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Cite as: AIP Advances 10, 035316 (2020); https://doi.org/10.1063/1.5143429
Submitted: 23 December 2019 . Accepted: 29 February 2020 . Published Online: 19 March 2020

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ABSTRACT
An analytical formula for the diatomic R-branch emission lines that was recently tested as a universal expression has been further modified based on the difference algebraic converging method. The tiny experimental line errors that may lead to amplified errors in the determination of high $J$ lines were taken into account in the formula. Applications are presented for the R-branch emission spectra of (2-0), (3-1), (6-4), and (7-5) overtone bands of the ground electronic state of $^{12}\text{C}^{16}\text{O}$. The rotational constants and band origins that are consistent with those reported previously are determined through the analytical formula for predicting frequency for emission lines up to $J = 110$. The results are shown to not only compare favorably with available lower $J$ lines, but also generate reasonable higher $J$ lines for the overtone bands, which agree with data from the HITRAN database and other works.

I. INTRODUCTION
Accurate spectroscopic parameters for carbon monoxide (CO) are of great need in studies of astrochemistry, planetary atmospheres, atmospheric carbon cycle, and thermodynamic properties. There has been a growing interest in the first overtone transitions in the ground electronic state of CO. The spectroscopic parameters of carbon monoxide, such as transition frequencies and rotational constants, are extensively studied with sufficient accuracy, where methods from both experiment and theory are well developed.

For example, in early 1965, Rank et al. published heated absorption tube measurements of rotational lines of the 2-0, 3-1, and 4-2 overtone bands of $^{12}\text{C}^{16}\text{O}$ to an accuracy of $\pm 0.0032$ cm$^{-1}$ when compared with the calculated data. The overtone $\Delta \nu = 2$ sequence bands are recorded up to $\nu' = 7$ in the $\text{X}^{\text{1}\Sigma^+} - \text{X}^{\text{1}\Sigma^+}$ transition of $^{12}\text{C}^{16}\text{O}$, in which the R- and P-branches were observed by Mantz and Maillard in 1974 with a high-resolution Fourier-transform Spectrometer (FTS). Later in 1983, the heterodyne frequency measurements of the 2-0 band in $\text{X}^{\text{1}\Sigma^+}$ of CO were performed by Pollock et al., which give accurate line positions for R- and P-branches and improved centrifugal distortion constants. In addition, extensive line lists for rovibrational transitions of the first overtone bands up to $\nu' = 22$ have been recorded by Goorvitch for astrophysical applications. Recently, the "hot" overtone 2-0 band was measured for rovibrational analyses over a wide spectral coverage by Zou, Sung, Mishra, Malathy Devi, Hashemi, and Esteki. On the other hand, the HITRAN (HIgh-resolution TRANsmission) and HITEMP (HIgh-TEMPerature) molecular spectroscopic databases provide line lists of high-resolution spectral parameters for molecules of atmospheric science.
Spectroscopic constants for different transitions in the observed states can be determined by fitting the rotational or vibrational lines using the corresponding term energy expressions. Thus, it is believed that extrapolation of the experimental lines to the higher rotational quantum numbers in these cases can also be achieved using spectroscopic constants that have sufficient accuracy. Based on this assumption, previous work has been directed toward predicting the high-lying transitional emission spectral lines using the difference converging method (DCM) for diatomic molecules.\(^{26-28}\) The results from these works yielded not only deeper insights into the delicate relationship between the rotational constants and the transitional lines, but also generated the formulae that can give high-lying transitional lines with precision. Despite these remarkable achievements, previous research was limited in two key ways: (a) In order to give accurate lines up to high \( J \), power series expansions in \( J (J + 1) \) for rotational energy part of the Herzberg expansion were set to be unchangeable in the DCM treatment of our past work\(^{27-28}\) and (b) the uncertainty of each experimental line is neglected, which may mainly affect the predictions of the weaker high \( J \) transitions.

The present study will introduce an algebraic technique in the DCM procedure to evaluate the contribution of the rotational constants \([B_\nu, D_\nu, H_\nu, \ldots]\), which are used to obtain high-lying transitional lines toward improved precision assisted by variational treatment during the calculation process. Our work will focus on several \( \Delta \nu = 2 \) bands of the \( X^1 \Sigma^+ \) ground electronic state of \( ^{12}\text{C}^{16}\text{O} \) and spectroscopic information concerning this state could also be derived from these bands. This paper is organized as follows. The theoretical details will be described briefly in Sec. II. In Sec. III, the theoretical applications to some overtone bands in the ground electronic state of \( ^{12}\text{C}^{16}\text{O} \) are given and discussed. Section IV summarizes this study.

