Spectroscopic parameters for silacyclopropynylidene, SiC$_2$, from extensive astronomical observations toward CW Leo (IRC +10216) with the *Herschel* satellite[☆,☆☆]

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Abstract

A molecular line survey has been carried out toward the carbon-rich asymptotic giant branch star CW Leo employing the HIFI instrument on board of the *Herschel* satellite. Numerous features from 480 GHz to beyond 1100 GHz could be assigned unambiguously to the fairly floppy SiC$_2$ molecule. However, predictions from laboratory data exhibited large deviations from the observed frequencies even after some lower frequency data from this survey were incorporated into a fit. Therefore, we present a combined fit of all available laboratory data together with data from radio-astronomical observations.

Keywords:
rotational spectroscopy, interstellar molecule, silicon compound, centrifugal distortion

1. Introduction

Silacyclopropynylidene, SiC$_2$, somewhat better known as silicon dicarbide, is a fascinating molecule for spectroscopists, structural and quantum chemists as well as astronomers. In 1926, uncataloged bands near 500 nm were discovered in the spectra of several carbon-rich asymptotic giant branch (AGB) stars [1, 2]. These are late-type stars which produce elements heavier than helium and which eject large quantities of gaseous material as well as dust which form a circumstellar envelope (CSE). Thirty years later, laboratory spectroscopy established that the molecule SiC$_2$ is the carrier of these bands [3]. It was assumed that the molecule has a linear SiCC structure (silapropadienediylidene) in analogy with the isoelectronic propadienediylidene, C$_3$. Although some later studies cast doubt on the linear structure of the molecule, it took almost another 30 years until the analysis of the rotational structure of the electronic origin band unmistakably determined the structure as silacyclopropynylidene [4]. In the course of their analysis, the authors instigated quantum chemical calculations which provided evidence that the cyclic isomer of SiC$_2$ may be lower in energy than the linear form [5].

A plethora of quantum chemical calculations on various properties of SiC$_2$ have been published later, yielding energy differences between the linear and the cyclic form which depended strongly on the level of the calculation and the size of the basis set. A high level ab initio calculation concluded that the cyclic isomer of SiC$_2$ is the only minimum on the potential energy surface and that the linear transition state is 24.3 kJ/mol higher in energy [6]. However, the authors attached a caveat to this value as an anharmonic force field calculation provided a much too small value for the vibrational energy of $v_3 = 1$ and much too large anharmonicity constants. Therefore, some of the authors revisited the problem of the energy difference between the two SiC$_2$ structures, the last time in 2003 when very high level calculations combined with very large basis sets, basis set extrapolation to infinite size as well as additional corrections yielded a value of 26.5 kJ/mol [7].

The SiC$_2$ molecular parameters obtained in Ref. [4] laid the foundation for progress in laboratory spectroscopy. The $J = 1 - 0$ rotational transition frequencies of the three isotopologs SiC$_2$[1], ^{29}SiC$_2$, and ^{30}SiC$_2$, as well as the permanent electric dipole moment were measured using Fourier transform microwave spectroscopy [8]. Subsequently, 34 additional transition frequencies were measured for the main isotopic species between 93 and 370 GHz [9]. Even though a comparatively large number of 15 spectroscopic parameters of a standard Watson-type Hamiltonian in the A-reduction, all parameters up to sixth order, were employed in the fit, the transition frequen-

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[1]Unlabeled atoms refer to ^{12}C and ^{28}Si.

cies were reproduced on average to only four times the experimental uncertainties.

Similarly large bodies of laboratory transition frequencies were obtained for $SiC^{13}C$ between 339 and 405 MHz [10] and, only very recently, for $^{29}SiC_2$ and $^{30}SiC_2$ between 140 and 360 GHz [11].

Higher excited vibrational states have been studied for the main isotopolog. Rotational transitions in its low-lying $v_3 = 1$ vibrational state between 186 and 399 GHz [12] and in $v_3 = 1$ and 2 were obtained between 140 and 400 GHz [13]. The symmetry of $v_3 = 1$ is b_2 and can be viewed as an asymmetric bending state which facilitates internal rotation of the C_2 unit with respect to the Si atom. Its vibrational energy has been determined as 196.37 cm^{-1} from an investigation into the laser-induced and the dispersed fluorescence of a jet-cooled sample of SiC_2 [14].

