Detection of C$_{60}$ in embedded young stellar objects, a Herbig Ae/Be star and an unusual post-asymptotic giant branch star

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1 INTRODUCTION

Although considered a candidate carrier for a few infrared (IR) astronomical emission features, as noted in Werner et al. (2004b) and discussed by Sellgren, Uchida & Werner (2007), confirmation of C$_{60}$ together with C$_{70}$ in the planetary nebula (PN) Tc 1 (Cami et al. 2010) and C$_{60}$ in the reflection nebulae NGC 7023 and NGC 2023 (Sellgren et al. 2010, 2011) has only recently been achieved. Further discoveries of neutral C$_{60}$ have since been reported in PNe in the Milky Way and the Magellanic Clouds (García-Hernández et al. 2010, 2011b), weakly H-deficient R Coronae Borealis (RCB) type stars (García-Hernández, Kameswara Rao & Lambert 2011a), a protoplanetary nebula (PPN; Zhang & Kwok 2011), across the ‘veil’ region of the Orion nebula (Rubin et al. 2011), in several post-asymptotic giant branch (post-AGB) objects (Gielten et al. 2011a,b) and possibly in the binary XX Oph (Evans et al. 2011). There is therefore now unambiguous evidence for neutral C$_{60}$ in objects in the later stages of stellar evolution and in the interstellar medium (ISM).

We report here the first detection of C$_{60}$ in two young stellar objects (YSOs) located in the Central Molecular Zone (CMZ) of the Milky Way, in a YSO candidate in the Rosette nebula and in a Herbig Ae/Be star. Taken with earlier reports, these findings show that neutral C$_{60}$ exists over a very wide spectrum of stellar and interstellar evolution, encompassing star-forming regions and young stars, mass-losing evolved stars, PPN, PNe and the ISM. We also report the detection of C$_{60}$ in the post-AGB star HR 4049 which, like HD 97300, is also reported. These observations extend the range of astrophysical environments in which C$_{60}$ is found to YSOs and a pre-main-sequence star. C$_{60}$ excitation and formation mechanisms are discussed in the context of these results, together with its presence and processes in post-asymptotic giant branch objects such as HR 4049.

Key words: astrochemistry – circumstellar matter – stars: pre-main-sequence – stars: winds, outflows – ISM: molecules – Galaxy: centre.

2 BACKGROUND

Astronomical conditions analogous to those of the early laboratory experiments in which C$_{60}$ is formed (Kroto et al. 1985; Krätschmer et al. 1990) might have been expected to favour C$_{60}$ formation, with H-poor RCB stars being good candidates. However, this has not been borne out by observation (Clayton et al. 1995) except in the case of one or possibly two less H-poor RCB stars (García-Hernández et al. 2011a). Alternatively, laser-induced decomposition of hydrogenated amorphous carbon (HAC) is known to produce fullerenes (Scott, Duley & Pinho 1997) and HAC decomposition has been referred to as a possible astrophysical C$_{60}$ formation route (Moutou et al. 1999; Ehrenfreund & Charnley 2000;
Table 1. Coordinates and photometry for the targets with C\textsubscript{60} emission bands. Right ascension, declination and near-infrared magnitudes are taken from the 2MASS catalogue (Skrutskie et al. 2006); mid-infrared magnitudes (where available) are from the Spitzer Infrared Array Camera survey of the Galactic Centre (Ramírez et al. 2008). Spitzer programme numbers and Principal Investigator (PI) names are given for the IRS observations used in this study.

| Name            | RA          | Dec         | J            | K            | [3.6] | [4.5] | [5.8] | [8.0] | Programme (PI) |
|-----------------|-------------|-------------|--------------|--------------|-------|-------|-------|-------|----------------|
| Embedded YSOs   |             |             |              |              |       |       |       |       |                |
| ISOGAL-P J174639.6–284126 | 17:46:39.60  | −28:41:27.00 | >13.8        | 12.95        | 10.28 | 8.83  | 7.38  | 5.58  | 40230 (Ramírez) |
| SSTGC 372630    | 17:44:42.76  | −29:23:16.2  | >16.0        | 12.87        | 10.31 | 8.82  | 7.67  | 6.48  | 40230 (Ramírez) |
| 2MASS J06314796+0419381 | 06:31:47.96  | +04:19:38.2  | 14.01        | 10.67        | –     | –     | –     | –     | 50146 (Keane)   |
| Other targets   |             |             |              |              |       |       |       |       |                |
| HD 97300 (Herbig Ae/Be star) | 11:09:50.03  | −76:36:47.7  | 7.64         | 7.15         | –     | –     | –     | –     | 2 (Houck)       |
| HD 52961 (post-AGB object) | 10:18:07.52  | −28:29:30.7  | 16.06        | 15.42        | –     | –     | –     | –     | 3274 (Van Winckel) |
| HR 4049 (post-AGB object) | 07:03:39.63  | +10:46:13.1  | 6.32         | 5.53         | –     | –     | –     | –     | 93 (Cruikshank)  |

