

Analytic representations of rovibrational dipole matrix elements for the CO molecule and its isotopomers^{*}

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Abstract. — We report new calculations of transition matrix elements for more than thirty thousand infrared lines of the CO molecule and its isotopomers inside the $X^1\Sigma^+$ ground electronic state. These lines belong to the $\Delta v=1, 2, 3$ bands involving very high excited states such as $v' \leq 41$ and $J' \leq 133$. The transition matrix elements have been calculated from an accurate solution of the Schrödinger equation by using two different theoretical electric dipole moment functions (Werner 1981; Langhoff & Bauschlicher 1995). For low lying levels, our data compare satisfactorily with experimental ones and related works (Goorvitch & Chackerian 1994a, b; Chackerian et al. 1994, Goorvitch 1994). Moreover, we make predictions for oscillator strengths and Einstein coefficients involving high excited transitions. In addition, we report simple analytic formulae that fit our results for $^{12}\text{C}^{16}\text{O}$ with an accuracy better than 10^{-2} as a function of $m = [J'(J' + 1) - J''(J'' + 1)]/2$ for each vibrational sequence and band. They offer an easy way to compute the various intensities of these rovibrational transitions whose transition energies may be introduced via the available Dunham coefficients.

Key words: molecular data — ISM: molecules

1. Introduction

The determination of the rovibrational intensities of carbon monoxide is important in our understanding of various astrophysical media such as stellar and planetary atmospheres, circumstellar envelopes and interstellar clouds. Amongst the recent attempts (Huré & Roueff 1993; Goorvitch & Chackerian 1994a, b; Chackerian et al. 1994; Goorvitch 1994) to get systematic results of the intensities of fundamental and overtone rovibrational bands, significant discrepancies have been found. As discussed in Chackerian et al. (1994), these differences come from different choices of the Electric Dipole Moment Function (EDMF hereafter) - the behaviour of which is very uncertain far from the equilibrium internuclear separation.

Laboratory measurements may provide the most accurate constraints on the EDMF from infrared emission line intensity ratios for low rovibrational states. However, their reliability is less obvious for intermediate and high energy levels which imply high excitation conditions and large internuclear separations. Alternatively, the accuracy of theoretical calculations for the EDMF is not limited at interatomic distances far from the equilibrium distance.

We present in this paper two new sets of infrared dipolar transition matrix elements with $v' \leq 41$ and $J' \leq 133$ for $^{12}\text{C}^{16}\text{O}$, $^{13}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$ and $^{12}\text{C}^{17}\text{O}$ molecules in their electronic ground state. The calculations are performed by using the two theoretical ab-initio EDMFs of Werner (1981) and Langhoff & Bauschlicher (1995). Both these EDMFs are in very good agreement with the experimental results for low excitation transitions of the fundamental band (Goorvitch & Chackerian 1994a, b). In addition, our transition matrix elements are fitted with fourth degree polynomial expansions which reproduce the original data with an accuracy of the order of 10^{-3} for most of the transitions.

Using the energy terms given by the mass independent Dunham coefficients (Farrenq et al. 1991; Authier et al. 1993), these new sets allow straightforward calculations of rovibrational intensities of the infrared transitions of CO and its minor isotopomers.

2. Theoretical background

In the Born-Oppenheimer approximation, the energy levels $E_{v,J}$ of a molecule in a $^1\Sigma^+$ ground state and the corresponding radial wave functions $\Psi_{v,J}(R)$ are solutions of the Schrödinger nuclear equation (see Steinfeld 1989):

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^{*}Tables 5 to 7 only available in electronic form at CDS via ftp 150.79.128.5

$$\left[-\frac{\hbar^2}{8\pi^2\mu} \left(\frac{d^2}{dR^2} + \frac{J(J+1)}{R^2} \right) + V(R) \right] \Psi_{v,J}(R) = E_{v,J} \Psi_{v,J}(R) \quad (1)$$

Here, μ is the reduced mass of the two nuclei, $V(R)$ is the electronic potential depending on the radial distance R , and v and J denote respectively the vibrational and the rotational quantum numbers. We point out that this equation does not assume any separation between rotation and vibration motions. It remains valid as far as the Born-Oppenheimer approximation holds.

Table 1. EDMF and its first derivative at equilibrium distance for EDMF1 (Werner 1981), EDMF2 (Langhoff & Bauschlicher 1995) and EDMF3 (Chackerian et al. 1984)

	EDMF1	EDMF2	EDMF3
$M(R_e)$ (D)	-0.237	-0.123	-0.123
$dM/dR _{R_e}$ (D/a ₀)	+1.682	+1.693	+1.674

Table 2. Values of the reduced masses for the different isotopes of CO

Isotope	Reduced mass (amu)
¹² C ¹⁶ O	6.856208709
¹³ C ¹⁶ O	7.172412452
¹² C ¹⁸ O	7.199865602
¹² C ¹⁷ O	7.034334287

Both absorption oscillator strengths (or f -values) and emission Einstein A coefficients depend on the energy levels *and* on the rovibrational matrix elements (or D -values). For a given transition involving a lower level (v'', J'') and an upper one (v', J'), the f -value and the A coefficient are respectively:

$$f_{v'',J''}^{v',J'} = \frac{8\pi^2 m_e}{3h^2 e^2} \frac{E_{v',J'} - E_{v'',J''}}{2J'' + 1} S_{v'',J''}^{v',J'} \left| D_{v'',J''}^{v',J'} \right|^2 \quad (2)$$

$$A_{v'',J''}^{v',J'} = \frac{64\pi^4}{3h^4 c^3} \frac{E_{v',J'} - E_{v'',J''}}{2J'' + 1} S_{v'',J''}^{v',J'} \left| D_{v'',J''}^{v',J'} \right|^2 \quad (3)$$

In these formulae, $S_{v'',J''}^{v',J'}$ is the Hönl-London factor resulting from the angular integrations ($S_{v'',J''}^{v',J'} = J''$ for P branches and $J'' + 1$ for R branches).

