The Astrophysical Journal, 630:1217–1223, 2005 September 10

LABORATORY STUDIES ON THE INFRARED ABSORPTIONS OF HYDROGENATED CARBON-SILICON CLUSTERS: DIRECTING THE IDENTIFICATION OF ORGANOMETALLIC $SiCH_x$ SPECIES TOWARD IRC +10216

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Received 2005 April 15; accepted 2005 May 10

ABSTRACT

Silicon-bearing species of the molecular formula $SiCH_x$ ($x = 1-6$) are plausible candidates for organometallic molecules that might be present in the circumstellar envelope of IRC +10216. Combining matrix-isolation laboratory experiments with computed vibrational spectra of these molecules, we have observed several fundamentals of the new silicon-containing radicals $SiCH_3$ and $SiCH_5$, in addition to the well-known $SiCH_4$ and $SiCH_6$ species, via infrared spectroscopy. These bands can now be used to search for hydrogen-deficient silicon-carbon–carrying molecules in the circumstellar envelope of the carbon star IRC +10216; the column densities of these species will yield valuable clues to the formation of silicon carbide molecules (SiC), together with their aggregates and partially hydrogenated clusters in the interstellar medium.

Subject headings: astrochemistry — ISM: molecules — methods: laboratory — molecular processes

1. INTRODUCTION

During the last decade, the search for interstellar carbon- and silicon-bearing molecules has received special attention in connection with the study of the atmospheres of dying carbons stars (Rittby 1992; Van Orden et al. 1994; Nielsen et al. 1997; Gordon et al. 2000; Botschwina et al. 2002). Since the identification of silane (SiH_4) in the circumstellar envelope of the carbon star IRC +10216 (CW Leo) (Barrett 1978; Goldhaber & Betz 1984), astronomers have identified 10 silicon-bearing molecules in the gas phase of cold molecular clouds, star-forming regions, and circumstellar envelopes of evolved carbons stars. These species of molecules can be classified into simple diatomic molecules of the general chemical formula SiX (group 1), silicon carbides holding the generic composition SiC_n (group 2), and silicon cyanides (group 3). The diatomic species silicon carbide (SiC), silicon sulfide (SiS), and silicon nitride (SiN) are important constituents of the circumstellar envelope of CW Leo (Cernicharo et al. 1989; Speck et al. 1997; Bieging & Nguyen 1989; Turner 1992; Wienkoop et al. 1997; Grutter et al. 1997). The second group, silicon carbides, contains three members: the cyclic C_{2v} symmetric silicon dicarbide molecule, SiC_2 (Thaddeus et al. 1984; Sarre et al. 1996; Chandra & Sahu 1993; Gensheimer & Snyder 1997; Lloyd Evans et al. 2000); a polar, rhomboidal bicyclic SiC_3 species (McCarthy et al. 1999; Apponi et al. 1999); and a closed-shell linear chain molecule of SiC_4 (Ohishi et al. 1989). Silicon carbide and silicon dicarbide have similar column densities, whereas the higher members silicon tricarbide (SiC_3) and silicon tetracarbide (SiC_4) are 200 times less abundant, with silicon tricarbide 50% more copious than silicon tetracarbide. The last group contains the SiCN and SiNC isomer pair (silicon monocyanide and silicon monoisocyanide), which have also been detected in the envelope of this carbon star (Guelin et al. 2000, 2004). Diatomics such as SiS were also detected in vibrationally excited ($\nu = 1$) states (Turner 1987); silicon monoxide (SiO) has only been observed in star-forming regions such as Sagittarius B2 (Peng et al. 1995; Schilke et al. 1997) and to a lesser extend in cold molecular clouds (Ziurys et al. 1989), but not in circumstellar envelopes of carbon-rich stars.

In addition to molecular lines, broad infrared emission features peaking between 11 and 11.5 μm have been observed (Goebel et al. 1995; Mutschke et al. 1999; Papoular et al. 1998; Blanco et al. 1998; Speck et al. 1997, 1999). They have been attributed to silicon carbide grains, which are believed to be significant constituents of circumstellar envelopes of dying carbons stars; alternatively, Blanco et al. (1994) suggested amorphous carbon and silicon carbide mixtures as potential carriers. Pillinger & Russel (1993) also identified silicon carbide particles in meteorites, and their role as cometary dust particles should be pointed out as well (Orofino et al. 1994). This is remarkably distinct from oxygen-rich evolved stars, which show broad 18 μm peaks from silicate–metal oxide dust grains (Wada et al. 2003; Greenberg 2002; Draine 2003).

