testing our understanding of chemistry since the long path lengths through the coma allow relatively small gas densities to produce significant column densities.

We are interested in the oxygen lines for several reasons. First, oxygen is one of the most abundant elements in the Universe after hydrogen and helium and it readily bonds with other atoms and molecules. Indeed, 80% of cometary ices are H₂O, so oxygen is a critical component of comets. Water is hard to detect spectrally from the ground so daughter products of water have traditionally been used as a proxy to study the water. Since the OH fluorescent bands are in the UV region of the spectrum, where there is low detector quantum efficiency and high atmospheric extinction, they are difficult to study. The three forbidden oxygen lines discussed in this paper are in the optical and have been used as a water proxy.
Figure 8: The green line (solid; labels left and bottom) and the 6300 Å line (dotted; labels right and top) from the 30 Mar 1996 R=200,000 spectrum of Hyakutake are plotted together. The spectra are normalized to the same relative intensity and the wavelength scales are the same number of Å/inch. The profiles are the convolution of the instrumental and intrinsic line widths. The instrumental width is wider for the red line but the observed green line is much wider. Thus, the green line must be intrinsically a wider line.
Figure 9: The flux in the green and red line was extracted in seven pieces along the slit from the R=200,000 spectra of comet Hyakutake and is plotted against cometocentric distance. The closed symbols are the data on one side of the opptocenter and the open symbols the other (the comet was not centered in the slit). The open data points at 215 km appear low, possibly due to vignetting at the end of the slit. The red line data shows a much flatter trend with cometocentric distance than does the green line.

Unfortunately for studies of atomic oxygen in comets, the telluric spectrum has strong atomic oxygen emissions which are always present and are quite variable. Thus, until the advent of the era of high resolution spectroscopy of comets, contamination of the cometary lines by the telluric lines was always an issue. Even with high resolving powers, the green line in cometary spectra has proved to be a difficult target since it sits within the spectral region of the C$_2$ (1,2) P-branch. Despite that, there have been some observations of the detection of the green line in cometary spectra previously reported. These are listed in Table V.

The three oldest observations all suffered from non-simultaneity of the observations of the three lines. Indeed, the Halley and Hyakutake observations reported in Table V
Table V: Previously Reported Green Line Detections

| Comet               | Date(s)          | Heliocentric Distance (AU) | Geocentric Distance (AU) | \(\frac{I_{5577}}{I_{6300}+I_{6364}}\) | Ref.               |
|---------------------|------------------|---------------------------|--------------------------|------------------------------------------|--------------------|
| C/1983 H1 (IRAS-Araki-Alcock) | 6, 8 May 1983 | 1.02                      | 0.13, 0.09               | 0.022–0.034                              | 1                  |
| 1P/Halley           | 5 Apr 1986       | 1.25                      | 0.45                     | 0.05 – 0.1                               | 2                  |
| C/1996 B2 (Hyakutake) | 23, 27 Mar 1996 | 1.08, 1.00                | 0.12                     | 0.13 – 0.16                              | 3                  |
| C/1995 O1 (Hale-Bopp) | 26, 28 Mar, 22 Apr 1997 | 0.92, 0.99 | 1.33, 1.63              | 0.18 – 0.22                              | 4                  |
| 153P/Ikeya-Zhang    | 20 Apr 2002      | 0.89                      | 0.43                     | 0.12±0.1                                 | 5                  |
| 9P/Tempel 1         | 2 – 6,9 Jul 2005 | 0.89–0.92                | 1.51                     | 0.056-0.13±0.1                           | 6                  |

References – 1: Cochran (1984) - red and green lines observed different nights; 2: Smith and Scheppe (1989) - 6364 line not observed; 3: Morrison et al. (1997) - 6300 line not observed; 4: Zhang et al. (2001); 5: Capria et al. (2005); Capria et al. (2008)

Each contain observations of only 1 line of the red doublet. Thus, these observations should be used cautiously. The ratios of the green line to the sum of the red line fluxes for Hale-Bopp, Ikeya-Zhang and Tempel 1 are consistent with the values we found for our 8 comets reported in this paper. Hale-Bopp seems to have the highest ratio. This might be because Hale-Bopp had extremely high water production rates and a very large collisional zone. However, there are not a great deal of details in the Zhang et al. (2001) paper so it is difficult to judge why this ratio might be higher. Hale-Bopp had a very strong continuum and \(C_2\) band so there may have been issues correcting for these factors.

Comparing these remaining three comets with the 8 observations presented here, it is obvious that the green line is typically about 10% the summed intensity of the red doublet. If there is collisional quenching, as implied in Fig. 9, the red line fluxes might be lower than without quenching so the \(1S/1D\) ratio in the absence of quenching might be even lower. All of the authors referenced in Table V and indeed our previous paper on 1999 S4 (LINEAR) (Cochran and Cochran 2001), have used this ratio along with Table 3 of Festou and Feldman (1981) to conclude that water is the source of the green atomic oxygen line.

In this paper, we reported on the widths of the oxygen lines in addition to their intensities and found that the green line was consistently wider than the red lines. Since 90–95% of the photons in the \(1S\) state decay to the ground state via the \(1D\) state, the higher velocity photons should widen the red lines. We examined how this would affect our measurements by generating two Gaussian line profiles with FWHM values appropriate for the green line and assuming the red line FWHM was the “correct” value. These two lines were then combined with the same average flux ratio observed in the comets reported in this paper. We then measured the properties of this artificially generated line against a red line generated by assuming none of the red line comes from
photons which were first excited to the $^1S$ state. We find the combined line has 2% lower flux than a pure line but that the FWHM of the lines agree to 0.001 Å, or at least as good as our measurement accuracy. Therefore, based on the relative intensity of the green and red lines, we would not have been able to measure any broadening of the red lines and the measured red line widths can be assumed to be indicative of excitation in the $^1D$ state only.

The wider green line leads to two possibilities for the production of photons in the $^1S$ state. The first is that there is a parent other than H$_2$O that dissociates into photons in the $^1S$ state. As discussed above, CO can be eliminated based on its bonding and on observations of comet 1999 S4. OH can be eliminated because it decays more slowly than the green line. Thus, CO$_2$ would be the likely alternative parent.

The other possibility is that H$_2$O is the parent for both the $^1S$ and $^1D$ states. This would imply that the energy of the photons responsible for the production of the $^1S$ state is higher than that for the production of the $^1D$ state. As Huestis (2006) pointed out, these excitation rates are not calibrated. The laboratory measurement of the production of the green line from H$_2$O has never been made. Nor has the production of the red lines from CO$_2$. Until the point that these rates are known with any certainty, all we can definitely conclude is that the green line flux is about 10% that of the combined red line flux in all comets.

However, this in itself may offer a clue. The observations of the 8 comets reported here span 11 years, or a full solar activity cycle. They also span heliocentric distances from 0.66 to 1.54 au. We see no difference in either the relative line intensities nor in the line widths from one comet to another. Thus, whatever photodissociative process(es) produce these lines, their relative importance does not change with solar UV flux or from comet to comet. Inspection of Table I of Bockelée-Morvan et al. (2004) shows that the abundances of minor species such as CO and CO$_2$ relative to water are quite variable. The constancy of the green line to the red line flux thus suggests a single parent for both states with different energies responsible for the production of the different states. Clearly, more laboratory work is needed but comets are lending clues to the processes involved.

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