Interpolation of Phosphorus, Chlorine and Potassium Emissivity for Coronal Thermal Plasmas I: He -like resonance lines

by

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Abstract

A number of peculiar spectral features is present on the solar flare X-ray spectra observed recently by RESIK bent crystal spectrometer aboard *CORONAS-F* satellite (Sylwester and Sylwester, 2003). The wavelengths of these features closely correspond to resonance transitions of highly ionized potassium and chlorine.

In this paper, we estimate the temperature dependence of line intensities contributing to the observed features. As chlorine and potassium belongs to the group of poorly abundant elements with their respective photospheric abundances relative to H below 10^{-6} in the solar plasma, their emissivity has not yet been directly calculated. Therefore, we present here the results of isoelectronic sequence interpolations of the intensity vs. temperature dependence for the strong lines corresponding to $1s^2\ ^1S_0\ -\ 1s2p\ ^1P_1$ ("w" line) transition in He-like ions. Results of the calculations will be useful for the final identification of the lines observed and for determination of the absolute abundance of chlorine and potassium in solar corona.

Key words: Sun, solar physics, X-ray spectroscopy, emission functions, chlorine, phosphorus and potassium.

1 Introduction

It is of general astrophysical interest to predict spectra of hot multimillion degree coronal plasma. A number of calculations and tabulations are presently available in this respect. Mewe, Gronenschild and van den Oord(1985) and Mewe, Lemen and Gronenschild and van den Oord (1986) tabulations and formulas have frequently been used in order to synthesise spectra of coronal active regions and flares. Presently there are at least four numerical codes available CHIANTI (Dere et al., 1997), PINTofAle (Kashyap, 2000), XSPEC (Arnaud, 1996) for calculations of the X-ray line and continuum emissivity for astrophysical plasma under various assumptions. However, these tables and codes incorporate the most abundant plasma species only. Chlorine, phosphorus and potassium line spectra are missing in all these sources. Therefore we decided to interpolate these missing spectra of interest for us. Here we focus our attention on the strongest transitions forming in He-like ions, which fall into the spectral region being observed by RESIK spectrometer. The approach we have used in the interpolations can easily be extended to the other elements and lines (papers are in preparation). We shall be repeating this work with data from the Chianti code.
The RESIK (REntgenowsky Spektrometr s Izognutymi Kristalami) spectrometer is placed aboard *CORONAS-F* satellite (cf. Sylwester et al., 2003) and observes solar X-ray spectra in four channels between $\sim$ 3.37 Å and $\sim$ 6.08 Å. In this spectral range we observe K XVIII, Ar XVIII, Ar XVII, S XV, Si XIV, and Si XVIII lines (Phillips et al., 2003). An example of a flare spectrum is shown in Fig. 1.

Figure 1: RESIK spectrum in all four channels, with stronger lines identified. The spectrum has been observed near the peak of the flare observed on 9 May 2003 at approximately 00:40 UT. Wavelength ranges are: 3.37 Å - 3.88 Å, 3.82 Å - 4.33 Å, 4.31 Å - 4.89 Å and 4.96 Å - 6.09 Å for channels 1, 2, 3 and 4 respectively. The spectrum presented has been corrected for the orbital background and the instrumental "notch" effect.

The knowledge of temperature dependence of line emissivity (called emission functions) is indispensable not only for purposes of proper line identification, but mainly for determination of elemental abundances (or their respective upper limits). For chlorine and potassium with their low solar abundances there do not appear to be available at present sufficient atomic data allowing direct calculations of line emissivity, so we performed interpolation along the He-like isoelectronic sequence in order to obtain temperature dependence of line intensities for the strongest resonance transitions (w line in notation of Gabriel, 1972).