Although the presence of silicon carbide in the circumstellar outflow of carbon-rich stars is well established (Clement et al. 2003), surprising little is known about the formation mechanism and chemistry of these stars. Walmsley et al. (1999) investigated the silicon chemistry in photodissociation regions (PDRs), but included predominantly silicon-oxygen chemistry. Similarly, chemical models of hot molecular cores have not coupled the silicon and carbon chemistry, but focus predominantly on silicon-oxygen and silicon-nitrogen chemical processing (MacKay 1995). The sole exceptions have been the postulated formation of silicon carbide via the reaction of silicon atoms with methyl (CH_3) and/or carbene (CH_2) followed by a stepwise photodissociation of the initial products to yield silicon carbide. Unfortunately, despite the incorporation of small hydrogenated

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silicon carbon clusters such as HCSi and $SiCH_2$, the models of Willacy & Cherchneff (1998) and Walmsley et al. (1999) could not yield conclusive evidence as to how silicon carbide grains are actually formed in circumstellar envelopes. This suggests that crucial formation routes are lacking. From the chemical viewpoint, it is quite surprising that with the exception of HCSi and $SiCH_2$, hydrogenated binuclear carbon-silicon clusters of the generic formula $SiCH_x$ ($x = 6-3$) have neither been incorporated into chemical models of, for instance, the carbon star IRC +10216, nor searched for in extraterrestrial environments. In the circumstellar envelope, a rich silane and methane chemistry can be driven by a photolysis of the silane and methane precursor molecule, thus forming the methyl (CH_3) and silyl (SiH_3) radicals. The latter could recombine to form the fully hydrogenated, binuclear carbon-silicon cluster silylmethane, $SiCH_6$, in a three-body reaction; if the reaction zone is too far from the central star, the $SiCH_6$ molecule cannot be stabilized by a three-body collision and decomposed to $SiCH_5$ isomers (recall that the number density drops with the inverse square of the radius from the centrals star). Successive photolysis of these species can yield silicon carbide (SiC) as a final product via stepwise atomic and/or molecular hydrogen elimination.

To test the validity of this hypothesis, it is important to search for $SiCH_x$ ($x = 6-3$) species in circumstellar envelopes of carbons stars. One drawback of a potential astronomical observation is the relatively small dipole moments of these molecules, less than 1.5 debye (Bennett et al. 2005a, 2005b). Therefore, an infrared spectroscopic search of the $SiCH_x$ species might present a viable alternative. Unfortunately, their infrared spectra—with the exception of silylmethane (CH_3SiH_3)—are elusive. In this paper, we present a matrix-isolation study of the infrared spectra of various $SiCH_x$ isomers ($x = 6-3$). This will assist an astronomical search for hydrogenated carbon-silicon clusters in the circumstellar envelope of IRC +10216 and provides valuable information on potential intermediates to finally synthesize silicon carbide in the interstellar medium.

2. EXPERIMENTAL PROCEDURE

Our experiments were carried out in a contamination-free ultrahigh vacuum (UHV) matrix-isolation chamber that can be evacuated down to 5×10^{-11} torr by a magnetically suspended turbopump backed by an oil-free scroll pump. A rotatable, two-stage closed-cycle helium refrigerator is attached to the lid of the machine and holds a polished silver single crystal. The latter is cooled to 10.2 ± 0.3 K and serves as a substrate for the silane-methane ices. The ices were prepared at 10 K by depositing silane (99.99%) and methane (99.99%) at pressures of 8×10^{-8} torr for 20 minutes onto the cooled silver crystal. Figure 1 shows a typical infrared spectrum of the frost at 10 K; the absorptions are summarized in Table 1. To determine the ice thickness quantitatively, we integrated the infrared absorption features at 2164 and 883 cm^{-1} (silane) as well as 4200, 3852, and 2815 cm^{-1} (methane). The ice thicknesses are then calculated via the Lambert-Beers relationship. Considering the integrated absorption coefficients of these fundamentals, i.e., 2.5×10^{-17} and 2.0×10^{-17} cm (silane) as well as 1.6×10^{-18}, 2.0×10^{-19}, and 2.3×10^{-18} cm (methane), this gives column densities of $2.0 \pm 0.1 \times 10^{17}$ and $1.5 \pm 0.2 \times 10^{17}$ cm^2, respectively. Taking the densities of the silane and methane ices to be 0.77 ± 0.03 and 0.53 ± 0.02 g cm^{-3} (Sears & Morrison 1975), this translates into thicknesses of 140 ± 15 nm silane and 70 ± 20 nm methane. The ices were irradiated at 10 K with 5 keV electrons generated in an electron gun at beam currents of 100 and 1000 nA by scanning the electron beam over an area of 3.0 ± 0.4 cm^2. Here the electron beam is used to cleave the carbon-hydrogen and silicon-hydrogen bonds of the methane and silane molecules and hence to initiate the formation of reactive radical precursors. Accounting for irradiation times of 60 minutes and the extraction efficiency of 78.8% of the electrons, this exposes the targets to up to 1.8×10^{16} electrons. To guarantee an identification of the reaction products in the ices and those subliming into the gas phase on line and in situ, a