II. THEORETICAL DETAILS

A. Method for R-branch transition lines

For a given transition band of the CO system in the \( X^1 \Sigma^+ \) state, which would be considered Hund’s case \((b)\), the R-branch transition lines and molecular constants can be expressed by using the well-known formula,\(^{22}\)

\[
v = v_0 + \left[ B_\nu J(J + 1)(J + 2) - D_\nu J(J + 1)^2(J + 2)^2 + H_\nu J(J + 1)^3(J + 2)^3 + \cdots \right] \quad \text{(1)}
\]

where \(v_0 = v_\nu = \{ (T_\nu’ - T_\nu”) + (G” - G”) \}) \) is the origin of the \( v’ - v” \) band, and \([B, D, H, L, \ldots]\) are the rotational constants. One can rewrite Eq. (1) as a series expression as

\[
v = v_0 + \left[ B_\nu \pi_{1,l} + D_\nu \pi_{2,l} + H_\nu \pi_{3,l} + \cdots \right] \quad \text{(2)}
\]

where \( \pi_{i,j} \) are the expansion coefficients that are the functions of the rotational quantum number \( J \),

\[
\pi_{i,j} = [J(J + 1)]^i.
\]

Based on Eq. (2), the 1st transition line difference between two rotational states \( J_1 \) and \( J_2 \) is

\[
v_{J_1} - v_{J_2} = \left[ B_\nu \pi_{1,l_1} + D_\nu \pi_{2,l_1} + H_\nu \pi_{3,l_1} + \cdots \right] \quad \text{(3)}
\]

Rearranging it, the inertial rotational constant \( B_\nu \) from Eq. (5) can be expressed as

\[
B_\nu = \left( v_{J_1} - 2v_{J_l} + v_{J_2} \right) \pi_{1,l_1} + D_\nu \pi_{1,l_2} - D_\nu \pi_{1,l_2} - H_\nu \pi_{1,l_3} + \cdots
\]

where the expansion coefficients \( \pi_{1,l_1} \) and \( \pi_{1,l_2} \) are given written as

\[
\pi_{1,l_1} = \frac{1}{\pi_{1,l_1} + \pi_{1,l_2} + \pi_{1,l_3} + \cdots} \quad \text{(4)}
\]

Then, one can substitute \( B_\nu \) in Eq. (6) into Eq. (2)

\[
v = v_0 + \left[ B_\nu \pi_{1,l_1} + D_\nu \pi_{1,l_2} + H_\nu \pi_{1,l_3} + \cdots \right] \quad \text{(5)}
\]
Next, a further modification is possible to simplify Eq. (8) giving

\[ v_0 + B_{\nu} \delta(J)_2 + D_{\nu} \delta(J)_3 + (-D_{\nu}) \delta(J)_4 + (-H_{\nu}) \delta(J)_5 + H_{\nu} \delta(J)_6 + (-L_{\nu}) \delta(J)_7 + L_{\nu} \delta(J)_8 + \cdots = v - (v_{ij} - 2v_{ij} + v_{ij})\pi_{11}^{j+1} \pi_{1j+1}. \]  

(9)

Equation (9) can be written in a matrix form as

\[ \delta \chi = k, \]  

(10)

in which the expansion coefficient matrix \( \delta \), the molecular constants matrix \( \chi \), and the matrix \( k \) of the transition lines are given by

\[
\begin{align*}
X & = \begin{pmatrix}
\begin{bmatrix}
v_0 \\ B_{\nu} \\ D_{\nu} \\ -D_{\nu} \\ -H_{\nu} \\ \cdots \\
\end{bmatrix}, & k = \begin{pmatrix}
v_{ij}' - (v_{ij} - 2v_{ij} + v_{ij})\pi_{11}^{j+1} \pi_{1j+1} + 1 \\
v_{ij}' - (v_{ij} - 2v_{ij} + v_{ij})\pi_{11}^{j+1} \pi_{1j+1} + 1 \\
v_{ij}' - (v_{ij} - 2v_{ij} + v_{ij})\pi_{11}^{j+1} \pi_{1j+1} + 1 \\
v_{ij}' - (v_{ij} - 2v_{ij} + v_{ij})\pi_{11}^{j+1} \pi_{1j+1} + 1 \\
\cdots \\
\chi_{\text{max}} \\
\end{pmatrix} \\
\end{align*}
\]

\[ \delta (J)_j = \begin{cases} \\
\pi_{11}^{j+1} \pi_{1j+1} - \pi_{1j}^{j+1} \pi_{1j+1}, & i = 3, 5, 7, \ldots, \text{odd} \\
\pi_{1j}^{j+1} \pi_{1j+1} - \pi_{1j}^{j}, & i = 2, 4, 6, \ldots, \text{even} \\
\end{cases} \]  

(11)

Note that, in the matrix \( k \) in Eq. (11), the \( v_{ij}' \) could be any one of the \( m \) known experimental lines \( (v_{ij})_m \) other than \( v_{ij}, i = 1, 2, 3 \). Thus, the exact experimental lines used in each algebraic procedure of Eq. (10) will be \((i_{\text{max}} + 3)(i_{\text{max}} = \text{even})\).

