Section III

Dust in Dense Clouds

THE HEATING OF INTERSTELLAR GAS BY DUST

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ABSTRACT. Interstellar grains serve as an intermediary in transferring stellar radiant energy or gas chemical energy into the heating of interstellar gas. Grain photoelectric heating, a process in which ultraviolet photons eject energetic electrons from grains into the gas, dominates the gas heating of the intercloud medium, diffuse clouds, and most photodissociation regions (PDRs); it is also significant in HII regions. Grain photoelectric heating in PDRs can explain the observed correlations of CII(158 μ m) with CO J=1-0 intensities and CII(158 μ m) + OI(63 μ m) with infrared continuum (grain) luminosities. Gas-grain collisions and the infrared emission from grains can dominate the gas heating in molecular clouds with embedded stars. The ejection of newly-formed, vibrationally-excited H₂ molecules from grains behind dense, dissociative shocks leads to postshock gas heating which produces strong far-infrared and millimeter line emission as well as H₂O maser emission.

1. INTRODUCTION

The interstellar medium (ISM) is far from Local Thermodynamic Equilibrium; in addition to the blackbody radiation field of 3 K there are generally present dilute fields of highly energetic particles and, especially, photons. The gas and dust temperatures can therefore exceed 3 K to the extent that they couple with these energetic particles and photons. The predominant source of the photons are stars, and interstellar gas does not couple well with starlight; it is especially transparent to photons with energies less than the Lyman limit of 13.6 eV. Therefore, outside of HII regions, the gas is quite cool relative to the temperature of the stellar radiation field. The gas would be cooler still if dust grains did not serve as an intermediary in the energy flow from stellar radiation to gas heating. Four mechanisms couple the gas to starlight via grains.

- 1. Gas-grain collisions (cf., Burke and Hollenbach, 1983). Deep in opaque molecular gas associated with a nearby star, starlight is absorbed by grains, the energy is reradiated in the infrared and reabsorbed by grains thereby heating the grains to temperatures typically $\sim 30 100$ K. The cooler gas collides with the warm grains and is heated "conductively".
- 2. Grain-IR (cf., Takahashi et al., 1983, 1985; Tielens and Hollenbach, 1985). Under the same conditions as in (1), the IR photons radiated by the warm grains are absorbed by, for example, H_2O molecules or O atoms in the opaque, molecular gas. Collisional deexcitation of these excited molecules and atoms with other gaseous components transfers the excitation energy to gas heating.

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Grain Heating of ISM Gas					
ISM State	Intercloud	Diffuse	HII	PDR	Molecular
Gas Density (cm ⁻³) Gas Temperature (K) Heating by Grains	0.1 7000 PE	30 100 PE	10-10 ⁴ 10 ⁴ PE	10-10 ⁶ 30-10 ³ PE Grain IR Gas-grain	10 ³ -10 ⁷ 10-3000 <i>H</i> ₂ Form Grain IR Gas-grain

TABLE 1

- 3. Grain photoelectric (PE) (cf., Watson, 1972; Jura, 1976; Draine, 1978; deJong, 1980; Tielens and Hollenbach, 1985*a*; d'Hendecourt and Léger, 1987). For grains which lie at $A_v < 1-5$ from stars with significant UV fluxes (in photodissociation regions or "PDRs"), the UV absorbed by the grains results in the emission of energetic electrons into the gas. If these ejected electrons carry more energy than the electrons recombining on the grains, there is a net heating.
- 6. Desorption from thermally fluctuating small grains (cf. Duley, 1976). Gas heating results from the desorption of "hot" atoms and molecules from small grains following a temperature spike occurring after the absorption of a single stellar photon. Under special circumstances, this process may be of comparable importance to grain photoelectric heating.

Grains can also serve as intermediaries in the heating of interstellar gas by catalyzing the release of the chemical heat of H_2 formation to the gas. Interstellar H_2 molecules form primarily on interstellar grains (cf., Hollenbach and Salpeter, 1971; Hollenbach and McKee, 1979). Hydrogen atoms stick to grain surfaces and migrate across the surfaces to combine with other hydrogen atoms. The 4.48 eV of binding energy which is released upon the formation of the molecule is distributed into: (i) heating of the grain, (ii) ejection, or translational, energy of the newly-formed molecule, and (iii) rotational and especially vibrational energy of the molecule. Although there is some controversy over the relative proportion of this three-way energy split (see discussion in Section 4 below), the predominant view is that a large fraction of the 4.48 eV goes into the vibrational excitation of the newly-ejected molecule. This energy can be delivered as heat to the gas if subsequent collisional deexcitations (by H atoms and H_2 molecules) of this excitation energy occur before it is radiated away.

