ABSTRACT

Many sulfur-bearing species have been detected in different astronomical environments and have allowed us to derive important information about the chemical and physical composition of interstellar regions. In particular, these species have also been shown to trace and probe hot-core environment time evolution. Among the most prominent sulfur-bearing molecules is SO, the sulfur monoxide radical, one of the more ubiquitous and abundant, which is also observed in its isotopic substituted species such as $^{34}\text{SO}$ and $^{18}\text{O}$. Due to the importance of this simple diatomic system, and in order to face the challenge of modern radioastronomical facilities, an extension to the THz range of the rare isotopologues of sulfur monoxide has been performed. High-resolution rotational molecular spectroscopy has been employed to extend the available data set of four isotopic species, SO, $^{34}\text{SO}$, $^{33}\text{SO}$, and $^{18}\text{O}$, up to the 1.5 THz region. The frequency coverage and spectral resolution of our measurements allowed a better constraint of the molecular constants of the four species considered, specifically focusing on the two oxygen-substituted isotopologues. Our measurements were also employed in an isotopically invariant fit including all of the available pure rotational and ro-vibrational transitions for all of the SO isotopologues, thus enabling accurate predictions of the rotational transitions at higher frequencies. We also provide comparisons with recent works performed on the same system, demonstrating the quality of our experiment and the improvement of the data sets for all of the species considered. Transition frequencies for this system can now be used with confidence by the astronomical community well into the THz spectral region.

Key words: ISM: molecules – line: identification – methods: data analysis – molecular data

1. INTRODUCTION

Molecules with sulfur account for about 10% of the species identified in interstellar gas and circumstellar envelopes. Of these species, sulfur monoxide (SO) is the most prominent. Since its first detection by Gottlieb & Ball (1973) toward Orion A, many astronomical studies have been dedicated to this molecule, including studies on gas kinematics (Plambeck et al. 1982), molecular abundances (Blake et al. 1987), and spatial distribution (Sutton et al. 1995). Sulfur-bearing species are considered good probes of hot-core time evolution because they are highly sensitive to the physical and chemical variations of these regions (Hatchell et al. 1998; Viti et al. 2001). Thus, they can be used as tools for investigating the chemistry and physical properties of complex star-forming regions located in dense molecular clouds. On the other hand, it is known that some molecules (SiO, H$_2$CS, SO, and SO$_2$) show increased abundances in regions affected by shocks (Bachiller 1996) as a result of the action of outflows on the surrounding gas. Studying the molecular lines from shocked areas provides valuable information about the chemical processes and physical conditions of the shocked components.

Recently, Esplugues et al. (2013) dedicated an entire study to the sulfur oxide species in Orion KL, detecting 68 lines of SO, $^{34}\text{SO}$, $^{33}\text{SO}$, and $^{18}\text{O}$ and providing upper limits for the abundances of rarer isotopologues, such as S$^{17}$O, $^{36}\text{SO}$, and $^{34}\text{S}^{18}\text{O}$. Using the IRAM-30 m antenna and analyzing SO non-LTE excitation, they found that most of the SO emission arises from the high velocity plateau (column density $N = (5 \pm 1) \times 10^{16} \text{cm}^{-2}$) and the hot core. These results confirm that SO (and SO$_2$) is a good tracer of not only shock-affected areas, but also hot dense gas. The analysis of the abundance ratios of the SO isotopologues compared to that of SO$_2$ for the different components of the observed region has shown that the latter is five times more abundant than SO in the high velocity plateau and the hot core. Esplugues et al. (2013) clearly demonstrated the importance of isotopic analysis in the interstellar medium for deriving information concerning both the abundances of optically thick parent species and the evolution of the isotopic ratio in different astronomical environments.

More recently, Martin-Drumel et al. (2015, hereafter MD) published a new extensive laboratory spectroscopic characterization of sulfur monoxide isotopologues. In their work, the authors provided new high-frequency measurements of the main isotopic species and its sulfur isotopic substitutes ($^{34}\text{SO}$ and $^{33}\text{SO}$) using continuous-wave terahertz photomixing based on a frequency comb, with a frequency accuracy ranging from 10 to 800 kHz. Furthermore, the authors combined their measurements with all available pure rotational and ro-vibrational transitions of different SO isotopologues in an isotopically invariant fit.