Several attempts have been made to model rotational and sometimes also rovibrational data to a varying extent and accuracy. A semirigid bender (SRB) Hamiltonian was employed [16] to reproduce $v_3 = 0$ and 1 rotational transition frequencies [9, 12] as well as rovibrational data from their previous [14] and present work [16]. The analysis suggested that the linear configuration is not a local minimum, and the cyclic form is 22.5 kJ/mol lower than the linear form; the estimated uncertainty was 2.4 kJ/mol. They found the energy difference to be in good agreement with results from their own ab initio calculations; their highest level value being 21.8 kJ/mol. The reproduction of the vibrational data was reasonable, that of the rotational data was only qualitative and thus of no use for radio-astronomical purposes.

The $v_3 = 0$ and 1 state rotational data [9, 12] were also modeled with a dedicated internal rotation Hamiltonian [15]. A greatly improved reproduction, within 1.5 times the experimental uncertainties, was achieved for the ground vibrational state, albeit at the expense of 16 spectroscopic parameters compared to 15 previously [9]. The barrier to linearity was derived as ~54 kJ/mol, more than twice the value from ab initio calculations of that time.

A reasonably successful result has been obtained by employing a conventional Watson-type Hamiltonian in the S-reduction [17]. The reproduction of the ground state rotational data [8, 9] was converged after varying 17 spectroscopic and keeping one fixed. The data were reproduced on average as well as in the fit which employed an internal rotation Hamiltonian [15]; the number of varied parameters, however, was larger by still another one. After scaling of the parameters, the transition frequencies of $^{29}SiC_2$ and $^{30}SiC_2$ available at that time, mostly from astronomical observation [10, 17], could be reproduced well after releasing only 5 spectroscopic parameters [17]; 13 parameter were released in the fit for $SiC^{13}C$ because of the large amount of accurate laboratory data [10].

The unambiguous assignment of a spectroscopic feature observed in space relies on reliable predictions which are usually based on laboratory data which, for the most part, have been obtained in approximately the same frequency domain. The predictions may also be based in part on data from astronomical observations, recent examples include $H^{13}CO^+$ [18],

DCO^+ [19, 20], DNC and $HN^{13}C$ [20], C_2H [21], and $C^{13}CH$ [22]. Sometimes, identifications are even possible in the absence of laboratory data, as demonstrated recently by the detection of C_5N^- in the CSE of CW Leo [23]. Frequencies have to be predicted with accuracies better than around one tenth of the line width to permit extraction of dynamical information. Some type of intensity information, such as that at a certain temperature, the line strength, or the Einstein A-value is needed as is additional auxiliary information such as quantum numbers, lower or upper state energies etc. Pickett's SPCAT and SPFIT programs [24] have been developed for that purpose and have evolved over time, see e. g. Ref. [25]. These programs are routinely used in the Cologne Database for Molecular Spectroscopy[2], CDMS [26, 27], to provide in its catalog section[3] predictions of (mostly) rotational spectra of molecules which may be found in various environments in space.

The spectroscopic parameters from the first rotational analysis of the electronic spectrum of SiC_2 [4] were accurate enough to identify nine unassigned emission features, previously observed between 93 and 171 GHz toward the carbon-rich AGB star CW Leo, also known as IRC +10216, as belonging to SiC_2 and improved the SiC_2 structural parameters [28]. Using the structural parameters from that work, the three $J = 4 - 3$, $\Delta K_a = 0$ transitions of $^{29}SiC_2$ and $^{30}SiC_2$ were detected toward the same source very soon thereafter [29]; two of these transitions were marginally detected for $SiC^{13}C$. Extensive sets of transition frequencies of $^{29}SiC_2$, $^{30}SiC_2$, and $SiC^{13}C$ were obtained from radio-astronomical observation between 90 and 241 GHz together with laboratory rest frequencies for the latter isotopolog [10].