2 THE INTERPOLATION

It has been shown by many authors (cf. Sylwester et al, 1998), that the temperature behaviour of the line intensity (sometimes called line emissivity or emission function or contribution function) $G_i(T_e)$ for a thermal, optically thin coronal plasma in ionization equilibrium can be expressed as:

$$G(T) = \frac{1}{4\pi \mathrm{R}^2} \frac{N_2 \mathrm{A}_{21}}{N_\mathrm{e}} = \frac{1}{4\pi \mathrm{R}^2} \frac{N(\mathrm{H})}{N_\mathrm{e}} \frac{N(\mathrm{El})}{N(\mathrm{H})} \frac{N_{ion}}{N(\mathrm{El})} \frac{N_2}{N_{ion}} \frac{\mathrm{A}_{21}}{\mathrm{N_e}} \; ; \quad [\mathrm{phot./cm^2/s}] \tag{1}$$

where R is 1 a.u., N_2 is the number density (in units of cm^{-3}) of ions excited with the electron in the upper energy level 2, A_{21} is the spontaneous transition probability from level 2 to the ground level. N_e and $N(\mathrm{H})$ are the electron and hydrogen number densities, respectively. $N(\mathrm{H})/N_e$ is the proton/electron number density ratio appropriate for a fully ionized solar plasma. $N(\mathrm{El})/N(\mathrm{H}) = \mathrm{A_{El}}$ is the abundance of line parent element, $N_{ion}/N(\mathrm{El})$ is the fractional (at a given temperature) population of the ion forming the line (taken from so-called ionization balance calculations). T stands for electron temperature.

For purposes of this paper, we have used the emission function values $G_i(T_e)$ as given by Mewe et al., (1985) in the form of tabulations for elements i = Ne, Na, Mg, Al, Si, S, Ar, Ca, Fe and Ni. Respective values for P, Cl and K have been determined by means of the interpolation procedure described below. It should be noted that Mewe values have been calculated using Arnaud and Raymond (1992) ionization balance. We have found it convenient to perform interpolation along the isoelectronic sequence using normalized $G_i^*(T)$ functions, as they represent elasticities scaled to the unit elemental abundance i.e. $\mathrm{A_{El}} = 1$.

Figure 2: **a)** Emissivity $G^*(T)$ of the thermal plasma in w (resonance) lines as plotted from tabulations of Mewe et al., (1985). The emissivity (per unit elemental abundance and emission measure $\mathrm{EM} = 10^{48}\,\mathrm{cm}^{-3}$) are plotted for elements: Ne, Na, Mg, Al, Si, S, Ar, Ca, Fe and Ni. The curves are of similar shape. For purpose of plotting, the emissivity have been interpolated piece by piece using 4[th] degree interpolation expression of the form $y = a\,x^b\,e^{(c\,x + d\,x^2)}$ drawn exactly through the points available from Mewe tabulations. **b)** When plotted on reduced (see the text) temperature scale T^*, the similarity of temperature behaviour of emissivity curves becomes less apparent. It is seen (cf. Table 1), that the maximum efficiency of emission depends on the atomic number.

In Fig. 2, we show $G_i^*(T)$ emissivity for the He-like w resonance transitions ($1s^2\ {}^1S_0 - 1s2p\ {}^1P_1$) plotted against the temperature T (left) and the reduced temperature T^* (right). The reduced temperature is taken as a ratio $T^* = T/T_m$, where T_m represents the temperature where the emissivity function reaches maximum (in other words T_m represents the temperature of maximum efficiency of line formation). The systematic behaviour shown in Fig. 2 is predicted from atomic theory (Gabriel, 1972). In Table 1, we put selected characteristics of the emission function used as input for the interpolations as well as those (for P, Cl and K) obtained from the interpolation. In the Table z stands for the atomic number, T_1 and T_2 are the low and high temperatures at which the plasma emits at half the maximum efficiency and T_{FWHM} is the temperature width of this temperature interval.