The radial transition matrix element $D_{v'',J''}^{v',J'}$ is:

$$D_{v'',J''}^{v',J'} = \int_0^\infty \Psi_{v'',J''}(R) M(R) \Psi_{v',J'}(R) dR \quad (4)$$

Figure 1

M (in Debye) is the EDMF of the molecule in its ground electronic state $X^1\Sigma^+$. (1D=10⁻¹⁸ esu, 1 au=2.541726645D and 1 C.m=2.99792458 10¹¹ esu).

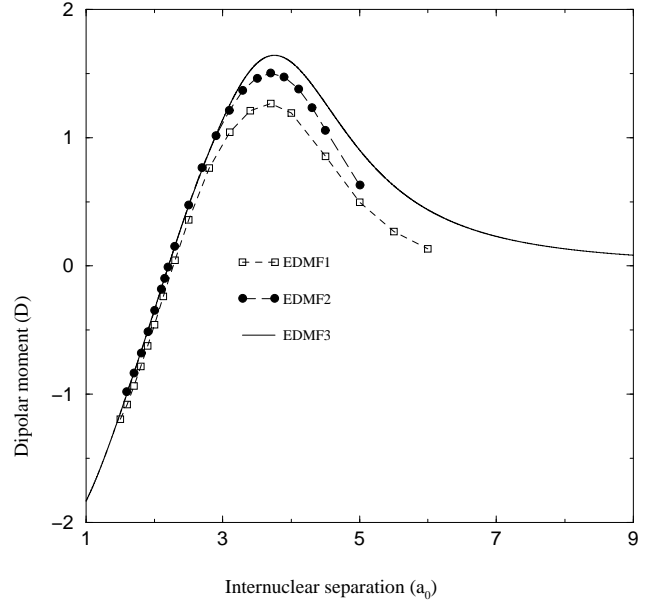


Fig. 1. The three EDMFs (in Debye) used in this work as a function of the internuclear distance (in a_0). EDMF1 = Werner (1981); EDMF2 = Langhoff & Bauschlicher 1995; EDMF3 = Chackerian et al. 1984

3. About the choice of the dipole moment function

The theoretical determination of the permanent dipole moment of CO at equilibrium (when $R = R_e$ and $R_e \approx 2.132a_0$) is a very difficult task since it involves cancellation of terms of about the same order of magnitude. Its experimental value is nowadays determined from Stark effect measurements on pure rotational transitions (Muenter 1975) and is equal to -0.123 D. Rovibrational transition probabilities ($\Delta v \geq 1$) on the other hand are most sensitive to the actual dependence of the EDMF with internuclear distance.

In a preliminary paper (Huré & Roueff 1993), we have reported a set of D -values using the EDMF of Cooper & Kirby (1987). This first investigation showed significant differences of the order of 10% with experimental determinations (Chackerian et al. 1984), even for low lying vJ -states. We have repeated our calculations with two different theoretical ab-initio EDMFs. The first one, named EDMF1, has been computed by Werner (1981). The second one, named EDMF2, has been recently published by Langhoff & Bauschlicher (1995). In addition, as we shall see below, EDMF1 and EDMF2 allow very satisfactory agreement with experimental results obtained at low excitations by Goorvitch & Chackerian (1994a, b). We have indeed reproduced the values obtained by these authors by

Table 3. D -values for some specific transitions. Values in the rectangles correspond to some transitions which are observed in the sun: 1–0 to 20–19 ($J' \leq 133$); 2–0 to 14–12 ($J' \leq 110$) for $^{2}\text{C}^{16}\text{O}$ e.g. (Numbers in parenthesis refer to the power of ten involved)

