On emission measures and element densities and masses inferred from XSPEC

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INTRODUCTION

Spectral model fits to observed spectra of hot (X-ray emitting) plasmas provide us crucial information on the state and amount of hot plasma. The spectral fits inform us of the elemental composition of the plasma and its temperature and, in the case of non-equilibrium ionization plasmas, tell us the age of the plasma by the parameter τ = ne t, with t the age since the plasma was shock heated.

The most common modeling software for X-ray spectra is the XSPEC software package (Arnaud 1996). The purpose of the current work is to explain the assumptions and provide corrections for cases where the assumptions are not accurate.

Definition of emission measure (EM)and definition of abundance factors (A_Z)) given below, with A_sol a solar abundance set:

$$EM_e = \int n_e(\vec{r})^2 dV = n_e^2\ V \quad \text{(if uniform)}$$

$$EM_H = \int n_e(\vec{r}) n_H(\vec{r}) dV = n_e\ n_H\ V \quad \text{(if uniform)}$$

$$EM_Z = \int n_e(\vec{r}) n_Z(\vec{r}) dV = n_e\ n_Z\ V \quad \text{(if uniform)}$$

$$n_H = A_1\ n_{H,0} \qquad\qquad n_Z = A_{sol,Z}\ A_Z\ n_{H,0}$$

For XSPEC, the value of the electron density, $n_{e,X}$, is tied to the hydrogen density, $n_{H,X}$, by:

$$n_{e,X} = 1.2\ n_{H,X}$$

ANALYSIS

The variation with solar abundance set is small (~3.5%). However the variation of the electron density between the different abundance sets (A_Z) is large, with a number of examples given in Table 1. The ionization state and composition gives the ratio ne/nH,0. The variation is nearly a factor of 1000, instead of the single value assumed by XSPEC.

Table 1. Electron-to-(fiducial)hydrogen density ratio $n_e/n_{H,0}$ for different cases of composition and different temperatures.

kT(keV):	0.10	0.25	0.50	1.0	2.0	4.0	10.0	40.0
COMPOSITION								
SOLAR CASES[a]								
angr	1.20532	1.20652	1.20769	1.20836	1.20866	1.20880	1.20885	1.20886
aspl	1.17672	1.17756	1.17829	1.17871	1.17893	1.17903	1.17907	1.17908
feld	1.20536	1.20647	1.20765	1.20829	1.20856	1.20867	1.20872	1.20873
aneb	1.16981	1.17092	1.17198	1.17258	1.17285	1.17297	1.17302	1.17303
grsa	1.17861	1.17962	1.18058	1.18113	1.18138	1.18149	1.18154	1.18155
wilm	1.20152	1.20224	1.20295	1.20335	1.20354	1.20362	1.20365	1.20366
lodd	1.16470	1.16552	1.16625	1.16666	1.16686	1.16696	1.16670	1.16670
lpgp	1.17506	1.17589	1.17668	1.17713	1.17736	1.17746	1.17775	1.17775
lpgs	1.20159	1.20254	1.20342	1.20394	1.20420	1.20431	1.20436	1.20437
NON-SOLAR CASES								
H 0[b]	0.20532	0.20652	0.20769	0.20836	0.20866	0.20880	0.20885	0.20886
(H,He) 0.1[b]	0.12946	0.13066	0.13183	0.13250	0.13280	0.13294	0.13299	0.13300
(H,He) 0[b]	0.00992	0.01112	0.01229	0.01296	0.01326	0.01340	0.01345	0.01346
(H to N) 0[b]	0.00743	0.00833	0.00935	0.01000	0.01030	0.01043	0.01049	0.01050
(H to Al) 0[b]	0.00093	0.00142	0.00155	0.00168	0.00183	0.00192	0.00195	0.00196
N100Fe1[c]	0.00108	0.00157	0.00172	0.00186	0.00202	0.00211	0.00215	0.00215
N100Fe1HHe[d]	1.1965	1.1970	1.1971	1.1973	1.1974	1.1975	1.1975	1.1976
N100Fe10[e]	0.01080	0.01574	0.01720	0.01862	0.02021	0.02112	0.02150	0.02152
N100Fe10HHe[f]	1.2062	1.2111	1.2126	1.2140	1.2156	1.2165	1.2169	1.2169

[a] Abundance references given in the XSPEC manual- see the abund command.
[b] All other elements taken to have solar abundance factors, $A_Z = 1$.
[c] N100 model (Seitenzahl et al. 2013) with A_{Fe}=1.
[d] N100 model with A_{Fe}=1, H He added at solar abundance.
[e] N100 model with A_{Fe}=10.
[f] N100 model with A_{Fe}=10, H He added at solar abundance.