In this work, we report an extension of the available data set to the THz range for sulfur monoxide and the minor isotopologues $^{34}\text{SO}$ (4.2%), S$^{18}$O (0.2%), and S$^{17}$O (0.04%) through laboratory absorption spectroscopy in order to improve the available spectroscopic parameters and determine the centrifugal-distortion terms. Our determination of the latter is also supported by high-level quantum-chemical calculations. Finally, we supply a detailed comparison with previous available spectroscopic data in the discussion section, together with the results from an isotopic invariant fit involving all of the available rotational and ro-vibrational frequencies for all SO isotopologues.
and the electronic spin momentum 

Due to the modulation and detection scheme employed, the instrumental line shape is approximately the second derivative of a Lorentzian. No averaging time was required for obtaining a good signal-to-noise ratio.

2. EXPERIMENT

All the measurements were carried out using a frequency-modulated, computer-controlled spectrometer (65 GHz–1.6 THz; Cazzoli & Puzzarini 2006, 2013; Puzzarini et al. 2012); the range considered was 200 GHz–1.5 THz. Frequency multipliers driven by Gunn diode oscillators, phase-locked to a rubidium frequency standard, have been employed as the millimeter and sub-millimeter-wave sources. Frequency modulation was obtained by sine-wave modulating the 72 MHz local oscillator of the synchronization loop at 16.66 kHz with the modulation depth varying from 400 kHz to 2.4 MHz according to the transition frequency under consideration. Liquid-He-cooled InSb and Schottky diode detectors were used and their output processed by means of a lock-in amplifier tuned to twice the modulation frequency (i.e., second harmonic detection was performed). Previous, unrelated experiments performed in the cell with sulfur-bearing chemicals allowed us to obtain very good signals of sulfur monoxide using the flow of \( \sim 30 \) mTorr of \( \text{O}_2 \) and a DC discharge of 12 mA at room temperature. The measurements of the \( ^{34}\text{S} \) isotopic species were carried out in natural abundance (4.22%), while an isotopically enriched oxygen sample, a mixture of 10% \( ^{17}\text{O}_2 \) and 90% \( ^{18}\text{O}_2 \), was employed for the experiment of the two oxygen minor isotopologues. A few-Gauss magnetic field, parallel to the radiation source, was used to disentangle the free-radical signal from those of the closed-shell species whose transitions contaminated the spectral window. Subtraction of the on-field spectrum from the off-field spectrum allowed for a perfect zeroing of the effect of the undesired non-magnetic species (see Figure 1).

3. COMPUTATIONS

As mentioned in the Introduction, to guide the analysis and experimental determination of the sextic centrifugal-distortion constant, we performed quantum-chemical calculations at the coupled-cluster singles and doubles (CCSD) approach augmented by a perturbative treatment of triple excitations (CCSD(T); Raghavachari et al. 1989) using the cc-pCVQZ basis set (Dunning 1989; Woon & Dunning 1995; Peterson & Dunning 2002). All electrons were included in the correlation treatment.

For each isotopic species considered (SO, \( ^{34}\text{SO} \), \( ^{17}\text{O}, \text{S}^{19}\text{O} \)), the harmonic force field was obtained using analytic second derivatives (Gauss & Stanton 1997), whereas the cubic force field was determined in a normal-coordinate representation via numerical differentiation of the harmonic force constants (Schneider & Thiel 1989; Stanton et al. 1998). The quartic and sextic centrifugal-distortion constants were then determined by means of the vibrational perturbation theory (Mills 1972; Puzzarini et al. 2012).

All of the computations were performed with the CFour program package (2012).

