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Fullerenes in Circumstellar and Interstellar Environments

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Abstract. In recent years, the fullerene species C_{60} (and to a lesser extent also C_{70}) has been reported in the mid-IR spectra of various astronomical objects. Cosmic fullerenes form in the circumstellar material of evolved stars, and survive in the interstellar medium (ISM). It is not entirely clear how they form or what their excitation mechanism is.

Keywords. Astrochemistry, (stars:) circumstellar matter, ISM: molecules, infrared: ISM

1. Fullerenes in astrophysical environments

Fullerenes (such as the buckminsterfullerene C_{60}) are large carbonaceous molecules in the shape of a hollow sphere of ellipsoid. They are very stable, and thus it was suggested early on that they could also form in space and be abundant and widespread in the Universe (Kroto *et al.* 1985). Astronomical searches for the electronic bands of neutral C_{60} were unsuccessful though (for an overview, see Herbig 2000); and the detection of two diffuse interstellar bands near the predicted wavelengths of C_{60}^{+} awaits confirmation from a gas-phase laboratory spectrum (Foing & Ehrenfreund 1994). C_{60} also has 4 IR active vibrational modes at 7.0, 8.5, 17.4 and 18.9 μm. Dedicated searches for these bands did not result in a detection either (Clayton *et al.* 1995; Moutou *et al.* 1999).

Recently, we reported the detection of the IR active modes of C_{60} and C_{70} in the *Spitzer*-IRS spectrum of the young, low-excitation planetary nebula (PN) Tc 1 (Cami *et al.* 2010). Since then, fullerenes have been found in many more PNe (García-Hernández *et al.* 2010, 2011a), a proto-PN (Zhang & Kwok 2011), a few R Cor Bor stars (García-Hernández *et al.* 2011b; Clayton *et al.* 2011) and even in O-rich binary post-AGB stars (Gielen *et al.* 2011). In addition, fullerenes have turned up in interstellar environments (Sellgren *et al.* 2010; Rubin *et al.* 2011; Boersma *et al.* 2012) and in young stellar objects (Roberts *et al.* 2012) as well. From these detections it is clear that fullerenes are formed in the circumstellar environments of evolved stars. They then either survive in the ISM (possibly incorporated into dust grains), or form there when conditions are right.

2. The fullerene excitation mechanism

To explain the IR emission of cosmic fullerenes, two mechanisms have been considered that offer quite different predictions about the relative band strengths (for a detailed comparison, see Bernard-Salas *et al.* 2012). Thermal C_{60} emission models show large variations in the relative strength of all bands as a function of temperature; for $T \leqslant 300$ K, the 7.0 and 8.5 μm bands are very weak compared to the 17.4 and 18.9 μm bands. For fluorescence on the other hand, the band strengths only depend on the average absorbed photon energy; in that case, the 17.4/18.9 μm band ratio is roughly constant (for reasonable photon energies) while the 7.0 and 8.5 μm bands should be fairly strong.

Observationally, the 7.0 and 8.5 μm bands are often very weak or even undetectable, while there are considerable variations in the 17.4/18.9 μm band ratio; this is more easily explained by thermal models than by fluorescence models. However, these variations could also be the consequence of contamination by PAH emission. In the three known uncontaminated fullerene-rich PNe on the other hand, the 7.0 μm band is far *too strong* to be explained by even fluorescence from C_{60} alone. As pointed out to the careful reader by Bernard-Salas *et al.* (2012), the 7.0 μm emission in those sources includes a significant contribution from C_{70}, provided at least that the emission is due to fluorescence. For one object (Tc 1), fluorescence is further supported by the observation that the C_{60} emission peaks at large distances ($\sim$ 8000 AU) from the central star. If fluorescence is also the excitation mechanism for the other astronomical sources where fullerenes have been detected, then the weak 7.0 and 8.5 μm bands indicate that the fullerene emission is not due to isolated, free C_{60} molecules in the gas-phase; there might be contributions from other species as well and/or the emission may be due to fullerene clusters or nanocrystals.

3. The formation of cosmic fullerenes

Several routes have been proposed to explain the formation of fullerenes in astrophysical environments. Densities in circumstellar and interstellar environments are too low for bottom-up fullerene formation on reasonable timescales (Micelotta *et al.* 2012). Fullerenes could form from the processing of PAHs (Berné & Tielens 2012), but this requires fine-tuned initial conditions. A promising route starts from *arophatics* – large clusters of aromatic rings with aliphatic and olefinic bridges that originate from a:C-H grains (Micelotta *et al.* 2012). UV irradiation first dehydrogenates and aromatizes such structures; subsequent C_2 ejection then shrinks down the resulting cages to C_{60}. Further shrinking is inhibited by a high energy barrier. The spectral imprint of the parent a:C-H grains in the IR spectra of fullerene-rich PNe offers some observational support for this mechanism (Bernard-Salas *et al.* 2012).

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