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Theoretical total cross sections for $e$-SO$_2$ scattering over a wide energy range (0.1–2000 eV) revealing a 3.4-eV shape resonance

Minaxi Vinodkumar,1,2 Chetan Limbachiya,2 Avani Barot,1 and Nigel Mason3

1V. P. & R. P. T. P Science College, Vallabh Vidyanagar–388 120, Gujarat, India
2P. S. Science College, Kadi–382 715, Gujarat, India
3Department of Physics and Astronomy, Open University, Milton Keynes, MK7 6AA, United Kingdom

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We have used the ab initio $R$-matrix formalism at low impact energies (below the ionization threshold of the target) and the spherical complex optical potential methodology above the ionization threshold to generate total cross sections for $e$-SO$_2$ scattering over the energy range from 0.1 to 2000 eV. The eigenphase diagram and total cross section indicate a structure at 3.4 eV which is ascribed to a shape resonance, evidence for which appears in earlier experimental studies.

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I. INTRODUCTION

Sulfur dioxide (SO$_2$) plays a key role in the formation of acid rain in the terrestrial atmosphere and, through the sulfate aerosols that it may form, produces cooling effects which can offset warming effects produced by CO$_2$ [1]. SO$_2$ has also been observed in the atmosphere of Venus and in the atmosphere of Jupiter and its satellite Io [2]. SO$_2$ has also been detected in the interstellar medium [3]. Owing to the structural similarities between SO$_2$ and ozone, SO$_2$ can also serve as a test molecule for understanding the dynamics of ozone production and decomposition in the earth’s atmosphere since experiments on O$_3$ are difficult [4] to perform due to the reactivity of ozone with atmosphere.

Electron interactions with SO$_2$ play an important role in magnetospheric plasma dynamics of the Jovian system, in the plasma-assisted treatment of biocompatible materials and biomedical surfaces, in models of diffuse discharge switches [5], and in understanding the underlying physics and chemistry of combustion processes. Low-energy collision processes are perhaps the most important phenomena since they underpin the physicochemical processes prevalent in the plasmas and many industrial discharges. At low energies (<10 eV) electrons may also cause short-lived anions (and thereby resonances) whose decay (to produce neutral and anionic fragments) may strongly influence the local chemistry.

Theoretical studies of low-energy electron scattering from SO$_2$ are nevertheless sparse and a critical review of such data reveals systematic discrepancies in the magnitude of the total cross section. Reviewing the literature on $e$-SO$_2$ scattering we can conveniently divide it into two regions of impact energies, one below and one above the ionization threshold (12.34 eV) of the target.

Concentrating first on a review of previous work conducted in the low-energy regime, several experimental measurements have been reported [6–10]. Gulley and Buckman [6] measured absolute differential cross sections for vibrationally elastic electron scattering using a crossed electron-molecular beam apparatus for incident energies of 1–30 eV. Zubek et al. [7], Szymtowski and Maciag [8], and Szymtowski et al. [9] have employed linear transmission experiments to measure total cross sections for impact energies 1.5–7 eV, 1.5–70 eV, and 6–370 eV, respectively, while Sokolov and Sokolova [10] measured total cross sections employing the electron cyclotron resonance technique in the energy range 1.5–10 eV. Sanche and Schulz [11] performed an electron transmission experiment to detect resonance structure in SO$_2$, identifying a broad shape resonance at 3.4 eV. This was subsequently confirmed by the measurements of Simon et al. [12] and Andric et al. [13], which showed the formation of a temporary SO$_2^-$ state which decays to leave the molecule excited in one of its vibrational modes.

There are only a few calculations of low-energy $e$-SO$_2$ scattering. Gupta and Baluja [14] have calculated total elastic cross sections using the $R$-matrix method for impact energies 0–15 eV. Gianturco et al. [15] performed ab initio calculations for the energy range 0–30 eV and Natalense et al. [16] employed the Schwinger multichannel method and computed rotationally summed inelastic, differential and integral, and momentum transfer cross sections for electron scattering for impact energies from 3 to 30 eV. Very recently Machado et al. [17] reported the results of a joint theoretical (1–1000 eV) and experimental (100–1000 eV) study to determine total cross sections for $e$-SO$_2$ scattering. It should be noted that these earlier theoretical works [14–17] were not able to predict the shape resonance reported in Refs. [12,13].

Reviewing the available high-energy work there are two experimental measurements reported in the literature. Zecca et al. [18] measured total cross sections for $e$-SO$_2$ using the Ramsauer technique over the energy range 90–4000 eV. Machado et al. [17] used the relative flow technique and measured total cross sections over the range of 100–1000 eV. High-energy theoretical formalisms of the total cross sections were reported by Shi et al. [19] using the Spherical Complex Optical Potential (SCOP) formalism over the energy range 30–4000 eV, and Raj and Tomar [20] used the additivity rule to derive cross sections for impact energies between 100 and 4000 eV.