Moreover, the error in Eq. (9) can be expressed as

\[ \partial v_0 + \partial B_{\nu} \delta(J)_2 + \partial D_{\nu} \delta(J)_3 + (-\partial D_{\nu}) \delta(J)_4 + (-\partial H_{\nu}) \delta(J)_5 + \partial H_{\nu} \delta(J)_6 + (-\partial L_{\nu}) \delta(J)_7 + L_{\nu} \delta(J)_8 + \cdots = \partial v - (\partial v_0 - 2v_{ij} + v_{ij})\pi_{11}^{j+1} \pi_{1j+1}. \]  

(12)

It can be seen in Eq. (12) that the errors to the molecular constants \( \chi \) are those from the experimental lines \( v_i \), which are mainly determined in the experimental procedure. Thus, to have minimum errors on the right sides of Eq. (12), one may minimize the coefficient \( \{\pi_{11}^{j+1} \pi_{1j+1} + 1, \pi_{11}^{j+1} \pi_{1j} + 1, \ldots, \pi_{11}^{j+1} \pi_{1j} \text{max} + 1\} \) [see Eq. (14)], which only depend on the chosen rotational quantum \( \nu \).

One may choose a subset of \((i_{\text{max}} + 3)\) transition lines that have sufficient spectral accuracy out of the \( m(!_{\text{max}} + 3) \) known experimental ones to solve Eq. (10). Then, \( C_{i_{\text{max}}}^{i_{\text{max}} + 3} \) sets of molecular constants \( (v_0, B_{\nu}, D_{\nu}, D_{\nu}, \ldots, \chi_{\text{max}}) \) can be obtained. The corresponding \( B_{\nu} \) of each set can be derived from Eq. (6). The best solution \((v_0, B_{\nu}, D_{\nu}, D_{\nu}, \ldots, \chi_{\text{max}})\) is determined by the following physical converging requirements:

\[ \Delta E_{\text{RMS}} = \sqrt{\frac{1}{m} \sum_{i=1}^{m} (v_{\text{exp}} - v_{\text{cal}})^2} \to 0, \]  

(13)

\[ \text{Max}(\pi_{11}^{j+1} \pi_{1j+1} + 1, \pi_{11}^{j+1} \pi_{1j} \text{max} + 1) \to \text{sufficiently small}, \]  

(14)

where the total accuracy for a transition band is given by the root mean square (rms) error \( \Delta E_{\text{RMS}} \) listed in Eq. (13), in which \( m \) stands for the number of known experimental R-branch lines for a given band. Equation (14) ensures that the computational errors in Eqs. (9) and (10) are as small as possible. Then, the converged molecular constants \((v_0, B_{\nu}, D_{\nu}, D_{\nu}, \ldots, \chi_{\text{max}})\) will be used to predict the unknown R-transition lines for a given band at higher \( f \). The typical workflow can be seen in Fig. 1.

According to the derivation above, a multi-difference method combined with an algebraic technique is found to

![FIG. 1. Workflow in the DACMt framework.](image-url)
obtain algebraic Eq. (10), and Eqs. (13) and (14) ensure that the calculated transition lines have sufficient spectral accuracy. Therefore, one may name this theoretical method as the difference algebraic converging method for transition lines (DACMt) and the converged transition lines as $\nu^\text{DACMt}
$. 

