

Deep Space 1 encounter with Comet 19P/Borrelly: Ion composition measurements by the PEPE mass spectrometer

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[1] We report *in situ* ion mass spectrometer measurements from the coma of Comet 19P/Borrelly, obtained during the flyby of the Deep Space 1 spacecraft on 22 September 2001. Cometary ions were detected at distances from $\sim 5.5 \times 10^5$ km to 2200 km from the nucleus of the comet. The predominant heavy ions observed during the seven minute interval about closest approach to Borrelly included OH^+ (at 57% of the total water-group density), H_2O^+ (at 29%), O^+ (at 13%), CH_3^+ (at 5%), and CH_2^+ (at 4%). Of particular note is the small amount of H_3O^+ (<9%), as this was the most abundant molecular ion observed at closest approach to Comet Halley. This difference is due to the difference in water production rates between the two comets. **INDEX TERMS:** 6005 Planetology: Comets and Small Bodies: Atmospheres—composition and chemistry; 6025 Planetology: Comets and Small Bodies: Interactions with solar wind plasma and fields; 6008 Planetology: Comets and Small Bodies: Composition. **Citation:** Nordholt, J. E., et al., Deep Space 1 encounter with Comet 19P/Borrelly: Ion composition measurements by the PEPE mass spectrometer, *Geophys. Res. Lett.*, 30(9), 1465, doi:10.1029/2002GL016840, 2003.

1. Introduction

[2] On 22 September 2001, the NASA-JPL Deep Space 1 (DS1) spacecraft encountered Comet 19P/Borrelly (hereafter “Borrelly”), passing within 2171 km of the comet and at a distance of 1.36 AU from the Sun. DS1 is only the second mission to carry instrumentation capable of determining the composition of cometary plasma. The spacecraft carries two primary scientific instruments: MICAS (Miniature Integrated Camera and Spectrometer) [Soderblom *et al.*, 2002], and PEPE (Plasma Experiment for Planetary Exploration) [Young *et al.*, 2000]. PEPE is capable of resolving ion energy, angle of incidence, and mass composition. PEPE measurements of plasma densities and flow velocities in the Borrelly environment are described elsewhere [Young *et al.*, 2003]; here, we report the initial analysis of PEPE ion composition observations in the near-Borrelly environment.

[3] Comets are thought to be the most primitive objects in the solar system. As such, they preserve information

about the state of the primordial solar nebula. They are primarily composed of dust and volatiles such as water, carbon monoxide, and carbon dioxide, as well as complex hydrocarbons. Volatiles are not found in primitive form elsewhere in the inner solar system due to the heating and collisional processing of planetary material during the early solar system. Comets, however, spend most of their lives far from the Sun, devolving their volatiles only as they briefly warm near perihelion.

[4] Borrelly (orbital period 7 years, perihelion of 1.36 AU, orbital inclination $\sim 30^\circ$) is a member of the Jupiter family of comets, which have histories significantly different from the Halley family. They are thought to have originated as long-period comets, but successive interactions with the strong gravitational field of Jupiter have pulled them into short-period orbits of less than 10 years. Because they have spent much more time in the warm near-Sun environment, Jupiter family comets evolve much more quickly than Halley-family comets, which spend most of their time far beyond Jupiter’s orbit. Therefore, the composition of Jupiter-family comets may be significantly different from Halley-family comets. Earth-based observations show that both the Halley and Jupiter cometary families have similar ratios of water and ammonia, but that many Jupiter-family comets are depleted in carbon chain molecules relative to the Halley family. Borrelly is an intermediate activity comet with a water production rate near perihelion of $Q_{\text{H}_2\text{O}} \sim 3.5 \times 10^{28}/\text{s}$ [Stern *et al.*, 2002]. This is comparable to the production rate of Giacobini-Zinner ($Q_{\text{H}_2\text{O}} \sim 5 \times 10^{28}/\text{s}$), but stands in contrast to highly active comets like Halley ($Q_{\text{H}_2\text{O}} \sim 10^{30}/\text{s}$), and to relatively quiescent comets such as Gregg-Skjellerup ($Q_{\text{H}_2\text{O}} \sim 7 \times 10^{27}/\text{s}$).

