PHYSICAL REVIEW A VOLUME 57, NUMBER 6 JUNE 1998

Optical and generalized oscillator strengths for the $B\,^1\Sigma^+$, $C\,^1\Sigma^+$, and $E\,^1\Pi$ vibronic bands in the CO molecule

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(Received 23 December 1997)

Theoretical results for the generalized oscillator strength and optical oscillator strength (OOS) have been obtained for the excitations from the ground vibronic state $X\,^1\Sigma^+$ ($\nu=0$) to the vibrational levels $v'=0,1$ of the $B\,^1\Sigma^+$, $C\,^1\Sigma^+$, and $E\,^1\Pi$ electronic states within the first Born approximation. The target electronic states were determined using the configuration-interaction method, with a Hartree-Fock basis for the occupied molecular orbitals, and improved virtual orbitals for the virtual space. We discuss recent optical and electron impact measurements and reexamine previous OOS results for these processes. [S1050-2947(98)02706-1]

PACS number(s): 34.80.Gs

I. INTRODUCTION

Valence spectra of CO have been intensively investigated both theoretically [1–10], and experimentally by optical [11–29] and electron impact [30–36] techniques. Although very much studied, we feel that basic questions are still not well understood concerning the electronic excitation of this molecule. As an example we mention the values of the optical oscillator strength for the vibronic ($v=0-v'=0$) and ($v=0-v'=1$) bands of the $B\,^1\Sigma^+$, $C\,^1\Sigma^+$, and $E\,^1\Pi$ electronic states. Also Zhong *et al.* [35] recently questioned the validity of the first Born approximation (FBA) results for these vibronic excitations even at 1500 eV electron impact energy. On the other hand, the optical oscillator strength (OOS) and generalized oscillator strength (GOS) results concerning the intense vibronic progression of the $A\,^1\Pi$ state are relatively well established [32,35].

One of the interesting questions about the OOS values for these vibronic bands is the poor agreement between the optical and electron impact results. The recent electron impact results of Zhong *et al.* [35], Ciocca *et al.* [34], Kanik *et al.* [33], Wu [36], Chan *et al.* [32], the photoabsorption experimental results of Stark *et al.* [15] and Eidelsberg *et al.* [13,14], together with the theoretical results of Chantranupong *et al.* [9,10] have brought some new elements to this discussion.

One of the problems related to this discussion is the disagreement between the measured values of the generalized oscillator strength, as a function of the transferred momentum, by Skerbele and Lassetre [30] at 300, 400, and 500 eV impact energies and those of Zhong *et al.* [35] at 1500 eV impact energy. The differences between the two sets of experimental results, particularly regarding the extrapolation to the OOS, seem to be mainly related to the method employed by Skerbele and Lassetre [30] to put their data on an absolute scale, as was shown in the work of Zhong *et al.* [35]. Nevertheless, the shape of the GOS as a function of the transferred momentum shows, in some cases, large differences. For example, the results for the GOS as a function of the squared transferred momentum (K^2), for the $B(v=0-v'=0)$ band of Zhong *et al.* [35] do not show the minimum near $K=0$, as observed by Skerbele and Lassetre [30]. This seems to be an indication that at the energies considered in Skerbele and Lassetre's [30] work, the impact energy region for which the validity of the first Born approximation had not been reached for this transition. Another problem concerns the disagreement between the recent GOS experimental results of Zhong *et al.* [35] and the calculations within the FBA of Chantranupong *et al.* [10]. These two questions gave rise, in the recent work of Zhong *et al.* [35], to the hypothesis of the inadequacy of the first Born approximation for these processes even at 1500 eV impact energy.

In the present work we have calculated the GOS for these vibronic bands using a methodology successfully applied before [37–40], and have come to a different conclusion. We have obtained a good general agreement between our calculations and the experimental results of Zhong *et al.* [35] except for very low scattering angles, where the agreement is only reasonable. As pointed out by Zhong *et al.* [35], the experimental results at very low scattering angle are subject to greater experimental errors.

