Previously unobserved water lines detected in the post-impact spectrum

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1 Water lines in Tempel 1

The team from UCL, monitored the Deep Impact event using the CGS4 spectrometer on the United Kingdom Infrared Telescope, UKIRT. Our principal objective was to determine the temporal development of solar pumped fluorescent (SPF) transitions of H$_2$O following impact, and to interpret the results using the recently published *ab initio* water line list, BT2 (Barber et al., 2006a). BT2 was produced at UCL using the DVR3D suite of programs (Tennyson et al., 2004), and is the most complete and most accurate water line list in existence.

Normal observing techniques were employed: these and other aspects of our work are fully reported in Barber et al. (2006b). We obtained spectra in the wavelength range centred on 2.894 $\mu$m, with a spectral range of $\pm 0.040$ $\mu$m. Apart from containing a number of SPF transitions (Dello Russo et al., 2004), it is largely devoid of other molecular lines (such as CO), which makes it possible to model the region using the BT2 line list without having to include other species. However, in the subsequent examination of the data, in order to maximise the S/N ratio, we restricted our analysis to a narrower wavelength range: 2.8945 - 2.8985 $\mu$m.

It had been our intention to obtain spectra of Tempel 1 on the night prior to impact, on impact night, and on the night after impact. However, prior to impact the comet was not sufficiently bright for us to be able to obtain useful data, and on the night after impact, reduced intensity and a deterioration in the observing conditions prevented us obtaining high quality data. Our results therefore relate only to the period of 143 minutes immediately following impact.

Our signal was effectively confined to one pixel row (we estimate that this contained $\sim 65\%$ of the signal), and it attests to the accuracy of the UKIRT tracking system that there was no detectable drift from this position over the whole observing session. No attempt was made to recover the small amount of signal from adjacent rows, as an analysis of the data revealed that this would
have resulted in a reduction in the overall S/N ratio. Moreover, because of
the weakness of the signal, it was necessary to combine the data for the whole
observing run in order to obtain a useful S/N ratio, which meant that, taking
the spectral region as a whole, no temporal resolution could be obtained (see
below for comments on temporal resolution for specific groups of lines).

The spectrum for the period July 4 05:54 to 08:17 U.T. is shown in Figure

The fact that some of the intensities are negative may in part be due to
our having over-corrected for the continuum, or more likely, is due to noise,
which we estimate to be in the region of $0.4 \times 10^{-16}$ Wm$^{-2}$ µm$^{-1}$.

Two bright fluorescent transitions at 2.89580 and 2.89831 cm$^{-1}$, stand out
against a background of weaker features. Many of these weaker features are
close to, or below, the noise threshold and these we disregard. However, there
are a several where we estimate the S/N ratio to be greater than 4 and which,
unlike noise, appear in the same place (albeit with differing intensities) in
many of the individual frames. We interpret these as also being genuine signals
and have marked them either SPF (where their wavelengths correspond to
known fluorescent transitions), or SH, (in those cases where transitions are

![Figure 1. Observed post-impact spectrum Tempel 1. Wavelength is in the rest frame. Reproduced from Barber et al. (2006b).](image-url)
Previously unobserved water lines detected in the post-impact spectrum thought to be by some other route). In the first column of Table 1 we give the observed wavelength of each of the features (adjusted for red shift).

The position of many of the spectral features in Figure 1 can be replicated using the BT2 synthetic water line list. Some of these are identified as being due to SPF transitions (sometimes blended). However, some of the features did not correspond to known SPF transitions, and moreover, as far as we are aware, have not previously been recorded in cometary spectra. We have labelled these ‘SH’ (the acronym is convenient as it can stand for ‘solar heating’, which is definitely true, or ‘stochastic heating’, which may also be an apt description). It should be noted that although the line positions derived from BT2 agree well with those of the observed features, the intensities are only approximate guides, as the LTE assumption used by BT2 is not generally valid for cometary spectra. Moreover, since the mechanism behind the formation of the SH transitions is not known, a precise match between the intensity of the observed features and the BT2 synthetic spectra is not to be expected.