García-Hernández et al. (2010; Sellgren et al. 2010). Following the identification of C\textsubscript{60} and C\textsubscript{70} in the particularly clean spectrum of Tc 1, Cami et al. (2010) suggested that these molecules were formed efficiently in this object because the circumstellar environment was H-poor. However, in their paper on C\textsubscript{60} emission in PNe García-Hernández et al. (2010) pointed out that neither the PN nor its compact core and the central star of Tc 1 are H-poor, and presented evidence in support of the idea that fullerenes are formed in astrophysical environments by the decomposition of HAC (García-Hernández et al. 2011b). They suggested that C\textsubscript{60} and polycyclic aromatic hydrocarbons (PAHs) were likely to be formed together from the decomposition of HAC due to ultraviolet (UV) processing and energetic phenomena such as shocks, and interpreted the deficiency of PAHs in Tc 1 in terms of longer survival times of fullerenes due to their high stability. C\textsubscript{60} formation issues are further explored in papers by Cami et al. (2011) and García-Hernández (2011), with the challenges being extended further by the detection of C\textsubscript{60} in mixed-chemistry post-AGB stars (Gien et al. 2011a) and reported for HR 4049 in this paper.

The phase (gas or solid) and excitation mechanism of C\textsubscript{60} in astrophysical sources are not firmly established and may vary between environments. From their analysis of spectral data for Tc 1 is consistent with high-energy (\sim \text{10 keV}) UV photoexcitation of gas-phase C\textsubscript{60}. At present we are not aware of predicted band strengths based on other possible excitation mechanisms. The discovery of C\textsubscript{60} in YSOs and a Herbig Ae/Be star provides additional environments with which proposed formation and excitation mechanisms can be evaluated.

3 OBSERVATIONS AND DATA REDUCTION

A search was undertaken for C\textsubscript{60} emission bands in spectra recorded with the Infrared Spectrograph (IRS; Houck et al. 2004) of the Spitzer Space Telescope (Werner et al. 2004a). We interrogated the Spitzer Heritage Archive (SHA)\footnote{http://archive.spitzer.caltech.edu} for objects observed at the wavelengths of the C\textsubscript{60} emission bands, concentrating on pre-main-sequence objects and examining several hundred spectra. Targets were selected by visual inspection of pipeline-reduced data in the spectral region around the 18.9-\mu m C\textsubscript{60} band, which is relatively strong and free from blending with atomic lines and PAH emission bands. Data for each object with a potential 18.9-\mu m detection were retrieved from the archive, together with additional targets selected for comparison. Observational details and photometry for the objects found to contain C\textsubscript{60} are given in Table 1.

All of the targets were observed using the IRS short-high (SH) module which covers the wavelength region 9.9–19.6 \mu m with resolving power R = \lambda / \Delta \lambda \sim 600. Some targets were also observed with the short-low (SL) module (5.2–14.5 \mu m, R \sim 60–120) and/or the long-high (LH) module (18.7–37.2 \mu m, R \sim 600).

Flux- and wavelength-calibrated post-Basic Calibrated Data produced by version S18.18.0 of the Spitzer Science Centre pipeline were obtained from the archive, with further analysis undertaken using IRAF.\footnote{IRAF is distributed by the National Optical Astronomy Observatories, which are operated by the Association of Universities for Research in Astronomy, Inc., under cooperative agreement with the National Science Foundation.} The observations were background-subtracted after inspection of Two Micron All Sky Survey (2MASS) K-band images (Skrutskie et al. 2006) for the presence of contaminating sources. Where no such sources were present, either the background subtraction performed by the pipeline was used (SL) or all of the background regions were combined and manual subtraction was employed (SH and LH). Where such sources were found to be present, only those background regions without significant contamination were combined and the background was subtracted manually. Multiple exposures were combined to increase the signal-to-noise ratio.

For targets observed with more than one IRS module, the spectra were combined by scaling the flux in overlapping wavelength regions. Where these were in disagreement, the flux from the SH observations was preferred and the other fluxes were scaled accordingly because the SH module has a smaller field of view and thus samples the flux from the target more reliably. In the final spectra, the wavelength ranges used from each module were 5.2–10 (SL), 10–19.5 (SH) and 19.5–36 \mu m (LH).

4 OBJECT CLASSIFICATION

Given the importance of determining that the YSOs discussed in this paper are embedded young objects, we review here the evidence that our two CMZ objects, ISOGAL-P J174639.6–284126 and SSTGC 372630, are indeed YSOs and not dust-enshrouded post-AGB sources. Based on the available data, we designate our third (Rosette nebula) object, 2MASS J06314796+0419381, as a candidate (but very likely) YSO. The attribution to YSOs rests principally on the steep smooth rise in the spectral energy distribution
in young stellar and other objects

Figure 1. Spitzer IRS spectra of the CMZ objects (a) ISOGAL-P J174639.6−284126 and (b) SSTGC 372630, illustrating the strong rise in the far-IR SED which is indicative of a YSO. The comparison traces are for (c) protoplanetary nebula IRAS 01005+7910 and (d) planetary nebula SMP SMC 016. These show a slower rise in SED (indicated by the dashed lines) and a broad 30-μm emission feature commonly seen in C_{60}-containing post-AGB objects. The spectra are normalized to the flux of ISOGAL-P J174639.6−284126 at 22.5 μm and vertical offsets applied.