4. ANALYSIS

The total angular momentum \( J \) for a diatomic molecule in the \( ^3\Sigma \) state is given by the coupling between the molecular angular momentum \( N \) and the electronic spin momentum \( S \). The effective Hamiltonian operator may be expressed as the sum of three terms:

\[
H = H_{\text{rot}} + H_{S-N} + H_{S-S}
\]

where

\[
H_{\text{rot}} = N^2 (B - D N^2 + HN^4)
\]

is the rotational Hamiltonian. For each \( N \) value (\( N \) being the associated quantum number to the angular momentum operator), there are three different energy levels corresponding to the three possible space orientations of the \( S \) vector (\( S = 0, \pm 1 \)).

\[
H_{S-N} = N \cdot S (\gamma_B + \gamma_D N^2)
\]

and

\[
H_{S-S} = \frac{2}{3} (\lambda_B + \lambda_D N^2) (3S^2 - S^2)
\]

are Hamiltonians describing the electron spin-rotation and spin–spin interactions, respectively. \( B, \gamma_B, \) and \( \lambda_B \) are the rotational, the electron spin-rotation, and the spin–spin interaction constants, and \( D, H, \gamma_D, \) and \( \lambda_D \) represent their centrifugal-distortion correction. The derived parameters of the Hamiltonian for each isotopic species are summarized in Tables 1–2.

The effective Hamiltonian of the \( ^{17}\text{O} \) species also includes nuclear hyperfine interactions with the overall rotation due to the \( ^{17}\text{O} \) nuclear spin (\( I = 5/2 \)).

\[
H_{\text{hfs}} = b_f I \cdot S + c \left( I \cdot S_z - \frac{1}{3} I \cdot S \right) + eQq \left( \frac{3I^2 - I^2}{4I(2I-1)} \right) + C_I I \cdot N,
\]

where \( b_f \) and \( c \) are the isotropic (Fermi contact interaction) and anisotropic parts of the electron spin-nuclear spin coupling, \( eQq \) is the nuclear quadrupole coupling constant, and \( C_I \) is the nuclear spin-rotation interaction constant.

Sulfur monoxide has been the subject of several laboratory studies. The Cologne Database for Molecular Spectroscopy (Müller et al. 2005) has been used as a review of previous works and to obtain a starting data set to flag transitions to re-measure with higher accuracy or to derive higher frequency predictions. The first spectroscopic study of the fundamental isotopic species dates back to the late 70s (Clark & De
Lucia 1976), followed over the years by many other works, including some THz measurements (Cazzoli et al. 1994). Also, for $^{34}$SO, previous laboratory data cover quite a large range of the millimeter/sub-millimeter wave spectrum, with some measurements taken at 1.05 THz by Klaus et al. (1996), allowing for a total of 42 rotational transition of the $X^{3}Σ^{−}$ electronic ground state to be cataloged. Somewhat more critical were in the past years measurements of the minor oxygen isotopic substituted species, such as $^{34}$S$^{18}$O and $^{34}$S$^{17}$O. Both species have been the subject of the same work studying the $^{34}$S species, but while for the former the measurements were carried out up to the THz region (1.03 THz), the rarer $^{17}$O species has been studied up to 620 GHz. In all the cases mentioned above, the accuracy of the measurements spans from 50 kHz in the lower frequency range up to 100 kHz in the THz region, values which our measurements can easily improve.

As briefly mentioned in our Introduction, during the conclusion of the present study, a new spectroscopic analysis of the SO isotopologue system was published (Martin-Drumel et al. 2015). The focus of this work is the extension of the absorption spectrum of SO, $^{34}$SO, and $^{33}$SO to 2.5 THz, allowing a global isotopically invariant to be performed.

In the present work, for the main isotopic species, 2 rotational transitions in the 340 GHz region have been remeasured and 10 new transitions have been detected in the 1.07–1.41 THz frequency range. The regions 200–500 GHz and 1.10–1.50 THz have been studied to detect 23 and 24 rotational transitions of the $^{34}$SO and $^{33}$SO isotopic species, respectively. Finally, the rarest isotopologue $^{31}$S$^{17}$O has been observed through 15 rotational transitions in the 1.10–1.50 THz region. The accuracy of our measurements is 20–30 kHz in the millimeter-/submillimeter-wave range and 50 kHz in the THz region. The measured frequencies will be made available to the spectroscopic community through the CDMS online catalog.

