The Rotationally Resolved Infrared Spectrum of TiO and Its Isotopologues

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ABSTRACT

In this study, we present the ro-vibrationally resolved gas-phase spectrum of the diatomic molecule TiO around 1000 cm\(^{-1}\). Molecules were produced in a laser ablation source by vaporizing a pure titanium sample in the atmosphere of gaseous nitrous oxide. Adiabatically expanded gas, containing TiO, formed a supersonic jet and was probed perpendicularly to its propagation by infrared radiation from quantum cascade lasers. Fundamental bands of \(^{46-50}\)TiO and vibrational hotbands of \(^{48}\)TiO are identified and analyzed. In a mass-independent fitting procedure combining the new infrared data with pure rotational and electronic transitions from the literature, a Dunham-like parameterization is obtained. From the present data set, the multi-isotopic analysis allows to determine the spin-rotation coupling constant \(\gamma\) and the Born-Oppenheimer correction coefficient \(\Delta_{\text{U10}}^{\text{Ti}}\) for the first time. The parameter set enables to calculate the Born-Oppenheimer correction coefficients \(\Delta_{\text{U02}}^{\text{Ti}}\) and \(\Delta_{\text{U02}}^{\text{O}}\). In addition, the vibrational transition moments for the observed vibrational transitions are reported.

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Keywords: spectroscopy — high-resolution — infrared — ro-vibrational — titanium monoxide — isotopologues — hotbands

1. INTRODUCTION

Since 1904, when the British astronomer Alfred Fowler (1868-1940) showed similarities between the spectra of Antarian stars\(^1\) and the arc spectrum of titanium oxide (TiO), TiO has become a molecule of astrophysical relevance (Fowler 1904). In the second half of the 20\(^{\text{th}}\) century, the blue-green emission in late-type stars were assigned to electronic transitions of TiO by Merrill et al. (1962). Since 1973, the strength of the prominent VIS-UV lines of TiO in spectra of late-type stars are used to classify stars within the Morgan-Keenan spectral classification scheme (Morgan & Keenan 1973). In rare cases, emission bands of TiO can be found in optical spectra of warm circumstellar environments (Barnbaum et al. 1996; Kamiński et al. 2010). Metal oxides, like TiO, are thought to play an important role in the change of the VIS-UV apparent magnitude in Mira-type variable stars at optical as well as infrared wavelengths, as has been demonstrated by Reid & Goldston (2002).

Up to now, TiO signatures in stellar spectra are the topic of many observational studies. Chavez & Lambert (2009) detected isotopologues of TiO towards local M-dwarf stars, such as GJ699 or GJ701, at optical wavelengths. The derived isotopic abundances in these objects are similar to the natural abundance found on earth. Kamiński et al. (2013) detected pure rotational transitions from TiO towards the oxygen-rich late-type star VY Canis Majoris for the first time using the submillimeter array (SMA) between 279.1 GHz and 335.1 GHz. In a follow-up study towards Mira (o-Ceti) at submm-wavelength, the detection of all stable titanium isotopologues was reported, with the exception of \(^{47}\)TiO (Kamiński et al. 2017). In these studies it was shown, that the titanium-bearing molecules, TiO and TiO\(_2\), are found outside the dust forming regions. From the high abundance, the authors concluded that a substantial fraction of titanium is present as gas-phase species and not as solid dust grains. This is an indication that titanium oxides do not initiate the dust formation - as

\(^1\) i.e. the spectrum of stars like Antares, \(\alpha\) Herculis or o Ceti
previously believed. The authors added that titanium might still support the formation of silicate
dust. Recently, pure rotational transitions of vibrationally excited TiO were identified towards the
AGB stars R Dor and IK Tau by Danilovich et al. (accepted 2020).

First evidence for signs of TiO in atmospheres of extrasolar planets (exoplanets) were found in the
atmosphere of the ultra-hot jupiter WASP-121b (Evans et al. 2016), while earlier studies indicated
no presence of TiO in the atmosphere of other investigated exoplanets (Huitson et al. 2013; Sing
et al. 2013). TiO is proposed to contribute to thermal inversion in the atmospheres of hot Jupiters,
which is in good agreement with self-consistent atmospheric models Piette et al. (2020). Recently,
an improved TiO line list was added to the ExoMol database (Tennyson et al. 2016; McKemmish
et al. 2019), which contains molecules associated with atmospheres of exoplanets. Based on this line
list, Pavlenko et al. (2020) investigated the spectra of the M dwarfs GJ15A and GJ15B, revealing
non-solar isotopic titanium ratios deduced from synthetic spectra of the TiO isotopologues. Using
the Spitzer (IR) Space Telescope, Smolders et al. (2012) published a paper, where they assigned an
infrared emission band of the S-type star NP Aurigae to TiO. The spectrum was taken at a resolution
of $2\text{ cm}^{-1}$ and no individual ro-vibrational transitions could be resolved. In the same work, further
candidates of TiO emission bands were suggested in the spectra of RX Psc and V899 Aql, but could
not be verified.

In terms of laboratory investigations, TiO has been intensively studied in various experiments. An
overview of the works targeting the main isotopologue $^{48}\text{Ti}^{16}\text{O}$ is given by McKemmish et al. (2017).
In the early stages, TiO was commonly produced from modulated high-voltage arc discharge sources,
like in the work of Phillips (1950). J. Phillips identified the $^{1}\Pi - ^{1}\Delta$ and the $^{1}\Phi - ^{1}\Delta$ bands of the
main isotopologue of TiO in the spectra using a grating spectrograph. Initially, it was mistakenly
assumed that the triplet electronic state $^{3}\Pi$ is the ground-state (Lowater 1929; Phillips 1951). In
1969, the $^{3}\Delta$ state was correctly assigned as electronic ground-state (Phillips 1969). Fletcher et al.
(1993) investigated the hyperfine splitting of $^{47}\text{TiO}$, that originates from the $I = 5/2$ spin of the
rare titanium isotope, using laser induced fluorescence spectra from the $^{3}\Pi - ^{3}\Delta$ transition. Amiot
et al. (1995, 1996) performed crossed beam experiments between a molecular beam of TiO and
a continuous wave tunable laser to study the $^3\Pi - ^3\Delta$ and the $^1\Phi - ^1\Delta$ bands at sub-Doppler resolution. The laser induced fluorescence spectra led to a comprehensive determination of the rotational molecular constants, as well as spin-orbit- and spin-spin-coupling constants, $A$ and $\lambda$. A few years later, two bands, $^3\Phi - ^3\Delta$ and $^1\Pi - ^1\Delta$ of the TiO main isotopologue, were identified in sunspots by Ram et al. (1996, 1999). This observation was based on laboratory measurements conducted between 10,000 and 16,000 cm$^{-1}$, where TiO was produced using a hollow cathode lamp. The same authors also improved the $^3\Delta$ ground-state rotational constants of $^{48}$TiO by including pure rotational transitions from jet cooled-measurements. Namiki & Ito (2002) and Namiki et al. (2003, 2004) analyzed several vibronic transitions of $^{48}$TiO of the $^3\Delta$ electronic ground-state in the optical frequency range. Measurements of the $^3\Pi - ^3\Delta$ transition of all TiO isotopologues in a jet-cooled experiment were performed by Kobayashi et al. (2002). Pure rotational transitions of laser ablated TiO were measured by Kania et al. (2008) in a supersonic-jet expansion utilizing millimeter-wave spectroscopy. Recently, Lincowski et al. (2016) presented a spectroscopic analysis of the rare isotopologues of TiO by means of high-resolution millimeter/submillimeter spectroscopy. From this study hyperfine constants of $^{47}$TiO and $^{49}$TiO were determined. The results agree well with those obtained by Fletcher et al. (1993). Lincowski et al. (2016) also obtained rotational constants, including centrifugal distortion constants for spin-spin and spin-orbit parameters, for all stable titanium isotopologues. Breier et al. (2019) conducted measurements for all stable titanium isotopologues of TiO around 300 GHz. The data were analyzed using a mass-independent Dunham approach, which allows to investigate all isotopologues in a global fit, thus combining measurements at microwave and optical wavelengths. In turn, the Dunham analysis allowed to predict frequencies for the radioactive molecule $^{44}$TiO within a sub-MHz uncertainty. This unstable isotopologue decays with a half-life of 60 years and is of particular interest in the context of young supernova remnants (Siegert et al. 2015; Tsygankov et al. 2016; Austin et al. 2017). The titanium isotope $^{44}$Ti is synthesized in core-collapse supernovae during helium burning reactions.

In this study, we present the first measurement of the infrared spectra of TiO and of all stable titanium isotopologues as well as the spectra of the vibrational hotbands of $^{48}$TiO. In total 1034
transitions have been assigned and a line list with data of accuracy better than $10^{-3}\text{cm}^{-1}$ was assembled to guide future astronomical observations. Transitions from vibrationally excited states of up to $v = 3$ have been observed in our experiments. Together with data from the literature (Breier et al. 2019; Lincowski et al. 2016; Fletcher et al. 1993; Ram et al. 1999; Amiot et al. 1995), a mass-independent Dunham analysis, based on that presented in Breier et al. (2019), was performed, which results in new insights into the vibrational potential of TiO.

2. EXPERIMENTAL APPROACH

The experiments in this work have been performed using a laser ablation technique combined with a supersonic jet expansion, intersected with infrared radiation from a quantum cascade laser (QCL), see Witsch et al. (2019) for a detailed description of the experimental setup. Here, only a brief description is given. A highly intense laser pulse of 7 ns pulse duration with an output power of up to 33.5 mJ/pulse produced by a Nd:YAG laser from Continuum Lasers (Inlite II-20 Series) was focused onto the surface of a pure titanium sample rod and produced a hot titanium plasma ($\sim 10,000\text{K}$). The sample rod with a diameter of 1 cm and a length of 5 cm containing titanium isotopes in natural abundances (see Table 1) was rotated and translated in order to continuously provide a pristine surface for the ablation processes. A helium buffer gas containing 3% of nitrous oxide (N$_2$O) as an oxygen donor was used as a carrier gas, for picking up parts of the ablated material. A Parker Series 9 General Valve was used to produce carrier gas pulses of 500 $\mu$s duration. In a subsequent reaction channel of 4 mm length and 12 mm $\times$ 1 mm cross section, TiO was formed and finally adiabatically expanded into a vacuum chamber of $1.2 \times 10^{-1}\text{mbar}$ background pressure. As a result, a supersonic jet was formed, which was probed by a quantum cascade laser (QCL) beam perpendicular to its propagation. A Herriott-type multi-pass cell (Herriott et al. 1964) guided the radiation 40 times through the jet to increase the absorption length. The experiment was operated at a repetition rate of 20 Hz. The delay between the gas flow and the ablation laser pulse was controlled by a trigger pulse generator (Quantum Composers 9300 series) to optimize the TiO yield.

In the frequency range between 984 and 992 cm$^{-1}$, spectra were measured in a step-scan mode (Witsch et al. 2019), using a narrow linewidth distributed feedback (DFB) QCL (Alpes Lasers).
After 40 ablation processes the QCL was stepped by $1.62 \times 10^{-4} \text{cm}^{-1}$. A liquid nitrogen cooled mercury cadmium tellurid (MCT) detector with 300 kHz response was used to record absorption signals of TiO.

Furthermore, experiments were performed between 971 cm$^{-1}$ and 1032 cm$^{-1}$ using a mode-hop-free external cavity (ec) QCL from Daylight Solutions. The infrared radiation was detected by a fast liquid nitrogen cooled 1 GHz-response-MCT detector. By applying a 200 kHz frequency modulation to the ec-QCL, spectral intervals of 0.03 cm$^{-1}$ width were acquired 600 times before stepping to the next spectral interval.

All spectra were calibrated by simultaneously measuring the spectrum of an internally coupled etalon with a free spectral range of 0.006 cm$^{-1}$ (0.01 cm$^{-1}$ in step scan measurements) and the spectrum of methanol (CH$_3$OH) in a Herriott-type multi-pass gas cell. The pressure in the cell was reduced until the Doppler width dominated the line broadening. The reference spectrum was calibrated using line positions from the Hitran database (Xu et al. 2004). The calibration accuracy was better than $2.8 \times 10^{-4} \text{cm}^{-1}$.

3. THE IR SPECTRUM OF TiO

In this study, we present the first rotationally resolved infrared spectrum of TiO between 971.2 cm$^{-1}$ and 1031.9 cm$^{-1}$, as shown in Figure 1. The laser ablation source does not provide a constant molecular yield, which causes intensity fluctuations in the observed spectrum. A total of 1034 transitions were assigned to the fundamental bands of TiO and its stable titanium isotopologues, $^{46-50}$TiO, as well as vibrational hotbands of the main isotopologue $^{48}$TiO. The typical linewidth is $2 \times 10^{-3} \text{cm}^{-1}$ (60 MHz). The band centers are listed in Table 1. A detailed list of transitions is provided in the supplemental material in Tables 5 to 12.

For the main isotopologue, $^{48}$TiO, ro-vibrational transitions in the $^3\Delta$ electronic ground state of $J''$ up to 25 and 32 have been assigned to the P- and the R-branch, respectively. In addition, 63 Q-branch transitions were assigned. As listed in Table 1, several hotband transitions of $^{48}$TiO and transitions originating from $^{46}$TiO, $^{47}$TiO, $^{49}$TiO and $^{50}$TiO are identified (see Figure 1) and appear in natural abundance. Transitions of $^{47}$TiO (nuclear spin $I = 5/2$) and $^{49}$TiO ($I = 7/2$) with low $J''$
values exhibit larger linewidths of up to $2.5 \times 10^{-3}$ cm$^{-1}$ (75 MHz), because of the unresolved hyperfine structure. Due to the spin-orbit coupling, energy levels split into three $\Omega$-components. Transitions between different $\Omega$ are prohibited by selection rules, resulting in three transitions for each $J''$ as can be seen in the upper plot in Figure 1. For $J'' > 6$ the splitting into three $\Omega$-components was observed for all isotopologues. However, as the total angular momentum can not be smaller than its components, only states with $J \geq \Omega$ exist, thus dissolving the triplet structure for the lowest $J''$ transitions. Furthermore, for $J'' \leq 5$, some $\Omega = 3$ transitions were too weak to be observed and for the lowest $J''$ values some $\Omega = 2$ components could not be detected due to the unfavorable partition function.

Finally, transitions belonging to higher vibrational states ($v'' \geq 1$) of $^{48}$TiO were found in the observed spectrum. In total 3 hotbands were assigned ($v = 2 \leftarrow 1, 3 \leftarrow 2$ and $4 \leftarrow 3$) indicating that the vibrational excitation of TiO is not effectively cooled in the supersonic jet expansion – contrary to the rotational excitation. The most populated hotband ($v = 2 \leftarrow 1$) exhibits Q-branch transitions at 990.9 cm$^{-1}$, while the Q-branches from the other hotbands are too weak to be observed in our spectrum.