Figure 2. Continuum-normalized spectrum of ISOGAL-P J174639.6−284126 between 10 and 19.5 μm showing the presence of silicate and CO_2 ice absorption.

ultracompact H II region that is likely to have higher UV flux (see Section 4.4).

From Fig. 1 it is clear that there is no 30-μm emission feature as seen in the C_{60}-containing PPN IRAS 01005+7910 (Zhang & Kwok 2011) and PN SMP SMC 016 (García-Hernández et al. 2010). Fig. 2 shows the continuum-normalized spectrum of ISOGAL-P J174639.6−284126 between 10 and 19.5 μm with two silicate absorption bands, and absorption by CO_2 ice is indicated. Based on these spectral characteristics, together with the presence of PAH and [Ne II] emission in this YSO (and our other YSOs) which is generally absent in low-mass YSOs (van Dishoeck 2004; Geers et al. 2009), it is concluded that ISOGAL-P J174639.6−284126 is a high-mass YSO.

4.1 ISOGAL-P J174639.6−284126

ISOGAL-P J174639.6−284126 is located in the CMZ of the Milky Way (see Table 1). It was identified as a massive YSO by Felli et al. (2002) based on ISO mid-IR photometry. Its Spitzer IRS spectrum is shown in Fig. 1 as trace (a) and it illustrates a steep rise in SED with increasing wavelength, an SED peaking to the red of ∼45 μm being indicative of a young object (e.g. Simpson et al. 2012). The figure shows that the SED of ISOGAL-P J174639.6−284126 has a much faster rise at longer wavelengths than those of the two sample post-AGB objects shown in traces (c) and (d). An et al. (2011) identified ISOGAL-P J174639.6−284126 as a candidate YSO based on 2MASS and Spitzer photometry, but excluded it from their final list of YSOs due to the lack of a ∼15.4 μm shoulder on the CO_2 ice absorption feature. The presence of a shoulder at ∼15.4 μm, thought to be due to methanol–CO_2 ice complexes, was used as the YSO selection criterion principally to distinguish between YSOs and field stars behind molecular clouds. However, other authors (e.g. Seale et al. 2009; Simpson et al. 2012) have identified massive YSOs which do not have CO_2 ice absorption features, or have different peak wavelengths and profiles from those used by An et al. (2011) for selecting YSOs. Also, Ehrenfreund et al. (1999) have shown that photolysis of methanol-containing CO_2 ice mixtures decreases the strength of the shoulder on the CO_2 ice band; this could lead to disappearance of the shoulder from spectra of the more evolved YSOs, such as those associated with a compact or

4 The 30-μm feature has been ascribed to MgS (Goebel & Moseley 1985; Hony, Waters & Tielens 2002) but may, perhaps more probably, be due to carbonaceous material (Zhang, Jiang & Li 2009; Zhang & Kwok 2011) such as HAC (Grishko et al. 2001).

4.2 SSTGC 372630

SSTGC 372630 is also located in the CMZ (see Table 1). Based on its SED and position in an IR colour–magnitude diagram, it was identified as a massive YSO by Yusef-Zadeh et al. (2009). Its Spitzer IRS spectrum between 5 and 36 μm is given in Fig. 1(b) and, like ISOGAL-P J174639.6−284126, shows a steeply rising continuum in the far-IR. An et al. (2011) listed this object as a possible YSO based on photometric data and their analysis of the shape of its strong CO_2 ice feature at ∼15.2 μm. Our own data reduction does suggest an absorption component near 15.4 μm. There is very strong absorption due to silicates, CO_2 ice at ∼15 μm, ices at 6.0, 6.8 and 7.3 μm and PAH emission. There is also H_2 rotational emission which is an indicator of an embedded YSO which has not yet developed an ultracompact H II region (Varricatt et al. 2010). It appears to have the spectral characteristics of an ‘outflow’ YSO as described by Simpson et al. (2012). We conclude that SSTGC 372630 is also a massive YSO.

4.3 2MASS J06314796+0419381

2MASS J06314796+0419381 lies in the outskirts of the Rosette nebula, which is a site of recent star formation (Kuchar & Bania 1993). Invisible in optical images, this object only becomes detectable in the near-IR (see Table 1) and brightens rapidly longward of 15 μm. The heavy extinction of this object, together with CO_2 ice and silicate absorption (see Fig. 3), the presence of H_2 rotational

5 Spectra of PNe (Bernard-Salas et al. 2009) and PPNe (Volk et al. 2011) provide further examples.
emission and PAH features are supportive of it being classified as a massive YSO. There are no photometric or spectroscopic data available beyond 21 µm so the presence or absence of a 30-µm emission feature is not known. As there are no directly relevant photometric data and the longer wavelength SED is not established, we treat 2MASS J06314796+0419381 as a candidate massive YSO.

