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A new method for calculating the CO-factored force constants of pentacarbonyliron

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Abstract

Using an analytical approach we were able to obtain a valid solution to the CO-factored force field of Fe(CO)₅. The solution led to the relations which allow direct calculation of the CO-factored force constants from C–O stretching frequencies of the all- $^{12}C^{16}O$ molecule. The force constants calculated from these relations were used to estimate C–O stretching frequencies of $^{13}C^{16}O$ -substituted species of Fe(CO)₅. The results were found to be in very close agreement with those obtained from isotopic spectra. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Pentacarbonyliron; Infrared spectra; CO-factored force field; Force constants

1. Introduction

For trigonal-bipyramidal Fe(CO)₅, under the D_{3h} local symmetry of the carbonyls, group theory predicts four C–O stretching modes $(2a_1'+e'+a_2'')$. The e' mode is both infrared and Raman-active, whereas the a_1' modes are only Raman-active and the a_2'' mode is only infrared active [1,2]. On the basis of the CO-factored force field [3–6] which neglects anharmonicity and all coupling except CO–CO interaction, trigonal-bipyramidal Fe(CO)₅ has two carbonyl stretching force constants $(k_1 \text{ and } k_2)$ and three physically different CO–CO interaction constants $(k_t, k_c' \text{ and } k_c)$, as shown Fig. 1. Since there are five force constants to be calculated and only four observable C–O stretching modes, the COfactored force field for Fe(CO)₅ is underdetermined.

Several methods that enable us to determine the COfactored force constants for $Fe(CO)_5$ have been reported in the literature. The method developed by Haas and Sheline [1] is based on the assumption that the effects of ligands on force constants are additive. However, this method necessitates the use of C–O stretching frequen-

* Corresponding author *E-mail address:* nzengin@cumhuriyet.edu.tr (N. Zengin). cies of all $Fe(CO)_{5-n}L_n$ (n = 0, 1, 2, 3, 4), species, not only those of Fe(CO)₅. Dalton et al. [7], using two relationships between the interaction constants $k_t/k_c =$ 1.74 and $k_c'/k_c = 1.58$, derived from orbital overlap theories [8], have calculated CO-factored force constants for Fe(CO)₅. In the cos β parameter method proposed by Bor [9], the solution of the force field was reduced to the problem of finding the value of the $\cos \beta$ parameter. Bor made use of isotopic data to obtain a suitable value for $\cos \beta$. Another method that can be used to determine CO-factored force constants for $Fe(CO)_5$ was suggested by Timney [10]. This method is based on several empirical relationships expressed in terms of ligand effect constants and bond angles. In our previous work [11–13] on solving the CO-factored force fields of complexes of the types $cis-L_2M(CO)_4$, $M(CO)_4$ and LM(CO)₅, we have developed some analytical approaches. These approaches enabled us to calculate force constants from C-O stretching frequencies of the all-¹²C¹⁶O molecule.

In the present report, a new analytical approach was employed in obtaining a valid solution to the COfactored force field for $Fe(CO)_5$. This approach led to the relations by which carbonyl stretching force constants and interaction constants can be calculated directly from ${}^{12}C{}^{16}O$ stretching frequencies.

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Fig. 1. Definition of CO-factored force constants for trigonal-bipyramidal Fe(CO)₅.

2. Derivations of relations

The secular equations for $Fe(CO)_5$, which are given elsewhere [1,2,9], are presented in Table 1. Since there are five unknowns (force constants) and only four equations, it is mathematically evident that an infinite number of solutions to the secular equations will be possible. In order to reduce the number of the unknowns we have employed the following substitutions:

$$k_1 + 2k'_c = \delta_1 k_c \tag{1}$$

$$k_2 + k_t = \delta_2 k_c \tag{2}$$

$$k_2 + k_t = \delta_2 k_c \tag{2}$$

With these substitutions, the following relations are obtained from the secular determinant given in Table 1.

$$\lambda_1 = (\mu/2)[(\delta_1 + \delta_2) + \sqrt{(\delta_1 - \delta_2)^2 + 24}]k_c$$
(3)

$$\lambda_2 = (\mu/2)[(\delta_1 + \delta_2) - \sqrt{(\delta_1 - \delta_2)^2 + 24}]k_c$$
(4)

where λ_1 and λ_2 are the λ parameters of the a'_1 modes. λ_1 denotes the mode at the higher frequency, and λ_2 the mode at the lower frequency. From Eqs. (3) and (4) two relations for k_c are obtained:

$$k_{\rm c} = \frac{\lambda_1 + \lambda_2}{\mu(\delta_1 + \delta_2)} \tag{5}$$

$$k_{\rm c} = \frac{\lambda_1 - \lambda_2}{\mu \sqrt{\left(\delta_1 - \delta_2\right)^2 + 24}} \tag{6}$$

These relations indicate that k_c can be calculated from observed frequencies of the a'_1 modes if δ_1 and δ_2 are known. Combining them gives:

$$\frac{\sqrt{\left(\delta_1 - \delta_2\right)^2 + 24}}{\delta_1 + \delta_2} - \frac{\lambda_1 - \lambda_2}{\lambda_1 + \lambda_2} = 0 \tag{7}$$

Table 1

Secular equations	for	Fe(CO) ₅	with	D_{3h}	symmetry
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Symmetry species	Secular equation	s ^a
$\overline{a'_1} a'_1$	$ \begin{vmatrix} \mu(k_1 + 2k'_c) - \lambda \\ \sqrt{6}\mu k_c \end{vmatrix} $	$ \begin{array}{c} \sqrt{6}\mu k_{\rm c} \\ \mu (k_2 + 2k_{\rm t}) - \lambda \end{array} = 0 $
e'	$\lambda = \mu (k_1 - k_{\rm c}')$	
a_2''	$\lambda = \mu(k_2 - k_{\rm t})$	

^a The various k are defined in Fig. 1; μ represents the reciprocal of the CO group; $\lambda = 4\pi^2 e^2 v^2$ where v is the frequency in cm⁻¹.

This resulting equation enables us to conclude that the determination of k_c is reduced to the problem of finding the values of δ_1 and δ_2 which satisfy it. For a given molecule the left-hand side of Eq. (7) has two variables, δ_1 and δ_2 , and may therefore be regarded as a function of δ_1 and δ_2 , which is represented by $f(\delta_1, \delta_2)$. When the function $f(\delta_1, \delta_2)$ is plotted against δ_2 for various values of δ_1 , such as δ'_1 , δ''_1 , δ''_1 , the curves shown in Fig. 2 are obtained.

As can be seen from Fig. 2, one of the solutions of Eq. (7) corresponds to the point at which the δ_2 -axis is tangential to the curve obtained for $\delta_1 = \delta_1''$. Since the curve considered has a minimum at the point, we may make use of the partial derivative of the function $f(\delta_1, \delta_2)$ with respect to δ_2 for obtaining the solution mentioned. With the use of $\partial f(\delta_1, \delta_2) / \partial \delta_2 = 0$ and $f(\delta_1, \delta_2) = 0$, we have

$$\delta_1 = \frac{2\sqrt{6}\sqrt{\lambda_1\lambda_2}}{(\lambda_1 - \lambda_2)} \tag{8}$$

$$\delta_2 = \frac{\sqrt{6}(\lambda_1^2 + \lambda_2^2)}{(\lambda_1 - \lambda_2)\sqrt{\lambda_1\lambda_2}} \tag{9}$$

Substituting these relations into Eqs. (5)–(6) gives:

$$k_{\rm c} = \frac{(\lambda_1 - \lambda_2)\sqrt{\lambda_1\lambda_2}}{\sqrt{6}\mu(\lambda_1 + \lambda_2)} \tag{10}$$

This equation shows that k_c can be calculated from observed frequencies of the a'_1 modes. Once k_c has been determined, the other four force constants $(k_1, k_2, k_t \text{ and } k_1, k_2, k_t \text{ and } k_1, k_2, k_1 \text{ and } k_2, k_2 \text{ and } k_2, k_3 \text{ and } k_3 \text{ and } k_4 \text{ a$ $k_{\rm c}$) can be found from the secular equations. Further-



Fig. 2. Model graphs of the function of (δ_1, δ_2) vs. δ_2 for various values of δ_1 .

Table 2 CO-factored force constants ^a for Fe(CO)₅ calculated by various methods

Methods ^b	k_1	k_2	$k_{\rm t}$	k'c	kc
A	16.559	16.964	0.422	0.386	0.283
В	16.54	16.95	0.43	0.39	0.28
С	16.57	16.95	0.41	0.40	0.28

^a Force constants are given in mdyn $Å^{-1}$.

^b A, B and C, respectively, represent our method, the method described by Dalton et al. and the $\cos \beta$ parameter method.