### Table 1

Spectroscopic Constants$^a$ of SO and $^{34}$SO (in MHz)

|        | SO | $^{34}$SO |
|--------|----|----------|
| $B$    | 21523.55568(26) | 21102.73094(43) |
| $10^3D$ | 33.91431(60) | 32.59862(90) |
| $10^3H$ | $−7.73(37)$ | $−7.22(49)$ |
| $\gamma_B$ | 158254.3860(80) | 158249.715(12) |
| $\lambda_D$ | 0.30662(12) | 0.30030(38) |
| $10^3\lambda_H$ | ... | ... |
| $\gamma_D$ | $−168.3045(22)$ | −164.9863(33) |
| $10^3\gamma_D$ | $−0.5239(46)$ | $−0.5181(61)$ |
| $\sigma^2$ | 0.62 | 0.86 |

Notes.

$^a$ Uncertainties (1σ) are in units of the last significant digit.

$^b$ Martin-Drumel et al. (2015).

### Table 2

Spectroscopic Constants$^a$ of Sulfur Monoxide Oxygen Minor Isotopologues (in MHz)

|        | $^{31}$S$^{18}$O | $^{31}$S$^{17}$O |
|--------|-----------------|-----------------|
| $B$    | 19929.27860(42) | 20677.80826(76) |
| $10^3D$ | 29.06925(96) | 31.29739(82) |
| $10^3H$ | $−5.10(60)$ | $−6.31(28)$ |
| $\gamma_B$ | 158236.114(40) | 158244.8126(26) |
| $\lambda_D$ | 0.283118(39) | 0.25955(26) |
| $\gamma_D$ | $−155.8017(61)$ | $−161.660(24)$ |
| $10^3\gamma_D$ | $−0.4366(78)$ | $−0.4889(83)$ |
| $b_E$ | ... | ... |
| $c$ | ... | ... |
| $\epsilon_Q$ | ... | ... |
| $10^3C_I$ | ... | ... |
| $\sigma^2$ | 0.74 | 0.54 |

Notes.

$^a$ Uncertainties (1σ) are in units of the last significant digit.

$^b$ Martin-Drumel et al. (2015).

$^c$ Klaus et al. (1996).

$^d$ Kept fixed at the computed value. See the text.

$^e$ Spectroscopic parameters are computed values derived from the isotopically invariant fit.
5. DISCUSSION

The results of these new measurements are summarized in Tables 1 and 2 for SO and $^{34}$SO (rms = 0.62 and 0.86), and $^{31}$O and $^{18}$O (rms = 0.74 and 0.54), respectively, and are compared with the data obtained by MD. From this comparison, we observe that our laboratory data for SO and $^{34}$SO are in very good agreement with the corresponding constants derived from an effective-fit for the same species (see Table 2 of MD). The higher frequency measurements performed in the previous work for the main species allowed the authors to constrain the second-order centrifugal-distortion correction of the spin–spin interaction constant, $\lambda_2$, which remains undetermined in our analysis. All of the other terms show an agreement of better than 1%, except for the sextic centrifugal-distortion parameter, $H_i$; in this case, our parameters are larger than those derived previously by 11 and 19%, respectively, for SO and $^{34}$SO. To inspect this large deviation, we make use of our computed values and of an empirical, well-tested scaling procedure:

$$H_{\text{scal}} = H_{\text{calc}} \times \left( \frac{H_{\text{exp}}}{H_{\text{main}}^{\text{MD}}} \right),$$

where the superscripts iso and main refer to a specific isotopic species and the main isotopologue, respectively; scal, exp, and calc denote the scaled, experimental, and quantum-chemically calculated values for $H$, respectively. Using the value of $-6.974(22) \times 10^{-9}$ MHz for SO, we obtain a scaled value of $-6.56 \times 10^{-9}$ MHz for $^{34}$SO, which is roughly in between our and MD values and well within the confidence range of our data. This outcome suggests that the fit of MD might benefit from the inclusion of the present measurements. In Table 2, the results for the two oxygen-substituted species are collected. Here, the literature values reported for the comparison are those predicted from the isotopically invariant fit available in MD. As for the previous table, the agreement for all of the parameters is better than a few percent. The only relevant deviation is noted for the $H$ constant of the $^{31}$O species: $-6.31(28) \times 10^{-9}$ MHz versus $-5.74 \times 10^{-9}$ MHz. Once again, we resort to the scaled computed value ($-6.18 \times 10^{-9}$ MHz) to a deeper understanding of such a discrepancy. The latter value agrees well with our data, within the given uncertainty, but it suggests that the $H$ constant from the isotopically invariant fit is underestimated. Therefore, this fit would largely benefit from the inclusion of our recorded frequencies. Since the Dunham expansion model MD used to determine the predicted parameter does not include hyperfine interactions, in Table 2 the corresponding parameters are compared with the results from Klaus et al. (1996). Very good agreement is observed. The only comment concerns the $^{17}$O spin-rotation constant, which is badly determined by the fit: we decided to keep it fixed at the quantum-chemical value, computed at a level of theory known to provide quantitative agreement with experiment (Puzzarini et al. 2010). For $^{34}$SO, we note that in comparison with the scaled value of $H (-5.53 \times 10^{-8}$ MHz) both our and MD parameters seem to be underestimated. On the other hand, our data are affected by a large uncertainty and the scaled value is within the upper limit.