TABLE 1

Infrared Absorptions of the Methane-Silane Matrix

Frequency (cm^{-1})	Assignment	Carrier
4523	$\nu_2 + \nu_3$	CH_4
4364	$2\ \nu_3$	SiH_4
4358	$\nu_3 + \nu_4$	CH_4
4298	$\nu_3 + \nu_4$	CH_4
4292	$\nu_1 + \nu_3$	SiH_4
4200	$\nu_1 + \nu_4$	CH_4
4112	$\nu_2 + 2\nu_4$	CH_4
3852/3895	$3\ \nu_4$	CH_4
	$\nu_3 + \nu_4 + \beta$	SiH_4
3139	$\nu_2 + \nu_3$	SiH_4
	$\nu_3 + \nu_4 + \alpha$	SiH_4
3074	$\nu_3 + \nu_4$	SiH_4
3011	ν_3	CH_4
2815	$\nu_2 + \nu_4$	CH_4
2595	$2\nu_4$	CH_4
2306	$\nu_3 + \gamma$	SiH_4
	$\nu_3 + \beta$	SiH_4
2193	$\nu_3 + \alpha$	SiH_4
2164	ν_3	SiH_4
1878	$\nu_2 + \nu_4 + \alpha$	SiH_4
1300	ν_4	CH_4
1032	$\nu_2 + \beta\ /\ \nu_4 + \gamma$	SiH_4
1032	$\nu_2 + \beta\ /\ \nu_4 + \gamma$	SiH_4
961	ν_2	SiH_4
930	$\nu_4 + \beta$	SiH_4
914	$\nu_4 + \alpha$	SiH_4
883	ν_4	SiH_4

Note.—Here α, β, and γ denote lattice modes.

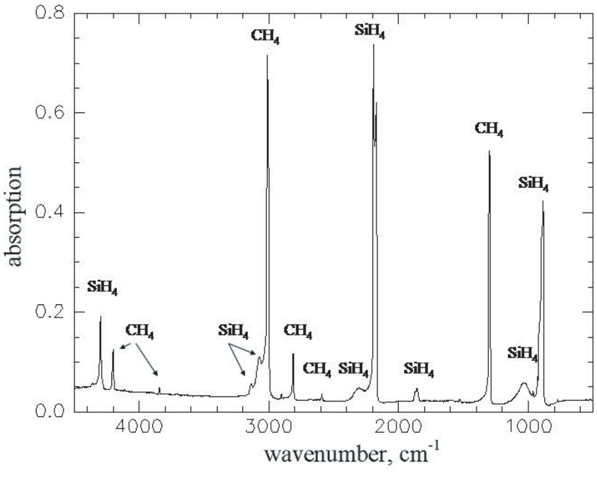

Fig. 1.—Infrared spectrum of the silane-methane sample at 10 K.

Fourier transform infrared spectrometer (FTIR; solid state) and a quadrupole mass spectrometer (QMS; gas phase) were used. The Nicolet 510 DX FTIR spectrometer operates in an absorption-reflection-absorption mode (reflection angle $\alpha = 75°$; resolution 0.5–2 cm^{-1}; spectra were averaged for 180 s). The infrared beam is coupled via a mirror flipper outside the spectrometer, passes through a differentially pumped potassium bromide (KBr) window, is attenuated in the ice sample before and after reflection at a polished silver waver, and exits the main chamber through a second differentially pumped KBr window before being monitored via a liquid-nitrogen–cooled detector. The gas phase is sampled by a quadrupole mass spectrometer (Balzer QMG 420; 1–200 amu mass range) with electron impact ionization of the neutral molecules.

3. RESULTS

Infrared spectroscopic studies of the irradiation phase suggest that the reaction of the silane-methane matrix to electron bombardment is dictated by the initial formation of the silyl, SiH$_3$ ($X\,^2A_1$), and methyl, CH$_3$($X\,^2A_2''$), radicals plus atomic hydrogen (reactions [1] and [2])

$$\mathrm{CH_4}(X\,^1A_1) \rightarrow \mathrm{CH_3}(X\,^2A_2'') + \mathrm{H}(^2S_{1/2}), \tag{1}$$

$$\mathrm{SiH_4}(X\,^1A_1) \rightarrow \mathrm{SiH_3}(X\,^2A_1) + \mathrm{H}(^2S_{1/2}). \tag{2}$$