The discussion related to the GOS is also important to understand the different predictions for the OOS of these vibronic bands. The differences between the experimental results of the OOS for the $B\,^1\Sigma^+$, $C\,^1\Sigma^+$, and $E\,^1\Pi$ vibronic bands [12–29,31–36] have been subjected to an intense discussion in the literature over the last few years. As we have already pointed out, the electron impact results are usually higher than the optical ones. A very interesting discussion about these experimental results is presented in the work of Chan *et al.* [32]. Three basic assertions are addressed in their work. First, the predictions of the OOS from lifetime measurements [17–29] depend critically on the branching ratios between the $B\,^1\Sigma^+$, $C\,^1\Sigma^+$, and $E\,^1\Pi$ vibronic bands to the

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$A\,^1\Pi$ vibronic bands, and depending on the branching ratio used, the same measurement can produce different values for the OOS. Second, the photoabsorption measurements suffer from line saturation effects resulting in incorrectly low measured OOS. Third, the electron impact measurements do not suffer from these two effects and are, consequently, more reliable. Chan *et al.* [32] and recently Zhong *et al.* [35] pointed out that line saturation effects should be stronger for intense and peaked bands. Following this argument the vibronic progressions of the $A\,^1\Pi$ electronic state should be more affected but the optical results of Letzelter *et al.* [12] agree very well with those obtained through electron impact techniques, including those of Chan *et al.* [32].

In the present work we discuss the questions related both to the OOS and GOS results based on our calculated values and the recent optical and experimental results for the $B\,^1\Sigma^+$, $C\,^1\Sigma^+$, and $E\,^1\Pi$ vibronic bands, and suggest an interpretation for these data.

II. CALCULATION DETAILS

The calculations considered the Born-Oppenheimer approximation for the target wave functions and the first Born approximation for the collision process. Briefly, within the Born-Oppenheimer approximation the target wave functions are written as

$$\Psi_{n\nu}(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N;R)=\psi_n(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N;R)\chi_{n\nu}(R), \tag{1}$$

where $\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N$ are the coordinates of the N electrons of the molecule, R the internuclear distance, ψ_n the electronic wave function, and $\chi_{n\nu}(R)$ the discrete ν vibrational function of the n electronic state. The spin functions are factored out in Eq. (1) since we do not consider spin-orbit interactions.

The generalized oscillator strength $f(K,E)_{00\rightarrow n\nu'}$ for the excitation from the $\nu=0$ vibrational level of the ground $n=0$ electronic state to the ν' vibrational level of the n electronic excited state is written, in atomic units, as [41]

$$f(K,E)_{00\rightarrow n\nu'}=\frac{2E}{K^2}\frac{g_n}{4\pi}\int\left|\int\chi^*_{n\nu}(R)\chi_{00}(R)\varepsilon_{0n}(K,R,\Omega)dR\right|^2 d\Omega, \tag{2}$$

where $\mathbf{K}$ is the transferred momentum and is equal to $\mathbf{k}_{00}-\mathbf{k}_{n\nu}$, $\mathbf{k}_{00}$ and $\mathbf{k}_{n\nu}$ being the momenta of the incident and scattered electron, respectively, g_n is the degeneracy of the final state (1 for Σ, 2 for Π) and E is the transferred energy (i.e., the vibronic transition energy). The integration over Ω in Eq. (2) results from averaging over the orientation of the molecular axis with respect to $\mathbf{K}$, i.e., the classical average. ε_{0n} is the electronic scattering amplitude in the first Born approximation [41–43]:

$$\begin{aligned}\varepsilon_{0n}(K,R,\Theta,\Phi)&=\varepsilon_{0n}(K,R,\Omega)\\&=-\int\psi^*_n(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N;R)\left(\sum_{i=1}^{N}e^{i\mathbf{K}\cdot\mathbf{r}_i}\right)\\&\quad\times\psi_0(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N;R)dr_1dr_2\cdots dr_N,\end{aligned} \tag{3}$$

where Θ and Φ ($\equiv\Omega$) specify the relative orientation between $\mathbf{R}$ and $\mathbf{K}$.

