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Cometary X-Rays: Line Emission Cross Sections for Multiply Charged Solar Wind Ion Charge Exchange.

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Absolute line emission cross sections are presented for 1 keV/amu charge exchange collisions of multiply charged solar wind ions with H₂O, H, O, CO₂, and CO cometary targets. The present calculations are contrasted with available laboratory data. A parameter-free model is used to successfully predict the recently observed x-ray spectra of comet C/LINEAR 1999 S4. We show that the resulting spectrum is extremely sensitive to the time variations of the solar wind composition. Our results suggest that orbiting x-ray satellites may be a viable way to predict the solar wind intensities and composition on the Earth many hours before the ions reach the earth.

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State-selective single electron capture cross sections for highly stripped multiply charged ions colliding with atoms and molecules are of particular importance not only in basic atomic physics research, but have direct applications to magnetic fusion plasma diagnostics [1–3], to heliospherical and planetary science, [4–6], and to astrophysical observations [7, 8]. In general, such reactions lead to an excited ion which decays via photon emission.

Motivation for the present work is provided by recent observations of x-ray emission from comets as they transit our solar system. In 1996 the Röntgen satellite (ROSAT) focused on the comet P/Hyakutake and observed x-ray emission of unexpected intensity between the comet and the Sun, out to a distance on the order of 10⁶ km from the comets nucleus [9]. It is now recognized that this emission is due to electron capture between heavy solar wind ions and the gas surrounding the comet [10, 11].

Since solar wind events on the comet and the Earth can be subject to a delay determined by the difference in the speed of light versus that of the solar wind ions, the measurement of x-ray emission from a comet that is situated inside the orbit of the Earth provides warning of the solar wind ion intensity and composition many hours in advance of these ions' arrival. In this sense, the observation of cometary x-ray emission by earth orbiting satellites can be used as solar wind weather stations. It is well known that solar wind bursts can impact computer operation by generating "phantom commands" from upsets in the memory chips. Other deleterious effects can impact astronauts' health and cause degradation of communication and the global positioning system. Moreover, since solar wind bursts induce current in long conductors on the ground, they can cause blackouts over major areas, as occurred, for example, in southern Canada and the eastern US in 1989 [12].

To date, astrophysical models for the electron capture reactions have assumed an equal population of the l -values, or statistical populations [10, 13, 14]. There is

also a model based on Landau-Zener calculations where the l -values are adjusted to reproduce available data [15]. Other analyses have fit the measurements of the Chandra X-ray Observatory (CXO) by means of six to nine emissions, adjusting their positions and intensities [11, 16, 17].

Initially, analyses have been based on low resolution laboratory data available for the reactants and collision energies encountered in comet x-ray emission [18, 19]. However, for hydrogenic projectiles one must be careful to recognize that the $2^3S \rightarrow 1^1S$ transition in the helium-like product ion, which will represent about 50 % of the x-ray emission in these systems for comets, is incompletely observed in beam measurements due to their long $\sim 10^{-3}$ sec 2^3S lifetime. More recently, laboratory work performed at EBIT with an x-ray micro-calorimeter spectrometer (XRS) provides spectra with an unprecedented ~ 10 eV FWHM resolution [20]. These x-ray spectra are useful as critical benchmarks of theoretical models, and include the forbidden triplet transitions for hydrogenic ions due to the long observation time scale of the trap measurements. They have been used to successfully fit the spectrum of C/Linear 1999 S4 [20]. However, these data are collected at ~ 0.01 keV/amu impact energy, while solar wind ion impact energies are 0.8 - 3.0 keV/amu. For analyzing cometary spectra it would be better to rely on data appropriate for higher collision energies, since the line emission changes over such a large energy range [21].

In this Letter we combine calculated emission cross sections together with the ion abundances measured by the Advanced Composition Explorer (ACE) to predict cometary spectra. We then show the sensitivity of the spectra that arise from various estimated time delays between the solar wind events at the comet and at the location of the Earth-orbiting ACE satellite.

For cometary observations, the classical trajectory Monte Carlo (CTMC) model [22] provides a tractable calculational method to study these involved charge-exchange systems. Within the CTMC method, semiclas-

sical methods have been developed to predict the n , l and m_l electron capture excited levels [23] of the projectile, and have lead over the years to capture and emission cross sections which are in good agreement with experimental data (see for example [23, 24]). After electron capture to excited nl levels of the projectile ion, absolute line emission cross sections are determined using a hydrogenic branching and cascading model.

In Table I the CTMC line emission cross sections for 1 keV/amu solar wind ions colliding with H_2O are presented. The H_2O molecule was approximated by a hydrogenic potential with an effective charge provided by its ionization energy of 12.6 eV. This approximation considers the problem within a 3-body theory. It must be noted that the CTMC method neglects the detailed molecular states associated with the product molecular ions. However, it reasonably predicts the projectile product states. The cross sections in Table 1 are insensitive (within $\pm 20\%$) to small changes in collision energy and are appropriate for both slow and fast solar wind speeds (0.8 to 3.0 keV/amu). The H_2O molecule was utilized since it makes up approximately 90 % of comet gases [25].

