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Grain photoelectric ionisation rates, heating rates, and charge as functions of visual extinction

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Abstract. Recombination onto grain surfaces is important in determining the fractional ionisation and the depletions of elements. The recombination rates of ions depend on the grain charges. We calculate the dependence of the grain charge distribution function on visual extinction for each of a number of cloud models in order to obtain the mean grain charge as a function of visual extinction. We give simple fits to the dependences on grain charge and visual extinction of photoionisation and photoelectric heating rates which may be used in the modelling of photon dominated regions.

Key words. astrochemistry – ISM: dust, extinction

1. Introduction

Ruffle et al. (1999) proposed an explanation for the large sulphur depletion in dense cores in which carbon, oxygen, and nitrogen are only moderately depleted. The issue of sulphur depletion is important for the ionisation structure in translucent regions and low-density dark regions (e.g. Ruffle et al. 1998, Fig. 3), which in turn affects the dissipation scale of waves and the rate of ambipolar diffusion, both of which influence collapse dynamics. The sulphur depletion is also relevant for observations of star formation, particularly as CS was at one time a species commonly observed in efforts to detect spectral signatures of infall (e.g. Zhou et al. 1993).

The explanation of Ruffle et al. (1999) was based on the supposition that as a dense core forms, most of the material in it evolves through a stage during which sulphur is contained mainly in S^+ but the grains are primarily negatively charged. The principal motivation behind the study reported here is the verification of that supposition.

Relevant work had been done by Bel et al. (1989), who calculated the average charge carried by a grain as a function of position in a cloud for a number of cloud parameters. However, the results that they presented in detail did not include results for translucent regions with values of n_{H}, the hydrogen nucleus number density, in the range of 300 cm^{-3} to 3000 cm^{-3}, which we would expect to be relevant for sulphur depletion. Also they restricted attention to clouds irradiated by UV fields roughly comparable to the typical interstellar background UV field. In some star-forming regions, the UV fields may be considerably stronger. Furthermore, Bel et al. (1989) appear to have assumed that all grains have the same electric potential, which is reasonable for regions in which the mean number of charges on a grain is large compared to unity. However, we are interested in regions where the mean number of charges on a grain is between 1 and –1, and a calculation of the grain charge distribution function, similar to that of Gail & Sedlmayr (1975), is required.

Like Bel et al. (1989), we have employed a chemical model to calculate the fractional ionisation. The network used is a combination of the combined networks identified by Rae et al. (2002). With the exception of the CO photodissociation rate, all gas phase photoreactions were taken from van Dishoeck (1988) and Roberge et al. (1991). The rates taken from van Dishoeck (1988) were modified to contain a quadratic visual extinction, A_{v}, term like the rates taken from Roberge et al. (1991). We made the modification of a rate from van Dishoeck (1988) by selecting a rate in the Roberge et al. (1991) paper having a similar dependence on A_{v} at large A_{v}. We then adopted the same dependence on A_{v} for the rate of the reaction listed by van Dishoeck (1988) as the dependence given by Roberge et al. (1991) for the selected reaction listed in their paper. All rates referred to in the Roberge et al. (1991) paper are for a cloud with a total A_{v} of 10. Our modifications of the van Dishoeck (1988) rates were made in an attempt to use rates that are more accurate at modest values of A_{v}. All other gas phase rates were calculated from the expressions in the UMIST database, as they were in the work of Rae et al. (2002).

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The depth dependent radiation field used in the evaluation of the rates of grain photoprocesses is that used by Roberge et al. (1991) for a cloud with a total edge-to-centre A_v of 10. The quantum data for the grains were taken from Weingartner & Draine (2001, hereafter WD). Thus, we have tried to use as reliable gas phase and solid state photorates as possible.

In Sect. 2 we give simple fits to the A_v- and charge-dependant grain photoionisation and photoelectric heating rates that we used. Our hope is that these fits will be useful to others. Section 3 contains results characterising the dependance of the average grain charge on A_v for equilibrium models of clouds. The fraction of sulphur in S^+ at points where the average grain charge switches sign is also given for each of the models. Section 4 concludes the paper.