In the limit when the transferred momentum K goes to zero (or the scattering angle goes to zero—forward scattering), the generalized oscillator strength goes to the optical oscillator strength $f(E)$,

$$\lim_{K\rightarrow0}f(K,E)=f(E)=\frac{2}{3}g_nE|M_{no}|^2, \tag{4}$$

where

$$\begin{aligned}M_{0n}(R)=-\int\int&\psi^*_n(\{\mathbf{r}_i\},\mathbf{R})\chi^*_{n\nu}(R)\chi_{00}(R)\\&\times\left(\sum_{i=1}^{N}x_i\right)\psi_0(\{\mathbf{r}_i\},\mathbf{R})\chi_{00}(R)d\{\mathbf{r}_i\}d\mathbf{R}\end{aligned} \tag{5}$$

is the usual dipole transition moment [41], including vibrational degrees of freedom ($\{\mathbf{r}_i\}=\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N$). This property of the GOS connects electron impact with optical experiments.

The electronic wave functions $\Psi_{n\nu}(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N,R)$ were determined with the configuration-interaction (CI) method, using Hartree-Fock molecular orbitals expanded in Gaussian-type basis functions. We built a $(12s,6p,1d)/[10s,4p,1d]$ basis set in the following way. First, we constructed a $(10s,5p)/[8s,3p]$ basis set by partially uncontracting s functions in the $(10s,5p)/[3s,3p]$ basis set of Dunning and Hay [44]. Next, we added two diffuse s-type functions, one diffuse p-type function, and a d polarization function producing the $(12s,6p,1d)/[10s,4p,1d]$ basis set used. This basis set was used previously to study inner-shell excitations of the CO_2 molecule [39].

The virtual space for the CI calculations was built using improved virtual orbitals (IVO) [45], in which the virtual orbitals were determined in the self-consistent field (SCF) of $N-1$ electrons where N is the number of electrons of the neutral target. The IVO thus provided orbitals corresponding more closely to the excited state molecular orbitals, resulting in improved convergence of the CI calculations [46], which is crucial to obtain GOS and OOS values close to experimental values, as was shown before for several molecules and atoms [37–40]. For the the vibronic excitation to the $B\,^1\Sigma^+$ and $C\,^1\Sigma^+$ electronic states, the frozen core approximation (FC) was used, that is, the occupied and virtual orbitals determined for the ground $X\,^1\Sigma^+$ state were also used in the excited state.

In the calculations concerning the excitation to the vibronic states of the $E\,^1\Pi$ electronic state, the frozen core approximation was not used. In this case, the occupied and virtual orbitals (IVO) were optimized independently for the ground and excited state of the target. This means that in this case relaxation effects are considered directly in the molecular basis set.

The $B\,^1\Sigma^+$ and $C\,^1\Sigma^+$ electronic states have the same symmetry of the ground state and, due to a problem of ground state collapse, it was not possible to converge accurately these states through independent Hartree-Fock (HF) calculations. Nevertheless, it was shown before [40] that, for valence excitations, the CI calculations with IVO recovers relatively well the relaxation effects not considered in the frozen core approximation.

The virtual space for the CO molecule, in the ground and excited states, was built with 18 IVO of $\sigma(6)$, $\Pi_x(6)$, and $\Pi_y(6)$ symmetries. The CI calculation considered single, double, triple, and quadruple excitations (SDTQ-CI) from all the occupied molecular orbitals to the IVO, allowing only two excitations from the innermost 1σ, 2σ, and 3σ molecular orbitals.

Convergence in what concerns the influence of the Gaussian basis, molecular orbitals, and CI expansions on the OOS and GOS was carefully tested.

For the $E\,^1\Pi$ final state, the electronic wave functions of the ground and excited state were not orthogonal, and the matrix elements related to the scattering amplitude ε_{0n} between nonorthogonal wave functions was done using a biorthogonalization procedure [40]. For this purpose, unitary transformations are applied on the two sets of N nonorthogonal molecular orbitals, turning $(N-1)$ of them orthogonal.