We note that the basic input to the calculations is the ionization potential of the target. Thus, the calculations also provide first order estimates of the x-ray line emission cross sections for the major comet gases and their photo-dissociated atoms such as CH_4 (12.6 eV), CO_2 (14.4 eV), atomic O (13.6 eV), atomic H (13.6 eV), and CO (14.1 eV) at energies close to 1 keV amu^{-1} (440 km/sec). In a previous publication we have shown that experimental and theoretical cross sections obtained for H_2O , CH_4 , and CO_2 at 0.01 keV/amu were almost identical [21]. It should be also noted that the electron capture CTMC cross sections for O^{8+} impact on atomic H also compare well with the quantum mechanical calculations of Shipsey et al. [26] at the energies considered here. Further support is given by other experimental measurements where at energies around 1 keV/amu, the electron capture cross sections for collisions on H_2O , CH_4 and CO_2 are functions of only the projectile charge [21]. Measurements for atomic H are also consistent with the scaling for the above molecular targets [27].

To obtain the emission cross sections for the hydrogenic projectiles presented in Table 1, we have used those corresponding to a bare projectile with the same charge state. From statistical weight considerations, the singlet spectra were obtained by multiplying the calculated $np \rightarrow 1s$ cross sections by 25 %. The remaining x-ray flux then resides in the $n = 2$ triplet states. This is partitioned as 1/3 to the $2^3\text{P} \rightarrow 1^1\text{S}$ transition and 2/3 to the forbidden $2^3\text{S} \rightarrow 1^1\text{S}$ transition. The ratios were derived from the high resolution measurements of Beiersdorfer on the $\text{Ne}^{9+} + \text{Ne}$ electron capture system [21].

To benchmark the calculations, the only absolute line emission cross sections available for Lyman transitions are those for $\text{He}^{2+} + \text{H}_2\text{O}$. The photon energies are in the 40 to 51 eV range, and, thus, are not directly applicable to the cometary x-ray emission, but will be very

important for EUV observations. In Figure 1 we compare our calculated line emission cross sections with the recent laboratory data of Serezyuk et al. [28]. The calculations overestimate the Lyman- α transition at the lowest energies and they underestimate the Lyman- β at the highest energies, but overall the absolute magnitudes and energy trends are very similar. We should note that the molecular product states produced in these collisions are very complex, as documented in the review by Stolterfoht et al. [29]. To emphasize the relative insensitivity to other targets having similar ionization potentials, we also display experimental results for CH_4 , CO_2 and CO [30]. In general, there is very little difference between them except at the lowest energies for the Lyman-alpha transition.

From the tabulated cross sections of Table I, the charge exchange produced x-ray emission for cometary spectra can be constructed. In order to compare to the Chandra X-ray Observatory (CXO) data, the emission lines were multiplied by the ACIS-S spectrometer effective area and then convoluted with a 100 eV FWHM Gaussian function [17]. The lines corresponding to each solar wind ion are weighted by the corresponding abundance in the solar wind appropriate for the time during which the x-ray measurements took place.

The solar wind ion abundances are available in two-hour intervals in terms of $[\text{C}/\text{O}]$, $[\text{C}^{q+}/\text{C}]$ and $[\text{O}^{q+}/\text{O}]$ ratios [31] and are based on ACE/SWICS-SWIMS (the latter for Solar Wind Ion Mass Spectrometer) satellite measurements. The accuracy of the ion observations is estimated to be 10 - 15 % [31]. In Figure 2 we show the ion abundances for the C^{5+} , C^{6+} , O^{7+} and O^{8+} ions appropriate for the period (from 4:30 to 8:04 UT) in which the spectrum of comet C/LINEAR 1999 S4 was measured by the CXO on July 14 2000. The figure also clearly illustrates the large variations in ion composition as a function of the hour of the day.

A critical point when the measured ion abundances are used to describe cometary spectra is the difference in time between the solar wind events at the Earth-orbiting satellite measuring the ion abundances and those at the comet coma. In the following we have used the full solar wind delay estimation of +0.7 days. To illustrate the sensitivity of the spectrum to time variations, we display how it would appear if the solar wind conditions are shifted ± 1 days.

In Figure 3, we present calculated x-ray spectra for C/Linear 1999 S4 considering a collisionally thin target with solar wind delays given in the caption. For x-ray emission energies between 200 eV and 300 eV, we have included lines of $\text{Mg}^{8+,9+}$ and Si^{8+} . Here, we have used the CTMC intensities of the Balmer transitions corresponding to a bare projectile with charge equal to that of the projectile. After averaging the solar wind abundances provided by Schwadron and Cravens [32], the Mg^{9+} and Si^{9+} projectiles have been assumed to have equal abundances, about 20 % less than that of Mg^{10+} . In the present case, a Mg^{10+} abundance of 0.38 was used.

