Vibrational–rotational spectra of ^{13}CS and global multi-isotopologue analysis

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Abstract

In total, 626 vibrational–rotational spectral lines of the Δv=1 transitions of $^{13}C^{32}S$ up to band v=5–4 have been measured with a Fourier-transform spectrometer at resolution 0.010 cm^{-1}. To calibrate accurately the spectral lines, a separate observation of the vibrational-rotational bands of $^{12}C^{32}S$ was made with simultaneous recording of the N_2O spectrum in absorption, to serve as wavenumber standards, with dual sample cells at resolution 0.008 cm^{-1}. The spectral wavenumbers of $^{12}C^{32}S$ in turn become calibration standards. All present vibrational–rotational spectra of $^{13}C^{32}S$ and $^{12}C^{32}S$, the reported vibrational–rotational spectra of $^{12}C^{32}S$, $^{12}C^{33}S$, $^{12}C^{34}S$, and $^{13}C^{32}S$, and the reported rotational spectra of $^{12}C^{32}S$, $^{12}C^{33}S$, $^{12}C^{34}S$, $^{12}C^{36}S$, $^{13}C^{32}S$, $^{13}C^{33}S$ and $^{13}C^{34}S$ were subjected to a global multi-isotopologue analysis, which reduced them to molecular parameters in a single set. The wavenumbers of 3974 spectral lines, in total, comprising data of seven isotopologues were fitted with 22 isotopically invariant, traditional molecular parameters in a single set. As the normalized standard deviation is 1.38, the obtained fit is satisfactory. To facilitate the calculation of spectral wavenumbers, the values of the Dunham coefficients of 42 Y_{ij} for each of $^{12}C^{32}S$, $^{12}C^{33}S$, $^{12}C^{34}S$, $^{12}C^{36}S$, $^{13}C^{32}S$, $^{13}C^{33}S$, $^{13}C^{34}S$, $^{13}C^{36}S$, $^{14}C^{32}S$, $^{14}C^{33}S$, $^{14}C^{34}S$ and $^{14}C^{36}S$, of which the spectra of the latter five isotopologues are not yet reported, were back-calculated with uncertainties using the evaluated 22 molecular parameters. The physical significance of the conventional treatments of the adiabatic and nonadiabatic corrections for $\mathit{\Delta}_{01}{}^{C}$ and $\mathit{\Delta}_{01}{}^{S}$ is discussed.

Keywords: CS; vibrational–rotational; high-resolution; breakdown; Born–Oppenheimer approximation.

1. Introduction

The dissociation of carbon disulfide to form CS was one of the earliest reactions to be reported in an electric discharge [1, 2]. After condensation in a trap cooled with liquid nitrogen, CS polymerizes readily on warming to $(CS)_n$ with the evolution of considerable heat, which might cause an explosion [3]. Because CS has a lifetime of order 1 s in the gaseous phase, its rotational and vibrational–rotational spectra have been extensively studied.

The first microwave measurements of the *J*=1–0 transitions of $^{12}C^{32}S$ (*v*=0, 1), $^{12}C^{33}S$ (*v*=0), $^{12}C^{34}S$ (*v*=0) and $^{13}C^{32}S$ (*v*=0) were reported by Mockler and Bird [4] following their brief report [5], which was an observation of rotational transitions *J*=1–0 of $^{12}C^{32}S$ and $^{12}C^{34}S$. Kewley *et al*. [6] subsequently observed millimeter-wave rotational transitions up to *J*=5–4 for $^{12}C^{32}S$ and *J*=3–2 for $^{12}C^{34}S$ using a free-space absorption cell. Bustreel *et al*. [7] observed the *J*=1–0 rotational transition in vibrationally excited states of $^{12}C^{32}S$ ($v \le 14$), $^{12}C^{34}S$ ($v \le 5$) and $^{13}C^{32}S$ ($v \le 3$). Bogey *et al*. [8] reported the millimeter-wave rotational spectra of rare isotopologues in the *v*=0 states of $^{12}C^{36}S$ ($J'' \le 4$), $^{13}C^{34}S$ ($J'' \le 3$), and $^{13}C^{33}S$ ($J'' \le 3$) as well as in the *v*=0 and 1 states of $^{12}C^{33}S$ ($J'' \le 4$). The measurements were extended by Bogey et al. [9] in the millimeter and submillimeter ranges to the vibrationally excited states of $^{12}C^{32}S$ ($v \le 20$), $^{12}C^{34}S$ ($v \le 7$) and $^{13}C^{32}S$ ($v \le 3$) for up to *J*=11–10 for $^{12}C^{32}S$ (*v*=0). Ahrens and Winnewisser [10] reported sub-millimeter-wave spectra of $^{12}C^{32}S$, $^{12}C^{33}S$, $^{12}C^{34}S$, $^{13}C^{32}S$, $^{13}C^{33}S$, $^{13}C^{34}S$ and $^{12}C^{36}S$. The rotational transitions up to *J*=23–22 included some of $^{12}C^{32}S$ ($v \le 16$), $^{12}C^{33}S$ ($v \le 2$), $^{12}C^{34}S$ ($v \le 8$), $^{12}C^{36}S$ ($v \le 1$), $^{13}C^{32}S$ ($v \le 5$), $^{13}C^{33}S$ (*v*=0) and $^{13}C^{34}S$ ($v \le 2$) in vibrationally excited states. Kim and Yamamoto [11] observed the *J*=1–0 transition in vibrational states up to *v*=39, 16, 7, and 9 for $^{12}C^{32}S$, $^{12}C^{34}S$, $^{12}C^{33}S$ and $^{13}C^{32}S$, respectively; the *J*=2–1 transition was observed for $^{12}C^{32}S$ in vibrational states from 18 to 20.

In 1977, Todd [12] reported vibrational–rotational bands *v*=2–0 of $^{12}C^{32}S$ and $^{12}C^{34}S$, recorded with a grating spectrometer with resolution 0.045 cm^{-1}; 70 spectral lines were reported for $^{12}C^{32}S$ and 31 for $^{12}C^{34}S$. Using a tunable diode-laser spectrometer, Todd and Olson [13] observed 115 vibrational–rotational transitions that were assigned to bands *v*=1–0, 2–1, 3–2 and 4–3 of $^{12}C^{32}S$, bands 1–0 and 2–1 of $^{12}C^{34}S$ and $^{13}C^{32}S$, and band 1–0 of $^{12}C^{33}S$. Yamada and Hirota [14] also reported 57 diode-laser spectral lines that were assigned to bands *v*=1–0 and 2–1 of $^{12}C^{32}S$ and 1–0 of $^{12}C^{34}S$, $^{12}C^{33}S$ and $^{13}C^{32}S$. Winkel *et al*. [15] observed the Δv=2 emission bands of $^{12}C^{32}S$ and $^{12}C^{34}S$ with *v*" up to 8 for $^{12}C^{32}S$. Using a Fourier-transform spectrometer at resolution 0.004 cm^{-1}, Burkholder *et al*. [16] measured bands v=1–0 of $^{12}C^{32}S$, $^{12}C^{33}S$, $^{12}C^{34}S$ and $^{13}C^{32}S$ and band 2–1 of $^{12}C^{32}S$. Ram *et al*. [17] measured the Δv=1 emission bands for $^{12}C^{32}S$ up to v=9–8 and J" up to 113 for band v=2–1; they observed the emission from samples at high temperatures with a Fourier-transform spectrometer at resolution 0.01 cm^{-1}.

To date, the vibrational–rotational spectra for transitions up to large v and J have been reported for only $^{12}C^{32}S$ and $^{12}C^{34}S$. Here we report the observation of the vibrational-rotational bands of $^{13}C^{32}S$ up to v=5–4 using a Fourier-transform spectrometer at resolution 0.010 cm^{-1}; we report also a separate observation of the vibrational-rotational bands of $^{12}C^{32}S$ up to v=7–6. The measurements were made on recording simultaneously the N_2O spectrum to provide wavenumber standards with dual sample cells at resolution 0.008 cm^{-1}; this resolution is slightly better than that (0.010 cm^{-1}) for the measurements of Ram *et al*. [17] As our measured vibrational–rotational wavenumbers for $^{12}C^{32}S$ are slightly more accurate than those of Ram *et al*. [17], both sets of values were included in the data set that was subjected to a global multi-isotopologue spectral analysis.

The global analysis employed here, which was comprehensively reviewed [18], is based on a non-Born–Oppenheimer effective Hamiltonian expressed with determinable molecular parameters in a set [19–21] as follows:

$$H = -B_e(1+\delta\Delta_B)\frac{d^2}{d\xi'^2} + \frac{B_e(1+\delta\Delta_B)}{(1+\xi')^2}\left(1+\sum_{i=1}\delta r_{iq}(\xi')^i\right)J(J+1)$$
$$+\frac{[\omega_e(1+\delta\Delta_\omega)]^2}{4B_e(1+\delta\Delta_B)}\xi'^2\left(1+\sum_{i=1}a_i(1+\delta\Delta_{aiq})(\xi')^i\right), \quad (1)$$

in which

$$\xi' = (1+\delta\Delta_B/2)\xi + \delta\Delta_B/2$$
$$= (1+\delta\Delta_B/2)\frac{r-r_e}{r_e} + \delta\Delta_B/2, \quad (2)$$

and $B_e=h/(8\pi^2 c\mu r_e^2)$ and $\omega_e=(1/2\pi c)(k/\mu)^{1/2}$, both in unit cm^{-1}. Quantity μ denotes the reduced mass of a molecule: $(1/\mu)=(1/M_a)+(1/M_b)$, in which M_a and M_b are masses of *atoms* A and B, respectively. All molecular parameters B_e, ω_e, a_1, … are those of the traditional concept in the Born–Oppenheimer scheme whereas the non-Born–Oppenheimer effects are all included in correction parameters; r_e is the equilibrium internuclear distance and k is the force coefficient at r_e of the Born–Oppenheimer potential. The notation $\delta x_i = (m_e/M_a)x_i^a + (m_e/M_b)x_i^b$ for the correction parameter is used throughout for the couple of arbitrary quantities x_i^a and x_i^b; m_e is the mass of the electron.

The Dunham-like treatment of the Schrödinger equation of the Hamiltonian (1) generates analytical expressions for the vibrational–rotational term values [19, 20, 22], which enable an analysis of a spectral data set of CS with a single set of Born–Oppenheimer fitting parameters, U_ω ($=\mu^{1/2}\omega_e$), U_B ($=\mu B_e$), a_i (i=1, 2, …), and isotopically invariant non-Born–Oppenheimer correction parameters $\Delta_\omega^{\mathrm{C,S}}$, $\Delta_B^{\mathrm{C,S}}$, $\Delta_{aiq}^{\mathrm{C,S}}$ (i=1, 2, …) and r_{iq}^{C} ($=r_{iq}^{\mathrm{S}}$) (i=1, 2, …) that are based on the traditional concept of the molecular parameters. Parameters a_i (i=1, 2, …) are those in the Dunham potential energy.

The definition and expressions with expansion coefficients $q_i^{a,b}$, $r_i^{a,b}$ and $s_i^{a,b}$ of the non-Born–Oppenheimer parameters are summarized in Tables 1 and 2 of Ref. [20], respectively.

2. Experiments

The ^{13}CS molecule was generated on passing a gaseous mixture of ^{13}C-enriched CS_2 (43 %, 1.8 hPa) and Ne (27-hPa) through a waveguide cavity (2450-MHz) for microwave discharge. As a cold trap made of Pyrex glass was broken frequently because of the unintended explosion of the deposited discharge product, a stainless-steel cold trap was used instead. At one end of the silica discharge tube was mounted a BaF_2 window to transmit the infrared radiation of CS from the discharged gas. The radiation was focused on the emission port of a Fourier-transform spectrometer (Bruker IFS-125HR). Using a KCl beam splitter and a HgCdTe detector (77 K), we detected the vibrational–rotational transitions for Δv=1 of $^{13}C^{32}S$ and $^{12}C^{32}S$ at unapodized resolution 0.010 cm^{-1} in the range 1090–1370 cm^{-1}. During integration for 135 min, 224 scans were accumulated; this spectrum is hereafter termed measurement 010. The $^{13}C^{32}S$ transitions were measured up to band v=5–4. Figure 1 shows a portion of this spectrum.

To calibrate the wavenumbers of the CS spectrum, we performed a separate experiment in which we recorded simultaneously the spectra of $^{12}C^{32}S$ and N_2O at unapodized resolution 0.008 cm^{-1} as a calibration standard. A sample of pure CS_2 with isotopes in natural abundance replaced the ^{13}C-enriched CS_2. A gas sample cell (length 15 cm) containing N_2O (33 Pa) was located in the sample compartment of the spectrometer to absorb the incident emitted radiation, generating the N_2O spectrum in the range 1240–1320 cm^{-1}. Figure 2 shows a portion of the simultaneous recording of the observed spectra of CS and N_2O. During integration for 132 min, 176 scans were added; we refer to this spectrum as measurement 008.

3. Spectral calibration

All spectral line centers were determined on fitting the measured line profiles to pseudo-Voigt functions with OPUS (Bruker software supplied with the spectrometer); a pseudo-Voigt function is a weighted sum of Gaussian and Lorentzian contributions. The spectral positions of bands v=1–0 and 2–1 of $^{12}C^{32}S$ in measurement 008 were calibrated with the simultaneously recorded N_2O spectrum for which the wavenumbers were adopted from the calibration tables provided by NIST [23].

Ram *et al*. [17] calibrated their CS spectrum using the CS spectrum measured by Burkholder *et al*. [16]. Our determined line positions of CS calibrated with the N_2O spectrum agree satisfactorily with those of Burkholder *et al*. [16]; the standard error is 0.00030 cm^{-1}; 15 outliers have been excluded from the lines, 142 in total, of bands v=1–0 and 2–1 reported by Burkholder *et al*. [16]. The details of the agreement between our measurements of bands v=1–0 and 2–1 and those of Burkholder *et al*. [16] are shown in Fig.S1 in Supplementary material; dots for 127 (=142 − 15) transitions are plotted on the vertical scale to show the differences (this work – Burkholder*et al*.). The abscissal axis indicates spectral wavenumbers; the straight line obtained in a least-squares fit of these differences is also shown. Although that straight line that shows differences +0.00011 cm^{-1} at 1330 cm^{-1} and −0.00017 cm^{-1} at 1200 cm^{-1}, revealing a slight but systematic deviation from the measurements of Burkholder *et al*. [16], we followed Ram *et al*. [17] in calibrating our CS measurements using the spectral wavenumbers published by Burkholder *et al*. [16]. Use of the same calibration as that of Ram *et al*. [17] enables a direct comparison of our measurements of $^{12}C^{32}S$ with theirs [17]. If necessary, one can readily recalibrate the spectrum using the straight line given in Fig. S1 in Supplementary material.

Our calibrated spectral lines for bands v=1–0 to 5–4 of $^{13}C^{32}S$ of measurement 010 and bands v=1–0 to 7–6 of $^{12}C^{32}S$ of measurement 008 are listed in Tables 1(a) and 1(b), respectively. The uncertainties for the measurements of bands v = 1–0 to 5–4 of $^{13}C^{32}S$ and v = 1–0 to 6–5 of $^{12}C^{32}S$ are estimated to be ±0.0003 cm^{-1}; those for band v = 7–6 of $^{12}C^{32}S$ are ±0.0015 cm^{-1}.

Spectra of bands v=2–1 to 5–4 of $^{13}C^{32}S$ were observed for the first time. For band v=1–0, Burkholder *et al*. [16] reported 50 transitions, which we extended to 150. Compared with the present work, Ram *et al*. [17] reported many more vibrational-rotational bands and transitions for $^{12}C^{32}S$, but we found our measurements to be slightly more accurate than theirs [17] because our spectral resolution was greater than theirs. A portion of the *R*-branch region of measurement 008 of CS, the same as that shown in Fig. 2 of Ram *et al*. [17], is shown in Fig. 2. As our line width was smaller than theirs, our measurements of the vibrational–rotational transitions of $^{12}C^{32}S$ are included in Table 1(b) and the spectral fitting. In Tables S1(a), S1(b) and S1(c) in Supplementary material are listed the vibrational–rotational transitions reported by Burkholder *et al*. [16], by Ram *et al*. [17] and by Winkel*et al*. [15], respectively, that are included in the spectral fit. The reported microwave transitions are listed in Tables S1(d), S1(e) and S1(f) in Supplementary material.

4. Analysis

A global multi-isotopologue analysis of CS was made on fitting a spectral data set comprising transitions listed in Tables 1(a), 1(b), S1(a), S1(b), S1(c), S1(d), S1(e) and S1(f) to molecular parameters in the non-Born–Oppenheimer effective Hamiltonian (1). This method of analysis has been extensively reviewed [18]. The Dunham-like treatment of the Schrödinger equation with the non-Born–Oppenheimer Hamiltonian (1) yielded an analytical solution,

$$F_{vJ} = \sum_{i,j} Y_{ij}^{*}(v+1/2)^{i}[J(J+1)]^{j} , \qquad (3)$$

in which Y_{ij}* (= $Y_{ij}*^{(0)}$ + $Y_{ij}^{(2)}$ +…) includes Born–Oppenheimer corrections to Dunham's original notation Y_{ij}. Coefficients $Y_{ij}*^{(0)}$ expressed in terms of the non-Born–Oppenheimer correction parameters, $\delta\Delta_B$, $\delta\Delta_\omega$, $\delta\Delta_{a1q}$, $\delta\Delta_{a2q}$, $\delta\Delta_{a3q}$, δr_{1q}, δr_{2q}, δr_{3q} and δr_{4q}, are given for eleven $Y_{ij}*^{(0)}$ [19], *i.e.*, $Y_{01}*^{(0)}$, $Y_{02}*^{(0)}$, $Y_{03}*^{(0)}$, $Y_{04}*^{(0)}$, $Y_{05}*^{(0)}$, $Y_{10}*^{(0)}$, $Y_{11}*^{(0)}$, $Y_{12}*^{(0)}$, $Y_{13}*^{(0)}$, $Y_{20}*^{(0)}$ and $Y_{21}*^{(0)}$, shown in Eqs. 36–43 and Eqs.13–15 of Refs. [22] and [19], respectively. The correction terms in $Y_{ij}*^{(0)}$ are quantities of order $Y_{ij}^{(2)}$, *i.e.*, the Dunham correction [24].

All present and reported vibrational–rotational spectra of $^{12}C^{32}S$, $^{12}C^{33}S$, $^{12}C^{34}S$ and $^{13}C^{32}S$ and the reported rotational spectra of $^{12}C^{32}S$, $^{12}C^{33}S$, $^{12}C^{34}S$, $^{12}C^{36}S$, $^{13}C^{32}S$, $^{13}C^{33}S$ and $^{13}C^{34}S$ were subjected to a single fit to molecular parameters in the specified set. The present measurements of bands v=1–0 to 5–4 of $^{13}C^{32}S$ and bands v=1–0 to 7–6 of $^{12}C^{32}S$ listed in Tables 1(a) and 1(b), respectively, were included in the spectral fit, with the vibrational–rotational and rotational spectral lines listed in Table S1: vibrational–rotational bands v=1–0 to 3–2 for $^{12}C^{32}S$ and v=1–0 for $^{13}C^{32}S$, $^{12}C^{33}S$ and $^{12}C^{34}S$ reported by Burkholder *et al*. [16]; bands v=1–0 to 9–8 for $^{12}C^{32}S$ by Ram *et al*. [17]; band v=2–0 for $^{12}C^{32}S$ by Winkel*et al*. [15]; rotational transitions J=1–0 up to 11–10 for $^{12}C^{32}S$ ($v \leq 20$), $^{12}C^{34}S$ ($v \leq 7$) and $^{13}C^{32}S$ ($v \leq 3$) by Bogey *et al*. [9]; rotational transitions J=6–5 up to 23–22 for $^{12}C^{32}S$ ($6 \leq v \leq 16$), $^{12}C^{33}S$ ($v \leq 2$), $^{12}C^{34}S$ ($v \leq 9$), $^{12}C^{36}S$ ($v \leq 1$), $^{13}C^{32}S$ ($v \leq 5$), $^{13}C^{33}S$ (v= 0) and $^{13}C^{34}S$ ($v \leq$ 1) by Ahrens and Winnewisser [10], and transitions J=1–0 for $^{12}C^{32}S$ ($v \leq 26$) and J=2–1 for $^{12}C^{32}S$ (v=18–20) by Kim and Yamamoto [11], excluding transitions J=1–0 of $^{12}C^{32}S$ ($27 \leq v \leq 39$).

In total, 3961 spectral lines comprising the vibrational–rotational transitions for $^{12}C^{32}S$, $^{12}C^{33}S$, $^{12}C^{34}S$ and $^{13}C^{32}S$ and the rotational transitions for $^{12}C^{32}S$, $^{12}C^{33}S$, $^{12}C^{34}S$, $^{12}C^{36}S$, $^{13}C^{32}S$, $^{13}C^{33}S$ and $^{13}C^{34}S$ were simultaneously fitted with 22 isotopically invariant molecular parameters: U_ω, U_B, a_i (i=1 to 9), $\Delta_\omega{}^{C}$, $\Delta_\omega{}^{S}$, $\Delta_B{}^{C}$, $\Delta_B{}^{S}$, $\Delta_{a1q}{}^{C}$, $\Delta_{a1q}{}^{S}$,$\Delta_{a2q}{}^{C}$, $\Delta_{a2q}{}^{S}$, $r_{1q}{}^{C}$ (=$r_{1q}{}^{S}$),$r_{2q}{}^{C}$ (=$r_{2q}{}^{S}$) and $r_{3q}{}^{C}$ (=$r_{3q}{}^{S}$).

The choice of these 22 parameters was made as follows. The correction parameters, $\Delta_\omega{}^{C,S}$, $\Delta_B{}^{C,S}$, $\Delta_{aiq}{}^{C,S}$ (i=1, 2, …), $r_{iq}{}^{C}$ (=$r_{iq}{}^{S}$) (i=1, 2, …), make a layered structure of $Y_{ij}^{*(0)}$. The levels of correction of three, five, and eight $Y_{ij}^{*(0)}$ sets include correction parameters {$\delta\Delta_\omega$, $\delta\Delta_B$, δr_{1q}}, {$\delta\Delta_\omega$, $\delta\Delta_B$, $\delta\Delta_{a1q}$, δr_{1q}, δr_{2q}}, and {$\delta\Delta_\omega$, $\delta\Delta_B$, $\delta\Delta_{a1q}$, $\delta\Delta_{a2q}$, δr_{1q}, δr_{2q}, δr_{3q}}, respectively [25]. We fitted the molecular parameters to the data set on changing stepwise the level of correction. When all correction parameters were set adjustable for each level of the $Y_{ij}^{*(0)}$ set, the level of an eight $Y_{ij}^{*(0)}$ set [19] gave a smaller standard deviation of the fit.

An analysis was made connecting these 22 parameters with the vibrational–rotational term values through $Y_{ij}^{*(0)}$+$Y_{ij}{}^{(2)}$ and $Y_{ij}{}^{(0)}$; the level of correction of an eight $Y_{ij}^{*(0)}$ set [19] and Dunham parameters up to a_9 were applied. A set of 41 Y_{ij} coefficients for each of $^{12}C^{32}S$, $^{12}C^{33}S$, $^{12}C^{34}S$, $^{12}C^{36}S$, $^{13}C^{32}S$, $^{13}C^{33}S$ and $^{13}C^{34}S$ that connects the fitting parameters with the term values is given by $Y_{ij}^{*(0)}$+$Y_{ij}{}^{(2)}$ for ij = 01, 02, 03, 04, 10, 11, 12 and 20, $Y_{ij}{}^{(0)}$+$Y_{ij}{}^{(2)}$ for ij= 05, 13, and 21, and $Y_{ij}{}^{(0)}$ for ij = 06, 07, 08, 09, 010, 011, 14, 15, 16, 17, 18, 19, 22, 23, 24, 25, 26, 27, 30, 31, 32, 33, 34, 35, 40, 41, 42, 43, 50 and 51. References for the algebraic formulae for $Y_{ij}^{*(0)}$, $Y_{ij}{}^{(2)}$ and $Y_{ij}{}^{(0)}$, including the potential parameters up to a_9, are given in Ref. [19]; additional details of the analysis are provided in Ref. [20]. The spectral uncertainties, δ_{obs}, were those specified in each paper. The weights for the spectral fit of the data were assumed to be proportional to $(1/\delta_{obs})^2$. The fundamental physical constants were taken from the 2006 CODATA recommended values [26].

The fit of a single data set comprising the present measurements of $^{12}C^{32}S$ and $^{13}C^{32}S$ and the reported $^{12}C^{32}S$, $^{12}C^{33}S$, $^{12}C^{34}S$, $^{12}C^{36}S$, $^{13}C^{32}S$, $^{13}C^{33}S$ and $^{13}C^{34}S$ transitions is satisfactory; the normalized standard deviation is 1.3796 with 22 parameters. Values observed−calculated of the spectral wavenumbers are listed in Tables 1(a) and 1(b), and S1(a), S1(b), S1(c), S1(d), S1(e) and S1(f) for the portions of the present and reported measurements, respectively; the molecular parameters evaluated in the fit are presented in Fit 1 in Table 2.

For Δ_{a1q}^{C}, Δ_{a1q}^{S}, Δ_{a2q}^{S}, r_{2q}^{C} (=r_{2q}^{S}), and r_{3q}^{C} (=r_{3q}^{S}), the uncertainties were larger than the determined values of the parameters. We therefore set three parameters Δ_{a2q}^{S}, r_{2q}^{C} (=r_{2q}^{S}), and r_{3q}^{C} (=r_{3q}^{S}) equal to zero. The result of fitting with 19 adjustable parameters is shown in Fit 2 in Table 2. The normalized standard deviation is 1.3789. As is stated below, the evaluated molecular parameters in Table 2 generate band parameters in Table 5 for all isotopologues. The band parameters calculated for $^{12}C^{32}S$ using the values of the molecular parameters in Fits 1 and 2 in Table 2 are listed in Table 5(a) simultaneously with the reported calculated [27] and experimental [17] values. Judging from the agreement between the absolute values of the present and the reported [17, 27] ones of the band parameters, we decided to use the values in Fit 1 throughout this paper that are free from artifactual constraints. Although the band parameters in Table 5(a) calculated on using the values of Fit 2 have smaller uncertainties, these smaller values are due to the setting of the three parameters to zero without uncertainties.

As the values of 22 parameters in Fit 1 in Table 2 produce 42 Y_{ij} values and 351 band parameters with uncertainties for each of the 12 isotopologues of CS as are shown below, those 22 values are accompanied with uncertainties of 3 digits in order to reproduce the values of Y_{ij} and the band parameters accurately. Evaluated values listed in tables in this paper have uncertainties of 3 digits throughout.

Our expressions [22],

$$
\begin{aligned}
Y_{01}^{*(0)} + Y_{01}^{(2)} &= B_{\mathrm{e}}\left[(1+\delta\Delta_B) + \frac{B_{\mathrm{e}}^2}{2\omega_{\mathrm{e}}^2}(15+14a_1-9a_2+15a_3-23a_1a_2+21(a_1^2+a_1^3)/2)\right] \\
&= B_{\mathrm{e}}\left[(1+\delta\Delta_B) + \frac{m_{\mathrm{e}}}{\mu}\frac{\mu B_{\mathrm{e}}^2}{2m_{\mathrm{e}}\omega_{\mathrm{e}}^2}(15+14a_1-9a_2+15a_3-23a_1a_2+21(a_1^2+a_1^3)/2)\right] \\
&= B_{\mathrm{e}}\left[(1+\delta\Delta_B) + \frac{m_{\mathrm{e}}}{\mu}\frac{h^2}{32\pi^2 m_{\mathrm{e}} r_{\mathrm{e}}^4 k}(15+14a_1-9a_2+15a_3-23a_1a_2+21(a_1^2+a_1^3)/2)\right] \\
&= B_{\mathrm{e}}\left(1+\delta r_0 + \frac{4B_{\mathrm{e}}}{\omega_{\mathrm{e}}^2}\delta s_1 + \frac{m_{\mathrm{e}}}{\mu}D_{01}\right)
\end{aligned}
\tag{4}
$$

and

$$
\begin{aligned}
Y_{10}^{*(0)} + Y_{10}^{(2)} &= \omega_{\mathrm{e}}\left[(1+\delta\Delta_\omega) + \frac{B_{\mathrm{e}}^2}{4\omega_{\mathrm{e}}^2}(25a_4-95a_1a_3/2-67a_2^2/4+459a_1^2a_2/8-1155a_1^4/64)\right] \\
&= \omega_{\mathrm{e}}\left[(1+\delta\Delta_\omega) + \frac{m_{\mathrm{e}}}{\mu}\frac{\mu B_{\mathrm{e}}^2}{4m_{\mathrm{e}}\omega_{\mathrm{e}}^2}(25a_4-95a_1a_3/2-67a_2^2/4+459a_1^2a_2/8-1155a_1^4/64)\right] \\
&= \omega_{\mathrm{e}}\left[(1+\delta\Delta_\omega) + \frac{m_{\mathrm{e}}}{\mu}\frac{h^2}{64\pi^2 m_{\mathrm{e}} r_{\mathrm{e}}^4 k}(25a_4-95a_1a_3/2-67a_2^2/4+459a_1^2a_2/8-1155a_1^4/64))\right] \\
&= \omega_{\mathrm{e}}\left[1-\frac{B_{\mathrm{e}}}{\omega_{\mathrm{e}}^2}(3a_1\delta s_1 - 2\delta s_2) + \delta q_0/2 + \frac{m_{\mathrm{e}}}{\mu}D_{10}\right],
\end{aligned}
\tag{5}
$$

in which quantities D_{01} and D_{10} denote the isotopically invariant Dunham corrections $\Delta_{ij}^{\mathrm{Dunham}}$ are equivalent to the conventional empirical expressions [9, 17, 28, 29],

$$
\begin{aligned}
Y_{01} &= \mu^{-1}U_{01}\left(1+\frac{m_{\mathrm{e}}}{M_{\mathrm{C}}}\Delta_{01}^{\mathrm{C}} + \frac{m_{\mathrm{e}}}{M_{\mathrm{S}}}\Delta_{01}^{\mathrm{S}}\right) \\
&= \mu^{-1}U_{01}\left[1+\frac{m_{\mathrm{e}}}{M_{\mathrm{C}}}\left\{(\Delta_{01}^{\mathrm{nonad}})_{\mathrm{C}} + (\Delta_{01}^{\mathrm{ad}})_{\mathrm{C}} + (\Delta_{01}^{\mathrm{Dunham}})_{\mathrm{C}}\right\} + \frac{m_{\mathrm{e}}}{M_{\mathrm{S}}}\left\{(\Delta_{01}^{\mathrm{nonad}})_{\mathrm{S}} + (\Delta_{01}^{\mathrm{ad}})_{\mathrm{S}} + (\Delta_{01}^{\mathrm{Dunham}})_{\mathrm{S}}\right\}\right]
\end{aligned}
\tag{6}
$$

and

$$
Y_{10} = \mu^{-1/2}U_{10}\left(1+\frac{m_{\mathrm{e}}}{M_{\mathrm{C}}}\Delta_{10}^{\mathrm{C}} + \frac{m_{\mathrm{e}}}{M_{\mathrm{S}}}\Delta_{10}^{\mathrm{S}}\right), \tag{7}
$$

respectively.

The quantities U_B, U_ω, $\Delta_B^{\mathrm{C,S}}$ and $\Delta_\omega^{\mathrm{C,S}}$ are identical to the corresponding conventional quantities U_{01}, U_{10}, $\Delta_{01}^{\mathrm{C,S}}-D_{01}$ and $\Delta_{10}^{\mathrm{C,S}}-D_{10}$. The values of U_B $(=U_{01})$, U_ω $(=U_{10})$, $\Delta_B^{\mathrm{C,S}}$ $(=\Delta_{01}^{\mathrm{C,S}}-D_{01})$ and

$\Delta_{\omega}^{C,S}$ ($=\Delta_{10}^{C,S}-D_{10}$) given by Ram *et al.* [17] are also listed in Table 2. Our values are in agreement with their values of the unconstrained fit rather than those of the constrained fit; our fit is constrained.

5. Discussion

To facilitate calculations or predictions of spectral wavenumbers, the values of 42 Dunham coefficients 42 Y_{ij} including Y_{00} for each of $^{12}C^{32}S$, $^{12}C^{33}S$, $^{12}C^{34}S$, $^{12}C^{36}S$, $^{13}C^{32}S$, $^{13}C^{33}S$, $^{13}C^{34}S$, $^{13}C^{36}S$, $^{14}C^{32}S$, $^{14}C^{33}S$, $^{14}C^{34}S$ and $^{14}C^{36}S$ that connect the 22 molecular parameters to the vibrational–rotational term values of CS have been back-calculated using the values of the parameters given in Fit 1 in Table 2. Although the spectra of $^{13}C^{36}S$, $^{14}C^{32}S$, $^{14}C^{33}S$, $^{14}C^{34}S$ and $^{14}C^{36}S$ are unreported, the values of Y_{ij} were calculated with uncertainties for those species. The values of Y_{ij} in Table 3 are those of Y_{ij}* given in Eq. (3); we used Y_{ij} instead of Y_{ij}* for convenience. In total, 504 Y_{ij} values for 12 isotopologues of CS are listed in Table 3. Except Y_{32}, all Y_{ij} values for each isotopologue of CS were determined with smaller standard errors. In sum, only 22 parameters were required in the present approach to fit the spectral data in the present set; in contrast, the use of Y_{ij} as adjustable parameters required 41 Y_{ij} parameters for each isotopologue of CS to reproduce the data.

