N86-23517

THE EFFECTS OF CHARGED DUST GRAINS ON IR MOLECULAR EXCITATION. R. Puetter and I. Krinsky, Center for Astrophysics and Space Sciences, UCSD. In this abstract we discuss a number of issues involving grain charging in the interstellar medium. Such effects include (1) Stark broadening of molecular spectral features, (2) electrostatic grain rupturing, (3) enhancements in particle-grain collision cross sections, and (4) excitation of molecular rotations and/or vibrations.

It has long been know that interstellar grains have an electric charge (see, for example, Spitzer's book "Physical Processes in the Interstellar Medium"). Simple arguments give electrostatic potentials of a few times kT of the gas. (Here we will be largely concerned with grains charged by sticking collisions with hot electrons; consequently the grains will be negatively charged. The effects of positive, photoelectrically charged grains, however, can also be important and should not be ignored.) Thus, for grains with a radius of 0.03μm, the electric field, $\vec{\varepsilon}$, at the grain surface will be of the order 10^6 volts per centimeter or 3×10^3 in cgs units. Note that smaller particles would acquire an even higher surface field, resulting in the onset of significant field emission. Furthermore particle breakup will occur under such high fields, especially if the tensile strength of the particles is low such as in lose particle agregates. At the smallest sizes (e.g. a few times 10^{-3} μm) only strong refractory grain cores are able to survive particle potentials of a few volts (Hill and Mendis 1979, The Moon and the Planets, 21, 53).

The Stark broadening of a rigid rotator in an electric field can be easily calculated, giving a fractional shift in the rotational energy, E, of $\Delta E/E \approx d\vec{\varepsilon}/E$ where d is the permanent dipole of the molecule. Since molecules typically have permanent dipoles of the order of a few debyes (1 debye $\equiv$ 10^{-18} esu cm, and we shall assume throughout that d=3 debyes), we find $\Delta E/E$ to be roughly 30. Hence under these conditions the Stark effect is much more than a small perturbation on the quantum mechanical states and causes any rotational sub-structure to be "washed out".

It should be noted that through Stark broadening the large electric field will affect both gas phase rotators and molecular rotators trapped in ice mantles. Furthermore, the strong electric field may also affect the quantum mechanics of surface states and solid state transitions.

The presence of charged grains also affects the collision cross sections for charged particles. Quite obviously, grains and particles of like charge are repelled, while grains and particles of opposite polarity are attracted. The enhancement to the collision cross section over the geometric cross section is well known (again see, for example, Spitzer's book "Physical Processes in the Interstellar Medium") and is given by Q =

$1 + (2eZV/3kT)$, where e is the charge on the electron, Z is the charge on the particle, V is the potential of the grain, and T is the kinetic temperature of the particle. For example, for positive molecular ions with a kinetic temperature of 100 K passing by a negatively charged grain of 3 volt potential, the enhancement to the geometric cross section is Q = 233.

We would also like to point out that charged grains may give rise to the well known unidentified infrared emission features seen at wavelengths of 3.3, 3.4, 3.5, 6.2, 7.7, 8.6, and 11.3μm in a wide range of astrophysical objects (including the spectrum of the galaxy M82--Willner et al. 1977, Ap.J.(Letters), 217, L121). These features apparently originate in the interface regions between the hot H II gas and the molecular cloud material (see Willner, Puetter, Russell, and Soifer 1979, Astrophys.SpaceSci., 65, 95, and references therein). Such a spatial correlation naturally suggests a molecular origin for the observed emission. This explanation is further strengthened by the fact that the 2 to 20μm spectral region is the "molecular signature" region in which most molecules emit strong rotation-vibration spectra. Based on the observation that the 3.3μm feature does not break up into the standard rotation-vibration structure under high spectral resolution (Grasdalen and Joyce 1976, Ap.J.(Letters), 205, L11 and Tokunaga and Young 1980, Ap.J.(Letters), 237, L93), most authors currently agree that if molecules are responsible for the observed emission, then they occur in the solid state as volatile mantles on more refractory grain cores. Two competing theories of the origin of this molecular emission are presently in favor: (1) thermal emission from grains containing volatile mantles (see Dwek, Sellgren, Soifer, and Werner 1980, Ap.J., 238, 140) and (2) UV fluoresence of molecules in volatile mantles (see Allamandola, Greenberg, and Norman 1979, Astron.Astrophys., 77, 66). Both of these senarios face problems. In the thermal emission case, an astronomical object has been found which apparently requires dust temperatures which are quite high ($T_{dust} \simeq 10^3$ K), considerably higher than expected and which remain constant independent of the distance to the exciting source (Sellgren, Werner, and Dinerstein 1983, Ap.J.(Letters), 271, L13). In the UV fuoresence senario, on the other hand, the effeciency of the conversion of UV photons into IR transitions must be very high, perhaps unacceptably high (Dwek, Sellgren, Soifer, and Werner 1980, Ap.J., 238, 140).