Table 3 Secular equations for isotopically substituted species of $M(CO)_5$ molecules with D_{3h} symmetry^a

$$3a_{1} \begin{vmatrix} \mu^{*}k_{2} - \lambda & \mu k_{1} & \sqrt{3}\mu k_{c} \\ \mu^{*}k_{1} & \mu k_{2} - \lambda & \sqrt{3}\mu k_{c} \\ \sqrt{3}\mu^{*}k_{c} & \sqrt{3}\mu k_{c} & \mu (k_{1} + 2k_{c}') - \lambda \end{vmatrix} = 0$$

$$e$$
 $\lambda = \mu (k_1 - k_c)$
 $M(^{12}CO)_3(^{13}CO)_2, ax, eq, C_s$

 $M(^{12}CO)_4(^{13}CO)$, ax, C_{3v}

$$4a' \begin{vmatrix} \mu^{*}k_{2} - \lambda & \mu k_{1} & \mu^{*}k_{c} & \sqrt{2}\mu k_{c} \\ \mu^{*}k_{1} & \mu k_{2} - \lambda & \mu^{*}k_{c} & \sqrt{2}\mu k_{c} \\ \mu^{*}k_{c} & \mu k_{c} & \mu^{*}k_{1} - \lambda & \sqrt{2}\mu k_{c}' \\ \sqrt{2}\mu^{*}k_{c} & \sqrt{2}\mu k_{c} & \sqrt{2}\mu^{*}k_{c}' & \mu(k_{1} + k_{c}') - \lambda \end{vmatrix} = 0$$

$$a'' \qquad \lambda = \mu (k_1 - k_c')$$

 $M(^{12}CO)_2(^{13}CO)_3$, ax,eq,eq, C_s

$$4a' \begin{vmatrix} \mu k_2 - \lambda & \mu * k_1 & \mu k_c & \sqrt{2} \mu * k_c \\ \mu k_1 & \mu * k_2 - \lambda & \mu k_c & \sqrt{2} \mu * k_c \\ \mu k_c & \mu * k_c & \mu k_1 - \lambda & \sqrt{2} \mu * k_c' \\ \sqrt{2} \mu k_c & \sqrt{2} \mu * k_c & \sqrt{2} \mu k_c' & \mu * (k_1 + k_c') - \lambda \end{vmatrix} = 0$$

$$a'' \qquad \lambda = \mu^* (k_1 - k_c')$$

 $M(^{12}CO)(^{13}CO)_4$, ax, eq, eq, eq, C_{3v}

$$3a_{1} \begin{vmatrix} \mu k_{2} - \lambda & \mu^{*} k_{1} & \sqrt{3} \mu^{*} k_{c} \\ \mu k_{1} & \mu^{*} k_{2} - \lambda & \sqrt{3} \mu^{*} k_{c} \\ \sqrt{3} \mu k_{c} & \sqrt{3} \mu^{*} k_{c} & \mu^{*} (k_{1} + 2k_{c}') - \lambda \end{vmatrix} = 0$$

 $e \qquad \lambda = \mu^*(k_1 - k_c)$

$$M(^{12}CO)_4(^{13}CO), eq, C_{2v}$$

$$3a_{1} \begin{vmatrix} \mu(k_{2}+k_{1})-\lambda & \sqrt{2}\mu^{*}k_{c} & \sqrt{2}\mu k_{c} \\ \sqrt{2}\mu k_{c} & \mu^{*}k_{1}-\lambda & \sqrt{2}\mu k_{c}' \\ 2\mu k_{c} & \sqrt{2}\mu^{*}k_{c}' & \mu(k_{1}+k_{c}')-\lambda \end{vmatrix} = 0$$

$$b_1 \quad \lambda = \mu(k_2 - k_t)$$

$$b_2 \quad \lambda = \mu(k_1 - k_c)$$

$$M(^{12}CO) \quad (^{13}CO) \quad \text{an an } d$$

$$M(-CO)_{3}(-CO)_{2}, eq, eq, C_{2v}$$

$$3a_{1} \begin{vmatrix} \mu(k_{2}+k_{1})-\lambda & \sqrt{2}\mu k_{c} & 2\mu^{*}k_{c} \\ \sqrt{2}\mu k_{c} & \mu k_{1}-\lambda & \sqrt{2}\mu^{*}k_{c}' \\ 2\mu k_{c} & \sqrt{2}\mu k_{c}' & \mu^{*}(k_{1}+k_{c}')-\lambda \end{vmatrix} = 0$$

$$\begin{split} b_1 & \lambda = \mu(k_2 - k_1) \\ b_2 & \lambda = \mu^*(k_1 - k_c') \\ M(^{12}CO)_2(^{13}CO)_3, \ eq, eq, eq, eq, D_{3h} \end{split}$$

$$2a_{1}' \quad \begin{vmatrix} \mu(k_{2}+k_{1}) - \lambda & \sqrt{6}\mu^{*}k_{c} \\ \sqrt{6}\mu k_{c} & \mu^{*}(k_{1}+2k_{c}') - \lambda \end{vmatrix} = 0$$

$$\begin{array}{ll} a_{2}^{"} & \lambda = \mu (k_{2} - k_{t}) \\ e^{'} & \lambda = \mu^{*} (k_{1} - k_{c}^{'}) \end{array}$$

$$M(^{13}CO)_5, D_{3h}$$

$$2a_{1}' \begin{vmatrix} \mu^{*}(k_{2}+k_{1})-\lambda & \sqrt{6}\mu^{*}k_{c} \\ \mu^{*}(k_{1}+2k_{c}')-\lambda \end{vmatrix} = 0$$

$$a_{2}'' \lambda = \mu^{*}(k_{2}-k_{1})$$

$$e' \lambda = \mu^{*}(k_{1}-k_{c}')$$

$$M(^{12}CO)_{3}(^{13}CO)_{2}, ax, ax, D_{3h}$$

$$2a_{1}' \begin{vmatrix} \mu^{*}(k_{2}+k_{1})-\lambda & \sqrt{6}\mu k_{c} \\ \sqrt{6}\mu^{*}k_{c} & \mu(k_{1}+2k_{c}')-\lambda \end{vmatrix} = 0$$

$$a_{2}'' \lambda = \mu^{*}(k_{2}-k_{1})$$

$$e' \lambda = \mu(k_{1}-k_{c}')$$

$$M(^{12}CO)_{2}(^{13}CO)_{3}, ax, ax, eq, C_{2v}$$

$$3a_{1} \begin{vmatrix} \mu^{*}(k_{2}+k_{1})-\lambda & \sqrt{2}\mu^{*}k_{c} & 2\mu k_{c} \\ \sqrt{2}\mu^{*}k_{c} & \mu^{*}k_{1}-\lambda & \sqrt{2}\mu k_{c}' \\ 2\mu^{*}k_{c} & \sqrt{2}\mu^{*}k_{c}' & \mu(k_{1}+k_{c}')-\lambda \end{vmatrix} = 0$$

$$b_{1} \lambda = \mu^{*}(k_{2}-k_{1})$$

$$b_{2} \lambda = \mu(k_{1}-k_{c}')$$

$$M(^{12}CO)(^{13}CO)_{4}, ax, ax, eq, eq, C_{2v}$$

$$3a_{1} \begin{vmatrix} \mu^{*}(k_{2}+k_{1})-\lambda & \sqrt{2}\mu k_{c} & 2\mu^{*}k_{c} \\ \sqrt{2}\mu^{*}k_{c} & \sqrt{2}\mu^{*}k_{c}' & \mu(k_{1}+k_{c}')-\lambda \end{vmatrix} = 0$$

$$b_{1} \lambda = \mu^{*}(k_{2}-k_{1})$$

$$b_{2} \lambda = \mu^{*}(k_{2}-k_{1})$$

$$b_{1} \lambda = \mu^{*}(k_{2}-k_{1})$$

$$b_{2} \lambda = \mu^{*}(k_{1}-k_{c}')$$

^a μ^* denotes the reciprocal of the reduced mass of ¹³C¹⁶O.

more, inserting Eq. (10) into the secular equations presented in Table 1 gives the following relations by which k_1 , k_2 , k_t and k'_c can be calculated from the observed frequencies of the all-¹²C¹⁶O molecule:

$$k_{1} = (\lambda_{1} + \lambda_{2} + 4\lambda_{3} - \beta)/(6\mu)$$
(11)

$$k_2 = (\lambda_1 + \lambda_2 + 2\lambda_4 + \beta)/(4\mu) \tag{12}$$

$$k_{\rm t} = (\lambda_1 + \lambda_2 - 2\lambda_4 + \beta)/(4\mu) \tag{13}$$

$$k'_c = (\lambda_1 + \lambda_2 - 2\lambda_3 - \beta)/6\mu \tag{14}$$

Where λ_3 , λ_4 are the λ parameters of e' and a''_2 modes, respectively, and $\beta = (\lambda_1 - \lambda_2)^2 / (\lambda_1 + \lambda_2)$.