Ram *et al.* [17] reported the values of 15 Dunham coefficients for $^{12}C^{32}S$ evaluated on fitting the vibrational–rotational and rotational spectra to the Dunham expression [24]. Their values of Y_{ij}, which are generally in satisfactory agreement with ours, are included in Table 3. Our set of 41 values of Y_{ij} is more extensive and accurate than preceding sets.

For reference, the values of 42 Y_{ij} for $^{12}C^{32}S$ back-calculated using the values of the parameters given in Fit 2 in Table 2 are listed in column 3 of Table 3. The computer output of the Y_{ij} values for the other 11 isotopologues back-calculated by the values of Fit 2 in Table 2 are tabulated in Table S2 in Supplementary material.

The equilibrium internuclear distance r_e and force coefficient k of CS were obtained from U_B and U_{ω} as r_e = 153.482211(41) pm and k = 849.01429(187) N m^{-1}, respectively. These agree well with the values R_e^{BO} = 153.4818 pm and k^{BO} = 848.989 N m^{-1} given by Coxon and Hajigeorgiou [27] as well as the value R_e^{BO} = 153.48224(23) pm reported by Tiemann *et al.* [29]. Our results are presented with error limits. The notations r_e and k in this work imply the physical significance of R_e^{BO} and k^{BO}, respectively. The values of ω_e and B_e for $^{12}C^{32}S$, $^{12}C^{33}S$, $^{12}C^{34}S$, $^{12}C^{36}S$, $^{13}C^{32}S$, $^{13}C^{33}S$, $^{13}C^{34}S$, $^{13}C^{36}S$,

$^{14}C^{32}S$, $^{14}C^{33}S$, $^{14}C^{34}S$ and $^{14}C^{36}S$ obtained from Table 2 are listed in Table 4.

Coxon and Hajigeorgiou [27] numerically determined a curve for the effective potential energy of CS using the vibrational–rotational and rotational spectral transitions reported at that time. Rotational and centrifugal distortion parameters were calculated *a posteriori*. The band parameters for the selected isotopologues of $^{12}C^{32}S$, $^{13}C^{32}S$ and $^{14}C^{36}S$ that were calculated from the Y_{ij} values in Table 3 are shown in Tables 5(a), 5(b) and 5(c), respectively. For $^{12}C^{32}S$, the band parameters calculated from the Y_{ij} values from Fit 2 in Table 3 are listed also at the second-row entries in Table 5(a). Although the uncertainties of the values of the band parameters from Fit 2 are smaller than those from Fit 1, no improvement of the agreement between the absolute values of the band parameters from Fit 2 and the reported values is observed compared with the case from Fit 1.

The notations for the vibrational term values and the rotational parameters in Tables 5(a), 5(b) and 5(c) are given by the equation for the vibrational–rotational term values as follows:

$$F_v(J) = G_v + B_v J(J+1) - D_v[J(J+1)]^2 + H_v[J(J+1)]^3 + L_v[J(J+1)]^4 + M_v[J(J+1)]^5$$
$$+ N_v[J(J+1)]^6 + O_v[J(J+1)]^7 + P_v[J(J+1)]^8 + Q_v[J(J+1)]^9 + R_v[J(J+1)]^{10} + S_v[J(J+1)]^{11}. \qquad (8)$$

Term $Y_{00} = (B_e/8)(3a_2 - 7a_1^2/4)$, which is added at the bottom of Table 3, is included in the calculation of G_v. The molecular parameters reported by Coxon and Hajigeorgiou [27] and by Ram *et al*. [17] are also listed in Tables 5(a, b) and 5(a), respectively. The molecular parameters evaluated in the present work agrees atisfactorily with those of Coxon and Hajigeorgiou [27], although these authors provided no error limits for their molecular parameters. Our analytical approach provides molecular parameters of the same quality as those obtained by the numerical approach.

Although only the band parameters for isotopologues $^{12}C^{32}S$, $^{13}C^{32}S$ and $^{14}C^{36}S$ are shown in this work, one can readily calculate these parameters for any other isotopologue with the equation

$$X_v = \sum_{i=0}^{5} Y_{ij}\left(v + \frac{1}{2}\right)^i, \qquad (9)$$

in which j = 0, 1, 2, 3, …, 11, corresponding to $[X_v \equiv]$ G_v, B_v, $-D_v$, H_v, …, S_v, respectively. The values of Y_{ij} are those given in Table 3.

Herman and Ogilvie [30], Uehara and Ogilvie [22], and Uehara [18] published relations between the rotational g factor $g_J(\xi)$, the permanent electric dipole moment $M(\xi)$, and the nonadiabatic expansion coefficients $r_i^{a,b}$:

$$g_J(\xi) = \sum_{i=0} \{(m_\mathrm{p}/M_a) r_i^a + (m_\mathrm{p}/M_b) r_i^b\} \xi^i = (m_\mathrm{p}/m_\mathrm{e}) \sum_{i=0} \delta\, r_i \xi^i \, , \qquad (10)$$

and

$$2M(\xi)/\{e r_\mathrm{e}(1+\xi)\} = \sum_{i=0} (r_i^b - r_i^a) \xi^i \, . \qquad (11)$$

Equation (11) is defined for a molecule AB of relative polarity $^{-}\mathrm{AB}^{+}$.

If functions $g_J(\xi)$ and $M(\xi)$ for molecule AB are available from experiments with external fields or from calculations, we can estimate the values of $r_i^{a,b}$ (i =0, 1, …) from Eqs. (10) and (11). Fitting parameters $\Delta_\omega^{a,b}$, $\Delta_B^{a,b}$, $r_{iq}^{a,b}$ and $\Delta_{aiq}^{a,b}$ (i=1, 2, …) can then become resolved with these values to yield expansion coefficients $q_i^{a,b}$ (i=0, 1, …) and $s_i^{a,b}$ (i=1, 2, …). McGurk *et al*. [31] determined the sign of the electric dipole moment to be −CS+ from a measurement of the molecular Zeeman effect. Parameters $r_i^{\mathrm{C,S}}$ (i =0, 1, …), $q_i^{\mathrm{C,S}}$ (i=0, 1, …) and $s_i^{\mathrm{C,S}}$ (i=1, 2, …) are the expansion coefficients for the functions of the nonadiabatic rotational, $R_{\mathrm{C,S}}(\xi)$, nonadiabatic vibrational, $Q_{\mathrm{C,S}}(\xi)$ and adiabatic $S_{\mathrm{C,S}}(\xi)$ corrections, respectively, which are given in Eqs. 3–5 of Ref. [22].

The function $g_J(\xi)$ of CS is unknown, but experimental values of the rotational g factor for $^{12}\mathrm{C}^{32}\mathrm{S}$, $^{12}\mathrm{C}^{34}\mathrm{S}$ and $^{13}\mathrm{C}^{34}\mathrm{S}$ for rotational transition J=1–0 in state v=0 are reported [31]. Experimental values exist for the electric dipole moment for rotational transitions J=1–0 in states v=0 and 1 [32]. From those values, only the expansion coefficients s_1^{C} and s_1^{S} can be evaluated. The physical significance of the conventional calculation of nonadiabatic corrections to the Born-Oppenheimer approximation with known values of the rotational g_J factor and the electric dipole moment follows.

The reported experimental values [31, 32] of $g_J = -0.2702\pm0.0004$ for $^{12}\mathrm{C}^{32}\mathrm{S}$ and dipole moment M =1.958±0.005 D are those for state v=0; quantities $g_J(0)$ and $M(0)$, i.e., g_J and M at r_e, are approximated with these experimental values. From the relations

$$g_J(0) = m_p \left(\frac{r_0^{\mathrm{C}}}{M_{\mathrm{C}}} + \frac{r_0^{\mathrm{S}}}{M_{\mathrm{S}}} \right) \qquad (12)$$

and

$$\frac{2M(0)}{e r_\mathrm{e}} = r_0^{\mathrm{S}} - r_0^{\mathrm{C}} \, , \qquad (13)$$

the values of

$r_0^{\mathrm{C}} = -2.4855(35)$

and

$r_0^{\mathrm{S}} = -1.9543(37)$

are obtained for the nonadiabatic rotational corrections.

From Eqs. (4) and (6), the relations

$$r_0^{\mathrm{C,S}} = (\mathit{\Delta}_{01}^{\mathrm{nonad}})_{\mathrm{C,S}}, \qquad (14)$$

$$(4B_{\mathrm{e}}/\omega_{\mathrm{e}}^2)s_1^{\mathrm{C,S}} = (\mathit{\Delta}_{01}^{\mathrm{ad}})_{\mathrm{C,S}} \qquad (15)$$

and

$$D_{01} = (\mathit{\Delta}_{01}^{\mathrm{Dunham}})_{\mathrm{C}} = (\mathit{\Delta}_{01}^{\mathrm{Dunham}})_{\mathrm{S}} \qquad (16)$$

that indicate the physical significance of empirical quantities $(\mathit{\Delta}_{01}^{\mathrm{nonad}})_{\mathrm{C,S}}$, $(\mathit{\Delta}_{01}^{\mathrm{ad}})_{\mathrm{C,S}}$ and $(\mathit{\Delta}_{01}^{\mathrm{Dunham}})_{\mathrm{C,S}}$ are obtained.

We compare $\mathit{\Delta}_B^{\mathrm{C,S}}$ of this work with $(\mathit{\Delta}_{01})_{\mathrm{C,S}}$ given by Bogey *et al*. [9]. The experimental values $\mathit{\Delta}_B^{\mathrm{C}}$ [= −2.54790(829)] and $\mathit{\Delta}_B^{\mathrm{S}}$ [= −2.3636(248)] that are listed in Table 1with the values of r_0^{C} and r_0^{S} given above generate the adiabatic corrections as follows:

$$(4B_{\mathrm{e}}/\omega_{\mathrm{e}}^2)s_1^{\mathrm{C}} = -0.0624(90),$$

$$(4B_{\mathrm{e}}/\omega_{\mathrm{e}}^2)s_1^{\mathrm{S}} = -0.409(25),$$

$$s_1^{\mathrm{C}} = -0.314(45)\times 10^5\ \mathrm{cm}^{-1}$$

and

$$s_1^{\mathrm{S}} = -2.06(13)\times 10^5\ \mathrm{cm}^{-1}.$$

The values of $(4B_{\mathrm{e}}/\omega_{\mathrm{e}}^2)s_1^{\mathrm{C}}$ and $(4B_{\mathrm{e}}/\omega_{\mathrm{e}}^2)s_1^{\mathrm{S}}$ can be compared with $(\mathit{\Delta}_{01}^{\mathrm{ad}})_{\mathrm{C}} = -0.096(30)$ and $(\mathit{\Delta}_{01}^{\mathrm{ad}})_{\mathrm{S}} = -0.566(70)$ given in Ref. [9], respectively. The calculated value $D_{01} = -0.01012(18)$ plus $\mathit{\Delta}_B^{\mathrm{C}}$ and $\mathit{\Delta}_B^{\mathrm{S}}$ in Table 1 are −2.5580(83) and −2.374(25), corresponding to the experimental values $(\mathit{\Delta}_{01})_{\mathrm{C}} = -2.586(25)$ and $(\mathit{\Delta}_{01})_{\mathrm{S}} = -2.525(64)$ of Ref. [9], respectively. Ram *et al*. [17] presented values $\mathit{\Delta}_{01}^{\mathrm{C}} = -2.5520(179)$ and $\mathit{\Delta}_{01}^{\mathrm{S}} = -2.6832(481)$ from an unconstrained fit. Isotopically invariant values of r_0^{C} and r_0^{S} provide g_J values from Eq. (12) for $^{12}C^{34}S$ and $^{13}C^{32}S$ as

$g_J(^{12}C^{34}S) = -0.26658(31)$

and

$g_J(^{13}C^{32}S) = -0.25410(29)$;

these correspond to experimental values $g_J(^{12}C^{34}S) = -0.2659(7)$ and $g_J(^{13}C^{32}S) = -0.2529(5)$ [31], respectively. The calculated and experimental values of g_J for $^{13}C^{32}S$ differ slightly beyond the mutual error limits, but the difference likely originates from the values of $g_J(0)$ and $M(0)$ taken from those determined from rotational transition J=1–0 in state v=0. According to Kirschner *et al*. [33], because the expected variation of g_J between adjacent vibrational states is of order $(4B_{\mathrm{e}}/\omega_{\mathrm{e}})g_J(0)$, an additional error about 0.00034 is expected in the present discussion regarding $g_J(0)$. Similarly, from a theoretical treatment of the vibrational and rotational dependence of the electric dipole moment of CS given by Maroulis *et al*. [34], the assumed $M(0)$ value in the present discussion includes an additional error about 0.010 D.

The values of $\Delta_\omega^{C,S}$ of Ref. [17] in Table 2 were obtained from the reported values of $(\Delta_{10})_{C,S}$ [17] minus the Dunham correction $D_{10} = -0.01208(118)$. Relations similar to Eqs. (14)–(16) can be written as,

$$q_0^{C,S}/2 = (\Delta_{10}^{nonad})_{C,S}, \quad (17)$$

$$-(B_e/\omega_e^2)(3a_1s_1^{C,S} - 2s_2^{C,S}) = (\Delta_{10}^{ad})_{C,S}, \quad (18)$$

and

$$D_{10} = (\Delta_{10}^{Dunham})_C = (\Delta_{10}^{Dunham})_S. \quad (19)$$

Although the value of $s_1^{C,S}$ was obtained above from the experimental values of g_J and M, $(\Delta_{10}^{nonad})_{C,S}$ and $(\Delta_{10}^{ad})_{C,S}$, cannot be determined separately from the observed value $(\Delta_{10})_{C,S}$ because $(\Delta_{10})_{C,S}$ includes two unknowns $q_0^{C,S}$ and $s_2^{C,S}$. As Watson [35] found, only combinations of expansion coefficients $q_i^{C,S}$, $r_i^{C,S}$, and $s_i^{C,S}$ can be determined from energy levels unless $r_i^{C,S}$ (i = 0, 1, 2, …) are estimated from experiments with external fields or from theoretical calculation [22, 36].

In summary, the above discussion reveals the physical significance of the conventional treatments of the adiabatic and nonadiabatic corrections for Δ_{01}^C and Δ_{01}^S.

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Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at

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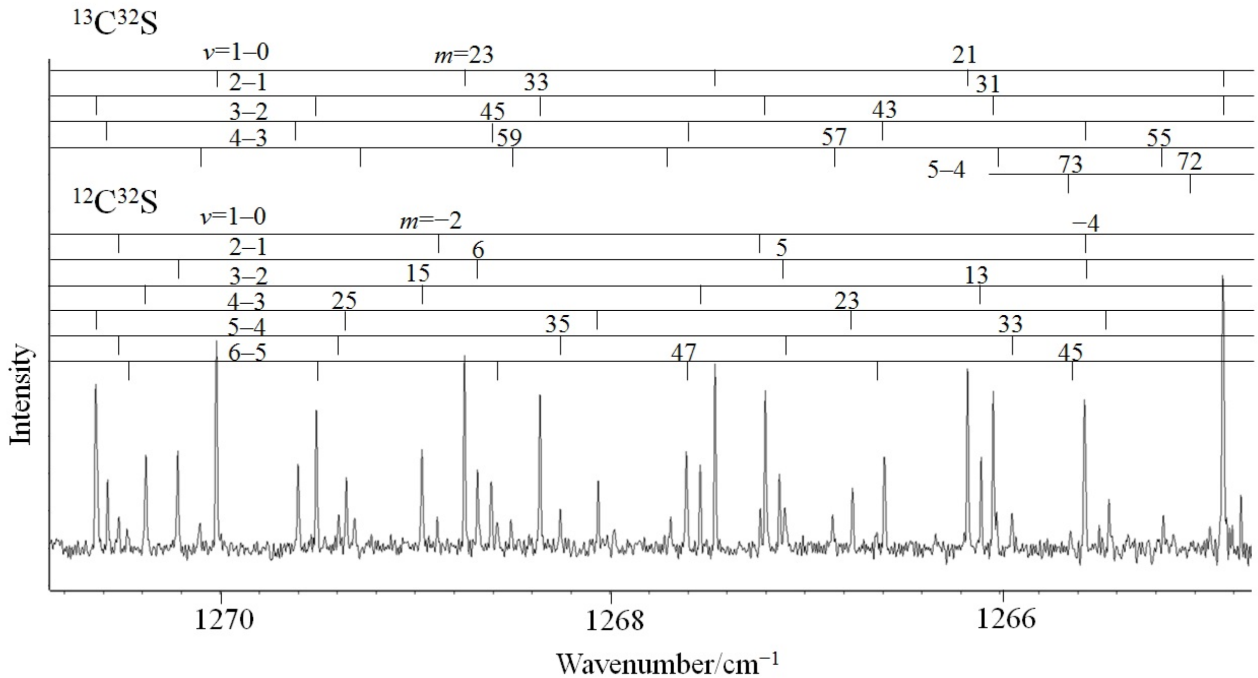
Captions of figures

Fig. 1. A portion of the vibrational-rotational spectra of $^{13}C^{32}S$ and $^{12}C^{32}S$.

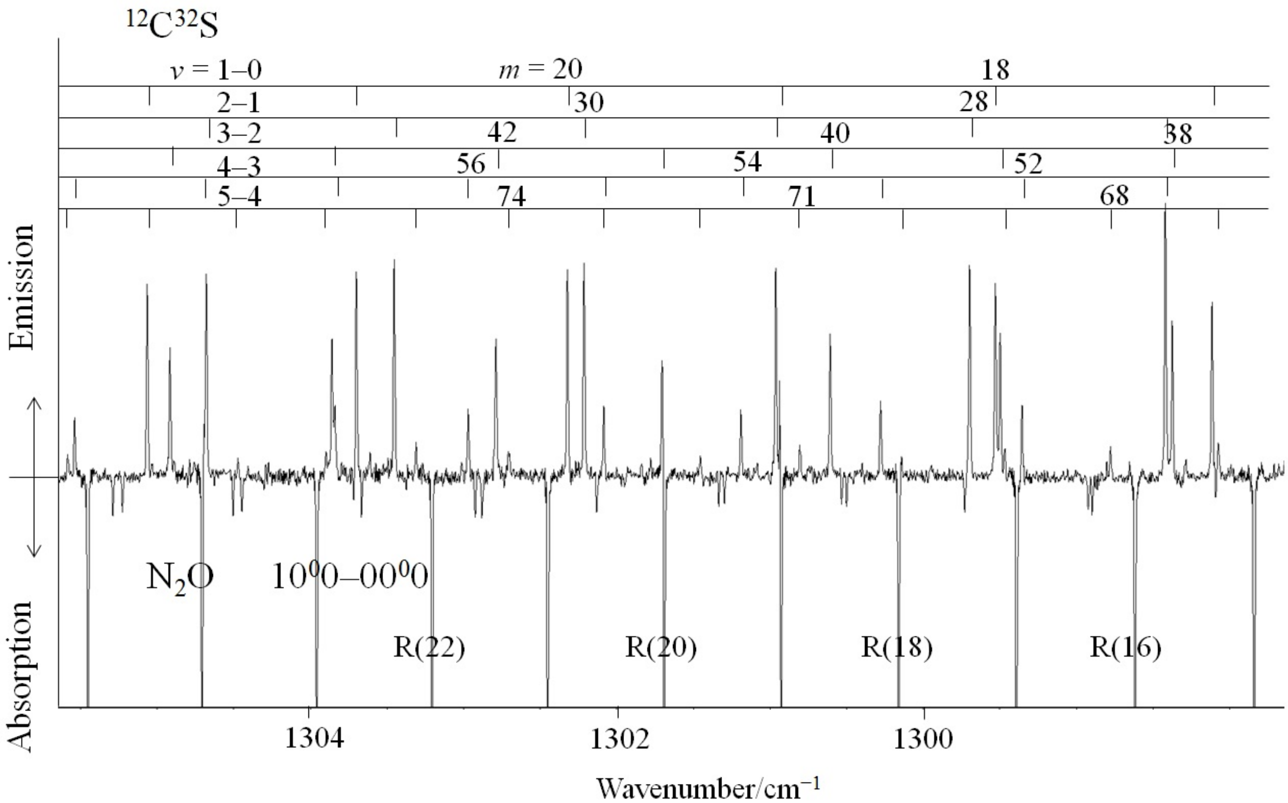
Fig. 2. Simultaneous recording of the spectra of CS and N_2O in emission and absorption, respectively. Spectral lines of N_2O were truncated graphically due to the range of the vertical scale shown in the figure.

Fig. 1.



$^{13}C^{32}S$
v=1–0
m=23
21
2–1
33
31
3–2
45
43
4–3
59
57
55
5–4
73
72
$^{12}C^{32}S$
v=1–0
m=−2
−4
2–1
6
5
3–2
15
13
4–3
25
23
5–4
35
33
6–5
47
45
Intensity
1270
1268
1266
Wavenumber/cm^{-1}

Fig. 2.



$^{12}C^{32}S$
v = 1–0
m = 20
18
2–1
30
28
3–2
42
40
38
4–3
56
54
52
5–4
74
71
68
Emission
Absorption
N_2O $10^00–00^00$
R(22)
R(20)
R(18)
R(16)
1304
1302
1300
Wavenumber/cm^{-1}

Table 1(a) Observed vibrational-rotational transitions (wavenumber/cm^{-1}) of $^{13}C^{32}S$.

m	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)
			-9	1222.045716	1.143	66	1312.730698	0.104
v = 1–0			-8	1223.672568	-0.499	67	1313.481268	0.181
-80	1080.972174	-1.332	-7	1225.291044	0.113	68	1314.217891	-0.847
-78	1085.590979	0.110	-6	1226.898987	0.852	69	1314.945520	2.004
-75	1092.449518	-1.765	-5	1228.493269	-1.383	71	1316.354802	0.471
-74	1094.719760	-0.725	2	1239.369011	0.380	72	1317.039609	-0.698
-73	1096.980634	-0.210	3	1240.880020	1.398	73	1317.714175	0.890
-72	1099.231087	-1.247	4	1242.379018	1.348	75	1319.020152	0.023
-70	1103.709687	1.083	5	1243.865071	-0.673	76	1319.654811	0.880
-68	1108.149471	0.380	6	1245.341521	-1.295	77	1320.275739	1.126
-67	1110.356179	0.327	7	1246.809131	0.273	78	1320.883166	1.025
-66	1112.553491	-0.099	8	1248.265224	1.383	79	1321.476003	-0.483
-65	1114.741451	-0.828	9	1249.708120	0.384	81	1322.625131	-0.368
-64	1116.922892	0.999	10	1251.140597	0.084	84	1324.251042	1.690
-63	1119.092861	0.455	11	1252.563032	0.887	85	1324.765011	1.079
-62	1121.253687	-0.105	12	1253.972381	-0.221	86	1325.265683	0.577
-61	1123.405213	-0.812	13	1255.371733	-0.123			
-60	1125.547984	-1.094	14	1256.760093	0.216	*v* = 2–1		
-59	1127.683165	0.238	15	1258.136828	0.192	-71	1089.992782	-0.644
-58	1129.808052	0.509	16	1259.502121	0.016	-70	1092.214903	-1.606
-57	1131.923069	0.168	17	1260.856427	0.172	-69	1094.431907	1.265
-56	1134.028927	-0.048	18	1262.198556	-0.500	-68	1096.636836	1.038
-55	1136.125591	-0.147	19	1263.530602	0.123	-67	1098.833443	1.492
-54	1138.213489	0.325	20	1264.848252	-2.243	-66	1101.019665	0.588
-53	1140.291608	0.383	21	1266.159054	-0.022	-65	1103.196960	-0.189
-52	1142.360174	0.278	22	1267.455939	-0.252	-64	1105.366585	0.444
-51	1144.420487	1.337	23	1268.741809	-0.003	-63	1107.526066	0.038
-50	1146.468876	-0.084	24	1270.015655	-0.254	-61	1111.817291	-1.089
-49	1148.509875	0.576	25	1271.278447	-0.007	-60	1113.952133	1.339
-48	1150.540552	0.411	26	1272.529341	-0.075	-59	1116.072368	-1.629
-47	1152.561625	0.166	27	1273.768651	-0.116	-58	1118.187927	-0.037
-46	1154.573914	0.689	28	1274.996444	-0.034	-57	1120.292799	0.130
-45	1156.574740	-0.673	29	1276.212574	0.056	-56	1122.388144	0.059
-44	1158.567873	-0.123	30	1277.416808	-0.050	-55	1124.474421	0.235
-43	1160.550691	-0.257	32	1279.790374	0.051	-54	1126.550237	-0.709
-42	1162.523482	-0.758	33	1280.959417	0.029	-53	1128.618739	0.402
-41	1164.487919	0.074	34	1282.116525	-0.111	-52	1130.676622	0.289
-40	1166.442481	0.743	35	1283.263002	0.965	-51	1132.724689	-0.219
-39	1168.385733	-0.156	36	1284.395641	0.080	-50	1134.764057	0.022
-38	1170.320583	0.310	37	1285.516984	-0.195	-49	1136.793169	-0.519
-37	1172.244819	-0.043	38	1286.626361	-0.501	-48	1138.814177	0.338
-36	1174.159533	-0.096	39	1287.726336	1.758	-47	1140.824483	0.021
-35	1176.064615	0.070	40	1288.810234	-0.066	-46	1142.825570	0.040
-34	1177.960094	0.509	41	1289.885023	1.027	-45	1144.817526	0.510
-33	1179.844731	0.012	42	1290.945480	-0.158	-44	1146.798418	-0.475
-32	1181.719729	-0.193	43	1291.995295	0.100	-43	1148.771105	-0.030
-31	1183.585163	-0.002	44	1293.032819	0.181	-42	1150.733575	-0.138
-30	1185.440214	-0.207	45	1294.057985	0.048	-41	1152.686598	-0.004
-29	1187.285700	0.038	46	1295.070272	-0.789	-40	1154.629849	0.076
-28	1189.120783	-0.078	47	1296.073950	1.969	-39	1156.564511	1.311
-27	1190.945945	-0.045	48	1297.060614	-0.053	-38	1158.486841	-0.015
-26	1192.761180	0.159	49	1298.036969	-0.120	-37	1160.401001	0.288
-25	1194.565728	-0.198	50	1299.002680	1.463	-36	1162.305028	0.283
-24	1196.360811	0.132	51	1299.952894	-0.127	-35	1164.198842	-0.080
-23	1198.145146	-0.104	52	1300.892350	-0.120	-34	1166.082980	-0.240
-22	1199.919878	0.266	53	1301.819674	0.139	-33	1167.957576	-0.033
-21	1201.683304	-0.433	54	1302.734255	0.070	-32	1169.821925	-0.137
-20	1203.437557	-0.041	55	1303.635898	-0.492	-31	1171.676492	-0.061
-19	1205.181714	0.548	56	1304.525487	-0.633	-30	1173.520232	-0.821
-18	1206.914566	0.153	57	1305.403517	0.172	-29	1175.355670	0.136
-17	1208.637336	0.025	58	1306.267757	-0.276	-28	1177.180213	0.243
-16	1210.350225	0.392	59	1307.120023	-0.133	-27	1178.994359	0.026
-15	1212.052053	0.103	60	1307.960330	0.649	-26	1180.798698	0.104
-14	1213.743575	-0.059	61	1308.786489	-0.090	-25	1182.592121	-0.605
-13	1215.425126	0.269	62	1309.601094	0.274	-24	1184.376256	-0.446
-12	1217.095827	0.236	63	1310.400133	-2.240	-23	1186.150540	0.047
-11	1218.755696	-0.111	64	1311.191412	0.206	-22	1187.913167	-0.905
-10	1220.405841	0.364	65	1311.968020	0.730	-21	1189.667493	0.082

Table 1(a) – Continued

m	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)
-20	1191.410242	-0.240	52	1288.077880	-0.095	-34	1154.228356	0.603
-19	1193.143449	0.192	53	1288.993613	-0.292	-33	1156.091307	-0.095
-18	1194.863404	-2.304	54	1289.897890	0.477	-32	1157.945145	0.033
-17	1196.577989	0.183	55	1290.787921	-0.547	-31	1159.788884	0.029
-16	1198.279389	-0.136	56	1291.666796	-0.243	-30	1161.622368	-0.235
-15	1199.969741	-1.094	57	1292.533000	-0.096	-29	1163.44656	0.230
-14	1201.651146	-0.563	58	1293.386280	-0.330	-28	1165.261501	1.494
-13	1203.322346	0.227	59	1294.227088	-0.460	-27	1167.064399	0.792
-12	1204.979915	-2.121	60	1295.056385	0.504	-26	1168.857409	0.307
-11	1206.630798	-0.634	61	1295.870845	-0.733	-25	1170.64043	-0.035
-10	1208.270617	0.338	62	1296.675855	1.246	-24	1172.413971	0.303
-9	1209.898978	0.430	63	1297.462150	-2.792	-23	1174.177053	0.371
-8	1211.516965	0.753	64	1298.241994	-0.552	-22	1175.929825	0.344
-7	1213.123080	-0.162	66	1299.759754	0.306	-21	1177.672834	0.799
-6	1214.718670	-0.939	67	1300.499020	0.337	-20	1179.403577	-0.742
-5	1216.305269	-0.016	68	1301.224953	-0.113	-19	1181.126459	0.157
-4	1217.880455	0.213	69	1301.939052	0.485	-18	1182.838362	0.404
-3	1219.442799	-1.652	70	1302.639607	0.453	-17	1184.540818	1.560
-2	1220.997035	-0.849	71	1303.323530	-3.265	-16	1186.229521	-0.653
2	1227.102643	-0.637	72	1304.000756	-0.705	-15	1187.913168	2.489
3	1228.600833	-1.569	74	1305.312395	0.656	-14	1189.579715	-1.028
5	1231.568302	0.529	76	1306.568336	-1.400	-13	1191.240342	0.002
6	1233.032327	-1.638	77	1307.178610	-0.441	-12	1192.890252	0.812
7	1234.488995	-0.127	78	1307.775396	0.194	-11	1194.527981	-0.034
8	1235.932463	-0.753	79	1308.357849	-0.308	-10	1196.155683	-0.355
9	1237.366738	0.519	80	1308.926089	-1.795	-9	1197.773569	0.089
10	1238.787600	-0.500	81	1309.482769	-1.583	-8	1199.383201	2.889
11	1240.198920	0.089	82	1310.026165	-1.364	-6	1202.56194	-0.094
12	1241.598127	-0.257	83	1310.558168	0.785	-5	1204.131159	-5.709
13	1242.986991	0.262	85	1311.577662	0.668	-4	1205.701798	0.820
14	1244.363808	-0.029	86	1312.067932	1.245	-3	1207.256334	1.997
15	1245.729510	-0.170				-2	1208.794229	-2.686
16	1247.083863	-0.365	*v* = 3–2			-1	1210.326563	-2.122
17	1248.427792	0.340	-70	1080.745971	1.033	2	1214.860411	1.556
18	1249.758705	-0.618	-69	1082.947042	-1.447	3	1216.344901	-2.202
19	1251.079667	-0.145	-68	1085.143375	0.318	4	1217.822299	-2.100
20	1252.388532	-0.357	-67	1087.325848	-2.770	5	1219.289993	-0.721
21	1253.686499	-0.027	-66	1089.505172	0.026	6	1220.746387	0.367
22	1254.972498	-0.195	-65	1091.672067	-0.548	7	1222.187764	-2.523
23	1256.247133	-0.229	-64	1093.830806	-0.193	9	1225.046863	1.273
24	1257.510141	-0.360	-63	1095.979274	-0.999	10	1226.456211	-0.357
25	1258.761251	-0.833	-62	1098.121259	0.849	11	1227.856718	0.326
26	1260.002047	-0.032	-61	1100.251101	-0.284	12	1229.24495	-0.083
27	1261.230373	-0.085	-60	1102.374194	1.023	13	1230.62185	-0.612
28	1262.447029	-0.162	-59	1104.487614	1.872	14	1231.98859	-0.059
29	1263.652616	0.368	-58	1106.588495	-0.577	15	1233.343802	0.235
30	1264.848252	2.651	-57	1108.683690	0.554	16	1234.686614	-0.571
31	1266.027188	-0.032	-56	1110.768614	0.709	17	1236.019591	0.117
32	1267.196883	-0.192	-55	1112.841995	-1.361	18	1237.340584	0.178
33	1268.354871	-0.265	-54	1114.908667	-0.793	19	1238.649966	0.015
34	1269.501547	0.172	-53	1116.965826	-0.365	20	1239.949053	0.974
35	1270.633399	-2.362	-52	1119.014442	0.919	21	1241.234917	0.154
36	1271.758010	-0.254	-51	1121.050586	-0.844	22	1242.509782	-0.189
37	1272.868942	0.086	-50	1123.080927	1.043	23	1243.773481	-0.195
38	1273.967492	-0.013	-49	1125.101456	2.596	24	1245.025123	-0.724
39	1275.053956	-0.228	-48	1127.109917	1.587	25	1246.266359	-0.096
40	1276.128803	-0.057	-47	1129.108180	-0.088	26	1247.495121	-0.350
41	1277.191389	-0.117	-46	1131.099074	0.428	27	1248.712078	-0.787
42	1278.241923	-0.167	-45	1133.079219	-0.220	28	1249.918142	-0.466
43	1279.280284	-0.300	-44	1135.050253	-0.365	29	1251.112368	-0.302
44	1280.306699	-0.257	-43	1137.014095	1.937	30	1252.294826	-0.196
45	1281.320941	-0.237	-42	1138.964071	0.040	31	1253.46542	-0.214
46	1282.323207	-0.011	-41	1140.906283	0.073	32	1254.624215	-0.261
47	1283.313337	0.289	-40	1142.838570	-0.098	33	1255.771165	-0.354
48	1284.289675	-0.961	-38	1146.674940	0.627	34	1256.906565	-0.169
49	1285.256291	0.338	-37	1148.576644	-0.801	35	1258.029389	-0.700
50	1286.208857	-0.112	-36	1150.470970	0.223	36	1259.141609	0.053
51	1287.149500	-0.153	-35	1152.355516	1.324	37	1260.241391	0.286

