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Excitation of the $C^1\Sigma^+ + c^3\Pi$ and $E^1\Pi$ electronic states of carbon monoxide by electron impact

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We report differential cross-section measurements for electron-impact excitation of the $C^1\Sigma^+ + c^3\Pi$ and $E^1\Pi$ electronic states in carbon monoxide. The energy range of this work is 30–200 eV. Where a comparison is possible, reasonable agreement is found with the earlier 20–50 eV results from Middleton *et al.* [J. Phys. B **26**, 1743 (1993)]. A generalized oscillator strength analysis of the present differential cross-section data enables us to determine estimates of the corresponding integral cross sections, which are compared to results from the BEf-scaling approach [Y.-K. Kim, J. Chem. Phys. **126**, 064305 (2007)] calculated as a part of this study. Very good agreement between them is in general found. Finally our 100-eV and 200-eV generalized oscillator strength data are also employed to determine values of the respective $C^1\Sigma^+$ and $E^1\Pi$ optical oscillator strengths, with excellent agreement being found between them and the previous dipole (e, e) results from Chan *et al.* [Chem. Phys. **170**, 123 (1993)].

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I. INTRODUCTION

In modeling the role that electron-driven processes play in technology and atmospheric phenomena (for instance), accurate integral cross sections (ICSs) for all relevant excitation, ionization, and dissociation processes are prerequisite if an understanding at the nanoscale is to be achieved. Such comprehensive sets of accurate integral cross sections, for even the simplest species, in general do not exist to an acceptable level of confidence. Recently, however, Kim and colleagues [1–4] have suggested that for an important subset of these processes—namely, for dipole-allowed electronic-state processes—a relatively simple technique known as the BEf-scaling approach [1] might provide accurate and reliable ICSs.

As a consequence in this short paper we further test the validity of the BEf-scaling procedure by comparing its integral cross sections, for the excitation of the $C^1\Sigma^+$ and $E^1\Pi$ electronic states in carbon monoxide (CO), to corresponding experimental ICS values determined as a part of this study. These experimental values were derived from our original differential cross section (DCS) measurements (see Sec. II), at five fixed energies between 30–200 eV, using a generalized oscillator strength analysis [1] (again see Sec. II for more details). The current DCS measurements are compared wherever possible to previous data, with a good summary of that available data being found in the review of Brunger and Buckman [5].

Optical oscillator strengths (OOSs) represent a fundamental test for the validity of the target description of a scattering system of interest [6]. Previous experimental determinations [7–9] of the OOSs for the respective $C^1\Sigma^+$ and $E^1\Pi$ electronic states have indicated some discrepancies between them. Therefore, we also use our 100-eV and 200-eV DCS data and the analysis procedure of Vriens [10] to derive OOSs for the C and E states. Note also that the present DCSs in principle represent a very sensitive test of any *ab initio* scattering theories applied to these systems, although as yet we know of no theories against which our present DCSs can be compared.

In the next section of this paper we present the details of our measurements and analysis procedures, while in Sec. III a brief description of the BEf-scaling approach is provided. Thereafter our results are outlined and discussed, before some conclusions from this work are drawn in Sec. V.

