A statistical comparison of the outflow of N_2^+ , NO^+ and O_2^+ molecular ions with that of atomic O^+ ions using Polar/TIMAS observations

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Abstract - Ion composition data from the first 22 months of operation (until the end of 1997) of the Polar/TIMAS instrument, covering the 15-eV/e to 33-keV/e energy range, have been surveyed to determine the typical abundance of N_2^+ , NO^+ and O_2^+ ions as a group ($M/Q \sim 30$) in the auroral ion outflow, as compared to that of the better known O^+ ions. The results, obtained at and near solar minimum, indicate that molecular ions have roughly the same energy distribution as the O^+ ions, with maximum differential flux occurring below 400 eV, but are far less abundant, by two orders of magnitude on average. The molecular ions also differ from the O^+ ions in that they seem more specifically associated with enhanced geomagnetic activity, possibly with some electrodynamic threshold being surpassed in the ionosphere. The most intense fluxes of molecular ions, 10^5 - 10^6 (cm² sec ster keV/e)⁻¹, are usually encountered near the Polar perigee in the southern auroral zone (at $R \sim 2$ R_E), but the longer lasting encounters, 30 min or more, are closer to the Polar apogee in the northern hemisphere, often well inside the polar cap (at $R \sim 4$ -9 R_E). The molecular ions are observed at varying local time but too infrequently to yield a significant measure of local time distribution.

INTRODUCTION

Since the discovery almost three decades ago (Shelley *et al.*, 1972) that singly charged atomic oxygen with keV energies is a large component of Earth's energetic plasma environment, O^+ ions have come to symbolize, more than any other ions, the strong and complex electrodynamic interaction between the solar wind and Earth's ionosphere. The focus on O^+ ions has been justified both by their great abundance and by their virtually certain terrestrial origin (e.g. Young *et al.*, 1982). However, with spaceborne ion mass spectrometers becoming increasingly sophisticated, the study of ionospheric ion outflow is beginning to include less abundant species, in particular the molecular N_2^+ , NO^+ and O_2^+ ions (e.g. Craven *et al.*, 1985; Klecker *et al.*, 1986; Yau *et al.*, 1993; Christon *et al.*, 1994; Peterson *et al.*, 1994; Wilson and Craven, 1998 and 1999). These molecular ions do provide a vital link in the magnetosphere-ionosphere coupling, being the principal carriers of Pedersen current (e.g. Hanson, 1965; Johnson, 1966), but they are chemically less stable than O^+ ions and therefore likely to contribute less to the ion outflow. On the other hand, when they are observed, they may be a more sensitive indicator of certain electrodynamic processes (Wilson and Craven, 1998 and 1999).

This paper reports on a statistical study of N_2^+ , NO^+ and O_2^+ ions using one of the latest generation instruments, one flown on the NASA GGS/Polar satellite called TIMAS. The focus here is on the overall abundance of these ions as a group, that is ions with $M/Q \sim 30$, in the ionospheric outflows, rather than the variables of specific events. Because the instrument monitors the entire M/Q range (from 1 to well beyond 32) continually at each E/Q, it is possible to make an essentially one-to-one comparison between this group and the well known O^+ component.

The reason for including O⁺ ions in this study is twofold: Because their statistical properties are already extensively documented from various parts of the magnetosphere, they do provide a global perspective

on the other terrestrial ions that are observed along the Polar orbit. In addition, having new O^+ data collected alongside the molecular ion data allows a more authentic measure of the relative abundance of the two groups of ions, since any sampling bias introduced in the molecular ion data by the operation of the TIMAS instrument, or by the shape of the Polar orbit, is likely to be the same, or very nearly the same, in the accompanying O^+ data.