**B. Variational treatment for the R-branch lines**

It has to be noted that tiny experimental line errors have a non-negligible impact in predicting the high-lying R-branch lines. Consequently, the uncertainty given to each observation should be taken into consideration as part of the process, and this can be done by varying each observation in the form of displacement from its initial value $\nu^\text{expt}$ by an increment $\delta\nu$, which has a numerical value within the uncertainty or error limit. The “true” experimental lines $\nu^\text{e}$ shown in Eq. (11) then become $\nu^\text{e} = \nu^\text{expt} - \Delta\nu^\text{e}$, where $\nu^\text{expt}$ is the error limit of the reported measurement $\nu^\text{expt}$. This corresponds to a spectral range of

$$
\nu^\text{e} \in \{ \nu^\text{expt} - \Delta\nu^\text{e}, \nu^\text{expt} + \Delta\nu^\text{e} \}
$$

or a Mathematical expansion

$$
\nu^\text{e} = \begin{cases} 
\nu^\text{expt} & \nu^\text{expt} + \Delta\nu^\text{e} \sum_{k=1}^{\infty} \frac{1}{2^k}, \ k = 1, 2, 3, \ldots 
\end{cases}
$$

For each $n_i$, $i$ can be 1 or –1. Then adjustments to each transition can be done in DACMt calculation, where the calculated variational transition lines are named $\nu_i^\text{DACMt}$. In Ref. 12, the difference between the experimental and calculated R-branch lines is at the $10^{-5}$ cm$^{-1}$ and $10^{-3}$ cm$^{-1}$ level, which is in good agreement with the experimental uncertainty. Thus, in this work, we set $\Delta\nu = 0.01$ cm$^{-1}$ as a tentative value for every R-branch line used in the DACMt calculation. Then, the final value of each $\Delta\nu$ is varied deterministically by applying the converging standards in Eqs. (13) and (14).

**III. APPLICATIONS AND DISCUSSIONS**

The DACMt of calculating the high-lying R-branch transitions by solving Eq. (10) is applied to the (2-0), (3-1), (6-4), and (7-5) overtone bands of the ground electronic state of CO. The DACMt calculated R-branch transition lines, which cover the range of 3935–4361 cm$^{-1}$ with $J$ values up to 110, are compared to the values from HITRAN,23 DCM, and available measurements. As can be seen from Table I, the rotational quantum numbers and the corresponding variational transition lines used in the DACMt process are listed for these overtone bands. The differences between our calculated band origins and experimental and theoretical values exhibit small absolute errors, and the rotational constants $B_0$, $D_0$, and $H_0$ (0 ≤ $\nu$ ≤ 7) are in good agreement with past works as can be seen in Tables II and III, respectively.

### Table I. The rotational quantum numbers $J_N$ and the corresponding variational transition lines $\nu_N$ for calculation of (2-0), (3-1), (6-4), and (7-5) overtone bands of the $X'$1$^1\Sigma^+ \rightarrow X'$1$^1\Sigma^+$ transition of CO (in cm$^{-1}$).

| Band   | $(J_N, \nu_N)$ | $(2-0)_N$ | $(3-1)_N$ | $(6-4)_N$ | $(7-5)_N$ |
|--------|---------------|-----------|-----------|-----------|-----------|
| (2-0)  | (34 274,740 969 28) (174 263,635 742 51) (604 137,395 097 06) (1 400 093,978 29) |
| (3-1)  | (254 335,031 083 10) (204 270,781 741 31) (624 135,490 053 57) (5 401,750 301 17) |
| (6-4)  | (474 359,596 752 82) (234 277,270 083 12) (644 133,267 662 71) (94 029,790 679 56) |
| (7-5)  | (304 343,806 833 95) (264 283,096 601 10) (604 052,934 611 13) (7 402,732 320 69) |

$^a$The m in $(1'-1')_m$ indicates that m transition lines are selected in the DACMt studies for this band to obtain the best predictions. Measurement lines used in the DACMt calculation of (2-0), (3-1), (6-4), (7-5) bands are from Ref. 12.

### Table II. Band origins of the $X'$1$^1\Sigma^+ \rightarrow X'$1$^1\Sigma^+$ system for the CO molecule (in cm$^{-1}$).

| Band origin | This work | Farrenq et al. | Rank et al. | Mantz and Maillard | Mishra et al. | Malathy Devi et al. | Coxon and Hajigeorgiou |
|-------------|-----------|---------------|------------|-------------------|---------------|------------------|-----------------------|
| 2-0         | 4 260,062 393 958 8 | 4 260,062 175 | 4 260,064 6 | 4 260,063 3 | 4 260,062 176 | 4 260,062 171 |
| 3-1         | 4 207,168 540 028 2 | 4 207,167 957 | 4 207,168 0 | 4 207,168 1 | 4 207,168 0 | 4 207,167 942 8 |
| 6-4         | 4 049,299 582 672 3 | 4 049,299 298 | 4 049,300 7 | 4 049,295 0 | 4 049,295 0 | 4 049,299 295 |
| 7-5         | 3 996,964 025 101 9 | 3 996,959 141 | 3 996,959 0 | 3 996,953 0 | 3 996,953 0 | 3 996,959 132 |
TABLE III. Rotational constants for the vibrational levels of the $X^1\Sigma^+$ state of CO (in cm$^{-1}$).