3. Results and discussion

When the secular equations given in Table 1 are rearranged so that four of the five force constants are expressed in terms of the fifth and the observed frequencies, it is obtained an algebraic system which consist of four equations in five unknowns. It is mathematically evident that for such a system that an infinite number of solutions will be possible. In fact, the

Table 4

Observed and calculated C-O stretching frequencies for ¹³CO-substituted species of Fe(CO)₅

$ \begin{split} \hline $	Species	Frequencies			Assignment
$ \begin{split} & Fq^{12}CO J_{4}^{13}CO, \ \mathcal{C}_{as}, \ ^{12}CO; \ ax & 2105.5 \ ^{\circ} & 2105.4 & 2105.1 & a_1 \\ & 2028.9 & 2028.9 & a_1 \\ & 2028.9 & 2028.9 & a_1 \\ & 2001. & 2000.9 & 2000.9 & e \\ & 2007.2 & 2027.1 & a_1 \\ & 2027.2 & 2027.6 & b_1 \\ & 2009.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & e' \\ & 1976 & 1978.5 & 1976.6 & a_1^2 \\ & 2062 & 2028.2 & a' \\ & 1988 & 1989.1 & 1987.6 & a' \\ & 2062 & 2028.2 & a' \\ & 1988 & 1989.1 & 1987.6 & a' \\ & 2062 & 2028.2 & a' \\ & 1988 & 1989.1 & 1987.6 & a' \\ & 2062 & 2028.2 & a' \\ & 1988 & 1989.1 & 1987.6 & a' \\ & 2029 & 2000.9 & 2000.9 & e' \\ & 1976 & 1978.5 & 1976.6 & a' \\ & 2029 & 2000.8 & a_1 \\ & 1964 & 1964.5 & 1962.8 & a' \\ & 2021 & 2020.8 & a_1 \\ & 1964 & 1964.5 & 1962.8 & a' \\ & 2021.0 & 2020.8 & a_1 \\ & 1976 & 1978.5 & 1976.6 & a_1 \\ & 1964 & 1964.5 & 1962.8 & a' \\ & 2021.0 & 2020.8 & a_1 \\ & 1976 & 1978.5 & 1976.6 & a_1 \\ & 2021.0 & 2020.8 & a_1 \\ & 1976 & 1978.5 & 1976.6 & a_1 \\ & 1964 & 1964.2 & 1962.5 & a_1 \\ & 1964 & 1964.5 & 1966.8 & a_1 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.8 & a_1 \\ & 1976 & 1978.5 & 1976.6 & b_1 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001.5 & 2001.6 & a_1 \\ & 1976 & 1978.5 & 1976.6 & b_1 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001.5 & 2001.6 & a_1 \\ & 1972 & 1974.0 & 1972.4 & a' \\ & 2021.5 & a' \\ & 1976 & 1978.5 & 1976.6 & b_1 \\ & 1975 & 1956.3 & 1954.5 & e' \\ & 2021.5 & a' \\ & 1976 & 1978.5 & 1976.6 & b_1 \\ & 1976 & 1978.5 & 1976.6 & b_1 \\ & 1976 & 1978.5 & 1976.6 & b_1 \\ & 1976 & 1978.5 & 1976.6 & b_1 \\ & 1976 & 1978.5 & 1976.6 & b_1 \\ & 1976 & 1978.5 & 1976.6 & b_1 \\ & 1976 & 1978.5 & 1976.6 & b_1 \\ & 1976 & 1978.5 & 1976.6 & b_1 \\ & 1972 & 1973.5 & 1972.0 & a_1 \\ & 1972 & 1973.5 & 1972.0 & a_1 \\ & 1975 & 1985.3 & 1954.5 & e' \\ & 2069 & 2064.9 & 2064.9 & a_1 \\ & 1975$		Observed	Calculated ^a	Calculated ^b	
$\begin{split} Fe({}^{12} CO)_4({}^{13} CO), C_{2n}, {}^{12} CO; eq & 2008, 0 & 2009, 0 & 2009, 0 & e^{-1} \\ 2010 & 2000, 9 & 2000, 9 & e^{-1} \\ 2027 & 2027, 1 & 2027, 1 & a^{-1} \\ 2027 & 2023, 6 & 2023, 6 & b^{-1} \\ 2028 & 2023, 6 & 2023, 6 & b^{-1} \\ 2029 & 2000, 9 & 2000, 9 & b^{-1} \\ 2010 & 2000, 9 & 2000, 9 & b^{-1} \\ 2010 & 2000, 9 & 2000, 9 & e^{-1} \\ 2010 & 2000, 9 & 2000, 9 & e^{-1} \\ 2010 & 2000, 9 & 2000, 9 & e^{-1} \\ 2010 & 2000, 9 & 2000, 9 & e^{-1} \\ 2010 & 2000, 9 & 2000, 9 & e^{-1} \\ 2010 & 2000, 9 & 2000, 9 & e^{-1} \\ 2010 & 2000, 9 & 2000, 9 & e^{-1} \\ 2010 & 2000, 9 & 2000, 9 & e^{-1} \\ 2010 & 2000, 9 & 2000, 9 & e^{-1} \\ 2010 & 2000, 9 & 2000, 9 & e^{-1} \\ 2010 & 2000, 9 & 2000, 9 & e^{-1} \\ 2010 & 2000, 9 & 2000, 9 & e^{-1} \\ 2010 & 2000, 9 & 2000, 9 & e^{-1} \\ 2028 & 2026, 2 & 2026, 2 & a^{-1} \\ 2029 & 2008, 8 & a^{-1} \\ 2029 & 2008, 8 & a^{-1} \\ 2029 & 2008, 8 & a^{-1} \\ 2020, 10 & 2000, 9 & 2000, 9 & a^{-1} \\ 2021, 0 & 2000, 9 & 2000, 9 & a^{-1} \\ 2021, 0 & 2000, 9 & 2000, 9 & a^{-1} \\ 2021, 0 & 2000, 9 & 2000, 9 & a^{-1} \\ 2021, 0 & 2000, 9 & 2000, 9 & a^{-1} \\ 2021, 0 & 2002, 8 & a_{1} \\ 2021, 0 & 2002, 9 & 2000, 8 & a_{1} \\ 2021, 0 & 2002, 9 & 2000, 9 & b_{2} \\ 2021, 0 & 2002, 9 & 2001, 6 & a_{1} \\ 2021, 0 & 2002, 9 & 2001, 6 & a_{1} \\ 2021, 0 & 2002, 9 & 2001, 6 & a_{1} \\ 2021, 0 & 2002, 9 & 2001, 6 & a_{1} \\ 2021, 0 & 2002, 9 & 2001, 6 & a_{1} \\ 2021, 0 & 2002, 9 & 2001, 6 & a_{1} \\ 2021, 0 & 2002, 9 & 2001, 6 & a_{1} \\ 2021, 0 & 2001, 9 & 2000, 9 & b_{2} \\ 2021, 0 & 2001, 0 & 2000, 9 & b_{2} \\ 2021, 0 & 2001, 0 & 2000, 9 & b_{2} \\ 2021, 0 & 2001, 0 & 2000, 9 & b_{2} \\ 2021, 0 & 2001, 0 & 2000, 0 & b_{2} \\ 2021, 0 & 2001, 0 & 2001, 0 & 2000, 0 & b_{2} \\ 2021, 0 & 2001, 0 & 2001, 0 & 2001, 0 & 2000, 0 & b_{2} \\ 2021, 0 & 2001, 0 & 2000, 0 & b_{2} \\ 2021, 0 & 2001, 0 & 2000, 0 & b_{2} \\ 2021, 0 & 2001, 0 & 2001, 0 & 2001, 0 & 2001, 0 & 2000, 0 & b_{2} \\ 2021, 0 & 2001, 0 & 2000, 0 & 2000, 0 & b_{2} \\ 2021, 0 & 2001, 0 & 2001, 0 & 2000, 0 & 2000, 0 & b_{2} \\ 2021, 0 & 2001, 0 & 2000, 0 & 2000, 0 $	$\overline{\text{Fe}(^{12}\text{CO})_4(^{13}\text{CO}), C_{3v}, ^{13}\text{CO}; \text{ax}}$	2105.5 °	2105.4	2105.1	a_1
Peq ¹² C0) ₄ (¹³ C0), C ₂ , ¹³ C0; eq Peq ¹² C0) ₄ (¹³ C0), C ₂ , ¹³ C0; ax, ax Peq ¹² C0) ₄ (¹³ C0), C ₂ , ¹³ C0; ax, ax Peq ¹² C0) ₄ (¹³ C0), C ₂ , ¹³ C0; ax, ax Peq ¹² C0) ₄ (¹³ C0), C ₂ , ¹³ C0; ax, ax Peq ¹² C0) ₄ (¹³ C0) ₂ , D _{3h} , ¹³ C0; ax, ax 2001 200.9<			2028.9	2028.9	a_1
2001 2000.9 9 e ⁻ 2108.0 ⁻⁵ 2108.5 ⁻ 2108.5 2108.5		1988	1988.7	1987.0	a_1
Fe(¹³ CO) ₄ (¹³ CO), C _{2x} , ¹³ CO; eq 208.0 * 200.1 200.1 200.1 6 1964 1965.1 1963.5 aq 2001 2000.9 200.9 b ₂ 2001 2000.9 200.9 b ₂ 2001 2000.9 200.9 c ₁ 2001 200.9 200.9 c ₁ 201 200.9 200.9 c ₁ 202.0 202.0 c ₁ c ₁ 202.0 202.0 202.0 c ₁ 202.1 202.1 202.0 202.0 c ₁ 200.1 200.1 200.0 200.9 a ¹ 201.1 201.0 202.0 202.0 202.0 a ¹ 202.1 202.1 202.0 202.0 a ¹ a ¹ 202.1 202.1		2001	2000.9	2000.9	e