4.4 YSO evolutionary stage

The three YSO targets are at different stages of evolution, and fall between the extremes represented by Cep A East and S106 IR which are examples of deeply embedded and more evolved massive YSOs, respectively (van den Ancker, Tielens & Wesselius 2000). In Cep A East there are strong silicate and ice absorption features but no PAHs, whereas S106 IR is characterized by emission in fine-structure lines of atomic ions and from PAHs, reflecting the impact of UV radiation on the environment and its capacity to create H II regions and photodissociation regions. Emission from atoms and molecules excited through shocks of various types is also expected to be prevalent. In broad terms SSTGC 372630 is relatively deeply embedded, 2MASS J06314796+0419381 is less so and ISOGAL-P J174639.6−284126 lies closer in form to the more evolved object S106 IR. The more evolved stage of ISOGAL-P J174639.6−284126 is supported through prominent [S II] (very weak in our other two objects), strong [Ne II] and PAH band ratios similar to those seen in H II regions. It is likely that both shocks and UV flux are present in the three young objects but to differing degrees.

5 SPECTRA OF C60-CONTAINING OBJECTS

In this section we describe an analysis of the C60 emission bands in the two YSOs and candidate YSO, the Herbig Ae/Be star HD 97300 and the post-AGB object HR 4049, spectra of which are shown in Figs 4–8. For each emission feature, fluxes (Table 2) were measured after subtraction of the nearby continuum which was fitted with a cubic spline. Whilst the C60 band at 18.9 µm is an isolated feature, the other three C60 bands are blended with atomic and/or PAH emission to varying degrees for each object. The 7.0-µm C60 band is sometimes contaminated by an [Ar II] emission line at 6.99 µm and potentially also by a band of C70, but as this region is only available in the low-resolution SL spectra deblending of these features is difficult. The 8.5-µm C60 band is heavily blended with a broad PAH feature peaking at 8.6 µm which has prevented the measurement of the flux in this band for all targets. The 17.4-µm C60 band may include some contribution from PAH emission. None of the spectra has the strongest C70 emission feature at 15.6 µm, suggesting that C70 is either absent or present in concentrations too low to be detected, and no evidence for bands of C24 as predicted by Kuzmin & Duley (2011) was found.

The YSOs with C60 bands (Sections 5.1–5.3) have a number of common spectral characteristics. All have PAH features and [Ne II] line emission, and two of the objects (SSTGC 372630 and 2MASS J06314796+0419381) have pure rotational H2 emission lines. In ISOGAL-P J174639.6−284126 there are also [Si II] (34.82 µm) and [S II] (18.71 and 33.48 µm) emission lines.

5.1 YSO ISOGAL-P J174639.6−284126

The spectrum of ISOGAL-P J174639.6−284126 covering the C60 bands is shown in Fig. 4 and the derived fluxes are listed in Table 2. In this and for all other objects, the flux quoted includes any [Ar II] contribution to the 7.0-µm band. The absence of the high-ionization lines – [Ne II] 15.55, [Ar III] 8.99 and [P II] 17.89 µm – which are seen in the PN Tc I (Camii et al. 2010) suggests that the UV radiation field is less harsh than in Tc 1. However, the observed [Ne II] 12.81-
μm and [S III] 18.71-μm lines do indicate the presence of a compact or ultracompact H II region (Seale et al. 2009). The PAH spectrum, and in particular the low 11.2-μm/12.7-μm band ratio (∼1:1), is also consistent with the presence of an H II region (Hony et al. 2001).

5.2 YSO SSTGC 372630

In addition to C60 emission in the 18.9- and 17.4-μm bands, the spectrum of SSTGC 372630 contains C60 emission at 7.0 μm, strong silicate, CO2 and other ice absorption features, and H2 S(1) and S(2) rotational emission lines (see Fig. 5). The 7.7-μm PAH emission band is distorted by the broad silicate absorption, but still appears very strong when compared to the other PAH bands. Although the [Ne II] line is much weaker than in ISOGAL-P J174639.6−284126, there may still be a small contribution to the 7.0-μm emission feature from [Ar II].

5.3 YSO candidate 2MASS J06314796+0419381

The spectrum of 2MASS J06314796+0419381 given in Fig. 6 has the weakest ionized atomic lines of the three objects, with barely discernible [SIII], weak [NeII] and hence likely negligible [ArII] at 6.99 μm. Strong C60 bands at 18.9, 17.4 and 7.0 μm are readily identifiable, together with PAH emission bands and the S(1), S(2) and S(3) lines of H2, where the S(3) line falls in the region of very strong silicate absorption.