To simplify notation, hereafter we define the electron density ratio as r_e, given by:

$$r_e = \frac{n_e}{1.2\ n_{H,0}} = \text{ ratio of electron density to XSPEC value}$$

the fiducial density is given in terms of $norm_X$ by:

$$n_{H,0} = r_e^{-1/2} \sqrt{10^{14}\ norm_X\ \frac{4\ \pi\ D_A^2}{1.2\ V}}$$

The XSPEC norm for hot plasma emission models is proportional to $EM_{H,X}$:

$$norm_X = 10^{-14}\ EM_{H,X}/(4\pi[D_A(1+z)]^2) \quad \text{with}$$
$$EM_{H,X} = \int n_{e,X}(\vec{r})\ n_{H,X}(\vec{r})\ dV = n_{e,X}\ n_{H,X}\ V \quad \text{(if uniform)}$$

From the detailed calculation (Leahy, Foster, Seitenzahl, 2024) we show the correct density of the plasma is given by:

$$n_H = A_1\ r_e^{-1/2}\ n_{H,X}$$
$$n_Z = A_Z\ A_{sol,Z}\ r_e^{-1/2}\ n_{H,X}$$

Element masses depend on the element densities and emitting volume,

$$\begin{aligned} M_Z &= m_Z \int n_Z(\vec{r}) dV = m_Z\ n_Z\ V \text{ (if uniform)} \\ &= m_Z\ EM_Z/n_e = m_Z\ A_{sol,Z}\ A_Z\ EM_{H,X}/n_e \\ &= m_Z\ A_{sol,Z}\ A_Z \sqrt{\frac{10^{14}\ norm_X\ 4\ \pi\ D_A^2\ V}{1.2\ r_e}} \end{aligned}$$

RESULTS

First, we review the contributions of various elements to the observed X-ray spectrum. In general, elements that strongly contribute (like Fe and Ni) are tightly constrained, but weakly contributing elements like H, He, Li, Be, B, C are poorly constrained, as shown in Fig,1 below.

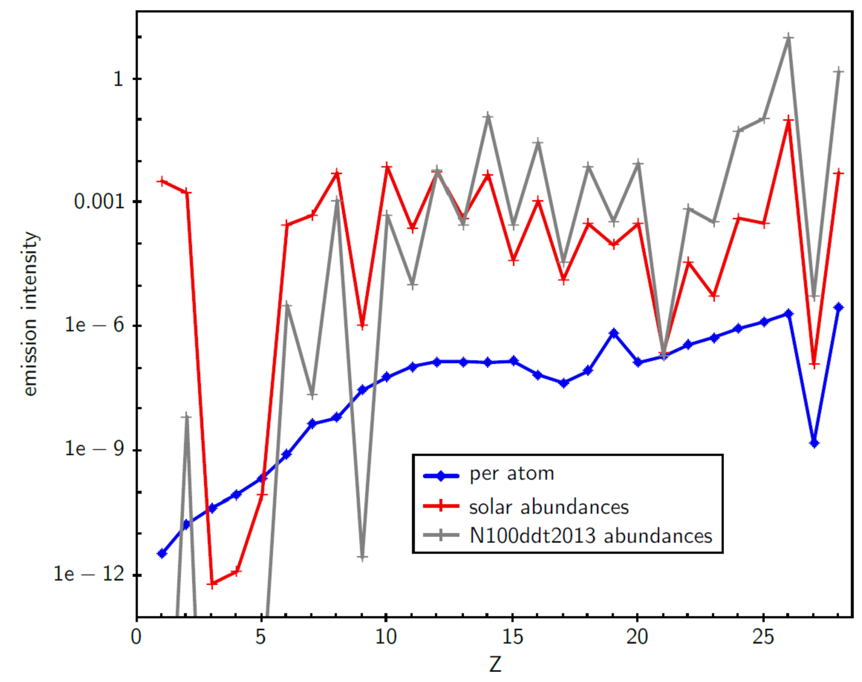

Figure 1. Illustration of the relative contributions of different elements to the 0.3 to 8 keV energy range for a spectrum, using the response matrices for the AstroSat SXT instrument (Singh et al. 2017). The maximum intensity in photons s^{-1} keV^{-1} is shown for elements $Z = 1$ to 28 for three cases: per atom, for solar abundances and for N100ddt2013 abundances. For each case the vertical scale is arbitrary. The XSPEC vvapec model was used with temperature of 1 keV. For N100ddt2013, H, Li, Be and B not shown because they are so small: they at 2.9×10^{-22}, 1.9×10^{-24}, 4.1×10^{-33}, and 1.2×10^{-16} respectively times the contribution of Fe.