II. EXPERIMENTAL DETAILS AND ANALYSIS TECHNIQUES

The present differential cross sections were measured using a crossed-beam apparatus [11], in which incident electrons are crossed with CO gas effusing from a single-capillary source. In this case the incident electron beam energy (E_0) was in the range 30–200 eV, the overall spectrometer energy resolution was about 35 meV [full width at half maximum (FWHM)], its angular resolution was $\pm 1.5^\circ$, and typical beam currents into the interaction region were ~ 4 nA. Electron energy loss spectroscopy (EELS) spectra, at specific electron scattering angles (θ) in the range 4° – 30° , were then put on an absolute scale using helium as a standard [12]. Full details of our EELS procedures can be found in Kitajima *et al.* [11] and so are not repeated here. A typical energy loss spectrum from the present study is given in Fig. 1, on which the vibrational sublevels of the $C^1\Sigma^+$, $c^3\Pi$, and $E^1\Pi$ states are clearly marked. Note, however, that the DCS or $\mathcal{D}\sigma$ we report here are for the $C^1\Sigma^+ + c^3\Pi$ and $E^1\Pi$ manifolds. In the present study spectral deconvolutions of the EELS spectra were not required to ensure there was not any contamination from other states to the channels of interest. Having said that, however, it is clear from Fig. 1 that the $c^3\Pi$ electronic state of CO is almost degenerate in energy with the $C^1\Sigma^+$ state. As there was no possibility, with the current energy resolution, of uniquely resolving these states, no attempt was made to do so. Therefore we must allow for some $c^3\Pi$ contribution to our $C^1\Sigma^+$ electronic-state DCSs and ICSs, a point which is examined in more detail in Sec. IV. Further note that the overall error on our DCS or $\mathcal{D}\sigma$ was typically $\sim 18\%$, which includes an estimate for the uncer-

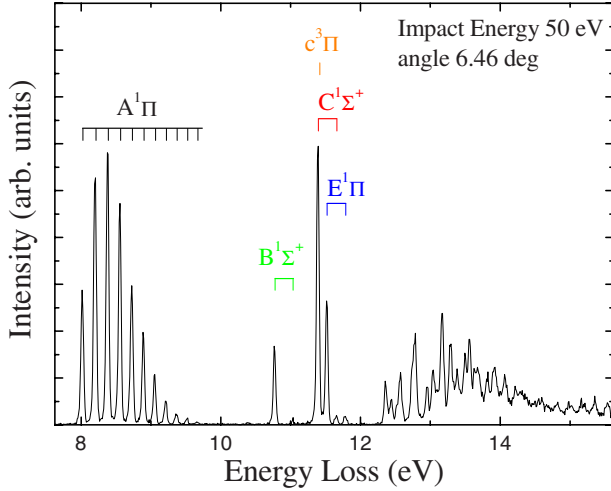


FIG. 1. (Color online) Typical energy-loss spectrum from the present study. The incident energy is 50 eV, and the electron-scattering angle is 6.46°. Relevant electronic states and their vibrational sublevels are indicated.

tainty in our analyzer transmission function and for the normalization we employed.

The so-determined values of $[\theta, D\sigma(\theta)]$, for each electronic state, are then transformed to (K^2, G_{expt}) using the standard formula [1]:

$$G_{\text{expt}}(K^2) = \frac{(E/R)k_i a_0}{4a_0^2 k_f a_0} K^2 D\sigma(E_0, \theta), \quad (1)$$

where k_i and k_f are the initial and final momenta of the incident electron, a_0 is the Bohr radius (0.529 Å), R is the Rydberg energy (13.6 eV), E is the excitation energy for each electronic state, $G_{\text{expt}}(K^2)$ is the experimental generalized oscillator strength, and K^2 is the momentum transfer squared defined by

$$K^2 = (k_i a_0)^2 + (k_f a_0)^2 - 2(k_i a_0)(k_f a_0) \cos \theta. \quad (2)$$

Vriens [10] proposed the following formula to represent the generalized oscillator strength for a dipole-allowed excitation, based on the analytic properties as identified by Lassette [13] and Rau and Fano [14]:

$$G(x) = \frac{1}{(1+x)^6} \left[\sum_{m=0}^{\infty} \frac{f_m x^m}{(1+x)^m} \right], \quad (3)$$

where

$$x = K^2/\alpha^2 \quad (4)$$

and

$$\alpha = \sqrt{B/R} + \sqrt{(B-E)/R}, \quad (5)$$

with B being the binding energy of the target electron being excited. In Eq. (3) the f_m are fitting constants to be determined in a least-squares fit analysis of the experimental generalized oscillator strengths. The beauty of Vriens' [10] formalism is that at the $x=0$ optical limit, the value of $G(0)$

$=f_0$ is the OOS. Note that full details of this analysis procedure can be found in Thorn *et al.* [2].