Table 1 provides an introductory overview of the role of grain heating in various states of the ISM; listed are the intercloud phase, the diffuse cloud phase, and then, three higher pressure states of the ISM associated with gravitationally-bound gas and/or star formation: HII regions, PDRs (HI regions where UV dominates the chemistry), and opaque molecular clouds (note that, although in molecular clouds the gas is generally at $T \sim 10 - 100$ K, postshock molecular gas can attain $T \lesssim 3000$ K). The numbers in Table 1 are all approximate. "PE" and " H_2 Form" refer to photoelectric heating and H_2 formation heating, respectively. This overview is discussed in more detail in the Sections below. Grain photoelectric heating (Section 5) may dominate in intercloud, diffuse and PDR gas and is an important contribution to HII regions. H_2 formation heating (Section 4) plays a major role in determining the structure of dense, dissociative shocks. Gas-grain collisions (Section 2) and the grain-IR mechanism (Section 3) can also dominate in certain portions of PDR regions and molecular gas.

2. GAS-GRAIN COLLISIONS

In order for a gas-grain collision to result in gas heating, an incident gas molecule usually H_2 - with average kinetic energy 2kT strikes a warmer grain and rebounds or is re-evaporated with higher average energy. The net energy input to the gas per collision is given by:

$$H_{GG} = \left[\frac{n_{gr}\sigma_{gr}}{n}\right]n^2 v_{th}\alpha \left(2kT_{gr} - 2kT\right), \qquad (1)$$

where n_{gr} is the grain density, *n* is the gas density, σ_{gr} is the average grain cross section, the term in brackets is the grain area per hydrogen nucleus which is ~ $2-3 \times 10^{-21}$ cm⁻² (cf., Omont, 1986), v_{th} is the thermal velocity of the colliding gas particle (hydrogen), α is the "accommodation coefficient" and T_{gr} is the grain temperature. The maximum value for α is unity and this is its typical value in cold $(T \leq 100 \text{ K})$, interstellar gas (cf., Burke and Hollenbach, 1983, who analyzed α as a function of T, T_{gr} , and the grain and gas composition).

This mechanism is dominant in opaque molecular gas $(A_v \gtrsim 3-5)$ near stars, where the radiation field has warmed grains above the gas temperature. It dominates cosmic ray heating when:

$$n (T_{gr} - T) T^{\frac{1}{2}} \gtrsim 10^5 \text{ cm}^{-3} \text{K}^{\frac{3}{2}}.$$
 (2)

This condition is fulfilled, for example, if $T_{gr} = 35$ K, T = 25 K, and $n \gtrsim 2 \times 10^3$ cm⁻³.

An interesting application of this mechanism was made by Krugel and Walmsley (1984), who noted that a size distribution of grains produces a temperature distribution in the grain material. The smaller, hotter grains dominate the surface area of the grains and therefore the heating. The larger, cooler particles, however, may dominate the color temperature observed in the far-infrared (e.g., the 80 μ m or 160 μ m to 640 μ m color temperatures). Therefore, one could potentially observe gas which *looks hotter* than the grains (a factor of ~ 1.2 when compared with the dust color temperature), yet the gas-grain collisional heating is still operative. The maximum T/T_{gr} is obtained for $n \gtrsim 10^5$ cm⁻³, so that the gas couples well to the grains. It appears marginally possible to explain the observed T/T_{gr} in B35 (Lada *et al.*, 1981) and the galactic center (Gusten *et al.*, 1981) by this mechanism. Strengthening this line of argument for the case of B35, Smith (1988) reports that IRAS data shows the presence of a large surface area of small, warm grains with temperatures $T_{gr} > T$ in addition to the cooler grains observed by Lada *et al.*, at longer wavelengths.