$ \begin{split} & \begin{array}{c} 2027, & 2027, & 0, \\ & 2023, & 2023, & 2023, & 0, \\ & 2023, & 2003, & 2000, 9 & b_2 \\ & 2001, & 2000, 9 & 2000, 9 & b_2 \\ & 2001, & 2000, 9 & 2000, 9 & b_2 \\ & 2003, & 2000, 9 & 2000, 9 & c_1 \\ & 2003, & 2000, 9 & 2000, 9 & c_1 \\ & 2003, & 2000, 9 & 2000, 9 & c_1 \\ & 2003, & 2000, 9 & 2000, 9 & c_1 \\ & 2003, & 2000, 9 & 2000, 9 & c_1 \\ & 2026, 2 & 2026, 2 & a_1 \\ & 2026, 2 & 2026, 2 & a_1 \\ & 2026, 2 & 2026, 2 & a_1 \\ & 2026, 2 & 2026, 2 & a_1 \\ & 2026, 2 & 2026, 2 & a_1 \\ & 2020, 2 & 2000, 9 & a_1 \\ & 1964 & 1964, 5 & 1962, 8 & a_1 \\ & 2020, 2 & 2000, 9 & a_1 \\ & 1964 & 1964, 5 & 1962, 8 & a_1 \\ & 2020, 2 & 2000, 9 & a_1 \\ & 2020, 2 & 2000, 9 & a_1 \\ & 2020, 2 & 2000, 9 & a_1 \\ & 2020, 2 & 2000, 9 & a_1 \\ & 2020, 2 & 2000, 9 & a_1 \\ & 2020, 2 & 2000, 6 & a_1 \\ & 2021, 0 & 2020, 8 & a_1 \\ & 1976 & 1978, 5 & 1976, 6 & b_1 \\ & 2021, 0 & 2020, 9 & 2000, 9 & b_2 \\ & 2021, 0 & 2020, 9 & 2000, 9 & b_2 \\ & 2021, 0 & 2020, 9 & 2000, 9 & b_2 \\ & 2021, 0 & 2000, 9 & 2000, 9 & b_2 \\ & 2001 & 2000, 1 & 0, 0 \\ & 2002, 1 & 2001, 1 & 0, 0 \\ & 2001, 1 & 2001, 1 & 0, 0 \\ & 2002, 1 & 2001, 1 & 0, 0 \\ & 2002, 1 & 2001, 1 & 0, 0 \\ & 2001, 1 & 2001, 1 & 0, 0 \\ & 1972 & 1973, 1 & 1976, 0 & a_1 \\ & 1972 & 1973, 1 & 1976, 0 & a_1 \\ & 1972 & 1973, 1 & 1976, 0 & a_1 \\ & 1988 & 1980, 1 & 108, 0 \\ & 1972 & 1976, 1 & 1983, 1 & 06 \\ & 1988 & 1980, 1 & 108, 0 \\ & 1976 & 1978, 1$	$Fe(^{12}CO)_4(^{13}CO), C_{2n}, ^{13}CO; eq$	2108.0 °	2108.5	2108.4	a_1
$\begin{split} & 964 \\ 965 \\ 966 \\ $			2027.2	2027.1	a_1
$\begin{split} & \begin{array}{c} & 2023 & 2023.6 & 2023.6 & 0 \\ & 2001 & 2009 & 0 \\ & 2005.7 & 2095.1 & a_1^{-1} \\ & 2003.1 & 2001.7 & a_1^{-1} \\ & 2003.1 & 2001.7 & a_1^{-1} \\ & 2003.1 & 2001.7 & a_1^{-1} \\ & 2003.1 & 2001.9 & e^{-1} \\ & 2003.1 & 2001.9 & 2008.9 & 2008.9 & a^{-1} \\ & 2026.2 & 2026.2 & a^{-1} \\ & 2021.0 & 2009.9 & 2000.9 & a^{-1} \\ & 2021.0 & 2020.9 & 2001.6 & a_1 \\ & 2021.0 & 2020.8 & a_1 \\ & 2023 & 2023.6 & 2023.6 & b_1 \\ & 2023 & 2023.6 & 2023.6 & b_1 \\ & 2029 & 2001.6 & a_1 \\ & 2009 & 2029.1 & 2001.8 & a_1 \\ & 2009 & 2009.9 & 2001.6 & a_1 \\ & 2001.9 & 2000.9 & b_2 \\ & 2021.7 & 2021.8 & a_1 \\ & 1976 & 1978.5 & 1976.6 & b_1 \\ & 1976 & 1978.5 & 1976.6 & b_1 \\ & 1976 & 1978.5 & 1976.6 & b_1 \\ & 1976 & 1978.5 & 1976.6 & a_1 \\ & 1976 & 1978.5 & 1976.6 & a_1 \\ & 2021 & 2021.7 & 2021.8 & a_1 \\ & 1972 & 1073.3 & 1976.8 & a_1 \\ & 1972 & 1073.5 & 1976.6 & a_1 \\ & 2021 & 2023.6 & 2023.6 & 2023.6 & a_2 \\ & 1976 & 1978.5 & 1976.5 & 1976.8 & a_1 \\ & 1976 & 1978.5 & 1976.8 & a_1 \\ & 1976 & 1978.5 & 1976.6 & b_1 \\ & 1976 & 1978.5 & 1976.6 & b_1 \\ & 1976 & 1978.5 & 1976.6 & b_1 \\ & 1976 & 1978.5 & 1976.8 & a_1 \\ & 1976 & 1978.5 & 1976.8 & a_1 \\ & 1976 & 1978.5 & 1976.8 & a_1 \\ & 1976 & 1978.5 & 1976.8 & a_1 \\ & 1976 & 1978.5 & 1976.8 & a_1 \\ & 1976 & 1978.5 & 1976.8 & a_1 \\ & 1976 & 1978.5 & 1976.8 & a_1 \\ & 1976 & 1978.5 & 1976.8 & a_1 \\ & 1976 & 1978.5 & 1976.8 & a_1 \\ & 1976 & 1978.5 & 1976.8 & a_1 \\ & 1976 & 1978.5 & 1976.8 & a_2 \\ & 1976 & 1978.5 & 1976.8 & a_1 \\ & 1976 & 1978.5 & 1976.8 & a_1 \\ & 1976 & 1978.5 & 1976.8 & a_1 \\ & 1976 & 1978.5 & 1976.8 & a_2 \\ & 1976 & 1978.5 & 1976.8 & a_2 \\ & 1$		1964	1965.1	1963.5	a_1
$\begin{split} & \begin{array}{ccccccccccccccccccccccccccccccccccc$		2023	2023.6	2023.6	b_1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		2001	2000.9	2000.9	b_2
$ Fe({}^{12}CO)_3({}^{13}CO)_2, C_s, {}^{13}CO; ax, eq Fe({}^{12}CO)_3({}^{13}CO)_2, C_s, {}^{13}CO; ax, eq Fe({}^{12}CO)_3({}^{13}CO)_2, C_s, {}^{13}CO; ax, eq Fe({}^{12}CO)_3({}^{13}CO)_2, C_{2s}, {}^{13}CO; eq, eq Fe({}^{12}CO)_3({}^{13}CO)_2, C_{2s}, {}^{13}CO; eq, eq Fe({}^{12}CO)_3({}^{13}CO)_2, C_{2s}, {}^{13}CO; eq, eq Fe({}^{12}CO)_3({}^{13}CO)_3, C_{2s}, {}^{13}CO; ax, ax, eq Fe({}^{12}CO)_3({}^{13}CO)_3, C_{2s}, {}^{13}CO; ax, eq, eq Fe({}^{12}CO)_3({}^{13}CO)_3, C_{2s}, {}^{13}CO; ax, eq, eq Fe({}^{12}CO)_3({}^{13}CO)_3, D_{2s}, {}^{13}CO; eq, eq Fe({}^{12}CO)_3({}^{13}CO)_3, {}^{13}CO; eq, eq Fe({}^$	$Fe({}^{12}CO)_3({}^{13}CO)_2, D_{3b}, {}^{13}CO; ax, ax$		2095.7	2095.1	
$\begin{split} & \begin{array}{ccccccccccccccccccccccccccccccccccc$			2003.1	2001.7	
$\begin{split} & Fe({}^{12}C0)_3({}^{13}C0)_2, \ C_s, \ {}^{13}C0; \ ax, \ eq} & 1976 & 1978.5 & 1976.6 & a^2 \\ 2097 & 208.9 & 2098.5 & a^7 \\ 2026.2 & 2026.2 & 2026.2 & a^2 \\ 2026.2 & 2026.2 & a^2 \\ 1988 & 1989.1 & 1987.6 & a^7 \\ 1988 & 1984.1 & 1987.6 & a^7 \\ 2001 & 2000.9 & 2000.9 & a^n \\ 2010 & 2000.9 & 2000.9 & a^n \\ 2010 & 2020.8 & a_1 \\ 2010 & 2020.8 & a_1 \\ 2021.0 & 2020.8 & a_1 \\ 2021.0 & 2020.8 & a_1 \\ 2021.0 & 2020.8 & a_1 \\ 2022.9 & 2021.6 & a_1 \\ 2022.9 & 2023.6 & 2023.6 & b_1 \\ 2022.9 & 2001.6 & a_1 \\ 2022.9 & 2000.9 & b_2 \\ 2022.1 & 2091.4 & a^2 \\ 2021.7 & 2021.5 & 2000.1 & a_1^2 \\ 2021.9 & 2021.9 & 2021.9 \\ 2022.9 & 2021.1 & 201.9 & 202.9 \\ 2022.9 & 2021.1 & 201.9 & 202.9 \\ 2021.9 & 2021.9 & 2021.9 & 202.9 \\ 2021.9 & 2021.9 & 2021.9 & 202.9 \\ 2021.9 & 2021.9 & 2021.9 & 202.9 \\ 2021.9 & 2021.9 & 2021.9 & 202.9 \\ 2021.9 & 2021.9 & 202.9 & 2021.9 & 202.9 \\ 2021.9 & 2021.9 & 202.9 & 202.9 & 202.9 \\ 2021.9 & 2021.9 & 202.9 & 202.9 \\$		2001	2000.9	2000.9	e'
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		1976	1978.5	1976.6	a2''
