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Comets

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ABSTRACT

Spectroscopy of comets, in the X-ray and far-ultraviolet from space, and in the near infrared and millimeter from the ground, have revealed a wealth of new information, particularly about the molecular constituents that make up the volatile fraction of the comet's nucleus. Interpretation of these data requires not only proper wavelengths for identification but also information about the photolytic and excitation processes at temperatures typical of the inner coma (70–100 K) that lead to the observed spectral signatures. Several examples, mainly from *Far Ultraviolet Spectroscopic Explorer* and *Hubble Space Telescope* spectra of comets observed during the last few years, will be given to illustrate some of the current issues.

1. Introduction

Cometary spectroscopy has long had a synergistic relationship with laboratory spectroscopy, particularly concerning free radicals that are unstable in the laboratory environment. Historical examples include the discovery of C_3 before its identification in terrestrial laboratories (recounted by Herzberg 1971), and the identification of H_2O^+ in the plasma tail of comet Kohoutek (Wehinger et al. 1974). Beginning in the 1970s, the window of the electromagnetic spectrum began to open, extending to the identification of parent molecules in the infrared and microwave (Bockelée-Morvan et al. 2004) and to the final atomic dissociation products in the ultraviolet (Feldman et al. 2004). Following the fortuitous apparitions of two bright comets, C/1996 B2 (Hyakutake) and C/1995 O1 (Hale-Bopp) in 1996 and 1997, more than two dozen parent molecules have been identified (Crovisier & Bockelée-Morvan 1999; Crovisier et al. 2004). Isotope ratios, particularly the D/H ratio, in molecules such as HDO have been determined from millimeter observations (Bockelée-Morvan et al. 2004). The same period saw the unexpected detection of soft X-ray emission from comets, followed by intense laboratory and theoretical activity to explain the features of the observed emission (Krasnopolsky et al. 2004).

In this brief overview, I will summarize some of the recent results that illustrate the importance of laboratory and theoretical data in interpreting a broad range of cometary observations. I will give these examples in order of increasing wavelength, with a bit more emphasis on the far ultraviolet with which I am most familiar. The references cited will be largely recent reviews, rather than the original papers. For a comprehensive bibliography, the reader is referred to the recently published *Comets II* book (Festou et al. 2004) and the relevant chapters therein.

2. X-Rays

Prior to 1996, X-rays had not been detected in comets and the conventional wisdom was that they were unlikely to be produced in the cold, rather thin cometary atmosphere. The discovery of soft X-ray emission ($E < 2$ keV) from comet C/1996 B2 (Hyakutake) by the *Röntgen Satellite* (*ROSAT*) thus came as a surprise. Since then, X-ray emission has been detected from over a dozen comets using *ROSAT* and four other space observatories, the *Extreme Ultraviolet Explorer*, *BeppoSAX*, the *Chandra X-ray Observatory* (*CXO*), and *Newton-XMM* (Krasnopolsky et al. 2004). The earliest observations were at very low spectral resolution making it difficult to select amongst the possible excitation mechanisms: charge exchange, scattering of solar photons by attogram dust particles, energetic electron impact and bremsstrahlung, collisions between cometary and interplanetary dust, and solar X-ray scattering and fluorescence. The more recent *CXO* observations, at somewhat higher spectral resolution, favor the charge exchange of energetic minor solar wind ions such as O^{6+}, O^{7+}, C^{5+}, C^{6+}, and others, with cometary gas, principally H_2O, CO, and CO_2, as the primary mechanism. This mechanism would explain why the X-ray intensity appears to be independent of the gas production rate of the comet and that the peak emission is offset from the location of the comet's nucleus. This conclusion is also supported by recent laboratory work on the charge transfer of highly ionized species with cometary molecules (Beiersdorfer et al. 2003) and by theoretical calculations of state specific cascades (Kharchenko & Dalgarno 2001). The X-ray emission thus tells us more about the solar wind than about the gaseous composition of comets. Nevertheless, cometary X-rays provide an excellent example of how laboratory astrophysics, in both laboratory experiments and theoretical modeling, were brought to bear on an unexpected observational phenomenon.

