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Ab initio calculation of the dipole transition moment and band oscillator strengths of the CO (A-X) transition

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Abstract. Band-integrated oscillator strengths of the CO $A^1\Pi - X^1\Sigma^+$ transition for $0 \leq v' \leq 23$ and $v'' = 0 - 1$ have been calculated from an ab initio dipole transition moment given by highly correlated electronic wave functions. The calculations were carefully optimized to represent the dipole transition moment in the large range of internuclear distances necessary to describe correctly high vibrational levels. The computed oscillator strengths agree well with the more recent experimental data available for $v'' = 0$. By comparing the present results with previous theoretical works, we estimate that the resulting line strengths for the higher v' vibrational levels should be the most accurate to date.

Key words: molecular data – ISM: molecules – ultraviolet: ISM

1. Introduction

The $A^1\Pi - X^1\Sigma^+$ absorption bands of carbon monoxide in the VUV are extensively used to determine the molecular density in a number of astrophysical media. In the interstellar medium, quantitative column densities in the line of sight of a given continuum source are obtained from optical absorption of CO in the VUV. Due to the advent of spectrographs on board of spatial satellites (IUE, HST), these observations have become feasible. A correct interpretation of the observations in terms of column densities requires that the observed lines are not saturated. As the band oscillator strengths of the CO $A^1\Pi - X^1\Sigma^+$ transition vary over six orders of magnitude for $0 \leq v' \leq 23$, CO offers the possibility to determine a large range of column densities. The relative abundance of different isotopic forms of CO may be deduced from the relative values of the oscillator strengths of the corresponding sets of bands.

Many laboratory investigations of the radiative transition in CO have been carried out these last ten years by various techniques (Chan et al. 1993, Eidelsberg et al. 1992, Federman et al. 1997, Field et al. 1983, Jolly et al. 1997, Smith et al. 1994, Zhong et al. 1997), a detailed analysis is given in Jolly et al. (1997) for $v' \leq 17$. Except for the data of Eidelsberg et al. (1992) above $v'=5$ and Federman et al. (1997), all these experi-

mental data agree within their error bars. Measurements of band oscillator strengths have become available very recently for the highest vibrational levels: Eidelsberg et al. (1998, this issue) for $v' \geq 11$ and Stark et al. (1998) for $v' = 13, 14, 16, 18-21$. For these very weak bands, accurate measurements are very difficult which justifies complementary theoretical investigations.

Previous theoretical calculations of the oscillator strengths of the lowest-lying optical transitions were performed by Kirby & Cooper (1989) and Chantranupong et al. (1992). These studies concern a number of transitions for which the upper states have predominantly a Rydberg character. The electronic properties such as the dipole transition moment are thus obtained in an average calculation using the same molecular orbitals for all the states. As we focus the present study on the A-X transition, our aim is to optimize the electronic calculation especially for these two low-lying valence states. First we present (Sect. 2) the summary of ab initio calculations of the electronic potential energies and the dipole transition moment. The corresponding results are given in Sect. 3. We then deduce the A-X oscillator strengths for $0 \leq v' \leq 23$ and $v'' = 0 - 1$ (Sect. 4). Sect. 5 deals with a discussion about the numerical accuracy given the large range of orders of magnitude in the oscillator strengths.

2. Summary of the ab initio calculation

The Gaussian basis sets employed are general contractions based on atomic natural orbitals. The basis sets include for both carbon and oxygen the primitive basis set [12s, 6p] of Dunning (1989) contracted to [5s, 4p] and [3d, 2f] polarization functions. This set was augmented by diffuse functions: the last s and p functions of Dunning were replaced by two s and p functions with exponents 0.16, 0.06 (s), 0.14, 0.05 (p) for carbon and 0.30, 0.12 (s), 0.25, 0.09 (p) for oxygen. The total number of contracted Gaussian functions was 102.