Table 1(a) – Continued

m	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)
38	1261.328767	0.062	-33	1144.247530	1.472	51	1261.603483	-0.266
39	1262.403597	-0.731	-31	1147.923312	1.282	52	1262.508300	-1.449
40	1263.467185	-0.758	-30	1149.744940	-0.092	53	1263.402387	-0.953
41	1264.519960	0.440	-29	1151.558428	0.420	54	1264.283898	-0.593
42	1265.558883	-0.146	-28	1153.361649	0.718	55	1265.154457	1.285
43	1266.586008	-0.432	-27	1155.152398	-1.375	57	1266.852699	-0.301
44	1267.602499	0.776	-26	1156.937129	0.623	58	1267.683216	-0.870
45	1268.604555	-0.294	-25	1158.709953	0.850	59	1268.502570	-0.009
46	1269.595806	0.020	-24	1160.470193	-1.342	60	1269.306960	-1.487
47	1270.574293	-0.211	-23	1162.224217	0.441	61	1270.101958	0.298
48	1271.541407	0.432	-22	1163.966191	0.394	62	1270.883342	1.155
49	1272.494700	-0.466	-20	1167.418764	-0.303	63	1271.650291	0.294
50	1273.436895	-0.153	-19	1169.130709	0.448	64	1272.404823	-0.236
51	1274.367132	0.541	-18	1170.829544	-1.579	65	1273.148678	1.337
52	1275.283270	-0.493	-17	1172.522723	1.097	66	1273.875753	-1.059
53	1276.188741	0.205	-16	1174.202398	0.657	67	1274.594576	1.135
54	1277.080060	-0.818	-15	1175.871465	0.025	68	1275.297314	0.117
55	1277.961594	0.836	-14	1177.530839	0.144	69	1275.989921	1.873
56	1278.828594	0.447	-13	1179.179956	0.477	70	1276.665027	-0.935
57	1279.683014	0.001	-11	1182.444988	-0.528	71	1277.330545	-0.364
58	1280.524160	-1.166	-10	1184.061898	-0.816	72	1277.984290	1.433
59	1281.354797	-0.258	-7	1188.850787	0.104			
60	1282.173278	1.108	-5	1191.989872	0.514	*v* = 5–4		
61	1282.975188	-1.451	-3	1195.086066	0.942	-46	1107.707636	0.596
62	1283.769715	1.283	4	1205.578304	-0.790	-44	1111.616769	0.482
63	1284.547194	-0.324	6	1208.480674	1.739	-43	1113.558812	2.362
64	1285.312130	-1.736	8	1211.335722	1.118	-42	1115.488597	1.659
65	1286.067008	-0.437	9	1212.744254	-1.548	-41	1117.409617	1.894
66	1286.806666	-1.558	10	1214.145288	-0.582	-40	1119.318081	-0.697
67	1287.536825	0.653	11	1215.534799	0.020	-38	1123.110301	-1.290
68	1288.250360	-0.898	12	1216.911140	-1.361	-37	1124.993903	0.609
69	1288.954423	0.973	13	1218.279427	0.422	-36	1126.866768	1.609
70	1289.643379	0.661	14	1219.632735	-1.529	-35	1128.725935	-1.224
71	1290.320033	1.004	15	1220.978941	0.694	-33	1132.419408	-2.044
73	1291.636796	4.138	16	1222.310366	-0.560	-32	1134.253468	-0.223
74	1292.270701	0.788	17	1223.632373	0.102	-31	1136.076601	0.646
75	1292.894243	0.157	18	1224.943305	1.051	-30	1137.888484	0.268
78	1294.687589	-0.208	19	1226.241945	1.101	-29	1139.689463	-0.984
80	1295.815917	-1.696	20	1227.527520	-0.494	-28	1141.481985	-0.635
81	1296.362985	0.357	21	1228.802621	-1.111	-27	1143.265733	1.025
85	1298.410306	0.983	22	1230.066235	-1.736	-25	1146.798409	-0.108
			24	1232.562456	0.566	-24	1148.550092	-0.091
v = 4–3			25	1233.793164	1.652	-23	1150.291454	-0.199
-65	1080.169544	0.931	26	1235.010133	0.597	-22	1152.023366	0.468
-64	1082.314940	-1.464	27	1236.216804	0.872	-21	1153.743441	-0.451
-63	1084.455570	0.490	28	1237.410811	0.140	-19	1157.154020	-0.992
-60	1090.816182	0.031	29	1238.593008	-0.716	-12	1168.767819	0.938
-58	1095.011968	1.158	30	1239.765010	-0.051	-10	1171.992110	1.925
-57	1097.093473	-0.772	31	1240.924243	-0.408	-9	1173.586456	0.489
-56	1099.170511	2.130	32	1242.071632	-0.834	-8	1175.171635	0.503
-54	1103.287351	-1.302	33	1243.209021	0.546	11	1203.232825	-1.040
-53	1105.333967	-0.769	34	1244.333737	1.088	12	1204.600661	0.003
-50	1111.416098	-0.360	35	1245.444030	-0.928	14	1207.300671	0.121
-49	1113.424102	-0.665	36	1246.544503	-0.868	18	1212.565766	1.032
-48	1115.422158	-1.408	37	1247.633850	-0.010	19	1213.852859	0.500
-46	1119.393068	0.541	38	1248.712092	1.697	20	1215.127927	-0.631
-45	1121.363074	0.439	39	1249.775217	0.273	21	1216.392577	-0.723
-44	1123.324691	1.565	40	1250.827726	0.248	22	1217.646748	0.192
-43	1125.275033	1.060	41	1251.868105	0.137	23	1218.888786	0.489
-42	1127.214573	-0.576	42	1252.895983	-0.399	24	1220.118953	0.459
-41	1129.149170	2.543	43	1253.911995	-0.696	25	1221.334922	-2.194
-40	1131.068945	0.566	44	1254.915836	-1.029	26	1222.543683	-0.451
-39	1132.980571	0.192	45	1255.909141	0.267	28	1224.921501	-1.739
-38	1134.882811	0.211	46	1256.888256	-0.430	29	1226.095248	-0.020
-37	1136.775638	0.624	47	1257.855614	-0.659	30	1227.256903	1.329
-36	1138.657008	-0.586	48	1258.811328	-0.275	31	1228.403825	-0.302
-35	1140.530277	-0.036	49	1259.754532	-0.114	33	1230.665675	-0.181
-34	1142.393974	0.831	50	1260.686060	0.689	34	1231.777195	-1.778

Table 1(a) – Continued

m	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)
35	1232.879917	-0.301	45	1243.234829	1.738	56	1253.210653	0.180
36	1233.969507	-0.054	46	1244.200685	-1.072	57	1254.041014	-1.861
37	1235.047578	0.606	48	1246.103738	1.384	60	1256.462645	-1.879
38	1236.111872	-0.548	49	1247.034796	0.571	61	1257.246331	-0.120
40	1238.206014	-1.297	50	1247.953819	0.049	69	1263.040751	-1.396
41	1239.236091	-0.602	51	1248.859818	-1.140	71	1264.361828	-0.390
42	1240.253108	-0.885	53	1250.637722	-0.419	72	1265.003243	0.491
44	1242.250884	-1.338	54	1251.508557	0.482	73	1265.630604	0.362

Table 1(b) Observed vibrational-rotational transitions (wavenumber/cm^{-1}) of $^{12}C^{32}S$.

m	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)
			-21	1235.410171	2.917	50	1338.096412	0.075
v = 1–0			-20	1237.271474	-0.069	51	1339.084733	-0.258
-90	1081.453379	-1.681	-19	1239.124779	0.154	52	1340.060129	0.004
-89	1084.019247	-0.295	-18	1240.966250	-0.221	53	1341.021893	0.190
-87	1089.121452	0.475	-17	1242.796667	-0.380	54	1341.969713	0.021
-86	1091.657471	-0.405	-16	1244.616424	0.101	55	1342.904511	0.453
-85	1094.188701	3.176	-15	1246.424067	-0.200	56	1343.824728	-0.039
-84	1096.704161	0.263	-14	1248.220785	-0.063	57	1344.731723	-0.061
-83	1099.215121	2.154	-13	1250.006059	0.024	58	1345.625221	0.145
-82	1101.715423	2.718	-12	1251.779756	-0.038	59	1346.504691	0.083
-81	1104.203868	0.785	-11	1253.542068	-0.028	60	1347.370602	0.255
-79	1109.156292	0.642	-10	1255.292814	-0.093	61	1348.222450	0.193
-78	1111.617647	-0.136	-9	1257.032291	0.093	62	1349.060701	0.397
-76	1116.515168	1.559	-8	1258.759888	-0.046	63	1349.884534	0.079
-75	1118.947639	0.394	-7	1260.476321	0.235	64	1350.694718	0.044
-74	1121.371268	-0.057	-6	1262.180748	0.127	65	1351.491011	0.083
-73	1123.786600	0.778	-5	1263.873286	-0.220	66	1352.272576	-0.605
-72	1126.190670	-0.037	-4	1265.556631	1.919	67	1353.041363	-0.035
-71	1128.586596	0.645	-3	1267.223849	-0.355	68	1353.795661	0.114
-70	1130.972340	0.814	-2	1268.882286	0.334	69	1354.535772	0.182
-69	1133.347980	0.577	2	1275.391760	-3.096	70	1355.261562	0.067
-68	1135.713808	0.255	3	1276.995263	1.863	71	1355.973513	0.288
-67	1138.070008	0.059	4	1278.580271	0.265	72	1356.670524	-0.222
-66	1140.416811	0.252	5	1280.154752	0.108	73	1357.353984	-0.039
-65	1142.753711	0.354	6	1281.717068	-0.211	75	1358.677671	-0.034
-64	1145.080067	-0.246	7	1283.267829	-0.052	76	1359.317975	-0.065
-63	1147.397687	0.290	8	1284.806401	-0.015	77	1359.944425	0.435
-62	1149.703416	-1.165	9	1286.335021	2.168	78	1360.555563	0.043
-61	1152.001689	-0.146	10	1287.847083	-0.076	80	1361.735986	0.806
-60	1154.291356	2.225	11	1289.350784	1.482	81	1362.303707	0.469
-59	1156.567356	0.918	12	1290.839238	-0.011	82	1362.857124	0.389
-58	1158.834144	0.416	13	1292.317024	0.056	84	1363.920231	0.331
-57	1161.091179	0.208	14	1293.782354	-0.072	86	1364.927338	2.949
-56	1163.338444	0.306	15	1295.235608	0.018	87	1365.404432	-0.108
-55	1165.575920	0.722	16	1296.676283	-0.146	88	1365.870344	0.430
-54	1167.801457	-0.666	17	1298.105336	0.427	89	1366.322305	1.829
-53	1170.018930	0.048	18	1299.520666	-0.333	90	1366.759365	3.178
-52	1172.225725	0.278	19	1300.924775	0.111	91	1367.176318	-0.696
-51	1174.421921	0.135	20	1302.315825	-0.048	92	1367.583451	0.533
-50	1176.607558	-0.312	21	1303.694439	-0.154	93	1367.973270	-0.594
-49	1178.783918	0.248	22	1305.060711	-0.080	94	1368.350315	0.501
-48	1180.948907	-0.247	23	1306.414419	-0.015	96	1369.056643	0.060
-47	1183.104259	-0.035	24	1307.755543	0.053			
-46	1185.248887	-0.172	25	1309.084121	0.196	*v* = 2–1		
-45	1187.383405	-0.014	26	1310.399670	-0.037	-102	1038.189353	-0.942
-44	1189.507101	-0.243	27	1311.702695	-0.108	-101	1040.852470	1.064
-43	1191.620878	0.075	28	1312.993186	0.006	-100	1043.504011	0.353
-42	1193.723505	-0.261	29	1314.270547	-0.257	-99	1046.146045	-0.98
-41	1195.816373	0.170	30	1315.535658	0.015	-97	1051.409838	2.836
-40	1197.898167	0.083	31	1316.787692	0.029	-95	1056.630054	-1.073
-39	1199.969367	-0.010	32	1318.026808	-0.025	-93	1061.819746	0.555
-38	1202.030149	0.096	33	1319.253275	0.157	-91	1066.974260	3.278
-37	1204.080271	0.191	34	1320.466349	-0.136	-89	1072.087367	1.081
-36	1206.119411	-0.018	35	1321.666145	-0.756	-88	1074.632325	2.136
-35	1208.148348	0.279	36	1322.854815	0.482	-87	1077.165503	0.614
-34	1210.165911	-0.057	37	1324.028456	-0.291	-86	1079.691496	1.136
-33	1212.172949	-0.147	38	1325.190255	0.144	-85	1082.206333	-0.241
-32	1214.169706	0.283	39	1326.338424	0.034	-84	1084.715388	1.884
-31	1216.154896	-0.021	40	1327.473488	-0.064	-83	1087.212636	1.514
-30	1218.129439	-0.109	41	1328.595724	0.161	-82	1089.700075	0.673
-29	1220.093209	-0.076	42	1329.704392	0.002	-81	1092.178287	-0.028
-28	1222.046113	0.017	43	1330.800102	0.103	-80	1094.647715	-0.120
-27	1223.988162	0.211	44	1331.882489	0.133	-79	1097.108622	0.690
-26	1225.918721	-0.097	45	1332.951476	0.047	-78	1099.560354	1.774
-25	1227.838583	-0.084	46	1334.007660	0.478	-77	1101.997841	-1.909
-24	1229.747432	-0.034	47	1335.049655	0.071	-76	1104.431685	0.271
-23	1231.645166	-0.019	48	1336.078821	0.222	-75	1106.853430	-0.115
-22	1233.531777	-0.014	49	1337.094261	0.066	-74	1109.266112	-0.002

Table 1(b) – Continued

m	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)
-73	1111.669942	0.849	-4	1252.631335	-0.260	66	1338.509755	0.933
-72	1114.064908	2.455	-3	1254.289132	-0.126	67	1339.264921	0.181
-71	1116.447059	0.892	-2	1255.935585	0.411	68	1340.006451	-0.125
-70	1118.819640	-0.565	-1	1257.570001	0.693	69	1340.734724	0.427
-69	1121.184978	0.438	2	1262.401087	0.381	70	1341.448005	0.140
-68	1123.539473	0.331	3	1263.987280	-0.117	71	1342.147763	0.515
-67	1125.883686	-0.297	4	1265.562468	0.322	72	1342.832514	0.105
-66	1128.219984	0.950	5	1267.124831	-0.091	73	1343.502953	-0.360
-65	1130.544330	0.064	6	1268.675407	-0.284	74	1344.159599	-0.326
-64	1132.859691	0.040	7	1270.214099	-0.324	75	1344.802439	0.230
-63	1135.165248	0.089	8	1271.740947	-0.136	76	1345.430152	0.021
-62	1137.461242	0.481	9	1273.255401	-0.240	77	1346.044248	0.593
-61	1139.746870	0.442	10	1274.757540	-0.523	78	1346.642938	0.194
-60	1142.022393	0.262	11	1276.248067	-0.251	79	1347.226952	-0.413
-59	1144.288041	0.200	12	1277.726328	-0.044	80	1347.798318	0.838
-58	1146.543892	0.364	13	1279.192046	-0.147	81	1348.352283	-0.771
-57	1148.789537	0.373	14	1280.645605	-0.144	82	1348.894780	0.729
-56	1151.025070	0.352	15	1282.087724	0.718	83	1349.420920	0.484
-55	1153.250329	0.169	16	1283.515858	-0.075	84	1349.931780	-0.392
-54	1155.465161	-0.302	17	1284.932114	-0.383	85	1350.429295	0.072
-53	1157.670601	0.006	18	1286.335012	-1.653	86	1350.911505	-0.048
-52	1159.865745	0.218	19	1287.728181	-0.222	87	1351.379506	0.380
-51	1162.050330	0.100	20	1289.107564	-0.116	88	1351.831989	0.084
-50	1164.224664	-0.009	21	1290.474286	-0.177	90	1352.694797	1.861
-49	1166.388768	-0.058	22	1291.828574	-0.145	91	1353.100756	-0.359
-48	1168.544387	1.726	23	1293.170097	-0.317	92	1353.494512	0.158
-47	1170.686366	0.220	24	1294.499444	-0.073	93	1353.873285	0.669
-46	1172.819479	0.228	25	1295.815902	-0.091	94	1354.236695	0.831
-45	1174.941990	0.042	26	1297.119689	-0.122	95	1354.586487	2.426
-44	1177.053659	-0.545	27	1298.410107	-0.830	96	1354.919167	1.997
-43	1179.155820	-0.171	28	1299.688753	-0.584	97	1355.235624	0.469
-42	1181.247421	0.143	29	1300.954795	-0.185	98	1355.537824	-0.152
-41	1183.328317	0.283	30	1302.207547	-0.284	99	1355.824000	-1.598
-40	1185.398614	0.384	31	1303.447815	-0.043	100	1356.098166	0.184
-39	1187.457622	-0.212	32	1304.675200	0.172	102	1356.595699	-1.187
-38	1189.507101	0.285	33	1305.889271	-0.036	104	1357.035777	1.391
-37	1191.545025	-0.122	34	1307.090477	-0.184	105	1357.232948	2.934
-36	1193.572825	0.031	35	1308.278943	-0.115	106	1357.411005	0.828
-35	1195.589570	-0.158	36	1309.454316	-0.148	107	1357.573943	-0.893
-34	1197.595918	0	37	1310.616951	0.104	108	1357.723374	-0.578
-33	1199.591274	-0.059	38	1311.767027	0.856	112	1358.162735	-1.481
-32	1201.575784	-0.159	39	1312.900488	-1.917	113	1358.234759	-0.278
-31	1203.549825	0.109	40	1314.025520	0.006	114	1358.290318	0.238
-30	1205.512547	-0.075	41	1315.135406	-0.059			
-29	1207.464504	-0.125	42	1316.232179	-0.045	*v* = 3–2		
-28	1209.405649	-0.059	43	1317.315791	0.033	-104	1021.100965	0.940
-27	1211.335731	-0.095	44	1318.386128	0.096	-103	1023.770660	3.130
-26	1213.254793	-0.160	45	1319.442769	-0.246	-102	1026.425647	-0.569
-25	1215.163219	0.161	46	1320.486801	0.131	-99	1034.349637	0.526
-24	1217.059928	-0.181	47	1321.517315	0.350	-98	1036.970870	-1.400
-23	1218.945970	-0.106	48	1322.533514	-0.353	-97	1039.588652	2.170
-22	1220.820952	0.025	49	1323.537329	-0.011	-96	1042.190861	-0.861
-21	1222.684638	0.008	50	1324.527304	-0.047	-92	1052.522062	-0.373
-20	1224.537054	-0.102	51	1325.505267	1.401	-91	1055.082204	-0.217
-19	1226.378470	-0.001	52	1326.466758	-0.093	-90	1057.634914	1.638
-18	1228.208593	0.048	53	1327.416559	0.287	-89	1060.177309	2.335
-17	1230.027277	-0.070	54	1328.349945	-2.150	-87	1065.230490	-0.303
-16	1231.834804	-0.041	55	1329.274482	0.196	-86	1067.745961	1.102
-15	1233.631167	0.160	56	1330.182988	0.178	-85	1070.250288	0.627
-13	1237.189006	-0.193	57	1331.077771	0.138	-84	1072.747004	1.833
-12	1238.951041	-0.124	58	1331.958816	0.095	-83	1075.233680	2.319
-11	1240.701484	-0.185	59	1332.826034	-0.005	-82	1077.707721	-0.485
-10	1242.440398	-0.281	60	1333.679540	-0.014	-81	1080.176727	1.051
-9	1244.169420	1.256	61	1334.519101	-0.129	-80	1082.635598	1.853
-8	1245.884430	0.338	62	1335.345161	0.128	-79	1085.082028	-0.356
-7	1247.588082	-0.349	63	1336.156802	-0.126	-78	1087.522511	0.944
-6	1249.281139	-0.010	64	1336.955133	0.252	-77	1089.951637	0.372
-5	1250.962713	0.499	65	1337.739001	0.144	-76	1092.374129	2.678

Table 1(b) – Continued

m	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)
-75	1094.781896	-0.200	-7	1234.722235	-1.390	72	1329.015826	0.315
-74	1097.183942	0.770	-6	1236.404263	-0.261	73	1329.674625	0.621
-73	1099.573591	-1.061	-5	1238.073796	0.030	74	1330.318479	0.288
-72	1101.956523	0.016	-4	1239.731256	-0.063	75	1330.949001	0.964
-71	1104.330274	1.566	-2	1243.011167	-0.063	76	1331.563339	-0.167
-70	1106.689377	-1.851	2	1249.429099	-0.275	77	1332.165043	0.481
-69	1109.045356	1.318	3	1251.004202	-0.005	78	1332.752685	1.516
-68	1111.387247	0.138	5	1254.118099	0.098	79	1333.325402	2.110
-67	1113.720766	0.353	6	1255.656954	0.056	80	1333.881336	0.441
-66	1116.044463	0.543	7	1257.184698	0.945	81	1334.424226	0.285
-65	1118.358048	0.444	8	1258.698397	-0.135	82	1334.950965	-1.430
-64	1120.661933	0.500	9	1260.201674	0.471	83	1335.466846	0.626
-63	1122.955601	0.221	10	1261.691715	-0.019	84	1335.967317	1.937
-62	1125.240213	0.797	11	1263.169766	-0.326	85	1336.449787	-0.051
-61	1127.514042	0.531	12	1264.637504	1.259	86	1336.920985	1.426
-60	1129.777999	0.362	13	1266.090349	0.189	87	1337.376522	2.017
-59	1132.031835	0.071	14	1267.531968	0.164	88	1337.815182	0.543
-58	1134.275512	-0.351	15	1268.961030	-0.115	89	1338.241686	1.760
-57	1136.510435	0.531	16	1270.378545	0.395	90	1338.652162	1.835
-56	1138.734010	0.151	18	1273.173793	-1.229	91	1339.045453	-0.354
-55	1140.947940	0.243	19	1274.555051	0.228	92	1339.424886	-1.442
-54	1143.151848	0.458	20	1275.922025	-0.132	93	1339.791141	-0.712
-53	1145.344323	-0.584	21	1277.276872	-0.118	94	1340.141797	-0.547
-52	1147.528532	0.312	22	1278.619244	-0.047	96	1340.797719	-0.359
-51	1149.703415	2.117	23	1279.948622	-0.404	98	1341.395037	1.810
-50	1151.864240	0.129	24	1281.266224	0.061	99	1341.669793	1.804
-49	1154.016910	0.280	25	1282.570745	0.078	100	1341.929683	2.192
-48	1156.158861	0.036	26	1283.861721	-0.786	101	1342.171316	-0.380
-47	1158.290774	0.108	27	1285.141341	-0.307			
-46	1160.411992	-0.131	28	1286.407073	-0.985	*v* = 4–3		
-45	1162.523469	0.303	29	1287.661903	0.199	-85	1058.31579	1.134
-44	1164.623712	-0.053	30	1288.902907	0.355	-84	1060.800251	1.479
-43	1166.714124	0.235	31	1290.130361	-0.209	-83	1063.274436	0.876
-42	1168.793505	-0.003	32	1291.345755	0.032	-82	1065.737137	-1.856
-41	1170.862778	0.185	33	1292.547986	0.008	-81	1068.194573	-0.472
-40	1172.921265	0.153	34	1293.737150	-0.153	-80	1070.642482	0.794
-39	1174.968970	-0.065	35	1294.913430	-0.234	-79	1073.081247	2.354
-38	1177.006593	0.260	36	1296.076933	-0.093	-78	1075.508463	1.829
-37	1179.033369	0.395	37	1297.227177	-0.180	-77	1077.926665	1.782
-36	1181.048623	-0.304	38	1298.364761	0.137	-76	1080.331686	-1.926
-35	1183.054353	0.190	39	1299.488711	-0.081	-75	1082.733488	0.694
-34	1185.048864	0.213	40	1300.599810	-0.018	-74	1085.122546	0.147
-33	1187.033087	0.728	42	1302.782684	0.315	-73	1087.501862	-0.539
-32	1189.005377	0.119	43	1303.853999	0.193	-72	1089.874145	1.374
-31	1190.967529	0.213	44	1304.911922	-0.054	-71	1092.235506	2.026
-30	1192.918820	0.318	45	1305.956859	0.013	-69	1096.925031	-0.775
-29	1194.858787	0.001	46	1306.988159	-0.221	-68	1099.254834	-2.531
-28	1196.788302	0.165	47	1308.006383	-0.163	-67	1101.580591	1.440
-27	1198.706772	0.249	48	1309.011170	-0.139	-66	1103.891373	0.239
-26	1200.613120	-0.794	49	1310.002683	0.047	-65	1106.191712	-1.574
-25	1202.510274	-0.004	50	1310.980664	0.173	-64	1108.486627	1.048
-24	1204.396182	0.597	51	1311.944791	-0.050	-63	1110.768537	0.555
-23	1206.269418	-0.386	53	1313.833053	0.163	-62	1113.040819	0.350
-22	1208.133702	0.800	54	1314.757763	1.243	-61	1115.302450	-0.558
-21	1209.984960	0.111	55	1315.666469	-0.039	-60	1117.556204	0.632
-20	1211.826115	0.502	56	1316.563032	0.213	-59	1119.798646	0.514
-19	1213.655266	0.102	57	1317.445505	0.085	-58	1122.031538	0.880
-18	1215.473459	-0.011	58	1318.313023	-1.252	-57	1124.253139	0.019
-17	1217.280649	0.151	59	1319.169152	-0.198	-56	1126.465443	-0.048
-16	1219.076312	0.093	60	1320.011124	0.514	-55	1128.668670	0.931
-15	1220.859767	-0.833	61	1320.837847	-0.174	-54	1130.861868	2.031
-14	1222.632619	-0.991	63	1322.451529	0.373	-53	1133.041927	0.174
-13	1224.395122	-0.095	64	1323.236834	0.024	-52	1135.213894	0.435
-12	1226.144885	-0.504	65	1324.008818	0.342	-51	1137.375537	0.612
-11	1227.884875	0.780	66	1324.766178	0.059	-50	1139.527276	1.154
-10	1229.611199	-0.105	68	1326.239049	-0.143	-49	1141.667655	0.636
-9	1231.327199	0.216	69	1326.954398	-0.156	-48	1143.798158	0.571
-8	1233.031177	0.077	70	1327.656472	0.721	-47	1145.917539	-0.256

Table 1(b) – Continued

m	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)
-45	1150.127681	0.666	28	1273.149486	0.217	-82	1053.792332	0.797
-44	1152.216280	0.314	29	1274.390930	0.028	-81	1056.237343	1.147
-42	1156.362512	0.113	30	1275.619743	0.013	-80	1058.671662	0.223
-41	1158.420132	0.310	31	1276.835960	0.239	-79	1061.097380	0.142
-40	1160.467084	0.410	32	1278.037691	-1.149	-78	1063.515491	1.927
-39	1162.503198	0.272	33	1279.229111	0.056	-76	1068.319982	2.295
-38	1164.528526	-0.020	34	1280.406428	0.096	-74	1073.081137	-2.451
-37	1166.542109	-1.397	35	1281.570442	-0.194	-72	1077.811942	0.898
-35	1170.541629	0.310	36	1282.722108	0.172	-71	1080.159711	-0.573
-34	1172.523957	-0.154	37	1283.861720	1.523	-70	1082.499285	-0.545
-33	1174.496040	-0.080	38	1284.985177	-0.208	-68	1087.150441	0.721
-32	1176.458062	0.748	39	1286.097563	0.097	-67	1089.459128	-0.880
-31	1178.408119	0.456	40	1287.196174	-0.234	-66	1091.762883	2.396
-30	1180.347231	0.096	41	1288.282549	0.374	-65	1094.052446	1.318
-29	1182.275841	0.140	43	1290.413209	-0.844	-63	1098.604124	1.342
-28	1184.194117	0.788	44	1291.459313	-0.783	-62	1100.864495	0.757
-27	1186.099836	-0.153	45	1292.492635	-0.194	-61	1103.115350	0.610
-26	1187.996418	0.770	46	1293.512685	0.467	-60	1105.357773	2.012
-25	1189.880220	-0.057	47	1294.518995	0.765	-59	1107.587543	0.772
-24	1191.753911	0.068	48	1295.511316	0.487	-58	1109.809037	1.297
-23	1193.616490	0.173	49	1296.489292	-0.691	-57	1112.019041	0.400
-22	1195.468028	0.363	50	1297.456281	0.625	-56	1114.221055	1.612
-21	1197.308511	0.652	51	1298.410107	2.293	-55	1116.409654	-0.463
-20	1199.137104	0.239	52	1299.346616	0.193	-54	1118.591410	0.775
-19	1200.954576	-0.077	53	1300.270889	-0.560	-53	1120.761340	0.375
-18	1202.761123	-0.069	54	1301.182637	-0.220	-52	1122.921627	0.547
-17	1204.557518	1.069	55	1302.078838	-1.775	-51	1125.071282	0.334
-16	1206.340167	-0.226	56	1302.964731	0.050	-50	1127.211012	0.470
-15	1208.113548	0.554	57	1303.834894	-0.134	-49	1129.341552	1.722
-14	1209.873661	-0.558	59	1305.534647	0.228	-48	1131.45935	0.567
-13	1211.624105	0.069	60	1306.363699	0.307	-47	1133.567564	0.192
-12	1213.362229	-0.186	61	1307.178579	0.074	-46	1135.666268	0.702
-11	1215.089006	-0.317	62	1307.979799	0.077	-45	1137.753243	-0.093
-10	1216.804550	-0.179	63	1308.767455	0.446	-44	1139.831129	0.478
-9	1218.507555	-1.045	64	1309.539416	-0.913	-43	1141.897601	0.120
-8	1220.201243	0.337	65	1310.299884	0.235	-42	1143.954864	1.068
-7	1221.882680	1.067	66	1311.045336	0.403	-41	1145.999968	0.401
-6	1223.553070	2.379	68	1312.492991	-0.260	-39	1150.060127	0.776
-5	1225.209620	1.512	69	1313.197289	1.074	-38	1152.074194	0.889
-4	1226.855184	1.354	70	1313.885349	0.348	-37	1154.076850	0.258
-3	1228.490213	2.386	71	1314.559855	0.281	-36	1156.069904	0.722
-2	1230.109636	-0.431	72	1315.219225	-0.673	-35	1158.052726	1.681
-1	1231.719037	-1.479	73	1315.866618	0.680	-34	1160.023224	1.074
2	1236.481686	0.882	75	1317.115293	0.271	-33	1161.982622	0.156
3	1238.043654	-0.118	76	1317.718849	0.855	-31	1165.871214	0.605
4	1239.596890	2.100	80	1319.986575	1.333	-29	1169.715799	0.571
5	1241.132581	-1.243	83	1321.531488	-1.302	-28	1171.620869	-0.270
6	1242.661801	0.958	84	1322.019007	-0.317	-27	1173.516654	0.577
8	1245.678871	0.168	85	1322.491426	0.288	-26	1175.399260	-0.749
9	1247.169530	0.050	86	1322.946315	-1.882	-25	1177.273530	0.624
10	1248.648516	0.405	87	1323.390961	0.498	-24	1179.135420	0.683
11	1250.114660	0.095	88	1323.819191	1.292	-23	1180.986261	0.792
12	1251.569800	0.993	90	1324.626380	-1.754	-22	1182.825668	0.596
13	1253.011575	0.769	91	1325.013206	2.348	-21	1184.652929	-0.585
14	1254.440241	-0.289	92	1325.378726	0.123	-20	1186.470914	0.149
15	1255.858218	0.274	96	1326.701582	2.537	-19	1188.276287	-0.506
16	1257.262386	-0.631	97	1326.993640	2.309	-18	1190.071527	-0.039
17	1258.656486	0.771	98	1327.269429	1.017	-17	1191.855553	0.500
18	1260.036494	0.488	100	1327.778048	1.245	-15	1195.388784	0.740
19	1261.403868	0.010				-14	1197.137822	0.338
20	1262.758926	-0.310	v = 5–4			-13	1198.875980	0.467
21	1264.103178	1.070	-95	1021.167707	1.483	-11	1202.317644	0.438
22	1265.430877	-1.564	-93	1026.287881	1.444	-10	1204.021104	0.296
23	1266.750885	0.683	-92	1028.831314	-1.598	-9	1205.712621	-0.250
24	1268.055376	0.018	-91	1031.372639	2.375	-8	1207.394320	0.958
25	1269.348263	0.387	-89	1036.417746	0.251	-7	1209.062538	0.287
26	1270.627878	0.155	-87	1041.426916	-1.001	-5	1212.366412	1.319
27	1271.894896	0.031	-84	1048.871704	-2.365	-4	1213.997542	-1.440