Isotopes	Δv	v''	J''	v'	J'	E (cm $^{-1}$)	D -values		
							D_1	D_2	D_3
12,16	1	0	0	1	0	2143.407	+1.069744 (-1)	+1.076565 (-1)	+1.063450 (-1)
		40	133	41	132	464.961	+3.888596 (-1)	+4.473379 (-1)	+5.076834 (-1)
		0	132	1	133	2285.640	+1.133904 (-1)	+1.122065 (-1)	+1.101410 (-1)
		2	133	3	132	1336.615	+1.966144 (-1)	+2.007720 (-1)	+1.971536 (-1)
		19	45	20	44	1477.437	+4.483567 (-1)	+4.640950 (-1)	+4.679886 (-1)
		0	0	2	0	4260.279	-6.340108 (-3)	-6.527777 (-3)	-6.670675 (-3)
	2	39	133	41	132	1199.611	-2.753283 (-1)	-2.955704 (-1)	-3.056673 (-1)
		0	109	2	110	4223.216	-9.620556 (-3)	-9.607787 (-3)	-9.705405 (-3)
		12	44	14	45	3714.386	-8.026599 (-2)	-7.617387 (-2)	-7.726195 (-2)
		0	0	3	0	6350.647	+3.609903 (-4)	+4.136643 (-4)	+4.273249 (-4)
		38	133	41	132	1960.119	+1.257997 (-1)	+1.267045 (-1)	+1.219023 (-1)
		0	0	1	0	2096.205	+1.057770 (-1)	+1.064516 (-1)	+1.051566 (-1)
13,16	1	40	133	41	132	496.790	+4.132171 (-1)	+4.720510 (-1)	+5.295498 (-1)
		0	102	1	103	2275.338	+1.106226 (-1)	+1.099103 (-1)	+1.081887 (-1)
		13	70	14	69	1473.339	+3.894796 (-1)	+3.988425 (-1)	+3.963493 (-1)
		0	0	2	0	4167.048	-6.194922 (-3)	-6.379481 (-3)	-6.519202 (-3)
		39	133	41	132	1255.368	-2.688827 (-1)	-2.866479 (-1)	-2.953231 (-1)
		0	0	3	0	6212.541	+3.484349 (-4)	+3.994183 (-4)	+4.122071 (-4)
	2	38	133	41	132	2044.644	+1.173594 (-1)	+1.169874 (-1)	+1.102474 (-1)
		0	0	1	0	2092.253	+1.056761 (-1)	+1.063502 (-1)	+1.050565 (-1)
		40	133	41	132	498.754	+4.152606 (-1)	+4.741270 (-1)	+5.314614 (-1)
		0	90	1	91	2272.724	+1.09834 (-1)	+1.093011 (-1)	+1.076784 (-1)
		7	45	8	44	1732.232	+2.968596 (-1)	+3.007020 (-1)	+2.950279 (-1)
		0	2	0	0	4159.241	-6.182778 (-3)	-6.367074 (-3)	-6.506529 (-3)
12,18	2	39	133	41	132	1259.908	-2.683949 (-1)	-2.859682 (-1)	-2.980042 (-1)
		0	0	3	0	6200.974	+3.473931 (-4)	+3.982350 (-4)	+4.109521 (-4)
		38	133	41	132	2050.719	+1.167619 (-1)	+1.162949 (-1)	+1.094245 (-1)
		0	0	1	0	2116.428	+1.062916 (-1)	+1.069694 (-1)	+1.056673 (-1)
		40	133	41	132	484.209	+4.030157 (-1)	+4.617415 (-1)	+5.202969 (-1)
		0	51	1	52	2261.660	+1.083181 (-1)	+1.083328 (-1)	+1.069200 (-1)
	2	2	20	3	19	1984.913	+1.834412 (-1)	+1.850181 (-1)	+1.824928 (-1)
		0	0	2	0	4206.996	-6.257093 (-3)	-6.442993 (-3)	-6.584076 (-3)
		39	133	41	132	1231.835	-2.707959 (-1)	-2.895178 (-1)	+5.378455 (-1)
		0	0	3	0	6271.722	+3.537873 (-4)	+4.054966 (-4)	+4.186553 (-4)
		38	133	41	132	2010.439	+1.207348 (-1)	+1.208871 (-1)	+1.149004 (-1)
		0	0	1	0	2116.428	+1.062916 (-1)	+1.069694 (-1)	+1.056673 (-1)
12,17	1	40	133	41	132	484.209	+4.030157 (-1)	+4.617415 (-1)	+5.202969 (-1)
		0	51	1	52	2261.660	+1.083181 (-1)	+1.083328 (-1)	+1.069200 (-1)
		2	20	3	19	1984.913	+1.834412 (-1)	+1.850181 (-1)	+1.824928 (-1)
		0	0	2	0	4206.996	-6.257093 (-3)	-6.442993 (-3)	-6.584076 (-3)
		39	133	41	132	1231.835	-2.707959 (-1)	-2.895178 (-1)	+5.378455 (-1)
		0	0	3	0	6271.722	+3.537873 (-4)	+4.054966 (-4)	+4.186553 (-4)
	2	38	133	41	132	2010.439	+1.207348 (-1)	+1.208871 (-1)	+1.149004 (-1)

using their analytical EDMF (see Chackerian et al. 1984), named EDMF3.

In a more recent paper (Roueff & Huré 1995), we have compared D -values using EDMF1 to those obtained from EDMF3. For the rotationless D -values involving the lowest levels of to $\Delta v = 1$ band, agreements are significantly better: less than 1% for v -numbers smaller than 10. But differences of the order of 3% and 20% remain for the $\Delta v = 2$ and 3 bands respectively in the same conditions. It appears that EDMF1 leads to better results than the EDMF of Cooper & Kirby (1987) does. However, EDMF2 might be preferable in some cases.

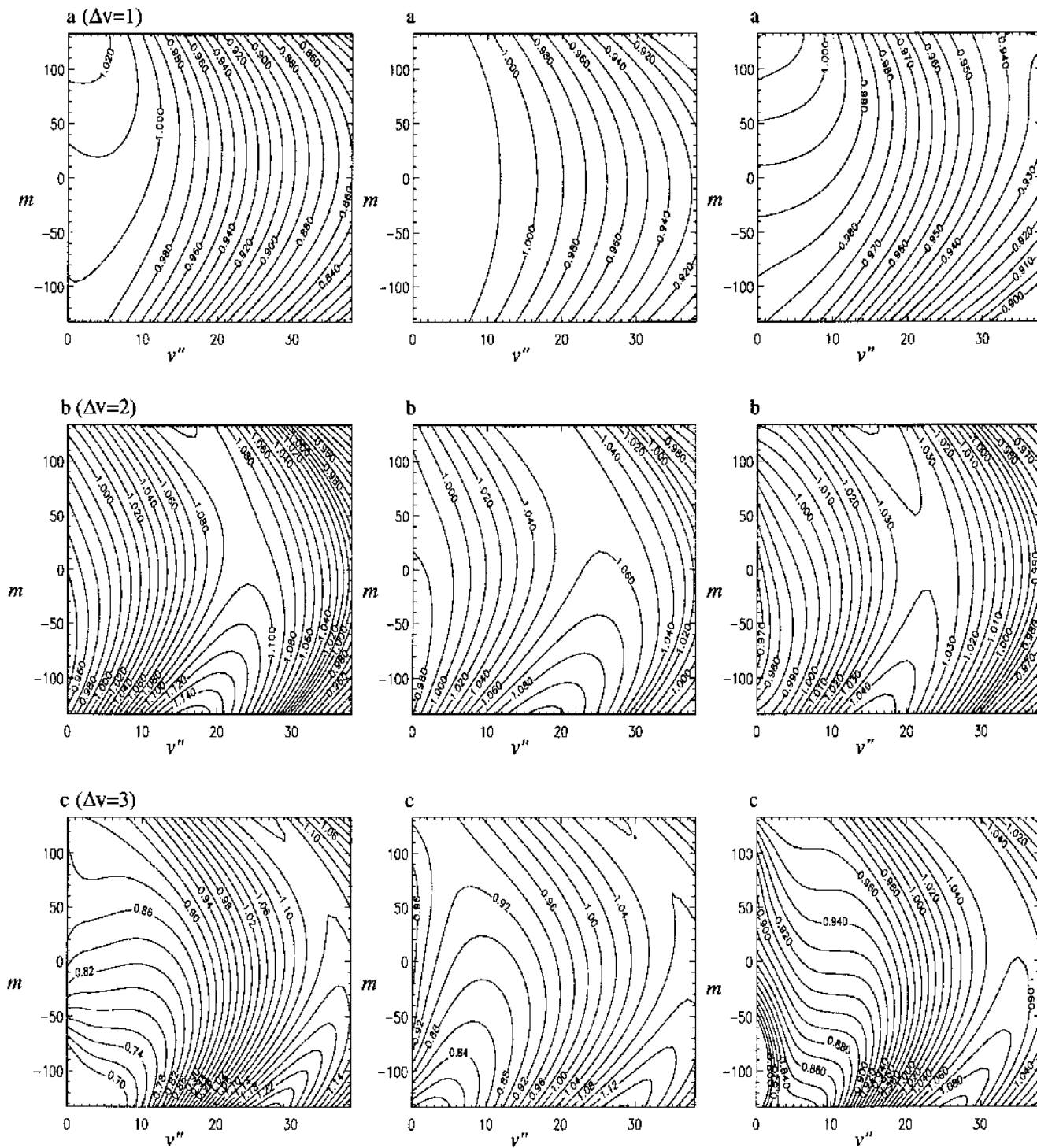
As shown in Table 1, EDMF2 and EDMF3 are identical at the equilibrium distance, but the first derivatives of