To obtain the best accuracy for both the potential energy and the dipole transition moment, multireference configuration interaction (MRCI) wave functions were constructed using multiconfiguration self-consistent field (MCSCF) active space (Werner & Knowles 1985, 1988, Knowles & Werner 1985, 1988) with valence and Rydberg orbitals ($3\sigma - 7\sigma, 1\pi - 3\pi$). Except for the core ($1\sigma - 2\sigma$) all valence and Rydberg electrons were correlated. The reference space was restricted to include

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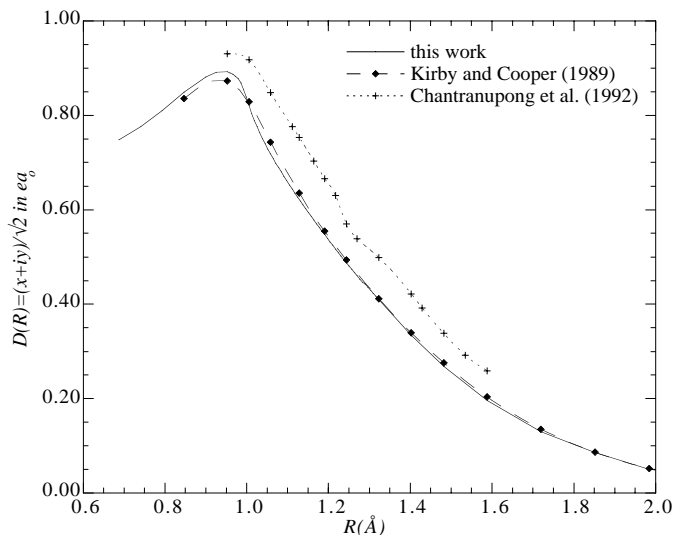


Fig. 1. Transition dipole moment (in atomic units ea_0 , $a_0 = 0.529177 \text{ Å}$) for the (A-X) transition from the present calculations (solid line), from Kirby & Cooper (1989) (dashed line) and from Chantranupong et al. (1992) (dotted line).

only occupations for which the absolute value of any determinant exceeded 0.005 for all interatomic distances. The MRCI wave functions accounted for more than 27 millions of configurations which were internally contracted to one million. All the calculations have been performed with the MOLPRO code¹.

3. Spectroscopic constants and dipole transition moment

In order to test the basis set and the active space, the $X^1\Sigma^+$ and $A^1\Pi$ electronic potential energy curves were obtained in separate optimization procedures. The minima R_e of the calculated potential energy curves and the excitation energy T_e of the A state have been determined. For each potential, a fit to the first vibrational levels gives the harmonic frequency ω_e and the anharmonicity constant $\omega_e x_e$. The vibrational levels were obtained from numerical integration of the radial Schrödinger equation using the Numerov method. The calculated values of these spectroscopic constants are given in Table 1 for comparison with the corresponding theoretical values of Cooper & Kirby (1987) et Chantranupong et al. (1992) as well as the experimental results (Huber & Herzberg 1979).

The present calculations show a very good overall agreement with the experimental data. This allows us to be confident in the high quality of the basis set.

To determine the electronic dipole transition moment $D(R) = (x + iy)/\sqrt{2}$ between X and A electronic states the MRCI wavefunctions were constructed from a common set of orbitals as a function of the nuclear separation R . A very small

¹ MOLPRO is a package of ab initio programs written by H. -J. Werner and P. J. Knowles, with contributions from J. Almlöf, R. D. Amos, A. Berning, M. J. O. Deegan, F. Eckert, S. T. Elbert, C. Hampel, R. Lindh, W. Meyer, A. Nicklass, K. Peterson, R. Pitzer, A. J. Stone, P. R. Taylor, M. E. Mura, P. Pulay, M. Schuetz, H. Stoll, T. Thorsteinsson, and D. L. Cooper.

