The Diffuse Interstellar Bands
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Formation, Evolution and Destruction of Possible DIB Carriers: Dirty Molecular Hydrogen Ice Clusters

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Abstract. We suggest that the diffuse interstellar bands (DIBs) are absorption lines arising from electronic transitions in molecular clusters primarily composed of a single molecule, atom, or ion ("seed"), embedded in a single-layer shell of H_2 molecules (Bernstein *et al.* 2013). We refer to these clusters as CHCs (Contaminated H_2 Clusters). CHCs arise from cm-sized, dirty H_2 ice balls, called CHIMPs (Contaminated H_2 Ice Macro-Particles), formed in cold, dense, Giant Molecular Clouds (GMCs), and later released into the interstellar medium (ISM) upon GMC disruption. Absorption by the CHIMP of a UV photon releases CHCs. CHCs produce DIBs when they absorb optical photons. When this occurs, the absorbed photon energy disrupts the CHC.

Keywords. ISM: clouds, ISM: lines and bands, ISM: molecules

1. Introduction

The raw material for CHCs is assembled in cold cores of molecular clouds or Giant Molecular Clouds (GMCs). GMCs contain copious, cold, dense, cores, with temperatures ranging over T $\sim$ 5-10 K and H_2 densities of $n_{H2} \leqslant 10^6$ cm^{-3}. H_2 and seed molecules aggregate to form CHC precursors, in the form of "dirty" H_2 ice balls, referred to as Contaminated H_2 Ice Macro-Particles (CHIMPs). The GMCs are disrupted by radiation pressure from the stars they spawn. Roughly $\sim$ 10% of the disrupted mass is in the form of dense molecular clumps of size $\sim$ 1pc, mass $\sim$ 10-1000 $M_\odot$, and velocity dispersion $\sim$ 10 km/sec (Oort 1954). These GMC cloud remnants serve as a reservoir for CHIMPs, which release CHCs that produce the DIBs. The life cycle of a CHC is illustrated in Figure 1, with quantitative analyses of the key formation and destruction processes presented in the following sections.

2. CHIMP and CHC Formation and Stability

CHIMP growth can be quantified under the following assumptions: (1) a growth rate limited by collisions of seeds with the CHIMP, (2) unity sticking coefficients for collisions between a seed and the CHIMP surface, (3) instantaneous coverage of a newly deposited surface seed by a layer of H_2 molecules, (4) no collisions between CHIMPs, and (5) no photo-destruction of CHIMPs in the core of a GMC due to absorption of energetic photons (i.e., ultraviolet photons do not penetrate into the cores). Then, the CHIMP radius, corresponding to a characteristic lifetime for the GMC, Δt_{GMC}, follows from the