| Vibrational level | $B_\nu$     | $D_\nu \times 10^6$ | $H_\nu \times 10^{12}$ | References |
|-------------------|-------------|----------------------|------------------------|------------|
| $\nu = 0$         |             |                      |                        |            |
| $\nu = 1$         |             |                      |                        |            |
| $\nu = 2$         |             |                      |                        |            |
| $\nu = 3$         |             |                      |                        |            |
| $\nu = 4$         |             |                      |                        |            |
| $\nu = 5$         |             |                      |                        |            |
| $\nu = 6$         |             |                      |                        |            |
| $\nu = 7$         |             |                      |                        |            |
A. (2-0) band

From Table IV [see Table A1 in the Appendix of the supplementary material (SM) for more transition lines], for the 2-0 band, there are eight relevant sets of data from previous calculations and measurements for comparison. It can be seen that, for the (2-0) overtone band, the best R-branch transition lines $v^{VDACMt}_{J,\text{cal}}(9)$ that are given to 8 decimal places up to $J = 110$ could be calculated using nine experimental transition lines (in bold-type) from the work by Mantz and Maillard, which has given satisfactory results with the error $AE_{\text{RMS}}$ of $1.945 \times 10^{-3}$ cm$^{-1}$. We have compared our transition lines $v^{VDACMt}_{J,\text{cal}}(9)$ to the HITRAN database and available measurements. For example, the benchmark values from Malathy Devi et al. have R-branch lines up to $J = 30$ that are listed in the third column. These lines are included as they have the most precise line positions to 6 decimal places for comparison of the low $J$ lines. The line positions recorded by the atmospheric chemistry experiment-Fourier transform spectrometer (ACE-FTS) are collected in the fourth column. The transition lines from HITRAN08 recorded by atmospheric trace molecule spectrometer-Fourier transform spectrometer (ATMOS-FTS), which were calculated by the PGOPHER program that is a general program for simulation molecular spectra, are listed in the fifth column. These two versions of HITRAN lines are presented here for comparison for high $J$ lines to validate the accuracy of the predicted transition lines beyond the observed ones. As seen in Table IV, the transition lines $v^{VDACMt}_{J,\text{cal}}(9)$ are found to be consistent with those measured by Malathy Devi et al., Mishra et al., Mantz and Maillard, Hashemi et al., Pollock et al., and Zou and Varanasi for the low $J$ lines. However, the calculated $v^{VDACMt}_{J,\text{cal}}(9)$ lines are slightly higher than the values from HITRAN for some higher rotational quantum numbers with $J$ values from 103 up to 110, which gives the difference errors at the $10^{-3}$ cm$^{-1}$ level (see Table A1 of the supplementary material). Moreover, plots of the differences between the $v^{VDACMt}_{J,\text{cal}}(9)$ values and lines of other works with $J$ values up to 80 are displayed in Fig. 2 in order to show the agreement and the small absolute error between them.
Additionally, to test the theoretical treatment of DACMt, we have shown variational (VDACMt) and non-variational (DACMt) treatments to yield results for the 2-0 overtone band. This allows us to compare the transition lines obtained from these two channels with the line values from the HITRAN database and some other works. However, along with a test for the variational and non-variational treatments in the calculation itself, there are also tests for the theoretical treatments of $\nu_{VDACMt J,cal}^{m,cal}(m) \mid m \neq 9$ calculation and DCM treatment of our recent work. Comparisons of the transition lines among these work are shown in Fig. 3 (these lines from Table A2 in the supplementary material), in which lines from $\nu_{VDACMt J,cal}^{9}$ show better agreement with the HITRAN08 database over the entire spectral region. Obviously, the calculated lines of $\nu_{VDACMt J,cal}^{9}$ for the higher $J$ lines.