There might be several ways in which charged grains could give rise to the unidentified emission features. First, charged molecular ions might be attracted to charged grains, accelerated to several electron volt kinetic energies, and collide into the grain. Such collisions would certainly have sufficient energy to excite vibrational transitions, if not sufficient to break up the molecule. Furthermore, due to the Stark effect, such emission would not show the typical rotational sub-structure since adjacent rotational states would be smeared together. A second senario would involve close passage of molecules and grains. Classical calculations of molecular proportioned, dipole rigid rotators demonstrate that the torques exerted on molecules during a grain passage can change the rotational energy of the molecule on the order of the dipole-electric field energy. Once the molecule is in such excited rotational states, it might be possible for rotation-vibration coupling to distribute the energy into vibrational motion.

Having proposed several mechanisms, we now turn to an analysis of the amount of observable emission that might result from these processes. The volume emissivity of both processes can be estimated from

$$4\pi j = h\nu\, N_{vib} v_{mole} n_{grain} \sigma$$

or

$$4\pi j = h\nu\, N_{vib} v_{mole} \sigma\, n_H^2\, (n_{mole}/n_H)(n_{grain}/n_H)$$

where N_{vib} is the number of vibrational transitions a molecule experiences in passing by or colliding with a grain, σ is the grain-molecule cross section ($\equiv \sigma_0$, the geometric cross section for neutral molecules; $\sigma_0 Q$ for charged molecular ions), and v_{mole} is the relative velocity of the molecule and grain. Assuming a gas to dust mass ratio of 100, we find

$$4\pi j = 2.8 \times 10^{-33}\, N_{vib} v_{mole} \sigma\, n_H^2\, Q(n_{mole}/n_H)\lambda^{-1}$$

where λ is the wavelength in microns of the feature.

We can now estimate the flux of radiation received at the telescope. Assuming the emission fills an angular beam, Ω, of 10"x10", that we are looking through a path length, L, of material 0.2 parsecs long, that the value of Q is 300, that the hydrogen abundance is 10^6 (the density that might be expected in some of the denser condensations near the Orion molecular ridge), that the abundance of the revelant molecular species is 10^{-4} relative to hydrogen, and that v_{moles} is 2.6×10^4 cm s^{-1} (i.e. the velocity corresponding to a molecule of molecular weight 25 and a kinetic temperature of 100 K), the observed flux, $F_{obs}(\equiv jLQ\Omega)$, received by the telescope is given by

$$F_{obs} = 2.4 \times 10^{-17} N_{vib}\lambda^{-1} \text{ W cm}^{-2}$$

Hence we see that the predicted brightness compares favorably with observed flux levels (a few times 10^{-17} W cm^{-2}, see, for example, the fluxes quoted in Dwek, Sellgren, Soifer, and Werner 1980). Slightly higher fluxes can be obtained by using smaller grains, although we must point out that this mechanism will only work with abundant molecular species in relatively dense regions. Still, small molecules and dust are known to exist in abundance in the gas phase in molecular cloud-H II region interfaces and shock processes in these regions will contribute to density enhancements. Thus, this interpretation of the unidentified emission features could be quite attractive.