3. Far-Ultraviolet

The *Far Ultraviolet Spectroscopic Explorer* (*FUSE*), launched in 1999, has provided access to the spectral region between 900 and 1200 Å at very high spectral resolving power (up to 20,000) although for comets, because of their extended nature, only a spectral resolution of ∼0.25 Å has been achieved. Four comets have been observed by *FUSE* and their spectra in this region are unexpectedly rich, dominated by three Hopfield-Birge band systems of CO and atomic O and H lines. In addition, H_2 fluorescence pumped by solar Lyman-β has been detected (Feldman et al. 2002) as well as some three dozen unidentified emission lines (Weaver et al. 2002). However, only upper limits on Ar I, N_2, and O VI were obtained, the latter despite the prediction of strong doublet emission at 1031.9 and 1037.6 Å from the X-ray model of Kharchenko & Dalgarno (2001). Emission of the 1031.9 Å line was initially detected in comet C/2000 WM1 (LINEAR), but increased signal-to-noise ratio in the spectra of comet C/2001 Q4 (NEAT), observed in 2004, enabled an accurate determination of the wavelength of this feature and identified it as the H_2 (1,1) Q(3) Werner band line, fluorescently pumped by solar O VI (Feldman 2005). The corresponding Q(3) lines of the (1,3) band at 1119.1 Å and the (1,4) band at 1163.8 Å are also detected.

The problem with this interpretation was that a large population of H_2 molecules in the $v = 1$ vibrational level was required. It was also noticed that there was a broad satellite feature centered near the position of the P(40) line of the $C\,^1\Sigma^+ – X\,^1\Sigma^+(0,0)$ band at 1087.9 Å that implied the presence of a hot, non-thermal population of CO rotational levels (Feldman et al., in preparation). Both populations result from the photodissociation of formaldehyde, the dynamics of which has been intensively studied, both experimentally and theoretically, for many decades (see, for example van Zee et al. 1993; Zhang et al. 2005, and references therein). The "molecular channel," leading to CO and H_2 as products, leaves the CO rotationally hot and the H_2 in several excited vibrational levels, the exact populations depending on the energy of the incident photon. H_2CO is also a minor comet species and has been detected in a number of recent comets both in the infrared and millimeter (Mumma et al. 2003; Biver et al. 2002, 2006) and its known abundance is able to account for the brightness of the observed CO and H_2 emissions. Moreover, the shape of the observed P-branch (the R-branch is at wavelengths below the detector cutoff) closely matches the population of J-levels seen in the laboratory spectra. A large population of higher H_2 vibrational levels can also account for some of the other unidentified features in the *FUSE* spectrum. As an example, pumping from the ground state $v = 2$ level of H_2 by solar Lyman-α photons can lead to a rich cascade spectrum from the $v = 1$ level of the excited B state (Lupu et al. 2006). The solar Lyman-β pumped lines described above require the H_2 to be in the ground vibrational level and these molecules are most likely produced in the secondary H_2O photodissociation branch to H_2 + O(^{1}D) (Slanger & Black 1982).

One of the initially unidentified features seen in the spectrum of comet C/2001 A2 (LINEAR) is at 1026.5 Å. This feature, together with a weaker feature at 1028.9 Å, appears as a satellite to the O I $2p^33d\ ^3D^o – 2p^4\ ^3P$ multiplet. It is identified as the O I intercombination multiplet $2p^33d\ ^5D^o – 2p^4\ ^3P$ (Feldman 2005). This multiplet does not appear at all in any of the terrestrial dayglow spectra recorded by *FUSE*, implying that electron impact excitation of atomic oxygen is negligible, and does not appear to have been reported in any astrophysical source to date. The $^5D^o$ state has two decay paths, the observed intercombination transition to the ground state, and cascade through allowed multiplets at 9261–9266 Å and 7772–