the three EDMF at $R = R_e$ differ by less than one percent. Figure 1 displays the 3 functions.

4. Calculations and discussion

The properties of the potential $V(R)$ as well as the integration method of the Schrödinger Eq. (1) have been described elsewhere (see Huré & Roueff 1993). Since numerous energy levels are well known from experiments, we have been able to check the accuracy of our calculations of the energy levels by comparing them with the spectroscopic determinations (see Farrenq et al. 1991; Sauval et al. 1992; Le Floch 1991; Authier et al. 1993).

We have considered the most abundant isotopomers, namely: $^{12}\text{C}^{16}\text{O}$, $^{13}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$ and $^{12}\text{C}^{17}\text{O}$. The elec-



Figures 2
(D_1/D_3)

Figures 3
(D_2/D_3)

Figures 4
(D_1/D_2)

Fig. 2. to 4. Contour maps displaying the ratios of D -values as a function of v'' and m for each band. D_1/D_3 are plotted in Fig. 2. D_2/D_3 are displayed in Fig. 3. D_1/D_2 are displayed in Figs. 4. From top to bottom: $\Delta v=1$ (case a), $\Delta v=2$ (case b) and $\Delta v=3$ (case c)

Table 4. a) Expansion coefficients of the polynomial expansion representing the transition D -values for the $\Delta v=1$ band and the $^{12}\text{C}^{16}\text{O}$ isotope. Results are obtained using EDMF2 (Langhoff & Bauschlicher 1995). The fits are better than 1% when $|m| \leq m_{\text{max}}$. The first column gives the lower vibrational quantum number v'' . The headers come from formula 5. The rotationless transition matrix element (in Debye) is displayed in the second column. Numbers in parenthesis refer to the power of ten involved