The vibrational wave functions were determined numerically from the potential curves of Cooper and Kirby [7], using the procedure developed by Le Roy *et al.* [47,48], also used to perform the R (internuclear distance) integration in Eq. (2).

The electronic transition amplitude $\varepsilon_{0n}(K,R,\Omega)$ was calculated in the internuclear distance interval $1.8 \leqslant R \leqslant 2.4$ bohrs (steps of 0.2 bohr including the equilibrium internuclear distance 2.132 bohrs), larger than the Franck-Condon region [9].

III. RESULTS

A. Generalized oscillator strengths

Figure 1 shows the GOS for the excitation to the $v'=0$ and $v'=1$ vibrational levels of the $B\,^1\Sigma^+$ electronic state, together with recent experimental results of Zhong *et al.* [35] and the theoretical results of Chantranupong *et al.* [10]. The experimental results of Skerbele and Lassetre [30] for the GOS of the $B\,^1\Sigma^+$ excitation process at the impact energies of 300, 400, and 500 eV do not converge to the Born limit, and consequently are not shown.

Figure 2 shows the GOS for the excitation to the $v'=0$ and $v'=1$ vibrational levels of the $C\,^1\Sigma^+$ electronic state, together with recent experimental results of Zhong *et al.* [35], the theoretical results of Chantranupong *et al.* [10], and the experimental results of Skerbele and Lassetre [30]. The experimental results of Skerbele and Lassetre were included because in this case the Born limit was reached.

Figure 3 shows the GOS for the excitation to the $v'=0$ and $v'=1$ vibrational levels of the $E\,^1\Pi$ electronic state, together with the recent experimental results of Zhong *et al.* [35] and the theoretical results of Chantranupong *et al.* [10]. As far as we are concerned, Skerbele and Lassetre did not obtain experimental results for these excitation processes.

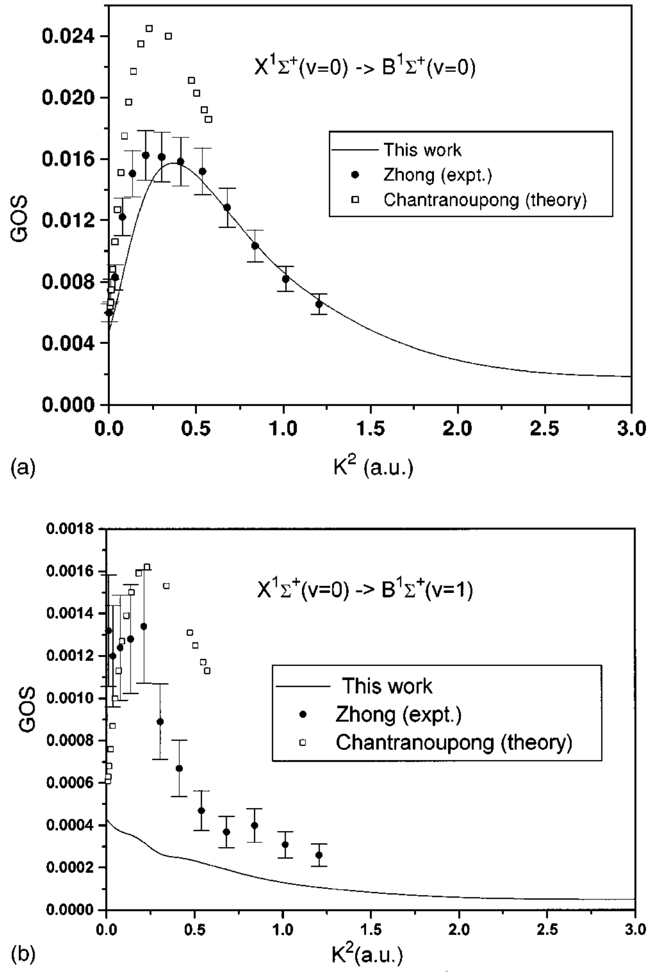

FIG. 1. Generalized oscillator strength for (a) $B(0-0)$ band, (b) $B(0-1)$ band. Both transitions are compared to Chantranupong *et al.*'s [10] theoretical and Zhong *et al.*'s [35] experimental results.