Finally, estimates of the ICS (σ) at each energy can be obtained from Eqs. (3)–(5) using the standard formulas [6]:

$$\sigma(E_0) = \frac{4\pi a_0^2}{E_0/R} \int_{K_{\text{min}}^2}^{K_{\text{max}}^2} \frac{G(K^2)}{E/R} d \ln(K^2), \quad (6)$$

with

$$K_{\text{min}}^2 = 2 \frac{E_0}{R} [1 - E/2E_0 - \sqrt{1 - E/E_0}], \quad (7)$$

$$K_{\text{max}}^2 = 2 \frac{E_0}{R} [1 - E/2E_0 + \sqrt{1 - E/E_0}]. \quad (8)$$

III. THEORY

A full description of the BE*f*-scaling approach for calculating integral cross sections can be found in Kim [1], so only a precis of the more important details are given here. Note that the scaled (plane-wave) Born cross sections used in this technique are not only subject to the approximations in the collision theory part, but also depend on the accuracy of the wave functions used for the initial and final states of the target molecule.

The *f*-scaled Born cross section (σ_f) is given by

$$\sigma_f(E_0) = \frac{f_{\text{accur}}}{f_{\text{Born}}} \sigma_{\text{Born}}(E_0), \quad (9)$$

where f_{accur} is an accurate dipole *f* value from accurate wave functions or experiments and f_{Born} is the dipole *f* value from the same wave functions used to calculate the unscaled Born cross section σ_{Born} . The *f*-scaling process has the effect of replacing the wave function used for σ_{Born} with accurate wave functions.

The BE-scaled Born cross section (σ_{BE}) is given by

$$\sigma_{\text{BE}}(E_0) = \frac{E_0}{E_0 + B + E} \sigma_{\text{Born}}(E_0). \quad (10)$$

The BE scaling corrects the deficiency of the Born approximation at low E_0 , without losing its well-known validity at high E_0 .

If an unscaled σ_{Born} is obtained from poor wave functions while an accurate *f* value is known, then both *f* scaling and BE scaling can be applied to obtain a BE*f*-scaled Born cross section ($\sigma_{\text{BE}f}$),

$$\sigma_{\text{BE}f}(E_0) = \frac{f_{\text{accur}} E_0}{f_{\text{Born}}(E_0 + B + E)} \sigma_{\text{Born}}(E_0). \quad (11)$$

We note that it is the $\sigma_{\text{BE}f}(E_0)$ integral cross sections that we later compare against corresponding experimental values derived from our DCS measurements and the earlier measurements of Zobel *et al.* [15], Lassette and Skerbele [8], Zhong *et al.* [9], Trajmar *et al.* [16], and a compilation proposed as part of a Landolt-Börnstein database [17].

Finally, we note that in the present calculations we chose the theoretical work of Chantranupong *et al.* [18] to generate

TABLE I. Differential cross sections for electron-impact excitation of the $C^1\Sigma^+ + c^3\Pi$ electronic states in CO. Results from the present measurements are shown. Errors on the present data are typically $\sim 18\%$.

θ (deg)	DCS (10^{-18} cm ² /sr)				
	30 eV	40 eV	50 eV	100 eV	200 eV
3.46			91.57		
4.34				160.09	
4.38					103.99
5		53.15			
5.34				110.95	
5.38					52.78
6	21.69	46.03			
6.34				75.37	
6.46			48.29		
7.34				51.54	
7.38					15.49
8	20.85				
8.46			32.51		
9.34				21.16	
9.38					4.49
10	15.21	27.31			
11.34				8.85	
11.38					1.59
13.46			8.872		
16.34				1.22	
18.46			2.660		
20	4.25				
29.4			1.049		
30	0.834	0.607			
39.4			0.706		

TABLE II. Differential cross sections for electron-impact excitation of the $E^1\Pi$ electronic state in CO. Results from the present measurements are shown. Errors on the present data are typically $\sim 18\%$.