step in R ($0.0125a_0$ i.e. 0.006 Å for $0.95 \leq R \leq 1.32 \text{ Å}$) has been used in order to represent correctly the variation of the transition moment near the equilibrium distance of the ground state where the $v''=0$ wave function has notable values. The calculated values are listed in Table 2 and compared in Fig. 1 with the theoretical results of Kirby & Cooper (1989) (hereafter KC) and Chantranupong et al. (1992) (hereafter Cha92). It first appears that the results by Cha92 are much larger than our calculated values and those obtained by KC. These two last calculations give very similar results although our calculated dipole transition moment is slightly larger for small R values and lower for large R values. Both of them exhibit a maximum around 0.95 Å , the most noticeable difference being located around 1 Å where its sign changes. As will be discussed in the Sect. 5, this point has consequences on the band oscillator strengths of ($v'-0$), especially for high v' corresponding to weak bands.

4. Oscillator strengths

The band oscillator strengths for absorption are expressed in terms of vibrationally averaged dipole transition moment $D_{v'v''}$ (in atomic units):

$$f(v', v'') = \left(\frac{2}{3}\right) \Delta E_{v'v''} g |D_{v'v''}|^2 \quad (1)$$

where $\Delta E_{v'v''}$ is the transition energy (in atomic units) between vibrational states v' and v'' associated with the initial and final electronic states Λ' and Λ'' respectively. The degeneracy factor g is given by:

$$g = \frac{2 - \delta_{0,\Lambda''+\Lambda'}}{2 - \delta_{0,\Lambda'}} \quad (2)$$

Here $g = 2$ for a $^1\Pi - ^1\Sigma^+$ transition. The vibrationally averaged dipole transition moment $D_{v'v''}$ is:

$$D_{v'v''} = \langle \Psi_{v'} | D(R) | \Psi_{v''} \rangle \quad (3)$$

where $\Psi_{v''}$ and $\Psi_{v'}$ are the rovibrational wave functions in the $X^1\Sigma^+$ state and in the $A^1\Pi$ state respectively. The $D_{v'v''}$ have been calculated without invoking the r-centroid approximation which breaks down for large v' values. As usual, for better precision, $D(R)$ has been taken equal to the ab initio dipole transition moment while the wave functions have been calculated solving the Schrödinger equation in RKR-potentials. These were generated from experimental molecular constants using the code RKR1 (Le Roy, 1992). For the $X^1\Sigma^+$ state, 9 vibrational and 7 rotational Dunham parameters were taken from Table 3 (Le Floch, 1991). For the $A^1\Pi$ state, we used 8 vibrational and 9 rotational constants (Field, 1971) derived from the deperturbed results of Field et al. (1972). To account for the selection rules, the calculations were carried out with $J'' = 0$ for the $X^1\Sigma^+$ state and $J' = 1$ for the $A^1\Pi$ state (very small differences have been found, less than 5.10^{-4} for $v' = 23$ and $v'' = 0$ when rotation is neglected).

One must be aware of the sensitivity of the Franck-Condon factors $q(v', v'') = |\langle \Psi_{v'} | \Psi_{v''} \rangle|^2$ and oscillator strengths relative to the potentials used for their calculation, especially

Table 1. Calculated and experimental spectroscopic constants for $^{12}\text{C}^{16}\text{O}$

State	Reference	R_e (a_0)	ω_e (cm^{-1})	$\omega_e x_e$ (cm^{-1})	T_e (eV)
$X^1\Sigma^+$	this work	2.136	2170	13.9	0
	Cooper & Kirby (1987)	2.153	2152	12.9	0
	Chantranupong et al. (1992)	2.137	2178	13.0	0
	EXP	2.132	2170	13.3	0
$A^1\Pi$	this work	2.332	1514	18.0	8.12
	Cooper & Kirby (1987)	2.362	1475	18.9	8.28
	Chantranupong et al. (1992)	2.349	1496	18.1	8.14
	EXP	2.334	1518	19.4	8.07

Table 2. Calculated dipole transition moment (in atomic units) as function of the internuclear distance R (in Å)