B. (3-1) band

It is also interesting to see the calculated R-branch transition lines for the (3-1) overtone band that are based on the measurement lines reported by Mantz and Maillard, which are collected in Tables A3 and A4 of the supplementary material. The best R-branch transition lines $\nu_{VDACMt J,cal}^{9}$ that give the lowest error $\Delta E_{RMS}$ of $1.52 \times 10^{-3} \text{ cm}^{-1}$ are calculated using the corresponding molecular constants $(v_0, B_\nu, D_\nu, H_\nu)$ listed in Tables II and III. Just as shown in Fig. 4, comparing $\nu_{VDACMt J,cal}^{9}$ with the lines of Mantz and Maillard, Hase et al., HITRAN08 database, and Mishra et al., we gain the conclusion that good agreement exists between them. Figure 5 illustrates the general trends in line differences between the DACMt, DCM treatments, and the values of HITRAN08 for the (3-1) overtone band. As can be seen in the inset of Fig. 5 (lines from Table A4), with increasing $J$, the absolute line differences of $[\nu_{VDACMt J,cal}^{9} \mid m = 7, 11]$-HITRAN08 and $[\nu_{DCMt J,cal}^{11} \mid m = 7, 11]$-HITRAN08 increase, which can be explained using the inappropriate expansions of rotational energy form for these three cases. In addition, the results of $\nu_{VDACMt J,cal}^{5}$, which are in poor agreement with the values of HITRAN08, should be abandoned. However, comparing with the results of $\nu_{DACMt J,cal}^{9}$, the $\nu_{VDACMt J,cal}^{9}$ treatment can be a better candidate to improve the accuracy of the predicted R-branch lines by utilizing the variational treatment (see the Fig. 5 inset).

C. (6-4) band

We also performed the DACMt method for the (6-4) transition band. This is illustrated in Fig. 6, where the differences between R-branch transition lines of $\nu_{VDACMt J,cal}^{9}$ and some other works are plotted against the rotational quantum number $J$ for this transition band.
band. The calculated precision of the (6-4) transition band is approximately $1.70 \times 10^{-3}$ cm$^{-1}$. It is clear that the $\nu_{VDACM}^{9}$ lines, and the lines of Mantz and Maillard,$^{12}$ Hase et al.$^{6}$ and HITRAN08$^{21}$ compare very well, but it is worth noting that the blended lines $R_{6,45,50}$ of Mishra et al.$^{17}$ used for comparison of $\nu_{VDACM}^{9}$ calculations are at $-0.0123$ cm$^{-1}$, $-0.0377$ cm$^{-1}$, and $0.0142$ cm$^{-1}$ in the line differences, slightly more than the values comparing the work of Mantz and Maillard,$^{12}$ Hase et al.$^{6}$ and HITRAN08.$^{21}$ Similarly, as can be seen in Fig. 7, the lines of $\nu_{VDACM}^{9}$ could enable a reasonable prediction of the behavior of high-lying transitional lines in the VDACMt approach, thus indicating a representation of its validity, while an obvious deviation can be seen between the $\nu_{VDACM}^{9}$ values and these HITRAN08 results$^{21}$ in the line differences as well as those for the $\nu_{VDACM}^{m}$ lines $m = 5, 7, 11$ and $\nu_{DCM}^{11}$.

D. (7-5) band

Figure 8 demonstrates the comparisons between our results and some other works for the (7-5) band with a $\Delta E_{RMS}$ of $3.72 \times 10^{-3}$ cm$^{-1}$. In the whole part of the line differences with $J$ values of 0–80, it appears that the lines of $\nu_{VDACM}^{9}$, available measurement lines, and the HITRAN08 database overlap, and a reasonable trend is visible. Most of these difference errors are at the $10^{-3}$ cm$^{-1}$ or $10^{-4}$ cm$^{-1}$ level, being consistent with the accuracy of the measurements or calculations, except for the line differences $[\nu_{VDACM}^{9} - \nu_{VDACM}^{9}]$, where the inconsistency is visible for most lines, given some differences at the $10^{-2}$ cm$^{-1}$ level. Another illustration of comparison is given in Fig. 9, which displays the line differences between the DACMt, DCM theoretical calculations, and the values of HITRAN08.$^{21}$ As it has been used above, the transition lines $\nu_{VDACM}^{9}$ will be a good interpretation
of the spectroscopic information for this band, other than the lines of \(v_{\text{DACMt}}(m)|m = 5, 7, 11, v_{\text{DACMt}}(9)\), and \(v_{\text{DACMt}}(11)\). Such a disagreement clearly expresses that among these approaches, difference in treatment for the experimental lines or polynomial truncation with respect to the \([J(J + 1)]^m\) indicates the failure of the prediction for high \(J\) R-branch transition lines for the (7-5) band.

It is worth to note that the matter of reassessing the predictions of the R-transition lines is not a simple one, and may arise from the accuracy of the experimental ones selected. As such, this is to say, the better representation of the data from the experiment could help us improve the accuracy of the DACMt prediction for higher \(J\) lines.