3. ABSORPTION OF GRAIN IR EMISSION

Grains also heat the gas by emitting continuum far-infrared photons which are absorbed by the gas. The excited atom or molecule is then collisionally deexcited, which transfers the energy into gas heating. Like gas-grain collisions, this mechanism works when $T_{gr} > T$ and only dominates in opaque molecular clouds, where grain photoelectric heating is negligible. Takahashi *et al.* (1983, 1985) showed that the grain IR mechanism with H_2O as the absorber dominates gas-grain collisions when $T_{gr} \gtrsim 40$ K and $x(H_2O) \gtrsim 5 \times 10^{-6}$. Tielens and Hollenbach (1985*a*) showed that this mechanism with OI as the absorber (the ${}^{3}P_{2} - {}^{3}P_{1}$ fine structure transition at 63 μ m) dominates deep ($A_{v} \sim 5 - 10$) in dense ($n \sim 10^{5}$ cm⁻³) PDRs illuminated by UV fields at least 100 times the ambient interstellar field.

4. H_2 FORMATION HEATING

The formation of H_2 on interstellar grains is likely followed by their ejection into the gas carrying much of their formation energy as translational energy E_{ej} and vibrational and rotational excitation energy E_{vr} . The former directly heats the gas while the latter is transformed to gas heat by collisional deexcitations. The heating rate is given (cf., Hollenbach, 1988):

$$H_{H_2} = 0.5 \left[\frac{n_{gr} \sigma_{gr}}{n} \right] n n_H v_{th} \beta \left[E_{ej} + E_{vr} \left(\frac{1}{1 + \frac{n_{ar}}{n}} \right) \right], \qquad (3)$$

where n_H is the atomic hydrogen density, the factor 0.5 reflects the fact that it takes 2 H atoms to make a molecule, the terms to the left of β represent one half the rate of H atom collisions with grains per unit volume, β is the probability of H_2 formation on the grain, and n_{cr} is the critical density for collisional deexcitation of rovibrationally-excited H_2 by impacts with hydrogen atoms (H atoms generally dominate over H_2 because of their much larger rate coefficients, see Hollenbach, 1988). The quantity in parenthesis in Equation 3 gives the fraction of excited H_2 molecules which are collisionally deexcited as opposed to radiatively deexcited. An accurate quantitative calculation of the H_2 formation heating mechanism is difficult because of uncertainties in the T and (especially) the T_{gr} dependence of β (see Hollenbach and McKee, 1979,1988), in the estimates of E_{ej} and E_{vr} (see discussion below), and in the collisional deexcitation rates (the H rates come from old, unpublished, theoretical work by S.-I. Chu (1977) and should be verified by the more accurate numerical treatments now possible).

Several authors (Hollenbach and Salpeter, 1971; Hunter and Watson, 1978; Duley and Williams, 1986) have made theoretical arguments that $E_{vr} \sim 4$ eV for refractory surfaces. Reliable laboratory confirmation is scanty, but generally supportive (cf., Lin and Somorjai, 1985; Comsa and David, 1985). Schutte *et al.* (1976) review earlier work and perform the most astrophysically relevant experiments; their conclusion is that roughly one half of the recombination energy emerges into the gas as ejection or rovibrational energy when the surface coverage of adsorbed H_2 is small (as is the case for most astrophysical applications). However, uncertainties in the recombining fraction could raise this estimate. Tielens and Allamandola (1987) warn that interstellar grain surfaces may contain functional groups such as OH and



Fig. 1. Postshock structure for dense $(n_o > 10^5 \text{ cm}^{-3})$, dissociative $(v_o > 40 \text{ km s}^{-1})$ shocks, showing T plateau at 300-400 K caused by H₂ formation heating.

CH groups with vibrational modes at about 3 μ m; these groups can accept the vibrational H_2 quanta, increase the fraction of the recombination energy transferred to the grain, and lower the fraction ejected into the gas.