4. ISOTOPICALLY INVARIANT FITTING PROCEDURE

The energy levels of the diatomic molecules, titanium monoxide and its isotopologues, can be described by the Dunham formalism (Dunham 1932a,b) to obtain a mass-independent molecular parameterization, according to Equation 1. Molecular parameters of TiO were derived from a global data set analysis using high-resolution data from Breier et al. (2019) and the here presented mid-IR measurements on multi-isotopologue ro-vibrational TiO transitions. The mass-independent molecular parameterization is described in detail by Breier et al. (2018, 2019). In short, the parameter description of TiO is obtained by an adjustment procedure of the following isotopically invariant equation of the molecular parameters,

$$X_{v,\alpha} = \sum_k \left\{ \eta \cdot \mu_{\alpha} \cdot \frac{2l+k}{2} \cdot \left( 1 + \sum_{i=Ti,O} \frac{m_i}{M_{\alpha}} \Delta_i \hat{O}_{k,i} \right) \cdot \hat{O}_{k,i} \cdot \left( v + \frac{1}{2} \right)^k \right\}. \quad (1)$$
Figure 1. The infrared spectrum of TiO. Lower plot: The measured spectrum is shown (upper trace, red) together with a simulated spectrum (lower trace, black) of the fundamental bands of $^{46-50}$TiO and hotbands of $^{48}$TiO up to $v = 4 \leftarrow 3$ assuming a rotational temperature of 247 K. In the simulation the vibrational temperature is assumed to be 1250 K and the isotopologues are simulated using their natural abundance values (De Laeter et al. 2003). Upper plot: A detailed view of the spectrum around 987.8 cm$^{-1}$. The three Ω components of the fundamental band of $^{48}$TiO are marked in red, fundamental transitions assigned to the rare isotopologues of TiO are labeled in green. Transitions assigned to the $^{48}$TiO hotbands are labeled in blue. The vibrational quantum numbers for hotband transitions are indicated.
Table 1. Number of assigned transitions in the observed spectrum of TiO, its isotopologues, and hot-bands together with measured band centers $\nu$ and calculated vibrational transition moments. The natural abundance of titanium isotopes is given in percent. A detailed list of transitions is given in Tables 5 to 12.

| Isotopologue/Transition | Natural abundance$^a$ | $\nu_{i\rightarrow i-1}$ (cm$^{-1}$) | P-branch | Q-branch | R-branch | $|\langle \nu_i |\mu| \nu_{i-1} \rangle|$(D) |
|-------------------------|----------------------|---------------------------------|----------|----------|----------|-----------------|
| $^{48}$TiO $v = 1 \leftarrow 0$ | 73.720(22) | 1000.0410(5) | 63 | 47 | 89 | 0.230 0.230 |
| $v = 2 \leftarrow 1$ | | 990.8839(5) | 41 | 32 | 103 | 0.323 0.323 |
| $v = 3 \leftarrow 2$ | | 981.7032(6) | 14 | 0 | 69 | 0.393 0.393 |
| $v = 4 \leftarrow 3$ | | 972.4989(7) | 0 | 0 | 42 | 0.452 0.451 |
| $^{46}$TiO $v = 1 \leftarrow 0$ | 8.249(21) | 1005.4076(5) | 73 | 0 | 69 | – – |
| $^{47}$TiO $v = 1 \leftarrow 0$ | 7.437(14) | 1002.6670(5) | 64 | 0 | 73 | – – |
| $^{49}$TiO $v = 1 \leftarrow 0$ | 5.409(10) | 997.5060(5) | 49 | 0 | 79 | – – |
| $^{50}$TiO $v = 1 \leftarrow 0$ | 5.185(13) | 995.0733(5) | 48 | 0 | 79 | – – |

$^a$Values taken from De Laeter et al. (2003)

$^b$Values are calculated according to McKemmish et al. (2019) using DUO (Yurchenko et al. 2016)

The isotopic invariant Dunham-like fitting parameter $\hat{O}_{k,l}$ takes a central role in Equation 1. The index $l$ describes the expansion of molecular parameters in terms of the the angular momentum operator $\hat{N}^2$, $\hat{N}^4$, $\ldots$, $\hat{N}^{2l}$ for the isotopologue $\alpha$ in its vibrational state $v$. For example, the molecular parameters $B_{v,\alpha}$, $D_{v,\alpha}$ and $H_{v,\alpha}$ for $l = 1$, 2, 3, respectively, are obtained from the Dunham parameters $\hat{O}_{k,l} = U_{k,l}$. The index $k$ is the ro-vibrational coupling order ($(v + 1/2)^k$). In the case of $l = 1$, the Dunham parameter $U_{k,l}$ are linked to the equilibrium rotational constant ($k = 0$) or the rotation-vibration interaction constants ($k = 1, 2, \ldots$). Analogous, Dunham-like parameters $\hat{O}_{k,l}$, such as $A_{k,l}$, $\gamma_{k,l}$ and $eQq_{0,k,l}$, are used to describe the fine- and hyperfine-structure, e.g. the spin-orbit coupling constant $A$, the spin-rotation coupling constant $\gamma$ or the electric hyperfine-structure parameter $eQq_0$. The coefficient $\eta$ in Equation 1 is a nucleus scaling factor being unity for rotational and fine-structure parameters. For hyperfine parameters, $\eta$ is set to be the nuclear $g_N$-factor for magnetic hyperfine parameters and the electric hyperfine parameters are scaled by the electric quadrupole moment $Q$. 

respectively. The scaling values of TiO are given in Breier et al. (2019). The isotopic invariance is introduced into Equation 1 by the reduced mass $\mu_\alpha$. To obtain a more precise description of the mass invariance, the Born-Oppenheimer breakdown (BO) correction is given as sum over parameters $\Delta^i_{O_k,l}$. Its mass dependency is given by the fraction of the electron mass $m_e$ and the mass of atom $M_i^\alpha$ ($i = \text{Ti}, \text{O}$). In this work, the BO correction parameters $\Delta^i_{O_k,l}$ are determined in addition to the first-order vibrational, rotational and spin-orbital expansion terms $U_{10}, U_{01}$ and $A_{00}$, respectively.

In our analysis we used the isotope masses of titanium and oxygen as published by AME2016 (Wang et al. 2017). The generalized equation is implemented in the program PGOPHER (Western 2017). Contrary to Breier et al. (2019), the weighting process of the various data sets is changed and the well-defined iterative re-weighting procedure introduced by Watson (2003) is used to improve the reproducibility. The ROBUST parameter value of PGOPHER was determined to be 0.1.

One advantage of a mass-independent analysis is that the effect of the spin-rotation interaction onto the energy level is distinguishable from the centrifugal distortion of the spin-orbital effects due to their difference in mass scaling behavior (Müller et al. 2015). In this work, two different fitting sets are obtained by excluding the spin-rotation interaction ("Fit A") or by including this contribution ("Fit B") in the parameter set. Both parameter sets describe the electronic ground-state ($X^3\Delta$) of TiO with 29 mass-independent Dunham-like molecular parameters, which are shown in Table 2. The confidence of parameter set "Fit B" is emphasized and its usage for TiO is recommended. This Dunham-like parameter set corresponds to 150 effective molecular parameters which describe the vibrational states $v = 0$ to 4 of $^{48}$TiO and the vibrational states $v = 0, 1$ of the observed rare isotopologues (including the hyperfine structure of $^{47}$TiO and $^{49}$TiO). Parameters for the $A^3\Phi$ and $B^3\Pi$ state, which are obtained from the global fit, are listed in Tables 13 and 14 of the supplementary material and are not further discussed. The uncertainty of the here measured IR data is $5.2 \times 10^{-4}$ cm$^{-1}$. The fitting routine within PGOPHER is available on request.
Table 2. Mass-invariant molecular parameters for the $X^3\Delta$ state of TiO based on the analysis of the six stable titanium isotopologues $^{46-50}\text{Ti}^{16}\text{O}$ and $^{48}\text{Ti}^{18}\text{O}$.

| Parameter | This work | Ref. \(^6\) |
|-----------|-----------|-------------|
| $\hat{O}_{k,l}$ | Fit A | Fit B | Fit A | Fit B | Units |
| $U_{00}$ | 0.0 | 0.0 | 0.0 | 0.0 | cm\(^{-1}\) |
| $U_{10} \times 10^{-3}$ | 3.4949905(13) | 3.4949915(13) | 3.4949966(26) | 3.4949959(26) | cm\(^{-1}\) u\(^{1/2}\) |
| $\Delta_{U_{10}}^{\text{Ti}}$ | 0.109(31) | 0.114(31) | – | – | |
| $U_{20} \times 10^{-1}$ | -5.470311(43) | -5.470315(43) | -5.47093(45) | -5.47063(46) | cm\(^{-1}\) u |
| $U_{30} \times 10^{1}$ | -1.6302(23) | -1.6300(23) | -1.587(22) | -1.596(22) | cm\(^{-1}\) u\(^{3/2}\) |
| $U_{01}$ | 6.4227147(57) | 6.42351367(72) | 6.4227037(25) | 6.4234987(74) | cm\(^{-1}\) u |
| $\Delta_{U_{01}}^{\text{Ti}}$ | -8.397(16) | -8.314(16) | -8.253(24) | -8.282(25) | |
| $\Delta_{U_{01}}^{\text{O}}$ | -6.116(25) | -9.769(31) | -6.112(8) | -9.722(29) | |
| $U_{11} \times 10^{1}$ | -1.255794(22) | -1.255799(21) | -1.255825(44) | -1.255631(69) | cm\(^{-1}\) u\(^{3/2}\) |
| $U_{21} \times 10^{3}$ | -1.3339(25) | -1.3337(25) | -1.3467(57) | -1.3542(61) | cm\(^{-1}\) u\(^2\) |
| $U_{02} \times 10^{5}$ | 8.67136(21) | 8.67227(26) | 8.67195(38) | 8.67186(38) | cm\(^{-1}\) u\(^2\) |
| $U_{12} \times 10^{6}$ | 1.7640(47) | 1.7608(47) | 1.7469(81) | 1.7469(81) | cm\(^{-1}\) u\(^{5/2}\) |
| $U_{03} \times 10^{10}$ | 2.08(14) | 2.29(14) | 1.95(17) | 2.05(17) | cm\(^{-1}\) u\(^3\) |
| $A_{00} \times 10^{-1}$ | 5.046090(88) | 5.0642587(62) | 5.065030(11) | 5.064254(14) | cm\(^{-1}\) |
| $\Delta_{A_{00}}^{\text{Ti}} \times 10^{-2}$ | 3.286(15) | – | – | – | |
| $A_{10} \times 10^{3}$ | 5.025(45) | 4.245(42) | 6.77(73) | 4.93(84) | cm\(^{-1}\) u\(^{1/2}\) |
| $A_{20} \times 10^{3}$ | -10.399(53) | -10.421(54) | -10.61(51) | -10.88(53) | cm\(^{-1}\) u |
| $A_{01} \times 10^{4}$ | -3.12190(99) | 1.895(24) | -1.797(10) | 1.722(56) | cm\(^{-1}\) u |
| $\Delta_{A_{01}}^{\text{Ti}} \times 10^{-4}$ | – | – | – | – | |
| $A_{11} \times 10^{5}$ | -3.958(63) | – | -4.25(22) | 7.3(28) | cm\(^{-1}\) u\(^{3/2}\) |
| $\gamma_{01} \times 10^{2}$ | – | 9.326(45) | – | 9.00(10) | cm\(^{-1}\) u |

Table 2 continued on next page
Table 2 (continued)

| Parameter      | This work | Ref.\(^a\) | Units           |
|----------------|-----------|------------|----------------|
| \(\hat{O}_{k,l}\) | Fit A     | Fit B      | Fit A          | Fit B          | Units       |
| \(\gamma_{11} \times 10^2\) | –         | 0.952(12)  | –              | 2.36(52)       | cm\(^{-1}\) \(u^{3/2}\) |
| \(\gamma_{02} \times 10^7\) | –         | 5.10(191)  | –              | –              | cm\(^{-1}\) \(u^2\)   |
| \(\lambda_{00}\) | 1.749446(62) | 1.745255(65) | 1.74974(16)   | 1.74584(18)   | cm\(^{-1}\)       |
| \(\lambda_{10} \times 10^2\) | -1.5066(29) | -1.5454(22) | -1.81(11)     | -2.00(12)     | cm\(^{-1}\) \(u^{1/2}\) |
| \(\lambda_{20} \times 10^3\) | –         | –          | 3.19(85)      | 3.13(85)      | cm\(^{-1}\) \(u\)    |
| \(\lambda_{01} \times 10^6\) | 5.65(20)  | -48.60(29) | 6.64(15)      | -47.76(44)    | cm\(^{-1}\) \(u\)    |
| \(\lambda_{11} \times 10^8\) | 4.7(10)   | –          | –             | –             | cm\(^{-1}\) \(u^{3/2}\) |
| \(a_{00} \times 10^3\) | 5.6198(21) | 5.6136(22) | 5.6220(45)    | 5.6133(46)    | cm\(^{-1}\) \(g_N^{-1}\) |
| \(\Delta a_{00} \times 10^3\) | 4.613(16) | 4.647(16)  | 4.620(31)     | 4.684(31)     | cm\(^{-1}\) \(g_N^{-1}\) \(u^{1/2}\) |
| \(b_{00} \times 10^2\) | 2.7470(11) | 2.7658(12) | 2.7481(30)    | 2.7653(26)    | cm\(^{-1}\) \(g_N^{-1}\) |
| \(c_{00} \times 10^3\) | -2.9640(87) | -3.1638(91) | -2.971(20)    | -3.160(20)    | cm\(^{-1}\) \(g_N^{-1}\) |
| \(c_{01} \times 10^4\) | 1.239(17)  | 1.204(17)  | 1.257(37)     | 1.205(38)     | cm\(^{-1}\) \(g_N^{-1}\) \(u\) |
| \(eQ_{d00} \times 10^3\) | -6.03184(55) | -6.03246(56) | -6.0320(11)  | -6.0322(11)  | cm\(^{-1}\) \(b\) |

\(^a\)Values taken from Breier et al. (2019)

5. MASS-INDEPENDANT DUNHAM-LIKE PARAMETERIZATION

The addition of new mid-IR ro-vibrational transitions confirm and improve the former mass-independent Dunham-like parameterization (Breier et al. 2019), see Table 2. This can be seen, when comparing the equilibrium bond length of \(^{48}\)Ti\(^{16}\)O (\(r_e^{48}\)) with previous works, see Table 3. The here derived value of \(r_e^{48} = 1.62033700(14) \text{ Å}\) is in perfect agreement with the single isotopologue study of Ram et al. (1999) (\(r_e^{48} = 1.62033709(25) \text{ Å}\)) and with the former multi-isotopologue study of Breier et al. (2019) (\(r_e^{48} = 1.62033696(7) \text{ Å}\)). The agreement with the previous works, is also reflected by the
Table 3. Comparison of bond length model values for TiO.

| Bond length (Å) | Ref.               |
|-----------------|--------------------|
| $r_e^{48}$      | 1.62033709(25)     | Ram et al. (1999) |
|                 | 1.62033696(7)      | Breier et al. (2019) |
|                 | 1.62033700(14)     | this work          |
| $r_e^{BO}$      | 1.61999035(93)     | Breier et al. (2019) |
|                 | 1.61998846(90)     | this work          |

$a$ Derived from parameter $U_{01}$ of Fit B listed in Tab. 11 (Breier et al. 2019)

Born-Oppenheimer corrected bond length of TiO $r_e^{BO}$, evaluated from the $U_{01}$ parameter, see Table 3. The difference between the here derived $r_e^{BO}$ and $r_e^{48}$ is solely related to BO correction terms.

5.1. Born-Oppenheimer correction coefficients

With the present TiO parameterization (“Fit B”), three mass-dependent BO correction parameters, namely $\Delta_{U_{01}}^{Ti}$, $\Delta_{U_{01}}^{O}$, and $\Delta_{U_{10}}^{Ti}$, are determined, see Table 4. By comparing the derived $U_{01}$ correction values with those derived from theoretical calculations ($\Delta_{U_{01}}^{Ti} = -4.9$ and $\Delta_{U_{01}}^{O} = -6.7$, Breier et al. (2019)), an almost constant shift of 3 to 3.4 is observed. Besides this difference in absolute values, the experimental results follow the same trend as the calculated $\Delta_{U_{01}}^{Ti}$ and $\Delta_{U_{01}}^{O}$ values, i.e., in both cases the contribution to the mass shift of rotational energy levels is stronger for oxygen than for titanium. The same trend is also observed in the case of ZrO and HfO (Table 4). Furthermore, the vibrational mass correction value of $U_{10}$ for titanium is derived here in the same order as expected from CO and SiO, see Table 4.

By using the Born-Oppenheimer mass correction values $\Delta_{U_{10}}^{A}$ and $\Delta_{U_{01}}^{A}$ for an atom A, Ogilvie (1989) derived an empirical relation to estimate the mass correction value $\Delta_{U_{02}}^{A}$ for the first order centrifugal distortion term $U_{02}$. In case of titanium it is as follows

\[
\Delta_{U_{02}}^{Ti} \approx 3\Delta_{U_{01}}^{Ti} - 2\Delta_{U_{10}}^{Ti},
\]
Table 4. Comparison of Born-Oppenheimer correction values for diatomic molecules of the form AB, i.e., TiO, CO, SiO, ZrO and HfO.

|          | This work | Ref.\textsuperscript{a} | Ref.\textsuperscript{b} | Ref.\textsuperscript{c} | Ref.\textsuperscript{d} |
|----------|-----------|-------------------------|-------------------------|-------------------------|-------------------------|
| TiO      | \( \Delta A_{U_{10}} \) | 0.114(31)               | 0.69547(7)              | 0.567(37)               | –                       | –                       |
| CO       | \( \Delta B_{U_{10}} \) | –                       | -0.16886(7)             | –                       | –                       | –                       |
| SiO      | \( \Delta A_{U_{01}} \) | -8.314(16)              | -2.0567(2)              | -1.2976(44)             | -4.872(39)              | -3.40(57)               |
| ZrO      | \( \Delta B_{U_{01}} \) | -9.769(31)              | -2.1047(2)              | -2.0507(16)             | -6.1888(25)             | -5.656(23)              |

\( \text{a} \) Values taken from Velichko et al. (2012)

\( \text{b} \) Values taken from Müller et al. (2013)

\( \text{c} \) Values taken from Beaton & Gerry (1999)

\( \text{d} \) Values taken from Lesarri et al. (2002)

yielding \( \Delta_{Ti}^{U_{02}} = -25.2(1) \). By applying the Kratzer-Pekeris relation (Kratzer 1920; Pekeris 1934) to \( U_{01} \) and \( U_{10} \), the mass independent first order centrifugal distortion term \( U_{02}^{BO} = 8.67932(3) \times 10^{-5} \text{ cm}^{-1} \text{ u}^{-2} \) is calculated according to:

\[
U_{02}^{BO} = \frac{4U_{01}^3}{U_{10}^2}
\]  

(3)

In contrast to \( U_{02} \), the BO correction is considered for \( U_{02}^{BO} \), and consequently their combination with \( \Delta_{Ti}^{U_{02}} \) allows to calculate the corresponding oxygen Born-Oppenheimer correction value \( \Delta_{U_{02}}^{O} = -15(1) \) according to Equation 1.