2. Description of the PEPE Instrument

[5] The miniaturized mass analyzer included in PEPE is a time-of-flight (TOF) mass spectrometer capable of determining the mass-per-charge (M/Q) of plasma ions by both conventional TOF analysis and by linear electric field (LEF) TOF analysis [McComas and Nordholt, 1990; McComas *et al.*, 1990]. The LEF mode, in which the ion TOF is approximately independent of energy and charge, was designed with a mass resolution $(M/Q)/\Delta(M/Q) \sim 20$, where M and Q are the ion mass and charge, respectively. This mode allows relatively high mass resolution analysis of that portion of the ions that pass through the thin carbon foil at the entrance of the PEPE TOF section and retain their initial positive charge. The fraction of ions exiting the foil positively charged is an increasing function of the incident ion energy. Under normal operation, a -15 kV potential is used

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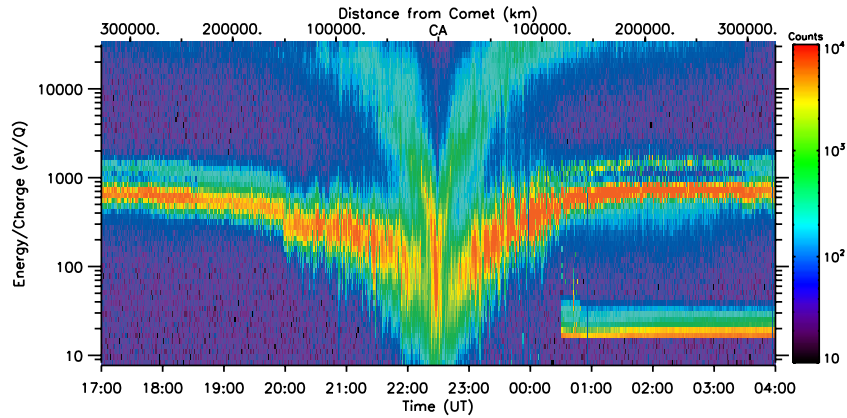


Figure 1. A spectrogram of ion energy/charge summed over all viewing angles versus time from PEPE during the DS1 encounter with Comet P19/Borrelly.

to accelerate ions into the foil for this very reason. During the Borrelly encounter, it was necessary to operate the spectrometer at the reduced voltage of -11 kV, resulting in a significantly reduced positive-ion yield. PEPE analyzes the incident ions that exit the foil as neutrals or negative ions using a conventional mode in which spectra are functions of both the ion energy and mass; this mode has a lower resolution, $(M/Q)/\Delta(M/Q) \sim 10$, and this was the mass peak resolution achieved during encounter.

[6] The PEPE energy-per-charge (E/Q) range is 8 eV to 33.5 keV, sampled in 120 logarithmically spaced steps every 65.5 seconds, with an energy resolution ($\Delta E/E$) of 5% . PEPE utilizes a top-hat design using angular deflectors with a total field-of-view covering a solid angle of 2.8π steradians, continuously sampling 360° in the azimuthal direction around the analyzer axis, and sweeping through ± 45 degrees in the instrument elevation direction.

3. The Borrelly Encounter

[7] PEPE made both electron and ion measurements in the environment of Comet Borrelly; here we primarily address measurements of ions heavier than protons. Figure 1 shows an overview of PEPE ion observations during the encounter. The colors represent intensity of counts as functions of E/Q and time over the full range of PEPE energy levels and summed over all angles. Far from the comet, the solar wind protons (lower horizontal band at ~ 700 eV/q on both the left and right sides of the figure) and alpha particles (upper horizontal band at about 1.4 keV/q) showed relatively undisturbed flow of ~ 370 km/s. PEPE detected heavy ions of cometary origin from $\sim 13:15$ to $\sim 6:45$ UT on 23 September, corresponding to spacecraft-comet distances of $r = 5.5 \times 10^5$ and 4.9×10^5 km, respectively.