The ν_2 vibrations of both the silyl and methyl radicals are visible at 723 and 609 cm^{-1}, respectively. These data agree very well with previous matrix studies (Andrews & Wang 2002). Very strong features of well-known ethane [C$_2$H$_6$($X\,^1A_{1g}$)] and disilane [Si$_2$H$_6$($X\,^1A_{1g}$)] molecules—typical recombination products of methyl (Bennett et al. 2005a, 2005b) and silyl radicals (Sillars et al. 2004) as observed in pure methane and silane ices—showed up as well (Table 2; reactions [3] and [4]):

$$\mathrm{CH_3}(X\,^2A_2'') + \mathrm{CH_3}(X\,^2A_2'') \rightarrow \mathrm{C_2H_6}(X\,^1A_{1g}), \tag{3}$$

$$\mathrm{SiH_3}(X\,^2A_1) + \mathrm{SiH_3}(X\,^2A_1) \rightarrow \mathrm{Si_2H_6}(X\,^1A_{1g}). \tag{4}$$

With increasing irradiation time, the ethane molecules are radiolyzed stepwise via the ethyl radical [C$_2$H$_5$($X\,^2A'$)], ethylene [C$_2$H$_4$ ($X\,^1A_g$)], and the vinyl radical [C$_2$H$_3$($X\,^2A'$)] to finally form acetylene [C$_2$H$_2$($X^1\Sigma_g^+$)]; disilane was found to degrade via the disilyl radical [Si$_2$H$_5$($X\,^2A'$)], two Si$_2$H$_4$ isomers, silylsilylene [H$_3$SiSiH($X\,^1A'$], disilene [H$_2$SiSiH$_2$($X\,^1A_g$)], and disilenyl [H$_2$SiSiH($X\,^2A$)], to yield the bridged disilicondihydride [SiH$_2$Si($X\,^1A_1$)]. These reaction sequences were also observed in neat methane and silane matrices at 10 K (Sillars et al. 2004, 2005; Kaiser & Osamura 2005). In addition to the absorption present in the methane and silane matrices, we also detected six prominent features of the well-known methylsilane molecule, CH$_3$SiH$_3$($X\,^1A_1$; see Table 2), which is formed via the recombination of a methyl with a silyl radical (reaction [5]):

$$\mathrm{SiH_3}(X\,^2A_1) + \mathrm{CH_3}(X\,^2A_2'') \rightarrow \mathrm{CH_3SiH_3}(X\,^1A_1). \tag{5}$$

We also identify two new SiCH$_5$ isomers: methylsilyl, CH$_3$SiH$_2$($X\,^2A'$), and silylmethyl, SiH$_3$CH$_2$($X\,^2A'$), via their absorptions at 1251 cm^{-1} (ν_5), 1414 cm^{-1} (ν_{12}), and 653 cm^{-1} (ν_8), as well as 645 cm^{-1} (ν_8) (see Figs. 2 and 3). These findings are in excellent agreement with computed frequencies of both isomers (Bennett et al. 2005a, 2005b).

TABLE 2

Compilation of Newly Observed Species in the Methane-Silane Matrix upon Electron Irradiation

Frequency (cm^{-1})	Fundamental	Carrier
Hydrogenated Carbon Species		
609	ν_2	CH$_3$
826	ν_{12}	C$_2$H$_6$
1380	ν_{16}	C$_2$H$_6$
1462	ν_{11}	C$_2$H$_6$
2880	ν_5	C$_2$H$_6$
2973	ν_{10}	C$_2$H$_6$
530	ν_9	C$_2$H$_5$
2848	ν_3	C$_2$H$_5$
2939	ν_2	C$_2$H$_5$
1440	ν_{12}	C$_2$H$_4$
960	ν_7	C$_2$H$_4$
826	ν_{10}	C$_2$H$_4$
897	ν_8	C$_2$H$_3$
688	ν_7	C$_2$H$_3$
3282	ν_3	C$_2$H$_2$
736	ν_5	C$_2$H$_2$
Hydrogenated Silicon Species		
722	ν_2	SiH$_3$
826	ν_6	Si$_2$H$_6$
934	ν_{11}	Si$_2$H$_6$
2142	$\nu_{5/4}$	Si$_2$H$_6$
852	ν_6	Si$_2$H$_5$
856	ν_5	H$_3$SiSiH
897	ν_{11}	H$_2$SiSiH$_2$
933	ν_4	H$_2$SiSiH
Hydrogenated Carbon-Silicon Species		
691	ν_5	CH$_3$SiH$_3$
863	ν_{11}	CH$_3$SiH$_3$
946	ν_{10}	CH$_3$SiH$_3$
976	ν_4	CH$_3$SiH$_3$
1254	ν_3	CH$_3$SiH$_3$
2142	ν_2	CH$_3$SiH$_3$
654	ν_8	CH$_3$SiH$_2$
1414	ν_{12}	CH$_3$SiH$_2$
1251	ν_5	CH$_3$SiH$_2$
645	ν_8	CH$_2$SiH$_3$
740	ν_7	H$_2$CSiH$_2$
1947	ν_3	CH$_3$SiH
1211	ν_4	H$_3$CSi
1387	ν_3	H$_3$CSi
717	ν_8	H$_2$CSiH
688	ν_4	H$_2$CSi