Table 1(b) – Continued

m	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)
2	1223.554343	-0.503	76	1303.892674	-0.641	-15	1182.687734	2.223
4	1226.645285	0.198	77	1304.470067	0.768	-14	1184.424086	0.919
5	1228.173065	0.825	79	1305.578786	0.998	-13	1186.148720	-0.686
6	1229.687969	0.596	80	1306.109830	-0.391	-9	1192.940950	1.395
7	1231.188091	-2.361	81	1306.628751	0.687	-8	1194.606045	-2.186
8	1232.680353	-1.092	84	1308.092584	-1.101	4	1213.717231	-0.510
9	1234.161208	0.889	85	1308.554041	1.241	5	1215.230646	-2.360
10	1235.627556	0.514	87	1309.426579	-0.089	6	1216.735909	-0.336
11	1237.082653	1.072	89	1310.239607	-1.532	12	1225.500351	-0.936
12	1238.523925	0.021				13	1226.918037	-1.387
13	1239.953457	-0.520	*v* = 6–5			16	1231.100275	0.302
14	1241.373314	1.545	-79	1049.137636	0.546	17	1232.469223	0.464
15	1242.778335	1.089	-78	1051.542502	0.472	19	1235.169558	0.520
16	1244.169420	-0.955	-77	1053.939924	2.463	20	1236.500707	0.242
17	1245.551466	0.343	-76	1056.324932	1.576	21	1237.819388	0.016
18	1246.919862	0.403	-75	1058.700096	0.409	22	1239.124778	-0.949
19	1248.275100	-0.248	-74	1061.069399	2.973	23	1240.421808	2.312
20	1249.618111	-0.646	-73	1063.425392	1.846	24	1241.700505	-0.141
21	1250.950746	1.092	-72	1065.771244	0.225	25	1242.969818	0.675
22	1252.268012	0.006	-71	1068.110798	1.982	26	1244.224971	0.016
23	1253.573437	-0.341	-70	1070.438028	1.118	27	1245.469074	1.026
24	1254.867246	0.307	-68	1075.064905	1.030	28	1246.698667	0.279
25	1256.147848	0.393	-66	1079.651629	-0.058	29	1247.915976	0.034
26	1257.415914	0.621	-65	1081.931779	0.939	30	1249.122069	1.393
27	1258.671681	1.262	-64	1084.201895	1.776	31	1250.314542	1.984
28	1259.91320	0.400	-62	1088.708070	-0.871	32	1251.491872	0.320
29	1261.142552	0.149	-61	1090.948633	0.206	33	1252.658179	0.553
30	1262.358478	-0.716	-59	1095.398385	0.982	34	1253.810674	-0.071
31	1263.562444	-0.696	-58	1097.606470	-0.366	35	1254.950095	-0.781
33	1265.932689	0.327	-57	1099.810062	3.869	36	1256.079345	1.359
34	1267.095931	-1.639	-56	1101.996795	1.350	38	1258.293002	-0.001
35	1268.249921	0.122	-55	1104.174560	-0.002	39	1259.380680	-0.163
36	1269.388756	-0.259	-54	1106.343525	0.008	40	1260.456875	1.350
37	1270.516007	0.824	-53	1108.505030	2.752	41	1261.518027	1.012
38	1271.628714	0.443	-52	1110.650322	-0.495	42	1262.567318	2.039
39	1272.728750	0.506	-51	1112.790821	1.717	43	1263.602367	2.084
40	1273.815379	0.311	-50	1114.916224	-0.885	45	1265.630493	0.119
41	1274.888781	0.071	-49	1117.035395	0.591	46	1266.626226	0.835
42	1275.948902	-0.233	-48	1119.142503	0.346	47	1267.606646	-0.365
43	1276.995262	-1.047	-47	1121.240286	1.146	48	1268.576780	1.581
45	1279.050639	-0.131	-46	1123.325931	0.209	49	1269.531939	2.019
46	1280.059741	1.754	-45	1125.401394	-0.480	51	1271.398366	-0.458
47	1281.052378	0.561	-44	1127.468524	0.958	52	1272.312392	-0.545
48	1282.032340	0.114	-43	1129.522703	-0.064	53	1273.212980	-0.465
49	1282.998816	-0.362	-42	1131.568293	0.846	55	1274.973745	0.239
50	1283.952350	-0.290	-41	1133.602352	0.775	56	1275.833621	0.632
51	1284.892524	-0.054	-40	1135.625320	0.194	57	1276.678371	-0.355
52	1285.819549	0.594	-39	1137.638861	0.797	58	1277.511586	0.902
53	1286.732047	0.308	-38	1139.639856	-0.504	59	1278.328768	-0.058
54	1287.631024	0.130	-37	1141.631045	-0.939	60	1279.134760	1.643
55	1288.517085	0.700	-36	1143.613419	0.513	61	1279.925106	1.583
56	1289.388373	0.194	-35	1145.586222	3.127	62	1280.702361	2.354
57	1290.247333	1.094	-34	1147.543942	1.421	63	1281.464010	1.475
58	1291.090675	0.144	-33	1149.490707	-0.446	64	1282.211364	0.294
59	1291.920835	-0.186	-32	1151.428578	-0.381	65	1282.947960	2.382
60	1292.738322	0.649	-30	1155.272308	0.332	67	1284.373168	0.801
61	1293.541016	0.565	-29	1157.177298	0.174	68	1285.063789	-0.788
62	1294.329346	0.024	-28	1159.071557	0.233	70	1286.407074	0.625
63	1295.104216	-0.034	-27	1160.954637	0.092	71	1287.057352	1.314
64	1295.865288	0.090	-26	1162.826645	-0.112	72	1287.690586	-0.762
65	1296.613709	1.576	-25	1164.689707	1.780	73	1288.314419	2.076
66	1297.345267	0.248	-23	1168.378173	1.153	75	1289.512350	1.108
67	1298.063846	0.026	-22	1170.204970	0.089	76	1290.087810	-1.263
68	1298.768892	0.392	-21	1172.020927	-0.649			
71	1300.799524	2.062	-20	1173.827315	0.241	*v* = 7–6		
72	1301.447736	2.433	-19	1175.621472	0.129	-64	1072.087367	-2.471
73	1302.078837	-0.009	-18	1177.406670	2.317	-63	1074.336198	-1.538
75	1303.304780	1.892	-17	1179.175132	-0.940	-62	1076.577910	2.215

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Table 1(b) – Continued

m	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)	*m*	obs.	10^3(o−c)
-61	1078.801856	-1.831	-25	1152.126067	1.064	23	1227.288223	1.223
-59	1083.230612	0.959	-24	1153.959817	-3.557	25	1229.814996	2.413
-58	1085.425434	-2.136	-23	1155.790672	0.035	26	1231.059044	2.694
-57	1087.614626	-0.778	-22	1157.610418	3.659	27	1232.287442	0.051
-56	1089.794115	0.990	-21	1159.411649	-0.061	28	1233.505871	0.201
-55	1091.962856	2.150	-20	1161.206031	0.573	29	1234.709387	-1.768
-54	1094.116756	-1.360	-19	1162.988091	0.118	30	1235.899649	-4.163
-53	1096.267037	1.711	-18	1164.758312	-0.910	31	1237.082870	-0.737
-51	1100.530376	1.346	-16	1168.270092	2.293	32	1238.251562	1.055
-50	1102.644701	-0.764	-15	1170.002979	-2.084	33	1239.403606	-0.871
-47	1108.932458	-0.285	-14	1171.733027	2.091	34	1240.545590	0.106
-46	1111.007438	-0.291	-13	1173.446271	0.885	35	1241.674929	1.435
-45	1113.072651	0.374	-12	1175.148069	-0.312	37	1243.891547	1.161
-44	1115.121080	-5.279	-11	1176.836843	-3.047	38	1244.978617	-0.584
-43	1117.172098	2.153	-10	1178.520539	0.659	39	1246.054807	-0.074
-42	1119.202821	-0.182	-9	1180.182830	-5.491	40	1247.117761	0.366
-41	1121.224694	-0.811	-7	1183.487754	-2.670	41	1248.165001	-1.705
-40	1123.239365	1.945	8	1206.751021	-2.543	42	1249.202502	-0.279
-39	1125.240211	1.493	9	1208.209033	0.428	43	1250.226203	0.617
-38	1127.231663	2.295	10	1209.650197	-1.285	44	1251.233955	-1.130
-37	1129.208706	-0.634	11	1211.080695	-1.467	45	1252.231751	0.505
-36	1131.178542	-0.062	12	1212.501035	0.422	46	1253.213513	-0.519
-35	1133.138337	1.208	13	1213.908292	1.490	47	1254.183213	-0.197
-34	1135.086389	1.504	14	1215.301867	1.172	48	1255.136934	-2.410
-33	1137.022456	0.615	15	1216.680436	-1.825	49	1256.079357	-2.444
-32	1138.950370	2.404	16	1218.053593	2.128	50	1257.011057	0.312
-31	1140.860941	-2.290	17	1219.409800	1.525	51	1257.926130	-0.011
-30	1142.765958	-1.645	18	1220.750577	-2.081	52	1258.828796	0.841
-29	1144.664118	3.066	19	1222.081916	-2.664	53	1259.715777	-0.374
-28	1146.543894	0.346	20	1223.404791	0.783	54	1260.592112	1.417
-27	1148.413317	-1.742	21	1224.711845	0.935	56	1262.300604	1.919
-26	1150.275884	0.330	22	1226.007849	2.597	57	1263.133788	1.727

Table 2 Molecular parameters of CS

Parameters	Fit 1	Fit 2	Ref. [17][a]	
			Unconstrained	Constrained
$U_\omega (= U_{10})$ /cm^{-1} u$^{1/2}$	3796.05431(417)[b]	3796.05328(404)	3796.06354(407)	3796.08507(446)
$U_B (= U_{01})$ /cm^{-1} u	7.15616586(384)	7.15616657(345)	7.15620308(936)	7.1560789(101)
a_1	−2.8848755(652)	−2.8849146(408)		
a_2	5.118402(544)	5.118730(185)		
a_3	−7.10501(275)	−7.105680(744)		
a_4	8.4363(215)	8.4487(113)		
a_5	−8.723(131)	−8.8475(774)		
a_6	8.785(430)	8.702(270)		
a_7	−21.98(178)	−14.77(200)		
a_8	75.5(112)	26.4(114)		
a_9	46.7(287)	193.1(261)		
$\Delta_\omega^{\mathrm{C}}$	0.7766(132)	0.7766(130)	0.7598(139)	0.7013(157)
$\Delta_\omega^{\mathrm{S}}$	−0.6250(470)	−0.6033(441)	−0.7108(419)	−0.8962(473)
Δ_B^{C}	−2.54790(829)	−2.55180(698)	−2.5419(179)	−2.3627(204)
Δ_B^{S}	−2.3635(247)	−2.3584(199)	−2.6731(481)	−2.1228(541)
$\Delta_{a1q}^{\mathrm{C}}$	0.260(557)	0.109(199)		
$\Delta_{a1q}^{\mathrm{S}}$	1.07(133)	1.683(607)		
$\Delta_{a2q}^{\mathrm{C}}$	−3.05(210)	−3.751(635)		
$\Delta_{a2q}^{\mathrm{S}}$	−1.07(411)	0.0[c]		
r_{1q}^{C} $(=r_{1q}^{\mathrm{S}})$	−2.332(133)	−2.391(117)		
r_{2q}^{C} $(=r_{2q}^{\mathrm{S}})$	−2.42(432)	0.0[c]		
r_{3q}^{C} $(=r_{3q}^{\mathrm{S}})$	6.2(168)	0.0[c]		
Reduced standard deviation	1.3796	1.3789		

[a]Only molecular parameters that can be compared are listed.
[b]The uncertainty (one standard error) in the last digits is given in parentheses.
[c]Fixed.

Table 3 Values of Dunham coefficients Y_{ij}/cm^{-1} for 12 isotopologues of CS back-calculated from 22 molecular parameters given by Fit 1 in Table 2.

Coeff.	$^{12}C^{32}S$	$^{12}C^{32}S^{a}$	$^{12}C^{32}S^{b}$	$^{12}C^{33}S$	$^{12}C^{34}S$
Y_{10}	1285.1543857(718)^{c}	1285.1545523(663)	1285.15464(10)	1279.8285003(653)	1274.8102411(722)
Y_{20}	-6.5023054(415)	-6.5024378(359)	-6.502605(53)	-6.4485101(417)	-6.3980266(438)
$10^2 Y_{30}$	0.37782(114)	0.381860(937)	0.38873(94)	0.37315(113)	0.36877(111)
$10^5 Y_{40}$	0.739(160)	0.225(131)	-0.853(54)	0.727(157)	0.716(155)
$10^6 Y_{50}$	-0.7759(833)	-0.5457(705)		-0.7600(816)	-0.7452(800)
Y_{01}	0.8200433747(207)	0.8200433819(166)	0.820043559(42)	0.8132611415(175)	0.8068964187(196)
$10^2 Y_{11}$	-0.59184849(168)	-0.59184902(122)	-0.5918345(49)	-0.58452054(160)	-0.57767144(177)
$10^6 Y_{21}$	-0.90190(504)	-0.90049(393)	-0.983(13)	-0.88687(490)	-0.87288(488)
$10^7 Y_{31}$	-0.27401(580)	-0.27541(473)	-0.124(12)	-0.26838(568)	-0.26316(557)
$10^{10} Y_{41}$	-0.635(272)	-0.580(229)	-11.05(36)	-0.620(265)	-0.605(259)
$10^{10} Y_{51}$	-0.24048(442)	-0.24121(381)		-0.23359(429)	-0.22726(418)
$10^5 Y_{02}$	-0.13357485(112)	-0.133575311(982)	-0.1335514(65)	-0.13137441(109)	-0.12932606(106)
$10^8 Y_{12}$	-0.132424(148)	-0.1324460(375)	-0.13110(76)	-0.129695(145)	-0.127164(143)
$10^{10} Y_{22}$	-0.38866(434)	-0.38221(289)	-0.381(15)	-0.37910(423)	-0.37027(414)
$10^{13} Y_{32}$	0.222(490)	-1.358(427)	-6.4(12)	0.216(476)	0.210(463)
$10^{13} Y_{42}$	-0.3999(364)	-0.3041(319)		-0.3868(352)	-0.3748(341)
$10^{12} Y_{03}$	0.250095(406)	0.2503226(253)	0.2068(56)	0.243945(391)	0.238267(378)
$10^{13} Y_{13}$	-0.165443(421)	-0.165490(120)	-0.1969(47)	-0.160700(404)	-0.156338(389)
$10^{15} Y_{23}$	-0.23555(436)	-0.24143(308)		-0.22786(422)	-0.22081(409)
$10^{17} Y_{33}$	-0.6120(562)	-0.4301(435)		-0.5895(542)	-0.5690(523)
$10^{19} Y_{43}$	0.839(485)	-0.397(417)		0.805(466)	0.774(448)
$10^{17} Y_{04}$	-0.228252(226)	-0.2283448(161)		-0.220792(216)	-0.213959(206)
$10^{19} Y_{14}$	-0.73102(729)	-0.72231(463)		-0.70421(702)	-0.67974(678)
$10^{21} Y_{24}$	-0.648(127)	-1.090(121)		-0.621(122)	-0.597(117)
$10^{21} Y_{34}$	-0.1942(142)	-0.1630(127)		-0.1855(136)	-0.1776(130)
$10^{23} Y_{05}$	-0.47550(121)	-0.475708(214)		-0.45615(114)	-0.43857(109)
$10^{24} Y_{15}$	-0.34539(477)	-0.35134(312)		-0.32997(456)	-0.31602(437)
$10^{25} Y_{25}$	-0.1956(136)	-0.1478(114)		-0.1861(129)	-0.1776(123)
$10^{27} Y_{35}$	0.927(218)	0.417(190)		0.878(206)	0.834(196)
$10^{28} Y_{06}$	-0.247788(903)	-0.246516(585)		-0.235744(859)	-0.224889(820)
$10^{29} Y_{16}$	-0.14572(638)	-0.16892(632)		-0.13807(604)	-0.13119(574)
$10^{30} Y_{26}$	-0.2451(131)	-0.2244(116)		-0.2312(124)	-0.2188(117)
$10^{33} Y_{07}$	-0.104102(417)	-0.104474(274)		-0.098223(393)	-0.092967(372)
$10^{34} Y_{17}$	-0.14341(503)	-0.12515(434)		-0.13475(472)	-0.12704(445)
$10^{36} Y_{27}$	0.653(195)	0.232(171)		0.611(183)	0.574(171)
$10^{39} Y_{08}$	-0.48425(471)	-0.50100(450)		-0.45312(441)	-0.42552(414)
$10^{39} Y_{18}$	-0.11150(349)	-0.10685(308)		-0.10390(325)	-0.09719(304)
$10^{44} Y_{09}$	-0.27469(178)	-0.26778(154)		-0.25491(165)	-0.23751(154)
$10^{45} Y_{19}$	-0.1209(382)	-0.1984(335)		-0.1117(353)	-0.1037(328)
$10^{49} Y_{010}$	-0.16047(149)	-0.15836(133)		-0.14768(137)	-0.13652(127)
$10^{55} Y_{011}$	-0.7427(100)	-0.76205(864)		-0.67789(918)	-0.62177(842)
Y_{00}	0.081076(180)	0.0811365(711)		0.080405(178)	0.079776(177)

Table 3 – Continued

Coeff.	$^{12}C^{36}S$	$^{13}C^{32}S$	$^{13}C^{33}S$	$^{13}C^{34}S$	$^{13}C^{36}S$
Y_{10}	1265.528130(106)	1248.5795836(695)	1243.0970131(701)	1237.9298672(816)	1228.369112(118)
Y_{20}	-6.3051723(512)	-6.1374715(377)	-6.0836770(384)	-6.0331943(408)	-5.9403414(484)
$10^2 Y_{30}$	0.36078(109)	0.34648(105)	0.34194(103)	0.33769(102)	0.32993(100)
$10^5 Y_{40}$	0.695(150)	0.659(142)	0.647(140)	0.636(138)	0.617(133)
$10^6 Y_{50}$	-0.7185(771)	-0.6717(721)	-0.6571(705)	-0.6435(691)	-0.6190(664)
Y_{01}	0.7951896811(318)	0.7740427358(255)	0.7672603846(226)	0.7608955510(235)	0.7491886098(325)
$10^2 Y_{11}$	-0.56514430(243)	-0.54275409(229)	-0.53563543(201)	-0.52898355(190)	-0.51682127(211)
$10^6 Y_{21}$	-0.84744(508)	-0.80027(563)	-0.78615(529)	-0.77302(504)	-0.74916(480)
$10^7 Y_{31}$	-0.25372(537)	-0.23719(502)	-0.23203(491)	-0.22725(481)	-0.21861(462)
$10^{10} Y_{41}$	-0.579(248)	-0.534(229)	-0.520(223)	-0.508(217)	-0.484(207)
$10^{10} Y_{51}$	-0.21592(397)	-0.19649(361)	-0.19053(350)	-0.18506(340)	-0.17528(322)
$10^5 Y_{02}$	-0.12560052(102)	-0.119010027(944)	-0.116933497(919)	-0.115001421(897)	-0.111489753(857)
$10^8 Y_{12}$	-0.122588(139)	-0.114578(128)	-0.112077(126)	-0.109760(124)	-0.105575(120)
$10^{10} Y_{22}$	-0.35438(396)	-0.32686(365)	-0.31835(355)	-0.31049(347)	-0.29638(331)
$10^{13} Y_{32}$	0.200(440)	0.182(400)	0.176(388)	0.171(377)	0.162(357)
$10^{13} Y_{42}$	-0.3536(322)	-0.3174(289)	-0.3064(279)	-0.2964(270)	-0.2786(253)
$10^{12} Y_{03}$	0.228054(355)	0.210341(319)	0.204864(307)	0.199811(296)	0.190736(276)
$10^{13} Y_{13}$	-0.148537(364)	-0.135119(354)	-0.131018(338)	-0.127251(324)	-0.120525(301)
$10^{15} Y_{23}$	-0.20827(385)	-0.18699(346)	-0.18052(334)	-0.17460(323)	-0.16410(304)
$10^{17} Y_{33}$	-0.5328(490)	-0.4720(434)	-0.4536(417)	-0.4370(401)	-0.4075(374)
$10^{19} Y_{43}$	0.720(416)	0.629(364)	0.602(348)	0.577(334)	0.534(309)
$10^{17} Y_{04}$	-0.201806(190)	-0.181179(168)	-0.174910(160)	-0.169176(152)	-0.159000(139)
$10^{19} Y_{14}$	-0.63648(635)	-0.56380(562)	-0.54191(540)	-0.52197(520)	-0.48680(485)
$10^{21} Y_{24}$	-0.555(109)	-0.4856(953)	-0.4647(912)	-0.4457(875)	-0.4125(810)
$10^{21} Y_{34}$	-0.1639(120)	-0.1413(103)	-0.13471(989)	-0.12867(945)	-0.11815(868)
$10^{23} Y_{05}$	-0.407662(996)	-0.356179(914)	-0.340841(862)	-0.326931(816)	-0.302535(738)
$10^{24} Y_{15}$	-0.29161(403)	-0.25145(347)	-0.23957(331)	-0.22884(316)	-0.21013(290)
$10^{25} Y_{25}$	-0.1626(113)	-0.13841(965)	-0.13129(916)	-0.12489(871)	-0.11379(794)
$10^{27} Y_{35}$	0.759(178)	0.637(149)	0.601(141)	0.569(134)	0.515(121)
$10^{28} Y_{06}$	-0.206010(751)	-0.175259(639)	-0.166245(606)	-0.158141(576)	-0.144093(525)
$10^{29} Y_{16}$	-0.11930(522)	-0.10014(438)	-0.09457(414)	-0.08958(392)	-0.08100(354)
$10^{30} Y_{26}$	-0.1976(106)	-0.16363(878)	-0.15386(825)	-0.14514(779)	-0.13021(698)
$10^{33} Y_{07}$	-0.083927(336)	-0.069501(278)	-0.065349(262)	-0.061648(247)	-0.055307(221)
$10^{34} Y_{17}$	-0.11385(399)	-0.09302(326)	-0.08708(305)	-0.08180(287)	-0.07282(255)
$10^{36} Y_{27}$	0.510(152)	0.411(123)	0.383(114)	0.359(107)	0.3171(949)
$10^{39} Y_{08}$	-0.37857(368)	-0.30516(297)	-0.28442(277)	-0.26608(259)	-0.23504(228)
$10^{39} Y_{18}$	-0.08584(268)	-0.06827(213)	-0.06335(198)	-0.05902(184)	-0.05173(161)
$10^{44} Y_{09}$	-0.20824(135)	-0.16340(106)	-0.150958(982)	-0.140055(911)	-0.121814(793)
$10^{45} Y_{19}$	-0.0902(285)	-0.0698(221)	-0.0642(203)	-0.0593(187)	-0.0512(162)
$10^{49} Y_{010}$	-0.11796(109)	-0.090104(839)	-0.082513(768)	-0.075918(707)	-0.065015(605)
$10^{55} Y_{011}$	-0.52944(717)	-0.39364(533)	-0.35732(484)	-0.32604(441)	-0.27491(372)
Y_{00}	0.078618(174)	0.076527(170)	0.075856(168)	0.075227(167)	0.074069(164)

Table 3 – Continued

Coeff.	$^{14}C^{32}S$	$^{14}C^{33}S$	$^{14}C^{34}S$	$^{14}C^{36}S$
Y_{10}	1216.4754370(984)	1210.847515(102)	1205.542155(112)	1195.722470(144)
Y_{20}	-5.8259125(373)	-5.7721186(383)	-5.7216366(407)	-5.6287848(479)
$10^2 Y_{30}$	0.320451(972)	0.316024(959)	0.311888(946)	0.304329(923)
$10^5 Y_{40}$	0.593(128)	0.583(126)	0.572(124)	0.554(120)
$10^6 Y_{50}$	-0.5897(633)	-0.5762(618)	-0.5636(605)	-0.5411(581)
Y_{01}	0.7347583270(391)	0.7279758750(369)	0.7216109469(369)	0.7099038316(419)
$10^2 Y_{11}$	-0.50196426(307)	-0.49502934(276)	-0.48855065(255)	-0.47670888(245)
$10^6 Y_{21}$	-0.71858(626)	-0.70523(584)	-0.69282(549)	-0.67029(502)
$10^7 Y_{31}$	-0.20824(440)	-0.20346(430)	-0.19905(421)	-0.19107(404)
$10^{10} Y_{41}$	-0.457(196)	-0.444(190)	-0.433(185)	-0.412(176)
$10^{10} Y_{51}$	-0.16375(301)	-0.15852(291)	-0.15372(282)	-0.14517(267)
$10^5 Y_{02}$	-0.107237072(808)	-0.105266359(786)	-0.103433586(766)	-0.100104569(731)
$10^8 Y_{12}$	-0.100551(114)	-0.098240(111)	-0.096101(109)	-0.092240(106)
$10^{10} Y_{22}$	-0.27958(312)	-0.27191(304)	-0.26484(296)	-0.25216(281)
$10^{13} Y_{32}$	0.151(334)	0.146(323)	0.142(313)	0.134(296)
$10^{13} Y_{42}$	-0.2577(234)	-0.2483(226)	-0.2398(218)	-0.2246(204)
$10^{12} Y_{03}$	0.179925(257)	0.174992(247)	0.170445(237)	0.162288(220)
$10^{13} Y_{13}$	-0.112562(304)	-0.108965(290)	-0.105665(277)	-0.099782(255)
$10^{15} Y_{23}$	-0.15183(281)	-0.14630(271)	-0.14125(261)	-0.13230(245)
$10^{17} Y_{33}$	-0.3734(343)	-0.3581(329)	-0.3442(316)	-0.3198(294)
$10^{19} Y_{43}$	0.485(280)	0.463(267)	0.443(256)	0.408(236)
$10^{17} Y_{04}$	-0.147099(129)	-0.141741(122)	-0.136847(116)	-0.128178(106)
$10^{19} Y_{14}$	-0.44602(445)	-0.42779(426)	-0.41121(410)	-0.38204(381)
$10^{21} Y_{24}$	-0.3743(735)	-0.3573(701)	-0.3420(671)	-0.3151(618)
$10^{21} Y_{34}$	-0.10617(780)	-0.10089(741)	-0.09614(706)	-0.08786(645)
$10^{23} Y_{05}$	-0.274447(710)	-0.262008(668)	-0.250748(630)	-0.231052(566)
$10^{24} Y_{15}$	-0.18882(261)	-0.17943(248)	-0.17097(236)	-0.15626(216)
$10^{25} Y_{25}$	-0.10126(706)	-0.09578(668)	-0.09087(634)	-0.08237(574)
$10^{27} Y_{35}$	0.454(106)	0.427(100)	0.4038(950)	0.3631(854)
$10^{28} Y_{06}$	-0.128228(467)	-0.121289(442)	-0.115064(419)	-0.104308(380)
$10^{29} Y_{16}$	-0.07138(312)	-0.06720(294)	-0.06348(277)	-0.05707(249)
$10^{30} Y_{26}$	-0.11365(610)	-0.10650(571)	-0.10015(537)	-0.08932(479)
$10^{33} Y_{07}$	-0.048270(193)	-0.045237(181)	-0.042540(170)	-0.037938(152)
$10^{34} Y_{17}$	-0.06294(220)	-0.05871(206)	-0.05497(192)	-0.04862(170)
$10^{36} Y_{27}$	0.2714(812)	0.2520(754)	0.2349(703)	0.2061(617)
$10^{39} Y_{08}$	-0.20119(196)	-0.18680(181)	-0.17413(169)	-0.15277(148)
$10^{39} Y_{18}$	-0.04385(137)	-0.04053(126)	-0.03761(117)	-0.03273(102)
$10^{44} Y_{09}$	-0.102261(665)	-0.094073(612)	-0.086925(566)	-0.075026(488)
$10^{45} Y_{19}$	-0.0426(134)	-0.0390(123)	-0.0358(113)	-0.03072(972)
$10^{49} Y_{010}$	-0.053528(498)	-0.048788(454)	-0.044686(416)	-0.037944(353)
$10^{55} Y_{011}$	-0.22199(300)	-0.20046(271)	-0.18200(246)	-0.15203(205)
Y_{00}	0.072643(161)	0.071972(160)	0.071343(158)	0.070185(156)

[a]Back-calculated from parameters given by Fit 2.

[b]Ref. [17].

[c]The uncertainty (one standard error) in the last digit is given in parentheses.

Table 4 Values of ω_e and B_e for 12 isotopologues of CS

Isotopologues	ω_e/cm^{-1}	B_e/cm^{-1}	Isotopologues	ω_e /cm^{-1}	B_e/cm^{-1}
$^{12}C^{32}S$	1285.12351(141)[a]	0.820172689(441)	$^{13}C^{34}S$	1237.90267(136)	0.761006849(409)
$^{12}C^{33}S$	1279.79733(141)	0.813388382(437)	$^{13}C^{36}S$	1228.34142(135)	0.749296599(402)
$^{12}C^{34}S$	1274.77879(140)	0.807021729(433)	$^{14}C^{32}S$	1216.45229(133)	0.734861897(395)
$^{12}C^{36}S$	1265.49619(139)	0.795311478(427)	$^{14}C^{33}S$	1210.82408(133)	0.728077590(391)
$^{13}C^{32}S$	1248.55295(137)	0.774157810(416)	$^{14}C^{34}S$	1205.51845(132)	0.721710937(388)
$^{13}C^{33}S$	1243.07009(136)	0.767373503(412)	$^{14}C^{36}S$	1195.69827(131)	0.710000686(381)

[a]The uncertainty (one standard error) in the last digit is given in parentheses.