Radio lines of SiC_2 have also been detected in the CSEs of other C-rich AGB stars, e. g. toward II Lup, which is also known as IRAS 15194-5115 [30]. However, SiC_2 features are particularly strong toward CW Leo, which, to a large extent, is due to its proximity to our Solar system. CW Leo has been studied extensively, and many molecular species, such as CN^- [31] and FeCN [32], have been detected toward its CSE exclusively or for the first time, including many Si-containing ones, such as SiCN and SiNC [33]. The source is a subject of observations in several key projects carried out with the recently launched *Herschel* satellite [34]. One of these projects is a molecular line survey carried out with the Heterodyne Instrument for the Far-Infrared (HIFI) [35]. This high-resolution instrument covers, in several bands, the 480−1250 and 1410−1910 GHz regions. A preliminary analysis of a lower frequency region (554−637 GHz) revealed that a rather small number of molecules account for a large fraction of the emission features [36]. These molecules are CS, SiO, SiS, HCN, and, in particular, SiC_2. Predictions of the rotational spectrum based on Ref. [17] turned out to be very good for transitions with higher values of K_a, but showed increasing deviations of up to 10 MHz for transitions with decreasing K_a, contrary to common expectations. A combined fit of these transitions frequencies together with those from laboratory spectra [8, 9] re-

quired only one additional parameter [36] to reproduce the astronomical data within uncertainties, and the laboratory data about as well as before [17]. Predictions of the SiC_2 rotational spectrum based on these results are currently available as version 2 in the CDMS[4]. Since they were still not appropriate to predict the observed emission features satisfactorily to high frequencies (beyond 1100 GHz), we present here a combined fit using these as well as laboratory data, supplemented with data from additional astronomical observations.

2. Observed spectrum

Silacyclopropynylidene, SiC_2, is a triangular, fairly asymmetric rotor with $\kappa = (2B - A - C)/(A - C) = -0.7117$. Its dipole moment of 2.393 (6) D [8] is along the a-axis. Only even K_a exist because of the two equivalent C nuclei with zero spin. R-branch transitions ($\Delta J = J' - J'' = +1$) with $\Delta K_a = 0$ are the strongest ones, and most of the transitions observed in the laboratory [8, 9] and in space, see e. g. Refs. [28, 29, 10], fall into this category. Q-branch transitions with $\Delta K_a = 0$ and transitions with $\Delta K_a = \pm 2$ also have considerable intensities because of κ being very different from -1. The former type of transitions was detected in space, the latter both in the laboratory [9] and in space.

The line survey of CW Leo was carried out with the HIFI instrument [35] on board of the *Herschel* satellite [34] May 11−15 2010 employing all six bands. Some details on the observations and on the data reduction have been given earlier [36], and additional information will be provided in a subsequent manuscript on the whole line survey. The lower resolution mode provides a point spacing of about 1.1 MHz which is well sufficient even at low frequencies. A fair fraction of the moderately strong to weak lines in the four lowest bands from 480 to 1120 GHz could be assigned to SiC_2. No lines were observed with sufficient signal-to-noise ratio in bands 5 to 7 (1120−1250 GHz and 1410−1910 GHz). The center frequencies were determined from a fit to the observed line profile using the CLASS program of the GILDAS package[5]. The rotational temperature of SiC_2 was determined as ~204 K; the Boltzmann peak at this temperature is near 500 GHz. 261 distinct features have been identified in the HIFI spectra corresponding to 319 rotational transitions with $19 \leq J \leq 53$ and $K_a \leq 16$. All transitions were R-branch transitions with $\Delta K_a = 0$. The accuracies of the frequencies range from 1.5 MHz for relatively strong, isolated lines at low frequencies to 20 MHz for lines with low signal-to-noise ratio at high frequencies. Selected SiC_2 transitions from the HIFI molecular line survey are shown in Fig. 1.