R	$D(R)$	R	$D(R)$	R	$D(R)$	R	$D(R)$
0.68793	0.7482	1.03851	0.7510	1.16419	0.5779	1.29648	0.4359
0.74085	0.7757	1.04512	0.7396	1.17080	0.5701	1.30310	0.4293
0.79377	0.8098	1.05174	0.7284	1.17742	0.5624	1.30971	0.4228
0.84668	0.8486	1.05835	0.7180	1.18403	0.5550	1.31633	0.4163
0.89960	0.8814	1.06497	0.7078	1.19065	0.5475	1.32294	0.4093
0.92606	0.8912	1.07158	0.6983	1.19726	0.5396	1.40232	0.3341
0.95252	0.8921	1.07820	0.6898	1.20388	0.5319	1.48170	0.2680
0.95913	0.8899	1.08481	0.6802	1.21049	0.5245	1.58753	0.1958
0.96575	0.8869	1.09143	0.6710	1.21711	0.5167	1.71983	0.1296
0.97236	0.8831	1.09804	0.6613	1.22372	0.5093	1.85212	0.0855
0.97898	0.8776	1.10466	0.6524	1.23034	0.5020	1.98441	0.0502
0.98559	0.8685	1.11127	0.6439	1.23695	0.4948	2.11671	0.0299
0.99221	0.8547	1.11789	0.6354	1.24357	0.4879	2.38130	0.0159
0.99882	0.8389	1.12450	0.6269	1.25018	0.4809	2.64589	0.0078
1.00544	0.8206	1.13112	0.6186	1.25680	0.4738	3.17506	0.0025
1.01205	0.8042	1.13773	0.6105	1.26341	0.4669	3.70424	0.0017
1.01867	0.7891	1.14435	0.6022	1.27002	0.4601	4.23342	0.0013
1.02528	0.7759	1.15096	0.5939	1.27664	0.4528	6.35012	0.0004
1.03190	0.7631	1.15757	0.5860	1.28325	0.4463	7.93766	0.0001

when high vibrational levels are involved. In an early stage of this work, we used for the X state a slightly different RKR potential generated from only 3 vibrational and 2 rotational constants from Table 4 of Le Floch (1991). Compared with the final results given in Table 3, the relative change varies from 0.4% (0-0) to 7% (23-0) for the two sets of A-X Franck-Condon factors, and from 0.4% to 4% for the corresponding oscillator strengths. The changes could be even larger if a slightly different A state potential were used. Furthermore, the numbers obtained for high v' are also sensitive to the extrapolations of the A state beyond the RKR well. Our choice of the *best potentials* is based on the best overall agreement between the calculated vibrational energies and rotational constants and the experimental results.

Our calculated band oscillator strengths for $0 \leq v' \leq 23$ ($v'' = 0$) as well as other calculated f-values are listed in Table 3 and presented in Fig. 2. Recent measurements available for high v' values (Jolly et al. 1997, Eidelsberg et al. 1998, Stark et al. 1998, noted Jol97., Eid98, Sta98 respectively in Table 2) are also given for comparison. As the oscillator strengths vary by several orders of magnitude between $v' = 0$ and $v' = 23$, the f-

values have been scaled in Fig. 2 by the Franck-Condon factors $q(v', 0)$ to give reduced oscillator strengths as first proposed by Jolly et al. (1997). The Franck Condon factors were calculated from the same vibrational wave functions as those used for band oscillator strengths. We have recalculated the f-values derived from the tabulated ab initio electronic dipole transition moment of Kirby & Cooper (1989) by using the above RKR potentials and extended them to include bands with $v' \geq 10$.