7775 Å to the ^{5}S^o level followed by the 1356 Å intercombination transition to the ground state. Recent calculations suggest that the branching ratio of the intercombination lines to the cascade lines is of the order 10^{-5} (Tachiev & Froese Fischer 2002), which would make observation of this multiplet extremely unlikely, contrary to this observation. This discrepancy remains to be resolved. We note that two lines of the cascade ^{5}P – ^{5}S^o multiplet at 7771.9 and 7774.2 Å appear (the third is blended), listed as unidentified, in the high resolution spectral atlas of comet 122P/de Vico (Cochran & Cochran 2002). The source of the ^{5}D^o excitation remains unknown, although charge exchange of oxygen ions degraded through successive charge transfers is a possibility that warrants further investigation.

4. Atomic Deuterium

Isotope ratios, particularly the abundance of D relative to H in water, are relevant to planetary formation scenarios and to the question of the delivery of water to the Earth's oceans (Owen & Bar-Nun 2002). The ratio of HDO to H_2O has been measured in only three very active comets; in 1P/Halley by *in situ* mass spectrometry, and by microwave spectroscopy in comets C/1996 B2 (Hyakutake) and C/1995 O1 (Hale-Bopp) (Bockelée-Morvan et al. 2004). The value of this ratio was found to be about twice that of terrestrial sea water for these three comets, but this represents a very small, biased sample. Except for a marginal detection of DCN, no other deuterated molecules have been detected in comets.

Weaver et al. (2004) reported the first direct detection of D I Lyman-α in comet C/2001 Q4 (NEAT) using the echelle mode of the Space Telescope Imaging Spectrograph (STIS) on *HST*. This line, ∼0.3 Å to the blue of the H I line, is clearly separated from both the cometary and geocoronal H I lines and appears at the correct geocentric velocity of the comet. One difficulty in interpreting the observed brightness is that the OD/OH branching ratio in HDO photodissociation varies with the energy of the incident photon (Vander Wal et al. 1991). OD was searched for but not found in longer wavelength STIS spectra. However, using a mean branching ratio there are still difficulties in modeling both the spectral and spatial profiles of the D I line. These difficulties may be related to the excess velocity of the D photofragment and suggest a closer look at the photodissociation dynamics of HDO.

5. Infrared and Microwave

We have already noted the direct detection of two dozen parent molecules, all but S_2 by means of infrared and radio frequency spectroscopy (Bockelée-Morvan et al. 2004; Crovisier et al. 2004). S_2 was first detected in the ultraviolet (A'Hearn et al. 1983) (its origin remains uncertain) while CO is the only parent observable in both the ultraviolet, infrared, and millimeter. This number of molecules is small compared with the known inventory of molecules in interstellar clouds. Upper limits for an additional two dozen species searched for in comet Hale-Bopp have been given by Crovisier et al. (2004). Many of these are likely to be detected when a new facility, the *Atacama Large Millimeter Array* (*ALMA*) becomes operational. Crovisier et al. also list 16 unidentified radio lines in this comet.

Microwave spectroscopy has also provided measurements of a number of isotope ratios of molecules containing C, N, O and S atoms (Bockelée-Morvan et al. 2004). These measurements are complemented by very high resolution ground-based spectroscopy of visible band systems of CN and C_2. Another recent measurement is that of the ortho-to-para population ratios in the ground states of H_2O and NH_3, all of which seem to be lower than the statistical values, implying spin temperatures in the range of 25–35 K (Kawakita et al. 2004). The spin temperatures, which appear to be similar for all comets observed to date, are interpreted in terms of the temperature of the comet formation region in the protosolar nebula.

6. Outlook

Traditional cometary spectroscopy has expanded in recent years to include the spectral domains of X-rays, far-ultraviolet, infrared and millimeter. Significant contributions to cometary science have been made by orbiting observatories spanning this spectral range: *CXO*, *FUSE*, *HST*, *SWAS*, and *Odin*, amongst others. Recent (*Stardust, Deep Impact*) and current (*Rosetta*) comet missions will provide ground truth for the interpretation of spectroscopic data. New facilities, such as *ALMA*, will greatly enhance our ability to determine the volatile composition of comets and to trace their evolution from interstellar matter. There are still significant challenges in understanding the atomic and molecular physics of the cometary atmosphere, a long term issue being the identification of the large number of unidentified lines seen in high resolution spectra across the entire electromagnetic spectrum.