5.2. Spin-rotation coupling constant

For a diatomic molecule in a multiplet state \( \Lambda > 0 \), the contribution of the spin-rotation interaction and the centrifugal correction of the spin-orbit coupling to the energy levels are only distinguishable in a multi-isotopic fitting procedure (Müller et al. 2013). In this work, the spin-rotation coupling constant \( \gamma \) for the \( X^\Delta \) ground-state of TiO was determined for the first time. Brown & Watson (1977) have shown that the spin-rotation interaction \( \gamma \hat{N} \cdot \hat{S} \) consists of two contributions \( \gamma^{(1)} \) and \( \gamma^{(2)} \), with \( \gamma^{(1)} \) describing the first-order dipole-dipole interaction contribution of electronic spin and the
rotating charges and $\gamma^{(2)}$ introduces the second-order spin-orbit interaction contribution (Brown & Watson (1977)). The term $\gamma^{(2)}$ dominates in case of molecules with a large spin-orbit interaction. According to Lefebvre-Brion & Field (1986) and assuming a microscopic description of the spin-orbital operator in a single configuration representation for the electronic states, the spin-rotation coupling constant $\gamma$ can be estimated to be

$$\gamma = \gamma^{(1)} + \gamma^{(2)} \approx 2 \frac{A \cdot \bar{B}}{E_{E^3\Pi} - E_{X^3\Delta}} = \gamma^{E-X}. \quad (4)$$

If we consider only contributions from the two lowest lying triplet configuration state $X^3\Delta$ and $E^3\Pi$ ($E_{E^3\Pi} - E_{X^3\Delta} = 11826.9548(5) \text{cm}^{-1}$) of TiO (Kobayashi et al. (2002)) and assume an average spin-orbital contribution of both states of $\bar{A} = 94.0513(5) \text{cm}^{-1}$ as well as an average rotational constant of $\bar{B} = 0.524442(4) \text{cm}^{-1}$, we obtain a spin-rotation coupling constant of $\gamma^{E-X} = 250.058(2) \text{MHz}$ from Equation 4. This value is in fairly good agreement with our experimental value of $\gamma = 236.5(11) \text{MHz}$ suggesting that the strongest contribution of the spin-rotation coupling occurs from the interaction between the states of $E^3\Pi$ and $X^3\Delta$.

5.3. Vibrational Transition Moments

Finally, the vibrational transition moments for the observed vibrational transitions $\nu_{i \rightarrow i-1}$ are calculated. We have utilized the Dunham-like parameterization of TiO to generate the electronic ground-state potential of TiO using the Rydberg-Klein-Rees description (Rydberg 1932, 1933; Klein 1932; Rees 1947). The potential constants are generated with the RKR1 program from Le Roy (2017). The potential is combined with diagonal elements of the dipole moment curve of the $X^3\Delta$ electronic ground-state taken from McKemmish et al. (2019) to determine the vibrational transition moments with the DUO software (Yurchenko et al. 2016). The results are listed in Table 1 and are in excellent agreement with the values reported in the literature. Furthermore, the calculated vibrational transition moments allow to reproduce the line intensities measured in our experiments very well, as depicted in Figure 1.

6. CONCLUSION
In this work, we report on 1034 ro-vibrational transitions of TiO around 1000 cm$^{-1}$. Accurate experimental frequency positions with an uncertainty of better than 10$^{-3}$ cm$^{-1}$ are provided in the supplementary material, see Tables 5 to 12. We have identified the fundamental bands of the stable isotopologues $^{46-50}$TiO, as well as the three lowest lying vibrational hotbands of the main isotopologue $^{48}$TiO. Our data can be used to guide the astronomical search for TiO at infrared frequencies. The tentative detection of TiO towards the S-type star NP Aurigae using low resolution spectra at 1000 cm$^{-1}$ from the Spitzer Space Telescope (Smolders et al. 2012) could be reexamined, using telescopes with high spectral resolution instruments such as EXES or TEXES ($R \sim 100,000$) to unambiguously verify this assignment.

The previous mass-independent Dunham-like parameterization of TiO (Breier et al. 2019) is improved by including experimental mid-IR data of the present study. Our analysis yields a reliable parameterization of the spin-rotation coupling constant $\gamma$ with strong contributions occurring between the states $E^3\Pi$ and $X^3\Delta$. Furthermore, additional Born-Oppenheimer correction coefficients $\Delta^{T_i}_{U_{01}}$, $\Delta^{T_i}_{U_{02}}$, and $\Delta^{0}_{U_{02}}$ have been determined. This enables accurate predictions of highly excited ro-vibrational states of rare TiO isotopologues, such as $^{44}$TiO, within the uncertainty accuracy of the main isotopologue. In addition, the vibrational transition moments are calculated from the Dunham-like parameterization using a RKR potential description as input for the DUO software.

ACKNOWLEDGMENT

This paper is dedicated to the 60th birthday of Stephan Schlemmer from the Universität zu Köln. His friendship and inspiring work in the field of molecular spectroscopy benefited us all. The authors gratefully acknowledge many fruitful discussions, support and advices from Stephan on various occasions. This work is supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) project number 328961117 - SFB 1319 ELCH and project number 326572190 - FU 715/2-1.

SUPPLEMENTARY MATERIALS
The supplementary materials contain lists of the observed infrared transitions for $^{46-50}\text{TiO}$ and the molecular parameters for the electronic states $A^3\Phi$ and $B^3\Pi$.

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Table 5. Observed transitions for $^{48}$TiO, $v = 1 \leftarrow 0$. Experimental errors for line positions are better than $1 \times 10^{-3}$ cm$^{-1}$.

| $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency | Obs-Calc | $E_{\text{lower}}$ | $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency | Obs-Calc | $E_{\text{lower}}$ |
|------|----------|------|----------|-----------|----------|-------------------|------|----------|------|----------|-----------|----------|-------------------|
| 25   | 3        | 24   | 3        | 971.264   | 1.1      | 954.0184          | 25   | 1        | 24   | 1        | 971.8669   | 4.76     | 748.4708          |
| 24   | 2        | 23   | 2        | 972.7568  | 1.2      | 922.4359          | 23   | 3        | 22   | 3        | 973.7034   | 4.13     | 901.2496          |
| 23   | 1        | 22   | 1        | 974.253   | 2.79     | 696.7772          | 22   | 3        | 21   | 3        | 974.9134   | -4.19    | 876.4754          |
| 22   | 2        | 21   | 2        | 975.1595  | 1.08     | 772.2968          | 22   | 1        | 21   | 1        | 975.4376   | 3.41     | 672.51           |
| 21   | 3        | 20   | 3        | 976.119   | 1.24     | 852.7754          | 21   | 2        | 20   | 2        | 976.3521   | 0.68     | 748.8236          |
| 21   | 1        | 20   | 1        | 976.6167  | 6.57     | 649.2964          | 20   | 3        | 19   | 3        | 977.3183   | 3.03     | 830.1499          |
| 20   | 2        | 19   | 2        | 977.5393  | 3.34     | 726.4151          | 20   | 1        | 19   | 1        | 977.7897   | 5.84     | 627.1364          |
| 19   | 2        | 18   | 2        | 978.7201  | 0.33     | 705.0716          | 18   | 3        | 17   | 3        | 979.6993   | 4.15     | 788.1239          |
| 18   | 2        | 17   | 2        | 979.8953  | -0.47    | 684.7934          | 18   | 1        | 17   | 1        | 980.1181   | 2.72     | 585.9782          |
| 17   | 3        | 16   | 3        | 980.8808  | 3.42     | 768.7242          | 17   | 2        | 16   | 2        | 981.0645   | -2.78    | 665.5808          |
| 17   | 1        | 16   | 1        | 981.2736  | 1.88     | 566.9805          | 16   | 3        | 15   | 3        | 982.0568   | 6.2      | 750.4003          |
| 16   | 2        | 15   | 2        | 982.2284  | -0.61    | 647.434           | 16   | 1        | 15   | 1        | 982.4235   | 2.04     | 549.0372          |
| 15   | 3        | 14   | 3        | 983.226   | 0.31     | 733.1527          | 15   | 2        | 14   | 2        | 983.3862   | 0.04     | 630.3534          |
| 15   | 1        | 14   | 1        | 983.568   | 6.5      | 532.1485          | 14   | 3        | 13   | 3        | 984.3897   | -0.15    | 716.9817          |
| 14   | 2        | 13   | 2        | 984.5379  | -1.95    | 614.3391          | 14   | 1        | 13   | 1        | 984.7058   | 1.5      | 516.3146          |
| 13   | 3        | 12   | 3        | 985.5479  | 2.56     | 701.8874          | 13   | 2        | 12   | 2        | 985.684    | -1.04    | 599.3914          |
| 13   | 1        | 12   | 1        | 985.8377  | -2.97    | 501.5357          | 12   | 3        | 11   | 3        | 986.6995   | -0.01    | 687.8703          |
| 12   | 2        | 11   | 2        | 986.824   | -2.6     | 585.5105          | 12   | 1        | 11   | 1        | 986.9651   | 4.5      | 487.8118          |
| 11   | 3        | 10   | 3        | 987.8461  | 6.38     | 674.9304          | 11   | 2        | 10   | 2        | 987.9587   | 3.12     | 572.6966          |
| 11   | 1        | 10   | 1        | 988.0858  | 3.81     | 475.1431          | 10   | 3        | 9    | 3        | 988.9854   | 1.21     | 663.0681          |

*Table 5 continued on next page*
| $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency $E_{lower}$ | Obs-Calc $E_{lower}$ |
|-----|----------|-----|-----------|----------------|------------------|
|     |          |     |           | cm$^{-1}$ | 10$^{-4}$ cm$^{-1}$ | K | cm$^{-1}$ | 10$^{-4}$ cm$^{-1}$ | K |
| 10  | 2        | 9   | 2         | 989.0861 | -5.71          | 560.9499          | 10  | 1        | 9   | 1         | 989.2003 | 0.0          | 463.5298          |
| 9   | 3        | 8   | 3         | 990.1195 | 3.48           | 652.2835          | 9   | 2        | 8   | 2         | 990.2087 | -3.86        | 550.2705          |
| 9   | 1        | 8   | 1         | 990.3095 | 1.56           | 452.9718          | 8   | 3        | 7   | 3         | 991.248   | 9.56         | 642.5769          |
| 8   | 2        | 7   | 2         | 991.3252 | -1.66          | 540.6587          | 8   | 1        | 7   | 1         | 991.4121 | -4.28        | 443.4694          |
| 7   | 3        | 6   | 3         | 992.3694 | 6.53           | 633.9483          | 7   | 2        | 6   | 2         | 992.4361 | 2.9          | 532.1144          |
| 7   | 1        | 6   | 1         | 992.5104 | 6.0            | 435.0226          | 6   | 3        | 5   | 3         | 993.4851 | 6.74         | 626.398           |
| 6   | 2        | 5   | 2         | 993.5402 | -0.01          | 524.638           | 6   | 1        | 5   | 1         | 993.6015 | 3.17         | 427.6315          |
| 5   | 3        | 4   | 3         | 994.5948 | 7.83           | 619.9261          | 5   | 2        | 4   | 2         | 994.6389 | 2.3          | 518.2294          |
| 5   | 1        | 4   | 1         | 994.6874 | 6.33           | 421.2961          | 4   | 3        | 3   | 3         | 995.6978 | 3.7          | 614.5326          |
| 4   | 2        | 3   | 2         | 995.7311 | 0.13           | 512.8887          | 4   | 1        | 3   | 1         | 995.7668 | 3.9          | 416.0165          |
| 3   | 2        | 2   | 2         | 996.8176 | 1.46           | 508.6161          | 3   | 1        | 2   | 1         | 996.8409 | 7.29         | 411.7928          |
| 2   | 1        | 1   | 1         | 997.9085 | 5.14           | 408.625           | 21  | 3        | 21  | 3        | 998.6149 | 10.54        | 852.7754          |
| 20  | 3        | 20  | 3         | 998.7449 | 5.83           | 830.1499          | 19  | 3        | 19  | 3         | 998.8694 | 7.57         | 808.5993          |
| 18  | 3        | 18  | 3         | 998.9869 | 1.09           | 788.1239          | 18  | 2        | 18  | 2         | 998.9989 | 5.81         | 684.7934          |
| 18  | 1        | 18  | 1         | 999.0086 | 2.56           | 585.9782          | 17  | 3        | 17  | 3         | 999.0994 | 7.4          | 768.7242          |
| 17  | 2        | 17  | 2         | 999.1084 | 4.0            | 665.5808          | 17  | 1        | 17  | 1         | 999.1157 | 1.1          | 566.9805          |
| 16  | 3        | 16  | 3         | 999.2049 | 5.64           | 750.4003          | 16  | 2        | 16  | 2         | 999.2116 | 0.58         | 647.434           |
| 16  | 1        | 16  | 1         | 999.2175 | 7.41           | 549.0372          | 15  | 3        | 15  | 3         | 999.3039 | 1.87         | 733.1527          |
| 15  | 2        | 15  | 2         | 999.3093 | 1.55           | 630.3534          | 15  | 1        | 15  | 1         | 999.312   | 0.0          | 532.1485          |
| 14  | 3        | 14  | 3         | 999.3973 | 3.18           | 716.9817          | 14  | 2        | 14  | 2         | 999.4008 | 2.67         | 614.3391          |
| 14  | 1        | 14  | 1         | 999.4013 | 0.5            | 516.3146          | 13  | 1        | 13  | 1         | 999.485  | 4.38         | 501.5357          |
| 13  | 2        | 13  | 2         | 999.485  | -7.96          | 599.3914          | 13  | 3        | 13  | 3         | 999.485  | 10.24        | 701.8874          |
| 12  | 1        | 12  | 1         | 999.5618 | -1.66          | 487.8118          | 12  | 2        | 12  | 2         | 999.565  | -0.26        | 585.5105          |
| 12  | 3        | 12  | 3         | 999.565  | 2.12           | 687.8703          | 11  | 1        | 11  | 1         | 999.6333 | -0.31        | 475.1431          |
| 11  | 2        | 11  | 2         | 999.6381 | -0.77          | 572.6966          | 11  | 3        | 11  | 3         | 999.64   | 5.95         | 674.9304          |

Table 5. continued on next page
Table 5. (continued)

| $J'$ | $Ω'$ | $J''$ | $Ω''$ | Frequency | Obs-Calc | $E_{lower}$ | $J'$ | $Ω'$ | $J''$ | $Ω''$ | Frequency | Obs-Calc | $E_{lower}$ |
|------|------|------|------|-----------|---------|------------|------|------|------|------|-----------|---------|------------|
| 10   | 1    | 10   | 1    | 999.6992  | 4.29    | 463.5298   | 10   | 2    | 10   | 2    | 999.7048  | -3.78   | 560.9499   |
| 10   | 3    | 10   | 3    | 999.7078  | 0.69    | 663.0681   | 9    | 1    | 9    | 1    | 999.7581  | -0.78   | 452.9718   |
| 9    | 2    | 9    | 2    | 999.7659  | -2.12   | 550.2705   | 9    | 3    | 9    | 3    | 999.7702  | 2.67    | 652.2835   |
| 8    | 1    | 8    | 1    | 999.8121  | 3.75    | 443.4694   | 8    | 2    | 8    | 2    | 999.8207  | -1.7    | 540.6587   |
| 8    | 3    | 8    | 3    | 999.8264  | 5.66    | 642.5769   | 7    | 1    | 7    | 1    | 999.8598  | 4.55    | 435.0226   |
| 7    | 2    | 7    | 2    | 999.8699  | 3.05    | 532.1144   | 7    | 3    | 7    | 3    | 999.8763  | 7.82    | 633.9483   |
| 6    | 1    | 6    | 1    | 999.9013  | 3.97    | 427.6315   | 6    | 2    | 6    | 2    | 999.9124  | 1.56    | 524.638    |
| 6    | 3    | 6    | 3    | 999.9199  | 7.99    | 626.398    | 5    | 1    | 5    | 1    | 999.9368  | 1.93    | 421.2961   |
| 5    | 2    | 5    | 2    | 999.9488  | -0.77   | 518.2294   | 5    | 3    | 5    | 3    | 999.9569  | 5.44    | 619.9261   |
| 4    | 1    | 4    | 1    | 999.9668  | 4.25    | 416.0165   | 4    | 2    | 4    | 2    | 999.9793  | 0.15    | 512.8887   |
| 4    | 3    | 4    | 3    | 999.9879  | 4.46    | 614.5326   | 3    | 1    | 3    | 1    | 999.9899  | -2.44   | 411.7928   |
| 3    | 2    | 3    | 2    | 1000.0034 | -2.74   | 508.6161   | 2    | 1    | 2    | 1    | 1000.0081 | 1.52    | 408.625    |
| 3    | 3    | 3    | 3    | 1000.0127 | 4.47    | 610.2177   | 1    | 1    | 1    | 1    | 1000.0215 | 16.7    | 406.5131   |
| 2    | 2    | 2    | 2    | 1000.0215 | -4.25   | 505.4116   | 1    | 1    | 2    | 1    | 1002.12   | 1.6     | 406.5131   |
| 2    | 1    | 3    | 1    | 1003.1582 | 2.4     | 408.625    | 2    | 2    | 3    | 2    | 1003.2084 | 2.07    | 505.4116   |
| 3    | 1    | 4    | 1    | 1004.1906 | 5.64    | 411.7928   | 3    | 2    | 4    | 2    | 1004.252  | 0.61    | 508.6161   |
| 3    | 3    | 4    | 3    | 1004.3031 | 8.44    | 610.2177   | 4    | 1    | 5    | 1    | 1005.2166 | 3.75    | 416.0165   |
| 4    | 3    | 5    | 3    | 1005.3491 | -7.1    | 614.5326   | 5    | 1    | 6    | 1    | 1006.2367 | 4.12    | 421.2961   |
| 5    | 2    | 6    | 2    | 1006.3208 | -0.54   | 518.2294   | 5    | 3    | 6    | 3    | 1006.3916 | 6.12    | 619.9261   |
| 6    | 1    | 7    | 1    | 1007.2508 | 3.59    | 427.6315   | 6    | 2    | 7    | 2    | 1007.3461 | 0.03    | 524.638    |
| 6    | 3    | 7    | 3    | 1007.4263 | 4.76    | 626.398    | 7    | 1    | 8    | 1    | 1008.2592 | 6.22    | 435.0226   |
| 7    | 2    | 8    | 2    | 1008.365  | -1.11   | 532.1144   | 7    | 3    | 8    | 3    | 1008.4551 | 6.9     | 633.9483   |
| 8    | 1    | 9    | 1    | 1009.261  | 3.74    | 443.4694   | 8    | 2    | 9    | 2    | 1009.3779 | 0.0     | 540.6587   |
| 8    | 3    | 9    | 3    | 1009.4772 | 6.22    | 642.5769   | 9    | 1    | 10   | 1    | 1010.257  | 3.58    | 452.9718   |
| 9    | 2    | 10   | 2    | 1010.3847 | 1.57    | 550.2705   | 9    | 3    | 10   | 3    | 1010.4931 | 8.24    | 652.2835   |