Table 5(a) Band parameters (unit cm^{-1}) for $^{12}C^{32}S$ calculated from 42Y_{ij} given in Table 3.

v	G_v	G_v–G_0	B_v	10^6D_v	$10^{13}H_v$	$10^{18}L_v$
0	641.033165(184)[a]	0.0	0.8170839033(224)	1.3364203(112)	2.41763(407)	−2.31926(229)
	641.0332807(709)	0.0	0.8170839082(178)	1.33642491(983)	2.419872(261)	−2.319857(284)
	641.02943		0.817084091	1.336472	2.418	−2.32
			0.817084141(31)	1.336182(65)	1.974(56)	
1	1913.195250(233)	1272.162085(297)	0.8111635250(347)	1.3378224(114)	2.24728(411)	−2.39429(253)
	1913.195375(150)	1272.162094(169)	0.8111635270(264)	1.33782641(986)	2.249411(319)	−2.394800(764)
	1913.19157	1272.16214	0.811163777	1.337877	2.247	−2.39
		1272.162055(43)	0.811163722(43)	1.337566(63)	1.777(53)	
2	3172.386880(410)	2531.353715(449)	0.8052410923(573)	1.3393032(121)	2.07169(402)	−2.47236(302)
	3172.386981(327)	2531.353701(336)	0.8052410932(433)	1.3393064(100)	2.073723(444)	−2.47339(140)
	3172.38327	2531.35384	0.805241383	1.339357	2.071	−2.47
		2531.353665(59)	0.805241221(60)	1.339021(61)	1.568(50)	
3	4418.630881(809)	3777.597715(830)	0.7993164319(914)	1.3408645(136)	1.89054(436)	−2.55465(380)
	4418.630980(674)	3777.597700(679)	0.7993164326(697)	1.3408673(107)	1.892530(615)	−2.55661(227)
	4418.62743	3777.59800	0.799316746	1.340917	1.890	−2.55
		3777.59739(10)	0.799316671(70)	1.340605(62)	1.383(51)	
4	5651.95002(154)	5010.91685(155)	0.793389361(139)	1.3425090(164)	1.70352(460)	−2.64230(492)
	5651.95014(128)	5010.91686(129)	0.793389362(107)	1.3425120(122)	1.705546(967)	−2.64543(342)
	5651.94682	5010.91739	0.793389690	1.342557	1.702	−2.64
		5010.91646(13)	0.793389601(75)	1.342244(61)	1.177(49)	
5	6872.36693(278)	6231.33376(278)	0.787459686(205)	1.3442404(210)	1.51034(497)	−2.73650(645)
	6872.36706(230)	6231.33378(230)	0.787459688(160)	1.3442442(153)	1.51247(143)	−2.74084(494)
	6872.36399	6231.33456	0.787460026	1.344283	1.507	−2.73
		6231.33336(15)	0.787459946(88)	1.344023(68)	1.024(60)	
6	8079.90399(473)	7438.87082(473)	0.781527198(292)	1.3460635(279)	1.31073(552)	−2.83841(847)
	8079.90410(391)	7438.87082(391)	0.781527201(229)	1.3460685(205)	1.31300(208)	−2.84381(689)
	8079.90126	7438.87183	0.781527547	1.346098	1.306	−2.83
		7438.87038(29)	0.781527353(11)	1.345849(80)	0.851(83)	
7	9274.58324(767)	8633.55008(767)	0.775591672(405)	1.3479837(375)	1.10446(636)	−2.9491(110)
	9274.58331(633)	8633.55002(633)	0.775591676(320)	1.3479900(282)	1.10683(300)	−2.95532(934)
	9274.58068	8633.55125	0.775592031	1.348005	1.097	−2.93
		8633.54915(29)	0.77559205(11)	1.347867(89)	0.734(98)	
8	10456.4263(119)	9815.3931(119)	0.769652862(548)	1.3500078(504)	0.89129(759)	−3.0699(143)
	10456.42636(985)	9815.39307(985)	0.769652866(437)	1.3500147(388)	0.89362(424)	−3.0763(123)
	10456.4240	9815.39457	0.76965324	1.35001	0.879	−3.04
		9815.39254(41)	0.76965316(15)	1.34993(15)	0.61(27)	
9	11625.4542(179)	10984.4211(179)	0.763710497(728)	1.3521432(671)	0.67101(932)	−3.2020(182)
	11625.4544(148)	10984.4212(148)	0.763710501(583)	1.3521492(530)	0.67304(588)	−3.2078(160)
	11625.4524	10984.4230	0.76371089	1.3521	0.653	−3.16
		10984.42006(53)	0.76371073(17)	1.351811(22)		
10	12781.6876(262)	12140.6545(262)	0.757764283(951)	1.3543984(886)	0.4434(116)	−3.3463(231)
	12781.6884(216)	12140.6551(216)	0.757764286(764)	1.3544008(713)	0.44476(802)	−3.3508(204)
	12781.6869	12140.65747	0.7577647	1.3543	0.416	−3.29
11	13925.1462(374)	13284.1130(374)	0.75181389(122)	1.356783(115)	0.2084(147)	−3.5042(288)
	13925.1483(309)	13284.1151(309)	0.751813897(987)	1.3567778(945)	0.2084(107)	−3.5063(256)
	13925.148	13284.119	0.7518144	1.3567	0.169	−3.43
12	15055.8489(521)	14414.8157(521)	0.74585897(155)	1.359307(148)	−0.0341(187)	−3.6769(355)
	15055.8538(431)	14414.8205(431)	0.74585897(125)	1.359288(123)	−0.0363(142)	−3.6752(317)
	15055.855	14414.826	0.7458595	1.3591	−0.089	−3.59
13	16173.8138(713)	15532.7807(713)	0.73989913(194)	1.361982(189)	−0.2845(237)	−3.8653(432)
	16173.8236(590)	15532.7904(590)	0.73989913(158)	1.361943(158)	−0.2899(184)	−3.8584(388)
	16173.826	15532.797	0.7398997	1.3617	−0.361	−3.75
14	17279.0581(958)	16638.0250(958)	0.73393395(241)	1.364821(239)	−0.5426(298)	−4.0708(522)
	17279.0759(793)	16638.0426(793)	0.73393395(197)	1.364752(202)	−0.5527(237)	−4.0571(469)
	17279.081	16638.052	0.7339346	1.3644	−0.648	−3.93

15	18371.597(126) 18371.627(105) 18371.637	17730.564(126) 17730.594(105) 17730.608	0.72796294(297) 0.72796294(242) 0.7279637	1.367837(298) 1.367726(253) 1.3673	−0.8087(373) −0.8250(300) −0.950	−4.2945(623) −4.2722(560) −4.13
16	19451.447(165) 19451.495(137) 19451.51	18810.414(165) 18810.462(137) 18810.48	0.72198560(362) 0.72198560(296) 0.7219863	1.371044(369) 1.370877(315) 1.3703	−1.0828(462) −1.1074(376) −1.270	−4.5376(738) −4.5046(664) −4.35
17	20518.621(212) 20518.695(176) 20518.71	19877.588(212) 19877.662(176) 19877.68	0.71600138(438) 0.71600137(359) 0.7160021	1.374457(452) 1.374217(387) 1.3735	−1.3649(568) −1.4001(466) −1.610	−4.8011(868) −4.7553(780) −4.59
18	21573.130(270) 21573.240(225) 21573.26	20932.097(270) 20932.207(225) 20932.23	0.71000966(526) 0.71000965(432) 0.7100102	1.378092(549) 1.377760(472) 1.3769	−1.6550(693) −1.7036(571) −1.973	−5.086(101) −5.0253(910) −4.85
19	22614.987(341) 22615.144(284) 22615.16	21973.954(341) 21974.111(284) 21974.13	0.70400978(627) 0.70400977(517) 0.7040099	1.381967(662) 1.381519(571) 1.3805	−1.9532(838) −2.0184(695) −2.360	−5.394(117) −5.315(105) −5.14
20	23644.199(425) 23644.420(354) 23644.43	23003.166(425) 23003.386(354) 23003.400	0.69800103(744) 0.69800103(614) 0.6980004	1.386100(792) 1.385509(685) 1.3843	−2.259(100) −2.3448(838) −2.775	−5.726(134) −5.627(121) −5.47
21	24660.775(526) 24661.077(439)	24019.742(526) 24020.044(439)	0.69198263(876) 0.69198264(725)	1.390509(941) 1.389746(815)	−2.573(120) −2.683(100)	−6.084(154) −5.960(138)
22	25664.720(646) 25665.126(539)	25023.687(646) 25024.093(539)	0.6859537(102) 0.68595377(851)	1.39521(111) 1.394246(964)	−2.895(142) −3.034(119)	−6.467(175) −6.317(157)
23	26656.039(786) 26656.575(656)	26015.006(786) 26015.542(656)	0.6799135(119) 0.67991353(994)	1.40024(130) 1.39902(113)	−3.225(167) −3.398(140)	−6.878(198) −6.699(178)
24	27634.734(950) 27635.431(794)	26993.701(950) 26994.397(794)	0.6738609(139) 0.6738609(115)	1.40560(152) 1.40410(132)	−3.563(195) −3.776(164)	−7.318(224) −7.105(201)
25	28600.80(114) 28601.698(954)	27959.77(114) 27960.665(954)	0.6677949(160) 0.6677950(133)	1.41133(176) 1.40949(153)	−3.909(227) −4.168(191)	−7.788(251) −7.537(225)
26	29554.24(136) 29555.38(114)	28913.21(136) 28914.34(114)	0.6617145(185) 0.6617145(154)	1.41744(203) 1.41522(177)	−4.262(263) −4.574(222)	−8.289(280) −7.997(252)

v	$10^{23}M_v$	$10^{28}N_v$	$10^{33}O_v$	$10^{39}P_v$	$10^{44}Q_v$	$10^{49}R_v$	$10^{55}S_v$
0	−0.49325(123) −0.493640(267) −0.495	−0.255688(959) −0.255523(666)	−0.111110(489) −0.110673(352)	−0.54000(503) −0.55442(476)	−0.28074(261) −0.27770(228)	−0.16047(149) −0.15836(133)	−0.7427(100) −0.76205(864)
1	−0.53140(144) −0.531594(580) −0.534	−0.27516(134) −0.27690(114)	−0.124144(968) −0.122723(806)	−0.65151(704) −0.66128(645)	−0.29283(601) −0.29755(525)	−0.16047 −0.15836	−0.7427 −0.76205
2	−0.57263(193) −0.57212(112) −0.576	−0.29954(200) −0.30277(183)	−0.13587(180) −0.13430(155)	−0.76302(991) −0.76813(892)	−0.30492(973) −0.31740(815)	−0.16047 −0.15836	−0.7427 −0.76205
3	−0.61639(281) −0.61499(197) −0.621	−0.32881(289) −0.33313(269)	−0.14629(300) −0.14542(261)	−0.8745(130) −0.8749(116)	−0.3170(135) −0.3372(118)	−0.16047 −0.15836	−0.7427 −0.76205
4	−0.66211(420) −0.65993(323) −0.671	−0.36300(401) −0.36798(374)	−0.15540(458) −0.15608(400)	−0.9860(164) −0.9818(145)	−0.3291(173) −0.3570(151)	−0.16047 −0.15836	−0.7427 −0.76205
5	−0.70924(621) −0.70670(501) −0.725	−0.40208(538) −0.40732(499)	−0.16321(654) −0.16626(572)	−1.0975(197) −1.0887(175)	−0.3412(211) −0.3769(184)	−0.16047 −0.15836	−0.7427 −0.76205
6	−0.75723(896) −0.75505(743) −0.784	−0.44606(699) −0.45114(644)	−0.16971(890) −0.17599(779)	−1.2090(231) −1.1955(205)	−0.3532(249) −0.3967(218)	−0.16047 −0.15836	−0.7427 −0.76205
7	−0.8055(125) −0.8047(105) −0.849	−0.49495(885) −0.49946(812)	−0.1749(116) −0.1852(102)	−1.3205(266) −1.3024(235)	−0.3653(287) −0.4166(251)	−0.16047 −0.15836	−0.7427 −0.76205
8	−0.8535(171) −0.8554(146) −0.921	−0.5487(109) −0.5522(100)	−0.1787(147) −0.1940(129)	−1.4320(300) −1.4092(265)	−0.3774(325) −0.4364(285)	−0.16047 −0.15836	−0.7427 −0.76205
9	−0.9007(228) −0.9070(196) −1.00	−0.6074(133) −0.6095(121)	−0.1813(182) −0.2023(160)	−1.5435(334) −1.5161(296)	−0.3895(363) −0.4563(318)	−0.16047 −0.15836	−0.7427 −0.76205
10	−0.9465(298) −0.9591(256) −1.09	−0.6710(160) −0.6713(144)	−0.1826(222) −0.2102(194)	−1.6551(369) −1.6229(326)	−0.4016(402) −0.4761(352)	−0.16047 −0.15836	−0.7427 −0.76205
11	−0.9905(381) −1.0116(329) −1.19	−0.7395(189) −0.7376(170)	−0.1826(265) −0.2176(232)	−1.7666(404) −1.7298(357)	−0.4137(440) −0.4960(385)	−0.16047 −0.15836	−0.7427 −0.76205
12	−1.0319(480) −1.0642(415) −1.30	−0.8129(220) −0.8083(198)	−0.1812(312) −0.2245(273)	−1.8781(438) −1.8366(387)	−0.4258(478) −0.5158(419)	−0.16047 −0.15836	−0.7427 −0.76205
13	−1.0703(595) −1.1165(515) −1.42	−0.8912(254) −0.8836(229)	−0.1786(363) −0.2310(318)	−1.9896(473) −1.9435(418)	−0.4379(516) −0.5357(452)	−0.16047 −0.15836	−0.7427 −0.76205
14	−1.1051(727) −1.1685(631) −1.56	−0.9744(291) −0.9633(262)	−0.1746(417) −0.2370(366)	−2.1011(508) −2.0503(448)	−0.4500(555) −0.5555(486)	−0.16047 −0.15836	−0.7427 −0.76205
15	−1.1357(879) −1.2197(764) −1.71	−1.0625(331) −1.0476(297)	−0.1694(476) −0.2425(418)	−2.2126(543) −2.1572(479)	−0.4621(593) −0.5754(519)	−0.16047 −0.15836	−0.7427 −0.76205
16	−1.161(105) −1.2700(914) −1.89	−1.1555(373) −1.1363(334)	−0.1628(539) −0.2476(473)	−2.3241(577) −2.2641(510)	−0.4742(631) −0.5952(553)	−0.16047 −0.15836	−0.7427 −0.76205
17	−1.182(124) −1.319(108) −2.09	−1.2534(418) −1.2295(374)	−0.1549(605) −0.2522(531)	−2.4356(612) −2.3709(540)	−0.4863(669) −0.6151(586)	−0.16047 −0.15836	−0.7427 −0.76205

18	−1.197(146)	−1.3562(465)	−0.1457(676)	−2.5471(647)	−0.4983(708)	−0.16047	−0.7427
	−1.366(127)	−1.3272(416)	−0.2563(593)	−2.4778(571)	−0.6349(620)	−0.15836	−0.76205
	−2.32						
19	−1.205(170)	−1.4639(515)	−0.1352(750)	−2.6586(682)	−0.5104(746)	−0.16047	−0.7427
	−1.412(148)	−1.4294(460)	−0.2600(658)	−2.5846(602)	−0.6548(653)	−0.15836	−0.76205
	−2.58						
20	−1.207(196)	−1.5765(568)	−0.1234(828)	−2.7701(717)	−0.5225(784)	−0.16047	−0.7427
	−1.457(171)	−1.5360(507)	−0.2632(727)	−2.6915(633)	−0.6746(687)	−0.15836	−0.76205
	−2.89						
21	−1.201(226)	−1.6940(623)	−0.1103(910)	−2.8817(751)	−0.5346(822)	−0.16047	−0.7427
	−1.499(197)	−1.6472(556)	−0.2660(799)	−2.7983(663)	−0.6945(720)	−0.15836	−0.76205
22	−1.187(258)	−1.8165(681)	−0.0959(996)	−2.9932(786)	−0.5467(861)	−0.16047	−0.7427
	−1.538(225)	−1.7628(608)	−0.2682(875)	−2.9052(694)	−0.7143(754)	−0.15836	−0.76205
23	−1.164(293)	−1.9438(741)	−0.080(108)	−3.1047(821)	−0.5588(899)	−0.16047	−0.7427
	−1.575(255)	−1.8830(661)	−0.2700(954)	−3.0120(725)	−0.7342(787)	−0.15836	−0.76205
24	−1.132(331)	−2.0760(805)	−0.063(118)	−3.2162(856)	−0.5709(937)	−0.16047	−0.7427
	−1.609(289)	−2.0076(718)	−0.271(103)	−3.1189(756)	−0.7540(821)	−0.15836	−0.76205
25	−1.091(372)	−2.2131(870)	−0.044(127)	−3.3277(891)	−0.5830(975)	−0.16047	−0.7427
	−1.639(325)	−2.1367(776)	−0.272(122)	−3.2257(786)	−0.7739(854)	−0.15836	−0.76205
26	−1.039(417)	−2.3552(939)	−0.025(138)	−3.4392(926)	−0.595(101)	−0.16047	−0.7427
	−1.667(364)	−2.2703(837)	−0.272(121)	−3.3326(817)	−0.7937(888)	−0.15836	−0.76205

[a] The uncertainty (one standard error) in the last digit is given in parentheses. The second-row entries are the calculated values from the Y_{ij} values in column 3 in Table 3 given by the parameters of Fit 2. The third- and fourth-row entries are the values reported in Refs. [27] and [17], respectively.

Table 5(b) Band parameters (unit cm^{-1}) for $^{13}C^{32}S$ calculated from $42Y_{ij}$ given in Table 3.

v	G_v	G_v-G_0	B_v	10^6D_v	$10^{13}H_v$	$10^{18}L_v$
0	622.8323850(360)[a] 622.82861	0.0	0.7713287623(280) 0.77132910	1.19068133(946) 1.1907	2.03537(320) 2.036	- 1.84012(170) - 1.84
1	1859.148314(139) 1859.14452	1236.315929(143) 1236.31591	0.7658995433(447) 0.76589990	1.19189259(967) 1.1919	1.89636(324) 1.897	- 1.89793(189) - 1.89
2	3083.220620(340) 3083.21895	2460.388235(342) 2460.39034	0.7604685071(723) 0.76046897	1.1931699(102) 1.1932	1.75321(332) 1.755	- 1.95799(228) - 1.95
3	4295.070237(724) 4295.07340	3672.237852(724) 3672.24479	0.755035503(111) 0.75503618	1.1945149(115) 1.1945	1.60565(346) 1.608	- 2.02114(287) - 2.01
4	5494.71805(140)	4871.88567(140)	0.749600376(162)	1.1959295(138)	1.45346(366)	- 2.08822(372)
5	6682.18484(252)	6059.35246(252)	0.744162958(230)	1.1974168(176)	1.29640(397)	- 2.16010(487)
6	7857.49116(427)	7234.65878(427)	0.738723070(316)	1.1989805(233)	1.13428(441)	- 2.23761(637)
7	9020.65729(691)	8397.82491(691)	0.733280520(425)	1.2006250(312)	0.96690(507)	- 2.32161(828)
8	10171.7031(107)	9548.8707(107)	0.727835099(560)	1.2023555(417)	0.79408(602)	- 2.4129(106)
9	11310.6481(161)	10687.8158(161)	0.722386579(726)	1.2041781(553)	0.61566(734)	- 2.5124(135)
10	12437.5113(235)	11814.6789(235)	0.716934708(928)	1.2060995(727)	0.43149(913)	- 2.6210(171)
11	13552.3109(334)	12929.4785(334)	0.71147921(117)	1.2081271(944)	0.2414(114)	- 2.7394(212)
12	14655.0646(464)	14032.2323(464)	0.70601980(146)	1.210269(121)	0.0454(144)	- 2.8685(261)
13	15745.7893(633)	15122.9569(633)	0.70055613(181)	1.212535(154)	- 0.1567(182)	- 3.0093(318)
14	16824.5010(849)	16824.5010(849)	0.69508786(222)	1.214934(194)	- 0.3650(228)	- 3.1624(384)
15	17891.214(112)	17268.382(112)	0.68961458(270)	1.217477(241)	- 0.5796(285)	- 3.3288(458)
16	18945.944(146)	18323.112(146)	0.68413588(326)	1.220175(298)	- 0.8005(352)	- 3.5094(542)
17	19988.703(187)	19365.871(187)	0.67865129(391)	1.223041(364)	- 1.0278(432)	- 3.7049(636)
18	21019.504(238)	20396.671(238)	0.67316030(467)	1.226087(442)	- 1.2614(526)	- 3.9162(741)
19	22038.355(300)	21415.523(300)	0.66766236(554)	1.229327(532)	- 1.5014(635)	- 4.1442(858)
20	23045.268(374)	22422.435(374)	0.66215689(653)	1.232775(636)	- 1.7478(762)	- 4.3897(987)
21	24040.249(462)	23417.416(462)	0.65664324(766)	1.236446(755)	- 2.0006(907)	- 4.653(112)
22	25023.305(567)	24400.472(567)	0.65112072(894)	1.240357(890)	- 2.259(107)	- 4.936(128)
23	25994.441(690)	25371.608(690)	0.6455885(103)	1.24452(104)	- 2.525(126)	- 5.239(145)
24	26953.659(833)	26330.827(833)	0.6400460(120)	1.24896(121)	-2.796(147)	- 5.563(163)
25	27900.96(100)	27278.12(100)	0.6344922(138)	1.25369(141)	- 3.074(171)	- 5.909(183)
26	28836.34(119)	28213.51(119)	0.6289263(159)	1.25873(163)	- 3.358(198)	- 6.278(205)

v	$10^{23}M_v$	$10^{28}N_v$	$10^{33}O_v$	$10^{39}P_v$	$10^{44}Q_v$	$10^{49}R_v$	$10^{55}S_v$
0	- 0.369090(930) - 0.368	- 0.180675(676)	- 0.074050(324)	- 0.33930(315)	- 0.16689(153)	- 0.090104(839)	- 0.39364(533)
1	- 0.39679(107) - 0.396	- 0.193962(938)	- 0.082528(628)	- 0.40757(437)	- 0.17388(348)	- 0.090104	- 0.39364
2	- 0.42669(141) - 0.426	- 0.21052(138)	- 0.09018(115)	- 0.47585(611)	- 0.18087(562)	- 0.090104	- 0.39364
3	- 0.45841(203) - 0.458	- 0.23035(198)	- 0.09701(191)	- 0.54412(804)	- 0.18786(781)	- 0.090104	- 0.39364
4	- 0.49155(299)	- 0.25345(273)	- 0.10302(291)	- 0.6123(100)	- 0.1948(100)	- 0.090104	- 0.39364
5	- 0.52574(438)	- 0.27983(364)	- 0.10820(414)	- 0.6806(121)	- 0.2018(122)	- 0.090104	- 0.39364
6	- 0.56060(628)	- 0.30948(472)	- 0.11256(563)	- 0.7489(142)	- 0.2088(144)	- 0.090104	- 0.39364
7	- 0.59574(878)	- 0.34241(596)	- 0.11610(736)	- 0.8172(163)	- 0.2158(166)	- 0.090104	- 0.39364
8	- 0.6307(119)	- 0.37860(738)	- 0.11882(933)	- 0.8854(184)	- 0.2228(188)	- 0.090104	- 0.39364
9	- 0.6653(159)	- 0.41807(897)	- 0.1207(115)	- 0.9537(205)	- 0.2297(210)	- 0.090104	- 0.39364
10	- 0.6990(207)	- 0.4608(107)	- 0.1217(140)	- 1.0220(226)	- 0.2367(232)	- 0.090104	- 0.39364
11	- 0.7315(264)	- 0.5068(126)	- 0.1220(167)	- 1.0903(247)	- 0.2437(254)	- 0.090104	- 0.39364
12	- 0.7623(332)	- 0.5561(147)	- 0.1214(196)	- 1.1585(268)	- 0.2507(276)	- 0.090104	- 0.39364
13	- 0.7911(411)	- 0.6086(170)	- 0.1200(229)	- 1.2268(290)	- 0.2577(298)	- 0.090104	- 0.39364
14	- 0.8175(502)	- 0.6645(195)	- 0.1178(263)	- 1.2951(311)	- 0.2647(320)	- 0.090104	- 0.39364
15	- 0.8412(607)	- 0.7236(221)	- 0.1147(300)	- 1.3633(332)	- 0.2717(342)	- 0.090104	- 0.39364
16	- 0.8617(725)	- 0.7859(249)	- 0.1108(339)	- 1.4316(353)	- 0.2787(365)	- 0.090104	- 0.39364
17	- 0.8786(858)	- 0.8516(279)	- 0.1061(381)	- 1.4999(375)	- 0.2856(387)	- 0.090104	- 0.39364
18	- 0.891(100)	- 0.9205(311)	- 0.1006(426)	- 1.5682(396)	- 0.2926(409)	- 0.090104	- 0.39364
19	- 0.900(117)	- 0.9927(344)	- 0.0943(473)	- 1.6364(417)	- 0.2996(431)	- 0.090104	- 0.39364
20	- 0.904(135)	- 1.0682(379)	- 0.0871(522)	- 1.7047(439)	- 0.3066(453)	- 0.090104	- 0.39364
21	- 0.903(155)	- 1.1469(416)	- 0.0791(574)	- 1.7730(460)	- 0.3136(475)	- 0.090104	- 0.39364
22	- 0.896(177)	- 1.2289(455)	- 0.0703(628)	- 1.8413(481)	- 0.3206(497)	- 0.090104	- 0.39364
23	- 0.884(201)	- 1.3142(495)	- 0.0606(685)	- 1.9095(503)	- 0.3276(519)	- 0.090104	- 0.39364
24	- 0.866(228)	- 1.4028(538)	- 0.0502(744)	- 1.9778(524)	- 0.3346(541)	- 0.090104	- 0.39364
25	- 0.840(256)	- 1.4946(582)	- 0.0389(806)	- 2.0461(545)	- 0.3416(563)	- 0.090104	- 0.39364
26	- 0.808(287)	- 1.5897(627)	- 0.0268(870)	- 2.1143(567)	- 0.3485(586)	- 0.090104	- 0.39364

[a] The uncertainty (one standard error) in the last digits is given in parentheses. The second-row entries are the values reported in Ref. [27].

Table 5(c) Band parameters (unit cm^{-1}) for $^{14}C^{36}S$ calculated from $42Y_{ij}$ given in Table 3.

v	G_v	G_v-G_0	B_v	10^6D_v	$10^{13}H_v$	$10^{18}L_v$
0	596.5246052(731)	0.0	0.7075201173(436)	1.00151320(733)	1.57266(221)	- 1.30097(107)
1	1780.999420(243)	1184.474815(254)	0.7027516255(569)	1.00248611(751)	1.47012(224)	- 1.34009(121)
2	2954.244171(492)	2357.719566(498)	0.6979816187(808)	1.00350998(799)	1.36467(230)	- 1.38063(148)
3	4116.277246(888)	3519.752641(891)	0.693209976(114)	1.00458582(900)	1.25612(240)	- 1.42312(188)
4	5267.11700(152)	4670.59239(152)	0.688436573(160)	1.0057151(108)	1.14432(255)	- 1.46809(244)
5	6406.78171(252)	5810.25710(252)	0.683661276(218)	1.0069000(137)	1.02911(277)	- 1.51606(319)
6	7535.28946(405)	6938.76486(405)	0.678883944(292)	1.0081431(179)	0.91034(309)	- 1.56755(415)
7	8652.65816(632)	8056.13355(632)	0.674104425(384)	1.0094475(238)	0.78789(354)	- 1.62311(537)
8	9758.90537(957)	9162.38077(957)	0.669322553(497)	1.0108170(315)	0.66163(418)	- 1.68325(688)
9	10854.0483(141)	10257.5237(141)	0.664538151(634)	1.0122558(415)	0.53144(507)	- 1.74850(872)
10	11938.1039(203)	11341.5793(203)	0.659751025(800)	1.0137685(542)	0.39723(626)	- 1.8193(109)
11	13011.0884(286)	12414.5638(286)	0.654960961(999)	1.0153607(700)	0.25890(782)	- 1.8964(135)
12	14073.0176(395)	13476.4930(395)	0.65016773(123)	1.0170380(895)	0.11637(980)	- 1.9801(166)
13	15123.9066(535)	14527.3820(535)	0.64537107(151)	1.018806(113)	- 0.0304(122)	- 2.0711(201)
14	16163.7701(714)	15567.2455(714)	0.64057073(184)	1.020674(141)	- 0.1815(153)	- 2.1698(242)
15	17192.6217(940)	16596.0970(940)	0.63576639(222)	1.022647(176)	- 0.3371(190)	- 2.2768(288)
16	18210.474(122)	17613.949(122)	0.63095773(267)	1.024735(216)	- 0.4971(234)	- 2.3926(341)
17	19217.340(156)	18620.815(156)	0.62614439(319)	1.026945(264)	- 0.6616(286)	- 2.5177(400)
18	20213.230(198)	19616.705(198)	0.62132600(378)	1.029286(320)	- 0.8305(347)	- 2.6527(465)
19	21198.154(249)	20601.630(249)	0.61650214(447)	1.031769(384)	- 1.0040(419)	- 2.7981(538)
20	22172.122(309)	21575.597(309)	0.61167235(524)	1.034403(458)	- 1.1821(502)	- 2.9544(619)
21	23135.141(382)	22538.617(382)	0.60683616(613)	1.037199(543)	- 1.3646(597)	- 3.1221(707)
22	24087.219(467)	23490.694(467)	0.60199305(713)	1.040169(640)	- 1.5516(705)	- 3.3018(804)
23	25028.360(568)	24431.835(568)	0.59714246(826)	1.043324(750)	- 1.7432(829)	- 3.4939(909)
24	25958.568(685)	25362.044(685)	0.59228379(954)	1.046676(873)	- 1.9391(968)	- 3.699(102)
25	26877.848(821)	26281.323(821)	0.5874164(109)	1.05023(101)	- 2.139(112)	- 3.917(114)
26	27786.198(979)	27189.674(979)	0.5825396(125)	1.05402(116)	- 2.344(130)	- 4.150(128)

v	$10^{23}M_v$	$10^{28}N_v$	$10^{34}O_v$	$10^{39}P_v$	$10^{45}Q_v$	$10^{50}R_v$	$10^{55}S_v$
0	- 0.239066(577)	- 0.107385(400)	- 0.40318(175)	- 0.16914(157)	- 0.76563(689)	- 0.37944(353)	- 0.15203(205)
1	- 0.256223(666)	- 0.114880(544)	- 0.44768(328)	- 0.20187(213)	- 0.7963(153)	- 0.37944	- 0.15203
2	- 0.274700(871)	- 0.124161(790)	- 0.48806(595)	- 0.23461(296)	- 0.8270(247)	- 0.37944	- 0.15203
3	- 0.29428(123)	- 0.13522(112)	- 0.52432(975)	- 0.26734(388)	- 0.8578(343)	- 0.37944	- 0.15203
4	- 0.31474(179)	- 0.14808(153)	- 0.5564(147)	- 0.30007(484)	- 0.8885(440)	- 0.37944	- 0.15203
5	- 0.33587(260)	- 0.16272(203)	- 0.5844(209)	- 0.33281(582)	- 0.9192(537)	- 0.37944	- 0.15203
6	- 0.35745(370)	- 0.17914(262)	- 0.6083(283)	- 0.36554(682)	- 0.9500(633)	- 0.37944	- 0.15203
7	- 0.37927(513)	- 0.19736(330)	- 0.6281(370)	- 0.39827(782)	- 0.9807(730)	- 0.37944	- 0.15203
8	- 0.40109(696)	- 0.21736(408)	- 0.6437(469)	- 0.43101(883)	- 1.0114(827)	- 0.37944	- 0.15203
9	- 0.42271(922)	- 0.23914(495)	- 0.6552(580)	- 0.46374(984)	- 1.0421(925)	- 0.37944	- 0.15203
10	- 0.4439(119)	- 0.26271(591)	- 0.6626(703)	- 0.4964(108)	- 1.072(102)	- 0.37944	- 0.15203
11	- 0.4644(152)	- 0.28807(697)	- 0.6659(839)	- 0.5292(118)	- 1.103(111)	- 0.37944	- 0.15203
12	- 0.4841(191)	- 0.31522(812)	- 0.6651(987)	- 0.5619(128)	- 1.134(121)	- 0.37944	- 0.15203
13	- 0.5028(236)	- 0.34415(937)	- 0.660(114)	- 0.5946(139)	- 1.165(131)	- 0.37944	- 0.15203
14	- 0.5201(288)	- 0.3748(107)	- 0.651(132)	- 0.6274(149)	- 1.195(141)	- 0.37944	- 0.15203
15	- 0.5359(348)	- 0.4073(121)	- 0.637(150)	- 0.6601(159)	- 1.226(150)	- 0.37944	- 0.15203
16	- 0.5500(416)	- 0.4416(136)	- 0.620(170)	- 0.6928(169)	- 1.257(160)	- 0.37944	- 0.15203
17	- 0.5621(492)	- 0.4777(153)	- 0.599(191)	- 0.7256(179)	- 1.288(170)	- 0.37944	- 0.15203
18	- 0.5721(577)	- 0.5156(170)	- 0.573(213)	- 0.7583(190)	- 1.318(179)	- 0.37944	- 0.15203
19	- 0.5797(671)	- 0.5552(188)	- 0.543(237)	- 0.7910(200)	- 1.349(189)	- 0.37944	- 0.15203
20	- 0.5847(776)	- 0.5966(207)	- 0.509(261)	- 0.8238(210)	- 1.380(199)	- 0.37944	- 0.15203
21	- 0.5869(891)	- 0.6399(228)	- 0.471(287)	- 0.8565(220)	- 1.410(209)	- 0.37944	- 0.15203
22	- 0.586(101)	- 0.6849(249)	- 0.429(314)	- 0.8892(231)	- 1.441(218)	- 0.37944	- 0.15203
23	- 0.581(115)	- 0.7317(271)	- 0.383(343)	- 0.9220(241)	- 1.472(228)	- 0.37944	- 0.15203
24	- 0.574(130)	- 0.7803(294)	- 0.333(372)	- 0.9547(251)	- 1.503(238)	- 0.37944	- 0.15203
25	- 0.563(146)	- 0.8306(318)	- 0.278(403)	- 0.9874(261)	- 1.533(248)	- 0.37944	- 0.15203
26	- 0.547(164)	- 0.8828(343)	- 0.220(435)	- 1.0202(271)	- 1.564(257)	- 0.37944	- 0.15203

[a] The uncertainty (one standard error) in the last digits is given in parentheses. The second-row entries are the values reported in Ref. [27].

Fig. S1. Agreement between the measurements of this study of the v = 1–0 and 2–1 bands and those of Burkholder et al. [16]. The vertical and abscissa axes indicate the differences (this study – Burkholder et al.) and the spectral frequencies, respectively.