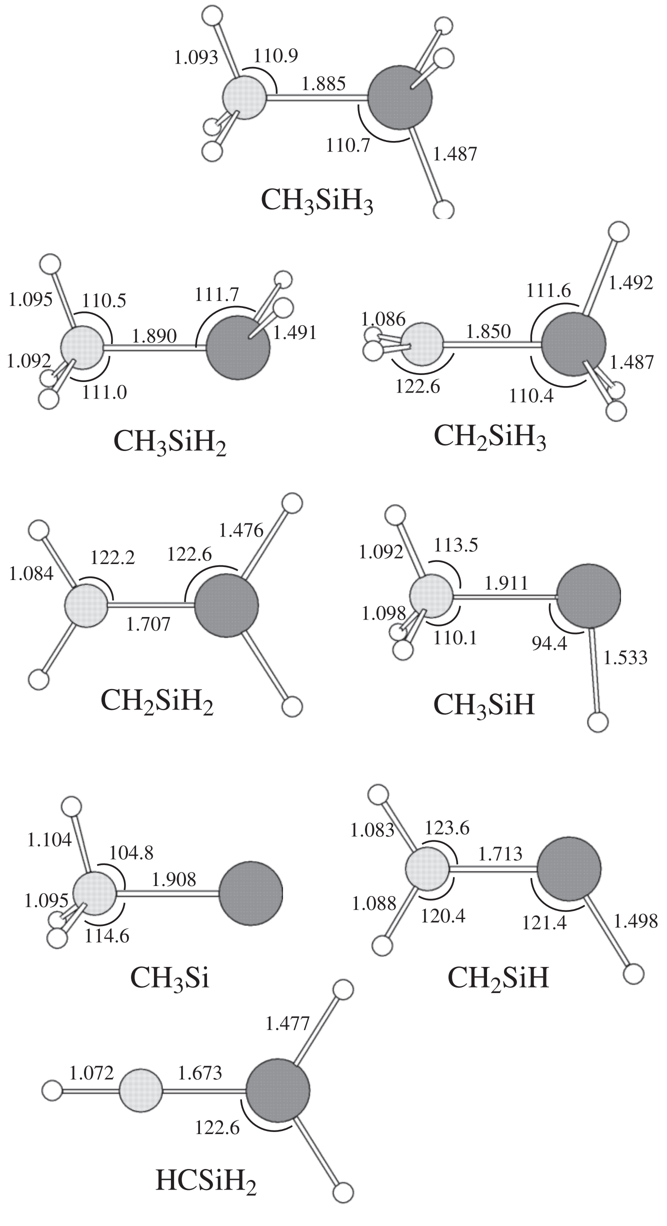

FIG. 2.—Structures of the hydrogenated silicon-carbon clusters. Bond lengths and bond angles are in Å and degrees (*dark gray*: silicon; *light gray*: carbon; *white*: hydrogen atoms). The computed frequencies and computational methods are listed in the Appendix.