By plotting the T_m values vs. z along the isoelectronic sequence, a clear linear dependence is noticeable. In Fig. 3 we present respective plot for the w line. Using the least squares algorithm we draw optimum line through the points. Obtained best fit relation between the T_m and z is given by:

$$log(T_m) = (3.06 \pm 0.04)\,log(z) + (3.505 \pm 0.008) \tag{2}$$

Table 1: **Basic characteristics of emission functions for** $1s^2\ {}^1S_0 - 1s2p\ {}^1P_1$ (w) **lines of selected elements.**

Element	z	λ^a [Å]	T_m [MK]	$log\ G^*_m$ [phot/cm^2/s]	T_1 [MK]	T_2 [MK]	$T_{\rm FWHM}$ [MK]
Ne	10	13.4401	3.87	8.922	2.6	6.0	3.4
Na	11	11.0027	5.10	8.896	3.3	7.9	4.6
Mg	12	9.1688	6.43	8.866	4.2	10.1	5.9
Al	13	7.7573	8.24	8.825	5.2	13.0	7.8
Si	14	6.6480	10.28	8.797	6.4	16.5	10.2
P†	15	5.7759	12.86	8.777	7.9	21.2	13.3
S	16	5.0387	15.07	8.759	9.2	25.5	16.3
Cl†	17	4.4560	18.9	8.721	11.3	32.3	21.0
Ar	18	3.9488	21.98	8.701	12.6	38.0	25.4
K†	19	3.5384	26.5	8.667	15.3	47.2	31.8
Ca	20	3.1773	29.5	8.639	16.9	54.7	37.8
Fe	26	1.8504	70.5	8.481	35.8	145	110
Ni	28	1.5885	92.0	8.448	45.7	201	155

λ^a - line wavelengths are taken from CHIANTI;

G^*_m - value of maximum efficiency of emission [phot./cm^2/s] as interpolated from Mewe et al., 1985; The uncertainty of this value is $\pm\, 0.01\, dex$

† values obtained as the results of present work.

Table 2: **Values of emission functions derived for w lines (He4 in notation of Mewe et. al., 1985) of elements P, Cl and K.**

Element	6.1	6.2	6.3	6.4	6.5	6.6	6.7	6.8	6.9	7.0
P	-	-	8.63	7.14	6.10	5.34	4.77	4.33	4.01	3.80
Cl	-	-	-	9.88	7.64	6.32	5.47	4.85	4.38	4.02
K	-	-	-	-	-	-	8.44	7.48	6.83	6.34

Element	7.1	7.2	7.3	7.4	7.5	7.6	7.7	7.8	7.9	8.0
P	3.72	3.78	3.95	4.21	4.49	4.78	5.07	5.34	5.61	5.86
Cl	3.76	3.61	3.58	3.67	3.86	4.10	4.37	4.64	4.90	5.17
K	5.97	5.69	5.52	5.44	5.47	5.59	5.79	6.03	6.28	6.53

Element	8.1	8.2	8.3	8.4	8.5	8.6	8.7	8.8	8.9	9.0
P	6.11	6.34	6.58	6.82	7.06	7.30	7.53	7.77	8.01	8.25
Cl	5.41	5.65	5.88	6.11	6.33	6.56	6.79	7.02	7.24	7.47
K	6.78	7.02	7.25	7.47	7.69	7.91	8.13	8.34	8.56	8.78

As the accuracy of Mewe tables extends to 3 digits (in logarithmic scale) we assume the uncertainty of any value given in the table to be $\pm\, 0.005 dex$. In order to assess the uncertainty of T_m determination based on the tabulated data, we have made a Monte Carlo simulation of the dependence of T_m independently for each line, allowing every entry from Mewe table to be randomly perturbed within the rounding error ($0.005\, dex$). The mean $\pm 1\,\sigma$ uncertainty obtained from 100 perturbation is indicated in Figure 2a. It is important to note that the uncertainty in T_m determination is of basic importance for the accuracy of interpolation method discussed in the present paper.