θ (deg)	DCS (10^{-18} cm ² /sr)				
	30 eV	40 eV	50 eV	100 eV	200 eV
3.46			37.28		
4.34				74.17	
4.38					49.40
5		21.40			
5.34				51.48	
5.38					23.44
6	7.41	19.00			
6.34				34.62	
6.46			21.38		
7.34				23.49	
7.38					6.34
8	7.52				
8.46			14.20		
9.34				9.13	
9.38					1.49
10	5.64	10.80			
11.34				3.45	
11.38					0.495
13.46			3.85		
16.34				0.635	
18.46			1.42		
20	1.84				
29.4			0.646		
30	0.518	0.398			
39.4			0.304		

the unscaled Born cross sections. While their OOS values do not agree with experiment [7], the f -scaled Born cross sections [$\sigma_{BEf}(E_0)$] in principle correct for this.

IV. RESULTS AND DISCUSSION

In Tables I and II and Figs. 2(a) and 2(b) we, respectively, present the current manifold differential cross sections for electron-impact excitation of the $C^1\Sigma^+ + c^3\Pi$ and $E^1\Pi$ electronic states. Also shown in the figures, where appropriate, are the earlier DCS results from Middleton *et al.* [19]. Note that the error bars plotted ($\pm 18\%$) in Figs. 2(a) and 2(b) represent plus and minus one standard deviation. It is clear from these figures that the DCSs for both the $C^1\Sigma^+ + c^3\Pi$ and $E^1\Pi$ electronic states are all strongly peaked towards forward-scattering angles, with the degree of forward peaking seeming to increase as the incident electron beam energy increases. This observation might reflect the fact that CO possesses both a permanent dipole moment and an important dipole polarizability. It also suggests that contributions from the $c^3\Pi$ state, which can only be populated from the ground

state via exchange, to the measured $C^1\Sigma^+ + c^3\Pi$ DCSs are likely to be small. This is particularly the case at 100 eV and 200 eV, although at 30 eV there is some evidence in the angular distribution (middle-angle structure) to suggest that a $c^3\Pi$ contribution is present. With one or two exceptions, we additionally see from Figs. 2(a) and 2(b) that the present DCSs and those of Middleton *et al.* are in reasonable agreement over the common scattered electron angular range and at each of 30, 40, and 50 eV. This provides an important cross-check for both sets of data and suggests that a consistent set of DCSs for both the $C^1\Sigma^+ + c^3\Pi$ and $E^1\Pi$ states now exists in the literature, against which scattering calculations can be tested for their validity. We note that at this time we know of no such calculations being available in the literature, a deficiency which we suggest should be looked at.

Using Eqs. (1) and (2) we can convert the measured DCS(θ) into $G_{\text{expt}}(K^2)$, with representative examples of our fits to the respective 100-eV and 200-eV $C^1\Sigma^+ + c^3\Pi$ and $E^1\Pi$ electronic-state generalized oscillator strength data, using Eqs. (3)–(5), being, respectively, given in Figs. 3(a) and 3(b). Note that in each plot the fits to the measured data are very good, which in the case of the $C^1\Sigma^+ + c^3\Pi$ states sug-