Table 1. Assignments of SPF and previously unobserved SH lines in the post-impact spectrum of Tempel 1. The first column gives the observed wavelength of each of the features (adjusted for red shift), the next column identifies the transition: the vibrational quantum numbers are given in round brackets and the rotational quantum numbers in square brackets. The last three columns give: the experimentally-determined wavelength of the listed transition, the Einstein A coefficient computed using BT2, and our designation of type: SPF or SH. Reproduced from Barber et al. (2006b).

| \( \lambda_{\text{observed}} \) (\( \mu\text{m} \pm0.00005 \)) | Identification | \( \lambda_{\text{laboratory}} \) (\( \mu\text{m} \)) | \( A_{\text{fi}} \) (s\(^{-1} \)) | Type |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| 2.89458         | (101)[211] - (001)[220] | 2.89462         | 1.9             | SPF             |
| 2.89527         | (103)[110] - (102)[110] | 2.89526         | 53.5            | SH              |
| 2.89527         | (211)[322] - (210)[211] | 2.89528         | 8.5             | SH              |
| 2.89573         | (210)[101] - (011)[000] | 2.89570         | 5.1             | SH              |
| 2.89580         | (200)[110] - (100)[221] | 2.89578         | 4.7             | SPF             |
| 2.89591         | (101)[202] - (100)[321] | 2.89590         | 1.7             | SPF             |
| 2.89723         | (220)[212] - (021)[111] | 2.89728         | 4.4             | SH              |
| 2.89831         | (200)[110] - (001)[111] | 2.89830         | 6.6             | SPF             |

In attempting to identify the non-SPF features in our observed spectrum, we generated a series of synthetic spectra using BT2, some of which are shown in Figures 3 and 4. In order to improve the signal to noise ratio and also to lessen the significance of errors in the wavelength calibration of our detector, estimated to be in the region of 0.00004 \( \mu\text{m} \) (slightly greater than a single pixel width, which is 0.000033 \( \mu\text{m} \)), we artificially reduced the resolution of our observed data from an instrument-limited ~37 000 to a pixel-averaged limited
value of $\sim 17500$ by taking a moving average of five pixels in the wavelength dimension in order to assist in matching the observed and synthetic data. Figure 2 shows our observed spectrum with this artificially de-graded spectral resolution. In this figure the vertical scale is terminated at a level well below the peak intensities of the two strongest SPF transitions. This was done to aid identification of the weak transitions.

Figure 2. Observed post-impact spectrum Tempel 1, moving average of 5 pixels. Wavelength is in the rest frame. The vertical scale has been limited to assist identification of the weaker features. Reproduced from Barber et al. (2006b).

Figure 3 shows three synthetic spectra generated at 3000, 4000 and 5000 K (assuming LTE), using the BT2 line list (with some corrections to the calculated wavelengths based on the available experimental data). In producing these spectra, we applied the restriction that only states with $J \leq 3$ are included. The resolution in Figure 3 was set to be the same as Figure 2. Figure 4 shows another set of synthetic BT2 spectra generated at the same three temperatures, but this time including all J levels (up to 50). Some of the same features are observed as in Figure 2, but we note that Figure 3 matches the observed spectrum better than Figure 4 does.
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Figure 3. BT2 synthetic spectra at 3 000 K, 4 000 K and 5 000 K, \( J_{\text{max}} \)=3. Reproduced from Barber et al. (2006b).

Figure 3 is therefore a high-v, low-J spectrum and it reproduces well the position (less-so, the intensities) of many of the non-SPF features in the low-resolution observed spectrum, Figure 2. It should be noted that similar features are observed in synthetic spectra generated for temperatures greater than 3 000 K and the appearances of the spectra vary little once \( T_{\text{vib}} > 4500 \) K, except for differences in the general levels of intensity. It is also noted that there are other features in our observed spectrum Figure 2 that are replicated in the synthetic spectrum Figure 3. These are also due to water emission and are produced by the blending of many overlapping transitions from different vibrational manifolds. They have not been included in Table 1 as it is not possible to assign them to one or two individual transitions.