Table 5 continued on next page
TiO and Its Isotopologues

Table 5. (continued)

| $J'$ | $Ω'$ | $J''$ | $Ω''$ | Frequency $E_{lower}$ |
|-----|------|------|------|----------------------|
|     |      |      |      | cm$^{-1}$ | 10$^{-4}$ cm$^{-1}$ | K |
| 10  | 1    | 11   | 1    | 1011.2468 | 0.84 | 463.5298 |
| 10  | 3    | 11   | 3    | 1011.5021 | 3.85 | 663.0681 |
| 11  | 2    | 12   | 2    | 1012.3779 | -10.6 | 572.6966 |
| 12  | 1    | 13   | 1    | 1013.2079 | -5.04 | 487.8118 |
| 12  | 3    | 13   | 3    | 1013.5016 | 4.45 | 687.8703 |
| 13  | 2    | 14   | 2    | 1014.3481 | -1.33 | 599.3914 |
| 14  | 1    | 15   | 1    | 1015.1463 | 4.01 | 516.3146 |
| 14  | 3    | 15   | 3    | 1015.4752 | 4.36 | 716.9817 |
| 15  | 2    | 16   | 2    | 1016.2924 | 1.9 | 630.3534 |
| 16  | 1    | 17   | 1    | 1017.0587 | -1.17 | 549.0372 |
| 16  | 3    | 17   | 3    | 1017.4229 | 3.92 | 750.4003 |
| 17  | 2    | 18   | 2    | 1018.2113 | 3.95 | 665.5808 |
| 18  | 1    | 19   | 1    | 1018.9477 | 4.66 | 585.9782 |
| 18  | 3    | 19   | 3    | 1019.3444 | 3.45 | 788.1239 |
| 19  | 3    | 20   | 3    | 1020.2954 | 4.35 | 808.5993 |
| 20  | 2    | 21   | 2    | 1021.0415 | 4.24 | 726.4151 |
| 21  | 1    | 22   | 1    | 1021.7335 | -0.1 | 649.2964 |
| 21  | 3    | 22   | 3    | 1022.1773 | 2.35 | 852.7754 |
| 22  | 2    | 23   | 2    | 1022.8958 | 0.8 | 772.2968 |
| 23  | 1    | 24   | 1    | 1023.56  | -0.21 | 696.7772 |
| 23  | 3    | 24   | 3    | 1024.0331 | 3.61 | 901.2496 |
| 24  | 2    | 25   | 2    | 1024.7244 | -1.6 | 822.4359 |
| 25  | 1    | 26   | 1    | 1025.3619 | 3.55 | 748.4708 |
| 25  | 3    | 26   | 3    | 1025.8622 | 3.85 | 954.0184 |
| 26  | 2    | 27   | 2    | 1026.5274 | -0.48 | 876.8295 |

Table 5 continued on next page
Table 5. (continued)

| $J'$ $\Omega'$ $J''$ $\Omega''$ | Frequency $E_{\text{lower}}$ $E_{\text{lower}}$ cm$^{-1}$ K | $J'$ $\Omega'$ $J''$ $\Omega''$ | Frequency $E_{\text{lower}}$ $E_{\text{lower}}$ cm$^{-1}$ K |
|-------------------------------|---------------------------------|-------------------------------|---------------------------------|
|                               | cm$^{-1}$ 10$^{-4}$ cm$^{-1}$    |                               | cm$^{-1}$ 10$^{-4}$ cm$^{-1}$    |
| 27 1 28 1                     | 1027.1382 2.57 804.3752          | 27 2 28 2                     | 1027.4191 -0.02 905.6208        |
| 27 3 28 3                     | 1027.6644 3.22 1011.0784         | 28 1 29 1                     | 1028.0171 4.55 833.9058         |
| 28 2 29 2                     | 1028.3042 -0.28 935.4746         | 28 3 29 3                     | 1028.5553 1.74 1041.2165        |
| 29 1 30 1                     | 1028.8895 3.92 864.4882          | 29 2 30 2                     | 1029.1829 1.53 966.3904         |
| 29 3 30 3                     | 1029.4395 0.18 1072.4258         | 30 1 31 1                     | 1029.7559 7.55 896.1221         |
| 30 2 31 2                     | 1030.0552 3.94 998.3678          | 30 3 31 3                     | 1030.3169 -1.18 1104.706        |
| 31 1 32 1                     | 1030.6152 3.56 928.8073          | 31 2 32 2                     | 1030.9202 0.51 1031.4064        |
| 31 3 32 3                     | 1031.1878 -0.85 1138.0565        | 32 1 33 1                     | 1031.4688 5.84 962.5434         |
| 32 2 33 2                     | 1031.7792 1.84 1065.5057         |                               |                                 |

Table 6. Observed transitions for $^{48}\text{TiO, }v = 2 \leftrightarrow 1$. Experimental errors for line positions are better than $1 \times 10^{-3}$ cm$^{-1}$.

| $J'$ $\Omega'$ $J''$ $\Omega''$ | Frequency $E_{\text{lower}}$ $E_{\text{lower}}$ cm$^{-1}$ K | $J'$ $\Omega'$ $J''$ $\Omega''$ | Frequency $E_{\text{lower}}$ $E_{\text{lower}}$ cm$^{-1}$ K |
|-------------------------------|---------------------------------|-------------------------------|---------------------------------|
|                               | cm$^{-1}$ 10$^{-4}$ cm$^{-1}$    |                               | cm$^{-1}$ 10$^{-4}$ cm$^{-1}$    |
| 17 3 16 3                     | 971.8212 4.61 1767.8228          | 17 2 16 2                     | 972.0063 3.94 1664.6888         |
| 17 1 16 1                     | 972.216 7.99 1566.096            | 16 2 15 2                     | 973.1647 6.6 1646.6456          |
| 16 1 15 1                     | 973.3607 9.54 1548.2539          | 15 3 14 3                     | 974.1554 4.42 1732.4565         |
| 15 2 14 2                     | 974.3167 4.42 1629.6625          | 14 3 13 3                     | 975.313 -0.26 1716.3786         |
| 14 2 13 2                     | 975.4643 17.63 1613.7396         | 14 1 13 1                     | 975.6325 13.79 1515.7159        |
| 13 2 12 2                     | 976.6038 8.18 1598.8772          | 13 1 12 1                     | 976.7589 8.28 1501.0202         |
| 12 3 11 3                     | 977.612 6.72 1687.435            | 12 2 11 2                     | 977.7382 7.96 1585.0755         |
| 12 1 11 1                     | 977.8802 10.38 1487.3737         | 11 3 10 3                     | 978.7517 2.07 1674.5698         |
| 11 2 10 2                     | 978.8665 6.16 1572.3347          | 10 3 9 3                     | 979.8855 0.08 1662.7758         |
| 10 2 9 2                      | 979.9889 4.71 1560.655           | 10 1 9 1                     | 980.1046 9.57 1463.2285         |

Table 6 continued on next page
| $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | $E_{\text{lower}}$ | Frequency | Obs-Calc | $E_{\text{lower}}$ | Frequency | Obs-Calc |
|-------|---------|-------|-----------|----------------|-----------|---------|----------------|-----------|---------|
| 9     | 3       | 8     | 3         | 981.0131      | -3.98     | 1652.0534| 981.1051      | 0.2       | 1550.0366|
| 9     | 1       | 8     | 1         | 981.2081      | 10.73     | 1452.73 | 982.1354      | 0.05      | 1642.4027|
| 8     | 2       | 7     | 2         | 982.2161      | 5.17      | 1540.4796| 982.3057      | 11.16     | 1443.2811|
| 7     | 3       | 6     | 3         | 983.2507      | -4.49     | 1633.8239| 983.3204      | 2.57      | 1531.9841|
| 7     | 1       | 6     | 1         | 983.3973      | 11.3      | 1434.8819| 984.3605      | -3.85     | 1626.3171|
| 6     | 2       | 5     | 2         | 984.4186      | -0.97     | 1524.5502| 984.4828      | 9.68      | 1427.5324|
| 5     | 3       | 4     | 3         | 985.4644      | -0.39     | 1619.8824| 985.5117      | 4.29      | 1518.1782|
| 5     | 1       | 4     | 1         | 985.5624      | 7.98      | 1421.2327| 986.5646      | 28.28     | 1614.52 |
| 4     | 2       | 3     | 2         | 986.5973      | -3.91     | 1512.8686| 986.6358      | 3.47      | 1415.9829|
| 3     | 2       | 2     | 2         | 987.6782      | 1.47      | 1508.6198| 987.7039      | 5.82      | 1411.7829|
| 2     | 1       | 1     | 1         | 988.7658      | 5.18      | 1408.6329| 990.139       | 0.46      | 1732.4565|
| 14    | 3       | 14    | 3         | 990.2322      | -6.08     | 1716.3786| 990.3192      | -11.39    | 1701.3714|
| 12    | 3       | 12    | 3         | 990.4013      | -3.03     | 1687.435 | 990.4054      | 8.6       | 1487.3737|
| 12    | 2       | 12    | 2         | 990.4054      | 8.03      | 1585.0755| 990.4771      | -11.37    | 1572.3347|
| 10    | 1       | 10    | 1         | 990.5407      | -15.72    | 1463.2285| 990.5456      | 2.26      | 1662.7758|
| 10    | 2       | 10    | 2         | 990.5456      | 0.08      | 1560.655 | 990.6027      | 6.52      | 1452.73 |
| 9     | 2       | 9     | 2         | 990.6074      | 4.45      | 1550.0366| 990.6082      | 2.2       | 1652.0534|
| 8     | 1       | 8     | 1         | 990.6569      | 9.98      | 1443.2811| 990.6629      | 8.3       | 1540.4796|
| 8     | 3       | 8     | 3         | 990.6644      | 1.74      | 1642.4027| 990.7048      | 9.7       | 1434.8819|
| 7     | 2       | 7     | 2         | 990.7115      | 4.25      | 1531.9841| 990.714       | -1.86     | 1633.8239|
| 6     | 1       | 6     | 1         | 990.7462      | 5.71      | 1427.5324| 990.7535      | -4.56     | 1524.5502|
| 6     | 3       | 6     | 3         | 990.7576      | -3.55     | 1626.3171| 990.7819      | 3.67      | 1421.2327|
| 5     | 2       | 5     | 2         | 990.7909      | 0.93      | 1518.1782| 990.7966      | 11.17     | 1619.8824|
| 4     | 1       | 4     | 1         | 990.812       | 5.25      | 1415.9829| 990.8213      | -1.27     | 1512.868|
| 4     | 3       | 4     | 3         | 990.8267      | -1.21     | 1614.52 | 990.8364      | 9.61      | 1411.7829|