$ Fe({}^{12}CO)_2({}^{13}CO)_3, C_{2n}, {}^{13}CO; eq, eq $ $ Fe({}^{12}CO)_2({}^{13}CO)_3, C_{2n}, {}^{13}CO; eq, eq $ $ 2001 2000.9 2000.9 a'' 2102.9 2102.6 a_1 2001 2000.9 2000.9 a'' 2102.9 2102.6 a_1 2021.0 2020.8 a_1 1976 1976.3 1974.9 a_1 2023 2023.6 2023.6 b_1 1955 1956.3 1954.5 b_2 2001 2000.9 b_3 Fe({}^{12}CO)_2({}^{13}CO)_3, C_{2n}, {}^{13}CO; ax, ax, eq 2001 2000.9 2000.6 a_1 1964 1964.2 1962.5 a_1 1976 1978.5 1976.6 b_1 1976 1978.5 1976.6 b_1 2001 2000.9 2000.9 b_3 Fe({}^{12}CO)_2({}^{13}CO)_3, C_s, {}^{13}CO; ax, eq, eq 2001 2000.9 2002.1 201.4 a' 1972 1974.0 1972.4 a' 1975 1985.1 1976.5 1980.1 a' 1975 1985.3 1954.5 a'' 201.5 2000.1 a'_1 1975 1955.3 1954.5 a'' 201.5 2000.1 a'_1 1975 1955.3 1954.5 a'' 2023 2023.6 2023.6 a_2'' Fe({}^{12}CO)_2({}^{13}CO)_3, D_{3n}, {}^{13}CO; eq, eq 2075 2097.3 2096.8 a_1' 201.5 2000.1 a'_1 1975 1955.3 1954.5 a'' 2023 2023.6 2023.6 a_2'' Fe({}^{12}CO)({}^{13}CO)_4, C_{2n}, {}^{13}CO; ax, ax, eq, eq 2076 2078.1 2076.9 a_1 1975 1955.3 1954.5 a'' 2021 5000.1 a'_1 1975 1955.3 1954.5 b_2 1975 1975.6 1972.0 a_1 1975 1975.6 1972.0 a_1 1975 1975.6 1972.0 a_1 1975 1975.3 1972.0 a_1 1975 1975.3 1972.0 a_1 1975 1975.6 1954.5 b_2 1975 1975.6 1974.6 a_1' 1975 1975.7 1983.9 a_1' 1975 1975.7 1974.5 a_2' 1975 1975.7 1974.5 a_2' 1975 1975.7 1974.5 a_2' 1975 1975.7 1974.5 a_1' 1975 1975.7 19$	$Fe(^{12}CO)_2(^{13}CO)_2$, C_{ab} , ^{13}CO ; ax, eq	2097	2098.9	2098.5	a'
$\begin{split} & \begin{array}{c} & 1988 & 1989.1 & 1987.6 & a' \\ & 1964 & 1964.5 & 1962.8 & a' \\ & 2001 & 2000.9 & 2000.9 & a'' \\ & 2102.9 & 2102.6 & a_1 \\ & 2021.0 & 2020.8 & a_1 \\ & 2021.0 & 2020.8 & a_1 \\ & 2021.0 & 2020.8 & a_1 \\ & 2023 & 2023.6 & 2023.6 & b_1 \\ & 2022 & 2001.6 & a_1 \\ & 2002.9 & 2001.6 & a_1 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2001.4 & a' \\ & 1975 & 1974.0 & 1972.4 & a' \\ & 1975 & 1956.3 & 1954.5 & a'' \\ & 2001.5 & 2000.1 & a_1' \\ & 1975 & 1956.3 & 1954.5 & a'' \\ & 2001.5 & 2000.1 & a_1' \\ & 1975 & 1975.0 & a_1 \\ & 1975 & 1975.0 & a_1 \\ & 1972 & 1973.5 & 1972.0 & a_1 \\ & 1972 & 1973.5 & 1972.0 & a_1 \\ & 1972 & 1973.5 & 1972.0 & a_1 \\ & 1972 & 1973.5 & 1976.6 & b_1 \\ & 1972 & 1973.5 & 1976.6 & b_1 \\ & 1972 & 1973.5 & 1976.6 & b_1 \\ & 1975 & 1985.3 & 1954.5 & b_2 \\ & 1976 & 1978.5 & 1976.6 & b_1 \\ & 1985.7 & 1983.9 & a_1' \\ & 1975 & 1985.3 & 1954.5 & e' \\ & 1985.7 & 1983.9 & a_1' \\ & 1975 & 1975.0 & 765.3 & 1954.5 & e' \\ & 1985.7 & 1983.9 & 361 \\ & 1975 & 1975.0 & 765.3 & 1954.5 & e' \\ & 1985.7 & 1983.9 & 361 \\ & 1975 & 1975.0 & 765.3 & 1954.5 & e' \\ & 1975 & 1975.0 & 765.3 & 1954.5 & e' \\ & 1985.7 & 1983.9 & a_1' \\ & 1975 & 1975.0 & 1985.5 & 1976.6 & a_2'' \\ & 1975 & 1975.0 & 1985.5 & 1976.6 & a_2'' \\ & 1975 & 1975.0 & 1978.5 & 1976.6 & a_2'' \\ & 1975 & 1975.0 & 1978.5 & 1976.6 & a_2'' \\ & 1975 & 1975.0 & 1978.5 & 1976.6 & a_2'' \\ & 1975 & 1975.0 & 1978.5 & 1976.6 & a_2'' \\ & 1975 & 1975.0 &$			2026.2	2026.2	a'
$\begin{split} & \begin{array}{c} & 1964 & 1964.5 & 1962.8 & a' \\ & 2001 & 2000.9 & 2000.9 & a'' \\ & 2010 & 2000.9 & 2000.9 & a'' \\ & 2010 & 2020.8 & a_1 \\ & 2021.0 & 2020.8 & b_1 \\ & 2022.0 & 2020.6 & b_1 \\ & 2022.0 & 2020.6 & b_1 \\ & 2022.0 & 2001.6 & a_1 \\ & 2002.0 & 2001.6 & a_1 \\ & 2002.0 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2001 & 2000.9 & 2000.9 & b_2 \\ & 2021.7 & 2021.5 & a' \\ & 1988 & 1990.5 & 1989.1 & a' \\ & 1972 & 1974.0 & 1972.4 & a' \\ & 2001.5 & 2001.1 & a' \\ & 2001.5 & 2000.1 & a'_1 \\ & 2001.5 & 2000$		1988	1989 1	1987.6	a'
$\begin{split} Fe(^{12}CO)_{3}(^{13}CO)_{2}, \ C_{2^{n}}, ^{13}CO; \ eq, \ eq & 2001 & 2000, 9 & 2000, 9 & 4^{n'} \\ & 2021 & 2020, 2000, 9 & 2010, 6 & 4_{1} \\ & 2021 & 2023 & 2023, 6 & 2023, 6 & b_{1} \\ & 2023 & 2023, 6 & 2023, 6 & b_{1} \\ & 2020, 9 & 2020, 6 & 4_{1} \\ & 2002, 9 & 2001, 6 & 4_{1} \\ & 2002, 9 & 2001, 6 & 4_{1} \\ & 2002, 9 & 2001, 6 & 4_{1} \\ & 2002, 9 & 2001, 6 & 4_{1} \\ & 2001 & 2000, 9 & 2000, 9 & b_{2} \\ & 1976 & 1978, 5 & 1976, 6 & b_{1} \\ & 2001 & 2000, 9 & 2000, 9 & b_{2} \\ & 1976 & 1978, 5 & 1976, 6 & b_{1} \\ & 2001 & 2000, 9 & 2000, 9 & b_{2} \\ & 1976 & 1978, 5 & 1976, 6 & b_{1} \\ & 2001 & 2000, 9 & 2000, 9 & b_{2} \\ & 1976 & 1978, 5 & 1976, 6 & b_{1} \\ & 2001 & 2000, 9 & 2000, 9 & b_{2} \\ & 2021, 7 & 2021, 5 & a' \\ & 2021, 7 & 2021, 5 & a' \\ & 1988 & 1990, 5 & 1989, 1 & a' \\ & 1988 & 1990, 5 & 1989, 1 & a' \\ & 1988 & 1990, 5 & 1989, 1 & a' \\ & 1988 & 1990, 5 & 1989, 1 & a' \\ & 2001 & 2002, 1 & 2091, 4 & a' \\ & 2001, 5 & 2000, 1 & a_{1} \\ & 1972 & 1973, 0 & 1972, 4 & a' \\ & 2001, 2000, 1 & a_{1} \\ & 1972 & 1973, 5 & 1976, 6 & b_{1} \\ & 1972 & 1973, 5 & 1976, 6 & b_{1} \\ & 1972 & 1973, 5 & 1976, 6 & b_{1} \\ & 1972 & 1973, 5 & 1976, 6 & b_{1} \\ & 1972 & 1973, 5 & 1976, 6 & b_{1} \\ & 1972 & 1973, 5 & 1976, 6 & b_{1} \\ & 1972 & 1973, 5 & 1976, 6 & b_{1} \\ & 1972 & 1973, 5 & 1976, 6 & b_{1} \\ & 1972 & 1973, 5 & 1976, 6 & b_{1} \\ & 1975 & 956, 3 & 1954, 5 & b_{2} \\ & 1976 & 1978, 5 & 1976, 6 & b_{1} \\ & 1975 & 1956, 3 & 1954, 5 & b_{2} \\ & 1976 & 1978, 5 & 1976, 6 & b_{1} \\ & 1975 & 1956, 3 & 1954, 5 & b_{2} \\ & 1985 & 956, 3 & 1954, 5 & b_{2} \\ & 1976 & 1978, 5 & 1976, 6 & b_{1} \\ & 1972 & 1973, 5 & 1976, 6 & b_{1} \\ & 1972 & 1973, 5 & 1976, 6 & b_{1} \\ & 1976 & 1978, 5 & 1976, 6 & b_{1} \\ & 1985 & 1956, 3 & 1954, 5 & e_{1} \\ & 2006, 9 & 2064, 9 & 4 & 4 \\ & 1985, 7 & 1983, 9 & 4 & 4 \\ & 1985, 7 & 1983, 9 & 4 & 4 \\ & 1985, 7 & 1983, 9 & 4 & 4 \\ & 1985, 7 & 1983, 9 & 4 & 4 \\ & 1985, 7 & 1983, 9 & 4 & 4 \\ & 1985, 7 & 1983, 9 & 4 & 4 \\ & 1985, 7 & 1983, 9 & 4 & 4 \\ & 1985, 7 & 1983, 9 & 4 $		1964	1964 5	1962.8	a'
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		2001	2000.9	2000.9	a"
