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Amorphous Hydrocarbon Optical Properties

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Abstract. Hydrogenated amorphous carbon materials, a-C(:H), whose optical properties evolve in response to UV irradiation processing are promising candidate materials for cosmic carbonaceous dust. The optical properties of a:C(:H) particles have been derived as a function of size, band gap and hydrogen content over a wide wavelength range (EUV-cm) and can be used to investigate the size-dependent evolution of a-C(:H) material properties in the ISM.

Keywords. (ISM:) dust, extinction, ISM: molecules, ISM: general

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1. Modelling amorphous hydrocarbon optical properties

The *exact* nature of interstellar carbonaceous dust is still something of a mystery. The evolution a-C:H, a-C or HAC solids is a complex subject that presents a particular challenge because these materials appear to be rather vulnerable to interstellar processing (*e.g.*, Serra Díaz-Cano & Jones 2008; Jones 2009; Jones & Nuth 2011) and to undergo complex, size-dependent evolution arising, principally, from UV photon-driven processing. Here we introduce the optEC$_{(s)}$(a) model for the optical properties of amorphous hydrocarbons, a-C(:H), from hydrogen-poor, a-C, to hydrogen-rich, a-C:H, carbonaceous solids. These data provide a tool that can be used to explore carbonaceous dust and its observable characteristics. The optEC$_{(s)}$(a) model for a-C(:H) materials is presented in a series of papers (Jones 2012b,c,a), which derive their size-dependent structure and their complex refractive indices, $m(n,k)$). These data are publicly-available through the CDS (see the links in papers). We note that the derived data are strongly-constrained by the available laboratory data and have *not* been adjusted to fit astronomical observations. The upper panels in Fig. 1 show the parent or bulk material optEC$_{(s)}$(a) values of n and k, from EUV to mm wavelengths, as a function of the bulk material Tauc band gap, $E_{\rm g}$, and the lower panels in Fig. 1 show the equivalent n and k data for 1 nm radius particles. The major changes that occur as particle size decreases (see Jones 2012a) are: 1) increased surface hydrogenation and CH$_n$ IR band intensities, and 2) a "collapse" of the continua for $\lambda \gtrsim 0.5\,\mu$m and $E_{\rm g} \lesssim 1.5$ eV. As shown by Jones (2012a), the latter effect is due to a reduction in the maximum-allowable, particle-radius-determined aromatic domain sizes as the particle radius decreases, which is clearly seen in the lower panels in Fig. 1. For particles with radii < 1 nm the optical properties begin to look rather similar.

As has been shown the derived optEC$_{(s)}$(a) data are qualitatively consistent with: the FUV-UV bump-visible extinction (non-)correlations, the IR absorption and emission bands in the $3.3 - 3.6\,\mu$m region, variations in the FIR-mm emissivity index (Jones 2012b,c,a). Further, the model predicts that: the $3.28\,\mu$m aromatic CH band will always be accompanied by aliphatic CH$_n$ bands and/or a plateau in the $3.35 - 3.55\,\mu$m region, the end of the road evolution for small a-C(:H) particles is probably aromatic/aliphatic cage-like structuresthat could provide a route to fullerene formation (Bernard-Salas *et al.* 2012; Micelotta *et al.* 2012) the UV-photolytic fragmentation of small a-C:H grains will lead to the formation of small hydrocarbon molecules (CCH, c-C$_3$ H$_2$, C$_4$H, etc.) in PDR

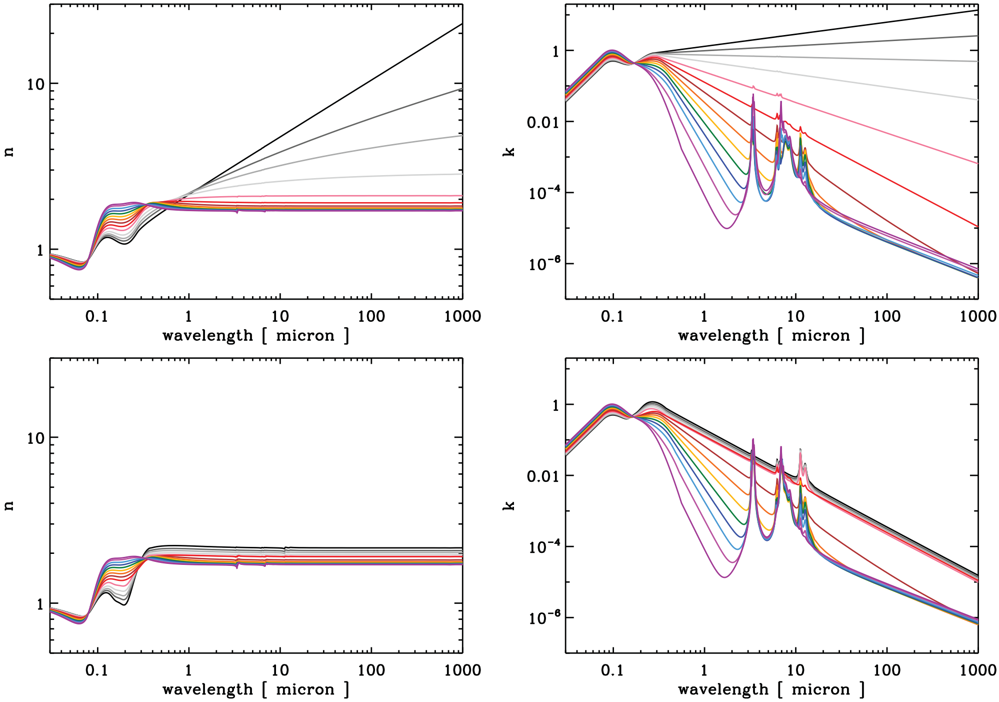

Figure 1. The optEC$_{(s)}$(a) model real and imaginary parts of the complex refractive index, n and k, for bulk a-C:H materials ($\equiv a > 100$ nm, upper) and for $a = 1$ nm particles (lower). The bulk material band gap, E_g, increases from -0.1 eV (top) to 2.67 eV (bottom) at $\lambda \sim 2\,\mu$m.

regions, and "pure" graphite grains and "perfect" PAHs are probably not important components of dust in the ISM (Jones 2012b,c,a).

2. Concluding remarks

A new data-set for the size-dependent optical properties of amorphous hydrocarbon particles, for the first time, provides a means to a detailed exploration of the evolution of these complex materials in the ISM. The principal drivers of their evolution would appear to be photon-induced processing, which results in de-hydrogenation and band gap closure that are coupled to significant changes in their IR spectra and their long wavelength emission.

References

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