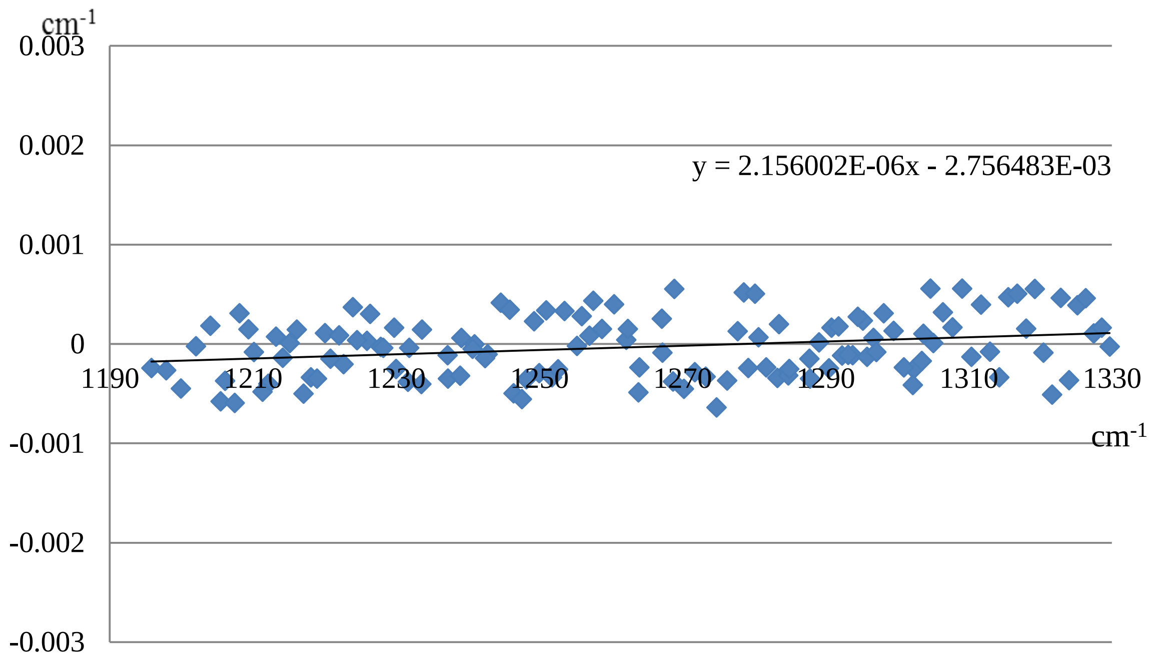

Table S1(a) Vibrational–rotational transitions (wavenumber/cm^{-1}) of $^{12}C^{32}S$, $^{13}C^{32}S$, $^{12}C^{34}S$, and $^{12}C^{33}S$ reported by Burkholder et al. [16].

m	obs.	10^3(o–c)
$^{12}C^{32}S$		
v = 1–0		
-41	1195.81647	0.267
-40	1197.89829	0.206
-39	1199.96968	0.303
-38	1202.03004	-0.013
-37	1204.07996	-0.12
-36	1206.11966	0.231
-35	1208.14792	-0.149
-34	1210.16588	-0.088
-33	1212.17324	0.144
-32	1214.16974	0.317
-31	1216.15465	-0.267
-30	1218.12968	0.132
-29	1220.09301	-0.275
-28	1222.04594	-0.156
-27	1223.98771	-0.241
-26	1225.91861	-0.208
-25	1227.83854	-0.127
-24	1229.7472	-0.266
-23	1231.64548	0.295
-22	1233.53212	0.329
-21	1235.40712	-0.134
-20	1237.27177	0.227
-19	1239.12467	0.045
-18	1240.96621	-0.261
-17	1242.79673	-0.317
-16	1244.61597	-0.353
-15	1246.42453	0.263
-14	1248.22111	0.262
-13	1250.00633	0.295
-12	1251.78007	0.276
-11	1253.54127	-0.826
-10	1255.29282	-0.087
-9	1257.0322	0.002
-8	1258.75973	-0.204
-7	1260.47592	-0.166
-6	1262.18071	0.089
-5	1263.87378	0.274
-4	1265.55435	-0.362
-3	1267.22395	-0.254
-2	1268.88175	-0.202
-1	1270.52768	-0.243
1	1273.78437	-0.037
2	1275.39516	0.304
3	1276.99351	0.11
4	1278.57979	-0.216
5	1280.15429	-0.354
6	1281.71735	0.071
7	1283.26822	0.339
8	1284.80677	0.354
9	1286.33319	0.337
10	1287.84749	0.331
11	1289.34892	-0.382
12	1290.83914	-0.109
13	1292.31721	0.242
14	1293.78254	0.114
15	1295.23545	-0.14
16	1296.6763	-0.129
17	1298.10511	0.201
18	1299.52062	-0.379
19	1300.92499	0.326
20	1302.31617	0.297
21	1303.69443	-0.163
22	1305.0608	0.009
23	1306.4142	-0.234
24	1307.75548	-0.01
25	1309.08367	-0.255
26	1310.39991	0.203
27	1311.70241	-0.393
28	1312.99338	0.2
29	1314.271	0.196
30	1315.53531	-0.333
31	1316.78731	-0.353
32	1318.02678	-0.053
33	1319.25285	-0.268
34	1320.46657	0.085
35	1321.66679	-0.111
36	1322.85449	0.157
37	1324.02896	0.213
38	1325.19001	-0.101
39	1326.33811	-0.28
40	1327.47353	-0.022
41	1328.59571	0.147
42	1329.70457	0.18
v = 2–1		
-30	1205.513	0.378
-29	1207.46498	0.351
-28	1209.40539	-0.318
-27	1211.3361	0.274
-26	1213.25462	-0.333
-25	1215.16311	0.052
-24	1217.06033	0.221
-23	1218.94622	0.144
-22	1220.82101	0.083
-21	1222.68478	0.15
-20	1224.53694	-0.216
-19	1226.37809	-0.381
-18	1228.20856	0.015
-17	1230.02746	0.113
-16	1231.83478	-0.065
-15	1233.63096	-0.047
-14	1235.416	0.198
-13	1237.18907	-0.129
-12	1238.95131	0.145
-11	1240.70149	-0.179
-10	1242.4405	-0.179
-9	1244.16806	-0.104
-8	1245.88405	-0.042
-7	1247.58861	0.179
-6	1249.28089	-0.259
-5	1250.96225	0.036
-4	1252.63176	0.165
-3	1254.28942	0.162
-2	1255.9353	0.126
-1	1257.56956	0.252
1	1260.80184	-0.267
2	1262.40094	0.234
3	1263.98756	0.163
5	1267.12462	-0.302
6	1268.6758	0.109
7	1270.21457	0.147
8	1271.74125	0.167
9	1273.25576	0.119
10	1274.75821	0.147
11	1276.24847	0.152
12	1277.72617	-0.202
13	1279.19233	0.137
14	1280.64558	-0.169
15	1282.08671	-0.296
16	1283.51571	-0.223
17	1284.93243	-0.067
19	1287.72839	-0.013
20	1289.10761	-0.07
21	1290.4746	0.137
22	1291.82847	-0.249
23	1293.17028	-0.134
24	1294.49924	-0.277
25	1295.81611	0.117
26	1297.11985	0.039
27	1298.41113	0.193
29	1300.95512	0.14
30	1302.20805	0.219
31	1303.44808	0.222
32	1304.67474	-0.288
$^{13}C^{32}S$		
v = 1–0		
-23	1198.14526	0.01
-22	1199.92011	0.498
-21	1201.68386	0.123
-20	1203.43726	-0.338
-19	1205.18075	-0.416
-18	1206.91416	-0.253
-17	1208.63736	0.049
-16	1210.3494	-0.433
-15	1212.05209	0.14
-14	1213.7439	0.266
-13	1215.42464	-0.217
-12	1217.0955	-0.091
-11	1218.75562	-0.187
-10	1220.40547	-0.007
-8	1223.67305	-0.017
-7	1225.29099	0.059
-6	1226.89821	0.075
-5	1228.49485	0.198
-4	1230.08031	-0.143
-2	1233.21973	-0.064
-1	1234.77402	0.743
1	1237.84702	-0.704
2	1239.36918	0.549
3	1240.87809	-0.532
4	1242.37747	-0.2
5	1243.86568	-0.064
6	1245.34271	-0.106
7	1246.80878	-0.078
8	1248.26368	-0.161
9	1249.70795	0.214
10	1251.14071	0.197
11	1252.56206	-0.085
12	1253.97287	0.268
13	1255.37207	0.214
14	1256.75972	-0.157
15	1258.13665	0.014
16	1259.50205	-0.055
17	1260.85604	-0.215
18	1262.19897	-0.086
19	1263.53036	-0.119
20	1264.85077	0.275
21	1266.15911	0.034
22	1267.45636	0.169

Table S1(a) – Continued

m	obs.	10^3(o–c)	*m*	obs.	10^3(o–c)	*m*	obs.	10^3(o–c)
23	1268.74194	0.128	2	1265.20766	0.138	-17	1237.82724	-0.22
24	1270.01593	0.021	3	1266.78054	-0.228	-16	1239.63078	-0.19
25	1271.27816	-0.294	4	1268.34232	-0.043	-15	1241.42322	-0.067
26	1272.52963	0.214	5	1269.89241	0.133	-14	1243.20442	0.04
27	1273.76789	-0.877	6	1271.43066	0.182	-13	1244.97409	-0.126
28	1274.99694	0.462	7	1272.95711	0.175	-12	1246.73282	0.053
29	1276.21231	-0.208	8	1274.47175	0.134	-11	1248.48019	0.191
			9	1275.97451	0.019	-10	1250.21586	-0.022
$^{12}C^{34}S$			10	1277.46536	-0.168	-9	1251.94083	0.445
v = 1–0			11	1278.94446	-0.236	-8	1253.65331	-0.167
-36	1197.09619	0.297	12	1280.41208	0.118	-7	1255.3549	-0.226
-35	1199.08962	0.535	13	1281.86733	0.033	-6	1257.0454	0.099
-34	1201.07223	0.445	14	1283.31045	-0.217	-5	1258.72386	-0.11
-32	1205.00537	-0.222	15	1284.74178	-0.263	-4	1260.39124	0.137
-31	1206.95596	-0.68	16	1286.16148	0.088	-3	1262.04631	-0.358
-30	1208.89742	0.343	17	1287.5689	0.218	-2	1263.69069	0.057
-29	1210.82674	-0.133	18	1288.96404	0.157	-1	1265.32321	0.243
-28	1212.74612	0.121	19	1290.34714	0.178	1	1268.55216	-0.455
-27	1214.65447	0.046	20	1291.71786	-0.028	2	1270.14961	-0.257
-26	1216.55215	0.032	21	1293.07634	-0.289	3	1271.73537	0.009
-25	1218.43898	-0.071	22	1294.42321	0.056	4	1273.3094	0.334
-24	1220.31482	-0.373	23	1295.75714	-0.291	5	1274.87084	-0.111
-23	1222.18044	-0.074	24	1297.07946	0.033	6	1276.42071	-0.273
-22	1224.03507	0.086	25	1298.3893	0.189	7	1277.95892	-0.211
-21	1225.87836	-0.212	26	1299.68689	0.438	8	1279.48535	-0.013
-20	1227.71119	-0.057	27	1300.97123	-0.187	9	1280.99968	0.032
-19	1229.53266	-0.321	28	1302.24409	0.115	10	1282.5021	0.147
-18	1231.34349	-0.251	29	1303.50427	0.177	11	1283.99226	0.013
-17	1233.14358	0.082	30	1304.75189	0.15	12	1285.47021	-0.287
-16	1234.93199	-0.231	31	1305.98647	-0.413	13	1286.93641	-0.262
-15	1236.71006	0.179	32	1307.20971	0.219	14	1288.39084	0.1
-14	1238.47619	-0.255	33	1308.41979	0.258	15	1289.83253	-0.139
-13	1240.23158	-0.304	34	1309.6166	-0.372	16	1291.26268	0.254
-12	1241.97635	0.183	35	1310.80236	0.579	17	1292.67995	-0.031
-11	1243.70941	0.147				18	1294.0852	-0.1
-10	1245.4313	0.158	$^{12}C^{33}S$			19	1295.47753	-0.821
-9	1247.14146	-0.313	*v* = 1–0			20	1296.85924	0.137
-8	1248.84089	-0.235	-26	1221.09717	-0.089	21	1298.22794	0.417
-7	1250.52895	-0.217	-25	1223.00025	0.129	22	1299.58349	-0.089
-6	1252.20596	0.091	-24	1224.8922	0.133	24	1302.25852	0.051
-5	1253.87137	0.17	-23	1226.773	-0.066	25	1303.57766	0.421
-4	1255.52532	0.191	-22	1228.64288	-0.208	26	1304.88361	0.094
-3	1257.16757	-0.055	-21	1230.50261	0.508	27	1306.17725	-0.017
-2	1258.79876	0.104	-20	1232.35026	0.183	28	1307.45882	0.36
-1	1260.41808	-0.113	-19	1234.18698	-0.002	29	1308.72699	-0.073
1	1263.62281	0.153	-18	1236.01265	-0.137			

Table S1(b) Vibrational–rotational transitions (wavenumber/cm^{-1}) of $^{12}C^{32}S$ reported by Ram et al. [17].

m	obs.	10^3(o–c)	*m*	obs.	10^3(o–c)	*m*	obs.	10^3(o–c)
$^{12}C^{32}S$			-44	1189.5069	-0.444	21	1303.6948	0.207
v = 1–0			-43	1191.6208	-0.003	22	1305.0606	-0.191
-106	1039.2019	3.55	-42	1193.7226	-1.166	23	1306.4142	-0.234
-105	1041.9091	3.201	-41	1195.8165	0.297	24	1307.7557	0.21
-104	1044.6013	-3.402	-40	1197.8986	0.516	25	1309.084	0.075
-103	1047.2868	-7.932	-39	1199.9688	-0.577	26	1310.4001	0.393
-102	1049.9743	-1.665	-38	1202.0296	-0.453	27	1311.7027	-0.103
-101	1052.6453	-3.074	-37	1204.0799	-0.18	28	1312.9932	0.02
-100	1055.3106	-1.334	-36	1206.1197	0.271	29	1314.2712	0.396
-99	1057.9677	1.082	-35	1208.1438	-4.269	30	1315.5357	0.057
-98	1060.6102	-2.202	-34	1210.1654	-0.568	31	1316.7873	-0.363
-97	1063.2494	0.143	-33	1212.1725	-0.596	32	1318.0272	0.367
-96	1065.8763	-0.859	-32	1214.1699	0.477	33	1319.2535	0.382
-95	1068.4972	1.119	-31	1216.1551	0.183	34	1320.4663	-0.185
-94	1071.1051	-0.896	-30	1218.1299	0.352	35	1321.6637	-3.201
-93	1073.7066	-0.279	-29	1220.0933	0.015	36	1322.8545	0.167
-92	1076.2977	-1.001	-28	1222.0455	-0.596	37	1324.0277	-1.047
-91	1078.8827	1.263	-27	1223.9874	-0.551	38	1325.1894	-0.711
-90	1081.4545	-0.56	-26	1225.919	0.182	39	1326.3381	-0.29
-89	1084.0189	-0.642	-25	1227.8384	-0.267	40	1327.4732	-0.352
-88	1086.5758	0.943	-24	1229.7474	-0.066	41	1328.5963	0.737
-87	1089.1203	-0.677	-23	1231.6449	-0.285	42	1329.7042	-0.19
-86	1091.6574	-0.476	-22	1233.5315	-0.291	43	1330.8003	0.301
-85	1094.1848	-0.725	-21	1235.4114	4.146	44	1331.8825	0.144
-84	1096.7033	-0.598	-20	1237.2719	0.357	45	1332.9517	0.271
-83	1099.2133	0.333	-19	1239.1252	0.575	46	1334.0075	0.318
-82	1101.713	0.295	-18	1240.9668	0.329	47	1335.0491	-0.484
-81	1104.2023	-0.783	-17	1242.7967	-0.347	48	1336.0786	0.001
-80	1106.6886	4.526	-16	1244.617	0.677	49	1337.0943	0.105
-79	1109.1572	1.55	-15	1246.4243	0.033	50	1338.0962	-0.137
-78	1111.6178	0.017	-14	1248.2208	-0.048	51	1339.0845	-0.491
-77	1114.0654	-5.045	-13	1250.0067	0.665	52	1340.0595	-0.625
-76	1116.5139	0.291	-12	1251.7804	0.606	53	1341.0218	0.097
-75	1118.9479	0.655	-11	1253.5415	-0.596	54	1341.9698	0.108
-74	1121.3712	-0.125	-10	1255.2927	-0.207	55	1342.9041	0.042
-73	1123.7862	0.378	-9	1257.0324	0.202	56	1343.8251	0.333
-72	1126.1907	-0.007	-8	1258.7594	-0.534	57	1344.7312	-0.584
-71	1128.586	0.049	-7	1260.4753	-0.786	58	1345.6242	-0.876
-70	1130.9711	-0.426	-6	1262.1809	0.279	59	1346.505	0.392
-69	1133.3471	-0.303	-5	1263.8744	0.894	60	1347.3696	-0.747
-68	1135.7119	-1.653	-4	1265.5564	1.688	61	1348.221	-1.257
-67	1138.0696	-0.349	-3	1267.2238	-0.404	62	1349.0604	0.096
-66	1140.4167	0.141	-2	1268.8818	-0.152	63	1349.8848	0.345
-65	1142.7558	2.443	-1	1270.5276	-0.323	64	1350.6949	0.226
-64	1145.0805	0.187	1	1273.783	-1.407	65	1351.4911	0.172
-63	1147.3972	-0.197	2	1275.3946	-0.256	66	1352.2725	-0.681
-62	1149.7027	-1.881	3	1276.9956	2.2	67	1353.0413	-0.098
-61	1152.002	0.165	4	1278.579	-1.006	68	1353.7956	0.053
-60	1154.2918	2.669	5	1280.1557	1.056	69	1354.5356	0.01
-59	1156.566	-0.438	6	1281.7174	0.121	70	1355.2614	-0.095
-58	1158.8336	-0.128	7	1283.2669	-0.981	71	1355.9732	-0.025
-57	1161.0911	0.129	8	1284.8064	-0.016	72	1356.6696	-1.146
-56	1163.3382	0.062	9	1286.3357	2.847	73	1357.3537	-0.323
-55	1165.5757	0.502	10	1287.847	-0.159	75	1358.6775	-0.205
-54	1167.8014	-0.723	11	1289.3516	2.298	76	1359.3167	-1.34
-53	1170.0186	-0.282	12	1290.8398	0.551	77	1359.9434	-0.59
-52	1172.2255	0.053	13	1292.3171	0.132	78	1360.5556	0.08
-51	1174.4215	-0.286	14	1293.7817	-0.726	80	1361.7347	-0.48
-50	1176.6079	0.03	15	1295.2348	-0.79	81	1362.302	-1.238
-49	1178.7836	-0.07	16	1296.6754	-1.029	84	1363.9202	0.3
-48	1180.9478	-1.354	17	1298.1048	-0.109	85	1364.4302	0.703
-47	1183.104	-0.294	18	1299.5204	-0.599	86	1364.9255	1.111
-46	1185.2492	0.141	19	1300.9231	-1.564	87	1365.4044	-0.14
-45	1187.3836	0.181	20	1302.3159	0.027	88	1365.8705	0.586

Table S1(b) – Continued

m	obs.	10^3(o–c)	*m*	obs.	10^3(o–c)	*m*	obs.	10^3(o–c)
89	1366.3206	0.124	-60	1142.0221	-0.031	5	1267.1243	-0.622
90	1366.7561	-0.087	-59	1144.2875	-0.341	6	1268.6758	0.109
91	1367.1777	0.686	-58	1146.5438	0.272	7	1270.2144	-0.023
92	1367.5835	0.582	-57	1148.789	-0.164	9	1273.2552	-0.441
93	1367.9732	-0.664	-56	1151.0248	0.082	10	1274.758	-0.063
94	1368.3485	-1.314	-55	1153.2503	0.14	11	1276.2481	-0.218
96	1369.0564	-0.183	-54	1155.4656	0.137	12	1277.7267	0.328
97	1369.3857	-1.628	-53	1157.6708	0.205	13	1279.1918	-0.393
99	1370.0057	2.347	-52	1159.8657	0.173	14	1280.646	0.251
100	1370.2899	1.342	-51	1162.0506	0.37	15	1282.086	-1.006
101	1370.557	-1.51	-50	1164.225	0.327	16	1283.516	0.067
102	1370.8134	0.23	-49	1166.3883	-0.526	17	1284.9323	-0.197
103	1371.0528	0.299	-48	1168.5449	2.239	18	1286.3357	-0.965
104	1371.2762	-0.265	-47	1170.6858	-0.346	19	1287.7281	-0.303
105	1371.4873	2.276	-46	1172.8193	0.049	20	1289.1072	-0.48
106	1371.6773	-0.842	-45	1174.9406	-1.348	21	1290.4734	-1.063
107	1371.855	-0.778	-44	1177.0538	-0.404	22	1291.829	0.281
108	1372.018	0.103	-43	1179.155	-0.991	23	1293.17	-0.414
111	1372.4116	0.843	-42	1181.2467	-0.578	24	1294.4994	-0.117
112	1372.5092	-1.217	-41	1183.3284	0.366	25	1295.8157	-0.293
113	1372.5983	3.935	-40	1185.3984	0.17	26	1297.1198	-0.011
			-39	1187.4578	-0.034	27	1298.4097	-1.237
v = 2–1			-38	1189.5069	0.084	28	1299.6886	-0.737
-101	1040.8516	0.194	-37	1191.5452	0.053	29	1300.9544	-0.58
-100	1043.5061	2.442	-36	1193.5725	-0.294	30	1302.2076	-0.231
-99	1046.1452	-1.825	-35	1195.5898	0.072	31	1303.4473	-0.558
-98	1048.7847	3.218	-34	1197.5962	0.282	32	1304.6757	0.672
-97	1051.4126	5.598	-33	1199.5912	-0.133	33	1305.8893	-0.007
-96	1054.0265	2.941	-32	1201.575	-0.943	34	1307.0901	-0.561
-95	1056.6308	-0.327	-31	1203.5503	0.584	35	1308.2796	0.542
-94	1059.2282	-1.48	-30	1205.513	0.378	36	1309.4544	-0.064
-93	1061.8191	-0.091	-29	1207.4638	-0.829	37	1310.6176	0.753
-92	1064.3986	-1.034	-28	1209.4058	0.092	38	1311.7682	2.029
-91	1066.969	-1.982	-27	1211.335	-0.826	39	1312.9022	-0.205
-90	1069.533	-0.208	-26	1213.2543	-0.653	40	1314.0257	0.186
-89	1072.0856	-0.686	-25	1215.1634	0.342	41	1315.1354	-0.065
-88	1074.6296	-0.589	-24	1217.0602	0.091	42	1316.2324	0.176
-87	1077.1644	-0.489	-23	1218.9464	0.324	43	1317.3158	0.042
-86	1079.6898	-0.56	-22	1220.8203	-0.627	44	1318.3859	-0.132
-85	1082.2087	2.126	-21	1222.6849	0.27	45	1319.4429	-0.115
-84	1084.7139	0.396	-20	1224.5368	-0.356	46	1320.4871	0.43
-83	1087.2105	-0.622	-19	1226.3789	0.429	47	1321.5189	1.935
-82	1089.7001	0.698	-18	1228.2082	-0.345	48	1322.5338	-0.067
-81	1092.1772	-1.115	-17	1230.0273	-0.047	49	1323.5367	-0.64
-80	1094.647	-0.835	-16	1231.835	0.155	50	1324.5274	0.049
-79	1097.1072	-0.732	-15	1233.6312	0.193	51	1325.5061	2.234
-78	1099.5571	-1.48	-14	1235.4114	-4.402	52	1326.4661	-0.751
-77	1101.9982	-1.55	-13	1237.1892	0.001	53	1327.416	-0.272
-76	1104.4318	0.386	-12	1238.9516	0.435	54	1328.3498	-2.295
-75	1106.8528	-0.745	-11	1240.702	0.331	55	1329.2743	0.014
-74	1109.2658	-0.314	-10	1242.44	-0.679	56	1330.183	0.19
-73	1111.6679	-1.193	-9	1244.1712	3.036	57	1331.0776	-0.033
-72	1114.0654	2.947	-8	1245.8838	-0.292	58	1331.9586	-0.121
-71	1116.4453	-0.867	-7	1247.5881	-0.331	59	1332.8259	-0.139
-70	1118.8207	0.495	-6	1249.2815	0.351	60	1333.6798	0.246
-69	1121.1839	-0.64	-5	1250.9612	-1.014	61	1334.519	-0.23
-68	1123.5393	0.158	-4	1252.6305	-1.095	62	1335.3453	0.267
-67	1125.8837	-0.283	-3	1254.2903	1.042	63	1336.1568	-0.128
-66	1128.2189	-0.134	-2	1255.9363	1.126	64	1336.9547	-0.181
-65	1130.5442	-0.066	-1	1257.5665	-2.808	65	1337.7387	-0.157
-64	1132.8597	0.049	1	1260.8031	0.993	67	1339.2642	-0.54
-63	1135.1648	-0.359	2	1262.4011	0.394	68	1340.0055	-1.076
-62	1137.461	0.239	3	1263.9874	0.003	69	1340.7341	-0.197
-61	1139.7463	-0.128	4	1265.5614	-0.746	70	1341.4478	-0.065

Table S1(b) – Continued

m	obs.	10^3(o–c)	*m*	obs.	10^3(o–c)	*m*	obs.	10^3(o–c)
71	1342.1462	-1.048	-76	1092.371	-0.451	-7	1234.7202	-3.425
72	1342.8317	-0.709	-75	1094.7815	-0.596	-6	1236.4052	0.676
73	1343.5032	-0.113	-74	1097.183	-0.172	-5	1238.0735	-0.266
74	1344.1597	-0.225	-73	1099.5729	-1.752	-4	1239.7321	0.781
75	1344.8014	-0.809	-72	1101.9542	-2.307	-3	1241.3739	-3.251
76	1345.4304	0.269	-71	1104.3282	-0.508	-2	1243.0082	-3.03
77	1346.0431	-0.555	-69	1109.0438	-0.238	2	1249.4282	-1.174
78	1346.6439	1.156	-68	1111.3872	0.091	3	1251.0033	-0.907
79	1347.2268	-0.565	-67	1113.7206	0.187	4	1252.5679	0.807
80	1347.7981	0.62	-66	1116.0432	-0.72	5	1254.1197	1.699
81	1348.3527	-0.354	-65	1118.3573	-0.304	6	1255.6571	0.202
82	1348.8944	0.349	-64	1120.6612	-0.233	7	1257.1884	4.647
84	1349.931	-1.172	-63	1122.9552	-0.18	8	1258.6971	-1.432
85	1350.4303	1.077	-62	1125.2391	-0.316	9	1260.2004	-0.803
86	1350.9107	-0.853	-61	1127.513	-0.511	10	1261.692	0.266
87	1351.3797	0.574	-60	1129.7783	0.663	11	1263.1703	0.208
88	1351.8315	-0.405	-59	1132.0306	-1.164	12	1264.6356	-0.645
89	1352.2725	2.646	-58	1134.2757	-0.163	13	1266.0909	0.74
90	1352.6941	1.164	-56	1138.7334	-0.459	14	1267.5318	-0.004
91	1353.1	-1.115	-55	1140.948	0.303	15	1268.9613	0.155
92	1353.4943	-0.054	-54	1143.1512	-0.19	16	1270.3785	0.35
93	1353.8713	-1.316	-53	1145.3446	-0.307	18	1273.1737	-1.322
94	1354.2364	0.536	-52	1147.5317	3.48	19	1274.5559	1.077
95	1354.5817	-2.361	-50	1151.864	-0.111	20	1275.9213	-0.857
97	1355.2356	0.445	-49	1154.0164	-0.23	21	1277.2768	-0.19
98	1355.5388	0.824	-48	1156.159	0.175	22	1278.619	-0.291
99	1355.8261	0.502	-47	1158.2908	0.134	23	1279.9485	-0.526
100	1356.097	-0.982	-46	1160.4117	-0.423	24	1281.2663	0.137
101	1356.3558	0.71	-45	1162.5224	-0.766	25	1282.5708	0.133
102	1356.599	2.114	-44	1164.6238	0.035	26	1283.8607	-1.807
103	1356.8232	-0.131	-43	1166.7138	-0.089	27	1285.1415	-0.148
104	1357.035	0.614	-42	1168.7935	-0.008	28	1286.4076	-0.458
105	1357.2298	-0.214	-41	1170.8628	0.207	29	1287.6614	-0.304
106	1357.4092	-0.977	-40	1172.921	-0.112	30	1288.9024	-0.152
107	1357.5752	0.364	-39	1174.9677	-1.335	31	1290.1305	-0.07
108	1357.7232	-0.752	-38	1177.0058	-0.533	32	1291.3458	0.077
109	1357.8564	-1.087	-37	1179.0332	0.226	33	1292.5478	-0.178
112	1358.1622	-2.016	-36	1181.0487	-0.227	34	1293.7361	-1.203
113	1358.2315	-3.537	-35	1183.0541	-0.063	35	1294.9136	-0.064
114	1358.2882	-1.88	-34	1185.0485	-0.151	36	1296.0772	0.174
			-32	1189.0045	-0.758	37	1297.2276	0.243
v = 3–2			-31	1190.9673	-0.016	38	1298.3639	-0.724
-98	1036.9714	-0.87	-30	1192.9175	-1.002	39	1299.4874	-1.392
-97	1039.5857	-0.782	-29	1194.8594	0.614	40	1300.6	0.172
-96	1042.1893	-2.422	-28	1196.7881	-0.037	41	1301.6978	0.102
-95	1044.7852	-2.763	-27	1198.7065	-0.023	42	1302.7825	0.131
-94	1047.3791	3.92	-26	1200.6122	-1.714	43	1303.8529	-0.906
-93	1049.9470	-6.346	-25	1202.5099	-0.378	44	1304.9119	-0.076
-92	1052.5216	-0.835	-24	1204.3955	-0.085	45	1305.9569	0.054
-91	1055.0828	0.379	-23	1206.2695	-0.304	46	1306.9883	-0.08
-90	1057.6319	-1.376	-21	1209.9846	-0.249	47	1308.0056	-0.946
-89	1060.1741	-0.874	-20	1211.8259	0.287	48	1309.0104	-0.909
-88	1062.7070	-0.489	-19	1213.6552	0.036	49	1310.0028	0.164
-87	1065.2297	-1.093	-18	1215.4729	-0.57	50	1310.9812	0.709
-86	1067.7451	0.241	-17	1217.2805	0.002	51	1311.9452	0.359
-85	1070.2485	-1.161	-16	1219.0763	0.081	52	1312.8951	-0.553
-84	1072.7482	3.029	-15	1220.8595	-1.1	53	1313.8329	0.01
-83	1075.2324	1.039	-14	1222.6322	-1.41	55	1315.6663	-0.208
-82	1077.7088	0.594	-13	1224.395	-0.217	56	1316.5623	-0.519
-81	1080.1706	-5.076	-12	1226.1446	-0.789	57	1317.4447	-0.72
-80	1082.6349	1.155	-11	1227.8838	-0.295	58	1318.3124	-1.875
-79	1085.0821	-0.284	-10	1229.6111	-0.204	59	1319.1689	-0.45
-78	1087.5208	-0.767	-9	1231.3278	0.817	61	1320.838	-0.021
-77	1089.9508	-0.465	-8	1233.0311	0	63	1322.451	-0.156

Table S1(b) – Continued

m	obs.	10^3(o–c)	*m*	obs.	10^3(o–c)	*m*	obs.	10^3(o–c)
64	1323.2361	-0.71	-56	1126.4651	-0.391	12	1251.5686	-0.207
65	1324.0064	-2.076	-55	1128.6685	0.761	13	1253.0106	-0.206
66	1324.7662	0.081	-54	1130.8589	-0.937	14	1254.4401	-0.43
68	1326.2391	-0.092	-53	1133.0419	0.147	15	1255.8582	0.256
69	1326.954	-0.554	-52	1135.213	-0.459	16	1257.263	-0.017
70	1327.656	0.249	-51	1137.3746	-0.325	17	1258.6555	-0.215
72	1329.0155	-0.011	-50	1139.5265	0.378	18	1260.0359	-0.106
73	1329.673	-1.004	-49	1141.667	-0.019	19	1261.4044	0.542
74	1330.3179	-0.291	-48	1143.7979	0.313	20	1262.7593	0.064
75	1330.9476	-0.437	-47	1145.9177	-0.095	21	1264.1032	1.092
76	1331.5632	-0.306	-46	1148.0296	1.985	22	1265.4328	0.359
78	1332.7513	0.131	-45	1150.1267	-0.315	23	1266.7508	0.598
79	1333.3233	0.008	-44	1152.216	0.034	24	1268.0555	0.142
80	1333.8813	0.405	-43	1154.294	-0.437	25	1269.3472	-0.676
81	1334.4243	0.359	-42	1156.363	0.601	26	1270.6282	0.477
82	1334.9525	0.105	-41	1158.42	0.178	27	1271.8956	0.735
83	1335.4658	-0.42	-40	1160.4661	-0.574	28	1273.148	-1.269
84	1335.9652	-0.18	-39	1162.5015	-1.426	29	1274.3909	-0.002
85	1336.4483	-1.538	-38	1164.5287	0.154	30	1275.6202	0.47
87	1337.3744	-0.105	-37	1166.5417	-1.806	31	1276.8347	-1.021
88	1337.8135	-1.139	-36	1168.5476	-0.174	32	1278.0386	-0.24
89	1338.2378	-2.126	-35	1170.5408	-0.519	33	1279.2283	-0.755
93	1339.7914	-0.453	-34	1172.5244	0.289	34	1280.4069	0.568
96	1340.7988	0.722	-33	1174.4945	-1.62	35	1281.5707	0.064
97	1341.103	-0.244	-32	1176.4565	-0.814	36	1282.7224	0.464
98	1341.3913	-1.927	-31	1178.4074	-0.263	38	1284.9851	-0.285
99	1341.6676	-0.389	-30	1180.3475	0.365	39	1286.0977	0.234
101	1342.1637	-7.996	-29	1182.2764	0.699	40	1287.1959	-0.508
102	1342.3991	-1.466	-28	1184.1935	0.171	42	1289.3548	0.065
103	1342.6139	-0.161	-27	1186.0999	-0.089	43	1290.4138	-0.253
			-26	1187.995	-0.648	44	1291.4602	0.104
v = 4–3			-25	1189.8802	-0.077	45	1292.4924	-0.429
-88	1050.8058	-0.817	-24	1191.7542	0.357	46	1293.5111	-1.118
-87	1053.3166	-1.952	-23	1193.6169	0.583	47	1294.5194	1.17
-86	1055.8211	-0.14	-22	1195.4675	-0.165	48	1295.5109	0.071
-85	1058.3132	-1.456	-21	1197.3074	-0.459	49	1296.4909	0.917
-84	1060.7995	0.728	-20	1199.1372	0.335	50	1297.4557	0.044
-83	1063.2723	-1.26	-19	1200.955	0.347	51	1298.4078	-0.014
-82	1065.7381	-0.893	-18	1202.7622	1.008	52	1299.346	-0.423
-81	1068.1939	-1.145	-17	1204.557	0.551	53	1300.2709	-0.549
-80	1070.6417	0.012	-16	1206.3411	0.707	54	1301.1833	0.443
-79	1073.0805	1.607	-15	1208.1138	0.806	55	1302.0805	-0.113
-78	1075.507	0.366	-14	1209.8745	0.281	56	1302.9645	-0.181
-77	1077.9236	-1.283	-13	1211.6242	0.164	57	1303.8332	-1.828
-76	1080.3324	-1.212	-12	1213.3628	0.385	58	1304.6914	-0.219
-75	1082.7327	-0.094	-11	1215.0888	-0.523	59	1305.5348	0.381
-74	1085.1229	0.501	-10	1216.8057	0.971	60	1306.3632	-0.192
-73	1087.5011	-1.301	-9	1218.5078	-0.8	61	1307.1786	0.095
-72	1089.8742	1.429	-8	1220.1999	-1.006	62	1307.979	-0.722
-71	1092.2323	-1.18	-7	1221.8811	-0.513	63	1308.7671	0.091
-70	1094.5834	-1.102	-6	1223.5492	-1.491	64	1309.54	-0.329
-69	1096.9262	0.394	-5	1225.2078	-0.308	65	1310.2999	0.251
-68	1099.2571	-0.265	-4	1226.8523	-1.53	66	1311.0443	-0.633
-67	1101.5794	0.249	-3	1228.4873	-0.527	69	1313.196	-0.215
-66	1103.8906	-0.534	-2	1230.1105	0.433	70	1313.8836	-1.401
-65	1106.1935	0.214	3	1238.0432	-0.572	71	1314.5595	-0.074
-64	1108.486	0.421	4	1239.5942	-0.59	72	1315.2201	0.202
-63	1110.7675	-0.482	5	1241.135	1.176	73	1315.8662	0.262
-62	1113.0403	-0.169	6	1242.6589	-1.943	74	1316.4978	0.142
-61	1115.3041	1.092	7	1244.175	-0.813	75	1317.1163	1.278
-60	1117.555	-0.572	8	1245.6793	0.597	76	1317.7182	0.206
-59	1119.7976	-0.532	9	1247.1692	-0.28	77	1318.3061	-0.438
-58	1122.031	0.342	10	1248.649	0.889	81	1320.515	-0.713
-57	1124.2528	-0.32	11	1250.1145	-0.065	82	1321.0323	0.726