Considering oscillator strengths for $v'' = 0$, all the results except the theoretical values of Chantranupong et al. (1992) agree reasonably well for $v' \leq 14$. For larger v' values, it appears from Fig. 2 that our results confirm the rapid increase with increasing v' of the reduced oscillator strengths as obtained in two recent experiments (Stark et al. 1998, Eidelsberg et al. 1998). These results differ significantly from KC's predictions. The difference between KC's and our results for large v' values may appear surprising since the two dipole transition moments differ by only a few percent in average. To explain these different behaviours, we have tested the numerical accuracy of the calculated band oscillator strengths.

Table 3. Comparison of experimental and theoretical band oscillator strengths for $v'' = 0$ and 1. Numbers in parentheses are the powers of 10 multiplying the results

v'	This work $v'' = 0$	KC $v'' = 0$	Cha92 $v'' = 0$	Eid98 $v'' = 0$	Sta98 $v'' = 0$	Jol97 $v'' = 0$	$q(v', 0)$	This work $v'' = 1$	$q(v', 1)$
0	1.50(-2)	1.55(-2)	1.48(-2)				1.22(-1)	2.84(-2)	2.70(-1)
1	3.13(-2)	3.23(-2)	3.56(-2)				2.28(-1)	1.72(-2)	1.47(-1)
2	3.59(-2)	3.72(-2)	4.73(-2)				2.35(-1)	9.00(-4)	7.02(-3)
3	3.02(-2)	3.15(-2)	4.62(-2)				1.80(-1)	4.39(-3)	3.01(-2)
4	2.09(-2)	2.20(-2)	3.71(-2)				1.13(-1)	1.63(-2)	1.02(-1)
5	1.27(-2)	1.34(-2)	2.62(-2)				6.30(-2)	2.31(-2)	1.32(-1)
6	7.03(-3)	7.48(-3)	1.68(-2)				3.20(-2)	2.23(-2)	1.16(-1)
7	3.64(-3)	3.90(-3)	1.0 (-2)				1.52(-2)	1.74(-2)	8.33(-2)
8	1.80(-3)	1.93(-3)					6.89(-3)	1.18(-2)	5.20(-2)
9	8.54(-4)	9.24(-4)				9.61(-4)	3.02(-3)	7.25(-3)	2.95(-2)
10	3.96(-4)	4.30(-4)				4.16(-4)	1.29(-3)	4.17(-3)	1.57(-2)
11	1.80(-4)	1.96(-4)		2.07(-4)		2.02(-4)	5.42(-4)	2.29(-3)	7.94(-3)
12	8.10(-5)	8.83(-5)		9.17(-5)			2.25(-4)	1.21(-3)	3.88(-3)
13	3.63(-5)	3.94(-5)		3.63(-5)	4.04(-5)	3.62(-5)	9.23(-5)	6.24(-4)	1.85(-3)
14	1.63(-5)	1.75(-5)		1.80(-5)	1.87(-5)	1.66(-5)	3.78(-5)	3.16(-4)	8.68(-4)
15	7.37(-6)	7.74(-6)		8.40(-6)		7.14(-6)	1.55(-5)	1.59(-4)	4.02(-4)
16	3.37(-6)	3.43(-6)		3.75(-6)	3.86(-6)	3.13(-6)	6.39(-6)	7.92(-5)	1.85(-4)
17	1.56(-6)	1.52(-6)		1.66(-6)		1.31(-6)	2.66(-6)	3.97(-5)	8.54(-5)
18	7.37(-7)	6.77(-7)		8.54(-7)	8.5 (-7)		1.12(-6)	2.01(-5)	3.94(-5)
19	3.53(-7)	3.02(-7)					4.80(-7)	1.03(-5)	1.84(-5)
20	1.72(-7)	1.350(-7)		1.93(-7)	1.87(-7)		2.10(-7)	5.42(-6)	8.64(-6)
21	8.60(-8)	6.07(-8)		1.06(-7)	9.9 (-8)		9.44(-8)	2.92(-6)	4.13(-6)
22	4.42(-8)	2.72(-8)					4.35(-8)	1.61(-6)	2.01(-6)
23	2.31(-8)	1.21(-8)		4.0 (-8)			2.03(-8)	8.89(-7)	9.81(-7)