THE TIMAS INSTRUMENT

The Toroidal Imaging Mass-Angle Spectrograph, or TIMAS, on the GGS Polar satellite (Shelley *et al.*, 1995) combines magnetic mass analysis with simultaneous recording of all species (all M/Q) and a nearly omnidirectional field of view. This is accomplished by accepting ions within a 10° by nearly 360° wide window and, following the energy selection, magnetically dispersing them radially on an annular detector (MCP) with position-sensitive wedge and strip anode. The total field of view scanned over the course of each 6-sec Polar spin cycle is 98% of the full 4π . The energy range is 15 eV/e to 33 keV/e, covered in 28 channels, of which the 14 even-numbered channels are used on even-numbered spins, and the 14 odd-numbered ones on odd spins. Each set of 14 channels (plus a pure background sampling) is swept 16 times per spin.

Data are partially processed onboard by binning and summing the detector counts into various arrays, in accordance with energy channel and view direction. These data arrays include 48 separate 64-step mass spectra, sorted by 8 selected energies, or energy bins, and 6 view angles. The angular bins used for mass spectra are roughly 90° by 90° solid angles centered on the despun Polar x-, y- and z-axes (parallel and antiparallel). Unlike the other data arrays, mass spectra are always summed over multiple spin cycles, often as many as 32.

The Polar satellite, with perigee and apogee at 1.9 and 9.0 $R_{\rm E}$ (geocentric), respectively, carries the TIMAS instrument through the auroral regions four times each 17.6-hour orbital revolution, at altitudes near perigee in the southern hemisphere (when these data were acquired) and at some 4 to 8 $R_{\rm E}$ in the northern hemisphere.

ILLUSTRATIVE EVENT

The upper panel of Figure 1 shows a somewhat extreme TIMAS recording of molecular ions (tallest peak), this one obtained inside the southern polar cap, but it illustrates the type of information contained in each set of 6 mass spectra of a given energy range, in this case the lowest four energy channels combined. The time label refers to the time of extraction of counts from a previously filled mass spectra buffer (two buffers alternating between accumulation and transmission), in this case about 6 s after the end of a 3.2-min (32-spin) accumulation interval. The counts are sorted by M/Q on a partially energy-dependent integer 64-bin scale, with mass increasing toward higher bin number. The $M/Q \le 32$ range is confined to the lower 2/3 of this scale for external $E/Q \le 364$ eV/e (lowest 8 energy channels) and held fixed by internal voltage adjustments. For higher external energies the M/Q scale is allowed to slide to higher bin number (reduced magnetic deflection; inward radial shift on detector), and the position of $M/Q \sim 30$ moves beyond bin number 50 at $E/Q \sim 30$ keV/e.

The peak counts at mass bin 34 in the upper panel of Figure 1 are extreme in four aspects: (1) The corresponding differential flux, about 7×10^6 (cm² sec ster keV/e)⁻¹ (averaged over about two steradians), is exceptionally large for molecular ions, (2) the counts are almost entirely confined to a single view direction (to within about 90° by 90° field of view), (3) the molecular ions are the dominant ion compo-

nent (virtually no ions at E/Q > 110 eV/e at this time), and (4) these molecular ions appear to be a single species, namely N_2^+ . Based on pre-flight calibration with certain other ions, it is expected that N_2^+ , NO^+ and O_2^+ ions in Figure 1 should appear, in terms of decimal centroids, at mass bins 34.4, 34.9 and 35.4, respectively. The symmetry and location of the main peak are thus best explained by N_2^+ ions alone. The geomagnetic Kp index at this time is 4, and its preceding four values (spanning 12 hours) were 3-, 3-, 3, and 3+, respectively.

The lower panel of Figure 1 shows more normal mass spectra, obtained 16 minutes later, well equatorward (by about 17° invariant latitude) and at greater altitude (by almost 2000 km). At this time there are, from left to right, H^+ , He^+ and O^+ ions in all 6 view directions at $E/Q \le 110 \, \mathrm{eV}/e$, and at least H^+ ions at all energies up to and beyond 25 keV/e (not shown), but the molecular ions have essentially vanished. The detector background counts, generated by penetrating energetic (MeV) electrons, are elevated about tenfold by now, because of the lower latitude, but not yet to the levels found in the radiation belts proper. It may be noted that the background is also a function of mass bin, albeit a rather smooth function, mainly because the MCP surface area associated with each bin varies with radial position in any given anode wedge.