Additional spectral data of IRC +10216 in the radio domain (90−358 GHz) were obtained with the IRAM[6] 30 m telescope,

located at Pico Veleta, Granada (Spain). Lines in the λ 2 mm wavelength domain have been previously reported [37], while those lying at λ 3 mm and 1 mm will be presented in detail in forthcoming papers. The center frequencies were determined in the same way as used for the lines observed with Herschel. A total of 59 SiC_2 lines were clearly observed in emission with a spectral resolution of 1−1.25 MHz below 260 GHz and of 2 MHz above this frequency. The 59 lines correspond to 75 rotational transitions with $K_a \leq 12$. Most of them are R-branch transitions with $\Delta K_a = 0$, but there were also five Q-branch transitions ($\Delta J = 0$) with $K_a = 2 - 0$ and two with $K_a = 2 - 2$. Although the observed lines are relatively wide, around 29 km s^{-1} in equivalent radial velocity, their edges are very sharp with a small broadening at the base due to micro turbulence velocities of 1.5 km s^{-1}. Hence, lines with a high signal-to-noise ratio can be fitted with an accuracy better than 1 km s^{-1}. Consequently, the experimental accuracies on the frequencies derived towards IRC +10216 depend on the line intensity, being around 1 MHz for the weakest lines and around 0.1 MHz for the strongest ones.

The transition frequencies from the HIFI and IRAM 30 m observations are given in the supplementary material together with those from laboratory experiments with quantum numbers, uncertainties, and residuals o−c between observed frequencies and those calculated from the final fit.

3. Spectroscopic analysis

The choice of spectroscopic parameters is often not unique if one has to reproduce a large set of transition frequencies, in particular in the case of floppy molecules, such as SiC_2. One way of getting a comparatively small and possibly even unique data set is to examine carefully which parameter improves the quality of the fit the most, as judged by the rms error, also known as reduced χ^2, and if one includes and keeps only parameters determined with a certain level of significance. However, this procedure may run into difficulties if parameters of a given order have rather similar magnitudes or if certain parameters are strongly correlated. Moreover, a particularly small parameter set or one yielding the smallest rms error does not always yield the most reliable predictions, in particular if the amount of transition frequencies is rather small.