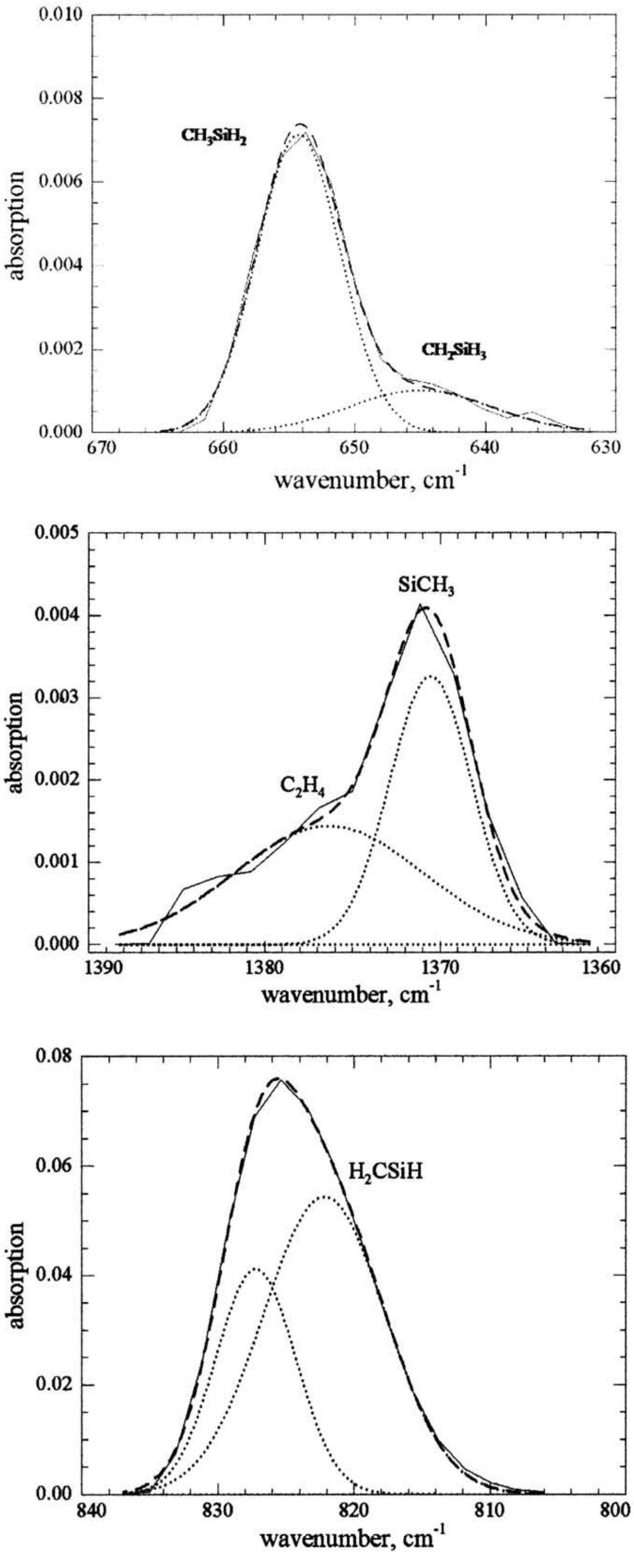

FIG. 3.—Absorption features of the newly silicon-carbon bearing species $SiCH_5$ and $SiCH_3$ in the silane-methane matrices.

The assignment of the methylsilyl and silylmethyl radicals raises the question whether, in a manner similar to the radiolysis of ethane and disilane, an enhanced electron exposure of the silane-methane matrices will lead to the formation of hydrogen-depleted silicon-carbon clusters of the formula $CSiH_n$ ($n = 4$, 3, 2). Indeed, with increasing irradiation time, new absorption features appear at 742 and 1947 cm^{-1}. These absorptions could not be assigned to any of the molecules discussed above. Instead, a comparison with computed vibration frequencies of the $SiCH_4$ isomers (Bennett et al. 2005a, 2005b) suggest the formation of the most thermodynamically stable silene molecule $[H_2CSiH_2(X\,^1A_1)]$ (ν_7) and the less stable methylsilylene isomer $[CH_3SiH(X\,^1A')]$ (ν_3). An enhanced irradiation times lead to the synthesis of $H_3CSi(X\,^2A'')$ and $H_2C{=}SiH(X\,^2A')$. Here, absorptions at 1226 cm^{-1} (ν_4) and 1371 cm^{-1} (ν_3) were assigned to the $H_3CSi(X\,^2A'')$ structure; the peak at 822 cm^{-1} (ν_6) could be attributed to the $H_2C{=}SiH(X\,^2A')$ isomer (Figs. 2 and 3, Table 2). These data are in excellent agreement with previous calculations (Bennett et al. 2005a, 2005b).

4. ASTROPHYSICAL IMPLICATIONS

Our studies provide reliable infrared absorptions of astrophysically important hydrogenated silicon-bearing molecules. Two classes of molecules can be identified from the present laboratory study. These are XH_3 species (X = C, Si) and XYH_x (X = C, Si; Y = C, Si; $x = 1-6$). The silicon-carbon–bearing dinuclear clusters $SiCH_x$ are of great interest in the potential formation of silicon carbide molecules and their aggregates in circumstellar envelopes of dying carbon stars such as of IRC +10216. Here, the fundamentals as observed in our experiments are compiled in Table 2 and serve as valuable guidelines for prospective astronomical identifications of these molecules. We would like to stress that the actual photodissociation of silane molecules in circumstellar envelopes is expected to preferentially yield the $SiH_2(X\,^1A_1)$ and $SiH(X\,^2\Pi)$ species. However, these radicals can react with ubiquitous methane molecules to form methylsilane and silylmethyl/methylsilyl isomers via insertion processes followed by isomerization:

$$SiH_2(X\,^1A_1) + CH_4(X\,^1A_1) \rightarrow CH_3SiH_3(X\,^1A_1), \qquad (6)$$

$$SiH(X\,^2\Pi) + CH_4(X\,^1A_1) \rightarrow SiH_2CH_3(X\,^2A'), \qquad (7)$$

$$SiH_3CH_2(X\,^2A') \rightarrow CH_3SiH_2(X\,^2A'). \qquad (8)$$

Considering the homologous C_2H_x ($x = 1-6$) series, we would like to point out that silicon-bearing species have not been detected in either the solar system or the interstellar medium so far. On the other hand, members of the homologous C_2H_x ($x = 1-6$) series are very abundant in our solar system and in the interstellar medium. Ethane (C_2H_6) and acetylene (C_2H_2) are actually present in the atmospheres of the giant planets Jupiter and Saturn (Fouchet et al. 1999; Courtin et al. 1984), as well as Uranus (Atreya et al. 1999; Bishop et al. 1990) and Neptune (Conrath et al. 1989; Orton et al. 1992). Ethylene (C_2H_4) was only observed in Jupiter and Neptune (Encrenaz et al. 2002; Fegley 1995). Ethane has been also identified in comets such as 153P/Ikeya-Zhang (Kawakita et al. 2003). Note that ethylene (Goldhaber et al. 1987), acetylene (Cernicharo et al. 1999), and the ethinyl radical (Fuente at al. 1998) have been detected in the circumstellar envelope of IRC +10216. We also computed the rotational constants and the dipole moments of the organosilicon species detected in our experiments (Table 3). Here the dipole moments are very small (only up to about 1 debye), so these molecules might be difficult to detect with microwave spectroscopy. Therefore, our laboratory investigations should be helpful in elucidating the hitherto poorly understood organosilicon chemistry in circumstellar envelopes of carbon-rich dying stars and also in prospective astronomical searches in the infrared regime using the NASA *Infrared Telescope Facility* and the *Spitzer Space Telescope*.

TABLE 3

Dipole Moments and Rotational Constants for $SiCH_6$, $SiCH_5$, $SiCH_4$, and $SiCH_3$ Calculated with the B3LYP/6-311G(d,p) Theory

Species	Dipole Moment (debye)	Rotational Constants (GHz)		
CH_3SiH_3..........	0.738	56.119	10.821	10.821
CH_3SiH_2..........	0.806	73.007	11.583	11.027
CH_2SiH_3..........	0.650	67.012	11.952	11.475
CH_2SiH_2..........	0.600	105.056	14.763	12.944
CH_3SiH	1.009	93.354	12.224	11.571
CH_2SiH	0.554	157.285	15.473	14.087
$HCSiH_2$	0.635	161.999	15.801	14.397

The experiments were supported by the University of Hawai'i at Manoa (R. I. K.) and by the Particle Physics and Astronomy Research Council (PPARC, UK) (R. I. K.). The computations were carried out at the computer center of the Institute for Molecular Science, Japan, and supported by the Grants-in-Aid for Scientific Research on Priority Areas from the Ministry of Education, Science, and Culture, Japan (Y. O.).

APPENDIX

COMPUTATIONAL METHOD

The vibrational frequencies and the molecular structures of the $CSiH_x$ ($x = 1-6$) isomers shown in Table 4 were computed in terms of ab initio molecular orbital methods. The geometries were optimized with the hybrid density functional B3LYP method, i.e., Becke's three-parameter nonlocal exchange functional (Becke 1993) with the nonlocal correlation functional of Lee et al. (1988) and the 6-311G(d, p) basis set (Krishnan et al. 1980). To assist spectroscopic identification in circumstellar envelopes, we also obtained vibrational frequencies and infrared intensities. The coupled cluster CCSD(T) calculations (Cizek 1969; Pople et al. 1987) with the aug-cc-pVTZ basis set (Kendall et al. 1992) were also performed for the optimized structures obtained with the B3LYP method. All computations were carried out using the GAUSSIAN 98 program package (Frisch et al. 2002).

TABLE 4

UNSCALED VIBRATIONAL FREQUENCIES (cm^{-1}) OF EXPERIMENTALLY OBSERVED HYDROGENATED CARBON-SILICON CLUSTERS CALCULATED WITH B3LYP/6–311G(d,p) THEORY