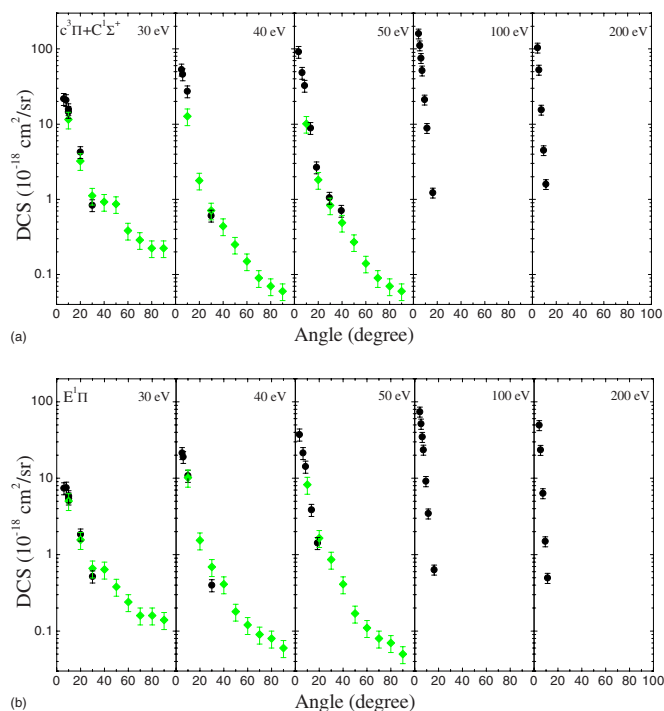


FIG. 2. (Color online) Differential cross sections ($10^{-18} \text{ cm}^2/\text{sr}$) for electron-impact excitation of the (a) $C^1\Sigma^+ + c^3\Pi$ and (b) $E^1\Pi$ electronic states. The present data (\bullet) are compared against earlier results from Middleton *et al.* [19] (\blacklozenge). Note that the respective incident electron energies are marked on each panel.

gests that any $c^3\Pi$ contamination is small at those higher energies. In other words, at these higher energies we are effectively dealing with excitation of the $C^1\Sigma^+$ state alone.

In Table III we present the current OOSs for the $C^1\Sigma^+$ and $E^1\Pi$ electronic states, as determined using the procedure outlined in Sec. II. Also shown in this table are corresponding experimental results from Chan *et al.* [7], Zhong *et al.* [9], and Lassetre and Skerbele [8] and results from the calculation of Chantranupong *et al.* [18]. It is clear from Table V, below, that the current OOSs, for both the $C^1\Sigma^+$ and $E^1\Pi$ states, are in very good agreement with relevant values from Zhong *et al.* [9] and the dipole (e, e) measurement from Chan *et al.* [7]. The results from Lassetre and Skerbele [8] are clearly too high for each state, while the calculated OOSs from Chantranupong *et al.* are manifestly low in each case. We believe that when the present results for the respective $C^1\Sigma^+$ and $E^1\Pi$ states are combined with those from Chan *et al.* [7] and Zhong *et al.* [9], reliable and accurate values for these OOSs can now be considered to be available in the literature. As noted previously, these values of the OOS represent a very good test for the validity of the structure part of a calculation involving the $C^1\Sigma^+$ and $E^1\Pi$ electronic states of CO.

If we now follow the prescription outlined in Sec. II, via Eqs. (3)–(8), the corresponding integral cross sections can be derived from our DCSs for both the $C^1\Sigma^+ + c^3\Pi$ and $E^1\Pi$ states. The results from these processes are tabulated in Tables IV and V and plotted in Figs. 4(a) and 4(b). Again the error bars in these latter figures represent plus and minus one standard deviation. Also shown in Figs. 4(a) and 4(b) are the