$ Fe(^{12}CO)_2(^{13}CO)_3, C_{2r}, ^{13}CO; ax, ax, eq, eq Fe(^{12}CO)_2(^{13}CO)_3, C_{2r}, ^{13}CO; ax, ax, eq, eq Fe(^{12}CO)_2(^{13}CO)_3, C_{2r}, ^{13}CO; ax, ax, eq, eq Fe(^{12}CO)_2(^{13}CO)_3, C_{3r}, ^{13}CO; eq, eq, eq Fe(^{12}CO)_2(^{13}CO)_4, C_{2r}, ^{13}CO; ax, eq, eq Fe(^{12}CO)_2(^{13}CO)_4, C_{2r}, ^{13}CO; ax, eq, eq Fe(^{12}CO)_2(^{13}CO)_4, C_{2r}, ^{13}CO; ax, eq, eq Fe(^{12}CO)(^{13}CO)_4, C_{3r}, ^{13}CO; ax, eq, eq Fe(^{12}CO)(^{13}CO)_5, D_{3h} Fe(^{12}CO)(^{13}CO)_5, D_{3h} Fe(^{12}CO) Fe(^{12}CO)_5, D_{3h} Fe(^{12}CO) Fe(^{12}C$	$Fe(^{12}CO)_{2}(^{13}CO)_{2}$ $C_{2} = ^{13}CO; eq. eq.$	2001	2102.9	2102.6	a.
$\operatorname{Fe}(^{12}\operatorname{CO})_2(^{13}\operatorname{CO})_3, C_{2^{\mu}}, ^{13}\operatorname{CO}; ax, ax, eq = 1976,$	$10(-20)_{3}(-20)_{2}, c_{2v}, -20, cq, cq$		2021.0	2020.8	<i>a</i> ₁
$\operatorname{Fe}({}^{12}\operatorname{CO})_2({}^{13}\operatorname{CO})_3, C_{2e}, {}^{13}\operatorname{CO}; ax, ax, eq = \begin{bmatrix} 1076 & 1076 & 2023.6 & 1074 & 0 & 1 \\ 1955 & 1956.3 & 1954.5 & b_2 \\ 2002.9 & 2001.6 & a_1 \\ 2002.9 & 2001.6 & a_1 \\ 2002.9 & 2001.6 & b_1 \\ 2001 & 2000.9 & 2000.9 & b_2 \\ 2001 & 2000.9 & 2000.1 & a_1 \\ 1976 & 1978.5 & 1976.6 & b_1 \\ 1972 & 1974.0 & 1972.4 & a_1 \\ 1972 & 1974.0 & 1972.4 & a_1 \\ 2001.5 & 2000.1 & a_1 \\ 2001 & 2002.4 & 2001.4 & a_1 \\ 2001 & 2002.4 & 2001.4 & a_1 \\ 2001 & 2002.4 & 2001.4 & a_1 \\ 1972 & 1973.5 & 1976.6 & b_1 \\ 1975 & 1956.3 & 1954.5 & b_2 \\ 2001 & 2002.4 & 2001.4 & a_1 \\ 1972 & 1973.5 & 1976.6 & b_1 \\ 1975 & 1975.5 & 1976.6 & b_1 \\ 1975 & 1975.5 & 1976.6 & b_1 \\ 1975 & 1956.3 & 1954.5 & b_2 \\ 2008.9 & 2007.9 & a_1 \\ 1975 & 1956.3 & 1954.5 & b_2 \\ 2008.9 & 2007.9 & a_1 \\ 1975 & 1956.3 & 1954.5 & b_2 \\ 2008.9 & 2007.9 & a_1 \\ 1975 & 1956.3 & 1954.5 & b_2 \\ 1976 & 1978.5 & 1976.6 & b_1 \\ 1985.7 & 1983.9 & a_1' \\ 1985.7 & 1985.9 & 1976.6 & a_2'' \\ 1976 & 1978.5 $		1976	1976 3	1974 9	<i>a</i> .
$Fe({}^{12}CO)_{2}({}^{13}CO)_{3}, C_{2n}, {}^{13}CO; ax, ax, eq = 2087.5 2086.6 a_{1} 2002.9 201.6 a_{1} 2002.9 2001.6 a_{1} 2002.9 2000.9 b_{2} 2001 2000.9 2000.9 b_{2} 2001 2000.9 2000.9 b_{2} 2001 2000.9 2000.9 b_{2} 2001 2002.1 2091.4 a_{1} 2001 2002.9 2001.4 a_{1} 2001 2002.9 2001.4 a_{1} 2001 2002.9 2001.4 a_{1} 2001 2002.1 2091.4 a_{1} 2001.5 2001.1 a_{1} 2001.5 2001.4 a_{1} 2001.5 2001.4 a_{1} 2001.5 2001.4 a_{1} 2001.2 2002.4 2001.4 a_{1} 2001.2 2002.4 2001.4 a_{1} 2001.2 2002.4 2001.4 a_{1} 2001.5 2001.4 a_{1} 2001.5 2001.4 a_{1} 2001.5 2000.1 a_{1} 2001.5 2001.4 a_{1} 2001.5 2000.5 2007.9 a_{1} 2000.5$		2023	2023.6	2023.6	a_1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		1055	1056 3	1054 5	b_1
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$E_2(^{12}CO)(^{13}CO) = C = ^{13}CO; as as as$	1955	2087.5	2086.6	02 a
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\Gamma(CO)_{2}(CO)_{3}, C_{2v}, CO, ax, ax, eq$		2007.5	2080.0	a_1
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		1064	2002.9	2001.0	a_1
$Fe({}^{12}CO)_{2}({}^{13}CO)_{3}, C_{s}, {}^{13}CO; ax, eq, eq = \begin{bmatrix} 1976 & 1978.3 & 1970.6 & 01 \\ 2001 & 2000.9 & 2000.9 & b_{2} \\ 2000 & 2092.1 & 2091.4 & a' \\ 2021.7 & 2021.5 & a' \\ 1988 & 1990.5 & 1989.1 & a' \\ 1972 & 1974.0 & 1972.4 & a' \\ 1975 & 1956.3 & 1954.5 & a'' \\ 2001.5 & 2000.1 & a_{1}' \\ 2001.5 & 2000.1 & a_{1}' \\ 2023 & 2023.6 & 2023.6 & a_{2}'' \\ 2023 & 2023.6 & 2023.6 & a_{2}'' \\ Fe({}^{12}CO)({}^{13}CO)_{4}, C_{2e}, {}^{13}CO; ax, ax, eq, eq & 2076 & 2078.1 & 2076.9 & a_{1} \\ 1976 & 1978.5 & 1976.6 & b_{1} \\ 1976 & 1978.5 & 1972.0 & a_{1} \\ 1976 & 1978.5 & 1972.0 & a_{1} \\ 1976 & 1978.5 & 1976.6 & b_{1} \\ 1976 & 1978.5 & 1976.6 & b_{1} \\ 1982.9 & 1981.1 & a_{1} \\ 1985.7 & 1983.9 & a_{1}' \\ 1976 & 1978.5 & 1976.6 & a_{2}'' \\ 1988 & 1988.7 & 1988.7 & 1988.7 \\ 1988 & 1988.7 & 1988.7 & 1988.7 & 1988.7 & 1988.7 & 1988.7 & 1988.7 & 1988.7 & 1988.7 & 1988.7 & 1988.7 & 1988.$		1904	1904.2	1902.5	a_1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		1976	19/8.5	1970.0	D_1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\Gamma_{12}(1200) = (1300) = C_{11}(1300)$	2001	2000.9	2000.9	<i>D</i> ₂
$\operatorname{Fe}({}^{12}\mathrm{CO})_{2}({}^{13}\mathrm{CO})_{3}, D_{3h}, {}^{13}\mathrm{CO}; eq, eq, eq = \begin{bmatrix} 2021, 7 & 2021, 3 & a \\ 1988 & 1990, 5 & 1989, 1 & a' \\ 1972 & 1974, 0 & 1972, 4 & a' \\ 1955 & 1956, 3 & 1954, 5 & a'' \\ 2007, 3 & 2096, 8 & a_{1}^{\prime} \\ 2001, 5 & 2000, 1 & a_{1}^{\prime} \\ 2001, 5 & 2000, 1 & a_{1}^{\prime} \\ 2023, 6 & 2023, 6 & 2023, 6 & a_{2}^{\prime\prime} \\ 2023 & 2023, 6 & 2023, 6 & a_{2}^{\prime\prime} \\ 2021, 5 & 2000, 1 & a_{1}^{\prime} \\ 2001 & 2002, 4 & 2001, 4 & a_{1} \\ 1972 & 1973, 5 & 1972, 0 & a_{1} \\ 1972 & 1973, 5 & 1972, 0 & a_{1} \\ 1972 & 1973, 5 & 1972, 0 & a_{1} \\ 1972 & 1973, 5 & 1976, 6 & b_{1} \\ 1975 & 1956, 3 & 1954, 5 & b_{2} \\ Fe({}^{12}\mathrm{CO})({}^{13}\mathrm{CO})_{4}, C_{3v}, {}^{13}\mathrm{CO}; ax, eq, eq & 2084 & 2084, 9 & 2084, 0 & a_{1} \\ 1975 & 1955 & 956, 3 & 1954, 5 & b_{2} \\ Fe({}^{12}\mathrm{CO})({}^{13}\mathrm{CO})_{4}, C_{3v}, {}^{13}\mathrm{CO}; ax, eq, eq & 2084 & 2084, 9 & 2084, 0 & a_{1} \\ 1975 & 1955, 3 & 1954, 5 & b_{2} \\ Fe({}^{12}\mathrm{CO})({}^{13}\mathrm{CO})_{5}, D_{3h} & 1 & 3 \\ Fe({}^{13}\mathrm{CO})_{5}, D_{3h} & 1954, 5 & e^{\prime} \\ Fe({}^{13}\mathrm{CO})_{5}, D_{3h} & 1954, 5 & e^{\prime} \\ 1975 & 1956, 3 & 1954, 5 & e^{\prime} \\ 1985, 7 & 1983, 9 & a_{1}^{\prime} \\ 1985, 7 & 1983, 9 & a_{1}^{\prime} \\ 1975 & 1956, 3 & 1954, 5 & e^{\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{2}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{2}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{2}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{2}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{2}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{2}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{2}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{2}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{2}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{2}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{2}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{2}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{2}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{2}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{2}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{2}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{2}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{2}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{1}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{1}^{\prime\prime} \\ 1976 & 1978, 5 & 1976, 6 & a_{1}^{\prime\prime} \\ 1976 & 19$	$Fe(CO)_2(CO)_3, C_s, CO; ax, eq, eq$	2090	2092.1	2091.4	a ='
$\operatorname{Fe}({}^{12}\operatorname{CO})_{2}({}^{13}\operatorname{CO})_{3}, D_{3h}, {}^{13}\operatorname{CO}; \operatorname{eq}, \operatorname{eq} = (20)_{2}({}^{13}\operatorname{CO})_{3}, D_{3h}, {}^{13}\operatorname{CO}; \operatorname{eq}, \operatorname{eq} = (20)_{2}({}^{13}\operatorname{CO})_{3}, D_{3h}, {}^{13}\operatorname{CO}; \operatorname{eq}, \operatorname{eq} = (20)_{2}({}^{13}\operatorname{CO})_{3}, D_{3h}, {}^{13}\operatorname{CO}; \operatorname{eq}, \operatorname{eq} = (20)_{2}(20)_{2}(20)_{2}(20)_{2}(20)_{3}, D_{3h}, {}^{13}\operatorname{CO}; \operatorname{eq}, \operatorname{eq} = (20)_{2}(2$		1000	2021.7	2021.5	a
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		1988	1990.5	1989.1	a'
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		1972	19/4.0	1972.4	a'
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	\mathbf{r} (l2aa) (l3aa) \mathbf{r} l3aa	1955	1956.3	1954.5	a"
$\operatorname{Fe}({}^{12}\mathrm{CO})({}^{13}\mathrm{CO})_4, C_{2v}, {}^{13}\mathrm{CO}; \text{ ax, ax, eq, eq} = \begin{bmatrix} 2001.5 & 2000.1 & a_1 \\ 1955 & 1956.3 & 1954.5 & e' \\ 2023 & 2023.6 & 2023.6 & a_2'' \\ 2026 & 2078.1 & 2076.9 & a_1 \\ 2001 & 2002.4 & 2001.4 & a_1 \\ 1972 & 1973.5 & 1972.0 & a_1 \\ 1976 & 1978.5 & 1976.6 & b_1 \\ 1955 & 956.3 & 1954.5 & b_2 \\ 1955 & 956.3 & 1954.5 & b_2 \\ 2008.9 & 2007.9 & a_1 \\ 1982.9 & 1981.1 & a_1 \\ 1985.7 & 1983.9 & a_1' \\ 1985.7 & 1983.9 & a_1' \\ 1955 & 1956.3 & 1954.5 & e' \\ 1976 & 1978.5 & 1976.6 & a_2'' \\ 1976 & 1978.5 & 1976.6 & 1978.5 \\ 1976 & 1978.5 & 1976.6 & 1978.5 \\ 1976 & 1978.5 & 1976.6 & 1978.5 \\ 1976 & 1978.5 & 1976.6 & 1978.5 \\ 1976 & 1978.5 & 1976.6 & 1978.5 \\ 1976 & 1978.5 & 1976.6 & 1978.5 \\ 1976 & 1978.5 & 1976.6 & 1978.5 \\ 1976 & 1978.5 & 1976.6 & 1978.5 \\ 1976 & 1978.5 & 1976.6 & 1978.5 \\ 1976 & 1978.5 & 1976.6 & 1978.5 \\ 1976 & 1978.5 & 1976.6 & 1978.5 \\ 1976 & 1978.5 & 1976.6 & 1978.5 \\ 1976 & 1978.5 & 1976.6 & 1978.5 \\ 1976 & 1978.5 & 1976.6 & 1978.5 \\ 1976 & 1978.5 & 1976.6 & 1978.5 \\ 1976 & 1978.5 & 1976.6 & 1978.5 \\ 1976 & 1978.5 & 1976.6 & 1978.5 \\ 1976 & 1978.5 & 1976.5 & 1976.5 \\ 1976 & 1978.5 & 1976.5 & 1976.5 \\ 1976 & 1978.5 & 1976$	$Fe(^{12}CO)_2(^{13}CO)_3, D_{3h}, ^{13}CO; eq, eq, eq$		2097.3	2096.8	a_1
$Fe(^{12}CO)(^{13}CO)_4, C_{2v}, ^{13}CO; ax, ax, eq, eq Fe(^{12}CO)(^{13}CO)_4, C_{2v}, ^{13}CO; ax, ax, eq, eq Fe(^{12}CO)(^{13}CO)_4, C_{2v}, ^{13}CO; ax, eq, eq Fe(^{12}CO)(^{13}CO)_4, C_{3v}, ^{13}CO; ax, eq, eq Fe(^{13}CO)_5, D_{3h} Fe(^{13}$			2001.5	2000.1	a_1
$Fe({}^{12}CO)({}^{13}CO)_4, C_{2v}, {}^{13}CO; ax, ax, eq, eq Fe({}^{12}CO)({}^{13}CO)_4, C_{2v}, {}^{13}CO; ax, ax, eq, eq Pe({}^{12}CO)({}^{13}CO)_4, C_{2v}, {}^{13}CO; ax, eq, eq Fe({}^{12}CO)({}^{13}CO)_4, C_{3v}, {}^{13}CO; ax, eq, eq Fe({}^{13}CO)_5, D_{3h} Fe({}^{13}$		1955	1956.3	1954.5	e'
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	- 12 12 12	2023	2023.6	2023.6	a_2
$Fe^{(12}CO)(^{13}CO)_4, C_{3v}, ^{13}CO; ax, eq, eq, eq$ $Pe^{(12}CO)(^{13}CO)_4, C_{3v}, ^{13}CO; ax, eq, eq$ $Pe^{(12}CO)(^{13}CO)_4, Pe^{(12}CO)_4, Pe^{(12}CO)_4, Pe^{(12}CO)_4, Pe^{(12}CO)_4, Pe^{(12}CO)_$	$Fe({}^{12}CO)({}^{13}CO)_4, C_{2v}, {}^{13}CO; ax, ax, eq, eq$	2076	2078.1	2076.9	a_1
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		2001	2002.4	2001.4	a_1
$Fe({}^{12}CO)({}^{13}CO)_4, C_{3v}, {}^{13}CO; ax, eq, eq, eq$ $Fe({}^{12}CO)({}^{13}CO)_4, C_{3v}, {}^{13}CO; ax, eq, eq, eq$ $Pe({}^{12}CO)({}^{13}CO)_4, C_{3v}, {}^{13}CO; ax, eq, eq, eq$ $Pe({}^{13}CO)_5, D_{3h}$ $Pe({}^{13}CO)_5, D_{3h$		1972	1973.5	1972.0	a_1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		1976	1978.5	1976.6	b_1
$\begin{array}{cccc} {\rm Fe}({}^{12}{\rm CO})({}^{13}{\rm CO})_4, C_{3v}, {}^{13}{\rm CO}; {\rm ax}, {\rm eq}, {\rm eq} & 2084 & 2084.9 & 2084.0 & a_1 \\ & & & & & & & & & & & & & & & & & & $		1955	956.3	1954.5	b_2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$Fe(^{12}CO)(^{13}CO)_4$, C_{3v} , ^{13}CO ; ax, eq, eq, eq	2084	2084.9	2084.0	a_1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			2008.9	2007.9	a_1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			1982.9	1981.1	a_1
Fe (^{13}CO) ₅ , D_{3h} 2066.92064.9 a_1' 1985.71983.9 a_1' 19551956.31954.5 e' 19761978.51976.6 a_2''		1955	1956.3	1954.5	е
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Fe $({}^{13}CO)_5$, D_{3h}		2066.9	2064.9	a_1'
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			1985.7	1983.9	a_1
1976 1978.5 1976.6 <i>a</i> ₂ "		1955	1956.3	1954.5	e'
		1976	1978.5	1976.6	$a_2^{"}$