By plotting values of G^*_m (from Table 1) we notice a clear dependence between G^*_m and z. This dependence is presented in Fig. 3b. Simple linear fit is not sufficient in this case, which is easy to observe. The null-hypothesis test of the quality of the fit gives value of $\chi^2_N = 3.5$ (per degree of freedom). Instead, satisfactory appears the parabolic fit through the points (also shown in Figure 2b as thicker line) which results in the value of $\chi^2_n = 0.45$. Obtained

Figure 3: **a**) Dependence of T_m (the temperature of maximum line formation) on the atomic number z. The optimum linear fit to the points is shown (see Eq. 2 for values and uncertainties). The emission lines considered represent $1s^2\ ^1S_0 - 1s2p\ ^1P_1$ resonance (w) transition in He-like ions of Ne, Na, Mg, Al, Si, S, Ar, Ca, Fe, Ni. **b**) Dependence of the maximum efficiency G^*_m of the emission (at T_m) on the atomic number z (see Eq. 3 for values and uncertainties). The uncertainties plotted has been estimated from simple Monte Carlo simulations (see the text).

Figure 4: Plots of the "cuts" through optimum emission function surface for selected values of reduced temperature T^*. The plots are complementary to that presented in Figure 3b and show the quality of parabolic interpolation along the isoelectronic sequence for a broad range of temperatures. It is seen that parabolic dependence (c.f. Eq. 3) is generally adequate to describe the observed $G^*(z)|_T$ dependence.

best fit formula describing relation between the G^*_m and z is:

$$log(G^*_m) = (-0.940 \pm 0.001)\, log^2(z) + (1.230 \pm 0.016)\, log(z) + (8.631 \pm 0.003) \tag{3}$$

With this (G^*_m) vs. z dependence, we observe that in general the shape of emission function can be described using the following parabolic dependence:

$$log(G^*_m) = r\, log^2(z) + q\, log(z) + p \tag{4}$$

It is worth noting that the above parabolic relation is not only adequate to approximate the z-dependence of (G^*_m) at the maximum of emission efficiency i.e. where $log(T^*) = 0$, but can also be used to approximate (G^*_m) vs T

Figure 5: Plots of the temperature dependence of parameters p, q and r defining the optimum emission function surface (c.f. Eq.3). The derived uncertainties are so small that are within the width of the line plotted. [They are better shown in the respective insets as shaded areas]. The optimum emission function surface itself is shown in Figure 6.

Figure 6: Interpolated emission function surface showing regular changes both in temperature and atomic number domains. The surface has been drawn using the parabolic parametric approximation (cf. Eq. 3 and Figure 4). Smooth black lines plotted on top of the surface represent these shown in Figure 2b.

variations in a broader range of $log(T^{*})$. This finding constitute a basis of the interpolation method adopted in the present paper.

While searching for the convenient algorithm to be used in the emission functions interpolation, we have tested a number of other approaches including fitting with different types of polynomials, exponential and power law formulas and orthogonal functions. These other approaches lack the necessary generality i.e. even when we managed to adequately fit the shape of emission function for a particular ion, we were unable to use the same parametric form to describe emission function variation for another. Scaling to normalized temperature T^{*}, useful by itself, did not help in this respect. The difficulty of the present interpolation problem is probably caused by the character of the $G(T)$ dependence. The function is asymmetric, steeply rising by several orders of magnitude over short interval of temperatures (due to contribution of excitation and ionization terms) with subsequent slower decrease due to (over)ionization. Our present approach making use of Eq. (3) appears to be flexible and accurate enough to be used in the interpolation of

Figure 7: The "interpolation consistency plot" showing the differences dex between the input tabulated values from Mewe et al. (1985) and these obtained from our interpolation. The plots are shown for two elements Ar and Ca which are the closest in the atomic number z to these of interest for us. In most cases, the observed differences are within the uncertainties of the interpolation method.

Figure 8: Comparison of the input normalized emission functions (light gray lines) with these obtained from the interpolation (black lines) as discussed in the text. Interpolated functions nicely fit into the observed pattern of variations.

such functions.

In Figure 4 we present examples of the best fitted parabolas drawn through the "known" points (taken from interpolated tabulated values). The lines drawn represent "cuts" through the optimum interpolation surface. The examples are shown for the four selected representative values of $log(T^*)$ (indicated in each panel) from the range of interest $log(T^*) \in [-1, 1]$. This range covers most part of the emission functions' variation (i,e. by at least three orders of magnitude down from the maximum).