5.4 Herbig Ae/Be star HD 97300

HD 97300 is an optically bright Herbig Ae/Be star of spectral type B9. It is a more evolved system than the YSOs and is approaching the stellar main sequence (Siebenmorgen et al. 1998). The IRS spectrum is shown in Fig. 7, where C60 emission in the 18.9-μm band is visible. Emission is also seen in the region of the 17.4-μm C60 band but this is heavily contaminated by PAH bands, so it is not possible to measure the flux from C60. No C60 feature is seen at 7.0 μm suggesting a low level of vibrational excitation, corresponding to a vibrational temperature of ≤200 K (Cami et al. 2011) – see also Section 6.1. Weak emission in the S(1), S(2) and S(3) lines of H2 is present. Although the identification of C60 in HD 97300 is based mostly on the 18.9-μm emission feature, it is reproducible as seen in other spectra (Keller et al. 2008; Manoj et al. 2011).

| Object               | 7.0 μm | 7.0 μm | 17.4 μm | 17.4 μm | 18.9 μm | 18.9 μm |
|----------------------|--------|--------|---------|---------|---------|---------|
|                      | λ      | FWHM   | Flux (mJy μm) | λ      | FWHM   | Flux (mJy μm) | λ      | FWHM   | Flux (mJy μm) |
| ISOGAL-P J174639.6−284126 | 7.01±0.09| 57.7±1.0 | 17.38 | 0.29 | 72.1±8.5 | 18.91 | 0.32 | 169.5±7.9 |
| SSTGC 372630          | 7.04   | 0.16   | 5.44±0.3 | 17.38 | 0.34 | 12.9±1.3 | 18.92 | 0.30 | 21.6±1.2 |
| 2MASS J06314796+0419381 | 7.01   | 0.11   | 6.47±0.14 | 17.38 | 0.22 | 40.550±1.9 | 18.94 | 0.30 | 61.7±2.7 |
| HD 97300              | −−−    | −−−    | −−−      | 17.32 | <1.24 | <1239±28 | 18.89 | 0.64 | 1565±48 |
| HR 4049               | −−−    | −−−    | −−−      | 17.39 | 0.28 | 37.5±2.2 | 18.91 | 0.35 | 99.0±1.9 |
| HD 52961              | −−−    | −−−    | −−−      | 17.32 | <1.24 | <1239±28 | 18.89 | 0.64 | 1565±48 |

a Includes a contribution from an [Ar II] line. b Includes a contribution from a PAH feature. c See also Gielen et al. (2011b).
5.5 Post-AGB star HR 4049

The Spitzer spectrum for this post-AGB object is shown in Fig. 8 together with our reduced spectrum of HD 52961, on which a study (Giielen et al. 2011a) was published after this paper was submitted. Although Giielen et al. (2011a) conclude that HR 4049 does not carry the signatures of C₆₀, our analysis indicates that there is evidence of C₆₀ emission as shown in the top-right inset of the figure. Due to some contamination of the 17.4-μm C₆₀ band from gas-phase CO₂ and PAH emission, only an upper limit on the flux in this band could be determined.

6 DISCUSSION

In this section, we discuss the appearance of C₆₀ in YSOs and other objects with particular emphasis on its excitation (Section 6.1) and formation (Section 6.2).

6.1 Excitation of C₆₀ IR emission bands

Two excitation mechanisms for C₆₀ IR emission with a quantitative basis have been discussed in the literature. Cami et al. (2010) put forward a model in which thermal equilibrium is assumed, which then allows a vibrational temperature to be deduced. In Tc 1 the temperature was found to be unexpectedly low at 330 K and led to the suggestion that the emitting C₆₀ molecules are attached to dust grains. In their study of C₆₀ emission from NGC 2023 and NGC 7023, Sellgren et al. (2011) invoked a gas-phase photoexcitation model commonly applied in interpreting astronomical IR emission spectra of PAH molecules. In this case, the absorption of a UV photon is followed by an internal redistribution of the energy leading to emission in the mid-IR.

Both of these quantitative approaches rely on the knowledge of intrinsic IR band intensities which are quite uncertain. For the 18.9-, 17.4-, 8.5- and 7.0-μm bands, Cami et al. (2010) used relative band strengths of 100:48:45:37.8 (Martin et al. 1993; Fabian 1996), whereas Sellgren et al. (2010) used those of Choi, Kertesz & Mihaly (2000): 100:26:31:46. Recently, Iglesias-Groth et al. (2011) measured relative band intensities of 100:43:26:26.9 at room temperature in a KBr matrix. The relative band intensities are also likely to be temperature dependent; notably, emission spectra at thermal equilibrium in the gas phase at ∼1000 K reveal the 18.9- and 17.4-μm emission features to have approximately the same intensity (Frum et al. 1991).