As indicated in section 1, the SiC_2 laboratory data from Ref. [9] were reproduced there to only four times the reported uncertainties employing Watson's A-reduction of the rotational Hamiltonian with a complete set of parameters up to sixth order. As will be shown later, the quality of the fit is a result of the particular choice of parameters, not a result of the choice of the reduction. In that fit, the residuals were distributed unevenly, and the K-ordering of the energy levels was incorrect starting at $J = 26$. Refs. [15, 17] used a dedicated internal rotation Hamiltonian with 16 parameters and Watson's S-reduction of the rotational Hamiltonian with 17 varied parameters, respectively, to reproduce these data within about 1.5 times the reported uncertainties. This suggests that the laboratory data [9] were estimated too optimistically. Here, as in previous fits [17, 36],
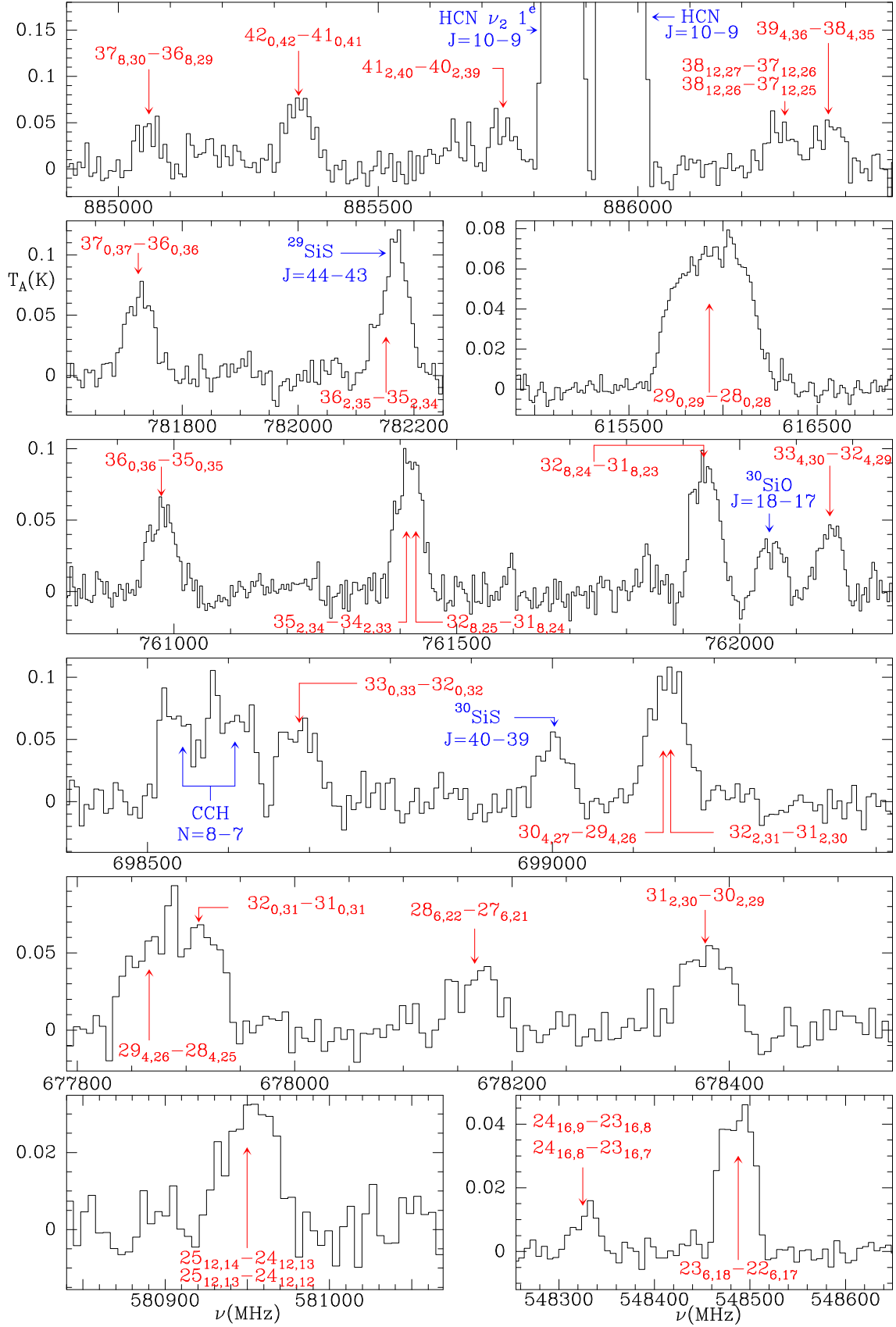

Figure 1: Sections of the molecular line survey of CW Leo displaying selected SiC_2 transitions. Their quantum numbers $J'_{K'_a,K'_c} - J''_{K''_a,K''_c}$ are given in red (grey). The formulae and quantum numbers of other lines are given in blue (black).

the uncertainties from that work were multiplied with 1.5 and rounded up.

Starting initially with the parameter set from Ref. [17], the complete list of transition frequencies from HIFI observations, from laboratory spectroscopy, and from selected additional astronomical observations could be reproduced well with the S-reduction of the rotational Hamiltonian. However, these fits required around 24 varied parameters compared with 17 and 18, respectively, in previous fits [17, 36]. Therefore, attempts were also made to fit the data employing the A-reduction. In one fit, the procedure described above was followed; a fit with only 18 spectroscopic parameters achieved an rms error of 0.77. However, comparatively many off-diagonal distortion parameters, such as ϕ_K, l_K, and p_K, were used in the fit. Moreover, the partition function values, calculated by including energy level up to $J = 90$ and $K_a = 40$ for convergence at 300 K, differed remarkably little between 10 K and 300 K. This was caused by decreasing energies, eventually turning negative, at low K_a. Since such energies are unphysical, the fit was therefore discarded.