It is also worth comparing, for the oxygen isotopologues of sulfur monoxide, all three available data sets, specifically ours, that of MD, and the catalog on the CDMS website (www.cdms.de). In Figure 2, this comparison is made for the predicted transitions in the frequency range 60–2000 GHz; in particular, it illustrates the difference of the strongest set of transitions ($\Delta N, \Delta J = +1$ with $J = N, N \pm 1$), the more relevant for the astrochemistry community, among our data set and the two previous ones. The need for new measurements is particularly evident when comparing our new predictions with those available on the CDMS catalog, which, in the high-frequency range ($\geq 1$ THz), differ by more than 1 MHz from ours for the $^{17}$O isotopic substituted species. Less significant but still sizeable is the comparison with the Dunham isotopically invariant results. First, it is important to point out the overall quality of these predictions, which make use of a very large data set of measurements of different isotopic species and several vibrational excited states. Second, it must be noted that, also in this case, although less prominent than in the previous one, the deviation at high-frequency might be worth considering and very likely is related to the discrepancy observed for the sextic centrifugal-distortion term. The two data sets show considerably better agreement for the other oxygen species, while a larger difference can be noted by comparing our predictions with the older data.

To conduct a more exhaustive comparison with the previous data and to inspect the impact of our new measurements, a multi-isotopologue Dunham analysis of the full data set has
been performed, using the known reduced mass dependences given by

\[ Y_{1,m} = U_{1,m} \left( 1 + \frac{\Delta_{V,m}^U}{M_S} + \frac{\Delta_{V,m}^X}{M_S} \right) \left( \frac{1}{\mu} \right)^{1+m} \]

for the rotational and vibrational parameters;

\[ X_{1,m} = U_{1,m}^X \left( 1 + \frac{\Delta_{V,m}^U}{M_S} + \frac{\Delta_{V,m}^X}{M_S} \right) \left( \frac{1}{\mu} \right)^{1+m} \]

with \( X = \lambda, b, c, eQq \); and

\[ X_{1,m} = U_{1,m}^X \left( 1 + \frac{\Delta_{V,m}^U}{M_S} + \frac{\Delta_{V,m}^X}{M_S} \right) \left( \frac{1}{\mu} \right)^{1+m} \]