Because the abundances of H and He are normally very large, they can contribute significantly to the X-rays spectrum. This is illustrated in Fig.2 below,
i.e. H abundance needs to be 30 times solar for H to contribute equally to Fe. Because solar abundance of some elements is very low (e.g. Li) the abundance relative to solar to contribute equally as Fe is large (~10^11).

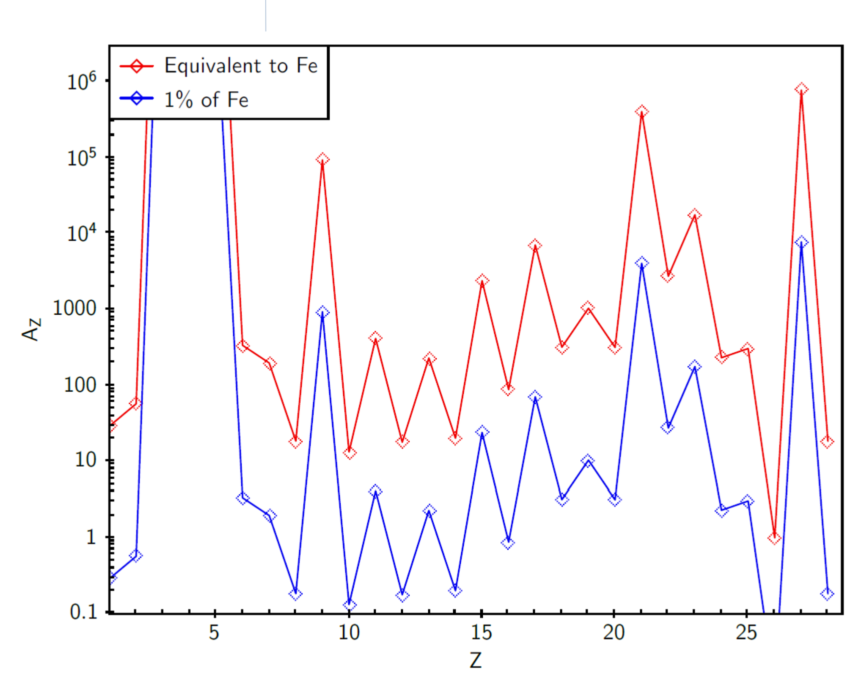

Figure 2. The abundance factors A_Z required to yield the same maximum contribution (red line) or to yield a contribution 1% as large (blue line) as the contribution from Fe to the 0.3 to 8 keV X-ray spectrum. The response matrices for the AstroSat SXT instrument was used and an equilibrium spectrum with temperature kT=2 keV and the abundance factor of Fe was set to 1 for the same-contribution line (or 0.01 for the 1% line). The abundance factors for Li, Be and B off scale, at values of 1.5×10^{11}, 7.8×10^{10}, and 1.1×10^{9} for equal contribution, with values 0.01 times as large for a 1% contribution.

We carried out a number of simulations in XSPEC simulating observed spectra using the Astrosat SXT response matrices. These were carried out for typical SNR fluxes, based on known type Ia SNRs with observed X-ray spectra, shown in Table 3.

Table 3. Measured temperatures and EM for type Ia SNRs[a]

SNR ID	type	D(kpc)	$EM(10^{58}cm^{-3})$	norm	kT(keV)	Age(yr)[b]	density(cm^{-3})[b]	$n_e\ t(cm^{-3}s)$[b]
G53.6-2.2	Ia	7.8	0.022	3.02E-04	3.9	44600	0.096	5.41E+11
G299.2-2.9	Ia	5	0.029	9.70E-04	1.36	8800	0.022	2.45E+10
G306.3-0.9	Ia	20	1.8	3.76E-03	1.51	12800	2.5	4.04E+12
G315.4-2.3	Ia	2.8	0.046	4.91E-03	3.04	11600	0.247	3.62E+11
G352.7-0.1	Ia?	7.5	0.11	1.64E-03	3.2	7600	1.66	1.59E+12
average:				2.32E-03	2.602			1.31E+12

[a] Values are from Tables 1 and 2 of Leahy et al. (2020), with references for EM, norm and kT given in Table 1.
[b] Values for age and density are from Table 2 of Leahy et al. (2020), with $n_e\ t$ calculated using post-shock density of $4n_e$.