Due to the poor description of the target wave functions, the early theoretical results of Chung and Lin [4] are not shown in these figures.

These figures show that the present theoretical results disagree, for some vibronic excitations, with the theoretical results of Chantranupong *et al.* [10] and agree, in a general way, with the experimental results of Zhong *et al.* [35], except for very low values of the transferred momentum.

We shall first examine the difference between the two sets of theoretical results, and later discuss the agreement with the experimental results.

Figures 1–3 show that the theoretical results of Chantranupong *et al.* [9] and the present work disagree, in general, both in the the absolute values of the GOS and on the shapes of the curves as a function of K^2. The two sets of calculations, used a CI target wave function, with the molecular orbitals expanded in Gaussian basis sets. They differed in the choice of the Gaussian basis set used in the Hartree-Fock calculations, the molecular basis set used in the CI calculations, and in the CI configurational space.

It is of interest to discuss the influence of these factors on the GOS calculations. Small values of the transferred momentum represent classically the scattered electron with a

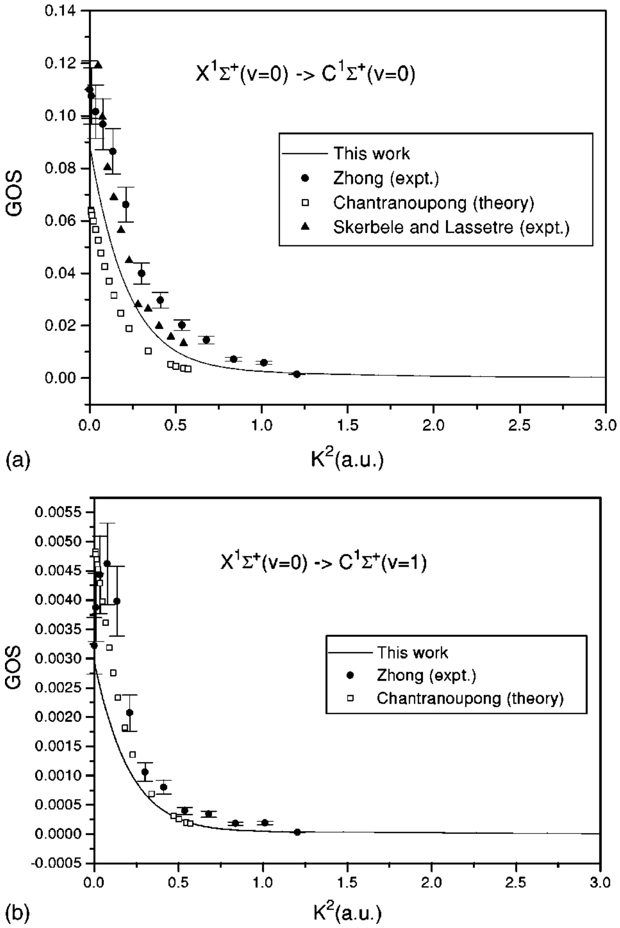

FIG. 2. Generalized oscillator strength for (a) $C(0-0)$ band, (b) $C(0-1)$ band. Both transitions are compared to Chantranupong *et al.*'s [10] theoretical, and Zhong *et al.*'s [35] and Skerbele and Lassetre's [30] experimental results.

large value of the impact parameter, and larger values of the transferred momentum represent classically smaller values of the impact parameter, that is, the incident electron penetrates deeper inside the molecular electron cloud. Therefore different values of the transferred momentum in the GOS calculations sample for different regions of the target wave functions making the GOS a very interesting property to the analysis of the differences between theoretical calculations with respect to the target wave functions. Let us examine this question in further detail.