Table 6 continued on next page
\begin{table}
\centering
\begin{tabular}{|c|c|c|c|c|c|c|}
\hline
\multicolumn{3}{|c|}{\textit{J}' \ \textit{\Omega}' \ \textit{J}'' \ \textit{\Omega}'' \ \text{Frequency} \ \text{Obs-Calc} \ \text{\textit{E}_{\text{lower}}} \ \text{\textit{K}}} & \multicolumn{3}{|c|}{\textit{J}' \ \textit{\Omega}' \ \textit{J}'' \ \textit{\Omega}'' \ \text{Frequency} \ \text{Obs-Calc} \ \text{\textit{E}_{\text{lower}}} \ \text{\textit{K}}} \\
\hline
3 & 2 & 3 & 2 & 990.8458 & -1.5 & 1508.6198 & 2 & 2 & 2 & 990.8643 & -0.13 & 1505.4335 \\
1 & 1 & 1 & 1 & 990.8655 & 1.49 & 1406.5329 & 1 & 1 & 2 & 1 & 992.9544 & 10.01 & 1406.5329 \\
2 & 1 & 3 & 1 & 993.9865 & 10.96 & 1408.6329 & 2 & 2 & 3 & 2 & 994.0315 & -6.4 & 1505.4335 \\
3 & 1 & 4 & 1 & 995.0123 & 8.61 & 1411.7829 & 3 & 2 & 4 & 2 & 995.0701 & 4.04 & 1508.6198 \\
3 & 3 & 4 & 3 & 995.1179 & 10.77 & 1610.23 & 4 & 1 & 5 & 1 & 996.0323 & 9.04 & 1415.9829 \\
4 & 2 & 5 & 2 & 996.101 & 0.88 & 1512.868 & 4 & 3 & 5 & 3 & 996.158 & 0.59 & 1614.52 \\
5 & 1 & 6 & 1 & 997.0462 & 8.25 & 1421.2327 & 5 & 2 & 6 & 2 & 997.1264 & 3.92 & 1518.1782 \\
5 & 3 & 6 & 3 & 997.1926 & -0.42 & 1619.8824 & 6 & 1 & 7 & 1 & 998.0544 & 10.48 & 1427.5324 \\
6 & 2 & 7 & 2 & 998.1452 & 2.21 & 1524.5502 & 6 & 3 & 7 & 3 & 998.2211 & 0.81 & 1626.3171 \\
7 & 1 & 8 & 1 & 999.0564 & 12.28 & 1434.8819 & 7 & 2 & 8 & 2 & 999.1582 & 6.2 & 1531.9841 \\
7 & 3 & 8 & 3 & 999.2428 & -2.83 & 1633.8239 & 8 & 1 & 9 & 1 & 1000.0518 & 8.17 & 1443.2811 \\
8 & 2 & 9 & 2 & 1000.1648 & 8.37 & 1540.4796 & 8 & 3 & 9 & 3 & 1000.2586 & -0.65 & 1642.4027 \\
9 & 1 & 10 & 1 & 1001.0417 & 9.99 & 1452.73 & 9 & 2 & 10 & 2 & 1001.1648 & 6.96 & 1550.0366 \\
9 & 3 & 10 & 3 & 1001.2682 & 3.92 & 1652.0534 & 10 & 1 & 11 & 1 & 1002.0251 & 7.12 & 1463.2285 \\
10 & 2 & 11 & 2 & 1002.1583 & 3.57 & 1560.655 & 10 & 3 & 11 & 3 & 1002.2706 & 0.56 & 1662.7758 \\
11 & 1 & 12 & 1 & 1003.0028 & 9.0 & 1474.7764 & 11 & 2 & 12 & 2 & 1003.1458 & 3.34 & 1572.3347 \\
11 & 3 & 12 & 3 & 1003.2669 & 0.66 & 1674.5698 & 12 & 1 & 13 & 1 & 1003.974 & 7.08 & 1487.3737 \\
12 & 2 & 13 & 2 & 1004.1273 & 6.17 & 1585.0755 & 12 & 3 & 13 & 3 & 1004.2565 & -1.4 & 1687.435 \\
13 & 1 & 14 & 1 & 1004.9396 & 10.41 & 1501.0202 & 13 & 2 & 14 & 2 & 1005.1022 & 6.98 & 1598.8772 \\
13 & 3 & 14 & 3 & 1005.2397 & -2.9 & 1701.3714 & 14 & 1 & 15 & 1 & 1005.8986 & 8.9 & 1515.7159 \\
14 & 2 & 15 & 2 & 1006.0709 & 8.4 & 1613.7396 & 14 & 3 & 15 & 3 & 1006.2169 & 0.62 & 1716.3786 \\
15 & 1 & 16 & 1 & 1006.8522 & 14.9 & 1531.4605 & 15 & 2 & 16 & 2 & 1007.0328 & 6.06 & 1629.6625 \\
15 & 3 & 16 & 3 & 1007.1869 & -2.01 & 1732.4565 & 16 & 1 & 17 & 1 & 1007.7987 & 11.61 & 1548.2539 \\
16 & 2 & 17 & 2 & 1007.9888 & 7.75 & 1646.6456 & 16 & 3 & 17 & 3 & 1008.151 & 1.98 & 1749.6046 \\
17 & 1 & 18 & 1 & 1008.7393 & 11.09 & 1566.096 & 17 & 3 & 18 & 3 & 1009.1083 & 3.69 & 1767.8228 \\
\hline
\end{tabular}
\caption{continued on next page}
\end{table}
| $J'$ | $Ω'$ | $J''$ | $Ω''$ | Frequency $E_{lower}$ | Obs-Calc $E_{lower}$ | $10^{-4}$ cm$^{-1}$ | cm$^{-1}$ |
|------|------|------|------|---------------------|---------------------|---------------------|---------|
| 18   | 1    | 19   | 1    | 1009.6739          | 12.07               | 1584.9866          | 1009.8809 |
| 18   | 3    | 19   | 3    | 1010.0582          | -3.22               | 1787.1107          | 1010.6018 |
| 19   | 2    | 20   | 2    | 1010.8171          | 1.57                | 1703.9541          | 1011.002  |
| 20   | 1    | 21   | 1    | 1011.5237          | 7.86                | 1625.9124          | 1011.7478 |
| 20   | 3    | 21   | 3    | 1011.9397          | -1.72               | 1828.8943          | 1012.439  |
| 21   | 2    | 22   | 2    | 1012.6717          | 10.94               | 1747.4562          | 1012.8705 |
| 22   | 1    | 23   | 1    | 1013.3494          | 11.98               | 1671.0299          | 1013.5884 |
| 22   | 3    | 23   | 3    | 1013.7946          | -0.25               | 1874.9525          | 1014.2522 |
| 23   | 2    | 24   | 2    | 1014.4996          | 10.99               | 1795.1925          | 1014.7113 |
| 24   | 1    | 25   | 1    | 1015.1496          | 11.57               | 1720.3372          | 1015.403  |
| 24   | 3    | 25   | 3    | 1015.623           | 2.97                | 1925.2823          | 1016.0399 |
| 25   | 2    | 26   | 2    | 1016.3008          | 5.69                | 1847.1604          | 1016.5263 |
| 26   | 1    | 27   | 1    | 1016.9245          | 10.36               | 1773.8323          | 1017.192  |
| 27   | 1    | 28   | 1    | 1017.8026          | 10.5                | 1802.1496          | 1018.3141 |
| 28   | 1    | 29   | 1    | 1018.6737          | 4.73                | 1831.5131          | 1018.9543 |
| 28   | 3    | 29   | 3    | 1019.1981          | -0.65               | 2038.7425          | 1020.075  |
| 30   | 1    | 31   | 1    | 1020.3982          | 8.18                | 1893.3772          | 1020.6906 |
| 30   | 3    | 31   | 3    | 1020.9454          | 0.57                | 2101.8653          | 1021.2507 |
| 31   | 2    | 32   | 2    | 1021.5487          | 7.73                | 2028.4226          | 1021.8082 |
| 32   | 1    | 33   | 1    | 1022.0968          | 7.18                | 1959.4222          | 1022.4    |
| 32   | 3    | 33   | 3    | 1022.6652          | -0.21               | 2169.2443          | 1022.9365 |
| 33   | 2    | 34   | 2    | 1023.2442          | 1.34                | 2097.2846          | 1023.5146 |
| 34   | 1    | 35   | 1    | 1023.7688          | -0.7                | 2029.6452          | 1024.0831 |
| 34   | 3    | 35   | 3    | 1024.3577          | -0.16               | 2240.8752          | 1024.596  |
| 35   | 2    | 36   | 2    | 1024.9138          | 1.8                 | 2170.3611          | 1025.1932 |

Table 6 continued on next page
Table 6. (continued)

| $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency $E_{\text{lower}}$ | Obs-Calc $E_{\text{lower}}$ | $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency $E_{\text{lower}}$ | Obs-Calc $E_{\text{lower}}$ |
|------|-----------|------|------------|----------------------------|---------------------------|------|-----------|------|------------|----------------------------|---------------------------|
| 36   | 1         | 37   | 1          | 1025.4167                  | 8.88 2104.0432            | 36   | 2         | 37   | 2          | 1025.739                   | 7.38 2208.4784            |
| 36   | 3         | 37   | 3          | 1026.0229                  | 1.75 2316.753             | 37   | 1         | 38   | 1          | 1026.2304                  | 8.71 2142.8069            |
| 37   | 2         | 38   | 2          | 1026.5566                  | 2.92 2247.6478            | 37   | 3         | 38   | 3          | 1026.8445                  | -3.68 2356.283            |

Table 7. Observed transitions for $^{48}$TiO, $v = 3 \leftarrow 2$. Experimental errors for line positions are better than $1 \times 10^{-3}$ cm$^{-1}$.

| $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency $E_{\text{lower}}$ | Obs-Calc $E_{\text{lower}}$ | $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency $E_{\text{lower}}$ | Obs-Calc $E_{\text{lower}}$ |
|------|-----------|------|------------|----------------------------|---------------------------|------|-----------|------|------------|----------------------------|---------------------------|
| 9    | 3         | 8    | 3          | 971.8842                   | -9.69 2642.6613           | 9    | 2         | 8    | 2          | 971.9776                   | -7.06 2540.6435           |
| 8    | 1         | 7    | 1          | 973.1733                   | -6.69 2433.9371           | 7    | 3         | 6    | 3          | 974.1096                   | -13.7 2624.5381           |
| 7    | 2         | 6    | 2          | 974.1823                   | 5.14 2522.6952            | 7    | 1         | 6    | 1          | 974.2611                   | 12.88 2425.5857           |
| 6    | 3         | 5    | 3          | 975.2129                   | -16.92 2617.0751          | 6    | 2         | 5    | 2          | 975.2747                   | 2.39 2515.3042            |
| 6    | 1         | 5    | 1          | 975.341                    | 12.74 2418.2781           | 5    | 3         | 4    | 3          | 976.3116                   | -4.8 2610.6779            |
| 5    | 2         | 4    | 2          | 976.3616                   | 5.66 2508.969             | 5    | 1         | 4    | 1          | 976.4151                   | 14.17 2412.0143           |
| 3    | 1         | 2    | 1          | 978.5438                   | 0.37 2402.6183            | 2    | 1         | 1    | 1          | 979.5989                   | -8.14 2399.4863           |
| 1    | 1         | 2    | 1          | 983.7641                   | 2.75 2397.3982            | 2    | 1         | 3    | 1          | 984.7904                   | 6.83 2399.4863            |
| 3    | 1         | 4    | 1          | 985.8106                   | 9.41 2402.6183            | 3    | 2         | 4    | 2          | 985.8639                   | -3.71 2499.4657           |
| 4    | 1         | 5    | 1          | 986.8233                   | -1.92 2406.7943           | 4    | 2         | 5    | 2          | 986.8888                   | -3.93 2503.6894           |
| 4    | 3         | 5    | 3          | 986.9419                   | -9.26 2605.3468           | 5    | 1         | 6    | 1          | 987.8323                   | 10.32 2412.0143           |
| 5    | 2         | 6    | 2          | 987.9078                   | -1.44 2508.969            | 5    | 3         | 6    | 3          | 987.97                     | -10.75 2610.6779          |
| 6    | 1         | 7    | 1          | 988.8344                   | 14.07 2418.2781           | 6    | 2         | 7    | 2          | 988.9211                   | 6.5 2515.3042             |
| 6    | 3         | 7    | 3          | 988.9912                   | -18.23 2617.0751          | 7    | 1         | 8    | 1          | 989.8298                   | 12.42 2425.5857           |
| 7    | 2         | 8    | 2          | 989.9274                   | 7.12 2522.6952            | 7    | 3         | 8    | 3          | 990.0074                   | -10.18 2624.5381          |
| 8    | 1         | 9    | 1          | 990.819                    | 9.11 2433.9371            | 8    | 2         | 9    | 2          | 990.9267                   | 1.45 2531.1416            |

Table 7 continued on next page
Table 7. (continued)

| $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency (cm$^{-1}$) | Obs-Calc ($10^{-4}$ cm$^{-1}$) | $E_{lower}$ (K) | $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency (cm$^{-1}$) | Obs-Calc ($10^{-4}$ cm$^{-1}$) | $E_{lower}$ (K) |
|------|-----------|------|-----------|-----------------------|--------------------------|-------------|------|-----------|------|-----------|-----------------------|--------------------------|-------------|
| 8    | 3         | 9    | 3         | 991.0164              | -10.2                    | 2633.0669   | 9    | 1         | 10    | 1         | 991.8032              | 18.05                    | 2443.3321   |
| 9    | 2         | 10   | 2         | 991.9204              | 2.49                     | 2540.6435   | 9    | 3         | 10    | 3         | 992.0187              | -13.13                   | 2642.6613   |
| 10   | 2         | 11   | 2         | 992.0982              | 7.21                     | 2551.2007   | 10   | 3         | 11    | 3         | 993.0149              | -11.59                   | 2653.3212   |
| 11   | 1         | 12   | 1         | 993.751               | 11.96                    | 2465.2528   | 11   | 2         | 12    | 2         | 993.8891              | 7.23                     | 2562.8129   |
| 11   | 3         | 12   | 3         | 994.0048              | -9.35                    | 2665.0464   | 12   | 1         | 13    | 1         | 994.716               | 12.88                    | 2477.7783   |
| 12   | 2         | 13   | 2         | 994.8633              | 2.99                     | 2575.4802   | 12   | 3         | 13    | 3         | 994.9875              | -13.14                   | 2677.8366   |
| 13   | 1         | 14   | 1         | 995.6747              | 11.19                    | 2491.347    | 13   | 2         | 14    | 2         | 995.8319              | 7.33                     | 2589.2022   |
| 13   | 3         | 14   | 3         | 995.9648              | -5.71                    | 2691.6917   | 14   | 1         | 15    | 1         | 996.6275              | 13.38                    | 2505.9588   |
| 14   | 2         | 15   | 2         | 996.7938              | 8.14                     | 2603.9787   | 14   | 3         | 15    | 3         | 996.9345              | -8.48                    | 2706.6114   |
| 15   | 1         | 16   | 1         | 997.5739              | 13.48                    | 2521.6136   | 15   | 2         | 16    | 2         | 997.7492              | 7.42                     | 2619.8097   |
| 15   | 3         | 16   | 3         | 997.8975              | -12.83                   | 2722.5954   | 16   | 1         | 17    | 1         | 998.5139              | 10.85                    | 2538.3112   |
| 16   | 2         | 17   | 2         | 998.6984              | 10.13                    | 2636.6947   | 16   | 3         | 17    | 3         | 998.8545              | -10.98                   | 2739.6435   |
| 17   | 1         | 18   | 1         | 999.4479              | 10.65                    | 2556.0515   | 17   | 3         | 18    | 3         | 999.8047              | -11.58                   | 2757.7554   |
| 18   | 1         | 19   | 1         | 1000.3755             | 9.23                     | 2574.8342   | 18   | 2         | 19    | 2         | 1000.5759             | -1.87                    | 2673.6262   |
| 18   | 3         | 19   | 3         | 1000.7488             | -6.52                    | 2776.9307   | 19   | 1         | 20    | 1         | 1001.2971             | 9.9                      | 2594.6593   |
| 19   | 2         | 20   | 2         | 1001.5057             | -0.07                    | 2693.6721   | 19   | 3         | 20    | 3         | 1001.6854             | -10.32                   | 2797.1692   |
| 20   | 2         | 21   | 2         | 1002.4301             | 11.56                    | 2714.771    | 20   | 3         | 21    | 3         | 1002.6157             | -10.48                   | 2818.4705   |
| 21   | 1         | 22   | 1         | 1003.1208             | 4.75                     | 2637.4354   | 21   | 2         | 22    | 2         | 1003.3467             | 11.57                    | 2736.9227   |
| 21   | 3         | 22   | 3         | 1003.539              | -13.73                   | 2840.8341   | 22   | 1         | 23    | 1         | 1004.0234             | 4.33                     | 2660.3861   |
| 22   | 3         | 23   | 3         | 1004.4561             | -12.95                   | 2864.2598   | 23   | 1         | 24    | 1         | 1004.9202             | 8.86                     | 2684.3782   |
| 23   | 3         | 24   | 3         | 1005.3685             | 8.83                     | 2888.7471   | 24   | 1         | 25    | 1         | 1005.8104             | 9.95                     | 2709.4114   |
| 24   | 2         | 25   | 2         | 1006.0573             | 10.21                    | 2809.691    | 25   | 1         | 26    | 1         | 1006.6946             | 15.54                    | 2735.4857   |
| 26   | 1         | 27   | 1         | 1007.5712             | 7.8                      | 2762.6006   | 26   | 2         | 27    | 2         | 1007.8307             | 0.54                     | 2863.4607   |
| 27   | 1         | 28   | 1         | 1008.4417             | 2.54                     | 2790.7558   | 27   | 3         | 28    | 3         | 1008.9416             | 5.78                     | 2997.3041   |
| 28   | 1         | 29   | 1         | 1009.3062             | 1.94                     | 2819.9512   | 28   | 2         | 29    | 2         | 1009.5799             | 12.19                    | 2921.4327   |

Table 7 continued on next page
$$J' \quad \Omega' \quad J'' \quad \Omega'' \quad \text{Frequency} \quad \text{Obs-Calc} \quad E_{\text{lower}}$$

| 28 | 3 | 29 | 3 | 1009.8168 | -6.55 | 3027.093 |
| 29 | 2 | 30 | 2 | 1010.4435 | 7.85 | 2951.9936 |
| 31 | 1 | 32 | 1 | 1011.8615 | 2.75 | 2913.7747 |
| 33 | 1 | 34 | 1 | 1013.5325 | 1.03 | 2981.5183 |

$$J' \quad \Omega' \quad J'' \quad \Omega'' \quad \text{Frequency} \quad \text{Obs-Calc} \quad E_{\text{lower}}$$

| 29 | 1 | 30 | 1 | 1010.1643 | 1.79 | 2850.1863 |
| 30 | 2 | 31 | 2 | 1011.2999 | -1.34 | 2983.6038 |
| 32 | 2 | 33 | 2 | 1012.9953 | 5.39 | 3049.9705 |

Table 8. Observed transitions for $^{48}$TiO, $v = 4 \leftarrow 3$. Experimental errors for line positions are better than $1 \times 10^{-3}$ cm$^{-1}$.

$$J' \quad \Omega' \quad J'' \quad \Omega'' \quad \text{Frequency} \quad \text{Obs-Calc} \quad E_{\text{lower}}$$

| 4 | 1 | 5 | 1 | 977.5936 | 12.31 | 3388.428 |
| 5 | 2 | 6 | 2 | 978.6653 | -13.62 | 3490.5787 |
| 6 | 2 | 7 | 2 | 979.671 | -17.2 | 3496.8769 |
| 7 | 2 | 8 | 2 | 980.6717 | -7.27 | 3504.2247 |
| 8 | 2 | 10 | 2 | 982.6525 | -3.11 | 3522.0682 |
| 9 | 1 | 11 | 1 | 983.7356 | -26.87 | 3634.6814 |

$$J' \quad \Omega' \quad J'' \quad \Omega'' \quad \text{Frequency} \quad \text{Obs-Calc} \quad E_{\text{lower}}$$

| 10 | 3 | 11 | 3 | 984.4751 | 7.24 | 3446.5494 |
| 11 | 2 | 12 | 2 | 985.4325 | -3.55 | 3459.0026 |
| 12 | 1 | 13 | 1 | 986.3852 | 1.41 | 3472.4931 |
| 13 | 1 | 14 | 1 | 987.3305 | -6.28 | 3487.0206 |
| 14 | 1 | 15 | 1 | 988.2711 | 0.96 | 3502.585 |
| 15 | 1 | 16 | 1 | 989.3827 | -2.71 | 3617.5581 |
| 16 | 2 | 17 | 2 | 990.3183 | -3.67 | 3635.3921 |
| 17 | 2 | 18 | 2 | 992.1699 | -5.89 | 3674.2023 |
| 18 | 2 | 19 | 2 | 993.0868 | 1.12 | 3695.1778 |