2 of the simulated X-ray spectra and their spectral fits are shown in Fig. 3. The results from a set of simulated spectra and fits to those spectra are shown in Table 4. These verify that the abundances A_Z derived from spectral fitting are quite uncertain, and the spectra are fit with significant changes in the H and He abundances.

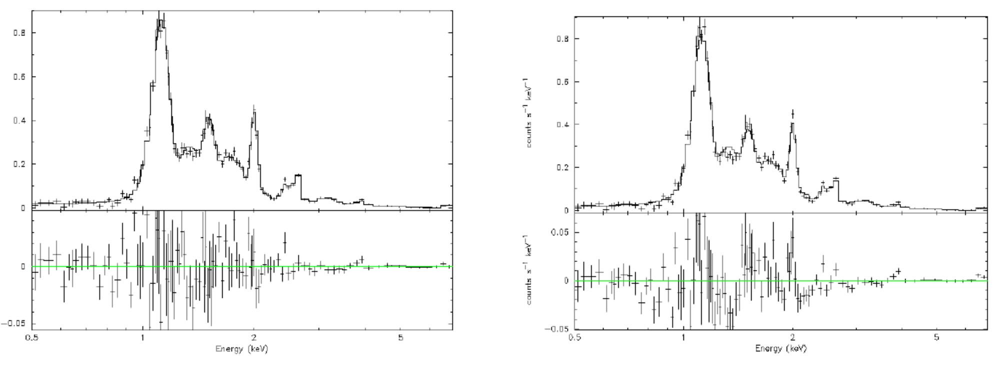

Figure 3. The HSN (high signal-to-noise, see text) simulated X-ray spectrum, which uses rmf, arf and background files for AstroSAT SXT, and abundances given by column 8 in Table 2 and model fits. The other spectrum parameters are $N_H = 10^{21}$ cm^{-2}, kT=2.6 keV, $n_e\ t = 1.31 \times 10^{12}$ cm^{-3} s and norm=2.32×10^{-2}. The fit model on the left has original N100 abundances, whereas the fit model on the right has added H and He with $A_H = A_{He} = 1$. Although the fit with solar H and He is statistically poor (probability=1.6E-06, Table 4), it is not clearly different except for larger residuals by a factor of ~1.2.

Table 4. Fits to simulated spectra with added H and He[a]

Spectrum	A_H, A_{He}	χ^2	probability	A_H, A_{He}	χ^2	probability
LSN	2.6E-16,7.5E-05	110.4	0.167	1, 1	109.8	0.177
	4,4	111.2	0.153	8,8	114.4	0.109
	16,16	119.2	0.063	24,24	122.4	0.042
	32,32	124.6	0.031	40,40	122.4	0.025
MSN	2.6E-16,7.5E-05	90.6	0.662	1, 1	105.6	0.258
	1.4,1.4	113.1	0.127	1.8,1.8	119.2	0.063
	2.2,2.2	124.7	0.033	2.6,2.6	128.5	0.018
HSN	2.6E-16,7.5E-05	93.2	0.590	2.6E-16,1	106.8	0.233
	1,7.5E-05	142.4	1.9E-03	1,1	176.1	1.6E-06
	0.1,0.1	96.0	0.509	0.2,0.2	100.3	0.390
	0.3,0.3	106.7	0.236	0.4,0.4	114.4	0.109
	0.5,0.5	123.0	0.038			

[a] LSN has exposure 10ks, norm 2.32 10^{-3}; MSN has exposure 20ks, norm 6.96 10^{-3}; HSN has exposure 20ks, norm 2.32 10^{-2}. All have kT=2.6 keV, $n_e\ t$ = 1.31 10^{12} and N100 abundances from column 8 of Table 2. H and He are added to the fit model, as listed.

A number of test cases with pre-specified abundances were carried out to illustrate the changes in density that results for non-solar abundance case, which are caused by the correction from including the correct values of electron density.