[8] In cometary environments, the heavy ion component is dominated by water group ions (O^+ , OH^+ , H_2O^+ , H_3O^+) formed from cometary gas by photoionization, charge exchange, and ion-neutral reactions. Once ionized, the ions are accelerated (“picked up”) by the $\mathbf{v} \times \mathbf{B}$ field of the solar wind, initially forming a ring/beam velocity distribution relative to the solar wind ions. Assuming a Parker spiral magnetic field geometry and using the measured solar wind speed, we estimate maximum pick-up energies from 31 keV for O^+ to 37 keV for H_3O^+ . Figure 1 shows that, far

from the comet, PEPE indeed observed ions up to the high-energy cutoff of the instrument, 33.5 keV. These are most likely O^+ ions, since at this distance the water-group ions are expected to be almost fully photo-dissociated. As the cometary ion density began to increase ($20:00$ UT), the pickup process slowed both the solar wind and cometary ion components until at closest approach ($22:29:33$ UT) the flow speeds were reduced to ~ 30 km/s. At closest approach, the solar wind protons and alphas all but disappear. As noted by *Young et al.* [2003], the distance of closest approach does not correspond to the ion density peak, which occurs 2 minutes before closest approach. *Young et al.* suggested that this is associated with a jet observed by MICAS [*Soderblom et al.*, 2002] that DS1 would have likely intercepted before closest approach. Figure 1 also shows a low energy band of ions (from ~ 15 eV to ~ 35 eV) starting after the encounter at about $00:30$ UT. These are Xe ions from the DS1 ion thruster, which was turned on at this time.

[9] PEPE observed He^+ , first detected above background at $21:37$ UT, or $r = 5.3 \times 10^4$ km. It appeared at the same energy (that is, at twice E/Q) as solar wind He^{++} ; presumably generated by charge transfer of solar wind He^{++} with cometary gases. The He^+ signal persisted at least until $23:15$ UT ($r = 4.5 \times 10^4$ km), but then became overwhelmed by the elevated detector background that arose due to higher pressure inside the detector following the encounter.

[10] Figure 2 depicts a portion of the time-of-flight spectrum (red dots) measured by PEPE during the 7 minutes centered on the time of the peak ion density observation. This corresponds to a $r = 6000$ km = 2171 km, the distance of closest approach, with the peak density occurring at 3000 km. The channels shown here, $150 = 450$, correspond to atomic and molecular ions of masses 12 through 28 amu. Two large peaks, at channels $210-250$ and $300-360$ respectively, dominate the spectrum. Each peak is a superposition of the water group ion mass ($16-19$ amu) peaks; the mass resolution of the instrument as operated at the encounter was too low to resolve the individual water group masses. The left-hand peak is formed by negative O ions exiting the foil as a result of the molecular dissociation and charge conversion within the foil of incident water group ions, and the right-hand peak is due to neutral O produced by the same mechanism. The fact that the parent molecules