As far as the statistical survey is concerned, the result of penetrating radiation is to reduce the effective daily observation time available for molecular ions by from several minutes to as much as four hours, depending on the size and intensity of the radiation belts. The effect is less on the O^+ observation time, owing to the generally greater flux of O^+ ions, but the resulting bias is modest and not relevant to the final conclusions.

Fig. 1. Top: Mass spectra in 6 view directions, one line each, at $E/Q \le 110 \text{ eV/}e$, recorded near the Polar perigee (~1.9 R_E) at about 80° invariant latitude and 0900 MLT. The solid line view direction is centered on the despun s/c x-axis. Bottom: Same but five accumulation periods later, at about 63° invariant latitude and 0900 MLT (see text for ion identification).

STATISTICAL SURVEY

The principal TIMAS data for this study have been the mass spectra, all summed over 32 spin cycles, either onboard (most commonly) or by a combination of onboard and ground processing. With the emphasis being placed on detection of molecular ions, rather than on detailed analysis of events, the spectra have been further summed on the ground over the 6 different view directions at each energy, so as to maximize the number of counts of an ion population that is expected (and found) to have mostly rather low density. It is presumed that all ions with M/Q in the 28- to 32-range are singly charged molecular ions $(N_2^+, NO^+ \text{ or } O_2^+)$ of terrestrial origin. The actual angular distribution has been found to agree, roughly, with a terrestrial source in all cases examined in some detail, although it may extend over several of the 6 solid angles at any one time.

For the most part, the mass spectra have been analyzed visually with the help of high-quality printouts of color-coded 24-hour plots of count rates versus time and mass step at each of 8 energies. This method allows clear separation of $M/Q \sim 30$ from M/Q = 16, for energies below 5 keV/e, at least, but does not generally allow N_2^+ , NO^+ and O_2^+ ions to be separated from each other. Gif file versions (of reduced image quality) can be found on the TIMAS WWW home page (ftp://timas.spasci.com/timas/survey_plots).

The color coding on these plots is such that a barely visible trace at low count rates corresponds fairly closely to the 3- σ level of Poisson statistics, that is 10 counts per 32-spin accumulation (per pixel). Due to residual weak detector background even far outside of Earth's radiation belts, it has proved necessary, however, to define the minimum "significant" count level about three times higher, or 30 counts per 32 spins. In a typical case, with the molecular ions essentially confined to the lowest energy bin (see below), this 30-count limit corresponds to a minimum detectable number density at $M/Q \sim 30$ of about 0.01 cm⁻³ and a flux of 1.5×10^4 (cm² sec ster keV/e)⁻¹ (averaged over 4π). The count rate of O⁺ ions, being the standard reference, has been recorded continually along with that of molecular ions. In the numerous cases where the O⁺ rate saturates the color coding (no saturation with molecular ions), actual numbers have been obtained from the raw data. Table 1 summarizes the known confines of this study.

Table_1.	Confines of Statistical Study
Ion energy range:	15 eV/e (+ s/c potential) to 33 keV/e
Time resolution:	3.2 minutes (32 spins)
Field of view:	98% of 4π (per spin)
Time span:	16 March 1996 through 31 December 1997
Total sampling time:	14,887 hours (95% coverage)
Average daily Σ Kp:	14-
Solar cycle phase:	passing through minimum

The sampling time in Table 1 refers, strictly speaking, to the O^+ ions and excludes actual data gaps as well as those periods within the radiation belts (~1 hour or less each) when it appears that the O^+ signal is obscured by a strongly elevated detector background count rate, BCR, because the O^+ is clearly present on either side at count rates < BCR. In principle, this sampling time may still include periods when otherwise significant molecular ion fluxes are obscured by elevated background, but that does not appear very likely, since the count rates of both the O^+ and the molecular ions tend to peak well poleward of the radiation belts. In any case, the effective coverage for molecular ion detection is at least about 85%.