In a subsequent fit, off-diagonal distortion parameters were avoided as far as possible. The fit achieved an overall rms error of 0.73 with 20 parameters. Three highly K-dependent off-diagonal distortion parameters and Φ_K, used in the previous fit, were replaced by l_{JK} and some additional diagonal distortion parameters. These parameters yielded partition function values similar to previous works [17, 36]. The laboratory data from Ref. [9] as well as astronomical observations up to 360 GHz were reproduced with partial rms errors marginally smaller than 1.0, while the transition frequencies obtained from HIFI observations had a partial rms error of 0.63, suggesting that, overall, they may have been judged slightly conservatively. The parameter Φ_K, determined insignificantly in the previous laboratory spectroscopic work [9] and judged to be rather large in a very recent laboratory study of $^{29}SiC_2$ and $^{30}SiC_2$ [11], was still not determined with significance in later fits and was therefore not included in the final fit. The resulting spectroscopic parameters are given in Table 1. The change in reduction of the rotational Hamiltonian prompted an attempt to fit the laboratory data [8, 9] with an A reduction parameter set. All transition frequencies from astronomical observations were eliminated from the line list, and all parameters with uncertainties not much smaller than the value were eliminated up to before the point at which the rms error increased substantially. The final fit consisted of 15 parameters which reproduced the data as well as the fits described in Refs. [15, 17], but actually with one and two varied parameters, respectively, less. The spectroscopic parameters from that fit have also been given in Table 1.

4. Discussion

The transitions of SiC_2, whose frequencies have been measured in the laboratory or in space, are almost all R-branch transitions, and most of them have $\Delta K_a = 0$. Spectroscopic parameters obtained from such a data set permit reasonable extrapolation up to around twice the highest frequencies in the line list even under favorable conditions. Favorable conditions are

Table 1: Spectroscopic parameters[a] (MHz) for SiC_2 obtained in the present investigation.

Parameter	All data	Lab. data only[b]
$A - (B + C)/2$	40673.821 (37)	40674.109 (60)
$(B + C)/2$	11800.14670 (66)	11800.14722 (89)
$(B - C)/4$	679.28139 (53)	679.28365 (87)
Δ_K	−1.2841 (89)	−1.2092 (153)
Δ_{JK}	1.538195 (69)	1.538100 (86)
$\Delta_J \times 10^3$	13.1962 (28)	13.2188 (38)
$\delta_K \times 10^3$	869.88 (20)	870.38 (29)
$\delta_J \times 10^3$	2.41187 (170)	2.42028 (374)
$\Phi_{KJ} \times 10^6$	381.0 (33)	426.9 (102)
$\Phi_{JK} \times 10^6$	−48.14 (81)	−61.19 (308)
$\Phi_J \times 10^9$	−84.9 (36)	
$\phi_K \times 10^3$	1.084 (16)	0.824 (59)
$\phi_{JK} \times 10^6$	−33.51 (43)	−29.96 (113)
$L_{KKJ} \times 10^9$	319.6 (225)	135.3 (207)
$L_{JK} \times 10^9$	−148.4 (43)	−92.9 (69)
$L_{JJK} \times 10^9$	−1.43 (31)	−5.94 (72)
$l_{JK} \times 10^9$	−1.575 (153)	
$P_{KKJ} \times 10^9$	−1.179 123)	
$P_{KJ} \times 10^{12}$	426.3 (271)	
$P_{JK} \times 10^{12}$	−49.50 (227)	

[a] Watson's A-reduction was used in the representation I^r. Numbers in parentheses are 1σ uncertainties in units of the least significant figures.
[b] Refs. [8, 9]

a good quantum number coverage (several transition frequencies for each spectroscopic parameter with a sufficiently representative range of J and K_a quantum numbers) and a Hamiltonian that converges sufficiently fast. A predicted transition frequency is deemed to be reasonable in this context if the measured line is found within three to five times the predicted uncertainties. The SiC_2 molecule is comparatively floppy. Moreover, the laboratory data set for the main isotopolog of SiC_2 is rather sparse and extends to 370 GHz. Nevertheless, the highest frequency transition in Ref. [36], which report a preliminary analysis of HIFI data, is $30_{0,30} - 29_{0,29}$ at 636346 MHz, and it shows among those lines the largest deviation from the predictions based on Ref. [17] with almost 10 MHz. However, this deviation corresponds to only 5.5 times the predicted uncertainty. Moreover, the frequency from the final analysis has been corrected to a slightly lower frequency, in better agreement with the initial predictions.