Table S1(b) – Continued

m	obs.	10^3(o–c)
84	1322.0188	-0.524
85	1322.491	-0.138
86	1322.9479	-0.297
87	1323.3904	-0.063
88	1323.8181	0.201
89	1324.2312	0.731
v = 5–4		
-88	1038.9286	1.28
-87	1041.4306	2.683
-86	1043.9177	-1.559
-85	1046.4002	-1.119
-84	1048.8734	-0.669
-83	1051.3371	-0.384
-82	1053.7881	-3.435
-81	1056.2346	-1.596
-79	1061.0944	-2.838
-78	1063.5111	-2.464
-77	1065.9199	-0.489
-76	1068.3185	0.813
-75	1070.706	0.571
-74	1073.0808	-2.788
-73	1075.4488	-3.336
-72	1077.8089	-2.144
-71	1080.1596	-0.684
-70	1082.5003	0.47
-69	1084.8288	-0.851
-68	1087.1482	-1.52
-67	1089.4606	0.592
-66	1091.7594	-1.087
-65	1094.0503	-0.828
-64	1096.3314	-0.503
-63	1098.6038	1.018
-62	1100.8621	-1.638
-61	1103.115	0.26
-60	1105.355	-0.761
-59	1107.5861	-0.671
-58	1109.808	0.26
-57	1112.018	-0.641
-56	1114.2192	-0.243
-55	1116.4096	-0.517
-54	1118.5914	0.765
-53	1120.761	0.035
-52	1122.921	-0.08
-51	1125.0714	0.452
-50	1127.2082	-2.342
-49	1129.3394	-0.43
-48	1131.4588	0.017
-47	1133.5668	-0.572
-46	1135.6677	2.134
-45	1137.7517	-1.636
-44	1139.831	0.349
-43	1141.8976	0.119
-42	1143.9531	-0.696
-41	1145.9993	-0.267
-40	1148.0339	-0.862
-39	1150.0597	0.349
-38	1152.0733	-0.005
-37	1154.0763	-0.292
-36	1156.0693	0.118
-35	1158.051	-0.045
-34	1160.0225	0.35
-33	1161.9825	0.034
-32	1163.9318	-0.162
-31	1165.8711	0.491
-29	1169.7161	0.872
-28	1171.6219	0.761
-27	1173.5169	0.823
-26	1175.4002	0.191
-25	1177.273	0.094
-24	1179.1346	-0.137
-23	1180.9847	-0.769
-22	1182.8244	-0.672
-21	1184.6535	-0.014
-20	1186.471	0.235
-19	1188.2761	-0.693
-18	1190.0726	1.034
-17	1191.8552	0.147
-15	1195.3881	0.056
-14	1197.1365	-0.984
-13	1198.8758	0.287
-11	1202.3185	1.294
-10	1204.0199	-0.908
-9	1205.7135	0.629
-8	1207.3938	0.438
-7	1209.0627	0.449
-6	1210.7205	0.994
-5	1212.365	-0.093
-4	1213.9971	-1.882
-3	1215.6222	1.059
4	1226.6442	-0.887
5	1228.1718	-0.44
6	1229.6876	0.227
7	1231.1905	0.048
8	1232.6821	0.655
9	1234.1603	-0.019
10	1235.6264	-0.642
11	1237.0826	1.019
12	1238.5236	-0.304
13	1239.9531	-0.877
15	1242.7773	0.054
17	1245.5513	0.177
18	1246.9201	0.641
19	1248.2743	-1.048
20	1249.6174	-1.357
21	1250.9502	0.546
22	1252.2676	-0.406
23	1253.573	-0.778
24	1254.8672	0.261
25	1256.1473	-0.155
26	1257.4147	-0.593
27	1258.6702	-0.219
28	1259.9129	0.1
29	1261.1423	-0.103
30	1262.3589	-0.294
31	1263.5627	-0.44
32	1264.7552	0.993
33	1265.9324	0.038
34	1267.0958	-1.77
35	1268.2493	-0.499
36	1269.388	-1.015
37	1270.5161	0.917
38	1271.6281	-0.171
39	1272.7283	0.056
40	1273.8148	-0.268
41	1274.8886	-0.11
42	1275.9476	-1.535
43	1276.9957	-0.609
45	1279.0506	-0.17
46	1280.0591	1.113
47	1281.0523	0.483
48	1282.032	-0.226
49	1282.9985	-0.678
50	1283.9529	0.26
51	1284.8919	-0.678
52	1285.8185	-0.455
53	1286.7319	0.161
54	1287.6301	-0.794
55	1288.5164	0.015
56	1289.3865	-1.679
57	1290.2468	0.561
58	1291.0906	0.069
59	1291.9208	-0.221
60	1292.737	-0.673
61	1293.5391	-1.351
62	1294.3298	0.478
63	1295.1046	0.35
64	1295.864	-1.198
65	1296.6123	0.167
66	1297.3448	-0.219
67	1298.0628	-1.02
68	1298.7679	-0.6
69	1299.4592	0.176
70	1300.1349	-0.457
71	1300.7976	0.138
72	1301.4444	-0.903
73	1302.0806	1.754
74	1302.6978	-0.252
75	1303.3036	0.712
76	1303.8916	-1.715
77	1304.47	0.701
78	1305.0301	-0.702
79	1305.5762	-1.588
80	1306.1096	-0.621
81	1306.6272	-0.864
82	1307.1335	2.219
83	1307.6197	-0.133
85	1308.5522	-0.6
87	1309.427	0.332
88	1309.8417	0.353
89	1310.2395	-1.639
v = 6–5		
-84	1036.9715	0.783
-83	1039.425	2.209
-82	1041.8643	-1.192
-81	1044.2961	-2.694
-80	1046.7212	-1.469
-79	1049.1363	-0.79
-78	1051.5462	4.17
-77	1053.936	-1.461
-76	1056.3241	0.744
-75	1058.6996	-0.087
-74	1061.0661	-0.326
-73	1063.4255	1.954
-72	1065.7694	-1.619
-71	1068.1101	1.284
-70	1070.4353	-1.61
-68	1075.0649	1.025
-67	1077.3606	-2.089
-66	1079.6527	1.013
-65	1081.9291	-1.74
-64	1084.2025	2.381
-63	1086.4597	0.205
-62	1088.7091	0.159

Table S1(b) – Continued

m	obs.	10^3(o–c)	*m*	obs.	10^3(o–c)	*m*	obs.	10^3(o–c)
-61	1090.9467	-1.727	19	1235.1689	-0.138			
-60	1093.1784	0.476	20	1236.4995	-0.965	*v* = 7–6		
-59	1095.3973	-0.103	21	1237.8192	-0.172	-76	1044.3488	-1.395
-58	1097.6071	0.264	23	1240.4195	0.004	-75	1046.714	-1.146
-57	1099.8069	0.707	24	1241.6987	-1.946	-74	1049.0701	-0.397
-55	1104.1724	-2.162	25	1242.9688	-0.343	-73	1051.4127	-3.519
-54	1106.3428	-0.717	26	1244.2247	-0.255	-72	1053.7545	2.214
-53	1108.5013	-0.978	27	1245.4676	-0.448	-71	1056.0753	-3.368
-52	1110.6523	1.483	28	1246.6979	-0.488	-70	1058.3941	-1.239
-51	1112.7889	-0.204	29	1247.9153	-0.642	-69	1060.7015	-0.77
-50	1114.9145	-2.609	30	1249.1209	0.224	-68	1062.9982	-1.233
-49	1117.0358	0.996	31	1250.3129	0.342	-67	1065.2835	-3.299
-48	1119.1442	2.043	32	1251.4914	-0.152	-66	1067.5652	0.859
-47	1121.2355	-3.64	33	1252.6564	-1.226	-65	1069.8288	-3.23
-46	1123.3256	-0.122	34	1253.8104	-0.345	-64	1072.0856	-4.238
-45	1125.4025	0.626	35	1254.9532	2.324	-62	1076.5773	1.605
-44	1127.4672	-0.366	36	1256.0788	0.814	-61	1078.8028	-0.887
-43	1129.5241	1.333	37	1257.1885	-3.539	-60	1081.0191	-2.582
-42	1131.5692	1.753	38	1258.293	-0.003	-59	1083.2331	3.447
-41	1133.6013	-0.277	39	1259.3809	0.057	-58	1085.4295	1.93
-40	1135.6228	-2.326	41	1261.517	-0.015	-57	1087.6168	1.396
-39	1137.6375	-0.564	42	1262.5648	-0.479	-56	1089.7929	-0.225
-38	1139.6399	-0.46	43	1263.6004	0.117	-55	1091.9621	1.394
-37	1141.6307	-1.284	44	1264.6236	1.607	-54	1094.1191	0.984
-36	1143.6135	0.594	45	1265.63	-0.374	-53	1096.2657	0.374
-35	1145.5829	-0.195	46	1266.6246	-0.791	-52	1098.4012	-1.108
-34	1147.5399	-2.621	47	1267.6069	-0.111	-51	1100.5296	0.57
-33	1149.4905	-0.653	48	1268.5755	0.301	-50	1102.6449	-0.565
-32	1151.4287	-0.259	49	1269.53	0.08	-48	1106.8478	0.449
-31	1153.3562	0.289	50	1270.4707	-0.44	-47	1108.9363	3.557
-30	1155.2728	0.824	51	1271.3959	-2.924	-46	1111.0088	1.071
-29	1157.1778	0.676	52	1272.3104	-2.537	-45	1113.0704	-1.877
-28	1159.0704	-0.924	53	1273.2129	-0.545	-44	1115.1271	0.741
-27	1160.9547	0.155	54	1274.0999	-0.413	-43	1117.1687	-1.245
-26	1162.8269	0.143	55	1274.9734	-0.106	-42	1119.2023	-0.703
-25	1164.6872	-0.727	56	1275.8322	-0.789	-41	1121.2215	-4.005
-24	1166.5418	3.775	57	1276.6784	-0.326	-40	1123.2367	-0.72
-23	1168.3777	0.68	58	1277.5102	-0.484	-39	1125.2391	0.382
-22	1170.2043	-0.581	59	1278.3292	0.374	-38	1127.2264	-2.968
-21	1172.0224	0.824	60	1279.132	-1.117	-37	1129.2108	1.46
-20	1173.8278	0.726	61	1279.9226	-0.923	-36	1131.1778	-0.804
-19	1175.6218	0.457	62	1280.6987	-1.307	-35	1133.1385	1.371
-18	1177.4032	-1.153	63	1281.4629	0.365	-34	1135.0833	-1.585
-17	1179.1794	3.328	64	1282.2093	-1.77	-33	1137.0224	0.559
-15	1182.6872	1.689	65	1282.945	-0.578	-32	1138.9498	1.834
-14	1184.4235	0.333	66	1283.6666	0.578	-31	1140.8628	-0.431
-13	1186.1481	-1.306	67	1284.3726	0.233	-29	1144.6613	0.248
-12	1187.8685	4.304	68	1285.0636	-0.977	-28	1146.5439	0.352
-10	1191.2618	2.498	69	1285.7426	-0.016	-27	1148.4166	1.541
-9	1192.9374	-2.155	70	1286.4077	1.251	-26	1150.2762	0.646
-8	1194.6079	-0.331	71	1287.0572	1.162	-25	1152.1272	2.197
-7	1196.2645	-0.799	75	1289.5106	-0.642	-24	1153.9636	0.226
6	1216.7366	0.355	76	1290.0899	0.827	-23	1155.7892	-1.437
7	1218.2287	1.276	77	1290.6531	0.657	-22	1157.6066	-0.159
8	1219.7063	-0.211	78	1291.2003	-1.015	-21	1159.4111	-0.61
9	1221.1751	1.626	79	1291.7369	1.248	-20	1161.2069	1.442
11	1224.0695	-1.394	80	1292.2547	-0.719	-19	1162.9848	-3.173
12	1225.4992	-2.087	81	1292.7595	-1.076	-18	1164.7573	-1.922
13	1226.9184	-1.024	84	1294.1885	0.471	-16	1168.2672	-0.599
14	1228.3253	0.028	85	1294.6357	1.318	-14	1171.7295	-1.436
15	1229.716	-2.8	86	1295.0632	-2.741	-13	1173.4435	-1.886
16	1231.1	0.027	87	1295.4808	-1.867	-12	1175.1482	-0.181
17	1232.4684	-0.359	88	1295.8895	4.977	-11	1176.8388	-1.09
18	1233.8257	0.575	89	1296.2749	3.428	-10	1178.5184	-1.48

Table S1(b) – Continued

m	obs.	10^3(o–c)	*m*	obs.	10^3(o–c)	*m*	obs.	10^3(o–c)
-9	1180.1853	-3.021	77	1276.8549	-0.556	-9	1167.4616	2.856
11	1211.0792	-2.962	78	1277.3898	-1.837	-8	1169.1101	6.318
12	1212.5014	0.787	79	1277.9127	-0.565	13	1200.9159	0.225
13	1213.9066	-0.202	80	1278.4194	-0.903	14	1202.2985	0.9
14	1215.2992	-1.495	81	1278.9105	-2.213	15	1203.6673	0.111
15	1216.6797	-2.561	83	1279.8495	-4	16	1205.025	0.59
16	1218.0504	-1.065	84	1280.3038	1.999	18	1207.7047	3.087
17	1219.4086	0.325	85	1280.7354	0.075	19	1209.0219	0.372
18	1220.7515	-1.158	88	1281.9452	-1.649	20	1210.3283	-0.642
19	1222.0853	0.72	89	1282.3246	3.719	21	1211.6242	0.379
20	1223.4024	-1.608				22	1212.9067	0.568
21	1224.7105	-0.41				24	1215.4326	-0.316
22	1226.006	0.748	*v* = 8–7			25	1216.6797	2.379
23	1227.2878	0.8	-70	1046.3743	-0.308	26	1217.9099	0.876
24	1228.5549	-1.222	-69	1048.6744	4.262	27	1219.1287	0.709
25	1229.8124	-0.183	-68	1050.9589	3.009	28	1220.3329	-1.289
26	1231.0566	0.25	-67	1053.229	-2.839	29	1221.5303	2.717
27	1232.2883	0.909	-66	1055.4948	-3.154	31	1223.876	0.174
28	1233.5041	-1.57	-65	1057.7542	-0.008	33	1226.1701	-2.349
29	1234.7114	0.245	-64	1059.9991	-1.471	34	1227.3025	1.181
30	1235.9032	-0.612	-63	1062.238	0.983	35	1228.416	-1.181
31	1237.0826	-1.007	-62	1064.465	1.485	36	1229.5225	2.497
32	1238.249	-1.507	-61	1066.6816	1.562	37	1230.6072	-2.549
33	1239.4053	0.823	-60	1068.8875	0.943	38	1231.685	-1.386
34	1240.5462	0.716	-59	1071.0801	-2.943	39	1232.7483	-1.579
35	1241.6735	0.006	-57	1075.4448	-1.001	40	1233.7978	-2.394
37	1243.8904	0.014	-56	1077.613	0.985	41	1234.8384	1.104
38	1244.9793	0.099	-55	1079.765	-3.08	42	1235.861	-0.151
39	1246.0559	1.019	-54	1081.9154	1.433	43	1236.8718	0.075
40	1247.1148	-2.595	-53	1084.0478	-1.847	44	1237.8676	-1.383
41	1248.166	-0.706	-52	1086.1757	0.609	45	1238.8536	0.71
42	1249.2047	1.919	-51	1088.29	-0.268	46	1239.8228	-0.611
43	1250.2256	0.014	-50	1090.3902	-4.951	47	1240.7799	-0.612
44	1251.2347	-0.385	-47	1096.6464	-1.33	48	1241.7228	-1.358
45	1252.2312	-0.046	-46	1098.7092	-1.935	49	1242.654	-0.314
46	1253.214	-0.032	-45	1100.7628	-1.296	50	1243.5708	-0.145
47	1254.1826	-0.81	-44	1102.807	0.416	51	1244.4744	0.385
48	1255.1392	-0.144	-41	1108.8698	-1.108	52	1245.3648	1.309
49	1256.0788	-3.001	-40	1110.8742	2.998	53	1246.2401	0.764
50	1257.0072	-3.545	-39	1112.865	4.128	54	1247.1031	1.584
51	1257.9257	-0.441	-38	1114.8381	-1.788	55	1247.9481	-1.894
52	1258.8269	-1.055	-36	1118.7652	-0.638	56	1248.7869	2.163
53	1259.7168	0.649	-35	1120.7117	-1.01	57	1249.6052	-0.507
54	1260.5911	0.405	-34	1122.65	1.194	58	1250.4157	2.83
55	1261.4535	1.948	-33	1124.5753	1.204	59	1251.2061	-0.09
56	1262.2982	-0.485	-32	1126.4881	-0.449	60	1251.9853	-0.332
57	1263.1294	-2.661	-31	1128.3927	0.565	61	1252.7513	0.141
58	1263.9534	1.757	-30	1130.2887	3.877	62	1253.5026	-0.135
59	1264.7552	-2.197	-29	1132.1657	-0.881	63	1254.2388	-1.526
60	1265.5481	-1.186	-28	1134.0361	-1.28	65	1255.6727	-0.703
61	1266.3268	-0.476	-26	1137.7464	0.426	66	1256.3718	2.981
62	1267.0908	-0.53	-25	1139.5816	-2.107	68	1257.7193	2.08
63	1267.8429	1.487	-24	1141.4132	2.843	69	1258.3701	-0.034
64	1268.5755	-1.99	-23	1143.2241	-1.791	70	1259.0081	-0.707
65	1269.3001	0.576	-22	1145.0306	0.32	71	1259.6315	-1.704
67	1270.7005	-0.821	-21	1146.826	2.509			
68	1271.383	1.989	-20	1148.6053	-0.193			
69	1272.048	1.485	-19	1150.3764	0.145	*v* = 9–8		
70	1272.6976	-0.196	-17	1153.8849	0.966	-59	1058.9531	-3.898
71	1273.3352	0.382	-16	1155.6212	0.412	-58	1061.1327	0.745
72	1273.9572	-0.344	-14	1159.0603	-0.065	-57	1063.2962	-0.614
74	1275.1598	-0.162	-13	1160.767	3.974	-56	1065.4505	-1.045
75	1275.7366	-2.981	-11	1164.1315	-2.434	-55	1067.5968	0.681
76	1276.3061	1.342	-10	1165.801	-1.117	-54	1069.7334	2.894

Table S1(b) – Continued

m	obs.	10^3(o–c)	*m*	obs.	10^3(o–c)	*m*	obs.	10^3(o–c)
-53	1071.8531	-1.579	-26	1125.2391	1.608	46	1226.4469	-6.027
-52	1073.9698	1.194	-25	1127.0627	-0.816	47	1227.3992	1.486
-51	1076.0747	2.44	-24	1128.8781	-0.35	48	1228.3253	-3.732
-50	1078.1703	4.689	-23	1130.6801	-2.162	49	1229.246	-0.848
-49	1080.2444	-4.23	22	1199.8301	2.276	50	1230.1525	1.375
-47	1084.3847	1.15	23	1201.0754	-10.075	51	1231.0407	-1.129
-46	1086.4361	0.707	24	1202.3185	-11.981	52	1231.9225	3.576
-45	1088.4741	-2.685	25	1203.5504	-12.409	53	1232.782	-0.375
-44	1090.5091	1.403	26	1204.7826	0.175	54	1233.6313	-0.846
-43	1092.5328	4.703	27	1205.9881	-1.197	55	1234.4686	0.399
-42	1094.535	-2.957	28	1207.1842	0.811	56	1235.2906	0.094
-41	1096.5341	-3.146	29	1208.3663	1.632	57	1236.0978	-1.224
-40	1098.5235	-2.434	30	1209.5269	-6.201	58	1236.897	3.28
-39	1100.5044	0.409	31	1210.6886	-0.052	59	1237.6787	4.143
-38	1102.4701	-1.287	33	1212.9611	0.123	60	1238.4408	-0.701
-37	1104.4285	0.408	34	1214.0743	-3.381	64	1241.3739	4.291
-36	1106.3745	0.425	36	1216.27	-2.003	65	1242.0667	0.161
-35	1108.3117	2.394	37	1217.3502	0.648	66	1242.7467	-2.657
-34	1110.237	3.246	39	1219.4639	-1.355	67	1243.4198	1.773
-33	1112.1496	2.211	40	1220.5022	-1.14	70	1245.3431	4.321
-30	1117.8175	-5.61	41	1221.5303	2.1	72	1246.547	-0.865
-29	1119.6913	-1.886	42	1222.5376	-2.202	74	1247.7015	2.028
-28	1121.5564	4.104	43	1223.5371	-1.01			
-27	1123.4027	2.292	45	1225.4992	4.492			

Table S1(c) Vibrational–rotational Δv = 2 transitions (wavenumber/cm^{-1}) of $^{12}C^{32}S$ reported by Winkel et al. [15].

m	obs.	10^3(o–c)	*m*	obs.	10^3(o–c)	*m*	obs.	10^3(o–c)
			-17	2500.378	0.335	48	2581.3327	0.455
v = 2–0			-16	2502.3912	4.717	49	2581.767	0.285
-83	2318.0167	-5.518	-15	2504.3719	-0.221	50	2582.1762	0.36
-82	2321.4983	1.393	-14	2506.3349	0.354	51	2582.5599	0.316
-79	2331.7935	0.701	-13	2508.2741	0.371	52	2582.9183	0.389
-78	2335.1841	2.142	-12	2510.1899	0.263	53	2583.2511	0.316
-77	2338.5496	-0.075	-11	2512.0838	1.56	54	2583.5586	0.431
-76	2341.8961	0.176	-10	2513.9511	-0.406	55	2583.8405	0.473
-75	2345.2222	1.517	-9	2515.7962	-1.204	56	2584.0965	0.176
-74	2348.5249	0.974	-8	2517.6203	0.397	57	2584.3273	0.277
-73	2351.8068	1.173	-7	2519.4193	0.329	58	2584.5329	0.814
-72	2355.0666	0.836	-6	2521.1942	-0.376	59	2584.7125	1.022
-71	2358.3039	-0.409	-5	2522.9478	1.113	60	2584.86	-5.162
-69	2364.7172	0.673	-4	2524.6759	0.628	61	2584.9891	-3.999
-67	2371.0425	0.423	-3	2526.3805	0.201	62	2585.0919	-3.355
-66	2374.171	-1.287	-2	2528.0629	1.163	63	2585.1691	-2.491
-65	2377.2811	0.347	-1	2529.7227	3.147	64	2585.2199	-2.17
-64	2380.3682	0.751	1	2532.9624	-1.792	65	2585.2466	-0.055
-63	2383.4319	-0.448	2	2534.5521	1.149	66	2585.2466	1.291
-62	2386.4757	0.276	3	2536.1147	0.74	67	2585.2199	1.907
-61	2389.4965	-0.15	4	2537.6535	0.313	68	2585.1691	4.43
-60	2392.4987	2.699	5	2539.1718	3.201	69	2585.0919	6.597
-59	2395.4739	0.451	6	2540.6603	0.136	70	2584.9891	9.247
-58	2398.4295	0.533	7	2542.1278	-0.05	71	2584.86	11.719
-57	2401.3625	-0.029	8	2543.572	0.377	72	2584.6875	-3.051
-56	2404.2745	0.392	9	2544.994	2.548	73	2584.506	-0.623
-55	2407.1641	0.425	10	2546.3874	0.097	74	2584.2973	0.841
-54	2410.0315	0.296	11	2547.7583	-0.845	75	2584.0614	1.379
-53	2412.8769	0.232	12	2549.1072	0.257	76	2583.7972	-0.069
-52	2415.7004	0.361	13	2550.4309	0.235	77	2583.5083	0.135
-51	2418.5016	0.311	14	2551.7309	0.621	78	2583.1939	1.231
-50	2421.281	0.61	15	2553.0063	0.55	79	2582.8505	-0.243
-49	2424.0373	-0.015	16	2554.2579	0.853	80	2582.4833	0.953
-48	2426.7724	0.364	17	2555.4845	0.365	81	2582.0877	0.259
-47	2429.4849	0.376	18	2556.6896	2.618	82	2581.6667	0.715
-46	2432.1752	0.449	19	2557.8645	-1.055	83	2581.2181	0.159
-45	2434.8479	5.21	20	2559.0201	0.281	84	2580.7441	0.832
-44	2437.4882	-0.11	21	2560.15	0.259	85	2580.2427	0.775
-43	2440.1119	0.315	22	2561.2556	0.311	86	2579.7144	0.527
-42	2442.7127	0.214	23	2562.3366	0.173	87	2579.1594	0.33
-41	2445.2915	0.517	24	2563.3933	0.177	88	2578.5781	0.623
-40	2447.8474	0.352	25	2564.4256	0.257	89	2577.9696	0.548
-39	2450.3807	0.048	26	2565.4333	0.247	90	2577.3346	0.845
-38	2452.8918	0.034	27	2566.4165	0.28	91	2576.672	0.457
-37	2455.3807	0.339	28	2567.3751	0.292	92	2575.9831	0.724
-36	2457.8475	1.092	29	2568.3091	0.315	93	2575.267	0.788
-35	2460.2902	0.323	30	2569.2184	0.285	94	2574.5239	0.89
-34	2462.7108	0.061	31	2570.1031	0.334	95	2573.7535	0.774
-33	2465.1095	0.535	32	2570.9631	0.398	96	2572.955	-0.32
-32	2467.4847	0.175	33	2571.7982	0.311	97	2572.1315	0.752
-31	2469.8378	0.41	34	2572.6086	0.307	98	2571.2796	0.632
-30	2472.1684	0.871	35	2573.3942	0.321	99	2570.4014	1.463
-29	2474.4752	0.287	36	2574.1549	0.287	100	2569.4946	0.987
-28	2476.7595	-0.012	37	2574.8907	0.24	101	2568.5604	0.449
-27	2479.0217	0.403	38	2575.6016	0.215	102	2567.5992	0.291
-26	2481.2608	0.564	39	2576.2876	0.246	103	2566.6112	0.758
-25	2483.4767	0.4	40	2576.9487	0.368	104	2565.5955	0.993
-24	2485.6695	0.041	41	2577.5845	0.217	105	2564.5548	3.74
-23	2487.8324	-7.282	42	2578.1955	0.328	106	2563.4845	4.445
-22	2489.9862	-0.739	43	2578.7813	0.335	107	2562.3868	5.351
-21	2492.1119	0.7	44	2579.3419	0.273	109	2560.0998	-1.452
-20	2494.213	0.567	45	2579.8675	-9.621	110	2558.9124	-7.17
-19	2496.2909	0.291	46	2580.3877	0.288	111	2557.7179	7.795
-18	2498.337	-8.697	47	2580.8728	0.335			

Table S1(d) Rotational transitions (wavenumber/cm^{-1}) of $^{12}C^{32}S$, $^{13}C^{32}S$, and $^{12}C^{34}S$ reported by Bogey et al. [9].

$^{12}C^{32}S$

v	*J*”	obs.	10^5(o−c)
0	0	1.634163125	0.066
1	0	1.622321566	-0.013
2	0	1.610477039	0.021
3	0	1.598628108	0.061
4	0	1.586773774	0.042
5	0	1.57491427	0.027
6	0	1.563048327	-0.069
7	0	1.551178182	0.023
8	0	1.539300899	0.057
9	0	1.527415843	0.026
10	0	1.51552385	0.07
11	0	1.503622716	0.035
12	0	1.49171281	0.029
13	0	1.479793064	0.023
14	0	1.467862977	0.053
0	1	3.268292693	-0.015
1	1	3.244610643	-0.065
2	1	3.220921588	0.008
3	1	3.197222693	-0.013
4	1	3.173515526	0.104
5	1	3.14979675	0.102
6	1	3.126067301	0.158
7	1	3.10232571	0.215
8	1	3.078570242	0.199
9	1	3.054800164	0.144
10	1	3.031015143	0.135
0	2	4.902359251	0.016
1	2	4.866839145	0.248
2	2	4.831303194	0.128
3	2	4.79575667	0.289
4	2	4.760193333	0.216
5	2	4.724615621	0.268
6	2	4.689019929	0.211
7	2	4.653406391	0.194
8	2	4.617772573	0.12
9	2	4.582119407	0.245
10	2	4.546441825	0.24
11	2	4.510739393	0.255
12	2	4.475009575	0.251
13	2	4.439250637	0.289
14	2	4.403458375	0.206
15	2	4.367632591	0.264
16	2	4.331768546	0.296
17	2	4.295864041	0.418
18	2	4.259912436	0.33
19	2	4.223910763	0.131
20	2	4.187857454	0.095
0	3	6.53632941	0.031
1	3	6.488966477	0.076
2	3	6.441588234	0.236
3	3	6.394193446	0.525
4	3	6.346772039	0.083
5	3	6.299335222	0.186
6	3	6.251879125	0.612
7	3	6.204389438	0.114
0	4	8.170137756	-3.307
1	4	8.110970323	0.398
2	4	8.051743717	0.244
3	4	7.992495662	0.177
4	4	7.933225392	0.303
0	5	9.803857174	0.499
1	5	9.732809689	0.326
2	5	9.66174049	0.453
3	5	9.590641737	0.305
4	5	9.519521368	0.895
5	5	9.448365009	1.019
0	6	11.43734577	0.466
1	6	11.35445776	0.388
0	7	13.07061	0.449
1	7	12.97588047	0.388
0	8	14.70361846	0.512
0	9	16.33633625	0.372
0	10	17.96872522	-0.579

$^{13}C^{32}S$

v	*J*”	obs.	10^5(o−c)
0	0	1.542652784	0.002
1	0	1.53179554	0.122
2	0	1.520933025	0.078
3	0	1.510065507	-0.072
0	1	3.085278016	0.107
1	1	3.063561492	0.146
2	1	3.041838397	0.255
3	1	3.020103461	-0.033
0	2	4.627846075	0.209
1	2	4.595271773	0.324
0	3	6.170327741	0.246
1	3	6.126893426	0.22
2	3	6.083445868	0.326
3	3	6.039983601	0.536
0	4	7.712702232	0.995
0	5	9.254918648	0.224
1	5	9.189770878	0.614

$^{12}C^{34}S$

v	*J*”	obs.	10^5(o−c)
0	0	1.608009598	-0.091
1	0	1.596453671	0.026
2	0	1.584892839	0.05
3	0	1.573327372	0.041
4	0	1.561758268	0.134
5	0	1.550182427	0.056
0	1	3.21598951	-0.044
1	1	3.192877954	0.223
2	1	3.169755425	0.187
3	1	3.146626357	0.359
4	1	3.123481512	-0.115
0	2	4.823907511	0.021
1	2	4.789238127	0.225
2	2	4.754554432	0.191
3	2	4.71985893	0.268
4	2	4.685147716	0.171
5	2	4.650424795	0.413
6	2	4.615684495	0.546
7	2	4.580925448	0.563
0	3	6.431731648	0.017
1	3	6.385505769	0.3
2	3	6.339260576	0.243
3	3	6.292998505	0.223
4	3	6.246718855	0.309
0	4	8.039434868	0.342
1	4	7.981651526	0.621
0	5	9.646981513	0.536
1	5	9.577636339	0.39
2	5	9.508265582	0.076

Table S1(e) Rotational transitions (wavenumber/cm⁻¹) of $^{12}C^{32}S$, $^{12}C^{33}S$, $^{12}C^{34}S$, $^{12}C^{36}S$, $^{13}C^{32}S$, $^{13}C^{33}S$, and $^{13}C^{34}S$ reported by Ahrens and Winnewisser [10].