The main difference between the Gaussian basis sets used in the two works consists in that we have considered s- and p-diffuse functions for each of the two atoms and Chantranupong *et al.* [10] considered s- and p-diffuse functions only on the center of the molecule. In our previous GOS and OOS calculations concerning valence and inner-shell excitations [37,39,40] we have used the diffuse functions centered in each atom of the molecule, obtaining a good agreement with the experimental results.

Concerning the molecular basis set, we have used improved virtual orbitals [45] to represent the excited and virtual orbitals used in all CI calculations. In the case of the $E\ {}^1\Pi$, the orbitals were independently optimized for the ground and excited state symmetries, within a nonorthogonal procedure. Chantranupong *et al.* [10] use the virtual orbitals obtained in the diagonalization of the Hartree-Fock matrix of the ground state. Physically, the molecular orbitals of the present work penetrate more deeply in the molecule than those of Chantranupong *et al.* [10], as expected by using IVO. Table I shows the virtual orbital eigenvalues of the Fock operator obtained in the present work, at the equilibrium distance, as compared to those of Chantranupong *et al.* [10].

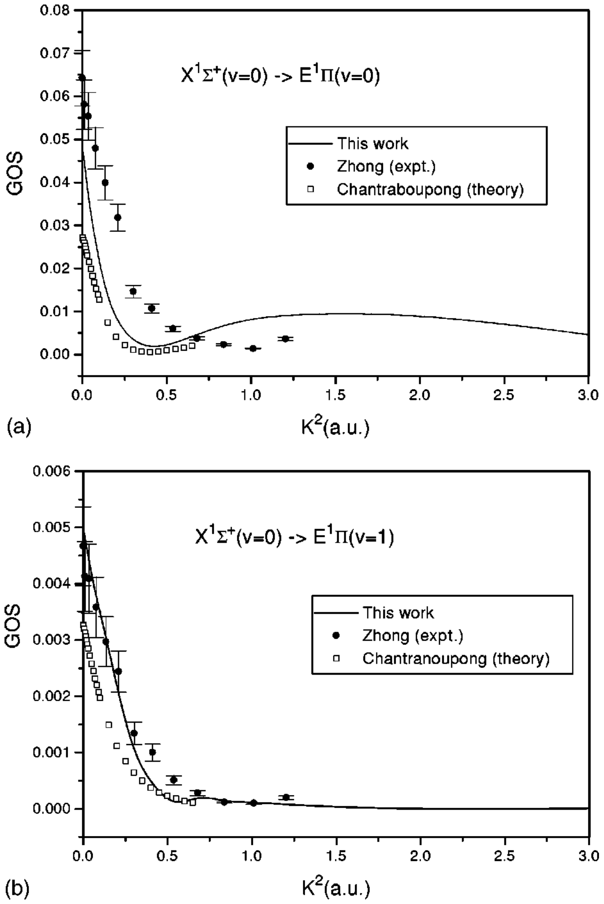

FIG. 3. Generalized oscillator strength for (a) $E(0-0)$ band, (b) $E(0-1)$ band. Both transitions are compared to Chantranupong *et al.*'s [10] theoretical and Zhong *et al.*'s [35] experimental results.

TABLE I. The virtual orbital eigenvalues (in hartrees) of the Fock operator at the internuclear equilibrium distance $R=2.132$ bohrs.

Orbital	Present	Chantranupong *et al.* [9]
6σ	-0.112773	0.010848
7σ	-0.088166	0.012559
8σ	-0.038238	0.079526
9σ	-0.022163	0.091961
10σ	0.047091	0.348297
11σ	0.100087	0.497984
2π	-0.206845	0.011975
3π	-0.086516	0.071491
4π	0.022389	0.148860
5π	0.194710	0.485883
6π	0.671668	0.821546
7π	1.365272	1.138791

TABLE II. Absolute optical oscillator strength for the vibronic bands from the ground state to the $B\ ^1\Sigma^+$, $C\ ^1\Sigma^+$, and $E\ ^1\Pi$ excited states of the CO molecule.