It is worth noting that the nominal lower end of the TIMAS energy range, 15 eV/e, falls below the minimum energy of escaping N_2^+ , NO^+ and O_2^+ ions at the Polar perigee, since the escape energy of N_2^+ ions, the lightest ones, is 10 eV at that altitude (0.9 R_E), and this energy, associated with upward motion, is added to the instrumental ram energy of 8 eV, associated with horizontal s/c motion. Although the

small surplus energy of 3 eV is often offset by a few volt positive s/c charging, it seems probable that a majority of escaping ions have more than the bare minimum energy and are therefore "visible" when present in statistically significant numbers.

RESULTS

Table 2 shows the overall occurrence rate of the molecular ions in relation to that of the O^+ ions. In this table the daily Σ Kp has been given a relative weight proportional to the length of time ions were present each day. The daily peak flux usually occurred in the southern auroral zone, at the closest approach to the terrestrial ion source. It is an average over the 3.2-min sampling, that is a spatial average across some 1400 km near perigee, and is an angular average over nearly 4π . The true differential flux may have reached substantially larger values along the upward magnetic field direction. In cases where the angularly averaged O^+ count rate saturates the color coding on the plots, for instance, examination of the raw O^+ data shows typically 2-4 times larger peak count rates among the 6 separated view directions.

Table 2. Comparison of Molecular Ions as a Group With the O⁺ Ions

	N_2^+ , NO^+ and O_2^+	$\overline{\mathbf{O}}^{+}$
At or above level of detection, in hours:	86.7 hrs	8,828 hrs
and in fraction of samplings:	< 1%	59%
Associated weighted daily Σ Kp:	22+	14+
Energy at daily peak flux, mostly:	$15 \text{ eV} \le E \le 110 \text{ eV}$	$15 \text{ eV} \le E \le 110 \text{ eV}$
and always:	$E \le 364 \text{ eV}$	$E \le 364 \text{ eV}$
Typical daily peak flux;	_	_
4π average in (cm ² sec ster keV) ⁻¹ :	$(1.3 \pm 0.6) \times 10^5$	$(1.0 \pm 0.5) \times 10^7$

Table 3 elaborates on the geomagnetic aspect. The average daily Σ Kp is unweighted here but is restricted to those days which had at least the required minimum ion abundance. Peak O⁺ fluxes exceeding 10^7 all occurred in the southern auroral zone.

Table 3. Average Daily ΣKp With Occurrence Rates at or Above Specified Limits

	N_2^+ , NO^+ and O_2^+	O ⁺
At or above level of detection, at least		
30 minutes /day:	27	14-
1 hour /day:	27-	14-
20 hours /day:	never	18-
Daily peak flux $> 10^7 \text{ (cm}^2 \text{ sec ster keV)}^{-1}$;		
4π average (typically $n > 5$ cm ⁻³ for O ⁺)	never	19-

The 30-minute limit on molecular ion detection was met or exceeded on 32 days in all. None of those were among the "Ten Quietest" days Q1-Q10 of each month (Coffey, 1996, and subsequent reports; see also Mayaud, 1980), but 6 were days with only modest activity. All of the other 26 days were among the "Five Most Disturbed" days of their respective month, D1-D5 (Coffey, 1996; Mayaud, 1980), and 8 were the single most disturbed day D1 of its month. Some of the longest cumulative encounters with molecular ions did take place on the most disturbed day or sequence of days, but others did not. For example, days 22 and 23 of November 1997, with Σ Kp = 37 and 38 and classified as D2 and D1, respectively, had about 1.8 and 2.7 hours of significant molecular ion flux, respectively, suggesting a strong geomagnetic link

and even a gradual buildup over time, but days 28 and 29 of March 1997, with $\Sigma Kp = 21+$ and 27- and also classified as D2 and D1, respectively, had about 1.3 hours and only 15 minutes, respectively, breaking with that trend.