v''	$ m_{\text{max}} $	$\alpha_{0,v'',1}$	$\alpha_{1,v'',1}$	$\alpha_{2,v'',1}$	$\alpha_{3,v'',1}$	$\alpha_{4,v'',1}$
00	133	+1.0765 (-01)	+1.14 (-05)	+3.85 (-07)	-1.39 (-09)	-1.48 (-12)
01	133	+1.5212 (-01)	+1.23 (-05)	+5.27 (-07)	-2.02 (-09)	-2.34 (-12)
02	133	+1.8610 (-01)	+1.03 (-05)	+6.25 (-07)	-2.53 (-09)	-3.23 (-12)
03	133	+2.1463 (-01)	+6.44 (-06)	+6.93 (-07)	-3.00 (-09)	-4.03 (-12)
04	133	+2.3959 (-01)	+8.96 (-07)	+7.50 (-07)	-3.44 (-09)	-5.17 (-12)
05	133	+2.6201 (-01)	-5.91 (-06)	+7.86 (-07)	-3.86 (-09)	-6.11 (-12)
06	133	+2.8244 (-01)	-1.39 (-05)	+8.08 (-07)	-4.27 (-09)	-6.98 (-12)
07	133	+3.0127 (-01)	-2.31 (-05)	+8.23 (-07)	-4.68 (-09)	-8.19 (-12)
08	133	+3.1874 (-01)	-3.33 (-05)	+8.30 (-07)	-5.08 (-09)	-9.54 (-12)
09	133	+3.3506 (-01)	-4.44 (-05)	+8.26 (-07)	-5.48 (-09)	-1.09 (-11)
10	133	+3.5035 (-01)	-5.65 (-05)	+8.14 (-07)	-5.89 (-09)	-1.23 (-11)
11	133	+3.6471 (-01)	-6.95 (-05)	+7.94 (-07)	-6.30 (-09)	-1.39 (-11)
12	133	+3.7823 (-01)	-8.33 (-05)	+7.67 (-07)	-6.71 (-09)	-1.57 (-11)
13	133	+3.9098 (-01)	-9.80 (-05)	+7.33 (-07)	-7.12 (-09)	-1.76 (-11)
14	133	+4.0299 (-01)	-1.14 (-04)	+6.91 (-07)	-7.54 (-09)	-1.97 (-11)
15	133	+4.1432 (-01)	-1.30 (-04)	+6.41 (-07)	-7.96 (-09)	-2.19 (-11)
16	133	+4.2499 (-01)	-1.47 (-04)	+5.83 (-07)	-8.39 (-09)	-2.44 (-11)
17	133	+4.3503 (-01)	-1.65 (-04)	+5.17 (-07)	-8.82 (-09)	-2.70 (-11)
18	133	+4.4446 (-01)	-1.84 (-04)	+4.44 (-07)	-9.26 (-09)	-3.00 (-11)
19	133	+4.5330 (-01)	-2.03 (-04)	+3.62 (-07)	-9.70 (-09)	-3.31 (-11)
20	133	+4.6155 (-01)	-2.23 (-04)	+2.72 (-07)	-1.02 (-08)	-3.66 (-11)
21	133	+4.6922 (-01)	-2.44 (-04)	+1.73 (-07)	-1.06 (-08)	-4.04 (-11)
22	133	+4.7632 (-01)	-2.66 (-04)	+6.48 (-08)	-1.11 (-08)	-4.46 (-11)
23	133	+4.8285 (-01)	-2.88 (-04)	-5.30 (-08)	-1.15 (-08)	-4.92 (-11)
24	133	+4.8881 (-01)	-3.11 (-04)	-1.81 (-07)	-1.20 (-08)	-5.42 (-11)
25	133	+4.9419 (-01)	-3.35 (-04)	-3.21 (-07)	-1.25 (-08)	-5.97 (-11)
26	133	+4.9899 (-01)	-3.59 (-04)	-4.72 (-07)	-1.29 (-08)	-6.58 (-11)
27	133	+5.0319 (-01)	-3.84 (-04)	-6.21 (-07)	-1.34 (-08)	-7.35 (-11)
28	133	+5.0663 (-01)	-4.09 (-04)	-6.91 (-07)	-1.40 (-08)	-8.83 (-11)
29	133	+5.0891 (-01)	-4.32 (-04)	-4.73 (-07)	-1.49 (-08)	-1.25 (-10)
30	133	+5.1008 (-01)	-4.51 (-04)	+3.90 (-08)	-1.64 (-08)	-1.86 (-10)
31	133	+5.1146 (-01)	-4.70 (-04)	+1.48 (-07)	-1.86 (-08)	-2.31 (-10)
32	133	+5.1330 (-01)	-4.96 (-04)	-3.73 (-07)	-2.00 (-08)	-2.41 (-10)
33	133	+5.1450 (-01)	-5.19 (-04)	-1.08 (-06)	-2.19 (-08)	-2.45 (-10)
34	133	+5.1552 (-01)	-5.30 (-04)	-2.38 (-06)	-2.48 (-08)	-2.10 (-10)
35	133	+5.1604 (-01)	-5.84 (-04)	-3.64 (-06)	-2.36 (-08)	-1.88 (-10)
36	133	+5.1244 (-01)	-6.52 (-04)	-4.01 (-06)	-2.18 (-08)	-2.13 (-10)
37	133	+5.0788 (-01)	-6.95 (-04)	-4.63 (-06)	-2.19 (-08)	-2.23 (-10)
38	129	+5.0196 (-01)	-7.40 (-04)	-5.25 (-06)	-2.15 (-08)	-2.30 (-10)
39	131	+4.9378 (-01)	-7.79 (-04)	-5.28 (-06)	-2.18 (-08)	-2.80 (-10)
40	130	+4.8536 (-01)	-8.15 (-04)	-5.69 (-06)	-2.22 (-08)	-3.09 (-10)

Table 4a - $\Delta v=1$ for $^{12}\text{C}^{16}\text{O}$.

tronic properties such as the interatomic potential and the EDMF are independent of the isotope. However the rovibrational energy levels and the corresponding wavefunctions, which are obtained from the solution of the Schrödinger equation, depend on the reduced mass of the system. Table 2 summarizes the values of the reduced mass for the various isotopomers.

We have computed D -values for transitions involving $v' \leq 41$ and $J' \leq 133$ for $\Delta v=1, 2$ and 3 using EDMF1, EDMF2 and EDMF3 (corresponding D -values are noted D_1, D_2 and D_3 respectively). A simple cubic spline has been applied to interpolate the ab-initio data points (except for EDMF3 which is analytical). The adopted limits

on v and J correspond to the highest (independently) observed levels for $^{12}\text{C}^{16}\text{O}$ molecule in the solar spectrum detected by the ATMOS experiment (Farmer & Norton 1989; Farrenq et al. 1991).

We point out that the computation of the D -values seems to be very sensitive to the interpolation method used to calculate the electric dipole moment functions between data points. Actually, severe differences appear on D -values when using a Padé approximant instead of a cubic spline procedure.

We display in Figs. 2 to 4 the contour plots of the ratios of the D -values calculated with the three EDMF's for the $\Delta v=1, 2$ and 3 bands (a, b and c respectively)