Whether our treatment of these lines is appropriate is not clear, due to the rapidly decreasing sensitivity of the spectrometer in this region. However, such a background must be included since their lines overlap those of the C ions because of the 100 eV CXO resolution. The lines corresponding to N^{6+} and N^{7+} were weighted by the solar wind abundance provided by Schwadron and Cravens [32].

In Figure 3a we compare the spectra obtained when considering the $C^{5+,6+}$ and $O^{7+,8+}$ abundances corresponding to the appropriate delay (measured on July 13) with those obtained for the ion abundances found one day before and one day after the spectral measurement. The spectra have been normalized to the O^{7+} line located at approximately 560 eV. As it can be seen, the time variation of the carbon to oxygen ion abundances gives rise to major changes in the spectra. We find that the spectra are not only sensitive to the overall intensity of the solar wind flux, but also to the hour-by-hour changes in the relative abundances of the solar wind ions.

In Figure 3b we display the spectral lines with 10 eV FWHM resolution, as might be realized in future XRS observations. A rich spectrum is obtained that will test our atomic physics knowledge. It is readily apparent that the high lying $np \rightarrow 1s$ transitions are very important and must be correctly portrayed in comet models. Furthermore, the spin forbidden $2^3S \rightarrow 1^1S$ and $2^3P \rightarrow 1^1S$ splitting is observed after capture by O^{7+} ions. The ion fractions X^{q+}/O used are presented by the insert in Fig. 3b.

To summarize, we have shown that CTMC calculated emission cross sections properly describe available laboratory measured x-ray line emission cross sections. These tabulated cross sections are then used to provide the first

theoretical spectrum of comet C/LINEAR 1999 S4 without any fitting of line positions or ion abundances for the C^{q+} and O^{q+} ions. Quantitative agreement is obtained with the CXO data. Furthermore, the underlying CXO spectra are presented with a 10 eV FWHM convolution to mimic the micro-calorimeter spectrometer such as the one launched on the Suzaku satellite in 2005. Unfortunately, the cryogenics failed after three weeks into the mission. These high resolution spectra clearly show the details of the charge exchange processes and resolve forbidden transitions for hydrogenic projectiles.

We note that the x-ray spectrum requires solar wind ion abundances measured on the same time scale as the x-ray observations. Based on the present results we conclude that in order to perform proper analyses on the solar wind ion abundances, future missions should be conceived to measure x-ray spectra continuously during a short period of time, instead of taking snapshots over several days. Furthermore, cases in which the solar wind ions hit the comet first and then the Earth can be used to provide timely information about the solar wind ion composition on the Earth several hours in advance. This would be of great importance in order to avoid or prevent space-weather related failures on satellites, communications and navigational systems among others.

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FIG. 1: Absolute line emission cross sections for Lyman transitions as a function of the projectile energy following charge exchange in He^{2+} collisions on H_2O , CH_4 , CO_2 and CO .

FIG. 2: Solar wind ion abundances as a function of time during the measurement of the spectrum of C/LINEAR 1999 S4 measured by ACE.

FIG. 3: (a) Calculated x-ray spectra for C/Linear 1999 S4 with FWHM of 100 eV. The full delay of solar wind events (+0.7 days) is compared with the predictions obtained with ion abundances from one day before and one day after the observation; (b) The calculated x-ray spectra is shown with FWHM of 100 eV and 10 eV to simulate the CXO ACIS-S and the XRS resolutions.

TABLE I: Line emission cross sections following single electron capture in 1 keV/amu collisions of ions with H_2O (10^{-15} cm^2). All the transitions are from the upper level indicated to the ground state. For hydrogenic projectiles the $n\text{p } ^1\text{P}_1$ levels represent the transitions $1\text{snp } ^1\text{P}_1 \rightarrow 1\text{s}^2 \text{ } ^1\text{S}_0$.

Upper level	C^{5+}	C^{6+}	N^{6+}	N^{7+}	O^{7+}	O^{8+}	Ne^{9+}	Ne^{10+}
$1\text{s}2\text{s } ^3\text{S}_1$	1.355	—	1.676	—	1.994	—	2.649	—
$1\text{s}2\text{p } ^3\text{P}_1$	0.678	—	0.838	—	0.997	—	1.325	—
$2\text{p } ^1\text{P}_1$	0.455	2.350	0.588	2.930	0.733	3.570	1.06	4.950
$3\text{p } ^1\text{P}_1$	0.144	0.363	0.091	0.373	0.093	0.396	0.101	0.407
$4\text{p } ^1\text{P}_1$	0.078	0.597	0.149	0.381	0.095	0.165	0.033	0.125
$5\text{p } ^1\text{P}_1$	0.001	0.043	0.011	0.297	0.074	0.479	0.075	0.107
$6\text{p } ^1\text{P}_1$	—	—	—	0.007	0.002	0.041	0.054	0.351
$7\text{p } ^1\text{P}_1$	—	—	—	—	—	—	0.002	0.025