v	*J*”	obs.	10^5(o−c)
$^{12}C^{32}S$			
6	5	9.37716458	0.119
7	5	9.30593661	0.119
8	5	9.23466904	0.109
9	5	9.16335894	0.122
10	5	9.09200318	0.198
11	5	9.02059648	0.199
12	5	8.94913557	0.227
13	5	8.87761523	0.231
14	5	8.80602967	0.145
15	5	8.73437613	0.259
16	5	8.66264224	-0.049
7	6	10.85643305	-0.095
8	6	10.77328703	-0.084
9	6	10.70393489*	1384.30
10	6	10.60684188	0.014
11	6	10.52353358	0.054
12	6	10.44016191	0.119
13	6	10.35672018	0.087
14	6	10.27320474	0.195
15	6	10.1896049	0.033
16	6	10.10591884	0.138
0	11	19.60077611	-0.059
1	11	19.45867814	0.023
2	11	19.31652904	-0.022
3	11	19.17432566	-0.093
0	12	21.23243741	-0.015
1	12	21.07849591	0.054
2	12	20.92449887	-0.02
3	12	20.77044346	-0.067
4	12	20.61632478	-0.102
5	12	20.46213834	-0.066
3	13	22.36614305	-0.032
4	13	22.20016622	-0.106
5	13	22.03411568	-0.164
0	18	31.01252551	-0.037
1	18	30.78751517	0.239
2	18	30.56241845	-0.1
3	18	30.337239	-0.025
4	18	30.11196416	-0.1
5	18	29.88658958	-0.015
1	19	32.40373512	0.014
2	19	32.16679003	0.008
3	19	31.92975205	-0.117
4	19	31.6926165	-0.091
5	19	31.45537254	-0.21
6	19	31.2180145	-0.192
7	19	30.98053354	0.001
8	19	30.74291649	0.057
9	19	30.505155	0.242
1	20	34.01931596	0.073
2	20	33.77051767	-0.011
3	20	33.52162031	-0.344
6	20	32.77428063	-0.132
7	20	32.52491629	-0.193
9	20	32.02575813	0.442
10	20	31.775934	0.539
0	21	35.89478308	0.471
1	21	35.63422199	0.052
2	21	35.37357384	0.302
3	21	35.11281778	-0.092
4	21	34.85195665	-0.032
5	21	34.5909761	-0.083
6	21	34.32986863	-0.059
7	21	34.06862307	-0.058
8	21	33.80723057	0.146
9	21	33.54567629	0.287
6	22	35.88475198	0.606
8	22	35.33833696	0.411
$^{12}C^{34}S$			
3	5	9.43887271	0.141
4	5	9.36945068	0.09
4	6	10.9308502*	29.856
5	6	10.8495216	-0.239
6	6	10.76845652	-0.171
7	6	10.68735191	0.057
8	6	10.60619727	-0.274
0	11	19.28724534	0.031
1	11	19.14855116	0.057
2	11	19.00980795	-0.001
0	12	20.89283327	-0.024
1	12	20.74257986	0.042
2	12	20.59227431	0.123
3	12	20.44190251	-0.755
4	12	20.29147978	-0.604
5	12	20.14099868	0.317
1	13	22.33620467	0.044
2	13	22.17433268	-0.1
3	13	22.01240833	0.634
4	13	21.85040509	0.082
5	13	21.6883358	0.055
0	18	30.51680189	0.016
1	18	30.29717946	-0.035
2	18	30.0774798	-0.055
3	18	29.85769258	-0.439
0	19	32.11891291	-0.011
1	19	31.88772848	0.069
2	19	31.65645882	-0.189
3	19	31.42510193	-0.312
4	19	31.19364947	-0.426
5	19	30.96209862	-0.06
6	19	30.73042935	-0.403
9	19	30.03467435	-0.135
0	20	33.7204035	0.005
1	20	33.47765456	0.03
2	20	33.23481707	-0.179
3	20	32.99188367	-0.651
4	20	32.74885838	-0.241
0	21	35.3212413	-0.071
2	21	34.81252404	0.034
3	21	34.5580193	-0.193
6	21	33.79384331	-0.172
$^{12}C^{33}S$			
0	5	9.72292422	0.009
1	5	9.65275868	0.054
0	11	19.43903138	-0.335
0	12	21.05724621	0.049
0	18	30.75679659	-0.088
1	18	30.53457285	0.183
2	18	30.31226806	0.233
0	19	32.37147714	0.095
1	19	32.13754847	-0.079
2	19	31.90354075	0.165
0	20	33.98552491	0.07
1	20	33.73989799	0.185
2	20	33.4941815	0.109
0	21	35.5989109	0.086
1	21	35.34158388	0.377
2	21	35.08414861	-0.944
$^{12}C^{36}S$			
0	5	9.50727903	-0.019
0	12	20.59041659	0.198
0	18	30.07534883	0.009
0	19	31.65434002	-0.192
0	20	33.23273413	0.197
0	21	34.81049063	0.134
1	21	34.561685	-0.686
$^{13}C^{32}S$			
0	5	9.25491611	-0.03
1	5	9.18976521	0.048
2	5	9.12459229	0.109
0	6	10.79696925	0.017
1	6	10.7209585	0.015
2	6	10.64492223	0.014
3	6	10.5688556	-0.26
0	12	20.04408263	-0.194
1	12	19.9029133	-0.09
2	12	19.76168827	-0.773
3	12	19.62042661	0.055
0	13	21.58413705	-0.003
1	13	21.43210871	0.31
2	13	21.28001916	-0.337
3	13	21.12788241	-0.122
0	19	30.81505923	0.665
1	19	30.59784746	0.266
2	19	30.38056698	0.478
3	19	30.16319927	0.053
0	20	32.35170513	-0.025
1	20	32.12363585	0.287
3	20	31.66724144	-0.402
5	20	31.21048662	-0.366
0	21	33.88775761	-0.07
5	21	32.692175	0.125
0	22	35.42318183	-0.097
1	22	35.17338068	0.144
2	22	34.92349014	0.128
3	22	34.67349952	-0.516
4	22	34.42341268	-0.669
5	22	34.1732231	-0.204
$^{13}C^{34}S$			
2	5	9.03451314*	6352.002
0	12	19.7044003	-0.028
1	12	19.56681545	0.294
2	12	19.4291729	-0.539
0	13	21.21838335	-0.085
1	13	21.07021451	0.385
0	19	30.29320054	-0.238
1	19	30.08150258	-0.474
0	20	31.80390165	0.031
1	20	31.58162938	1.248
1	21	33.08114826	0.205
0	22	34.82352965	-0.191
1	22	34.58006772	0.008
$^{13}C^{33}S$			
0	5	9.17397312	-0.019
0	6	10.70254459	0.156
0	12	19.86885007	-0.147
0	13	21.39545585	-0.016
0	19	30.54584449	-0.272

*Excluded from fitting.

Table S1(f) Rotational transitions (wavenumber/cm^{-1}) of $^{12}C^{32}S$ reported by Kim and Yamamoto [11].

v	*J”*	obs.	10^5(o−c)	*v*	*J”*	obs.	10^5(o−c)	*v*	*J”*	obs.	10^5(o−c)
0	0	1.634162354	-0.011	10	0	1.515522082	-0.107	20	0	1.395996496	-0.003
1	0	1.622321626	-0.007	11	0	1.503622393	0.003	21	0	1.383959759	0.004
2	0	1.610476822	-0.001	12	0	1.491712567	0.005	22	0	1.371902081	0.012
3	0	1.598627394	-0.011	13	0	1.479792871	0.004	23	0	1.359821644	0.019
4	0	1.586773227	-0.013	14	0	1.467862477	0.003	24	0	1.347716499	0.023
5	0	1.574913843	-0.015	15	0	1.455920429	0.001	25	0	1.335584486	0.014
6	0	1.563048874	-0.014	16	0	1.443965708	-0.003	26	0	1.323423303	-0.017
7	0	1.551177825	-0.013	17	0	1.431997212	-0.006	18	1	2.839994400	-0.015
8	0	1.539300252	-0.007	18	0	1.420013732	-0.008	19	1	2.815994801	-0.011
9	0	1.52741553	-0.006	19	0	1.408013973	-0.007	20	1	2.791959750	-0.003

Table S2 Computer output of Dunham coefficients Y_{ij}/cm^{-1} for 11 isotopologues of CS back-calculated by the values of Fit 2 in Table 2.

Coeff.	$^{12}C^{33}S$		$^{12}C^{34}S$	
	Values	Uncertainties[a]	Values	Uncertainties
Y_{10}	0.127982865152d+04	0.59636131d-04	0.127481037795d+04	0.65832962d-04
Y_{20}	-0.644863684406d+01	0.36014591d-04	-0.639814809968d+01	0.37653439d-04
Y_{30}	0.377133586531d-02	0.92628032d-05	0.372715091319d-02	0.91542832d-05
Y_{40}	0.221845527977d-05	0.12928215d-05	0.218386832161d-05	0.12726657d-05
Y_{50}	-0.534561982603d-06	0.69066070d-07	-0.524164787862d-06	0.67722741d-07
Y_{01}	0.813261146491d+00	0.13997379d-07	0.806896421628d+00	0.15754606d-07
Y_{11}	-0.584520913568d-02	0.12134694d-07	-0.577671664623d-02	0.12584458d-07
Y_{21}	-0.885658447013d-06	0.38678283d-08	-0.871843395837d-06	0.38077176d-08
Y_{31}	-0.269758865601d-07	0.46358818d-09	-0.264512073742d-07	0.45457159d-09
Y_{41}	-0.566388193286d-10	0.22361022d-10	-0.553194646903d-10	0.21840140d-10
Y_{51}	-0.234309203112d-10	0.37102964d-12	-0.227953953032d-10	0.36096623d-12
Y_{02}	-0.131374868713d-05	0.95864161d-11	-0.129326507945d-05	0.93624945d-11
Y_{12}	-0.129714420269d-08	0.37034242d-12	-0.127182096793d-08	0.36874137d-12
Y_{22}	-0.372809850479d-10	0.28229636d-12	-0.364125552126d-10	0.27572048d-12
Y_{32}	-0.131976075791d-12	0.41556611d-13	-0.128396442746d-12	0.40429456d-13
Y_{42}	-0.294244840320d-13	0.30934685d-14	-0.285141638297d-13	0.29977645d-14
Y_{03}	0.244166877871d-12	0.24588004d-16	0.238482564457d-12	0.23981291d-16
Y_{13}	-0.160748850611d-13	0.11723309d-16	-0.156388439847d-13	0.11406700d-16
Y_{23}	-0.233548145778d-15	0.29841575d-17	-0.226322748211d-15	0.28918374d-17
Y_{33}	-0.414403256515d-17	0.41976052d-18	-0.400008249127d-17	0.40517942d-18
Y_{43}	-0.381772711026d-19	0.40067580d-19	-0.367066434720d-19	0.38524136d-19
Y_{04}	-0.220880414685d-17	0.15697524d-21	-0.214043429090d-17	0.15341341d-21
Y_{14}	-0.695823465663d-19	0.44622967d-21	-0.671652844966d-19	0.43072887d-21
Y_{24}	-0.104638605299d-20	0.11623288d-21	-0.100607818925d-20	0.11175547d-21
Y_{34}	-0.155755829402d-21	0.12161466d-22	-0.149168837421d-21	0.11647154d-22
Y_{05}	-0.456358990580d-23	0.20600320d-26	-0.438777970379d-23	0.19807176d-26
Y_{15}	-0.335655886772d-24	0.29887523d-26	-0.321460831326d-24	0.28623604d-26
Y_{25}	-0.140618799541d-25	0.10933115d-26	-0.134143979164d-25	0.10429698d-26
Y_{35}	0.395922664035d-27	0.18086523d-27	0.376211585340d-27	0.17186083d-27
Y_{06}	-0.234534151840d-28	0.55735138d-31	-0.223734980532d-28	0.53168475d-31
Y_{16}	-0.160049116673d-29	0.59879537d-31	-0.152081043561d-29	0.56898405d-31
Y_{26}	-0.211778410098d-30	0.11020688d-31	-0.200446044034d-30	0.10430970d-31
Y_{07}	-0.985742843600d-34	0.25887095d-36	-0.932995263039d-34	0.24501926d-36
Y_{17}	-0.117593130691d-34	0.40855410d-36	-0.110864311006d-34	0.38517621d-36
Y_{27}	0.217700401979d-36	0.16072449d-36	0.204438668652d-36	0.15093359d-36
Y_{08}	-0.468798890103d-39	0.42183636d-41	-0.440240900280d-39	0.39613838d-41
Y_{18}	-0.995718888618d-40	0.28702969d-41	-0.931396415916d-40	0.26848808d-41
Y_{09}	-0.248499401771d-44	0.14363518d-46	-0.231535275834d-44	0.13382970d-46
Y_{19}	-0.183422916512d-45	0.30968256d-46	-0.170231301098d-45	0.28741042d-46
Y_{010}	-0.145747781233d-49	0.12290300d-51	-0.134735419700d-49	0.11361703d-51
Y_{011}	-0.695526392257d-55	0.78893630d-57	-0.637942372036d-55	0.72361644d-57

Table 3 – Continued

Coeff.	$^{12}C^{36}S$		$^{13}C^{32}S$	
	Values	Uncertainties	Values	Uncertainties
Y_{10}	0.126552824116d+04	0.98107549d-04	0.124857974356d+04	0.64736616d-04
Y_{20}	-0.630528418434d+01	0.43761012d-04	-0.613759417721d+01	0.32510166d-04
Y_{30}	0.364633541254d-02	0.89557969d-05	0.350187462255d-02	0.86009594d-05
Y_{40}	0.212096148258d-05	0.12360063d-05	0.200967824162d-05	0.11711552d-05
Y_{50}	-0.505360008616d-06	0.65293143d-07	-0.472437531118d-06	0.61039519d-07
Y_{01}	0.795189680371d+00	0.25552119d-07	0.774042753298d+00	0.18671702d-07
Y_{11}	-0.565144250218d-02	0.14538046d-07	-0.542755800275d-02	0.12464392d-07
Y_{21}	-0.846716986505d-06	0.36983789d-08	-0.798097522323d-06	0.36900553d-08
Y_{31}	-0.255022517652d-07	0.43826381d-09	-0.238408672164d-07	0.40971211d-09
Y_{41}	-0.529465532094d-10	0.20903313d-10	-0.488349766237d-10	0.19280062d-10
Y_{51}	-0.216587579359d-10	0.34296780d-12	-0.197095455079d-10	0.31210167d-12
Y_{02}	-0.125600954051d-05	0.89605433d-11	-0.119010417505d-05	0.82572158d-11
Y_{12}	-0.122602704262d-08	0.37358867d-12	-0.114587649293d-08	0.34341196d-12
Y_{22}	-0.348506498182d-10	0.26389348d-12	-0.321443147104d-10	0.24340149d-12
Y_{32}	-0.121994264028d-12	0.38413538d-13	-0.111015207137d-12	0.34956453d-13
Y_{42}	-0.268951366842d-13	0.28275525d-14	-0.241471894333d-13	0.25386541d-14
Y_{03}	0.228258830388d-12	0.23223709d-16	0.210513856687d-12	0.22104967d-16
Y_{13}	-0.148589872098d-13	0.10840336d-16	-0.135139128426d-13	0.10343037d-16
Y_{23}	-0.213472198737d-15	0.27276438d-17	-0.191661179573d-15	0.24489438d-17
Y_{33}	-0.374549100463d-17	0.37939114d-18	-0.331780886248d-17	0.33607011d-18
Y_{43}	-0.341201694950d-19	0.35809595d-19	-0.298197196099d-19	0.31296212d-19
Y_{04}	-0.201884031086d-17	0.14890434d-21	-0.181246066058d-17	0.13410846d-21
Y_{14}	-0.628904452482d-19	0.40331403d-21	-0.557092451568d-19	0.35726351d-21
Y_{24}	-0.935186524708d-21	0.10388079d-21	-0.817317157639d-21	0.90787818d-22
Y_{34}	-0.137648444136d-21	0.10747641d-22	-0.118689815192d-21	0.92673436d-23
Y_{05}	-0.407857451540d-23	0.18412298d-26	-0.356291957002d-23	0.16707768d-26
Y_{15}	-0.296634230363d-24	0.26413052d-26	-0.255778132491d-24	0.22774943d-26
Y_{25}	-0.122882795376d-25	0.95541414d-27	-0.104540121414d-25	0.81279999d-27
Y_{35}	0.342120232412d-27	0.15628724d-27	0.287157687588d-27	0.13117927d-27
Y_{06}	-0.204952767932d-28	0.48704511d-31	-0.174359536486d-28	0.41435645d-31
Y_{16}	-0.138299839760d-29	0.51742382d-31	-0.116081594763d-29	0.43429828d-31
Y_{26}	-0.180955079319d-30	0.94166901d-32	-0.149851894609d-30	0.77981152d-32
Y_{07}	-0.842272705559d-34	0.22119513d-36	-0.697499960655d-34	0.18317006d-36
Y_{17}	-0.993554618262d-35	0.34519108d-36	-0.811769963170d-35	0.28203374d-36
Y_{27}	0.181882001082d-36	0.13428039d-36	0.146615783691d-36	0.10824394d-36
Y_{08}	-0.391667077608d-39	0.35242924d-41	-0.315724344287d-39	0.28409464d-41
Y_{18}	-0.822598546107d-40	0.23712593d-41	-0.654227372969d-40	0.18859041d-41
Y_{09}	-0.203000561225d-44	0.11733626d-46	-0.159289732610d-44	0.92071505d-47
Y_{19}	-0.148165190864d-45	0.25015499d-46	-0.114706096451d-45	0.19366427d-46
Y_{010}	-0.116416688459d-49	0.98170031d-52	-0.889212027361d-50	0.74983995d-52
Y_{011}	-0.543210682319d-55	0.61615901d-57	-0.403885192418d-55	0.45812390d-57

Table 3 – Continued

Coeff.	$^{13}C^{33}S$		$^{13}C^{34}S$	
	Values	Uncertainties	Values	Uncertainties
Y_{10}	0.124309715802d+04	0.65786285d-04	0.123792999816d+04	0.76989922d-04
Y_{20}	-0.608379421351d+01	0.32655013d-04	-0.603330648058d+01	0.34324112d-04
Y_{30}	0.345595016894d-02	0.84881672d-05	0.341303697715d-02	0.83827707d-05
Y_{40}	0.197461510859d-05	0.11507219d-05	0.194199108843d-05	0.11317100d-05
Y_{50}	-0.462156816290d-06	0.59711240d-07	-0.452632146727d-06	0.58480642d-07
Y_{01}	0.767260399851d+00	0.17590135d-07	0.760895564259d+00	0.19674119d-07
Y_{11}	-0.535636973046d-02	0.12318285d-07	-0.528984946522d-02	0.12658081d-07
Y_{21}	-0.784166124572d-06	0.36259880d-08	-0.771204008336d-06	0.35663709d-08
Y_{31}	-0.233220660185d-07	0.40079652d-09	-0.228414175362d-07	0.39253659d-09
Y_{41}	-0.475625359079d-10	0.18777702d-10	-0.463887093566d-10	0.18314274d-10
Y_{51}	-0.191117155941d-10	0.30263515d-12	-0.185625748063d-10	0.29393960d-12
Y_{02}	-0.116933878837d-05	0.80413125d-11	-0.115001794930d-05	0.78424386d-11
Y_{12}	-0.112085287860d-08	0.33804816d-12	-0.109767197134d-08	0.33593451d-12
Y_{22}	-0.313067647073d-10	0.23705941d-12	-0.305341248355d-10	0.23120885d-12
Y_{32}	-0.107647893989d-12	0.33896153d-13	-0.104554825290d-12	0.32922208d-13
Y_{42}	-0.233119551910d-13	0.24508440d-14	-0.225480244902d-13	0.23705302d-14
Y_{03}	0.205031794280d-12	0.21375571d-16	0.199974493751d-12	0.20818219d-16
Y_{13}	-0.131039763555d-13	0.10030835d-16	-0.127274275336d-13	0.97440113d-17
Y_{23}	-0.185031754623d-15	0.23642386d-17	-0.178968280460d-15	0.22867646d-17
Y_{33}	-0.318898531783d-17	0.32302121d-18	-0.307166304833d-17	0.31113731d-18
Y_{43}	-0.285360435239d-19	0.29948976d-19	-0.273719707690d-19	0.28727265d-19
Y_{04}	-0.174973846808d-17	0.12989077d-21	-0.169237204828d-17	0.12666040d-21
Y_{14}	-0.535461722590d-19	0.34339151d-21	-0.515762169828d-19	0.33075800d-21
Y_{24}	-0.782133376448d-21	0.86879588d-22	-0.750227756684d-21	0.83335497d-22
Y_{34}	-0.113081797479d-21	0.88294691d-23	-0.108018033675d-21	0.84340899d-23
Y_{05}	-0.340953010372d-23	0.15990307d-26	-0.327043295060d-23	0.15339646d-26
Y_{15}	-0.243692779631d-24	0.21698873d-26	-0.232780301191d-24	0.20727233d-26
Y_{25}	-0.991633742208d-26	0.77099580d-27	-0.943291922275d-26	0.73341004d-27
Y_{35}	0.271192571783d-27	0.12388610d-27	0.256899858075d-27	0.11735691d-27
Y_{06}	-0.165391810643d-28	0.39304253d-31	-0.157329014080d-28	0.37387953d-31
Y_{16}	-0.109627802358d-29	0.41015243d-31	-0.103850067433d-29	0.38853596d-31
Y_{26}	-0.140899232276d-30	0.73322321d-32	-0.132918660740d-30	0.69169351d-32
Y_{07}	-0.655828938471d-34	0.17222732d-36	-0.618682605772d-34	0.16247273d-36
Y_{17}	-0.759920941220d-35	0.26401984d-36	-0.713899368658d-35	0.24803058d-36
Y_{27}	0.136648606534d-36	0.10088534d-36	0.127839495465d-36	0.94381730d-37
Y_{08}	-0.294260894766d-39	0.26478084d-41	-0.275291239891d-39	0.24771112d-41
Y_{18}	-0.607074846487d-40	0.17499817d-41	-0.565579076746d-40	0.16303655d-41
Y_{09}	-0.147160195861d-44	0.85060442d-47	-0.136531451831d-44	0.78916864d-47
Y_{19}	-0.105506233882d-45	0.17813163d-46	-0.974791486155d-46	0.16457907d-46
Y_{010}	-0.814302925192d-50	0.68667371d-52	-0.749222578436d-50	0.63179530d-52
Y_{011}	-0.366620453505d-55	0.41585341d-57	-0.334521520968d-55	0.37944278d-57

Table 3 – Continued

Coeff.	$^{13}C^{36}S$		$^{14}C^{32}S$	
	Values	Uncertainties	Values	Uncertainties
Y_{10}	0.122836921760d+04	0.11165605d-03	0.121647559125d+04	0.94969142d-04
Y_{20}	-0.594044442563d+01	0.40336888d-04	-0.582602692571d+01	0.32296666d-04
Y_{30}	0.333457424089d-02	0.81900629d-05	0.323871425171d-02	0.79545987d-05
Y_{40}	0.188269475355d-05	0.10971546d-05	0.181088570299d-05	0.10553073d-05
Y_{50}	-0.435422991293d-06	0.56257200d-07	-0.414764302421d-06	0.53588071d-07
Y_{01}	0.749188619340d+00	0.28296234d-07	0.734758352247d+00	0.30149364d-07
Y_{11}	-0.516822391512d-02	0.14247679d-07	-0.501966810496d-02	0.14363653d-07
Y_{21}	-0.747644909015d-06	0.34579958d-08	-0.715904825792d-06	0.35548625d-08
Y_{31}	-0.219729827430d-07	0.37761253d-09	-0.209304723033d-07	0.35969636d-09
Y_{41}	-0.442803998375d-10	0.17481913d-10	-0.417715349046d-10	0.16491413d-10
Y_{51}	-0.175820998960d-10	0.27841394d-12	-0.164254973887d-10	0.26009882d-12
Y_{02}	-0.111490112271d-05	0.74859804d-11	-0.107237409577d-05	0.70568681d-11
Y_{12}	-0.105579486564d-08	0.33841378d-12	-0.100553568634d-08	0.32216702d-12
Y_{22}	-0.291463865919d-10	0.22070066d-12	-0.274949934809d-10	0.20819660d-12
Y_{32}	-0.990322410563d-13	0.31183257d-13	-0.925176074811d-13	0.29131929d-13
Y_{42}	-0.211921152176d-13	0.22279804d-14	-0.196065408684d-13	0.20612849d-14
Y_{03}	0.190890836454d-12	0.20087138d-16	0.180059556375d-12	0.19824490d-16
Y_{13}	-0.120551134076d-13	0.92317739d-17	-0.112565437044d-13	0.90564244d-17
Y_{23}	-0.168206151340d-15	0.21492549d-17	-0.155621123550d-15	0.19884422d-17
Y_{33}	-0.286465723071d-17	0.29016911d-18	-0.262469124625d-17	0.26586234d-18
Y_{43}	-0.253301896030d-19	0.26584387d-19	-0.229838556574d-19	0.24121877d-19
Y_{04}	-0.159055467846d-17	0.12229525d-21	-0.147148870845d-17	0.11443913d-21
Y_{14}	-0.481003875059d-19	0.30846719d-21	-0.440711246967d-19	0.28262919d-21
Y_{24}	-0.694265366664d-21	0.77119170d-22	-0.629955607337d-21	0.69975626d-22
Y_{34}	-0.991886370258d-22	0.77446895d-23	-0.891302764852d-22	0.69593277d-23
Y_{05}	-0.302645834908d-23	0.14198265d-26	-0.274507149680d-23	0.13525753d-26
Y_{15}	-0.213752833820d-24	0.19033035d-26	-0.192076932894d-24	0.17102836d-26
Y_{25}	-0.859498361229d-26	0.66826056d-27	-0.764869371524d-26	0.59468656d-27
Y_{35}	0.232271585300d-27	0.10610624d-27	0.204699691290d-27	0.93510850d-28
Y_{06}	-0.143353321047d-28	0.34066359d-31	-0.127570417259d-28	0.30316605d-31
Y_{16}	-0.938942511563d-30	0.35128789d-31	-0.827484954768d-30	0.30958817d-31
Y_{26}	-0.119248097437d-30	0.62055389d-32	-0.104076205169d-30	0.54160083d-32
Y_{07}	-0.555051662763d-34	0.14576325d-36	-0.484432640640d-34	0.12721452d-36
Y_{17}	-0.635529599007d-35	0.22080258d-36	-0.549306398865d-35	0.19084606d-36
Y_{27}	0.112926824095d-36	0.83371962d-37	0.966617996732d-37	0.71363768d-37
Y_{08}	-0.243178098514d-39	0.21881440d-41	-0.208152782403d-39	0.18729849d-41
Y_{18}	-0.495745388794d-40	0.14290617d-41	-0.420238010524d-40	0.12113991d-41
Y_{09}	-0.118749376845d-44	0.68638557d-47	-0.996889160959d-45	0.57621674d-47
Y_{19}	-0.841285958741d-46	0.14203860d-46	-0.699420023496d-46	0.11808667d-46
Y_{010}	-0.641617280330d-50	0.54105776d-52	-0.528261985340d-50	0.44546740d-52
Y_{011}	-0.282069301129d-55	0.31994519d-57	-0.227764954921d-55	0.25834964d-57

Table 3 – Continued

Coeff.	$^{14}C^{33}S$		$^{14}C^{34}S$	
	Values	Uncertainties	Values	Uncertainties
Y_{10}	0.121084765544d+04	0.99314939d-04	0.120554228145d+04	0.10971693d-03
Y_{20}	-0.577222788246d+01	0.32440676d-04	-0.572174101334d+01	0.33964671d-04
Y_{30}	0.319397463610d-02	0.78447165d-05	0.315217825578d-02	0.77420630d-05
Y_{40}	0.177760897469d-05	0.10359151d-05	0.174666140291d-05	0.10178801d-05
Y_{50}	-0.405259242885d-06	0.52360007d-07	-0.396459292234d-06	0.51223043d-07
Y_{01}	0.727975898037d+00	0.29839692d-07	0.721610967886d+00	0.31227025d-07
Y_{11}	-0.495031720761d-02	0.14179028d-07	-0.488552881455d-02	0.14362272d-07
Y_{21}	-0.702743207051d-06	0.34899033d-08	-0.690502973586d-06	0.34294823d-08
Y_{31}	-0.204508134123d-07	0.35145342d-09	-0.200067368071d-07	0.34382195d-09
Y_{41}	-0.406254659700d-10	0.16038944d-10	-0.395691946587d-10	0.15621928d-10
Y_{51}	-0.159009405797d-10	0.25179255d-12	-0.154196619970d-10	0.24417158d-12
Y_{02}	-0.105266688492d-05	0.68627011d-11	-0.103433908543d-05	0.66840302d-11
Y_{12}	-0.982414718649d-09	0.31672265d-12	-0.961011200805d-09	0.31401503d-12
Y_{22}	-0.267406243164d-10	0.20248437d-12	-0.260453620312d-10	0.19721972d-12
Y_{32}	-0.895630095283d-13	0.28201586d-13	-0.868521788029d-13	0.27347999d-13
Y_{42}	-0.188925955666d-13	0.19862262d-14	-0.182405046861d-13	0.19176703d-14
Y_{03}	0.175121957983d-12	0.19153872d-16	0.170571145693d-12	0.18630028d-16
Y_{13}	-0.108970330837d-13	0.87686567d-17	-0.105671846784d-13	0.85045803d-17
Y_{23}	-0.149954393719d-15	0.19160375d-17	-0.144778615076d-15	0.18499057d-17
Y_{33}	-0.251741743224d-17	0.25499627d-18	-0.241987894718d-17	0.24511632d-18
Y_{43}	-0.219425078080d-19	0.23028968d-19	-0.209999301871d-19	0.22039719d-19
Y_{04}	-0.141788178146d-17	0.11063007d-21	-0.136892025602d-17	0.10763177d-21
Y_{14}	-0.422698927840d-19	0.27107768d-21	-0.406321265347d-19	0.26057450d-21
Y_{24}	-0.601413707027d-21	0.66805180d-22	-0.575578961695d-21	0.63935445d-22
Y_{34}	-0.846983584644d-22	0.66132829d-23	-0.807048744275d-22	0.63014711d-23
Y_{05}	-0.262068813915d-23	0.12915164d-26	-0.250810286072d-23	0.12362403d-26
Y_{15}	-0.182526090533d-24	0.16252437d-26	-0.173920079247d-24	0.15486164d-26
Y_{25}	-0.723474742042d-26	0.56250224d-27	-0.686343191302d-26	0.53363245d-27
Y_{35}	0.192725710137d-27	0.88040902d-28	0.182033279782d-27	0.83156392d-28
Y_{06}	-0.120666323107d-28	0.28675686d-31	-0.114473255901d-28	0.27203771d-31
Y_{16}	-0.779080928412d-30	0.29147860d-31	-0.735857486340d-30	0.27530726d-31
Y_{26}	-0.975349530154d-31	0.50756109d-32	-0.917201173939d-31	0.47730151d-32
Y_{07}	-0.453985757526d-34	0.11921934d-36	-0.426920049563d-34	0.11211201d-36
Y_{17}	-0.512400862722d-35	0.17802396d-36	-0.479741577069d-35	0.16667714d-36
Y_{27}	0.897504086031d-37	0.66261207d-37	0.836617845336d-37	0.61766081d-37
Y_{08}	-0.193269702568d-39	0.17390612d-41	-0.180158379943d-39	0.16210808d-41
Y_{18}	-0.388385719640d-40	0.11195811d-41	-0.360451739790d-40	0.10390580d-41
Y_{09}	-0.917067196525d-45	0.53007824d-47	-0.847380011275d-45	0.48979784d-47
Y_{19}	-0.640440385238d-46	0.10812882d-46	-0.589181293718d-46	0.99474467d-47
Y_{010}	-0.481477915338d-50	0.40601691d-52	-0.441001223602d-50	0.37188499d-52
Y_{011}	-0.205677432181d-55	0.23329540d-57	-0.186739603064d-55	0.21181398d-57

Table 3 – Continued

Coeff.	$^{14}C^{36}S$	
	Values	Uncertainties
Y_{10}	0.119572257154d+04	0.13931781d-03
Y_{20}	-0.562888054720d+01	0.39464112d-04
Y_{30}	0.307578231591d-02	0.75544314d-05
Y_{40}	0.169044862128d-05	0.98512172d-06
Y_{50}	-0.380575019863d-06	0.49170777d-07
Y_{01}	0.709903849041d+00	0.37035202d-07
Y_{11}	-0.476710827705d-02	0.15460381d-07
Y_{21}	-0.668270357816d-06	0.33197129d-08
Y_{31}	-0.192051602949d-07	0.33004684d-09
Y_{41}	-0.376744841018d-10	0.14873895d-10
Y_{51}	-0.145617436729d-10	0.23058656d-12
Y_{02}	-0.100104878391d-05	0.63642384d-11
Y_{12}	-0.922382615499d-09	0.31427741d-12
Y_{22}	-0.247982195804d-10	0.18777612d-12
Y_{32}	-0.820199019539d-13	0.25826412d-13
Y_{42}	-0.170853470032d-13	0.17962259d-14
Y_{03}	0.162407806365d-12	0.17909692d-16
Y_{13}	-0.997920548627d-14	0.80337183d-17
Y_{23}	-0.135609892368d-15	0.17327551d-17
Y_{33}	-0.224816933570d-17	0.22772337d-18
Y_{43}	-0.193509216675d-19	0.20309061d-19
Y_{04}	-0.128218901798d-17	0.10336458d-21
Y_{14}	-0.377489547675d-19	0.24208441d-21
Y_{24}	-0.530381925178d-21	0.58914940d-22
Y_{34}	-0.737618830833d-22	0.57593610d-23
Y_{05}	-0.231113984370d-23	0.11395155d-26
Y_{15}	-0.158957840431d-24	0.14153933d-26
Y_{25}	-0.622188506588d-26	0.48375217d-27
Y_{35}	0.163674066996d-27	0.74769545d-28
Y_{06}	-0.103773075971d-28	0.24660669d-31
Y_{16}	-0.661641583684d-30	0.24754063d-31
Y_{26}	-0.817978911432d-31	0.42566762d-32
Y_{07}	-0.380736099486d-34	0.99984270d-37
Y_{17}	-0.424358874607d-35	0.14743551d-36
Y_{27}	0.734009160244d-37	0.54190658d-37
Y_{08}	-0.158062491626d-39	0.14222546d-41
Y_{18}	-0.313667777856d-40	0.90419734d-42
Y_{09}	-0.731390679761d-45	0.42275404d-47
Y_{19}	-0.504392454968d-46	0.85159115d-47
Y_{010}	-0.374462085382d-50	0.31577573d-52
Y_{011}	-0.155991645407d-55	0.17693634d-57

[a]One standard error.