2. Grain photoelectric ionisation and heating rates

For a grain of radius a and charge $Z_g e$, the photoelectric charging rate is given by WD as

$$\Gamma_{\rm pe,i}(a, Z_g) = \pi a^2 \int_{\lambda_{\rm min}}^{\lambda_{\rm pet}} Y(a, \lambda, Z_g) Q_{\rm abs}(a, \lambda) \frac{\lambda F_\lambda}{hc} {\rm d}\lambda + \int_{\lambda_{\rm min}}^{\lambda_{\rm pdt}} \sigma_{\rm pd}(a, \lambda, Z_g) \frac{\lambda F_\lambda}{hc} {\rm d}\lambda \quad (1)$$

where the first term is for photoemission, and the second term is for photodetachment of attached electrons and is only present for $Z_g < 0$. The lower limit on the integration variable is $\lambda_{\rm min} = 912$ Å. The upper limits are the wavelengths corresponding to the threshhold energies for photoemission and photodesorption. These energies are given by the equations in the caption of Fig. 1 of WD, and by Eqs. (2), (4), (5) and (7) of that paper.

We assume that 50% of grains are carbonacious and 50% silicate (as did Laor & Draine 1993). We follow WD in taking work functions of 4.4 eV for graphite grains, and 8 eV for silicate.

The photoelectric yield $Y(a, \lambda, Z_g)$ is given by Eqs. (8) to (17) of WD. Dielectric tensors for graphite and silicates are given on Draine's webpage (`http://astro.princeton.edu/~drain/dust/dust.diel.html`). The absorption efficiency $Q_{\rm abs}(a, \lambda)$ is given by Draine (webpage). For silicate grains we used the "smoothed silicate" data. The photodetatchment cross-section, $\sigma_{\rm pd}(a, \lambda, Z_g)$, is given by Eq. (20) of WD.

We considered two separate grain radii, of 10^{-5} cm and 5×10^{-7} cm. For both of these grain radii we calculated $\Gamma_{\rm pe,i}$ at a large number of points in (A_v,Z_g)-space.

For each of the two grain radii, we obtained a least-squares fit for the dependence of $\ln\left(\Gamma_{\rm pe,i}(A_v)\right)$ on A_v for each Z_g under consideration. In each case we obtained two separate quadratic expressions – one for $A_v \leq 1$, and another for $A_v > 1$. We restricted ourselves to $A_v \leq 8$ in our calculations.

We then used least squares fitting again to obtain an expression for the dependence on Z_g of the coefficients of the quadratic fits. The photoelectric ionisation rate is then given by

$$\Gamma_{\rm pe,i} = \exp\left(C_0\left(Z_g\right) + C_1\left(Z_g\right) A_v + C_2\left(Z_g\right) A_v^2\right) \quad (2)$$

where $C_0\left(Z_g\right)$, $C_1\left(Z_g\right)$ and $C_2\left(Z_g\right)$ each have the form

$$C_i\left(Z_g\right) = a_i + b_i Z_g + c_i {Z_g}^2 + d_i {Z_g}^3. \quad (3)$$

The parameters a_i, b_i, c_i and d_i for $a_g = 5 \times 10^{-7}$ cm and $a_g = 10^{-5}$ cm are given in Tables 1 and 2 respectively.

We also obtained fits for the grain photoelectric heating rates in the same manner. The grain photoelectric heating rate is given by

$$\Gamma_{\rm pe,h}(a, Z_g) = \pi a^2 \int_{\lambda_{\rm min}}^{\lambda_{\rm pet}} Y(a, \lambda, Z_g) Q_{\rm abs}(a, \lambda) \frac{\lambda F_\lambda}{hc} \left(\frac{hc}{\lambda} - \frac{hc}{\lambda_{\rm pet}}\right) {\rm d}\lambda + \int_{\lambda_{\rm min}}^{\lambda_{\rm pdt}} \sigma_{\rm pd}(a, \lambda, Z_g) \frac{\lambda F_\lambda}{hc} \left(\frac{hc}{\lambda} - \frac{hc}{\lambda_{\rm pdt}}\right) {\rm d}\lambda. \quad (4)$$

Fit parameters for the heating rate for $a = 5 \times 10^{-7}$ cm and $a = 10^{-5}$ cm are given in Tables 3 and 4 respectively. The heating rate is

$$\Gamma_{\rm pe,h} = \exp\left(C'_0\left(Z_g\right) + C'_1\left(Z_g\right) A_v + C'_2\left(Z_g\right) A_v^2\right) \quad (5)$$

where $C'_i(Z_g)$ is given by an equation similar to Eq. (3), and a'_i, b'_i, c'_i and d'_i are given in Tables 3 and 4.