Figures 4 and 6 compare cases with solar abundance to those with light elements removed. With e.g H and He removed the element densities increase by factors of 10 and masses increase by the same factor.

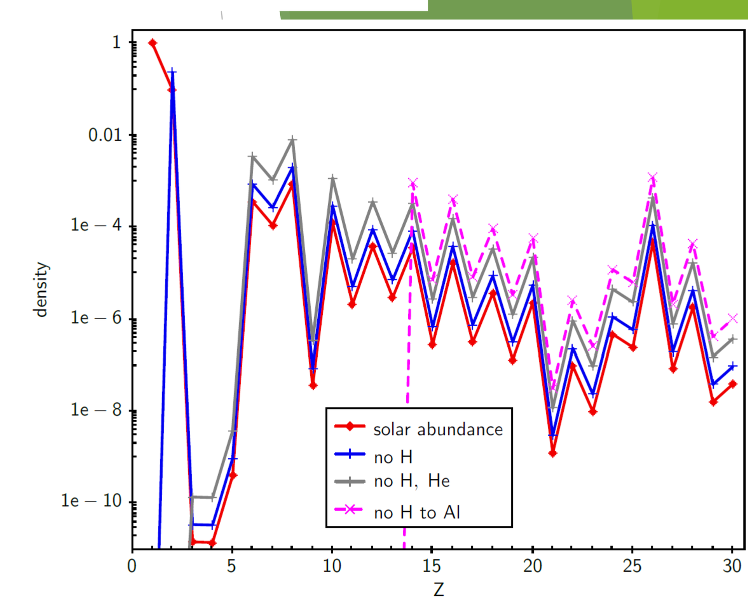

Figure 4. Element densities for different cases. The four cases shown are solar abundance, no H, no H and He, and no H through Al.

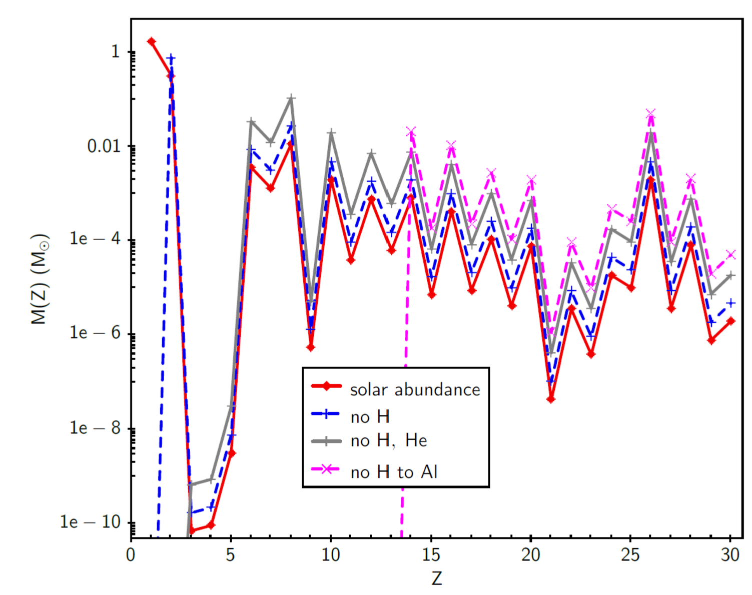

Figure 6. Masses for different cases. For calculation, the distance is 1 kpc, the emitting volume is a sphere of radius 2 pc, and the XSPEC norm is 0.1. The four cases shown are solar abundance, no H, no H and He and no H through Al.

Figures 5 and 7 compare cases with realistic type Ia abundances from the N100 model. The difference is that the spectral fit is normalized with Fe abundance =1 (red line) or Fe abundance = 10 (grey line). These two spectral fits are compared to the same abundance set but with added H and He at solar abundance, which is orders of magnitude large that that produced by the N100 model, but still comparable with what might be assumed for a spectral fit with XSPEC. The densities and masses for added H and He are lower by factors of ~30 to 60 than for the case using realistic H and He abundances. I.e. assuming too high H and He results in significant underestimate of densities and abundances, compared to the real physical case.