Vibrational temperatures for our objects have been estimated using the method described by Cami et al. (2010) by plotting ln(N_u/g_u) versus E_u/k in an excitation diagram; an example for ISOGAL-P J174639.6−284126 is shown in Fig. 9. Using the flux values given in Table 2, which as listed include the [Ar ii] contribution to the 7.0-μm band, the C₆₀ vibrational temperature for ISOGAL-P J174639.6−284126 is found to be ≤670 K (using band strengths taken from Cami et al. 2010) or ≤790 K (using band strengths of Iglesias-Groth et al. 2011). By applying the two-component deconvolution fitting in IRAF, the contribution of [Ar ii] is estimated to be ∼60 per cent and removal leads to lower vibrational temperatures of ≤450 K or ≤500 K, respectively. Vibrational temperatures for ISOGAL-P J174639.6−284126 and the other two YSOs are given in Table 3. The values are in the same range as determined for PN Tc 1 by Cami et al. (2010), PNe by Garcia-Hernández et al. (2010) and a PPN by Zhang & Kwok (2011), although the low signal-to-noise ratio of the C₆₀ bands in SSTGC 372630 renders the apparently slightly higher temperature values in this YSO less certain. We have not conducted our own photoexcitation calculations for IR emission from C₆₀, but predicted IR band intensity ratios for photoexcitation energies of 5, 10 and 15 eV are available from Sellgren et al. (2010) and are given in Table 3.

![Figure 9](https://academic.oup.com/mnras/article-abstract/421/4/3277/1093522/figure9)

**Figure 9.** Plot of ln(N_u/g_u) versus E_u/k, where N_u is the number of molecules in the upper (u) vibrational level, g_u is the upper level degeneracy, E_u is the level energy and k is the Boltzmann constant. For details see Cami et al. (2010). Data for the 18.9-, 17.4- and 7.0-μm bands of C₆₀ in the YSO ISOGAL-P J174639.6−284126 are shown. For this example the band strengths (Martin et al. 1993; Fabian 1996) were used. A vibrational temperature of ∼450 K is obtained from the slope.

Table 3. Observed vibrational band intensity ratios, inferred vibrational temperatures for YSOs and comparison with predicted photoexcited band ratios of Sellgren et al. (2010). T_vib^C(K) and T_vib^G(K) are the vibrational temperatures derived from the C₆₀ band strengths used by Cami et al. (2010) and obtained by Iglesias-Groth, Cataldo & Manchado (2011), respectively.

| Object | I_17.4/H_18.9 | I_17.4/H_18.9 | T_vib^C(K) | T_vib^G(K) |
|--------|---------------|---------------|------------|------------|
| ISOGAL-P J174639.6−284126 (CMZ) | ~0.42<sup>a</sup> | 0.53 | ≤450<sup>b</sup> | ≤500<sup>b</sup> |
| SSTGC 372630 (CMZ) | ≤0.70<sup>a</sup> | ~0.59<sup>b</sup> | ≤540<sup>b</sup> | ≤620<sup>b</sup> |
| 2MASS J06314796+0419381 | 0.29 | 0.48<sup>c</sup> | 410 | 450 |

*Photon energy (eV) 5 0.46–0.58 0.28–0.38 10 0.76–0.94 0.28–0.38 15 0.97–1.20 0.29–0.38

<sup>a</sup>Value when 60 per cent contribution to 7.0-μm feature from [Ar ii] is removed (see text).

<sup>b</sup>Silicate and ice absorptions affect continuum level definition.

<sup>c</sup>Ratio when the contribution of 20 per cent from PAH feature at 17.4 μm is removed.
We now consider whether the thermal or photoexcitation models hold for these YSOs. Examination of Table 3 shows that, with one possible exception ($I_{17}/I_{18.9}$ for SSTGC 372630), the $I_{17}/I_{18.9}$ and $I_{17}/I_{18}$ ratios fall outside the ranges calculated by Sellgren et al. (2010) for photons with 5, 10 and 15 eV. If the $C_60$ molecule were excited by UV radiation, the flux ratios derived for ISO-GALP J174639.6–284126 and 2MASS J06314796+0419381 (see Table 3) would suggest the need for photons with energies lower than 5 eV. A similar result is found for Tc 1 (Cami et al. 2011) and for a number of PNe (García-Hernández et al. 2011b). However, for the PPN IRAS 01005+7910 the band ratios can be satisfied within this model but with high-energy photons of around 10–15 eV (Zhang & Kwok 2011). The case of the pre-main-sequence Herbig Ae/Be star HD 97300 is notable because even for photon energies as low as 5 eV, a ratio of 0.46–0.58 for the 7.0/1.89 band ratio is predicted. While the 18.9-μm band of $C_{60}$ is clearly discernible in HD 97300, a band at 7.0 μm is not seen which implies emission from very cool $C_{60}$. Unfortunately, the 17.4-μm feature is too heavily contaminated by PAH features to allow a value for $T_{\nu,8}$ to be deduced.