Assuming $E_{vr} \sim 4 \text{ eV}$, Hollenbach and McKee (1988) and Neufeld and Dalgarno (1988) show that H_2 formation heating significantly affects the postshock structure of dense, dissociative shocks. Figure 1 shows a portion of the postshock temperature profile behind a dissociative shock with preshock density $n_o = 10^7 \text{ cm}^{-3}$ and shock velocity 100 km s⁻¹ as a function of the hydrogen column N behind the shock. This profile is obtained with minor variations for shocks with velocities 40 km s⁻¹ $< v_o < 200 \text{ km s}^{-1}$ and densities $10^5 \text{ cm}^{-3} < n_o < 10^8 \text{ cm}^{-3}$ (Hollenbach and McKee, 1988). The H_2 formation heating matches the postshock cooling and produces a temperature plateau at $T \sim 300 - 400 \text{ K}$. Large columns of warm atoms and molecules are produced, and observable emission is predicted, for example, from high J SiO, SI (25 μ m), and, behind $n_o \sim 10^7 \text{ cm}^{-3}$ shocks, water maser emission with brightness temperatures up to 10^{14-15} K (Elitzur, Hollenbach and McKee, 1988).

5. GRAIN PHOTOELECTRIC HEATING

5.1. PHYSICAL PROCESSES

Grain photoelectric heating (cf., Watson, 1972; Jura, 1976; Draine, 1978; deJong, 1980; d'Hendecourt and Léger, 1987) is initiated by the absorption by grains or "PAHs" (large polycyclic aromatic hydrocarbon molecules) of UV photons which eject energetic ($\sim eV$) electrons into the gas. In equilibrium the rate of electron ejections from grains equals the rate of recombination, and the grains assume a charge to insure this equality. Often the photoelectric effect dominates the charging and the grain charge is positive. The net rate of gas heating, H_{PE} , is then the energy input of ejected electrons minus the energy loss of recombining electrons. H_{PE} is a decreasing function of the positive charge of a grain, since the ejected electrons must overcome the grain Coulomb potential and emerge into the gas with reduced kinetic energy. H_{PE} depends on a number of parameters involving the grain material, the interstellar grain model, and the physical parameters of the gas and radiation field. The grain material properties include the "work function" or threshold E_{th} for photoelectric emission from a neutral grain (~ 6 - 10 eV, Draine, 1978; deJong, 1980), the photoelectric yield Y per absorbed UV photon(\sim 0.1 - 1 for photons above the threshold, Watson, 1972; Jura, 1976; Draine, 1978; deJong, 1980; d'Hendecourt and Léger, 1987), and the surface properties which determine the sticking probability s_e of an incident electron (s_e is usually taken as 0.3-1.0, see Draine, 1978). The interstellar grain model parameters required include $(n_{gr}\sigma_{gr}/n)$, the geometrical cross-sectional grain area per hydrogen nucleus, and the grain efficiency for UV absorption Q_{abs} (~ 0.75, Draine, 1978). The gas parameters required are the electron density n_e and the gas temperature T; these parameters determine the rate of electron recombinations with the grain and therefore the grain charge. Finally, and most obviously, H_{PE} depends on the UV flux G (from E_{th} to 13.6 eV in HI regions or molecular gas because the more energetic photons are absorbed in HII regions), since the UV photons initiate the process and determine the grain charge.

We can subsume much of the physics in a "heating efficiency" parameter ϵ , defined by the equation:

$$H_{PE} = \epsilon G n_{gr} \sigma_{gr} Q_{abs}. \tag{4}$$

Therefore, ϵ is the ratio of the heat input to the gas divided by the total UV energy absorbed by grains. Figure 2 schematically diagrams the photoelectric process. Typically, ~ 10 eV photons are absorbed inside a positively charged grain. One out of ten (Y ~ 0.1) photons leads to the ejection of an electron with kinetic energy (gas heat) $\lesssim 1$ eV, the remaining 9 eV of the photon being used to overcome the work function and Coulomb barrier of the grain and being dissipated as the electron scatters through the material to the surface. Therefore, typically,

$$\epsilon \lesssim \left(\frac{1eV}{10eV}\right) Y \sim 10^{-2}.$$
 (5)

About 1% of the UV energy heats the gas and the rest heats the grains and is reradiated as grain far-infrared continuum. Thus, ignoring photons below E_{th} which grains may also absorb, the ratio of the luminosities of the gas cooling lines [typically $OI(63 \ \mu m)$ and $CII(158 \ \mu m)$] to the IR continuum is of order $\lesssim 0.01$.



Fig. 2. Microphysics of grain photoelectric heating.