In most cases the use of the parameters in Tables 1 to 4 allows the photoelectric ionisation and heating rates to be calculated to within a factor of 2 of the values given by Eqs. (1) and (4). The only exception is for $a_g = 5 \times 10^{-7}$ when $Z_g = -1$. In this case, it is necessary to use

$$\ln\left(\Gamma_{\rm pe,i}\right) = -12.54 - 6.225 A_v + 2.515 A_v^2 \quad (6)$$

$$\ln\left(\Gamma_{\rm pe,h}\right) = -38.40 - 6.701 A_v + 2.707 A_v^2 \quad (7)$$

for $A_v \leq 1$, and

$$\ln\left(\Gamma_{\rm pe,i}\right) = -13.96 - 2.507 A_v + 0.040 A_v^2 \quad (8)$$

$$\ln\left(\Gamma_{\rm pe,h}\right) = -40.05 - 2.660 A_v + 0.054 A_v^2 \quad (9)$$

for $A_v > 1$.

3. Average grain charge

We calculated the average charge on a grain under different conditions, when both photoelectric and collisional charging are considered. We followed Rae et al. (2002) in using sodium as the representative metal. We used CO photodissociation rates given by

$$k_{\rm pd}({\rm CO}) = 5.32 \times 10^{-12} \exp\left(-5.663 A_v + 0.400 A_v^2\right) \quad (10)$$

which produces CO abundances in harmony with the results in Fig. 6 of van Dishoeck (1998).

We assumed that grains of only one size are present in a given cloud. For $a_g = 10^{-5}$ cm we assumed a dust-to-gas number density ratio of 1.07×10^{-12}. For smaller grains, we assumed the grain number density n_d was related to that at $a_g = 10^{-5}$ cm through the MRN Distribution (Mathis et al. 1977) so that

$$\frac{n_d\left(a_{g_1}\right)}{n_d\left(a_{g_2}\right)} = \left(\frac{a_{g_2}}{a_{g_1}}\right)^{\frac{5}{2}}. \quad (11)$$

Table 1. Ionisation rate fit parameters for $a_g = 5 \times 10^{-7}$ cm.

C_i	$A_v \leq 1$				$A_v > 1$			
	a_i	b_i	c_i	d_i	a_i	b_i	c_i	d_i
C_0	–12.64	–0.1795	3.285×10^{-3}	-1.427×10^{-4}	–14.12	–0.2244	1.949×10^{-3}	1.121×10^{-4}
C_1	–6.293	–0.1210	7.416×10^{-3}	-2.249×10^{-4}	–2.554	–0.04943	4.689×10^{-3}	-2.980×10^{-4}
C_2	2.512	0.04131	-3.934×10^{-3}	1.239×10^{-4}	0.04863	2.016×10^{-3}	-2.362×10^{-5}	-4.921×10^{-6}

Table 2. Ionisation rate fit parameters for $a_g = 10^{-5}$ cm.

C_i	$A_v \leq 1$				$A_v > 1$			
	a_i	b_i	c_i	d_i	a_i	b_i	c_i	d_i
C_0	−6.712	-9.508×10^{-3}	1.592×10^{-5}	-4.292×10^{-8}	−8.149	-9.924×10^{-3}	1.931×10^{-6}	1.267×10^{-8}
C_1	−6.153	-5.877×10^{-3}	2.573×10^{-5}	-4.578×10^{-8}	−2.457	-4.882×10^{-3}	3.607×10^{-5}	-9.322×10^{-8}
C_2	2.480	1.055×10^{-3}	-1.668×10^{-6}	-5.664×10^{-9}	0.03514	3.570×10^{-4}	-1.785×10^{-6}	1.583×10^{-9}

Table 3. Heating rate fit parameters for $a_g = 5 \times 10^{-7}$ cm.

C'_i	$A_v \leq 1$				$A_v > 1$			
	a'_i	b'_i	c'_i	d'_i	a'_i	b'_i	c'_i	d'_i
C'_0	–38.44	–0.2111	0.01220	-6.763×10^{-4}	–40.09	–0.263	0.01721	-7.269×10^{-4}
C'_1	–6.669	–0.1052	0.01048	-4.419×10^{-4}	–2.681	–0.05455	4.147×10^{-3}	-2.893×10^{-4}
C'_2	2.651	8.518×10^{-3}	-1.628×10^{-3}	7.051×10^{-5}	0.05953	2.491×10^{-3}	-1.982×10^{-4}	6.029×10^{-6}

Table 4. Heating rate fit parameters for $a_g = 10^{-5}$ cm

C'_i	$A_v \leq 1$				$A_v > 1$			
	a'_i	b'_i	c'_i	d'_i	a'_i	b'_i	c'_i	d'_i
C'_0	–32.55	-9.592×10^{-3}	2.582×10^{-5}	-9.483×10^{-8}	–34.11	–0.01021	2.476×10^{-5}	-8.451×10^{-8}
C'_1	–64.88	-2.846×10^{-3}	1.259×10^{-5}	-3.798×10^{-8}	–2.620	-2.778×10^{-3}	1.864×10^{-5}	-5.912×10^{-8}
C'_2	2.566	1.2560×10^{-4}	1.176×10^{-6}	-3.494×10^{-9}	0.04883	2.235×10^{-4}	-1.692×10^{-6}	3.461×10^{-9}