Larger deviations from the predictions were observed around 1 THz, but these had to be expected since the predicted transition frequencies have uncertainties of several tens to almost 100 MHz. In fact, predictions from Refs. [17, 36] are quite reasonable for the most part even if the deviations are large enough to be easily recognizable in the astronomical spectra.

Fits employing Watson's A-reduction of the rotational Hamiltonian reproduce the experimental transition frequencies with fewer parameters than those using the S-reduction and should thus be preferred as long as the energy ordering is correct up to sufficiently high quantum numbers. It may be interesting to compare the quality of the predictions of the transitions detected with HIFI from either laboratory fit from Refs. [17] or in Table 1. Predictions based on S-reduction parameters [17] are quite good for transitions having higher val-

ues of K_a (6 − 14), but deteriorate for lower K_a values. In contrast, predictions based on A-reduction parameters (Table 1 under heading "Lab. data only") are quite good for low-K_a transition, but deteriorate for higher K_a values, which is closer to common expectations. Both fits as well as both predictions, as well as additional fits are available in the archive section of the CDMS[7]. Overall, however, the quality of the predictions is quite similar and do not provide a reasoning which reduction should be preferred. A very recent laboratory study of $^{29}SiC_2$ and $^{30}SiC_2$ [11] also obtained fits of similar quality for the A- and the S-reduction, but only if one more parameter was used in the S-reduction and preferred thus the A-reduction.

The SiC_2 spectroscopic parameters in Table 1 from laboratory data only and from all data agree quite well as far as they have been determined, in particular for the lower order parameters, rotational and quartic distortion constants. The higher order parameters show larger deviations, possibly reflecting the floppy nature of the molecule. However, the deviations are in all instances, at most, barely significant, meaning larger than three times the initial uncertainties.

The measured transition frequencies have been reproduced well with parameter sets of conventional Watson-type Hamiltonians. The molecule is rather floppy already in its ground vibrational state such that a fairly large number of parameters were used. Additionally, the magnitudes of the parameters decrease slowly such that the contributions of the higher order parameters are fairly large at energy levels having high values of J or K_a. Extrapolations to slightly higher quantum numbers may be reasonable, but should be viewed with caution.

The dedicated internal rotation Hamiltonian [15] did not achieve a considerably more compact representation of the measured transition frequencies known at that time. Without any available predictions for transition frequencies or rotational energies it seems questionable if that model is more appropriate than a conventional Watson-type Hamiltonian, even more so as the predicted barrier to linearity was rather far from values from ab initio calculations [7] or from the SRB extrapolation from highly vibrationally excited levels [16]. Moreover, one may question if an internal rotation model is appropriate at all. On the other hand, the semirigid bender approach [16] may be a viable alternative, but only if it will achieve reproduction of the measured transition frequencies to within estimated uncertainties with a parameter set that is not much larger than those used previously.

Additional laboratory data for the main isotopolog of SiC_2 will be of great use in particular if these connect levels with $K_a \geq 2$ via transitions with $\Delta K_a \geq 2$. But even Q-branch transitions with $\Delta K_a = 0$ may be very useful as they sample higher J levels at comparatively low frequencies. Such higher excited transitions may well be observable with existing interferometric facilities such as PdBI, ATCA, or SMA, and even more so with upcoming instruments such as ALMA, NOEMA, or possibly EVLA.

5. Conclusions

Astronomical observations with *Herschel* have been used to improve spectroscopic parameters of SiC_2 in its ground vibrational state greatly. The transition frequencies obtained from laboratory data as well as from astronomical observations have been reproduced to within the estimated uncertainties employing a conventional Watson-type Hamiltonian. These data should be useful to test alternative models to describe the rotational or even rovibrational energy levels of this floppy molecule. Predictions of the rotational spectrum as well as line, parameter and other auxiliary files, both from present fits as well as previous ones, will be available in the CDMS [26, 27].

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Appendix A. Supplementary Material

Supplementary data associated with this article can be found, in the online version, at doi: 10.1016/j.jms.2011.11.006.

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