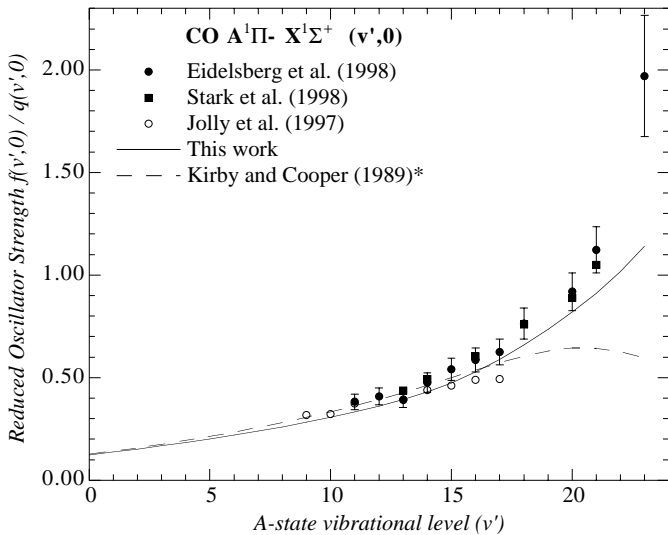


Fig. 2. Reduced oscillator strengths $f(v', 0)/q(v', 0)$ for $A^1\Pi-X^1\Sigma^+$ bands. * See text.

5. Numerical accuracy

The overlap integral of the $v'-v''$ radial wave functions varies approximately from 0.3 to 10^{-4} for $v''=0$, which implies a variation of the Franck Condon factor and of the oscillator strength over 7 and 6 orders of magnitude respectively. Cancellation effects may have a strong influence upon the small values cor-

responding to high v' levels. Thus it is necessary to check the reliability of these numbers.

We have first tested the accuracy of the radial wave functions and of the Franck Condon factors. For this, two different numerical methods were compared: the Gordon algorithm (Gordon 1969) and the renormalized Numerov method (Johnson 1977). We have found a very good agreement to the 10^{th} digit. For integration steps smaller than $2 \cdot 10^{-6} \text{ \AA}$, all the calculated Franck-Condon factors reach convergence within 10^{-6} in relative values and summing $q(v', v'' = 0)$ over v' up to $v'=23$ gives 0.999999956 with nine stable figures. According to the Franck-Condon factor sum rule (Nicholls, 1991), the complement to 1 of this sum represents the contribution of possible higher vibrational levels and of the continuum. However, for all the calculations performed in the present paper, we have chosen an integration step of 10^{-5} \AA which is sufficient to get eight stable figures for the largest FC factor $q(0-0)$ while the smallest FC factor $q(23-0)$, 7 orders of magnitude smaller, is given with five stable figures.

It appears to us that uncertainties in the determination of the ab initio electronic dipole transition moment $D(R)$ are the main cause of errors on the f -values. First, the absolute value of $D(R)$ is certainly correct to three significant digits and probably to four. To test the influence of the number of significant figures in $D(R)$, we have performed two different calculations of the reduced oscillator strengths: one with $D(R)$ from Table 1 (4