Table 8 continued on next page
### Table 8. Continued

| $J'$ | $Ω'$ | $J''$ | $Ω''$ | Frequency $E_{lower}$ | Obs-Calc | $E_{lower}$ |
|------|------|------|------|---------------------|----------|---------|
|      |      |      |      | cm$^{-1}$           | 10$^{-4}$ cm$^{-1}$ | K       |
| 21   | 2    | 22   | 2    | 993.9969           | 6.42     | 3717.1999|
| 22   | 1    | 23   | 1    | 994.6733           | -7.68    | 3640.5557|
| 23   | 1    | 24   | 1    | 995.5633           | -2.56    | 3664.409 |
| 25   | 1    | 26   | 1    | 997.3232           | -1.17    | 3715.2208|
| 26   | 1    | 27   | 1    | 998.1931           | -5.86    | 3742.1787|
| 28   | 2    | 29   | 2    | 1000.1805          | 16.36    | 3900.6296|

| $J'$ | $Ω'$ | $J''$ | $Ω''$ | Frequency $E_{lower}$ | Obs-Calc | $E_{lower}$ |
|------|------|------|------|---------------------|----------|---------|
|      |      |      |      | cm$^{-1}$           | 10$^{-4}$ cm$^{-1}$ | K       |
| 29   | 2    | 28   | 2    | 971.6409            | 0.7      | 1401.2293|
| 28   | 2    | 27   | 2    | 972.8882            | 2.81     | 1356.2784|
| 27   | 2    | 26   | 2    | 974.1296            | 3.95     | 1312.8716|
| 26   | 1    | 25   | 1    | 975.7062            | 5.34     | 1125.6935|
| 25   | 2    | 24   | 2    | 976.5948            | 3.73     | 1230.6929|
| 24   | 2    | 23   | 2    | 977.8185            | 2.25     | 1191.9221|
| 23   | 3    | 22   | 3    | 978.7729            | 2.54     | 1304.9548|
| 23   | 1    | 22   | 1    | 979.3348            | 2.2      | 1010.6672|
| 22   | 2    | 21   | 2    | 980.2486            | 1.21     | 1119.0205|
| 21   | 3    | 20   | 3    | 981.2163            | -0.78    | 1234.4666|
| 21   | 1    | 20   | 1    | 981.7251            | 4.69     | 941.6382 |
| 20   | 2    | 19   | 2    | 982.655             | -2.01    | 1052.3089|
| 19   | 3    | 18   | 3    | 983.637             | 6.52     | 1170.2281|

### Table 9. Observed transitions for $^{46}$TiO, $v = 1 \leftarrow 0$. Experimental errors for line positions are better than $1 \times 10^{-3}$ cm$^{-1}$.

| $J'$ | $Ω'$ | $J''$ | $Ω''$ | Frequency $E_{lower}$ | Obs-Calc | $E_{lower}$ |
|------|------|------|------|---------------------|----------|---------|
|      |      |      |      | cm$^{-1}$           | 10$^{-4}$ cm$^{-1}$ | K       |
| 20   | 1    | 19   | 1    | 982.655             | -2.01    | 1052.3089|
| 21   | 3    | 20   | 3    | 981.2163            | -0.78    | 1234.4666|
| 21   | 1    | 20   | 1    | 981.7251            | 4.69     | 941.6382 |
| 22   | 2    | 21   | 2    | 980.2486            | 1.21     | 1119.0205|
| 21   | 3    | 20   | 3    | 981.2163            | -0.78    | 1234.4666|
| 21   | 1    | 20   | 1    | 981.7251            | 4.69     | 941.6382 |
| 20   | 2    | 19   | 2    | 982.655             | -2.01    | 1052.3089|
| 19   | 3    | 18   | 3    | 983.637             | 6.52     | 1170.2281|

Table 9 continued on next page
| $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency (cm$^{-1}$) | Obs-Calc (10$^{-4}$ cm$^{-1}$) | $E_{\text{lower}}$ (K) | $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency (cm$^{-1}$) | Obs-Calc (10$^{-4}$ cm$^{-1}$) | $E_{\text{lower}}$ (K) |
|-----|-------|-----|-------|------------------|-----------------------|----------|-----|-------|-----|-------|------------------|-----------------------|----------|
| 19  | 1     | 18  | 1     | 984.0917         | 4.21                  | 878.7367 | 18  | 3     | 17  | 3     | 984.8366         | 8.77                  | 1140.4538   |
| 18  | 2     | 17  | 2     | 985.0379         | -4.18                 | 991.7911 | 18  | 1     | 17  | 1     | 985.2661         | 3.56                  | 849.5844    |
| 17  | 3     | 16  | 3     | 986.033          | 4.79                  | 1112.2436| 17  | 2     | 16  | 2     | 986.2211         | 0.5                   | 963.856     |
| 17  | 1     | 16  | 1     | 986.4343         | -0.18                 | 821.9649 | 16  | 3     | 15  | 3     | 987.2205         | -11.18                | 1085.5979   |
| 16  | 2     | 15  | 2     | 987.3973         | -4.36                 | 937.4706 | 16  | 1     | 15  | 1     | 987.5971         | 0.3                   | 795.8784    |
| 15  | 3     | 14  | 3     | 988.4052         | 5.17                  | 1060.5172| 15  | 2     | 14  | 2     | 988.5684         | -1.76                 | 912.6353    |
| 14  | 3     | 13  | 3     | 989.582          | 2.16                  | 1037.0019| 14  | 2     | 13  | 2     | 989.7333         | -0.92                 | 889.3505    |
| 14  | 1     | 13  | 1     | 989.905          | 2.72                  | 748.3054 | 13  | 3     | 12  | 3     | 990.7533         | 5.89                  | 1015.0525   |
| 13  | 2     | 12  | 2     | 990.892          | -2.66                 | 867.6165 | 13  | 1     | 12  | 1     | 991.0504         | 6.58                  | 726.8193    |
| 12  | 3     | 11  | 3     | 991.9184         | 6.81                  | 994.6692 | 12  | 2     | 11  | 2     | 992.0455         | 3.22                  | 847.4336    |
| 12  | 1     | 11  | 1     | 992.189          | 2.32                  | 706.8671 | 11  | 3     | 10  | 3     | 993.077          | 4.92                  | 975.8525    |
| 11  | 2     | 10  | 2     | 993.1925         | 4.42                  | 828.8022 | 11  | 1     | 10  | 1     | 993.3223         | 3.78                  | 688.449     |
| 10  | 3     | 9    | 3     | 994.2399         | 6.61                  | 958.6028 | 10  | 2     | 9    | 2     | 994.3331         | 2.84                  | 811.7224    |
| 10  | 1     | 9    | 1     | 994.498          | 7.09                  | 671.5652 | 9   | 3     | 8    | 3     | 995.377          | 11.87                 | 942.9202    |
| 9   | 2     | 8    | 2     | 995.4864         | 7.14                  | 796.1945 | 9   | 1     | 8    | 1     | 995.571          | 6.95                  | 656.2157    |
| 8   | 3     | 7    | 3     | 996.5171         | 8.56                  | 928.8051 | 8   | 2     | 7    | 2     | 996.5967         | 3.18                  | 782.2188    |
| 8   | 1     | 7    | 1     | 996.6866         | 10.5                 | 642.4008 | 7   | 3     | 6    | 3     | 997.6514         | 8.43                  | 916.2577    |
| 7   | 2     | 6    | 2     | 997.7193         | 2.04                  | 769.7954 | 7   | 1     | 6    | 1     | 997.7956         | 7.85                  | 630.1206    |
| 6   | 3     | 5    | 3     | 998.7798         | 11.48                 | 905.2783 | 6   | 2     | 5    | 2     | 998.8363         | 6.47                  | 758.9245    |
| 6   | 1     | 5    | 1     | 999.899          | 7.98                  | 619.3751 | 5   | 3     | 4    | 3     | 999.9004         | -1.64                 | 895.867     |
| 5   | 2     | 4    | 2     | 999.9358         | -3.22                 | 749.6064 | 5   | 1     | 4    | 1     | 999.996          | 4.68                  | 610.1645    |
| 4   | 3     | 3    | 3     | 1000.0162        | 0.08                  | 888.024  | 4   | 2     | 3    | 2     | 1001.0511        | 5.54                  | 741.841     |
| 4   | 1     | 3    | 1     | 1001.0878        | 9.58                  | 602.4889 | 3   | 1     | 2    | 1     | 1002.1727        | 5.6                   | 596.3484    |
| 2   | 1     | 1    | 1     | 1003.2524        | 8.43                  | 591.7249 | 1   | 1     | 2    | 1     | 1007.5091        | 5.84                  | 588.6726    |
| 2   | 1     | 3    | 1     | 1008.5581        | 5.11                  | 591.7249 | 2   | 2     | 3    | 2     | 1008.6093        | 5.33                  | 730.9692    |
| $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency | Obs-Calc $E_{lower}$ | $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency | Obs-Calc $E_{lower}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 1 | 4 | 1 | 1009.6014 | 7.26 | 596.3484 | 3 | 2 | 4 | 2 | 1009.6637 | 0.23 | 735.6286 |
| 3 | 3 | 4 | 3 | 1009.7136 | -16.61 | 881.7494 | 4 | 1 | 5 | 1 | 1010.6381 | 4.91 | 602.4889 |
| 4 | 2 | 5 | 2 | 1010.7125 | 1.6 | 741.841 | 4 | 3 | 5 | 3 | 1010.7747 | 6.48 | 888.024 |
| 5 | 1 | 6 | 1 | 1011.6692 | 6.7 | 610.1645 | 5 | 2 | 6 | 2 | 1011.7552 | 5.01 | 749.6064 |
| 5 | 3 | 6 | 3 | 1011.8271 | 6.33 | 895.867 | 6 | 1 | 7 | 1 | 1012.6942 | 9.54 | 619.3751 |
| 6 | 2 | 7 | 2 | 1012.7914 | 5.91 | 758.9245 | 6 | 3 | 7 | 3 | 1012.8734 | 10.04 | 905.2783 |
| 7 | 1 | 8 | 1 | 1013.7128 | 8.02 | 630.1206 | 7 | 2 | 8 | 2 | 1013.8207 | 0.49 | 769.7954 |
| 7 | 3 | 8 | 3 | 1013.9126 | 7.15 | 916.2577 | 8 | 1 | 9 | 1 | 1014.7249 | 3.97 | 642.4008 |
| 8 | 2 | 9 | 2 | 1014.8443 | 2.05 | 782.2188 | 8 | 3 | 9 | 3 | 1014.9448 | -0.74 | 928.8051 |
| 9 | 1 | 10 | 1 | 1015.7313 | 4.47 | 656.2157 | 9 | 2 | 10 | 2 | 1015.8614 | 1.96 | 796.1945 |
| 9 | 3 | 10 | 3 | 1015.9721 | 6.47 | 942.9202 | 10 | 1 | 11 | 1 | 1016.7316 | 4.27 | 671.5652 |
| 10 | 2 | 11 | 2 | 1016.8722 | 1.29 | 811.7224 | 10 | 3 | 11 | 3 | 1016.9922 | 7.28 | 958.6028 |
| 11 | 1 | 12 | 1 | 1017.7258 | 5.93 | 688.449 | 11 | 2 | 12 | 2 | 1017.8768 | 3.45 | 828.8022 |
| 12 | 1 | 13 | 1 | 1018.7136 | 4.62 | 706.8671 | 12 | 2 | 13 | 2 | 1018.8747 | 2.19 | 847.4336 |
| 12 | 3 | 13 | 3 | 1019.0124 | 5.06 | 994.6692 | 13 | 1 | 14 | 1 | 1019.6956 | 7.62 | 726.8193 |
| 13 | 2 | 14 | 2 | 1019.8664 | 2.2 | 867.6165 | 13 | 3 | 14 | 3 | 1020.0131 | 7.76 | 1015.0525 |
| 14 | 1 | 15 | 1 | 1020.671 | 6.43 | 748.3054 | 14 | 2 | 15 | 2 | 1020.8518 | 3.68 | 889.3505 |
| 14 | 3 | 15 | 3 | 1021.0068 | 6.77 | 1037.0019 | 15 | 1 | 16 | 1 | 1021.6395 | -2.01 | 771.3252 |
| 15 | 2 | 16 | 2 | 1021.8302 | -0.35 | 912.6353 | 15 | 3 | 16 | 3 | 1021.9935 | 1.44 | 1060.5172 |
| 16 | 1 | 17 | 1 | 1022.6035 | 6.99 | 795.8784 | 16 | 2 | 17 | 2 | 1022.8026 | 0.39 | 937.4706 |
| 16 | 3 | 17 | 3 | 1022.9743 | 3.7 | 1085.5979 | 17 | 2 | 18 | 2 | 1023.7689 | 4.8 | 963.856 |
| 17 | 3 | 18 | 3 | 1023.9481 | 2.13 | 1112.2436 | 18 | 1 | 19 | 1 | 1024.5105 | 2.76 | 849.5844 |
| 18 | 2 | 19 | 2 | 1024.7281 | 2.86 | 991.7911 | 18 | 3 | 19 | 3 | 1024.9157 | 5.78 | 1140.4538 |
| 19 | 1 | 20 | 1 | 1025.4549 | 3.72 | 878.7367 | 19 | 2 | 20 | 2 | 1025.6812 | 4.67 | 1021.2755 |
| 19 | 3 | 20 | 3 | 1025.8763 | 5.36 | 1170.2281 | 20 | 1 | 21 | 1 | 1026.3931 | 5.14 | 909.4214 |
Table 9. (continued)

| $J'$ $\Omega'$ $J''$ $\Omega''$ | Frequency $E_{\text{lower}}$ | Obs-Calc | | $J'$ $\Omega'$ $J''$ $\Omega''$ | Frequency $E_{\text{lower}}$ | Obs-Calc |
|---|---|---|---|---|---|---|
| 20 2 21 2 | 1026.6274 | 2.34 | 1052.3089 | 20 3 21 3 | 1026.8298 | 0.8 | 1201.5658 |
| 21 1 22 1 | 1027.3246 | 2.84 | 941.6382 | 21 2 22 2 | 1027.5671 | 0.78 | 1084.8907 |
| 21 3 22 3 | 1027.7775 | 5.77 | 1234.4666 | 22 1 23 1 | 1028.2502 | 4.18 | 975.387 |
| 22 2 23 2 | 1028.5004 | 0.64 | 1119.0205 | 22 3 23 3 | 1028.7173 | -0.78 | 1268.9298 |
| 23 1 24 1 | 1029.1695 | 6.9 | 1010.6672 | 23 2 24 2 | 1029.4272 | 1.24 | 1154.6978 |
| 23 3 24 3 | 1029.6514 | 3.78 | 1304.9548 | 24 1 25 1 | 1030.0824 | 7.69 | 1047.4786 |
| 24 2 25 2 | 1030.3475 | 2.21 | 1191.9221 | 24 3 25 3 | 1030.5782 | 1.54 | 1342.5411 |
| 25 1 26 1 | 1030.9885 | 5.24 | 1085.8208 | 25 2 26 2 | 1031.261 | 1.68 | 1230.6929 |
| 25 3 26 3 | 1031.4987 | 5.52 | 1381.6879 | | |

Table 10. Observed transitions for $^{47}$TiO, $v = 1 \leftarrow 0$. Experimental errors for line positions are better than $1 \times 10^{-3}$ cm$^{-1}$.

| $J'$ $\Omega'$ $J''$ $\Omega''$ | Frequency $E_{\text{lower}}$ | Obs-Calc | | $J'$ $\Omega'$ $J''$ $\Omega''$ | Frequency $E_{\text{lower}}$ | Obs-Calc |
|---|---|---|---|---|---|---|
| 27 3 26 3 | 971.255 | -3.79 | 1459.3858 | 27 1 26 1 | 971.9176 | 5.07 | 1161.9564 |
| 26 2 25 2 | 972.7939 | -3.72 | 1266.0184 | 26 1 25 1 | 973.1325 | 11.75 | 1120.7779 |
| 25 3 24 3 | 973.7306 | -8.89 | 1376.8277 | 24 3 23 3 | 974.9599 | -8.79 | 1337.9428 |
| 24 2 23 2 | 975.2332 | -4.04 | 1187.3642 | 24 1 23 1 | 975.5455 | 30.64 | 1042.9864 |
| 23 3 22 3 | 976.1835 | -8.45 | 1300.5649 | 23 2 22 2 | 976.4447 | 1.26 | 1150.3438 |
| 23 1 22 1 | 976.7397 | 3.41 | 1006.3743 | 22 3 21 3 | 977.3999 | -20.99 | 1264.7396 |
| 22 2 21 2 | 977.6503 | 5.73 | 1114.8621 | 22 1 21 1 | 977.9311 | 6.66 | 971.285 |
| 21 3 20 3 | 978.6135 | -3.55 | 1230.4677 | 21 2 20 2 | 978.8491 | 0.44 | 1080.9193 |
| 21 1 20 1 | 979.1164 | 6.22 | 937.719 | 20 3 19 3 | 979.8196 | -1.96 | 1197.7495 |
| 20 2 19 2 | 980.0427 | 1.74 | 1048.5162 | 20 1 19 1 | 980.2961 | 8.28 | 905.6765 |