with \( X = \gamma, \Gamma, \Delta_{i,m}^i \) and \( \Delta_{i,m}^X \) are unitless coefficients that account for the effect of Born–Oppenheimer breakdown. For a clearer relation of Dunham’s coefficients to the molecular energy levels and the rotational-vibrational parameters, see Townes & Schawlow (1975) Equations (1–35) and (1–36). The SPFIT/SPCAT software (Pickett 1991) has been used for this analysis and the corresponding parameters are shown in Table 3. The SPFIT parameters have been converted to the isotopically invariant terms \( U_{1,m} \) through the previously mentioned \( Y_{1,m} \) and \( X_{1,m} \) relations for a better comparison with the previous published data; more specifically, the parameters derived from the present work are set side by side with the ro-vibrational isotopic constants of MD, along with the relative reduced rms errors. Some high-order parameters derived in MD have been left out of our analysis because their inclusion in the global analysis did not contribute to the quality of the fit. This comparison shows a generally very good agreement for all of the parameters analyzed. Nevertheless, there are some discrepancies that required deeper investigation. The vibrational corrections to the rotational constants, \( U_{3,1}, U_{4,1} \), and \( U_{5,1} \), show a difference from a factor of a few to more than 10. Surprisingly, both of the former two parameters are in very good agreement (in 1σ deviation) with the isotopically invariant analysis performed by Klaus et al. (1996) to which MD compared their work (see Table 4 of MD). Unfortunately, this comparison cannot be addressed for the third parameter \( U_{5,1} \), which was first determined by MD. A similar situation can be seen for the higher-order vibrational corrections to the \( \lambda \) constant, namely, the \( U_{4,0}^{\lambda}, U_{5,0}^{\lambda}, \) and \( U_{6,0}^{\lambda} \) parameters. The former constant is the one showing the largest deviation, including a change in sign from \(-0.1057 \) to \(0.6547\) MHz amu\(^{-2}\). Again, as for the previous cases, a more accurate analysis reveals a good agreement (in 1σ deviation) with the value derived by Klaus et al. (1996). Similarly, the other two parameters, \( U_{4,0}^{\lambda} \) and \( U_{5,0}^{\lambda} \), were first determined by MD and cannot be compared to a third analysis; here, the difference is less critical among the two studies but is still a factor of \(\sim 4\) and \(\sim 10\), respectively.

Crucial parameters of an isotopically invariant analysis are the Born–Oppenheimer Breakdown (BOB) constants. In Table 4, the BOB constants derived from our work are compared with those from MD. The parameters for the correction to the rotational constants, \( \Delta_{i,1}^U \) and \( \Delta_{i,0}^U \), show very good agreement, with the latter slightly \(\sim 2\) improved with our global analysis. Similarly good agreement is found for the sulfur correction to the vibrational frequency, \( \Delta_{i,0}^\nu \), while a large discrepancy, including a change in sign, is shown for the oxygen correction, \( \Delta_{i,0}^\chi \). A future study including more ro-vibrational and vibrational transitions of oxygen-substituted species (currently there is only the first excited vibrational band of \(^{13}\)O\(_2\) in the analysis) might help to clarify this discrepancy and further constrain this important parameter. To compare the BOB coefficients of the fundamental \( \lambda \) constants, \( \Delta_{i,1}^{\lambda} \) and \( \Delta_{i,0}^{\lambda} \), the equation

\[ \Delta_{i,0}^{\lambda} = -\frac{M_0^\lambda}{m_e} \left( U_{0,0} + X_{0,0}^\lambda + X_{0,0}^\mu \right) X_{i,0}^{\lambda} \]

has been used. Here, \( A \) is the atom considered, \( M_0^\lambda \) is the atomic mass of the main isotopic species of the \( A \) atom, \( m_e \) is

| Parameter | This Work | MD* |
|-----------|-----------|-----|
| \( U_{1,0} \) | 3757.50375(287) | 3757.49542(195) |
| \( U_{2,0} \) | -68.3228(628) | -68.32167(622) |
| \( U_{3,0} \) | 0.47701(898) | 0.47558(818) |
| \( U_{4,0} \) | -0.04119(509) | -0.04041(463) |
| \( U_{5,0} \) | 0.00519(104) | 0.0050319(934) |
| \( U_{6,0} \) | 230416.7278(172) | 230387.59070(231) |
| \( U_{7,0} \) | -6001.5217(148) | -6001.6578(164) |
| \( U_{8,0} \) | 25.4579(211) | 25.7585(267) |
| \( U_{9,0} \) | -0.5585(120) | -0.8254(165) |
| \( U_{10,0} \) | -0.12215(270) | -0.1197(508) |
| \( U_{11,0} \) | -0.001253(218) | -0.2207(533) |
| \( U_{12,0} \) | -3.854293(244) | -3.854309(229) |
| \( U_{13,0} \) | -0.004668(126) | -0.004547(114) |
| \( U_{14,0} \) | -0.001072(628) | -0.001163(677) |
| \( U_{15,0} \) | -7.8512835(8E-06) | -7.8489791E-06 |
| \( U_{16,0} \) | -1.023(156)E-09 | -1.040(146)E-09 |
| \( U_{17,0} \) | -15775.875(303) | 157795.4203(201) |
| \( U_{18,0} \) | 2978.880(153) | 2979.597(136) |
| \( U_{19,0} \) | 114.524(188) | 112.732(159) |
| \( U_{20,0} \) | 11.905(107) | 13.6225(953) |
| \( U_{21,0} \) | 6.6537(290) | -0.10573(327) |
| \( U_{22,0} \) | 0.05997(282) | 0.22948(606) |
| \( U_{23,0} \) | -0.001964(177) | -0.018122(580) |
| \( U_{24,0} \) | 3.24178(138) | 3.24222(125) |
| \( U_{25,0} \) | 0.14168(874) | 0.14226(791) |
| \( U_{26,0} \) | 0.03660(511) | 0.03545(466) |
| \( U_{27,0} \) | 5.626(387)E-05 | 5.374(357)E-05 |
| \( U_{28,0} \) | -39.7904(214) | -39.7830(110) |
| \( U_{29,0} \) | 95.3590(315) | 95.3400(480) |
| \( 1.5 \times U_{e0}^q \) | -3.5687(859) | -3.6140(600) |
| \( U_{29,0}^q \times \mu^{1/2} \) | -0.00757 | -0.00440(150) |