From these comparisons, an emission mechanism based solely on the absorption of UV radiation followed by re-emission in the IR would seem unlikely for these four new $C_{60}$-containing young objects. However, within the thermal model, the derived temperatures (Table 3) for the three YSO objects are not inconsistent with the temperatures of up to ~1000 K for warm gas in massive YSOs (Luhuis & van Dishoeck 2000; Boonman et al. 2003; An et al. 2011). While the location of the $C_{60}$ in the YSOs is not yet established, and there is no evidence for gas-phase absorption by HCN, $C_2$H$_2$ or CO$_2$ in the spectra, warm gaseous regions could provide a suitable environment for thermal excitation of IR emission from $C_{60}$.

For SSTGC 372630 (CMZ) and 2MASS J06314796+0419381 (Rosette nebula), there are S(1) and S(2) pure rotational lines of molecular hydrogen. Assuming that the lines are optically thin and that thermal equilibrium holds both for the rotational levels and for the ortho/para ratio, the rotational temperatures can be deduced. We find $T_{\text{rot}}$ values of ~540 and ~370 K for SSTGC 372630 and 2MASS J06314796+0419381 which are within ~100 K of the vibrational temperatures for $C_{60}$ in these objects. In addition to the assumptions listed, this difference may have a number of contributing factors including the molecular physics of the excitation, the allowed vibrational transitions of $C_{60}$ and the strongly forbidden rotational ones of $H_2$, and uncertainty as to whether $C_{60}$ and $H_2$ share the same spatial distribution. Nevertheless, to our knowledge this is the first time that a $C_{60}$ vibrational temperature has been compared with the internal temperature of another molecule. Observations of other (polar) molecules through their rotational spectra in these objects would clearly be of interest.

Further possible $C_{60}$ vibrational excitation mechanisms include shock-induced excitation, possibly during $C_{60}$ formation from HAC in grain–grain collisions, or through dehydrogenation of HAC while on the grain surface (Cami et al. 2011; García-Hernández et al. 2011b). The YSOs SSTGC 372630 and 2MASS J06314796+0419381 show H$_2$ S(1) and S(2) lines, which are an indicator of shocked gas, while all three YSOs have strong [Ne ii], also an indicator of shocked gas, but no [Ne iii] emission. In their study of $C_{60}$-containing PNe, García-Hernández et al. (2011b) found very low [Ne ii]/[Ne iii] ratios. This result was considered incompatible with the predictions of photoionisation modelling, but one that could possibly be rationalized in terms of shocks. Shocks are expected in YSOs and so could provide $C_{60}$ vibrational excitation. In the case of SSTGC 372630, the H$_2$ lines are shifted by ~200 km s$^{-1}$ relative to the [Ne ii] line, strongly suggesting a strong outflow/shock which is consistent with the likelihood that this object is an ‘outflow’ source as mentioned in Section 4.2.

### 6.2 Formation of $C_{60}$

It is well established that $C_{60}$ is formed in the later stages of stellar evolution (see Cami et al. 2010; García-Hernández et al. 2010 and references in Section 1). Its presence in NGC 2023 and NGC 7023 (Sellgren et al. 2010) indicates that it might also be formed in situ in the ISM, where it may also exist in ionized form (Foing & Ehrenfreund 1994). Discovery of $C_{60}$ in the YSOs reported here makes the question as to the mechanism and location for $C_{60}$ formation an even wider one. In this section we discuss how $C_{60}$ could form in situ in pre-main-sequence objects or arise from earlier synthesis in post-AGB stars or the ISM (Section 6.2.1), and draw attention to a tentative link between $C_{60}$ and nanodiamonds (Section 6.2.2).

#### 6.2.1 $C_{60}$ in the YSOs and Herbig Ae/Be star HD 97300

A number of scenarios for the origin of $C_{60}$ in YSOs can be envisaged. Given that it is clearly formed in post-AGB objects, if the integrity of the $C_{60}$ structure was maintained on it being expelled to the ISM, it could then (re)appear in the spectrum of a YSO following cloud collapse. For a discussion on the evolution of organic material through these stages, see Ehrenfreund & Charnley (2000). Alternatively, $C_{60}$ in YSOs could originally have formed in the ISM as discussed by Bettens & Herbst (1996, 1997). A third scenario is that $C_{60}$ forms in situ in YSOs. Recent commentaries on the current challenges relating to both mechanistic and spatial aspects of $C_{60}$ formation have been published by Cami et al. (2011) and by García-Hernández (2011). Attention is focused here on the in situ formation of $C_{60}$ in YSOs.

We consider two main schemes. First, shock-induced formation of $C_{60}$ might occur in situ in YSOs through the decomposition of HAC, essentially as described by García-Hernández et al. (2010) for post-AGB objects. However, it is not clear whether HAC is present in YSOs. For post-AGB objects there is a very strong correlation between $C_{60}$ and the broad 30-μm feature that is commonly attributed to HAC. However, the $C_{60}$-containing reflection nebulae NGC 2023 and NGC 7023 do not have the 30-μm emission (see Zhang & Kwok 2011), and nor do the YSOs SSTGC 372630 and ISO-GALP J174639.6–284126, the Herbig Ae/Be star HD 97300 (Keller et al. 2008) or the mixed-chemistry post-AGB objects HR 4049 and HD 52961. Hence, if the 30-μm emission does indeed arise from HAC then it is hard to see how this particular shock-induced $C_{60}$ formation mechanism involving HAC could be operating in young stellar environments.

