

OPTICAL ABSORPTION AND EMISSION BANDS OF SiC₂ IN CARBON STARS

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ABSTRACT

Observations of the Merrill-Sanford bands of SiC₂ in the 4750–5050 Å spectral region, seen in absorption in some carbon stars and in emission in IRAS 12311–3509, are reported. Vibrational band assignments based on recent laser-based laboratory electronic spectroscopy of this molecule constitute substantial revisions compared with earlier work. Vibrational hot bands are very strong when present in carbon stars, but were greatly weakened in T Mus for a time in 1994, indicating that the bands were then formed in a cooler region than that typical of carbon star photospheres. Emission bands of SiC₂, with intensities that are consistent with optical excitation of cool gas, appear in IRAS 12311–3509 which is probably a J-type carbon star occulted by a dusty disk so that the star is seen by reflection from material out of the plane of the disk.

Subject headings: circumstellar matter — ISM: molecules — stars: carbon — stars: individual
(T Muscae, IRAS 12311–3509)

1. INTRODUCTION

It is 70 years since prominent unidentified molecular absorption bands in the blue-green spectra of some N- and J-type stars were first reported by Merrill (1926) and Sanford (1926). Additional bands were found by Shane (1928) and McKellar (1947), while observations at higher resolution were made by Sanford (1950). The crucial step in identifying the carrier was made by Klemm (1956), who recorded many of the bands in the laboratory in both emission and absorption. Based on the form of the spectrum and the chemical conditions under which the bands appeared, the spectrum was ascribed to the SiCC molecule, in part by analogy with the spectrum of C₃, which was known to be linear in its ground and excited electronic states. The notion that SiCC was a linear molecule persisted, though not without question (Bondybey 1982), until a laser experiment by Michalopoulos et al. (1984), who recorded rotationally resolved electronic spectra of the origin band near 4980 Å, analysis of which showed that the molecule was in fact T-shaped; theoretical calculation led to the same conclusion (Grev & Schaefer 1984). A detailed rotational analysis of two of the Merrill-Sanford bands has subsequently been published (Bredohl et al. 1988).

The rotational constants published by Michalopoulos et al. (1984) enabled Thaddeus, Cummins, & Linke (1984) to assign nine previously unidentified lines in the millimeter-wave spectrum of the circumstellar shell of the evolved carbon-rich star IRC +10216 to SiC₂. Further radioastronomical and laboratory studies of SiC₂ have ensued, including isotope ratio measurements (Cernicharo et al. 1986, 1991), mapping (Gensheimer, Likkell, & Snyder 1992, 1995; Takano, Saito, & Tsuji 1992), and chemical modeling (Takano et al. 1992) of SiC₂ in IRC +10216. Rotational spectra of SiC₂ in the carbon star IRAS 15194–5115 have also been reported (Nyman et al. 1993).

Intensity estimates of the strongest Merrill-Sanford bands in carbon stars were made by Yamashita (1967, 1972, 1975) and

by Walker (1976) and were found to be well correlated with *B*–*V* color, which Walker considered to be an indicator of the violet opacity in carbon stars. Tsuji (1981a, 1981b) used these data to show that the band strengths show a strong decrease in intensity with increase in photospheric temperature over the range 2400–3600 K, estimated from near-infrared photometry. The extreme redness of the cooler carbon stars makes it very hard to obtain spectra of even moderate resolution in the blue spectral region, so that most of the N stars observed in this region by Yamashita are hotter examples in which the SiC₂ bands are weak or absent. The majority of the cooler N stars were observed only in the red spectral region.

Laboratory study of the electronic spectrum of gas-phase SiC₂ has advanced further recently through the recording and assignment of extensive laser excitation and dispersed fluorescence spectra, yielding well-determined vibrational levels in both ground and excited electronic states (Butenhoff & Rohlfing 1991). These results form the basis for the assignments of the new astronomical absorption and emission spectra of SiC₂ reported in this Letter.

2. OBSERVATIONS

The publication of the *IRAS* Point Source Catalog, Version 2 (1988) and the Atlas of Low Resolution *IRAS* Spectra (1986) opened a new window on stars with circumstellar material. This stimulated an extension of the survey carried out by Yamashita (1967, 1972, 1975) to southern N stars. We have undertaken an initial survey of 200 N stars with the grating spectrograph and intensified Reticon (RPCS) detector (Jordan, Read, & van Breda 1982) at the Cassegrain focus of the 1.9 m Radcliffe reflector of the South African Astronomical Observatory at Sutherland. Two spectra were taken for each star, covering 5550–6750 Å at 2 Å resolution and 4650–5250 Å at 1 Å resolution. A small number of variable stars with strong SiC₂ bands or other interesting features were selected for spectroscopic monitoring that has continued for nearly

10 years; some of the later spectra of the blue region cover a wider band at 2 Å resolution. Examination of these spectra shows that the relative intensities of the Merrill-Sanford bands generally vary in lockstep as they increase in strength, but T Mus is a revealing counterexample which we discuss here.