Notes:
- * Uncertainties (1σ) are in units of the last significant digit.
- † The units for these constants have been corrected; in MD, these parameters were missing the amu dependencies.
- ‡ Martin-Drumel et al. (2015).
the electron mass, $U$ is the Dunham constant to which the BOB coefficient is related, and the $X$s are the parameters provided from the MDanalysis. The oxygen BOB coefficient is in very good agreement with that derived in the previous work, and is slightly improved ($\sim 2$); the sulfur one, $\Delta_{0,0}^{5}$, is dissimilar and, once again, opposite in sign. As seen previously for the discussion of $U$s, a comparison of our analysis with that of Klaus et al. (1996) reveals a better agreement for this parameter, with respect to its sign (now both positive) and its absolute values, although different to a few $\sigma$ deviation (0.886 and 0.221, our and Klaus et al. 1996, respectively).

The present laboratory work extends the spectroscopic study of a very simple and important diatomic radical well into the THz region, including some minor isotopic species. For such an important molecular system, widely distributed and very abundant in many different interstellar regions, the accuracy of the data set for less abundant isotopologues is also crucial. This is particularly true in an era in which high-sensitivity, high-spectral and spatial resolution radioastronomical facilities are becoming available to the scientific community. The ALMA interferometer has become the reference and most relevant observatory for the millimeter- and sub-millimeter-wave regions; its unprecedented properties will allow us to observe SO and its isotopologues in regions previously undetected. Above the THz threshold, the instruments of the airborne observatory SOFIA may also be able, in the near future, to extend the identification of this molecular system to interstellar environments at higher frequency.

This work has been supported in Bologna by “PRIN 2012” funds (project “STAR: Spectroscopic and computational Techniques for Astrophysical and atmospheric Research”) and by the University of Bologna (RFO funds). The authors would like to thank Marie Aline Martin-Drumel for providing the manuscript before its publication.

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Table 4

| Parameter | This work | MD\(^{b}\) | Klaus et al.\(^{c}\) |
|-----------|-----------|-----------|-----------------|
| $\Delta_{0,1}^{5}$ | -1.9737(16) | -1.9725(14) | -1.9772(58) |
| $\Delta_{0,0}^{5}$ | -2.7015(20) | -2.7175(57) | -2.7247(34) |
| $\Delta_{1,0}^{5}$ | 0.4093(35) | 0.3953(32) | ... |
| $\Delta_{0,0}^{1}$ | -0.2664(89) | 0.1338(40) | ... |
| $\Delta_{1,0}^{5}$ | 0.8686(55) | -0.1108(5) | 0.2118(89) |
| $\Delta_{0,0}^{7}$ | 1.4944(46) | 1.4278(7) | 1.3304(48) |

Notes.

\(^{a}\) Uncertainties ($1\sigma$) are in units of the last significant digit.

\(^{b}\) Martin-Drumel et al. (2015).

\(^{c}\) Klaus et al. (1996).