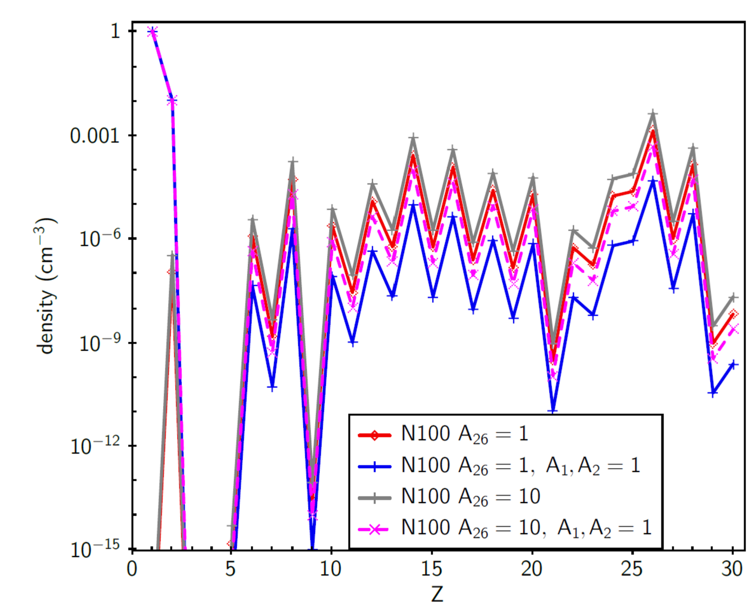

Figure 5. Element densities for N100 model (Seitenzahl et al. 2013), with and without added H and He. For calculation, the distance is 1 kpc, the emitting volume is a sphere of radius 2 pc, and the XSPEC norm is 0.1, which yields XSPEC $EM_X = 1.2 \times 10^{57}$ cm^{-3}. The four cases shown are N100 abundances normalized with A_{Fe}=1, N100 with A_{Fe}=1 and H and He added at solar abundances, N100 abundances normalized with A_{Fe}=10, and N100 with A_{Fe}=10 and H and He added at solar abundances.

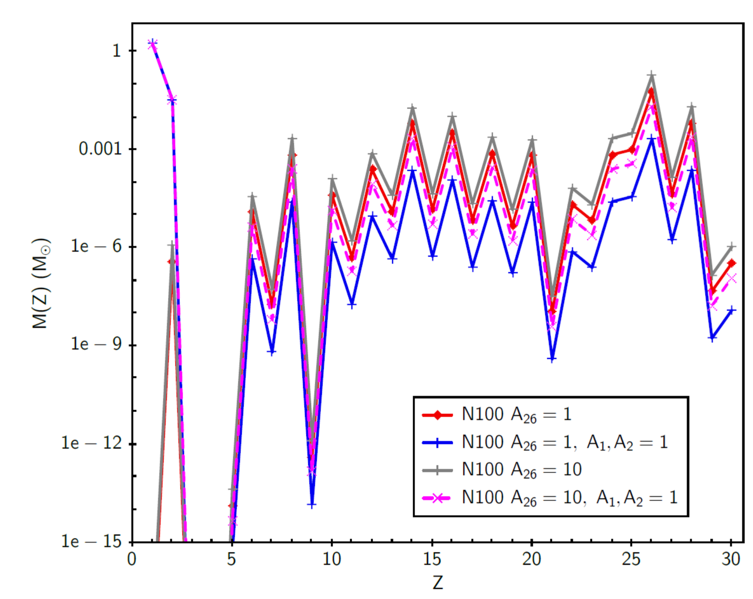

Figure 7. Masses for different cases. For calculation, the distance is 1 kpc, the emitting volume is a sphere of radius 2 pc, and the XSPEC norm is 0.1. The four cases shown are N100 abundances normalized with A_{Fe}=1, N100 with A_{Fe}=1 and H and He added at solar abundances, N100 abundances normalized with A_{Fe}=10, and N100 with A_{Fe}=10 and H and He added at solar abundances.

CONCLUSIONS/FUTURE WORK

For cases of non-solar abundances, with A1 or A2 different from 1, significant corrections are needed to the element densities to account for the difference between ne and ne,X . ne/ne,X can be much less than 1 as illustrated by the examples in Table 1. We define the electron density ratio re. The corrected densities are higher, by the factor re^−1/2, and the inferred element masses are corrected by the same factor (re^−1/2) thus can also be much larger. This implies that masses that may have been derived in the past using norm's from XSPEC spectral fitting on hydrogen poor plasmas, such as expected for Type Ia SNRs, may be significantly underestimated.