Table 4. b) Same as Table 4a for $\Delta v=2$

v''	$ m_{\max} $	$\alpha_{0,v'',2}$	$\alpha_{1,v'',2}$	$\alpha_{2,v'',2}$	$\alpha_{3,v'',2}$	$\alpha_{4,v'',2}$
00	133	-6.5274 (-03)	-1.68 (-05)	-9.23 (-08)	-2.67 (-11)	-5.42 (-13)
01	133	-1.1458 (-02)	-2.89 (-05)	-1.57 (-07)	-4.02 (-11)	-1.05 (-12)
02	133	-1.6391 (-02)	-4.06 (-05)	-2.25 (-07)	-4.50 (-11)	-1.36 (-12)
03	133	-2.1418 (-02)	-5.20 (-05)	-2.88 (-07)	-4.36 (-11)	-1.86 (-12)
04	133	-2.6540 (-02)	-6.31 (-05)	-3.52 (-07)	-3.81 (-11)	-2.30 (-12)
05	133	-3.1760 (-02)	-7.41 (-05)	-4.18 (-07)	-1.68 (-11)	-2.59 (-12)
06	133	-3.7088 (-02)	-8.47 (-05)	-4.83 (-07)	+5.89 (-12)	-2.87 (-12)
07	133	-4.2514 (-02)	-9.51 (-05)	-5.45 (-07)	+3.72 (-11)	-3.29 (-12)
08	133	-4.8036 (-02)	-1.05 (-04)	-6.09 (-07)	+8.10 (-11)	-3.59 (-12)
09	133	-5.3649 (-02)	-1.15 (-04)	-6.73 (-07)	+1.34 (-10)	-3.80 (-12)
10	133	-5.9356 (-02)	-1.25 (-04)	-7.35 (-07)	+1.97 (-10)	-4.04 (-12)
11	133	-6.5151 (-02)	-1.34 (-04)	-7.98 (-07)	+2.69 (-10)	-4.27 (-12)
12	133	-7.1032 (-02)	-1.43 (-04)	-8.59 (-07)	+3.57 (-10)	-4.46 (-12)
13	133	-7.6995 (-02)	-1.52 (-04)	-9.20 (-07)	+4.57 (-10)	-4.64 (-12)
14	133	-8.3036 (-02)	-1.60 (-04)	-9.80 (-07)	+5.69 (-10)	-4.81 (-12)
15	133	-8.9156 (-02)	-1.68 (-04)	-1.04 (-06)	+6.95 (-10)	-4.93 (-12)
16	133	-9.5350 (-02)	-1.76 (-04)	-1.10 (-06)	+8.38 (-10)	-5.09 (-12)
17	133	-1.0161 (-01)	-1.83 (-04)	-1.15 (-06)	+9.97 (-10)	-5.19 (-12)
18	133	-1.0794 (-01)	-1.90 (-04)	-1.21 (-06)	+1.17 (-09)	-5.31 (-12)
19	133	-1.1434 (-01)	-1.96 (-04)	-1.26 (-06)	+1.37 (-09)	-5.44 (-12)
20	133	-1.2079 (-01)	-2.02 (-04)	-1.31 (-06)	+1.59 (-09)	-5.52 (-12)
21	133	-1.2731 (-01)	-2.07 (-04)	-1.36 (-06)	+1.82 (-09)	-5.61 (-12)
22	133	-1.3387 (-01)	-2.12 (-04)	-1.41 (-06)	+2.09 (-09)	-5.64 (-12)
23	133	-1.4048 (-01)	-2.17 (-04)	-1.46 (-06)	+2.38 (-09)	-5.64 (-12)
24	133	-1.4714 (-01)	-2.21 (-04)	-1.51 (-06)	+2.70 (-09)	-5.56 (-12)
25	133	-1.5384 (-01)	-2.24 (-04)	-1.56 (-06)	+3.05 (-09)	-5.33 (-12)
26	133	-1.6057 (-01)	-2.27 (-04)	-1.61 (-06)	+3.44 (-09)	-4.75 (-12)
27	133	-1.6734 (-01)	-2.30 (-04)	-1.65 (-06)	+3.93 (-09)	-4.35 (-12)
28	133	-1.7438 (-01)	-2.35 (-04)	-1.57 (-06)	+4.63 (-09)	-1.16 (-11)
29	133	-1.8205 (-01)	-2.37 (-04)	-1.16 (-06)	+5.38 (-09)	-4.14 (-11)
30	131	-1.8962 (-01)	-2.38 (-04)	-7.23 (-07)	+6.07 (-09)	-8.01 (-11)
31	133	-1.9652 (-01)	-2.46 (-04)	-6.65 (-07)	+8.16 (-09)	-9.41 (-11)
32	127	-2.0251 (-01)	-2.70 (-04)	-1.31 (-06)	+1.08 (-08)	-7.01 (-11)
33	120	-2.0753 (-01)	-2.57 (-04)	-1.99 (-06)	+1.11 (-08)	-4.35 (-11)
34	113	-2.1360 (-01)	-2.39 (-04)	-2.64 (-06)	+1.11 (-08)	-8.01 (-12)
35	124	-2.2027 (-01)	-2.23 (-04)	-3.42 (-06)	+1.12 (-08)	+5.65 (-11)
36	133	-2.2963 (-01)	-2.19 (-04)	-3.28 (-06)	+1.32 (-08)	+6.61 (-11)
37	133	-2.3914 (-01)	-2.07 (-04)	-3.07 (-06)	+1.43 (-08)	+7.38 (-11)
38	133	-2.4876 (-01)	-2.02 (-04)	-2.70 (-06)	+1.62 (-08)	+6.92 (-11)
39	133	-2.5621 (-01)	-1.84 (-04)	-2.69 (-06)	+1.72 (-08)	+8.54 (-11)

Table 4b - $\Delta v=2$ for $^{12}\text{C}^{16}\text{O}$.

and the complete set of v'' and m values. The ratios are: D_1/D_3 in Fig. 2, D_2/D_3 in Fig. 3 and D_1/D_2 in Figs. 4. These plots concern the $^{12}\text{C}^{16}\text{O}$ molecule.

For low v and J transitions inside the fundamental band of the $^{12}\text{C}^{16}\text{O}$ molecule, the three EDMF lead to very similar results. Agreement is good to within less than 1%. EDMF1 leads to D -values slightly closer to the experimental results than EDMF2 according to the first derivatives at $R = R_e$. For extreme v and J transitions, differences appear as large as 20%, especially when using EDMF1 as shown in Roueff & Huré (1995). For intermediate v and J values, agreement between the EDMF's is quite good within a few percent. This is the case for most of the lines recently identified in the solar spectrum (see Table 3). For the first overtone band ($\Delta v=2$), we see that EDMF1 and EDMF2 lead to very close values of dipole matrix elements for the whole set of vJ -lines within 2–3%. Comparing with EDMF3, the shift is largest for intermediate

v -numbers ($v \approx 20$) and largest J -numbers. Finally, for the second overtone band ($\Delta v=3$), the three EDMF lead to very different D -values. As shown from Eq. (2), larger differences do exist between gf -values based on the three different EDMF.