Table 10 continued on next page
| \(J'\) | \(\Omega'\) | \(J''\) | \(\Omega''\) | Frequency \(cm^{-1}\) | Obs-Calc \(10^{-4} cm^{-1}\) | \(E_{lower}\) K | \(J'\) | \(\Omega'\) | \(J''\) | \(\Omega''\) | Frequency \(cm^{-1}\) | Obs-Calc \(10^{-4} cm^{-1}\) | \(E_{lower}\) K |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 19 | 3 | 18 | 3 | 981.0182 | -16.61 | 1166.5857 | 19 | 2 | 18 | 2 | 981.2304 | 1.6 | 1017.653 |
| 19 | 1 | 18 | 1 | 981.4697 | 7.9 | 875.1578 | 18 | 3 | 17 | 3 | 982.2141 | 0.15 | 1136.9769 |
| 18 | 2 | 17 | 2 | 982.412 | 0.1 | 988.3302 | 18 | 1 | 17 | 1 | 982.6374 | 6.98 | 846.1633 |
| 17 | 3 | 16 | 3 | 983.4018 | -4.7 | 1108.9236 | 17 | 2 | 16 | 2 | 983.5883 | 3.87 | 960.5484 |
| 17 | 1 | 16 | 1 | 983.7994 | 6.86 | 818.6932 | 16 | 3 | 15 | 3 | 984.5846 | 0.28 | 1082.4261 |
| 16 | 2 | 15 | 2 | 984.7578 | -1.77 | 934.3078 | 16 | 1 | 15 | 1 | 984.955 | 1.98 | 792.7478 |
| 15 | 3 | 14 | 3 | 985.7604 | -4.86 | 1057.4851 | 15 | 2 | 14 | 2 | 985.9217 | -3.59 | 909.6088 |
| 15 | 1 | 14 | 1 | 986.1057 | 5.48 | 768.3273 | 14 | 3 | 13 | 3 | 986.9296 | -16.08 | 1034.1009 |
| 14 | 2 | 13 | 2 | 987.0797 | -6.33 | 886.4518 | 14 | 1 | 13 | 1 | 987.2489 | -6.69 | 745.432 |
| 13 | 3 | 12 | 3 | 988.0951 | -4.62 | 1012.274 | 13 | 2 | 12 | 2 | 988.2324 | -1.95 | 864.8372 |
| 13 | 1 | 12 | 1 | 988.3885 | 3.8 | 724.062 | 12 | 3 | 11 | 3 | 989.2531 | -8.81 | 992.0047 |
| 12 | 2 | 11 | 2 | 989.3789 | -0.21 | 844.7652 | 12 | 1 | 11 | 1 | 989.5213 | 5.54 | 704.2176 |
| 11 | 3 | 10 | 3 | 990.4052 | -10.93 | 973.2935 | 11 | 2 | 10 | 2 | 990.5193 | 0.1 | 826.2361 |
| 11 | 1 | 10 | 1 | 990.648 | 5.04 | 685.8989 | 10 | 3 | 9 | 3 | 991.5515 | -11.61 | 956.1407 |
| 10 | 2 | 9 | 2 | 991.6545 | 7.59 | 809.2503 | 10 | 1 | 9 | 1 | 991.7695 | 10.81 | 669.1062 |
| 9 | 3 | 8 | 3 | 992.6921 | -8.8 | 940.5467 | 9 | 1 | 8 | 1 | 992.8843 | 9.61 | 653.8395 |
| 8 | 3 | 7 | 3 | 993.8248 | -25.21 | 926.5118 | 8 | 2 | 7 | 2 | 993.905 | 4.22 | 779.9093 |
| 8 | 1 | 7 | 1 | 993.9934 | 9.46 | 640.0989 | 7 | 3 | 6 | 3 | 994.954 | -17.41 | 914.0364 |
| 7 | 2 | 6 | 2 | 995.0213 | 2.24 | 767.5546 | 7 | 1 | 6 | 1 | 995.0966 | 10.64 | 627.8847 |
| 6 | 2 | 5 | 2 | 996.1312 | -2.93 | 756.7441 | 6 | 1 | 5 | 1 | 996.1933 | 5.91 | 617.1968 |
| 5 | 2 | 4 | 2 | 997.236 | 0.6 | 747.478 | 5 | 1 | 4 | 1 | 997.2851 | 12.73 | 608.0353 |
| 4 | 2 | 3 | 2 | 998.3368 | 22.44 | 739.7567 | 4 | 1 | 3 | 1 | 998.3703 | 15.2 | 600.4003 |
| 2 | 1 | 3 | 1 | 1005.7996 | -24.49 | 589.7082 | 3 | 1 | 4 | 1 | 1006.838 | -7.81 | 594.2913 |
| 3 | 2 | 4 | 2 | 1006.8991 | 15.58 | 733.5807 | 4 | 1 | 5 | 1 | 1007.87 | 1.48 | 600.4003 |
| 4 | 2 | 5 | 2 | 1007.943 | 17.65 | 739.7567 | 5 | 1 | 6 | 1 | 1008.895 | 0.3 | 608.0353 |

Table 10 continued on next page
| $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency | Obs-Calc | $E_{\text{lower}}$ |
|------|-----------|------|-----------|-----------|---------|----------------|
|      |           |      |           | cm$^{-1}$ |         | K             |
|      |           |      |           | 10$^{-4}$ cm$^{-1}$ |         |               |
| 6    | 1         | 7    | 1         | 1009.9141 | -1.69   | 617.1968      |
| 7    | 1         | 8    | 1         | 1010.9274 | -0.64   | 627.8847      |
| 8    | 1         | 9    | 1         | 1011.9348 | 1.99    | 640.0989      |
| 8    | 3         | 9    | 3         | 1012.1524 | 13.45   | 926.5118      |
| 9    | 2         | 10   | 2         | 1013.0635 | -2.8    | 793.8079      |
| 10   | 1         | 11   | 1         | 1013.9307 | 0.93    | 669.1062      |
| 10   | 3         | 11   | 3         | 1014.1881 | 10.87   | 956.1407      |
| 11   | 2         | 12   | 2         | 1015.0688 | 2.9     | 826.2361      |
| 12   | 1         | 13   | 1         | 1015.9024 | 1.67    | 704.2176      |
| 12   | 3         | 13   | 3         | 1016.1981 | 11.17   | 992.0047      |
| 13   | 2         | 14   | 2         | 1017.0482 | 3.7     | 864.8372      |
| 14   | 1         | 15   | 1         | 1017.8496 | 2.76    | 745.432       |
| 14   | 3         | 15   | 3         | 1018.1822 | 13.93   | 1034.1009     |
| 15   | 2         | 16   | 2         | 1019.0022 | 4.97    | 909.6088      |
| 16   | 1         | 17   | 1         | 1019.7721 | 3.47    | 792.7478      |
| 16   | 3         | 17   | 3         | 1020.1394 | 9.71    | 1082.4261     |
| 17   | 2         | 18   | 2         | 1020.9306 | 6.34    | 960.5484      |
| 18   | 1         | 19   | 1         | 1021.6691 | -3.42   | 846.1633      |
| 18   | 3         | 19   | 3         | 1022.0702 | 5.47    | 1136.9769     |
| 19   | 2         | 20   | 2         | 1022.8328 | 2.98    | 1017.653      |
| 20   | 1         | 21   | 1         | 1023.5421 | -2.4    | 905.6765      |
| 20   | 3         | 21   | 3         | 1023.9751 | 7.09    | 1197.7495     |
| 21   | 2         | 22   | 2         | 1024.7096 | 4.02    | 1080.9193     |
| 22   | 1         | 23   | 1         | 1025.3904 | 2.47    | 971.285       |
| 22   | 3         | 23   | 3         | 1025.8532 | 6.95    | 1264.7396     |

Table 10 continued on next page
### Table 10. (continued)

| $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency  | Obs-Calc | $E_{\text{lower}}$ |
|------|-----------|-------|-----------|------------|----------|------------------|
|      |           |       |           | cm$^{-1}$  | 10$^{-4}$ cm$^{-1}$ | K             |
| 23   | 2         | 24    | 2         | 1026.5603  | 3.18     | 1150.3438       |
| 24   | 1         | 25    | 1         | 1027.2126  | -2.36    | 1042.9864       |
| 24   | 3         | 25    | 3         | 1027.7048  | 9.47     | 1337.9428       |
| 25   | 2         | 26    | 2         | 1028.3846  | -0.13    | 1225.9225       |
| 26   | 1         | 27    | 1         | 1029.0103  | 0.3      | 1120.7779       |
| 26   | 3         | 27    | 3         | 1029.5283  | 0.17     | 1417.3539       |
| 27   | 2         | 28    | 2         | 1030.1835  | 5.17     | 1307.6511       |
| 28   | 1         | 29    | 1         | 1030.7822  | -2.25    | 1204.6563       |
| 28   | 3         | 29    | 3         | 1031.3258  | 1.56     | 1502.9676       |

### Table 11. Observed transitions for $^{49}$TiO, $v = 1 \leftarrow 0$. Experimental errors for line positions are better than $1 \times 10^{-3}$ cm$^{-1}$.

| $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency  | Obs-Calc | $E_{\text{lower}}$ |
|------|-----------|-------|-----------|------------|----------|------------------|
|      |           |       |           | cm$^{-1}$  | 10$^{-4}$ cm$^{-1}$ | K             |
| 22   | 2         | 21    | 2         | 972.7555   | 5.92     | 769.6305         |
| 20   | 3         | 19    | 3         | 974.9027   | -10.19   | 827.7024         |
| 20   | 1         | 19    | 1         | 975.3693   | 4.65     | 624.7359         |
| 19   | 2         | 18    | 2         | 976.2964   | -2.26    | 702.7481         |
| 18   | 1         | 17    | 1         | 977.6862   | 10.15    | 583.7847         |
| 17   | 2         | 16    | 2         | 978.6287   | -1.93    | 663.4588         |
| 16   | 3         | 15    | 3         | 979.6158   | -7.05    | 748.3659         |
| 15   | 1         | 15    | 1         | 979.979    | 4.04     | 547.0292         |
| 15   | 2         | 14    | 2         | 980.9373   | -7.15    | 628.4113         |
| 14   | 3         | 13    | 3         | 981.9379   | 1.01     | 715.1209         |

*Table 11 continued on next page*
Table 11. (continued)

| $J'$ | $Ω'$ | $J''$ | $Ω''$ | Frequency | Obs-Calc | $E_{lower}$ | $J'$ | $Ω'$ | $J''$ | $Ω''$ | Frequency | Obs-Calc | $E_{lower}$ |
|------|------|------|------|----------|----------|------------|------|------|------|------|----------|----------|------------|
| 14   | 1    | 13   | 1    | 982.2496 | 6.21     | 514.471    | 13   | 3    | 12   | 3    | 983.0885 | -12.12   | 700.1054   |
| 13   | 2    | 12   | 2    | 983.2229 | -9.0     | 597.6075   | 13   | 1    | 12   | 1    | 983.3759 | 4.38     | 499.7662   |
| 12   | 3    | 11   | 3    | 984.2338 | -17.94   | 686.1615   | 12   | 2    | 11   | 2    | 984.3576 | -4.31    | 583.7976   |
| 12   | 1    | 11   | 1    | 984.4966 | 4.55     | 486.1111   | 11   | 3    | 10   | 3    | 985.3739 | -16.67   | 673.2894   |
| 11   | 2    | 10   | 2    | 985.4859 | -4.02    | 571.0493   | 11   | 1    | 10   | 1    | 985.6118 | 7.7      | 473.5059   |
| 10   | 3    | 9    | 3    | 986.5073 | -24.53   | 661.4896   | 10   | 2    | 9    | 2    | 986.6078 | -9.63    | 559.3628   |
| 10   | 1    | 9    | 1    | 986.7204 | 2.36     | 461.9507   | 9    | 3    | 8    | 3    | 987.6364 | -15.15   | 650.7622   |
| 9    | 2    | 8    | 2    | 987.7247 | -5.53    | 548.7382   | 9    | 1    | 8    | 1    | 987.8242 | 8.14     | 451.4455   |
| 8    | 3    | 7    | 3    | 988.7589 | -14.14   | 641.1075   | 7    | 3    | 6    | 3    | 989.8433 | -16.46   | 632.5258   |
| 7    | 2    | 6    | 2    | 989.9404 | -4.33    | 530.6757   | 7    | 1    | 6    | 1    | 990.0134 | 9.71     | 433.5857   |
| 6    | 3    | 5    | 3    | 990.9872 | -7.42    | 625.0176   | 6    | 2    | 5    | 2    | 991.0391 | -7.84    | 523.2381   |
| 6    | 1    | 5    | 1    | 991.0995 | 13.58    | 426.2312   | 5    | 3    | 4    | 3    | 992.0848 | -89.1    | 618.5832   |
| 5    | 2    | 4    | 2    | 992.1313 | -17.08   | 516.8632   | 5    | 1    | 4    | 1    | 992.1791 | 10.52    | 419.9269   |
| 4    | 2    | 3    | 2    | 993.2196 | -8.86    | 511.5512   | 4    | 1    | 3    | 1    | 993.2536 | 19.54    | 414.6729   |
| 3    | 1    | 2    | 1    | 994.3213 | 19.62    | 410.469    | 2    | 1    | 3    | 1    | 1000.6064 | -31.27   | 407.315    |
| 5    | 1    | 6    | 1    | 1003.6711 | -1.62    | 419.9269   | 5    | 2    | 6    | 2    | 1003.7545 | 11.61    | 516.8632   |
| 6    | 1    | 7    | 1    | 1004.6798 | -4.49    | 426.2312   | 6    | 2    | 7    | 2    | 1004.7746 | 9.02     | 523.2381   |
| 7    | 1    | 8    | 1    | 1005.6835 | 2.49     | 433.5857   | 7    | 2    | 8    | 2    | 1005.7883 | 4.42     | 530.6757   |
| 8    | 1    | 9    | 1    | 1006.6809 | 5.47     | 441.9905   | 8    | 2    | 9    | 2    | 1006.7966 | 9.27     | 539.1758   |
| 9    | 1    | 10   | 1    | 1007.6716 | 1.21     | 451.4455   | 9    | 3    | 10   | 3    | 1007.9050 | 21.88    | 650.7622   |
| 10   | 1    | 11   | 1    | 1008.6565 | -0.82    | 461.9507   | 10   | 2    | 11   | 2    | 1008.7934 | 5.72     | 559.3628   |
| 11   | 1    | 12   | 1    | 1009.6362 | 4.89     | 473.5059   | 11   | 2    | 12   | 2    | 1009.7821 | 0.8      | 571.0493   |
| 11   | 3    | 12   | 3    | 1009.9069 | 12.75    | 673.2894   | 12   | 1    | 13   | 1    | 1010.6087 | -0.69    | 486.1111   |
| 12   | 2    | 13   | 2    | 1010.7652 | 1.16     | 583.7976   | 12   | 3    | 13   | 3    | 1010.8999 | 16.37    | 686.1615   |
| 13   | 1    | 14   | 1    | 1011.576  | 1.82     | 499.7662   | 13   | 2    | 14   | 2    | 1011.7418 | 0.64     | 597.6075   |

Table 11 continued on next page
| $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency $E_{\text{lower}}$ | Obs-Calc $E_{\text{lower}}$ |
|-----|---------|------|---------|----------------|----------------|
| 13  | 3       | 14   | 3       | 1011.8841 14.96 | 700.1054 |
| 14  | 2       | 15   | 2       | 1012.7129 6.91  | 612.4788 |
| 15  | 1       | 16   | 1       | 1013.4917 -0.65 | 530.2254 |
| 15  | 3       | 16   | 3       | 1013.8348 9.69  | 731.2079 |
| 16  | 2       | 17   | 2       | 1014.6345 1.77  | 645.4047 |
| 17  | 1       | 18   | 1       | 1015.3833 -0.94 | 564.8824 |
| 17  | 3       | 18   | 3       | 1015.76 7.16    | 766.5946 |
| 18  | 2       | 19   | 2       | 1016.5309 -2.1  | 682.5734 |
| 19  | 1       | 20   | 1       | 1017.2504 -1.22 | 603.7359 |
| 19  | 3       | 20   | 3       | 1017.6591 5.32  | 806.2632 |
| 20  | 2       | 21   | 2       | 1018.4022 -3.84 | 723.9828 |
| 21  | 1       | 22   | 1       | 1019.0934 1.79  | 646.7845 |
| 21  | 3       | 22   | 3       | 1019.5326 7.96  | 850.2109 |
| 22  | 2       | 23   | 2       | 1020.2486 0.64  | 769.6305 |
| 23  | 1       | 24   | 1       | 1020.9115 3.04  | 694.0264 |
| 23  | 3       | 24   | 3       | 1021.3789 0.59  | 898.4346 |
| 24  | 2       | 25   | 2       | 1022.0703 14.55 | 819.5139 |
| 25  | 1       | 26   | 1       | 1022.7047 3.75  | 745.4599 |
| 25  | 3       | 26   | 3       | 1023.1997 3.85  | 950.9312 |
| 26  | 2       | 27   | 2       | 1023.864 5.51   | 873.6303 |
| 27  | 1       | 28   | 1       | 1024.4729 2.45  | 801.083 |
| 27  | 3       | 28   | 3       | 1024.9937 3.33  | 1007.697 |
| 28  | 3       | 29   | 3       | 1025.881 6.18   | 1037.6798 |
| 30  | 1       | 31   | 1       | 1027.0778 -1.97 | 892.3682 |
| 30  | 3       | 31   | 3       | 1027.635 7.3    | 1100.8424 |