Mode	Frequency	Characterization
CH_3SiH_3		
ν_1 a_1	3031	CH_3 sym. stretch
ν_2 a_1	2221	SiH_3 sym. stretch
ν_3 a_1	1305	CH_3 umbrella
ν_4 a_1	949	SiH_3 umbrella
ν_5 a_1	690	C—Si stretch
ν_6 a_2	194	torsion
ν_7 e	3105	CH_3 asym. stretch
ν_8 e	2221	SiH_3 asym. stretch
ν_9 e	1469	CH_3 deformation
ν_{10} e	965	SiH_3 deformation
ν_{11} e	896	CH_3, SiH_3 rocking
ν_{12} e	525	CH_3, SiH_3 rocking
CH_3SiH_2		
ν_1 a'	3091	CH_3 asym. stretch
ν_2 a'	3021	CH_3 sym. stretch
ν_3 a'	2178	SiH_2 sym. stretch
ν_4 a'	1463	CH_3 deformation
ν_5 a'	1291	CH_3 umbrella
ν_6 a'	938	SiH_2 bending
ν_7 a'	851	CH_3, SiH_2 rocking
ν_8 a'	681	C—Si stretch
ν_9 a'	570	CH_3, SiH_2 rocking
ν_{10} a''	3112	CH_3 asym. stretch
ν_{11} a''	2203	SiH_2 asym. stretch
ν_{12} a''	1458	CH_3 deformation
ν_{13} a''	895	CH_3, SiH_2 deformation
ν_{14} a''	530	CH_3, SiH_2 deformation
ν_{15} a''	177	torsion
CH_2SiH_3		
ν_1 a'	3122	CH_2 sym. stretch
ν_2 a'	2221	SiH_3 sym. stretch
ν_3 a'	2185	SiH_3 asym. stretch
ν_4 a'	1405	CH_2 bending
ν_5 a'	951	SiH_3 umbrella
ν_6 a'	948	SiH_3 deformation
ν_7 a'	748	C—Si stretching
ν_8 a'	666	SiH_3 rocking
ν_9 a'	525	CH_2 umbrella
ν_{10} a''	3214	CH_2 asym. stretch
ν_{11} a''	2224	SiH_3 asym. stretch
ν_{12} a''	961	SiH_3 deformation
ν_{13} a''	847	CH_2, SiH_3 rocking
ν_{14} a''	526	CH_2, SiH_3 rocking
ν_{15} a''	17	torsion
$H_2C{=}SiH_2$		
ν_1 a_1	3143	CH_2 sym. stretch
ν_2 a_1	2265	SiH_2 sym. stretch
ν_3 a_1	1401	CH_2 scissor
ν_4 a_1	997	C—Si stretch
ν_5 a_1	943	SiH_2 scissor
ν_6 a_2	730	twist
ν_7 b_1	782	CH_2 out-of-plane
ν_8 b_1	455	SiH_2 out-of-plane
ν_9 b_2	3231	CH_2 asym. stretch
ν_{10} b_2	2288	SiH_2 asym. stretch
ν_{11} b_2	841	CH_2 rocking
ν_{12} b_2	485	SiH_2 rocking
$H_3C{-}SiH$		
ν_1 a'	3104	CH_3 asym. stretch
ν_2 a'	2993	CH_3 sym. stretch
ν_3 a'	2005	SiH stretch
ν_4 a'	1437	CH_3 deformation
ν_5 a'	1267	CH_3 umbrella
ν_6 a'	952	SiH bend, CH_3 rock
ν_7 a'	662	C—Si stretch
ν_8 a'	629	SiH bend
ν_9 a''	3045	CH_3 asym. stretch
ν_{10} a''	1453	CH_3 deformation
ν_{11} a''	578	CH_3 rocking
ν_{12} a''	150	torsion
$H_3C{-}Si$		
ν_1 a'	3040	CH_3 asym. stretch
ν_2 a'	2965	CH_3 sym. stretch
ν_3 a'	1445	CH_3 deformation
ν_4 a'	1259	CH_3 umbrella
ν_5 a'	665	C—Si stretch
ν_6 a'	528	CH_3 rocking
ν_7 a''	3072	CH_3 asym. stretch
ν_8 a''	1359	CH_3 deformation
ν_9 a''	598	CH_3 deformation
$H_2C{=}SiH$		
ν_1 a'	3223	CH_2 asym. stretch
ν_2 a'	3116	CH_2 sym. stretch
ν_3 a'	2128	SiH stretch
ν_4 a'	1368	CH_2 scissor
ν_5 a'	964	C—Si stretch
ν_6 a'	839	SiH bend, CH_2 rock
ν_7 a'	521	SiH bend, CH_2 rock
ν_8 a''	749	out-of-plane
ν_9 a''	256	torsion
$HC{=}SiH_2$		
ν_1 a_1	3343	CH stretch
ν_2 a_1	2254	SiH_2 sym. stretch
ν_3 a_1	1072	C—Si stretch
ν_4 a_1	958	SiH_2 scissor
ν_5 b_1	667	out-of-plane
ν_6 b_1	319	out-of-plane
ν_7 b_2	2265	SiH_2 asym. stretch
ν_8 b_2	606	SiH_2 rocking
ν_9 b_2	196	CH bend

NOTE.—Frequencies must to be scaled by a factor of 0.98–0.97 to be compared with experimental data.

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