In Figure 5, we show the z-dependence of p, q and r values defining the "optimum interpolation surface" together with respective formal error range representative of the $1\,\sigma$ uncertainties of the fit. It is seen, that the dependence of the best-fitted p, q and r values smoothly varies with z. Their formal uncertainties are rather low and can been on the blow-ups only. Therefore, the illustrated dependencies together with Eqs (2) and (3) can be directly used in order to predict corresponding unknown values for phosphorus, chlorine and potassium (see Table 2). The smooth character of the p, q and r

vs $log(z)$ behaviour allows also for easy interpolation of existing tabulated emission function, without using the other (formal) interpolation techniques.

The overall agreement between the input data and optimum interpolation surface is presented in Figure 6, where the interpolated surface is shown (in grey) with the lines drawn on top. These lines are drawn exactly through the tabulated Mewe points and lie on the interpolation surface (to plotting accuracy).

3 Verification of the interpolation approach

Finally, we have cross-checked the entire interpolation method by comparing the values arising from optimum interpolation surface with respective exact values tabulated by Mewe et al. (1985). In Figure 7 we present results of such a comparison for the elements Ar and Ca. These two elements have z values the closest to phosphorus, chlorine and potassium which are of interest for us. In the Figure, the differences (dex) are plotted between the tabulated and interpolated values. The temperatures for which the differences are plotted exactly correspond to these used by Mewe. The uncertainties represent values characteristic for the interpolation method, estimated assuming presence of the rounding errors ($0.005\,dex$) in the tabulated values. It is seen from Figure 7, that the difference between the interpolated and input values are mostly negligible within the uncertainties. They are less than $\sim 25\%$ except towards the end of the temperature interval). This makes us confident, that the our results of the emission function interpolations will have similar level of accuracy. Therefore, we claim that the interpolated values of emission functions for P, Cl and K given in Table 2 are accurate better than $25\,\%$ over entire range of temperatures, and better than $10\,\%$ in the temperature range around the maximum efficiency of line formation. The observed differences might relate not only to the interpolation procedure itself, but also might reflect presence of uncertainties in the atomic data used for making the tabulations. In this respect, the optimum interpolation surface represents the weighted w-line emission function, averaged over the individual shapes for many elements.

4 Results and discussion

In Figure 8 we show our interpolated emission functions for phosphorus, chlorine and potassium imbedded into the family of the parent emission functions normalized to unit abundance. The interpolated functions' shapes (in black) certainly appear to fit the z- dependent pattern. In order to make the results of interpolation easy to use, we put the interpolated value in Table 2. The Table is organized exactly the same as the original Mewe et al. (1985) line emissivity table. The values given in Table 2 have been calculated assuming the following elemental abundances (log $\mathrm{A_H} = 12$): $\mathrm{A_P} = 5.52$, $\mathrm{A_{Cl}} = 5.6$ and $\mathrm{A_K} = 5.57$. The former two represent cosmic abundances from Allen (1973). The potassium abundance is Taken three times the photospheric value as found by Phillips at al, (2003). The IDL code to calculate the $G(T, z)$ values from optimum interpolated surface is available on request from `ak@cbk.pan.wroc.pl`.

5 Summary

We present the interpolation method allowing for determination of unknown values for the emission functions given the atomic number of the element z and the temperature T for all elements between Ne and Ni. In the present research, using this method, the emission functions for the resonance transition $1s^2\ ^1S_0 - 1s2p\ ^1P_1$ (w line in notation of Gabriel, 1972) have been calculated for elements: phosphorus, chlorine and potassium. These lines are in the wavelength range of X-ray spectra being observed by RESIK bent crystal spectrometer presently on board the *CORONAS-F* solar observatory. The interpolated emission functions will further be used in a detailed analysis of coronal flare plasma composition. Presented method of interpolation can easily by adopted for the other important emission lines observed by RESIK. In the forthcoming papers, we will present the results obtained for highly ionized phosphorus, chlorine and potassium namely 1s2 - 1s(np) transitions in He-like ions, respective important satellite transitions, and the resonance and satellite lines forming in(to) the H-like ions of these elements.

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