An unrelated project involving the optical identification of much redder objects revealed IRAS 12311–3509, which has the Merrill-Sanford bands in emission. This object also has strong emission in atomic resonance lines and is thought (Lloyd Evans 1991) to share the interpretation given by Herbig (1970) for VY CMa, i.e., a star with a dusty circumstellar disk that is seen edge on and eliminates direct light from the star, which is visible only by reflection from material out of the plane of the disk. The spectrum of the underlying star is best matched by a J-type carbon star, probably of relatively warm spectral subtype, but no exact match has been found for the entire spectral energy distribution, distorted as it is by strong broad emission bands from presumably circumstellar material.

3. SPECTROSCOPIC ASSIGNMENTS

The SiC₂ molecule has an unusual equilibrium T-shaped geometry (C_{2v} symmetry) with a partially ionic electronic structure in the sense Si⁺C₂[−] (Thaddeus et al. 1984; Oddershede et al. 1985) in which the C₂ fragment undergoes hindered internal rotation (Coudert 1993; Ross et al. 1994). The vibrational analysis of the \tilde{A}^1B_2 – \tilde{X}^1A_1 electronic transition by Butenhoff & Rohlffing (1991) has led to accurate values of the vibrational constants. There are three vibrational modes in each electronic state: ν_1 is a C–C stretch (a_1), ν_2 is a Si(C₂) stretch (a_1), and ν_3 is an antisymmetric bending-type vibration (b_2). The well-determined value for the ν_3 fundamental of 196.4 cm^{−1} is of particular significance in relation to this work. This mode arises from a very low frequency motion which is an antisymmetric vibration of the Si atom with respect to the C–C entity. Its low value is of considerable astrophysical interest, as it corresponds to an excitation temperature of only 281 K and so vibrational hot bands can readily be observed in stellar absorption spectra.

Figure 1 shows spectra of the region 4750–5050 Å for T Mus in 1995 July and 1994 May where SiC₂ bands appear in absorption, and for IRAS 12311–3509 with bands in emission; the vibrational band assignments, energy levels, and transitions are also given. Concentrating initially on the absorption bands in T Mus, the main bands are red-degraded with a width governed by the rotational temperature, the determination of which will be discussed in detail elsewhere. Built on the origin band (0, 0, 0)–(0, 0, 0), or, in the preferred notation, 0₀⁰ (Brand et al. 1983), there is a vibrational progression in the ν_2 mode of the excited electronic state giving the 2₀¹ (0, 1, 0)–(0, 0, 0) and 2₀² (0, 2, 0)–(0, 0, 0) bands. All of the other absorption bands in Figure 1 and listed in Table 1 involve one or two quanta of the ν_3 mode in the ground electronic state. Some of these bands are very strong. There are specific and restrictive selection rules for changes in ν_3 which do not hold for the other two vibrational modes. The number of quanta must change by 0 or 2 only in the electronic transition (Butenhoff & Rohlffing 1991), so that the 3₁¹ and 3₂² bands appear but not the forbidden 3₀¹ or 3₁⁰ bands. This is not only crucial to the assignments but is also of interest in connection with the optical emission spectrum of IRAS 12311–3509, discussed in § 4.2. The absorption spectrum of T Mus in 1995 July shows a very strong 3₁¹ hot band with origin at 4911 Å, indicating that

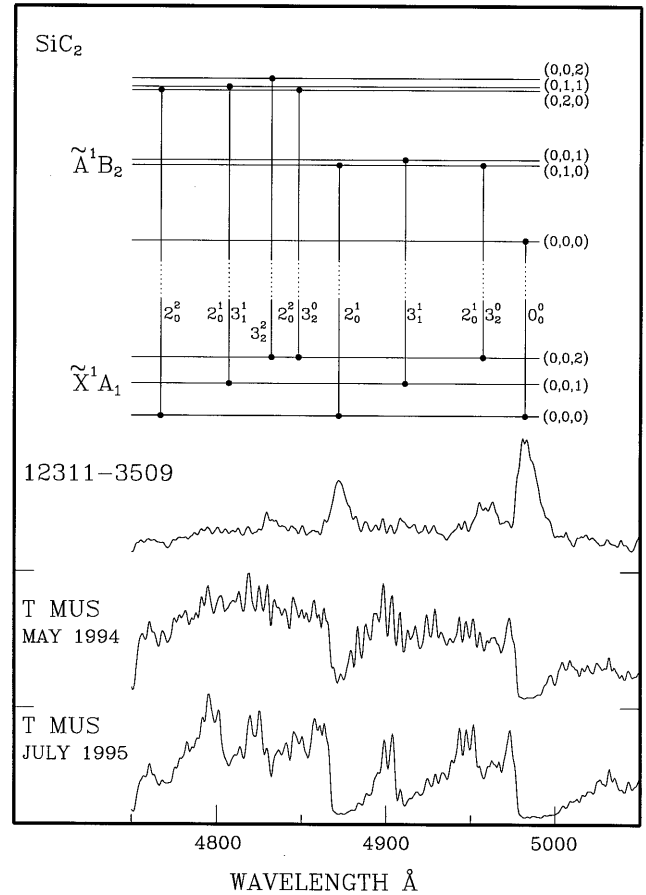


FIG. 1.—Spectra between 4750 and 5050 Å of T Mus in 1995 July and in 1994 May where SiC₂ is seen in absorption and IRAS 12311–3509 with emission bands of SiC₂. Vibrational band assignments, energy levels, and transitions are shown. The notation for the vibrational bands follows that of Brand et al. (1983).