The differences obtained from the three EDMFs remain of the same order of magnitude for the $^{13}\text{C}^{16}\text{O}$ molecule and other isotopomers, which reflects the coherence of the EDMF over all involved internuclear distances. This is not the case when two experimental EDMFs (Chackerian & Tipping 1983 and Chackerian et al. 1984) are compared as shows Goorvitch (1994) in his Table 5.

Globally, whereas the ratios D_1/D_3 , D_2/D_3 and D_1/D_2 remain close to 1 for most values of v'' and m of the $\Delta v=1$ band, we note that the discrepancies between both choices of EDMF increase as Δv , v' and m increase. We feel that these results show the remaining uncertainties in the D -values due to the different choices

Table 4. c) Same as Table 4a for $\Delta v=3$

v''	$ m_{\max} $	$\alpha_{0,v'',3}$	$\alpha_{1,v'',3}$	$\alpha_{2,v'',3}$	$\alpha_{3,v'',1}$	$\alpha_{4,v'',3}$
00	133	+4.1405 (-04)	+2.44 (-06)	+1.27 (-08)	+2.80 (-11)	+2.12 (-13)
01	133	+8.5412 (-04)	+4.91 (-06)	+2.67 (-08)	+5.47 (-11)	+3.58 (-13)
02	133	+1.3896 (-03)	+7.78 (-06)	+4.40 (-08)	+8.62 (-11)	+4.99 (-13)
03	133	+2.0375 (-03)	+1.10 (-05)	+5.90 (-08)	+1.21 (-10)	+9.13 (-13)
04	133	+2.7736 (-03)	+1.46 (-05)	+7.91 (-08)	+1.59 (-10)	+1.23 (-12)
05	133	+3.6091 (-03)	+1.85 (-05)	+1.02 (-07)	+2.02 (-10)	+1.51 (-12)
06	133	+4.5438 (-03)	+2.27 (-05)	+1.27 (-07)	+2.42 (-10)	+1.86 (-12)
07	133	+5.5794 (-03)	+2.72 (-05)	+1.54 (-07)	+2.86 (-10)	+2.23 (-12)
08	133	+6.7167 (-03)	+3.19 (-05)	+1.83 (-07)	+3.31 (-10)	+2.59 (-12)
09	133	+7.9571 (-03)	+3.69 (-05)	+2.15 (-07)	+3.76 (-10)	+2.96 (-12)
10	133	+9.3010 (-03)	+4.21 (-05)	+2.49 (-07)	+4.21 (-10)	+3.34 (-12)
11	133	+1.0750 (-02)	+4.75 (-05)	+2.85 (-07)	+4.66 (-10)	+3.73 (-12)
12	133	+1.2308 (-02)	+5.31 (-05)	+3.22 (-07)	+5.11 (-10)	+4.15 (-12)
13	133	+1.3975 (-02)	+5.89 (-05)	+3.61 (-07)	+5.54 (-10)	+4.58 (-12)
14	133	+1.5752 (-02)	+6.49 (-05)	+4.02 (-07)	+5.95 (-10)	+5.03 (-12)
15	133	+1.7642 (-02)	+7.10 (-05)	+4.44 (-07)	+6.34 (-10)	+5.49 (-12)
16	133	+1.9645 (-02)	+7.73 (-05)	+4.88 (-07)	+6.70 (-10)	+5.98 (-12)
17	133	+2.1762 (-02)	+8.37 (-05)	+5.33 (-07)	+7.04 (-10)	+6.48 (-12)
18	133	+2.3993 (-02)	+9.02 (-05)	+5.79 (-07)	+7.33 (-10)	+6.99 (-12)
19	133	+2.6340 (-02)	+9.69 (-05)	+6.27 (-07)	+7.58 (-10)	+7.51 (-12)
20	133	+2.8802 (-02)	+1.04 (-04)	+6.76 (-07)	+7.78 (-10)	+8.03 (-12)
21	133	+3.1381 (-02)	+1.10 (-04)	+7.27 (-07)	+7.93 (-10)	+8.55 (-12)
22	133	+3.4075 (-02)	+1.17 (-04)	+7.79 (-07)	+8.03 (-10)	+9.08 (-12)
23	133	+3.6887 (-02)	+1.24 (-04)	+8.31 (-07)	+8.06 (-10)	+9.71 (-12)
24	133	+3.9816 (-02)	+1.31 (-04)	+8.83 (-07)	+8.01 (-10)	+1.04 (-11)
25	133	+4.2860 (-02)	+1.38 (-04)	+9.36 (-07)	+7.84 (-10)	+1.11 (-11)
26	133	+4.6026 (-02)	+1.45 (-04)	+9.86 (-07)	+7.43 (-10)	+1.21 (-11)
27	133	+4.9375 (-02)	+1.52 (-04)	+1.00 (-06)	+6.75 (-10)	+1.57 (-11)
28	133	+5.3092 (-02)	+1.60 (-04)	+8.70 (-07)	+5.93 (-10)	+2.96 (-11)
29	126	+5.6617 (-02)	+1.66 (-04)	+8.79 (-07)	+5.47 (-10)	+3.68 (-11)
30	118	+6.0195 (-02)	+1.73 (-04)	+9.13 (-07)	+4.99 (-10)	+4.45 (-11)
31	111	+6.3957 (-02)	+1.79 (-04)	+8.77 (-07)	+4.46 (-10)	+6.26 (-11)
32	105	+6.7844 (-02)	+1.85 (-04)	+7.84 (-07)	+4.16 (-10)	+9.61 (-11)
33	110	+7.1774 (-02)	+1.86 (-04)	+7.90 (-07)	+1.22 (-09)	+1.35 (-10)
34	101	+7.4757 (-02)	+1.92 (-04)	+1.50 (-06)	+1.28 (-09)	+1.20 (-10)
35	92	+7.8791 (-02)	+2.01 (-04)	+2.29 (-06)	+1.13 (-09)	+8.43 (-11)
36	105	+8.3444 (-02)	+2.13 (-04)	+3.64 (-06)	-5.61 (-10)	-6.09 (-11)
37	110	+9.1414 (-02)	+2.24 (-04)	+3.21 (-06)	-1.58 (-09)	-3.38 (-11)
38	133	+9.9492 (-02)	+2.34 (-04)	+2.58 (-06)	-3.34 (-09)	+1.28 (-11)

Table 4c - $\Delta v=3$ for $^{12}\text{C}^{16}\text{O}$.

of the EDMF functions. Both $\Delta v = 1$ and 2 transitions are present in the infrared solar spectrum (Grevesse & Sauval 1991, 1993) and are often used to determine the temperature of the photosphere. In the particular case of $\Delta v=2$, we suggest that models of the photosphere should be performed with both sets of D -values to evaluate the uncertainties coming from the molecular data themselves.