^a Calculated without effective reduced mass ratio.

^b Calculated with an effective reduced mass ratio of 0.9768.

^c These frequencies were taken from Ref. [9].

solution corresponding to Eqs. (10)–(14) is the only one of possible solutions of the algebraic system.

In order to test the validity of the solution found here Eqs. (10)-(14) were first used to calculate force con-

stants of Fe(CO)₅ and then compared with those determined from the cos β parameter method [9] and those of Dalton et al. [7]. C–O stretching bands of Fe(CO)₅ were reported by many authors [14–17]. In our

calculations of force constants, we have employed the frequencies given in Ref. [18], $a'_1 = 2114$, $a'_1 = 2031$, e' = 20312000.9 and $a_2'' = 2023.6$ cm⁻¹. Our results, together with those of the two methods mentioned above, are presented in Table 2. Inspection of the table reveals that there exists a very good agreement between the force constants calculated by our method and the other two methods. It should also be noted that the method presented utilizes only ¹²C¹⁶O stretching frequencies whereas the application of the $\cos \beta$ parameter method [9] needs to use frequencies of isotopically enriched species for finding value of $\cos \beta$ and the method suggested by Dalton et al. [7] requires some relationships among the interaction constants derived from elementary bonding considerations [7,8]. Therefore, our method is easier to apply than the two methods.

As a further check upon the validity of Eqs. (10)–(14), the force constants calculated were employed to predict C-O stretching frequencies of isotopically enriched species of $Fe(CO)_5$ and the results obtained were compared with observed frequencies of the species. The reliability of such a comparison is based on the assumption that the force constants remain unchanged on isotopic substitution [19]. This also means that C-O stretching frequencies of isotopically substituted species can be determined by using the force constants of the all-¹²C¹⁶O molecule. For such a comparison we have made use of ¹³CO-substituted species, since the COfactored force field works best for ¹³C¹⁶O-substitution [6,20]. ¹³CO-substituted species of Fe(CO)₅ were prepared and their infrared spectra in the carbonyl stretching region were reported by Noack and Ruch [18].

The secular equations for isotopically enriched species of $M(CO)_5$ molecules having D_{3h} symmetry were derived by procedures given in Ref. [19] and are summarized in Table 3. With the use of these equations and the force constants calculated by Eqs. (10)–(14), the C–O stretching frequencies of ¹³CO-substituted species of the Fe(CO)₅ were estimated. The results obtained are given in Table 4 together with observed frequencies [18] of the species.

It can be seen from Table 4 that a rather good fit between observed and calculated frequencies was obtained for ¹³CO-substituted species of Fe(CO)₅, with a maximum error of 2.5 cm⁻¹. The mean error measured as $(\sigma^2/n)^{1/2}$ was calculated to be 1.41 cm⁻¹. A much better fit was obtained by using an 'effective reduced

mass ratio' [6,9] of 0.9768. The maximum and mean error were 1.5 and 0.71 cm⁻¹, respectively. The effective reduced mass ratio for Fe(CO)₅ was determined from observed frequencies of the e' and a''_2 modes of Fe(¹²C¹⁶O)₅ and Fe(¹³C¹⁶O)₅ species. It is noted that our value of the effective reduced mass ratio is very close to that of Bor, 0.9771 [9].

In conclusion, the data in Tables 2 and 4 show that Eqs. (10)–(14) correspond to a valid solution for the CO-factored force field of Fe(CO)₅. The relations make it easy to calculate force constants, allowing direct calculation of them from fundamental C–O stretching frequencies of the all-¹²C¹⁶O molecule. As can be seen from Table 4, a remarkably good agreement between observed and calculated frequencies of ¹³CO-substituted species was obtained using the set of force constants calculated from Eqs. (10)–(14). From this observation, one concludes that the method presented here may be employed to analyze isotopic spectra of Fe(CO)₅.

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