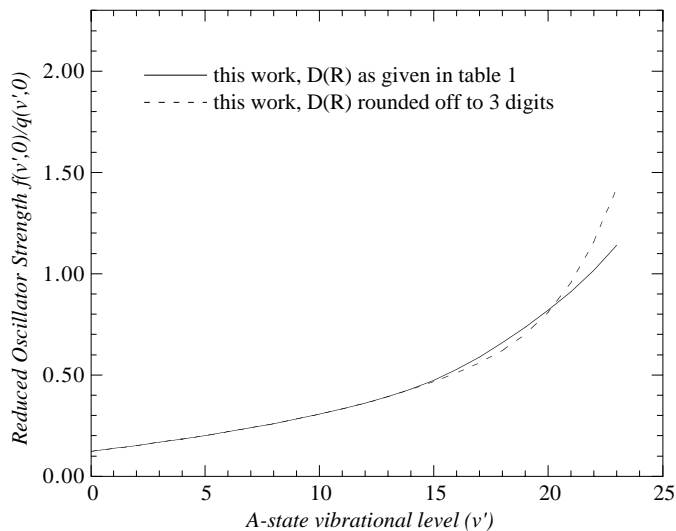


Fig. 3. $v''=0$: influence of the number of significant figures in $D(R)$.

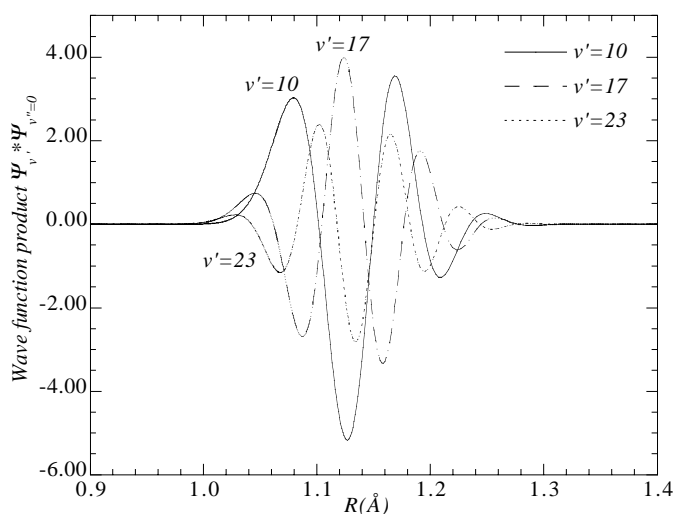


Fig. 4. Wave function product $\Psi_{v'} \Psi_{v''}$ as a function of the internuclear distance.

digits) and the other one with $D(R)$ rounded off to three digits. The results are compared in Fig. 3 for $v''=0$. The differences between the results give an estimate of the uncertainty due to the ab initio calculation of $D(R)$. One can see that it is very small up to $v'=20$ then increases for higher v' values up to 20% for $v'=23$, but that the global behaviour of the curves remains the same. For $v''=1$, the results of the two calculations are identical at the scale of the figure.

Two reasons may explain the difference between Kirby & Cooper's f -values and our results. First, the vibrational wave functions are oscillating functions and if we consider the overlap integral giving $D_{v'v''}$, the product of the vibrational wave functions oscillates for R distances where $\Psi_{v''}$ has significant values. We have plotted in Fig. 4 the product $\Psi_{v'} \Psi_{v''}$ for $v' = 10, 17, 23$ and $v'' = 0$ and in Fig. 5, the difference $diff(R)$ between our calculated dipole transition moment and the KC values.

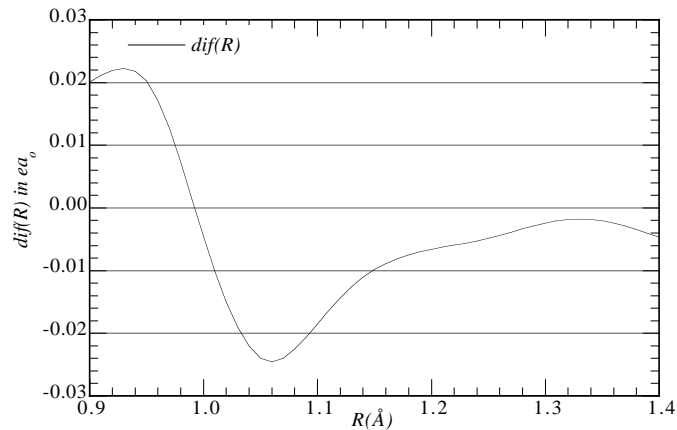


Fig. 5. Difference $diff(R)$ between our dipole transition moment and the KC results (Kirby & Cooper, 1989).