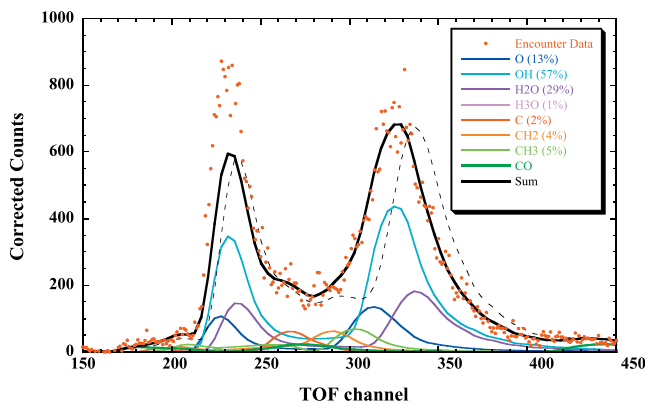


Figure 2. Initial analysis of PEPE time-of-flight spectra from channels 150 = 450 during the seven minutes of peak ion density ($2000 \text{ km} < r < 6000 \text{ km}$). The red points are the encounter TOF counts corrected for instrument noise. The solid black line is the total TOF count spectrum from the instrument simulation. All other curves represent simulated counts of incident ionic species as labeled. Two dominant peaks are apparent. This is because singly-charged positive atomic and molecular ions which enter PEPE are converted to negative, neutral, and positive atomic ions, resulting in multiple peaks for each incident ion; here the left-hand peaks for each species are due to negative ions, and the right-hand peaks are due primarily to neutralized ions. The ion simulations consisted of two steps. The first step was to compute the molecular and atomic ion interactions with the thin (80 \AA) carbon entrance foil. Second, the resulting energy and angular straggling distributions were used as input to a 3D instrument simulation. Trajectories ($n = 200,000$) of each species (C^+ , CH^+ , CH_2^+ , CH_3^+ , CO^+ , N^+ , O^+ , OH^+ , H_2O^+ , H_3O^+) were simulated using Monte Carlo techniques. The simulation's accuracy was verified via comparison of the computation output to laboratory calibration data. To determine detection efficiencies, the distributions were then weighted by empirical data on the fraction of each fragment species exiting the foil as negative, neutral, and positive atomic ions. These results were then used to fit the encounter data curve via a χ^2 -minimization technique, permitting us to determine the relative ion abundances. The dashed line represents a synthetic instrument response computed from a modeled mass spectrum (see text for details).

dissociate in the foil is not a concern for purposes of molecular mass identification. This is because the exit fragments have the same velocity as the incident parent molecule; thus they appear in the TOF spectrum at locations corresponding to the parent molecular masses. Although individual mass peaks cannot be resolved, we can calculate the spectrum through use of laboratory calibration data and instrument simulations. In this way, we can infer the abundances of the different parent molecular ions required to create the observed TOF spectrum. This procedure is described in the Figure 2 caption.

[11] Our initial ion abundance determinations are shown in Table 1, determined using a χ^2 -minimization technique. The fitting procedure excludes data in the core of the O^- peak (channels 211–249) because in the particular case

of oxygen, the relative exit yield of negative ions versus neutrals from the foil is quite sensitive to the thickness of the foil and to possible chemical changes in the foil since the launch of the spacecraft with an estimated uncertainty of about $\pm 25\%$.

[12] The dominant coma constituents in Table 1 are O^+ , OH^+ , and H_2O^+ , at 13%, 57%, and 29% of the total water group fraction, respectively. At these distances from the comet, H_3O^+ contributes only 1% although the uncertainty allows an upper limit of about 9%. Our calculations indicate that carbon-containing molecules (CH_n^+) also contribute significantly to the spectrum, with CH_3^+ being the most abundant, whereas N^+ does not. The instrument is capable of distinguishing between the two 14 amu species N^+ and CH_2^+ because carbon can exit the foil as a negative ion (contributing to the negative-ion signal at channel ~ 195), whereas nitrogen, or nitrogen bearing molecules, cannot. Ammonia products (NH_n^+), in the range 15–18 amu apparently do not contribute at detectable levels to the data, and we have not included them in the fit. Their inclusion would reduce the size of the simulated negative ion peak (channels 211–249) relative to the computed neutral peak (channels 300–370), further increasing the discrepancy with the observations. As it stands, the size of the simulated negative ion peak is already at the edge of the acceptance limit. The abundances reported here are only for the period around the peak ion density observation. In future work we intend to determine the composition variations as a function of encounter distance.

[13] It is important to point out that PEPE has significantly different sensitivities to different species, as the instrument response decreases as ion mass increases, due to increased angular scattering and energy straggling in the foil for higher mass ions. Thus, for example, simulations in combination with laboratory data show that the detection efficiency for C^+ is 3 times greater than for O^+ . Although the contribution of CH_n^+ to the fit is small compared to the contribution from the water group, the fit is much more sensitive to these minor species, and hence it is possible to constrain their abundances reasonably well in spite of the fact they are not well resolved in the spectrum. This also explains why, as shown in Table 1, the stated uncertainties tend to increase with mass.

[14] The instrument response becomes substantially diminished for heavy molecular ions such as CO^+ and CS^+ . Thus, for example, the detection efficiency for CO^+ is 12 times less than for O^+ . As a consequence it is difficult to do more than place upper limits on the abundance of

Table 1. Ion Composition From Coma of Comet Borrelly Over 2171–6000 km

Atomic Mass	Ion Species	Abundance ^a		
12	C^+	0.019	\pm	0.005 ^b
13	CH^+	<0.023		
14	N^+	<0.046		
	CH_2^+	0.036		0.010
15	CH_3^+	0.052		0.020
16	O^+	0.131		0.041
17	OH^+	0.566		0.087
18	H_2O^+	0.293		0.111
19	H_3O^+	0.010		0.078

^aNormalized to total water group abundance (16–19 amu).