1.1 Assigning the features

Among the assigned features are fluorescent emission lines from levels that have two quanta of \( \text{H}_2\text{O} \) stretching, such as \((2\ 0\ 0)\rightarrow(1\ 0\ 0)\) and \((1\ 0\ 1)\rightarrow(1\ 0\ 0)\); in the former transition, the emission involves one quantum of \( \nu_1 \), in the latter it involves one quantum of \( \nu_3 \). A quantum of \( \nu_1 \) and of \( \nu_3 \), have similar
energies $\sim 3450$ cm$^{-1}$. In both cases, the final state is the 1$\nu_1$ state. Because a quantum of $\nu_2$ carries less than half the energy of a $\nu_1$ or $\nu_3$ quanta, ($\sim 1500$ cm$^{-1}$), transitions involving a change of one quantum of $\nu_2$ are not observed in our selected wavelength range.

Our post-impact spectrum of Tempel 1 also includes several transitions from states that include one or more quanta of $\nu_2$, or that involve a total of 4 vibrational quanta. These are not SPF spectral features. It will be seen from Table 1 that these include the blend of (1 0 3)$\rightarrow$(1 0 2) and (2 1 1)$\rightarrow$(2 1 0) at 2.8953 $\mu$m, and (2 2 0)$\rightarrow$(0 2 1) at 2.8972 $\mu$m. It seems likely that upper levels with more than two vibrational quanta have not been populated by solar pumping from ground vibrational states, but by another mechanism. Whereas SPF transitions originate from upper states having energies in the region of 7300 cm$^{-1}$, the transitions that we have labelled ‘SH’ all originate from higher energy states (those upper states having four vibrational quanta are in the energy range 10300-14400 cm$^{-1}$). It is possible that the production route involves H$_2$O molecules that have sublimed from the freshly exposed icy grains ejected by the impact. However, an understanding of the precise nature of these SH lines will require further research. We have recently learned

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig4}
\caption{BT2 synthetic spectra at 3000 K, 4000 K and 5000 K, $J_{\text{max}}=50$. Reproduced from Barber et al. (2006b).}
\end{figure}
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that Villanueva et al. (2006) observed some previously unrecorded lines in the
2.8313 \( \mu \)m region in the post-impact spectrum of Tempel 1, which may be
due to transitions from higher energy ro-vibrational states of \( \text{H}_2\text{O} \).

1.2 Comparison with other spectra

We have compared our results with the spectra obtained by Mumma et al. (2005).

As far as the positions of the observed SPF transitions are concerned,
our results agree well with those of Mumma et al.. However, none of the
SH features that we identify appear in Mumma et al.'s spectrum D. One
possible reason for the difference between our results and those of Mumma
et al. is the difference in times when the spectra were obtained. Our results
were obtained between 05:54 and 08:17 U.T. on impact night, whilst Mumma
et al.'s spectrum in Figure 5 were obtained between 6:43 and 7:25 U.T.. By
summing the intensities of all the SH features, we were able to achieve a
degree of temporal resolution that was not possible for the individual lines.
We observed that the total intensity of the SH features was particularly strong
during the period 20–40 minutes after impact., but by 50 minutes after impact
had declined to a level that was only slightly above that of the background
noise. This could be the reason why the features are not observed in Mumma
et al.'s spectra.

Recently we have obtained UKIRT spectra of Comet 73P/Schwassmann-
Wachmann, fragment-C in order to investigate whether this recently frag-
mented comet exhibits similar SH features to those that we observed in Temple 1. Our preliminary investigation of the 73P spectra does not show any of
the SH features. Work on this is continuing.
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