	$B(0-0)$	$B(0-1)$	$C(0-0)$	$C(0-1)$	$E(0-0)$	$E(0-1)$
Theory						
Chantranupong *et al.* [9]	0.00508	0.00052	0.0647	0.0049	0.0274	0.00329
Kirby and Cooper [8]	0.0021	0.0003	0.1181	0.0018	0.049	0.0050
Present results	0.0048	0.00043	0.089	0.0029	0.049	0.0050
Electron impact						
Lassetre and Skerbele [31]	0.015	0.002	0.163	0.007	0.094	0.007
Chan *et al.* [32]	0.00803	0.00132	0.1177	0.00356	0.0706	0.00353
Kanik *et al.* [33]	0.0115		0.154			
Zhong *et al.* [35]	0.00598		0.114	0.00322	0.0642	0.00467
Wu [36]	0.00814		0.129	0.0035	0.065	0.00418
Ciocca *et al.* [34]					0.0708	
Optical						
Aarts and de Heer [11]	0.015		0.16			
Letzelter *et al.* [12]	0.0045	0.0007	0.0619	0.0028	0.0365	0.0025
Eidelsberg *et al.* [14]					0.0365	
Stark (photon) [15]					0.049	

All eigenvalues obtained in the work of Chantranupong *et al.* [10] are positive and do not represent bound states [45]. The importance of a realistic representation of the excited state molecular orbitals in the CI calculations of the GOS as a function of K^2 has been shown previously [37,39,40].

Concerning the CI calculations, we have used a SDTQ-CI allowing only two excitations from the innermost 1σ, 2σ, and 3σ molecular orbitals and Chantranupong *et al.* [10] used a multireference CI (MR-CI). We believe that both calculations consider the non-negligible contributions of the full CI configurational space and are similar in this aspect.

The disagreement between the theoretical results of Chantranupong *et al.* [10] and the experimental results of Zhong *et al.* [35] at 1500 eV impact energy gave rise, in the latter work, to the hypothesis that the Born limit was not reached even at 1500 eV. The comparison between the present results and the experimental results of Zhong *et al.* shows a different picture.

Figures 1(a), 2(a), 2(b), and 3(b) for the $B(0-0)$, $C(0-0)$, $C(0-1)$, and $E(0-1)$ transitions, respectively, show a good overall agreement between the present results and the experimental ones, except for very small values of the transferred momentum, where the agreement is only reasonable. Small values of the transferred momentum are related to small values of the scattering angle in electron impact experiments. In this region, the intensity of the scattered beam varies strongly with the scattering angle, introducing larger error bars in the GOS experimental values, as correctly considered in the work of Zhong *et al.* [35]. A possible explanation for this trend could be related to larger problems in the angular resolution and normalization procedures in this strongly angular dependent region. This question will be further discussed in Sec. III B where the theoretical OOS results are compared with other calculations and experiments.

Figure 1(b) shows that for the $B(0-1)$ the theoretical and experimental results disagree completely. The intensity of this vibronic state is very low, much lower than the other vibronic excitations considered in the present work and, consequently, subject to larger experimental errors.

Figure 3(a) shows that the theoretical results predict a minimum for the GOS of the $E(0-0)$ vibronic excitation around $K^2=0.4$ a.u. while the experimental results present a minimum around $K^2=1.0$ a.u. As the experimental determination of the minimum of the GOS as a function of K^2 is usually subject to small experimental errors, another possible explanation for this discrepancy may be in order. We have previously shown [38] that at the minimum of the GOS higher-order terms in the Born expansion become important and, consequently, at the minimum region for the GOS the FBA is not adequate to describe the collision process between the electron and the molecule. The use of the FBA in these cases may shift the minimum region and, as was shown before [38,40], underestimates the GOS values.