We calculated the photoelectric charging rates from Eqs. (2) and (3), with the parameters given in Tables 1 and 2. For the ion and electron grain collisional charging rates, Γ_i and Γ_e, we used Eqs. (26) and (28) to (30) of WD, and Eqs. (3.3) to (3.5) of Draine & Sutin (1987).

The rate of change of the fraction of grains carrying charge $Z_g e$, $x(Z_g)$,is

$$\begin{aligned}\frac{dx(Z_g)}{dt} = & \left(\Gamma_{pe,i}(Z_g-1)+\Gamma_i(Z_g-1)\right)x(Z_g-1) \\ & +\Gamma_e(Z_g+1)x(Z_g+1) \\ & -\left(\Gamma_{pe,i}(Z_g)+\Gamma_i(Z_g)+\Gamma_e(Z_g)\right)x(Z_g). \qquad (12)\end{aligned}$$

The values of the Γs in Eq. (12) are large compared to the inverse of the chemical timescale, so we assumed $x(Z_g)$ to be in quasi-steady state, i.e. that at any time $\frac{dx(Z_g)}{dt} = 0$, so that for each Z_g we calculated $x(Z_g)$ with an algebraic, rather than a differential equation.

The average grain charge is given by

$$\left\langle Z_g \right\rangle = \sum_{Z_{g_{min}}}^{Z_{g_{max}}} x(Z_g) Z_g. \qquad (13)$$

Table 5. Elemental abundances.

Element	Abundance
He	7×10^{-2}
C	1×10^{-4}
O	2×10^{-4}
N	2×10^{-5}
S	1×10^{-6}
Na	1×10^{-6}

We considered clumps of several uniform denities. We also considered several values of I_{UV}, a factor scaling the radiation field and all photorates and equal to unity for the radiation field used by Roberge et al. (1991). In each case, we did the calculation for a number of A_vs between 0 and 5. We used a set of elemental abundances in which the abundances of sulphur and metals were high, as is consistent with a region which has not yet undergone collapse. These abundances are shown in Table 5. We assumed a gas temperature of 10 K, and did the calculations for both $a_g = 5 \times 10^{-7}$ cm and $a_g = 10^{-5}$ cm.

Table 6. Results for a uniform static clump for $a_g = 10^{-5}$ cm.

Model	n_H cm^{-3}	I_{UV}	A_v $(\langle Z_g \rangle = 1)$	$\frac{x(S^+)}{x_S}$	A_v $(\langle Z_g \rangle = 0)$	$\frac{x(S^+)}{x_S}$	$\langle Z_g \rangle_{min}$	A_v $(\langle Z_g \rangle = \frac{1}{2}\langle Z_g \rangle_{min})$	$\frac{x(S^+)}{x_S}$
S1	100	1	0.39	0.99	0.88	0.99	−0.915	1.31	0.98
S2	300	1	0.16	0.99	0.48	0.99	−0.915	0.85	0.98
S3	1000	1	–	–	0.21	0.99	−0.930	0.44	0.98
S4	1000	10	0.39	0.99	0.89	0.99	−0.921	2.05	0.97
S5	1000	100	1.21	0.99	2.18	0.98	−0.849	3.03	0.97
S6	1000	1000	2.22	0.99	3.21	0.98	−0.534	3.82	0.97
S7	3000	1	–	–	0.02	0.98	−0.938	0.21	0.98
S8	10^4	1	–	–	–	–	−0.941	–	–