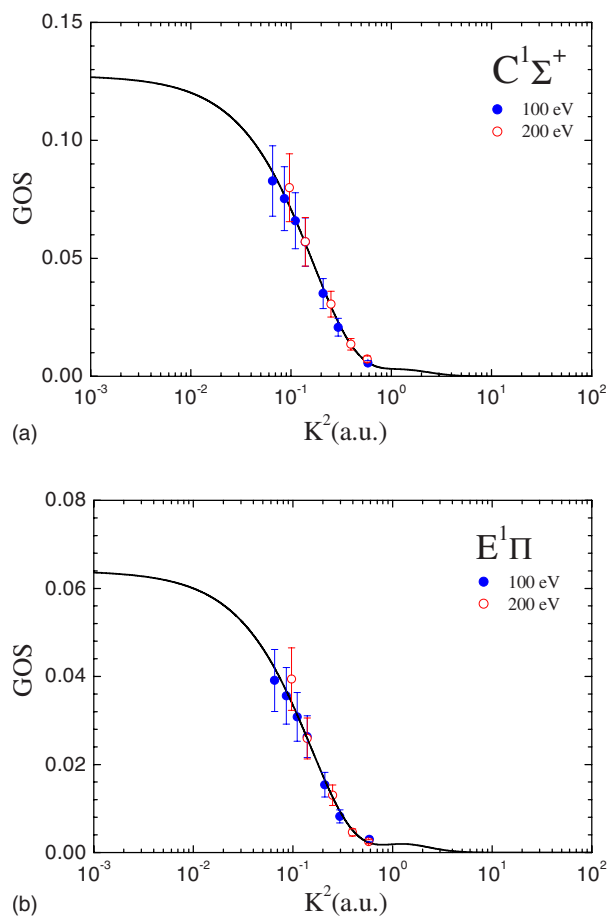


FIG. 3. (Color online) Fits (solid line) to our experimentally determined generalized oscillator strengths, using Eqs. (3)–(5), for the (a) $C^1\Sigma^+$ and (b) $E^1\Pi$ electronic states. The incident electron energies in each case were 100 eV (\bullet) and 200 eV (\circ), so that any $c^3\Pi$ contamination to $C^1\Sigma^+$ will be minimal.

previous ICS results from Zobel *et al.* [15], Trajmar *et al.* [16], Lassetre and Skerbele [8], and Zhong *et al.* [9] and data from a Landolt-Börnstein compilation [17]. Note that Trajmar *et al.* [16] never published their 20-eV CO DCSs; we took them from an ICPEAC abstract [21]. Trajmar [22] expressed some doubt as to the validity of that data [16], and this should be borne in mind in the comparisons that follow. In addition, Figs. 4(a) and 4(b) also contain the present

TABLE III. A comparison between the present optical oscillator strengths and a selection of those from previous workers. The error on the present OOSs is $\sim 20\%$.

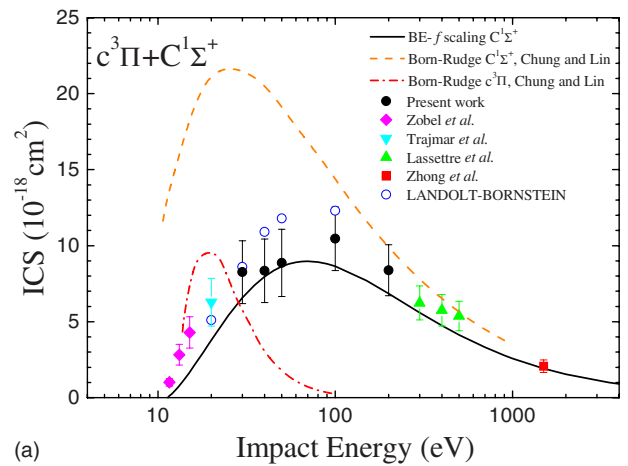
	$C^1\Sigma^+$	$E^1\Pi$
Experiment		
Present work	0.1275	0.0640
Chan <i>et al.</i>	0.1177	0.0706
Zhong <i>et al.</i>	0.114	0.0642
Lassetre and Skerbele	0.163	0.094
Theory		
Chantranupong <i>et al.</i>	0.0647	0.0274

TABLE IV. Integral cross sections for electron-impact excitation of the $C^1\Sigma^+ + c^3\Pi$ electronic states in CO. The present BEf-scaling calculation and data (present work) are compared against the previous experiments of Zobel *et al.* [15], Trajmar *et al.* [16], Lassette and Skerbele [8], and Zhong *et al.* [9]. Numbers in parentheses represent the absolute uncertainty on the data. Note that our BEf-scaling result is for the $C^1\Sigma^+$ state.