The heating efficiency decreases with increasing positive grain charge. For a specified grain material and model, the charge (and ϵ) depends mainly on the parameter $GT^{\frac{1}{2}}/n_e$, which is proportional to the ratio of the rate of photoionization of grains to the rate of recombinations. The heating efficiency ϵ is plotted as a function of $G_o T^{\frac{1}{2}}/n_e$ for four different grain models in Figure 3, assuming that the gas temperature is $<< 10^4$ K so that the recombination energy is negligible. $G_o = G/1.6 \times 10^{-3} \text{ erg cm}^{-2} \text{ s}^{-1}$ is a unitless flux normalized to the Habing (1968) field for the local ISM integrated from 6 eV to 13.6 eV. The four models shown include the grain models of Draine (1978) and deJong (1980) and the PAH models of d'Hendecourt and Léger (1987, dHL in Figure 3) and Lepp and Dalgarno (1988, LD in Figure 3). DeJong adjusted the grain work function and photoelectric yield in his model to values (6 eV and 0.1, respectively) which would produce gas heating rates in accordance with observed gas cooling rates in diffuse clouds. Draine utilized laboratory thresholds and yields in his model and assumed a grain model with a minimum grain size of 50-100 Å. Watson (1972) and Jura (1976) have shown that the inclusion of a population of small (<< 100 Å) grains can increase the photoelectric heating rate because of the increase in the photoelectric yield and in the grain cross sectional area per H nucleus. This is the fundamental reason why the Draine curve lies below the PAH curves in Figure 3. The main difference between dHL and LD is the PAH abundance, taken to be 4 times larger in dHL. $G_o T^{\frac{1}{2}}/n_e \sim 10^3 - 10^5$ in the intercloud phase, in diffuse clouds, or in molecular clouds near stars. Using Figure 3, we therefore predict $\epsilon \sim 10^{-2} - 10^{-3}$.



Fig. 3. Photoelectric heating efficiency as a function of $G_o T^{\frac{1}{2}}/n_e$ for HI gas at $T << 10^4$ K. Four models are plotted, see text.

5.2. APPLICATIONS

Maciel and Pottasch (1982) and Oliviera and Maciel (1986*a*,1986*b*) have shown that grain photoelectric heating can be significant in HII regions. They conclude that grain photoelectric heating exceeds gas photoelectric heating (photoionization of *H* and *He*) over a substantial portion of certain HII regions. The average gas temperature in HII regions is raised by ~ 10% and the local temperature can be raised by as much as 45% over models in which just gas photoelectric heating was included.

A number of researchers (cf., Tielens and Hollenbach, 1985*a* and references therein) have studied the photoelectric heating of the "surfaces" of molecular clouds by incident UV flux. "Surfaces" is a misleading term here since the regions of significant photodissociation and photoelectric heating extend to $A_v \sim 3-10$ into the cloud and include regions which are predominantly H_2 and CO. Since the average visual extinction through molecular clouds is ~10 (Solomon *et al.*, 1987), most of the molecular mass of the ISM is in these PDRs, and, of course, the atomic gas is also in PDRs. Thus, grain photoelectric heating dominates in most of the interstellar gas. In the PDR models, most of the observed ${}^{12}CO J=1-0$ as well as the fine structure emission (e. g., CII(158 μ m), OI(63 μ m), and S*i*II(35 μ m)) emerges from the grain photoelectrically heated region. Wolfire *et al.* (1988*a*) explain an observed correlation of CII(158 μ m) with ${}^{12}CO J=1-0$ (Crawford *et al.*, 1985) via PDR models.



Fig. 4. Correlation of grain IR luminosity with the $CII(158 \ \mu m) + OI(63 \ \mu m)$ luminosity from the gas. Arrows represent lower limits where only the $CII(158 \ \mu m)$ line has been observed.

Tielens and Hollenbach (1985b) construct a PDR model for gas behind the HII region in Orion, and obtain a good fit if $n \sim 10^5$ cm⁻³ and $G_o \sim 10^5$ (Θ^1 Ori C about 0.2 pc from the neutral gas). The gas attains temperatures of ~ 1000 K at $A_v \leq 2$, while the grain temperatures are ~ 75 K. This high T/T_{gr} ratio is a hallmark of grain photoelectrically heated regions, differentiating them from regions heated by gas-grain collisions or the grain IR radiation. PDR models, with grain photoelectric heating generally dominant, are being applied to a number of observed objects including the neutral gas surrounding HII regions and planetary nebulae (Burton et al., 1988; Lane et al., 1988), reflection nebulae (Chokshi et al., 1988), and the ISM as a whole in the nuclei of external galaxies (Wolfire et al., 1988b).