The most prolonged detection of molecular ions, a total of 4.7 hours, took place on April 21, 1997, a day with $\Sigma Kp = 22+$ and classified as D3. By comparison, the most disturbed day D1 of that same month, April 11 with $\Sigma Kp = 33-$, yielded less than half, or 1.9 hours. On both days the molecular ions appeared during some of the most active hours, between about 19:00 UT and 24:00 UT on April 21 and between 03:00 UT and 05:00 UT on April 11. This follows a general trend: If molecular ions appear along the Polar orbit on a given day, they tend to do so during the most disturbed part of that day. However, this correlation begins to break down at the level of individual 3-hour Kp indices, perhaps in part because of the shape of the Polar orbit, and the size of Kp is not a sure predictor of the length of ion detection.

In Figure 2 the occurrence of significant ion count rates is subdivided by months and plotted along with the monthly sunspot numbers and geomagnetic Ap indices.

Fig. 2. Average daily occurrence by month of molecular ions (solid line) and O⁺ ions (dots and dashes), along with the monthly sunspot numbers (long dashes) and Ap (short dashes), all on the same scale.

Although the molecular ions, when observed at all, usually had their daily peak flux in the southern auroral zone at $R \sim 2$ R_E, like the O⁺ ions (Table 2), they were found at all altitudes along the Polar orbit, sometimes around apogee at 9 R_E. In fact, most of the detection time referred to in Table 3 was met above the northern auroral zone and polar cap, at R > 4 R_E, which is where the Polar satellite spent 80% of the time. As far as their local-time distribution is concerned, these data are inconclusive. The ions were found marginally more often at some local times, but that is likely to have been coincidental and caused by increased geomagnetic activity. For example, three of the occurrence peaks in Figure 2, centered about the months of October 1996 and 1997 and April 1997, coincide with times when the Polar orbit is near the noon-midnight plane, where several extended observations were made, but they also coincide with local maxima in the Ap index. A fourth peak in Figure 2, about January 1997, coincides with orbits near

the dawn-dusk plane, where other extended observations were made, but also with another local maximum in the Ap. By comparison, in July 1997, when the orbit is again near the dawn-dusk plane, Figure 2 shows reduced occurrence and a minimum in the Ap.

CONCLUSIONS

Possibly the single most striking result above is the rarity of molecular ions in comparison with the virtual omnipresence of the O⁺ ions. The rather limited literature on molecular ion outflow acknowledges that these ions are a minor component of the total auroral ion outflow, but the previous emphasis on specific events might give the impression that these ions are somewhat more commonplace. Being that the magnetospheric content of O⁺ ions is positively correlated with solar activity, that is with the EUV radiation level (e.g. Young *et al.*, 1982), the strong presence of O⁺ ions in these data, taken at and near solar minimum, implies that the adopted limit for "significant" ion counts is indeed low and favorable for the detection of those ions and probably favorable for the detection of molecular ions, as well, since the two groups are counted at nearby positions on the TIMAS detector.

As expected, the daily occurrence of O⁺ ions in Figure 2 does suggest some long-term increase after solar minimum in May 1996, but some part of that may be due to the mass spectra collection being altered at the beginning of September 1996, in effect doubling the sensitivity at low energy. The occurrence of molecular ions is far too variable to allow an inference with respect to long-term trends this early in solar cycle 23.

The O⁺ and the molecular ions both show the influence of geomagnetic activity, as indicated in Table 3, for instance, but this effect seems significantly stronger with the molecular ions. In particular, in Figure 2 the monthly variation in the molecular ion occurrence is consistently in phase with the monthly Ap, sometimes vastly magnifying the variation in the Ap, whereas the O⁺ occurrence is partially out of phase. The peak occurrence rates of the molecular ions in Figure 2 reflect the contribution from relatively few days with exceptional abundance (30 min or more), measured mostly at high altitude above the northern auroral zone and polar cap (where Polar spent the most time), which may indicate that some ionospheric condition must reach beyond a threshold before the outflow of these ions becomes substantial (cf. Wilson and Craven, 1998 and 1999).

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