^bUncertainties and upper bounds quoted at the 90% confidence level.

heavy molecular ions that have been observed in previous cometary encounters [Balsiger et al., 1986; Neugebauer et al., 1991]. For CO^+ , our preliminary upper limit is $\sim 20\%$. We have not yet attempted to fit heavier molecular species, although there is a significant count rate in TOF channels 400 through 600; this corresponds to ion masses between 28 and 100, and occurs at solar wind pickup energies corresponding to masses heavier than water group ions. Analysis of this mass range is planned for the future, after a more detailed laboratory calibration is performed.

4. Discussion

[15] Observations from the Giotto flyby of comet Halley [Balsiger et al., 1986; Coates et al., 1989; Altwegg et al., 1993] showed that water-group ions were the predominant heavy ion in that cometary environment. Furthermore, while H_3O^+ was the most dense such ion from closest approach at 710 km out to about 20,000 km, at intermediate distances H_2O^+ and OH^+ were dominant, and beyond $\sim 10^5$ km, O^+ was the most dense water-group ion [Balsiger et al., 1986]. These observations are consistent with production of H_3O^+ due to molecular collisions between H_2O and H_2O^+ close to the nucleus, and with progressive photodissociation as the molecules traveled outward from the nucleus. The PEPE observations also show water-group ions to be the predominant heavy ion constituents in the Borrelly environment but, in contrast to the Halley data, show very little H_3O^+ near closest approach. This is to be expected since (1) the photo-ionization rate near Borrelly during the encounter (at 1.36 AU) should be lower than that during the Halley encounter (at 0.9 AU) since the solar UV flux was smaller by over a factor of 2, and (2) the activity level of Borrelly was about 30 times lower than observed at Halley.

[16] Our PEPE results were compared with a model of cometary environments that considered dusty, multifluid flow, detailed photolytic and gas-phase chemistry, transition to free molecular flow, and solar wind interaction [e.g., Benkhoff and Boice, 1996]. The volatile composition was estimated to be similar to Halley, adjusted to reflect depletions in C-chain molecules. The MHD model contains detailed chemistry for 82 ions and 69 neutrals, coupled by 871 reactions, and is axisymmetric about the comet-sun axis, so model results do not reflect the offset of peak ion abundance observed by DS1. The model, integrated along the spacecraft trajectory inside 6000 km from Borrelly, predicts abundances of water-related ions (O^+ , OH^+ , H_2O^+ , and H_3O^+) to be 1, 7, 82, and 10% of the total water-related fraction, respectively [Boice, Private Communication, 2002]. While decreased cometary activity and increased UV flux relative to Halley have been taken into account, the model results still differ from Table 1 by predicting higher hydrogen abundances in the water-group ions. We have computed a synthetic instrument response to the modeled water-group ion percentages stated above; the result is shown as a dashed line in Figure 2 and is clearly different from the observed mass spectrum. We intend to pursue and, if possible, to resolve this apparent discrepancy between the model and our observations.

[17] The minor peaks from 12 to 15 amu at Borrelly show a fairly similar composition to Halley. We see little or no N^+ and CH^+ , and small but measurable amounts of C^+ , CH_2^+

and CH_3^+ . The 5% CH_3^+ abundance is comparable to what was observed at Halley at closest approach [Altwegg et al., 1994]; thus our PEPE data confirms a relatively high CH_3^+ abundance in cometary environments. However, it is interesting that the abundance of CH_3^+ is elevated in spite of the relative absence of H_3O^+ . This is puzzling because CH_3^+ and H_3O^+ are postulated to be produced by collisions of H_2O with CH_2^+ and H_2O^+ , respectively, in the cometary environment at Halley [Altwegg et al., 1994]. In the absence of a similarly high H_3O^+ abundance, the origin of cometary CH_3^+ at Borrelly should be re-examined. Thus interpreting the presence of this ion is critical for understanding the differences between Halley-class and Jupiter-class comets specifically and the history of cometary volatiles in general.

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