IV. SUMMARY

The difference algebraic converging method (DACM) originates from a close cooperation between the theoretical method and experimental measurements. Based on some experimental lines, algebraic Eq. (10) and analytical formula Eq. (9) are used to predict R-branch transition spectral lines with variational treatment for (2-0), (3-1), (6-4), and (7-5) overtone bands in the \(X^1\Sigma^+ \rightarrow X^1\Sigma^+\) transition of CO. With \(J\) values up to 110, our results \(v_{\text{DACMt}}\) are in good agreement with the line values from HITRAN and some other experiments, and also are expected to give reliable predictions. In addition, an improved set of molecular constants is derived for vibrational analyses of the R-transition lines for these first overtone bands. In the case of each band of CO, there is a typically well-seen connection between transition lines and the molecular constants. Such deep insights shall undoubtedly enhance our understanding of how the diversities of molecular constants influence the transition lines, and of course, improve the development of a better method. Therefore, the DACMt suggested in this work for the calculation of the R-transition lines provides a promising method for diatomic molecules. In addition, the improved spectroscopic parameters of CO will be important to the astrophysical research and astronomical community.

SUPPLEMENTARY MATERIAL

See the supplementary material for the transition lines of (2-0), (3-1), (6-4), and (7-5) overtones bands of the ground electronic state of \(^{12}\text{C}\text{^16}\text{O}\).

ACKNOWLEDGMENTS

This work was supported by the Funds for Sichuan Distinguished Scientists of China (Grant Nos. 2019DJQ0050 and 2019DJQ0051), the National Natural Science Foundation of China (Grant Nos. 61722507, 11904295, and 11647058), Project (Grant No. 17ZA0369) of Education Department of Sichuan Province, the Outstanding Innovation Teams of Higher Learning Institutions of Shanxi (OIT), State Key Laboratory Open Fund of Quantum Optics and Quantum Optics Devices, Laser Spectroscopy Laboratory (Grant No. KF201811), and the fund of the Key Laboratory of Advanced Scientific Computation, Xihua University, China.