B. Optical oscillator strengths

As already pointed out in the Introduction, much work has been done on the optical oscillator strengths for the vibronic excitations to the $B\ ^1\Sigma^+$, $C\ ^1\Sigma^+$, and $E\ ^1\Pi$ electronic states. Table II shows our values for the optical oscillator strengths for these vibronic excitations, along with other theoretical results, photoabsorption, and electron impact experimental measurements. Among the theoretical results [1–10] we have selected those where a greater care was taken in the determination of the target wave function. Following the arguments of Chan *et al.* [32], related to the branching ratios between these processes and the $A\ ^1\Pi$ series, we do not show the results obtained by lifetime techniques [17–29]. We also do not present the early photoabsorption results of Lee and Guest [16], as also according to Chan *et al.* [32], they are subject to serious line saturation effects.

Table II shows a very good agreement between the present theoretical results and the photoabsorption ones for the $B(0-0)$, $C(0-1)$, and $E(0-0)$ vibronic bands, a reasonable agreement for the the $C(0-0)$ vibronic band, and a disagreement with the very low intensity $E(0-1)$ and $B(0-1)$ vibronic bands.

The results by electron impact techniques are higher than the theoretical and photoabsorption results. For instance, concerning the $B(0-0)$, the results of Zhong *et al.* [35] by energy loss technique are 33% higher than those of Letzelter *et al*. [12], those of Chan *et al.* [32] and Wu [36], both on dipole (e-e') techniques are about 80% higher, the results of Kanik *et al*. by electron impact combined with ultraviolet spectroscopy [33] 155% and those of Lassetre and Skerbele [31] 230%. Zhong *et al.* showed that the experimental results of Lassetre and Skerbele suffered from a negligence of the finite acceptance angle at zero scattering angle and, once corrected for that, they come closer to the present results. It is important to mention the difference between energy loss experiments and the dipole (e-e') technique concerning the determination of the optical oscillator strength. While energy loss techniques look for a large region of K^2 values and extrapolate the results to $K^2=0$, the dipole (e-e) experiments look for a selected scattering angle.

Chan *et al.* [32] have pointed out that the electron impact results are not subjected to line saturation effects and are consequently more precise. Nevertheless they show a good agreement with the optical result of Eidelsberg and Rostas [13] for the vibronic bands of the $A\,^1\Pi$ state. On the other hand, the optical result of Letzelter *et al.* [12] for the $E\ ^1\Pi$ band agrees with those of Eidelsberg *et al* [14].

In Sec. III A we compared the experimental results for the GOS of Zhong *et al.* [35] with the theoretical ones, concluding that the agreement was better for larger values of the transferred momentum. Another point that must be taken into account is that the experimental results for the OOS by different electron impact techniques in general do not agree among themselves.

IV. CONCLUSIONS

In the present work optical and generalized oscillator strengths have been calculated for vibronic excitations to the $B\,^1\Sigma^+$, $C\,^1\Sigma^+$, and $E\,^1\Pi$ electronic states of the CO molecule and compared with the available theoretical, electron impact, and photoabsorption experimental values.

We would like to emphasize the following aspects related to these vibronic excitations.

(1) There is a general agreement between the present theoretical and the photoabsorption measurements for the OOS results.

(2) There is a general agreement between the present theoretical results and the experimental results for the GOS at larger values of the transferred momentum.

(3) The photoabsorption and theoretical results for the OOS disagree, in general, with the electron impact values.

(4) There are large disagreements between the OOS values determined within different electron impact experimental techniques.

These facts suggest the need of more discussion about the correspondence between the electron impact measurements and the OOS values for these excitation processes. Thus additional electron impact experimental measurements with particular attention to the small scattering angle region and to the normalization procedure would be highly welcome.

ACKNOWLEDGMENTS

We thank Professor G. G. B. de Souza and Professor Edilson C. da Silva for helpful comments, and Professor R. J. Le Roy for providing us with the computer program to calculate the vibrational wave functions and perform the R integration. Fundação Universitária José Bonifácio and the Brazilian agencies CNPq and CAPES are acknowledged for partial financial support.

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