Figure 4 plots the $CII(158 \ \mu m) + OI(63 \ \mu m)$ luminosity (the dominant coolants in PDRs) versus the IR continuum luminosity for a number of galactic and extragalactic sources. For galactic sources, only those with measurements of both $CII(158 \ \mu m)$ and $OI(63 \ \mu m)$ are included (Genzel and Stacey, 1985; Tielens and Hollenbach, 1985*a*); for external galaxies, a number with just $CII(158 \ \mu m)$ measurements (arrows) have been included (Crawford *et al.*, 1985). Note that there is a good correlation over about 8 orders of magnitude in luminosity. This correlation corresponds to a heating efficiency ϵ of about $10^{-2} - 10^{-3}$, which is precisely the ratio predicted by the theory of grain photoelectric heating. The fact that the interstellar media in external galaxies follow the correlation emphasizes the point that grain photoelectric heating is an extremely important general heating mechanism in the ISM.



Fig. 5. The grain photoelectric heating rate per H atom as a function of the gas temperature, T, and n_e for three grain models (see text).

Figure 5 plots the heating rate per H atom as a function of T for various grain models (see Figure 3), for two electron densities ($n_e = 0.1$ and 0.01 cm⁻³) which span the range anticipated for diffuse clouds and the intercloud medium, and for the ambient interstellar radiation field analytically described by Draine (1978). The heating required to explain the observed temperatures of these regions is of order $10^{-26} - 10^{-25}$ erg s⁻¹ per H (cf., deJong, 1980). The steep decline at T ~ 10⁴ K occurs because the electrons recombining with the grains have comparable energies to the photoelectrically ejected electrons. Draine (1978, dotted lines in Figure 5) concluded that he could explain the heating in diffuse clouds but not that in the intercloud medium; his heating drop due to recombination occurred at temperatures typical of the intercloud temperature ($T \sim 7000$ K). The PAH models look promising to explain the intercloud heating (d'Hendecourt and Léger, 1987, solid lines; Lepp and Dalgarno, 1988, dashed lines). The lower E_{th} and the quantum nature of the charge on PAHs both serve to raise the heating rate in the 7000 K regime. However, deJong (1980) has pointed out that somewhat different assumptions on Y and E_{th} can provide a fit to intercloud heating with standard grains.

6. SUMMARY AND CONCLUSION

Grain and PAH photoelectric heating probably dominates the heating of intercloud gas, diffuse clouds, and substantial portions of molecular clouds (PDRs). It is also significant in HII regions. Grain photoelectric heating models have been constructed which explain observed fine structure and molecular emission from galactic clouds and external galaxies. Physical parameters such as the incident UV flux G, the gas density n, the clumpiness in the gas and the gas phase elemental abundances can be obtained. Grain photoelectric heating explains the observed correlations of CII(158 μ m) with ¹²CO J=1-0 and of the CII(158 μ m) + OI(63 μ m) luminosity with the IR continuum luminosity.

 H_2 formation heating is important in dense $(n_o \gtrsim 10^5 \text{ cm}^{-3})$, dissociating $(v_s \gtrsim 40 \text{ km s}^{-1})$ shocks, producing a large column $N \sim 10^{22-23} \text{ cm}^{-2}$ of warm $T \sim 300-400$ K gas. Strong IR and submillimeter line emission (e.g., high J SiO and SI(25 μ m)) is predicted. H_2O maser emission is produced behind very dense $(n_o \sim 10^7 \text{ cm}^{-3})$, dissociating shocks.

Gas-grain collisional heating and heating from grain IR emission is an important gas heating mechanism in opaque (insignificant UV for the grain photoelectric mechanism) molecular gas associated with stars which heat the grains to $T_{gr} > T$.

Future progress in the area of gas heating by interstellar grains depends on better laboratory measurements or interstellar observations which determine E_{vr} and E_{ei} , the internal and ejection energies of newly-formed H_2 molecules leaving interstellar grain surfaces and which determine grain material parameters relevant to the photoelectric heating process including Y, E_{th} , s_e and the photoionization thresholds and cross sections for ionizing neutral and singly ionized PAHs.

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