Secondly, in most astrophysical sources where $C_{60}$ has been found, PAH emission is also present. This raises the question as to whether there might be a link between PAHs (perhaps particularly in dehydrogenated form) and fullerene formation. Micelotta, Jones & Tielens (2010a,b) have argued from a theoretical standpoint that fullerene formation could occur through shock-driven processing of PAHs. They conclude that shock velocities of 75–100 km s$^{-1}$ can significantly modify the structure of PAHs, these speeds being comparable to those found in massive YSOs. Even at velocities as low as 50 km s$^{-1}$ some carbon atoms are expected to be removed from the carbon framework as could occur in C-type shocks (e.g. van den Falls et al. 2011 and references in Section 4.2).

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The anonymous referee has pointed out that the absence of a 30-μm feature could be related to the temperature of the bulk of the HAC material.
Ancker et al. 2000). Chuvilin et al. (2010) have recently shown that under highly energetic conditions small PAH-like graphene sheets can undergo rearrangement to form fullerenes.⁷ Although the laboratory experiments of Chuvilin et al. (2010) were conducted using transmission electron microscopy in which very high energy electrons induce dehydrogenation and loss of carbon atoms leading to C₆₀ formation, high-energy photons, X-rays and cosmic rays could play an equivalent role in astrophysical environments. These processes all proceed via initial dehydrogenation and loss of carbon atoms leading to the formation of five-membered rings. Curvature follows with the final stage being the closure of the fullerene structure. Given that PAHs are present in all of the YSOs, ‘top–down’ mechanisms starting from large PAHs would appear to be favoured as formation routes for C₆₀ in YSOs as well as in the Herbig Ae/Be star HD 97300.

6.2.2 C₆₀ in post-AGB stars: HR 4049 and HD 52961

During the search of Spitzer archival data two post-AGB sources with C₆₀ emission at 18.9 µm were found: HR 4049 and HD 52961 (see Table 1 and Fig. 8). These objects are unusual in that they have a mixed oxygen–carbon chemistry and so the presence of C₆₀ is perhaps unexpected. The presence of a band of C₆₀ in HD 52961 has also been recently reported by Gielen et al. (2011a).⁸ We include these objects in this paper because of the parallel between the outflows (jets and shocks) that are common in the later stages of stellar evolution and those occurring in young objects. It follows that C₆₀ formation processes in these two very different evolutionary stages may be quite similar. We suggest that the ‘top–down’ formation of C₆₀ from PAHs, as described by Micelotta et al. (2010a,b) and seen experimentally by Chuvilin et al. (2010), will likely apply also to C₆₀ formation in mixed-chemistry post-AGB objects such as HR 4049.

HR 4049 and HR 52961 exhibit the very rare C–H emission features at 3.43/3.53 µm from H-coated nanodiamonds (Geballe et al. 1989; Oudmaijer et al. 1995; Guillois, Ledoux & Reynaud 1999). Given that they also have C₆₀ emission, this suggests that there may be a connection between fullerene and nanodiamonds. Carbon onions are composed of fullerene-like concentric shells and due to their similarity with fullerenes may form together in astrophysical environments. It has been proposed that astrophysical carbon onions could act as pressure cells for the formation of nanodiamonds under highly energetic conditions (Goto et al. 2009). The fact that the only post-AGB objects with nanodiamond signatures also have C₆₀ bands provides indirect observational support for the nanodiamond formation proposal of Goto et al. (2009).

7 SUMMARY

This paper reports the first detection of the C₆₀ molecule in three YSOs and in a Herbig Ae/Be star using Spitzer IRS archive observations. Evidence that the three objects are YSOs is critically reviewed and their relative stage of evolution discussed. C₆₀ emission in two unusual mixed-chemistry post-AGB objects is also described as they share shock-induced processes similar to those active in YSOs. A common feature of all of the objects is emission from PAHs.

The origin of the C₆₀ emission is considered in detail. From the measured fluxes in the 7.0-, 17.4- and 18.9-µm bands, it is found that the band intensities can best be described by a thermal rather than a UV photoexcitation model and approximate vibrational temperatures were determined. These are similar to the rotational temperatures deduced from H₂ line emission found in two of the young objects.

C₆₀ formation mechanisms are evaluated, focusing particularly on photoinduced and shock-induced in situ formation from PAHs in YSOs. We suggest that the most likely formation mechanism is through dehydrogenation followed by carbon atom loss from PAHs resulting in five-membered ring formation, curvature and closure to make fullerenes. It is concluded that shock-induced and UV-stimulated decomposition are active in generating C₆₀ in the YSOs, with the relative contributions varying with evolutionary stage. It is thought that shocks play the dominant role in C₆₀ formation in the Herbig Ae/Be and post-AGB stars.

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