5. Polynomial fits

For an intensive use of this set of numerous lines and associated D -values, it is very useful to have an analytical formula. Consequently, we have fitted them with a fourth order polynomial form for each sequence and each vibrational band by using a numerical minimax procedure from the NAG mathematical library as a function of $m = [J'(J'+1) - J''(J''+1)]/2$, v'' and $\Delta v = n$:

$$D_n^{v''}(m) = \langle v'' + n, J' | M | v'', J'' \rangle = \alpha_{0,v'',n} + \alpha_{1,v'',n}m +$$

$$\alpha_{2,v'',n}m^2 + \alpha_{3,v'',n}m^3 + \alpha_{4,v'',n}m^4 \quad (5)$$

For the P-branch ($\Delta J = -1$), m is $(-J'')$ and for the R-branch ($\Delta J = +1$), m is $(+J')$.

This procedure is sufficient to reproduce most of the original values with a relative uncertainty less than 1%. The accuracy depends on the values of m and v'' involved. Figure 5 displays the results of the calculations for $v'' = 38$ and $\Delta v = 1, 2$ and 3 obtained with EDMF2 together with our obtained analytical fit. The relative error arising from the fitting procedure in logarithmic scale is also shown. Tables 4a-c give the polynomial expansion coefficients for the $\Delta v = 1, 2$ and 3 sequences for $^{12}\text{C}^{16}\text{O}$ corresponding to EDMF2 which gives the best agreement with the experiments. The range of values of m for which the error due to the fitting procedure is less than 1% is also listed (for example, we note that, for the fundamental ($\Delta v = 1$) band of the $^{12}\text{C}^{16}\text{O}$ molecule, this error is less than 10^{-2} for $v''=38$ and $|m|$ smaller than 129). We feel that this ac-

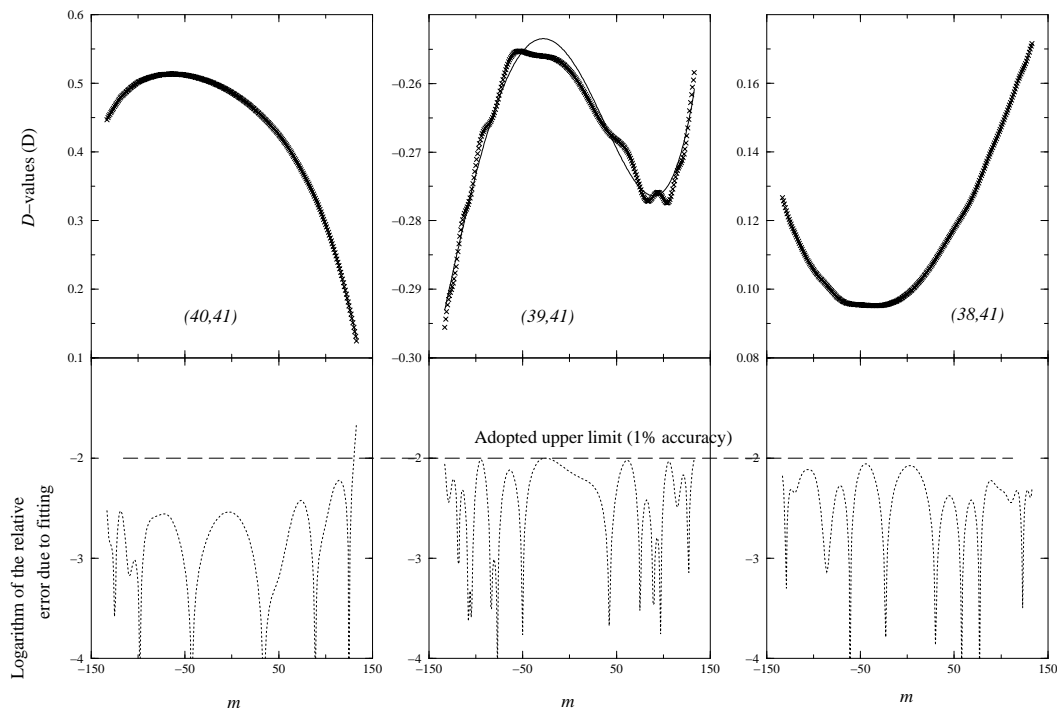


Fig. 5. D -values as a function of m for the highest vibrational sequences considered (top). Crosses are the data. Lines are the polynomial fittings. Logarithm of the relative errors due to the fitting procedure is also shown (dotted, bottom plots)

curacy is sufficient for most applications and still smaller than the uncertainty due to the choice of the EDMF as we point out later.

Though the square of the transition matrix elements is involved in f -values or A Einstein coefficients, we found that the errors arising from the fitting of the D -values squared were always larger than two times the error coming from the fitting of the D -values themselves for the whole set of data. We found that the isotopic substitution has only a small effect on D -values. Consequently, we have obtained very close polynomial forms for the different isotopomers. Tables 4a-c and similar tables for the $^{13}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$ and $^{12}\text{C}^{17}\text{O}$ isotopomers are available in electronic form at the CDS via anonymous ftp 130.79.128.5. The polynomial fits of D_1 -values (computed with EDMF1) can also be obtained via e-mail on request to the authors.

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