the $\nu_3 = 1$ level lying at 196 cm^{−1} is very substantially populated. Moreover, the adjacent 2₀¹ 3₂⁰ band near 4957 Å is also evident where the lower state level lies 353 cm^{−1} above the vibrationless ground state. The band intensities also depend on the Franck-Condon factors, but these are not known. The

TABLE 1
OBSERVED BANDS OF SiC₂

Band	$\lambda(\text{lab})$ (Å)	$\lambda(\text{obs})$ (Å)	Absorption	Emission	Comment
0 ₀ ⁰	4982	4982	vs	vs	Origin
2 ₀ ¹ 3 ₂ ⁰	4957	4957	w	m	HB
3 ₁ ¹	4911	4910	m	vw	HB
2 ₀ ²	4872	4871	s	s	
2 ₀ ² 3 ₂ ⁰	4848	4851	w	...	HB
3 ₂ ²	4832	4832	w	w	HB
2 ₀ ¹ 3 ₁ ¹	4807	4806	w	...	HB
2 ₀ ²	4767	4766	w	...	

NOTE.—Laboratory wavelengths are from the data of Butenhoff & Rohlffing (1991), who give the following fundamental vibrational frequencies: (ν_1 , ν_2 , ν_3): \tilde{X}^1A_1 , 1746.0, 840.6, 196.37 cm^{−1}; \tilde{A}^1B_2 , 1462, 455.04, 487 cm^{−1}. The observed wavelengths are those for absorption in T Mus in 1995 July. Qualitative estimates of the band intensities in T Mus (absorption) in 1995 July are given, with corresponding intensity data for IRAS 12311–3509 (emission). HB in the last column denotes a hot band as observed in absorption.

assignment of the 4954 Å feature to the $2_0^1 3_2^0$ band of SiC₂ removes the possibility that it might be due to TiO (McKellar 1947). We give a list of the observed peak wavelengths for the observed bands of SiC₂, together with the band origins, in Table 1.

4. DISCUSSION

4.1. *T Mus*

The semiregular variable *T Mus* has periods of 93 and 1082 days (Lysaght 1989). It is a J star with strong SiC₂ bands and has been classified as C–J 4.5, C₂ 5+, J 5.5, MS 6 (Keenan 1993; Barnbaum, Stone, & Keenan 1996). The spectrum changed radically during the 1994 season when it was on the fading branch of the longer cycle. The spectrum of 1994 May is compared with that of 1995 July in Figure 1 and shows abnormally weak hot bands, whereas the three bands involving absorption from the vibrational ground state remain strong, but with slightly narrower rotational contours. This contrasts with the usual situation in long-period variables where the hot bands retain the same strength relative to the other SiC₂ bands throughout the light cycle. The SiC₂ bands in *T Mus* in 1994 must have been formed in cooler material, possibly high above the photosphere. It is of interest that another doubly periodic semiregular variable, *V Hya*, shows indications of circumstellar material and mass loss during deep minimum (Lloyd Evans 1993, 1995) although in this case the notable spectroscopic features are emission of atomic lines and the Swan bands of C₂.

4.2. *IRAS 12311–3509*

The emission bands of SiC₂ in *IRAS 12311–3509* in Figure 1 may usefully be compared with those of the absorption bands

in *T Mus*. There are two important differences. First, the widths of the rotational contours in emission are narrower than those for *T Mus*; second, there are fewer strong vibrational bands in the emission spectrum than in the “normal” spectrum of *T Mus* (1995 July). The 3_1^1 band in particular is very weak in the spectrum of *IRAS 12311–3509*.

The strongest bands, after the origin band 0_0^0 , are the 2_0^1 and $2_0^1 3_2^0$ bands, both of which involve emission from the (0, 1, 0) level. It is therefore surprising that emission from the almost isoenergetic (0, 0, 1) level in the 3_1^1 band is so weak. This apparent anomaly is removed if the fluorescence results from photoexcitation of the molecule. The selection rule $\Delta v = 0$ or 2 implies that the $v'_3 = 1$ level can only be accessed efficiently via the 3_1^1 absorption band. However, the rotational contours of the emission bands are narrow, which suggests that the SiC₂ molecules are cool, so the populations of the vibrational levels $v'_3 = 1$ (and $v'_3 = 3$) of SiC₂ in *IRAS 12311–3509* will be low. Hence, minimal optical pumping in absorption in the 3_1^1 and 3_1^1 bands can occur, and so there will be little resultant fluorescence in the 3_1^1 band. Thus the appearance of the emission spectrum of *IRAS 12311–3509* is consistent with optical excitation of cool SiC₂ molecules.

Spectra of these and other stars, which also cover the regions where SiC₂ bands have been reported at both longer and shorter wavelengths, and the results of rotational contour calculations, will be discussed elsewhere.

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