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REFERENCES

A'Hearn, M. F., Schleicher, D. G., & Feldman, P. D. 1983, ApJ, 274, L99

Beiersdorfer, P., et al. 2003, Science, 300, 1558

Biver, N., et al. 2002, Earth Moon and Planets, 90, 323

Biver, N., et al. 2006, A&A, 449, 1255

Bockelée-Morvan, D., Crovisier, J., Mumma, M. J., & Weaver, H. A. 2004, in Comets II, ed. M. C. Festou, H. A. Weaver, & H. U. Keller (Tucson: Univ. of Arizona), 391

Cochran, A. L., & Cochran, W. D. 2002, Icarus, 157, 297

Crovisier, J., & Bockelée-Morvan, D. 1999, Space Science Reviews, 90, 19

Crovisier, J., Bockelée-Morvan, D., Colom, P., Biver, N., Despois, D., & Lis, D. C. 2004, A&A, 418, 1141

Feldman, P. D. 2005, Physica Scripta, T119, 7

Feldman, P. D., Cochran, A. L., & Combi, M. R. 2004, in Comets II, ed. M. C. Festou, H. A. Weaver, & H. U. Keller (Tucson: Univ. of Arizona), 425

Feldman, P. D., Weaver, H. A., & Burgh, E. B. 2002, ApJ, 576, L91

Festou, M. C., Keller, H. U., & Weaver, H. A. 2004, Comets II (Tucson: Univ. of Arizona)

Herzberg, G. 1971, The spectra and structures of simple free radicals. an introduction to molecular spectroscopy (Ithaca: Cornell University Press)

Kawakita, H., Watanabe, J.-I., Furusho, R., Fuse, T., Capria, M. T., De Sanctis, M. C., & Cremonese, G. 2004, ApJ, 601, 1152

Kharchenko, V., & Dalgarno, A. 2001, ApJ, 554, L99

Krasnopolsky, V. A., Greenwood, J. B., & Stancil, P. C. 2004, Space Science Reviews, 113, 271

Lupu, R. E., France, K., & McCandliss, S. R. 2006, ApJ, in press

Mumma, M. J., Disanti, M. A., dello Russo, N., Magee-Sauer, K., Gibb, E., & Novak, R. 2003, Advances in Space Research, 31, 2563

Owen, T. C., & Bar-Nun, A. 2002, in ASP Conf. Ser. 269: The Evolving Sun and its Influence on Planetary Environments, ed. B. Montesinos, A. Gimenez, & E. F. Guinan, 163

Slanger, T. G., & Black, G. 1982, J. Chem. Phys., 77, 2432

Tachiev, G. I., & Froese Fischer, C. 2002, A&A, 385, 716

van Zee, R. D., Foltz, M. F., & Moore, C. B. 1993, J. Chem. Phys., 99, 1664

Vander Wal, R. L., Scott, J. L., Crim, F. F., Weide, K., & Schinke, R. 1991, J. Chem. Phys., 94, 3548

Weaver, H. A., A'Hearn, M. F., Arpigny, C., Combi, M. R., Feldman, P. D., Festou, M. C., & Tozzi, G.-P. 2004, BAAS, 36, 1120

Weaver, H. A., Feldman, P. D., Combi, M. R., Krasnopolsky, V., Lisse, C. M., & Shemansky, D. E. 2002, ApJ, 576, L95

Wehinger, P. A., Wyckoff, S., Herbig, G. H., Herzberg, G., & Lew, H. 1974, ApJ, 190, L43

Zhang, X., Rheinecker, J. L., & Bowman, J. M. 2005, J. Chem. Phys., 122, 4313