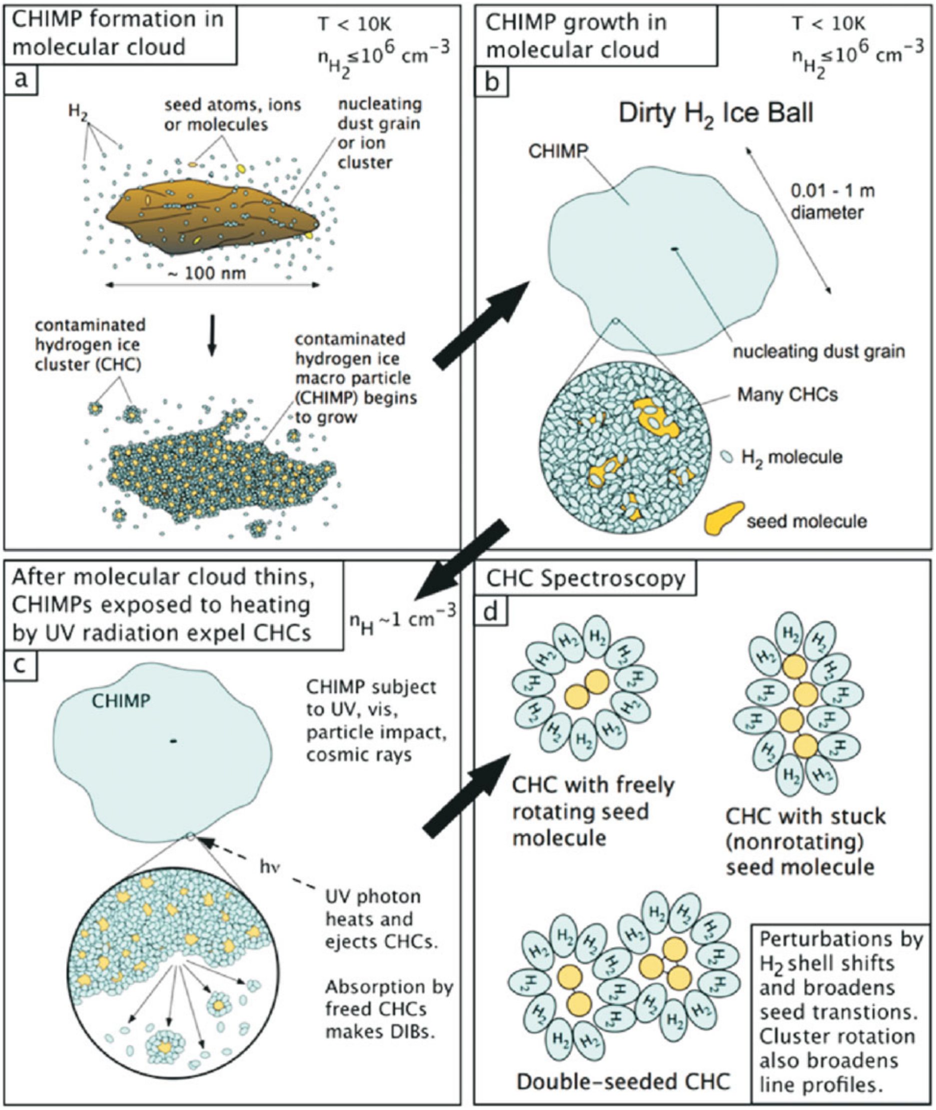

Figure 1. Life cycle of a CHC.

standard gas-kinetic expression for gas-surface collisions,

$$R_{CHIMP} = n_s \left(\frac{kT}{2\pi m_s} \right)^{1/2} \Delta t_{GMC} N_{H2} \sigma^3_{H_2},$$

where n_s is seed number density, m_s is seed mass, T is gas temperature, N_{H2} is the number of H_2 molecules bound by a seed, and σ_{H2} is the H_2 Van der Waals diameter.

Using characteristic values for GMC's, T = 10 K, $n_{H2} = 10^5$ cm^{-3}, Δt_{GMC} = 10 Myr, and for the seeds, m_S = 36 amu (e.g., C_3), N_{H2} = 60 H_2 molecules (~1.5 layers per seed), σ_{H2} = 3.4 Å, χ = 0.003 (seed mole fraction), we find $R_{\rm CHIMP}$ = 0.3 cm. Considering the variability of GMC dense cores (Murray *et al.* 2010), we suggest that the CHIMPs are produced over a range of diameters, 0.1-100 cm.

CHCs and CHIMPs are fragile because they are held together by weak Van der Waals and ion-induced dipole interactions for neutral and ionic seeds, respectively. Typical Van der Waals bond energies are 0.004 eV for H_2-H_2 and 0.07 eV for seed-H_2 interactions, and a typical ion-induced dipole interaction energy for ion-H_2 is 0.5 eV. When a UV photon (∼12 eV) is absorbed by an H_2 molecule, there is sufficient energy available to break all the local bonds associated with a neutral seed and its surrounding layer(s) of H_2 molecules and approximately 50% of the bonds for an ionic seed. Some of the energy, ∼ 4.5 eV, is used to break the H-H bond. The remainder, ∼ 7.5 eV, is quickly thermalized due to collisions of the high velocity H atoms, produced by the photo-dissociation process, with neighboring H_2 and seed molecules. In a CHIMP, the thermal energy is dissipated over many H_2 and seed molecules, resulting in mild heating of the CHIMP surface and the release of CHCs. In a CHC, the thermal energy is dissipated over a much smaller number of molecules, resulting in the complete dissociation of neutral-seeded CHCs and partial dissociation of ion-seeded CHCs.

When exposed to the ISM radiation field incident on the outer surface of a molecular cloud, CHIMPs begin to erode. We assume the primary erosion process is desorption of CHCs near the surface, from localized, transient heating upon absorption of energetic, far-UV photons below ∼ 1000 Å for H_2 (Jura 1974). The change in CHIMP radius with time is given by,

$$\Delta R_{CHIMP} = \varepsilon \frac{2\pi F_{UV}}{\rho_{H_2(S)}} \frac{h\nu}{D} \Delta t_{ISM},$$

where ϵ is an efficiency factor related to the penetration depth of the photon, F_{UV} is the integrated ISM UV flux below 1000 Å, $\rho_{H2(S)}$ is the density of solid H_2, hν is the average UV photon energy, and D is the energy required to desorb an H_2. The efficiency factor ϵ is determined by the requirement that absorption of a UV photon occur near the surface, within ∼40 Å, thereby heating the surface and promoting rapid desorption of CHCs. We assume that CHCs will be released with a variable number of shell H_2's, ranging from a single H_2 up to the maximum number supported by the seed-H_2 interaction potential. The variability in the number of shell H_2's may lead to many, distinct DIB features for a single seed. If the photon penetrates deeper, then its energy is diffused throughout the cluster, and the very small change in temperature is radiated back into the ISM, maintaining radiative equilibrium with the CMB at 2.7 K. Given the average UV absorption cross section for H_2 of ∼1x10^{-17} cm^2, the average penetration depth is ∼400 Å, thus, $\epsilon = 0.1$ (i.e., 40 Å / 400 Å). Using characteristic parameter values, $F_{UV} = 1.5 \times 10^5$ phot/sec/cm^2/sr (Draine 1978), and hν/D = 700, we find ΔR_{CHIMP} = 1 cm for Δt_{ISM} = 10 Myr. Thus, CHIMPs serve as a reservoir for CHCs, allowing CHCs to maintain a continuing presence in the ISM.

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