Table 11 continued on next page
Table 11. (continued)

| $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency | Obs-Calc | $E_{lower}$ | $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency | Obs-Calc | $E_{lower}$ |
|------|-----------|------|-----------|-----------|----------|------------|------|-----------|------|-----------|-----------|----------|------------|
| 32   | 1         | 33   | 1         | 1028.7833 | -1.69    | 958.4551   | 32   | 2         | 33   | 2         | 1029.0915 | 2.31     | 1061.3457  |
| 32   | 3         | 33   | 3         | 1029.3617 | 3.19     | 1168.2643  | 33   | 1         | 34   | 1         | 1029.6274 | 8.06     | 993.0666   |
| 33   | 2         | 34   | 2         | 1029.9403 | 5.69     | 1096.3263  | 33   | 3         | 34   | 3         | 1030.2144 | -4.27    | 1203.5712  |
| 34   | 2         | 35   | 2         | 1030.7822 | 6.83     | 1132.3612  | 34   | 3         | 35   | 3         | 1031.0616 | 1.9      | 1239.9412  |
| 35   | 1         | 36   | 1         | 1031.294  | 0.97     | 1065.4239  |       |           |      |           |           |          |            |

Table 12. Observed transitions for $^{50}$TiO, $v = 1 \leftarrow 0$. Experimental errors for line positions are better than $1 \times 10^{-3}$ cm$^{-1}$.

| $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency | Obs-Calc | $E_{lower}$ | $J'$ | $\Omega'$ | $J''$ | $\Omega''$ | Frequency | Obs-Calc | $E_{lower}$ |
|------|-----------|------|-----------|-----------|----------|------------|------|-----------|------|-----------|-----------|----------|------------|
| 21   | 1         | 20   | 1         | 971.8864  | 5.78     | 644.3644   | 20   | 2         | 19   | 2         | 972.8016  | -0.51    | 721.6488   |
| 19   | 3         | 18   | 3         | 973.767   | 10.05    | 804.0225   | 19   | 1         | 18   | 1         | 974.2022  | 3.26     | 601.5254   |
| 18   | 3         | 17   | 3         | 974.943   | 20.28    | 783.7534   | 18   | 2         | 17   | 2         | 975.1335  | 0.48     | 680.4423   |
| 18   | 1         | 17   | 1         | 975.3515  | 1.47     | 581.6713   | 17   | 3         | 16   | 3         | 976.1107  | 5.94     | 764.549    |
| 17   | 2         | 16   | 2         | 976.2907  | -0.46    | 661.4214   | 17   | 1         | 16   | 1         | 976.4951  | -0.22    | 562.8612   |
| 16   | 3         | 15   | 3         | 977.2739  | 3.64     | 746.4098   | 16   | 1         | 15   | 1         | 977.6338  | 6.65     | 545.095    |
| 15   | 3         | 14   | 3         | 978.4313  | 3.06     | 729.3361   | 15   | 2         | 14   | 2         | 978.5881  | -0.09    | 626.5455   |
| 15   | 1         | 14   | 1         | 978.7658  | 3.15     | 528.3731   | 14   | 3         | 13   | 3         | 979.5834  | 7.37     | 713.328    |
| 14   | 2         | 13   | 2         | 979.7278  | -1.97    | 610.6911   | 14   | 1         | 13   | 1         | 979.892  | -0.47    | 512.6955   |
| 13   | 3         | 12   | 3         | 980.7287  | 1.95     | 698.3859   | 13   | 2         | 12   | 2         | 980.8621  | -0.86    | 595.8925   |
| 13   | 1         | 12   | 1         | 981.0131  | 1.56     | 498.0625   | 12   | 2         | 11   | 2         | 981.9915  | 9.42     | 582.1502   |
| 12   | 1         | 11   | 1         | 982.1282  | 1.94     | 484.4741   | 11   | 3         | 10   | 3         | 983.0028  | 3.88     | 671.7006   |
| 11   | 2         | 10   | 2         | 983.1129  | -2.96    | 569.4642   | 11   | 1         | 10   | 1         | 983.2372  | -1.65    | 471.9305   |
| 10   | 3         | 9     | 3         | 984.1316  | 10.58    | 659.9579   | 10   | 2         | 9     | 2         | 984.2295  | -3.45    | 557.8348   |

Table 12 continued on next page
| \(J'\) | \(\Omega'\) | \(J''\) | \(\Omega''\) | Frequency (cm\(^{-1}\)) | Obs-Calc K | \(E_{\text{lower}}\) cm\(^{-1}\) | \(E_{\text{lower}}\) cm\(^{-1}\) K |
|------|------|------|------|----------------|----------|----------------|----------------|
| 10   | 1    | 9    | 1    | 984.3412       | 1.94     | 460.4318       | 469.2821       |
| 9    | 2    | 8    | 2    | 985.3399       | -6.77    | 547.262        | 449.9781       |
| 8    | 3    | 7    | 3    | 986.3695       | 6.08     | 639.6733       | 537.7461       |
| 8    | 1    | 7    | 1    | 986.5306       | -2.4     | 440.5695       | 631.1318       |
| 7    | 2    | 6    | 2    | 987.5442       | -5.81    | 529.2872       | 432.2061       |
| 6    | 3    | 5    | 3    | 988.5833       | 0.04     | 623.6576       | 521.8854       |
| 6    | 1    | 5    | 1    | 988.6971       | -5.67    | 424.8879       | 617.251        |
| 5    | 2    | 4    | 2    | 989.7255       | 1.72     | 515.5408       | 418.6151       |
| 4    | 2    | 3    | 2    | 990.8064       | -2.58    | 510.2535       | 413.3877       |
| 3    | 2    | 2    | 2    | 991.882        | -0.75    | 506.0235       | 409.2057       |
| 2    | 1    | 3    | 1    | 998.1604       | 6.98     | 406.0691       | 502.851        |
| 3    | 1    | 4    | 1    | 999.1822       | 4.79     | 409.2057       | 611.9119       |
| 4    | 2    | 5    | 2    | 1000.2697      | -1.93    | 510.2535       | 515.5408       |
| 5    | 1    | 6    | 1    | 1001.2089      | 7.47     | 418.6151       | 424.8879       |
| 5    | 3    | 6    | 3    | 1001.36        | 1.05     | 617.251        | 623.6576       |
| 6    | 2    | 7    | 2    | 1002.307       | 6.06     | 521.8854       | 537.7461       |
| 7    | 1    | 8    | 1    | 1003.2109      | -0.01    | 432.2061       | 684.51         |
| 8    | 1    | 9    | 1    | 1004.2037      | 4.05     | 440.5695       | 659.9579       |
| 8    | 3    | 9    | 3    | 1004.4157      | 5.6      | 639.6733       | 471.9305       |
| 9    | 2    | 10   | 2    | 1005.3135      | -18.78   | 547.262        | 577.414        |
| 10   | 1    | 11   | 1    | 1006.171       | 7.05     | 460.4318       | 557.8348       |
| 10   | 3    | 11   | 3    | 1006.4207      | 1.62     | 659.9579       | 471.9305       |
| 11   | 2    | 12   | 2    | 1007.2907      | 1.28     | 569.4642       | 671.7006       |
| 12   | 1    | 13   | 1    | 1008.1143      | 7.76     | 484.4741       | 582.1502       |
| 12   | 3    | 13   | 3    | 1008.4006      | -0.92    | 684.51         | 498.0625       |
Table 12. (continued)

| J' Ω' J'' Ω'' Frequency cm⁻¹ | Obs-Calc E_{lower} K | J' Ω' J'' Ω'' Frequency cm⁻¹ | Obs-Calc E_{lower} K |
|-----------------------------|----------------------|-----------------------------|----------------------|
| 1009.2409 -1.49 595.8925 K | 1009.3821 9.16 698.3859 K | 1010.0326 -0.49 512.6955 K | 1010.2068 -0.97 610.6911 K |
| 1010.3561 7.13 713.328 K | 1010.9832 0.71 528.3731 K | 1011.3222 -9.17 729.3361 K | 1011.9282 4.93 545.095 K |
| 1012.1202 0.84 643.4557 K | 1012.6109 2.24 746.4098 K | 1012.8666 4.28 562.8612 K | 1013.0666 -6.95 661.4214 K |
| 1013.2394 -0.45 764.549 K | 1013.799 4.35 581.7613 K | 1014.0082 0.51 680.4423 K | 1014.1881 1.88 783.7534 K |
| 1014.9424 -3.72 700.5182 K | 1015.130 0.27 804.0225 K | 1015.6455 4.39 622.4232 K | 1015.8712 1.11 721.6488 K |
| 1016.0658 2.94 825.356 K | 1016.5593 1.66 644.3644 K | 1016.9282 4.93 545.095 K | 1017.0788 1.51 767.0728 K |
| 1016.7925 -4.85 743.8337 K | 1016.995 4.2 847.7537 K | 1017.4676 4.17 667.3489 K | 1017.7088 1.51 767.0728 K |
| 1017.9177 6.43 871.2151 K | 1018.369 0.01 691.3765 K | 1018.618 0.72 791.3656 K | 1018.7633 1.8 895.7398 K |
| 1018.618 0.72 791.3656 K | 1018.8333 1.8 895.7398 K | 1019.2649 2.12 716.4468 K | 1019.5211 2.85 816.7119 K |
| 1019.7427 1.81 921.3274 K | 1020.1549 2.74 742.5598 K | 1020.4176 2.85 816.7119 K | 1020.6456 1.64 947.9776 K |
| 1020.4176 2.85 816.7119 K | 1020.7633 1.8 895.7398 K | 1021.307 -4.59 870.5632 K | 1021.542 2.49 975.6898 K |
| 1021.307 -4.59 870.5632 K | 1021.8333 1.8 895.7398 K | 1022.191 -0.82 899.0675 K | 1022.4313 -2.15 1004.4636 K |
| 1022.191 -0.82 899.0675 K | 1022.6333 -2.15 1004.4636 K | 1022.7856 -1.21 827.1514 K | 1023.0676 -7.55 928.6237 K |
| 1023.3141 -5.26 1034.2985 K | 1023.6505 0.22 857.432 K | 1023.9389 -1.91 959.2314 K | 1024.1906 -4.26 1065.194 K |
| 1024.5089 0.31 888.7537 K | 1024.8032 -7.55 928.6237 K | 1025.0604 -4.52 1097.1497 K | 1026.2068 -1.75 954.5195 K |
Table 13. Mass-invariant molecular parameters of the $A^3\Phi$ state of TiO. Two sets of parameters are obtained by excluding ("Fit A") and including ("Fit B") the spin-rotation interaction in the electronic ground state (see Table 2). In a global fit, the infrared data obtained in this work are combined with data for $^{46-50}\text{Ti}^{16}\text{O}$ and $^{48}\text{Ti}^{18}\text{O}$ at optical and microwave frequencies from the literature (Breier et al. 2019; Lincowski et al. 2016; Fletcher et al. 1993; Ram et al. 1999; Amiot et al. 1995).

| Parameter $\hat{O}_{k,l}$ | Fit A            | Fit B            | Units       |
|---------------------------|------------------|------------------|-------------|
| $U_{00} \times 10^{-4}$   | 1.41635548(5)    | 1.41635442(5)    | cm$^{-1}$   |
| $U_{10} \times 10^{-3}$   | 3.004397(3)      | 3.004397(3)      | cm$^{-1}u^{1/2}$ |
| $U_{20} \times 10^{-1}$   | -4.5972(5)       | -4.5972(5)       | cm$^{-1}u$   |
| $U_{30} \times 10^{1}$    | -4.88(2)         | -4.88(2)         | cm$^{-1}u^{3/2}$ |
| $U_{01}$                  | 6.084493(4)      | 6.084491(4)      | cm$^{-1}u$   |
| $U_{11} \times 10^{1}$    | -1.3146(2)       | -1.3145(2)       | cm$^{-1}u^{3/2}$ |
| $U_{21} \times 10^{4}$    | -9.2(4)          | -9.3(4)          | cm$^{-1}u^2$  |
| $U_{31} \times 10^{4}$    | -1.5(2)          | -1.4(2)          | cm$^{-1}u^{5/2}$ |
| $U_{02} \times 10^{5}$    | 9.9762(8)        | 9.9760(8)        | cm$^{-1}u^2$  |
| $U_{12} \times 10^{7}$    | 6.6(3)           | 6.8(3)           | cm$^{-1}u^{5/2}$ |
| $U_{22} \times 10^{7}$    | 1.8(3)           | 1.8(3)           | cm$^{-1}u^3$  |
| $U_{03} \times 10^{10}$   | 2.8(2)           | 2.8(2)           | cm$^{-1}u^3$  |
| $A_{00} \times 10^{-1}$   | 5.801031(10)     | 5.801012(10)     | cm$^{-1}$    |
| $A_{10} \times 10^{1}$    | -3.678(3)        | -3.678(3)        | cm$^{-1}u^{1/2}$ |
| $A_{20} \times 10^{2}$    | 1.48(2)          | 1.48(2)          | cm$^{-1}u$    |
| $A_{01} \times 10^{4}$    | -5.060(3)        | -5.033(5)        | cm$^{-1}u$    |
| $A_{11} \times 10^{5}$    | 1.43(9)          | 1.30(9)          | cm$^{-1}u^{3/2}$ |
| $\lambda_{00} \times 10^{1}$ | -5.163(2)    | -5.178(2)        | cm$^{-1}$    |
| $\lambda_{10} \times 10^{2}$ | 1.12(8)        | 1.23(8)          | cm$^{-1}u^{1/2}$ |
| $\lambda_{20} \times 10^{3}$ | -3.5(5)        | -3.7(5)          | cm$^{-1}u$    |
| $\lambda_{01} \times 10^{5}$ | -5.43(8)       | -3.74(8)         | cm$^{-1}u$    |
| $\lambda_{11} \times 10^{6}$ | 7(2)           | -3(2)            | cm$^{-1}u^{3/2}$ |
Table 14. Molecular parameters of the $B^3Π$ state of TiO in the singly excited vibrational state $v = 1$. All values are given in cm$^{-1}$. Two sets of parameters are obtained by excluding (“Fit A”) and including (“Fit B”) the spin-rotation interaction in the electronic ground state (see Table 2). In a global fit, the infrared data obtained in this work are combined with data for $^{46−50}$Ti$^{16}$O and $^{48}$Ti$^{18}$O at optical and microwave frequencies from the literature (Breier et al. 2019; Lincowski et al. 2016; Fletcher et al. 1993; Ram et al. 1999; Amiot et al. 1995).

| Parameter | Fit A | Fit B |
|-----------|-------|-------|
| $T \times 10^{-4}$ | $1.751591015(13)$ | $1.751589964(14)$ |
| $B \times 10^1$ | $5.028657(2)$ | $5.028657(2)$ |
| $D \times 10^7$ | $6.9128(8)$ | $6.9142(9)$ |
| $H \times 10^{13}$ | $1.90(13)$ | $2.02(13)$ |
| $A \times 10^{-1}$ | $2.07884(2)$ | $2.07883(2)$ |
| $A_D \times 10^4$ | $-1.15(2)$ | $-1.14(2)$ |
| $\gamma \times 10^2$ | $2.491(5)$ | $2.490(5)$ |
| $\lambda \times 10^1$ | $-9.305(2)$ | $-9.305(2)$ |
| $\lambda_D \times 10^6$ | $-3.7(6)$ | $-3.8(6)$ |
| $\lambda_H \times 10^{10}$ | $-6.0(1.4)$ | $-5.6(1.4)$ |
| $\sigma \times 10^1$ | $-6.185(2)$ | $-6.184(2)$ |
| $\sigma_D \times 10^6$ | $1.6(4)$ | $1.3(4)$ |
| $\sigma_H \times 10^{10}$ | $5.0(1.0)$ | $6.2(1.0)$ |
| $p \times 10^2$ | $2.6123(8)$ | $2.6121(8)$ |
| $p_D \times 10^7$ | $1.13(3)$ | $1.14(3)$ |
| $q \times 10^4$ | $2.963(3)$ | $2.964(3)$ |
| $q_D \times 10^{10}$ | $-7.2(8)$ | $-8.2(8)$ |