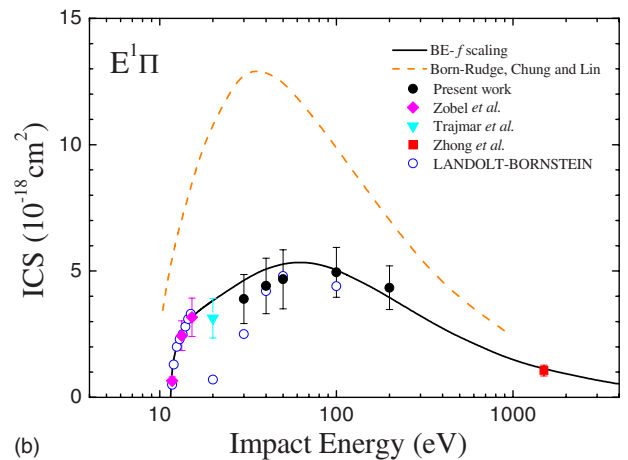
E_0 (eV)	BEf	Present work	Zobel <i>et al.</i>	ICS (10^{-18} cm 2)		
				Trajmar <i>et al.</i>	Lassette and Skerbele	Zhong <i>et al.</i>
11.3965	0					
11.5	0.072					
11.6	—		1.006 (0.241)			
12	0.265					
13	0.689					
13.2	—		2.825 (0.678)			
14	1.151					
15	1.624					
15.1	—		4.287 (1.029)			
16	2.092					
17	2.545					
18	2.980					
19	3.394					
20	3.785			6.279 (1.570)		
25	5.412					
30	6.574	8.255 (2.064)				
35	7.394					
40	7.967	8.345 (2.086)				
45	8.364					
50	8.632	8.868 (2.217)				
55	8.806					
60	8.911					
65	8.964					
70	8.978					
80	8.925					
90	8.803					
100	8.643	10.457 (2.301)				
150	7.699					
200	6.846	8.380 (1.844)				
300	5.587				6.229 (0.934)	
400	4.737				5.753 (0.863)	
500	4.127				5.376 (0.806)	
700	3.310					
900	2.783					
1000	2.583					
1500	1.921					2.075 (0.311)
2000	1.545					
3500	0.999					
5000	0.750					

TABLE V. Integral cross sections for electron-impact excitation of the $E^1\Pi$ electronic state in CO. The present BEf-scaling calculation and data (present work) are compared against the previous experiments of Zobel *et al.* [15], Trajmar *et al.* [16], and Zhong *et al.* [9]. Numbers in parentheses represent the absolute uncertainty on the data.

E_0 (eV)	BEf	ICS (10^{-18} cm 2)			
		Present work	Zobel <i>et al.</i>	Trajmar <i>et al.</i>	Zhong <i>et al.</i>
11.5219	0				
11.7	0.974				
11.77			0.655 (0.157)		
12	1.539				
13	2.423				
13.32			2.443 (0.586)		
14	2.856				
15	3.126				
15.22			3.169 (0.761)		
16	3.319				
17	3.472				
18	3.603				
19	3.719				
20	3.827			3.131 (0.783)	
25	4.283				
30	4.637	3.892 (0.973)			
35	4.900				
40	5.087	4.409 (1.102)			
45	5.213				
50	5.293	4.673 (1.168)			
55	5.337				
60	5.354				
65	5.351				
70	5.332				
80	5.261				
90	5.164				
100	5.052	4.948 (1.089)			
150	4.464				
200	3.966	4.336 (0.954)			
300	3.234				
400	2.757				
500	2.406				
700	1.969				
900	1.667				
1000	1.553				
1500	1.254			1.060 (0.159)	
2000	1.044				
3500	0.575				
5000	0.432				



(a)



(b)