REFERENCES

1. D. W. Savin, R. G. Bhaskar, S. Vissapragada, and X. Urbain, Astrophys. J. 844, 154 (2017).
2. B. Bézard, C. de Bergh, D. Crisp, and J.-P. Maillard, Nature 345, 508 (1990).
3. A. Faure, L. Wiesenfeld, B. J. Drouin, and J. Tennyson, J. Quant. Spectrosc. Radiat. Transfer 116, 79 (2013).
4. V. A. Krasnopolsky, icarus 228, 189 (2014).
5. R. Farrenq, G. Guelachvili, A. J. Saurau, N. Grevesse, and C. B. Farmer, J. Mol. Spectrosc. 149, 375 (1991).
6. F. Hase, L. Wallace, S. D. McLeod, J. J. Harrison, and P. F. Bernath, J. Quant. Spectrosc. Radiat. Transfer 111, 521 (2010).
7. P. F. Bernath, J. Quant. Spectrosc. Radiat. Transfer 186, 3 (2017).
8. P. A. Crutzen, L. E. Heidt, J. P. Krasnec, W. H. Pollock, and W. Seiler, Nature 282, 253 (1979).
9. P. Lyons, E. Gharib-Nezhad, and T. R. Ayres, Nat. Commun. 9, 908 (2018).
10. Z. Qin, J. M. Zhao, and L. H. Liu, J. Quant. Spectrosc. Radiat. Transfer 210, 1 (2018).
11. D. H. Rank, A. G. St. Pierre, and T. A. Wiggins, J. Mol. Spectrosc. 18, 418 (1965).
12. A. W. Manzt and J.-P. Maillard, J. Mol. Spectrosc. 53, 466 (1974).
13. C. R. Pollock, F. R. Petersen, D. A. Jennings, J. S. Wells, and A. G. Maki, J. Mol. Spectrosc. 99, 357 (1983).
14. D. Goorvitch, Astrophys. J., Suppl. Ser. 95, 535 (1994).
15. Q. J. Zou and P. Varanasi, J. Quant. Spectrosc. Radiat. Transfer 75, 63 (2002).
16. K. Sung and P. Varanasi, J. Quant. Spectrosc. Radiat. Transfer 91, 319 (2005).
17. A. P. Mishra, B. J. Shetty, and R. J. Khirsagar, J. Mol. Spectrosc. 232, 296 (2005).
18. V. Malathy Devi, D. Chris Benner, M. A. H. Smith, A. W. Manzt, K. Sung, L. Brown, and A. Predoi-Cross, J. Quant. Spectrosc. Radiat. Transfer 113, 1013 (2012).
19. B. Hashemi, A. Predoi-Cross, A. S. Dudaryonok, N. N. Lavrentievna, A. C. Vandaele, and J. Vander Auwera, J. Mol. Spectrosc. 326, 60 (2016).
20. K. Esteki, A. Predoi-Cross, C. Povey, S. Ivanov, A. Ghoulai, F. Thibault, and M. A. H. Smith, J. Quant. Spectrosc. Radiat. Transfer 203, 309 (2017).
21. L. S. Rothman, I. E. Gordon, A. Barbe, D. Chris Benner, P. F. Bernath, M. Birk, V. Boudon, L. R. Brown, A. Campargue, J.-P. Champion, K. Chance, L. H. Courdert, V. Dana, V. Malathy Devi, S. Fally, J.-M. Flaud, R. R. Gamache, A. Goldman, D. Jacquemart, I. Kleinier, N. Lacombe, W. J. Lafferty, J.-Y. Mandin, S. T. Massie, S. Mikhailenko, C. E. Miller, N. Moazzen-Ahmadi, O. V. Naumenko, A. Nikiitin, J. Orphal, A. Predoi-Cross, V. Perevalov, A. Perrin, C. P. Rinsland, M. Rotger, M. Šimecková, M. A. H. Smith, K. Sung, T. Tashkun, J. Tennyson, R. A. Toth, A. C. Vandaele, and J. Vander Auwera, J. Quant. Spectrosc. Radiat. Transfer 110, 533 (2009).
22. E. Gordon, L. S. Rothman, C. Hill, R. V. Kochanov, Y. Tan, P. F. Bernath, M. Birk, V. Boudon, A. Campargue, K. V. Chance, B. J. Drouin, J. M. Flaud, R. R. Gamache, J. T. Hodges, D. Jacquemart, V. I. Perevalov, A. Perrin, K. P. Shine, M.-A. H. Smith, J. Tennyson, G. C. Toon, H. Tran, V. G. Tyuterev, A. Barbe, A. G. Császárr, V. M. Devi, T. Furtenbacher, J. J. Harrison, J.-M. Hartmann, A. Jolly, T. J. Johnson, T. Karman, I. Kleinier, A. A. Kyuberis, J. Loos, O. M. Lyulin, S. T. Massie, S. N. Mikhailenko, N. Moazzen-Ahmadi, H. S. P. Müller, O. V. Naumenko, A. V. Nikiitin, O. L. Polynsky, M. Rey, M. Rotger, S. W. Sharpe, K. Sung, E. Stankóva, S. A. Tashkun, J. Vander Auwera, G. Wagner, J. Wilczewski, P. Wcislo, S. Yu, and J. J. Zak, J. Quant. Spectrosc. Radiat. Transfer 203, 3 (2017).
23. L. S. Rothman, R. B. Wattson, R. Gamache, J. Schroeder, and A. McCann, Proc. Soc. Photo-Opt. Instrum. Eng. 2471, 105 (1995).
24. L. S. Rothman, I. E. Gordon, R. J. Barber, H. Dothe, R. R. Gamache, A. Goldman, V. I. Perevalov, S. A. Tashkun, and J. Tennyson, J. Quant. Spectrosc. Radiat. Transfer 111, 2139 (2010).
25. Y. Zhang, W. G. Sun, J. Fu, Q. C. Fan, J. Ma, L. T. Xiao, and S. T. Jia, Sci. China: Phys., Mech. Astron. 62, 943011 (2019).
26. J. A. Coxon and P. G. Haiegeorgiou, J. Chem. Phys. 121, 2992 (2004).
27. W. G. Sun, Q. C. Fan, H. D. Li, and H. Feng, Spectrochim. Acta, Part A 79, 35 (2011).
28 H. D. Li, W. G. Sun, Q. C. Fan, and H. Feng, Spectrochim. Acta, Part A 83, 136 (2011).
29 Q. C. Fan, Q. Wang, W. G. Sun, H. D. Li, and H. Feng, Spectrochim. Acta, Part A 87, 199 (2012).
30 Y. H. Jiang, W. G. Sun, Y. Zhang, J. Fu, Q. C. Fan, H. D. Li, and H. Feng, Spectrochim. Acta, Part A 153, 87 (2016).
31 Q. C. Fan, C. P Hu, J. Fu, J. Ma, Z. X. Fan, Y. G. Xu, H. D. Li, and Yi. Zhang, Spectrochim. Acta, Part A 200, 290 (2018).
32 G. Herzberg, Molecular Spectra and Molecular Structure (I): Spectra of Diatomic Molecules (Nostrand D Van Printing, New York, 1953).
33 C. M. Western, J. Quant. Spectrosc. Radiat. Transfer 186, 221 (2017).