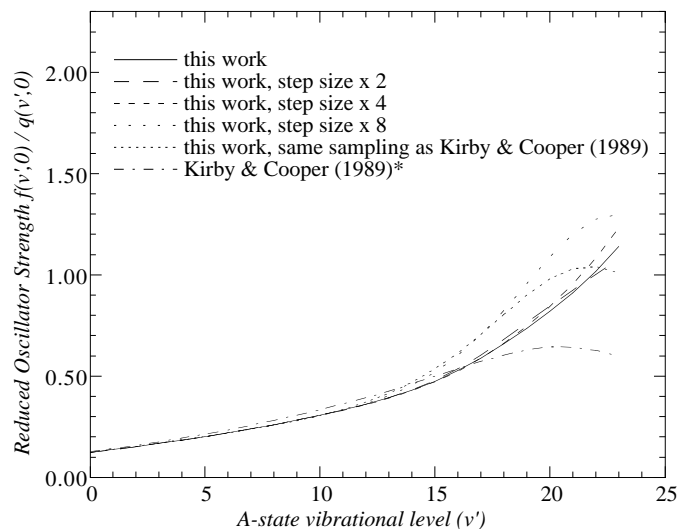


Fig. 6. Reduced oscillator strengths $f(v', 0)/q(v', 0)$: influence of the R sampling used in the calculation of the dipole transition moment. * Same remark as in Fig. 2.

It appears that the product of the vibrational wavefunctions oscillates like $\Psi_{v'}$ with R (since $\Psi_{v''}$ has no node for $v'' = 0$), and thus the critical R distances for the integral come from the region $1.0 \leq R \leq 1.32 \text{ \AA}$ where the difference $diff(R)$ is negative. For relatively low values of v' (up to $v' = 10$) the wave function product is positive which explains why our oscillator strengths are lower than those calculated by Kirby & Cooper (1989). The conclusion is opposite for large v' values since the wave function product is negative for the relevant R values. For $v' = 17$, the positive and negative parts of $\Psi_{v'} \Psi_{v''}$ compensate.

Secondly, it is very important that the dipole transition moment function $D(R)$ be determined precisely for a large number of R -values in the region where the overlap product $\Psi_{v'} \Psi_{v''}$ has notable values. For $v''=0$ and 1, this region overlaps the region $0.95 \leq R \leq 1.32 \text{ \AA}$ where our dipole moment function differs from the KC result as mentioned in Sect. 3. This point is illustrated in Fig. 6 where we compare our calculated reduced oscillator strengths with those derived from the dipole transition

moment by Kirby & Cooper (1989) and with those derived from our transition moment but selecting the same set of internuclear distances R as Kirby & Cooper (1989).

On the same figure we have plotted the f -values obtained by multiplying by two, four and eight the step size ($0.0125a_0$) in the critical region. In all cases, cubic spline functions are used for interpolation. Large differences appear immediately, in particular the reduced f -values calculated with the same sampling as Kirby & Cooper decrease for large v' values. A small step size ($\approx 0.02 \text{ \AA}$) is therefore necessary.

Numerical results concerning Franck-Condon factors, RKR potentials and oscillator strengths are available upon request to the authors (WLTB) and will be deposited in the CDS and the laboratory databases.

6. Conclusion

We have calculated very accurate oscillator strengths for vibrational bands in the CO $A^1\Pi - X^1\Sigma^+$ system up to $v' = 23$. Our results are consistent with the more recent experimental values of Eidelsberg et al. (1998) and Stark et al. (1998). For the highest values of v' , the calculated band f -values for $v'' = 0$ cannot be reproduced using the electronic dipole transition moment function of Kirby & Cooper (1989). We have pointed out that this discrepancy is partly due to a too sparse sampling of the transition moment function, especially near the R value corresponding to the maximum of the ground state wavefunction.

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