FIG. 4. (Color online) Integral cross sections (10^{-18} cm 2) for electron-impact excitation of the (a) $C^1\Sigma^+ + c^3\Pi$ and (b) $E^1\Pi$ electronic states. The present data (\bullet) and BEf-scaling calculation (solid) are compared against the earlier results from Zobel *et al.* [15] (\blacklozenge), Trajmar *et al.* [16] (\blacktriangledown), Lassetre and Skerbele [8] (\blacktriangle), Zhong *et al.* [9] (\blacksquare), and a Landolt-Börnstein [17] (\circ) compilation. Also shown are some Born-Rudge results (dashed line) or (dot-dashed) from Chung and Lin [20]. Note that in (a) the BEf-scaling result is for the $C^1\Sigma^+$ electronic state.

BEf-scaling results for the $C^1\Sigma^+$ and $E^1\Pi$ states, as well as some earlier Born-Rudge computations [20] for the $C^1\Sigma^+$ and $c^3\Pi$ states [Fig. 4(a)] and the $E^1\Pi$ state [Fig. 4(b)].

Considering Fig. 4(a) in more detail we see that for $E_0 \geq 30$ eV the present $C^1\Sigma^+$ BEf-scaling calculation is in very good agreement with our data and most of the other available data [8,9,15], at least to within the stated uncertainties on those ICSs. At energies < 30 eV, however, the available ICSs [15–17] tend to be somewhat higher in magnitude than our BEf-scaling result. We believe this discrepancy is due to the contribution from the $c^3\Pi$ state that cannot be experimentally resolved, a hypothesis that is supported by the Born-Rudge level calculations for the $C^1\Sigma^+$ and $c^3\Pi$ states from Chung and Lin [20]. As a consequence, we assert that the present BEf-scaling result for the $C^1\Sigma^+$ state would provide a reasonable representation for its ICS in any modeling studies that incorporated this electronic state. Finally we note that while the Landolt-Börnstein compilation [17] displays

the correct energy dependence for the $C^1\Sigma^+ + c^3\Pi$ ICSs, it appears to be uniformly a little high in magnitude.

For the $E^1\Pi$ integral cross section [see Fig. 4(b)] we find that there is excellent agreement between the present BEf-scaling result and all the available experimental data [9,15,16] including the current ICSs. The only exception to this is the 20-eV ICS from the Landolt-Börnstein compilation, which is much lower in magnitude than the present BEf-scaling result and the result derived from Trajmar *et al.* [16]. As the datum point at 20 eV from Trajmar *et al.* was derived from DCS data that Trajmar was not fully confident in [22] and as the BEf-scaling approach will fail if resonance effects in the scattering process are present, we cannot be definitive as to who is right or wrong here. However, as the Landolt-Börnstein compilation [17] was largely drawn from the data of Liu and Victor [23], who derived their ICS estimates from the DCS of Middleton *et al.* [19], then if the BEf-scaling result at 20 eV is correct, it would suggest problems in the 20-eV data of Middleton *et al.* These problems might be due to the absolute 20-eV elastic CO DCS that Middleton *et al.* used to normalize their data, or it could be indicative of an analyzer response problem with their 20-eV $E^1\Pi$ DCS.

V. CONCLUSIONS

We have reported measurements for absolute DCSs for electron-impact excitation of the $C^1\Sigma^+ + c^3\Pi$ and $E^1\Pi$ electronic states in CO, with incident electron energies in the range 30–200 eV. Where a comparison was possible, reasonable agreement between the present DCSs and those of Middleton *et al.* was generally seen. Integral cross sections were subsequently derived from these DCSs and also calculated using the BEf-scaling approach [1]. Good agreement was typically found between the BEf-scaling results and most of the available measurements including our own. Finally, optical oscillator strengths for the respective $C^1\Sigma^+$ and $E^1\Pi$ electronic states were determined as a part of this study. The present OOSs were seen to be in very good agreement with those from Chan *et al.* [7] and Zhong *et al.* [9].

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