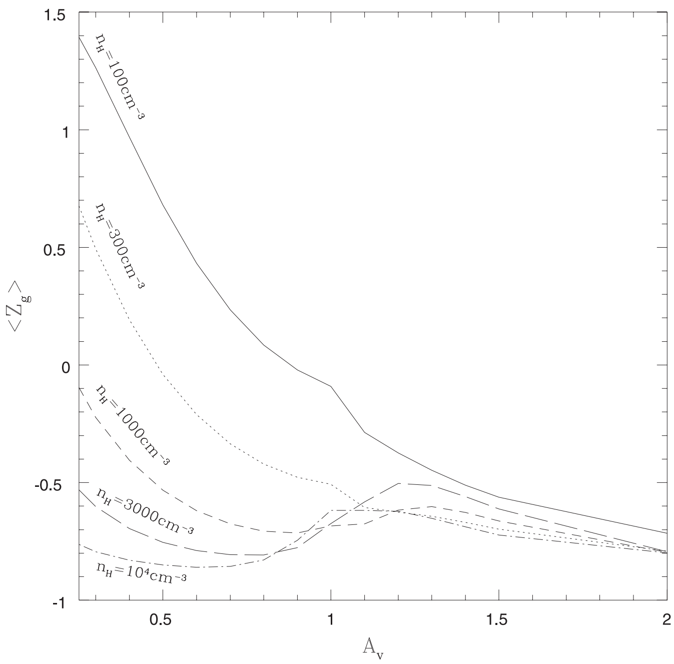

Fig. 1. Dependence of $\langle Z_g \rangle$ on A_v for different n_H, for $a_g = 10^{-5}$ cm and $I_{UV} = 1$.

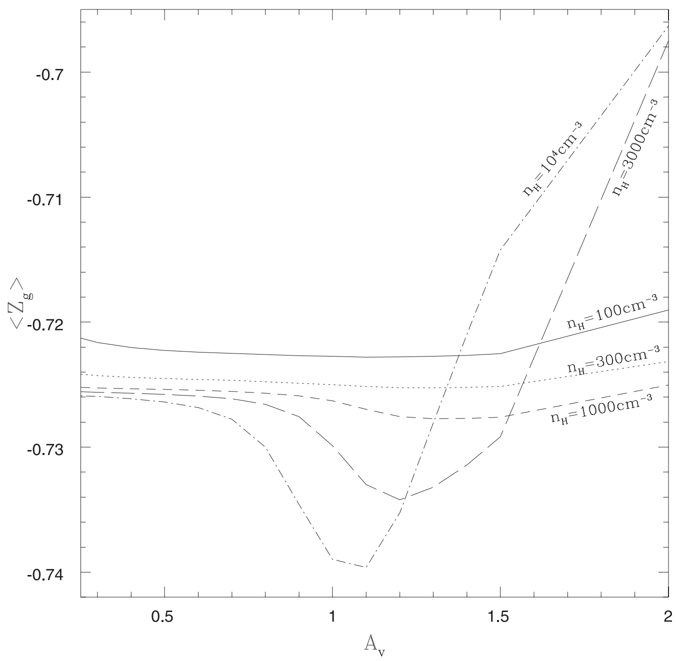

Fig. 2. Dependence of $\langle Z_g \rangle$ on A_v for different n_H, for $a_g = 5{\times}10^{-7}$ cm and $I_{UV} = 1$.

We integrated the differential rate equations of the species until the system reached chemical equilibrium.

For $a_g = 10^{-5}$ cm, we found for each (n_H, I_{UV}) pair the A_vs at which $\langle Z_g \rangle = 0$, $\langle Z_g \rangle = 1$, and $\langle Z_g \rangle = \frac{1}{2}\langle Z_g \rangle_{min}$, where $\langle Z_g \rangle_{min}$ is the minimum value of $\langle Z_g \rangle$ for that (n_H, I_{UV}) pair, i.e. the value at the centre of the clump. The results are shown in Table 6. A dash in a column indicates that the corresponding value of $\langle Z_g \rangle$ never occurs for that combination of n_H and I_{UV}. We also show the fraction of sulphur that is in the form of S^+ when $Z_g = 0$. In Fig. 1 we show the variation of $\langle Z_g \rangle$ with A_v for different n_H, for $a_g = 10^{-5}$ cm^{-3} and $I_{UV} = 1$. For $a_g = 5 \times 10^{-7}$ cm, the average grain charge is always negative, and indeed is always less than half of the minimum charge. Therefore, results for $a_g = 5 \times 10^{-7}$ are not shown in Table 6. However, we do show in Fig. 2 results for the variation of $\langle Z_g \rangle$ with A_v for different n_H, for $a_g = 5 \times 10^{-7}$ cm^{-3} and $I_{UV} = 1$. The values of Z_g for different n_H and A_v differ by no more than a few per cent.

4. Conclusions

We have established that the mean charge on grains is negative in equilibrium models for a range of visual extinctions at which the sulphur is contained primarily in S^+, as required in the explanation given by Ruffle et al. (1999) for the high sulphur depletions in dense cores. Small grains carry negative mean charge everywhere in all of the models in which we included them, ensuring that such grains will have substantial effects on ion abundances anywhere where they are present in high concentration (Lepp et al. 1988).

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