Thus reviewing previous work on $e$-SO$_2$ scattering it is notable that there are more experimental data [6–11,13,17] than theoretical investigations [11,12,14,15,17]. The other notable fact is that although $e$-SO$_2$ has been studied over

*minaxivinod@yahoo.co.in
TABLE I. Target properties of SO$_2$.

<table>
<thead>
<tr>
<th>Properties of SO$_2$</th>
<th>Present</th>
<th>Theoretical results</th>
<th>Expt. results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ground-state energy (Hartree)</td>
<td>−547.20</td>
<td>−547.28 (Ref. [14]); −547.28 (Ref. [17])</td>
<td>−567.23 (Ref. [15])</td>
</tr>
<tr>
<td>First excitation energy (eV)</td>
<td>3.794</td>
<td>3.75 (Ref. [14])</td>
<td>3.40 (Ref. [29]); 3.5 (Ref. [30])</td>
</tr>
<tr>
<td>Rotational constant (cm$^{-1}$)</td>
<td>2.025</td>
<td>3.0 (Ref. [15])</td>
<td>2.025 (Ref. [22])</td>
</tr>
<tr>
<td>Dipole moment (D)</td>
<td>2.1</td>
<td>2.4 (Ref. [14])</td>
<td>1.63 (Refs. [6,12,29])</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.92 (Ref. [16])</td>
<td></td>
</tr>
</tbody>
</table>
used method [31]. The ab initio $R$-matrix method relies on the division of configuration space into two spatial regions, viz., an inner region and an outer region. This spatial distribution is a consequence of electronic charge distribution around the center of mass of the system. The inner region is chosen such that it accommodates the total wave function of the target molecule. Thus all the $N + 1$ electrons are contained in the inner region which makes the problem numerically complex, but very precise. The interaction potential consists of short-range exchange and electron-electron correlation polarization potentials. Moreover the inner region problem is solved independently of the energy of the scattering electron. In the outer region exchange and correlation are assumed to be negligible and the only long-range multipolar interactions between the scattering electron and the target are included. A single-center approximation is assumed here since this enables simple and fast solutions in the outer region. For the present system the inner $R$-matrix radius is taken as 10$a_0$ while the outer region calculations are extended up to 100$a_0$.

The inner region wave function is constructed using the close-coupling approximation [32]. In the inner region the total wave function for the system is written as

$$
\psi_k^{N+1} = A \sum_i \psi_i^N(x_1, \ldots, x_N) \sum_j \xi_j(x_{N+1}) a_{ijk} 
+ \sum_m \chi_m(x_1, \ldots, x_{N+1}) b_{mk},
$$

(1)

where $A$ is the antisymmetrization operator, $x_N$ is the spatial and spin coordinate of the $n$th electron, $\xi_j$ is a continuum orbital spin-coupled with the scattering electron, and $a_{ijk}$ and $b_{mk}$ are variational coefficients determined in the calculation. The accuracy of the calculation depends solely on the accurate construction of this wave function given in Eq. (1). The first summation runs over the target states used in the close-coupled expansion and a static exchange calculation has a single Hartree-Fock target state in the first sum. The summation in the second term runs over configurations $\chi_m$, where all electrons are placed in target molecular orbitals. This sum runs over the minimal number of configurations, usually three or fewer, which are required to relax orthogonality constraints between the target molecular orbitals and the functions used to represent the configuration. Our fully close-coupled calculation uses the lowest number of target states, represented by a configuration interaction (CI) expansion in the first term and over 100 configurations in the second. These configurations allow for both orthogonality relaxation and short-range polarization effects.

The complete molecular orbital representation in terms of occupied and virtual target molecular orbitals are constructed using the Hartree-Fock self-consistent field method with Gaussian-type orbitals (GTOs) and the continuum orbitals of Faure et al. [33] and include up to $g (l = 4)$ orbitals. The benefit of employing partial wave expansion for low-energy electron molecule interaction is its rapid convergence. In the case of dipole-forbidden excitations ($\Delta J \neq 1$) the convergence of the partial waves is rapid, but in the case of dipole-allowed excitations ($\Delta J = 1$) the partial wave expansion converges slowly due to the long-range nature of the dipole interaction.

In order to account for the higher partial waves not included in the fixed-nuclei $T$ matrices, the Born correction is applied. For low partial waves ($l \leq 4$) $T$ matrices computed from the $R$-matrix calculations are employed to compute the cross sections. The low partial wave contribution arising from the Born contribution may be subtracted in order that the final rotational cross-section set only contains those partial waves due to $R$-matrix calculation. We have performed the calculations with and without a dipole Born correction.

The $R$ matrix provides the link between the inner region and outer region. For this purpose the inner region is propagated to the outer region potential until its solutions match with the asymptotic functions given by the Gailitis expansion [34]. Thus by generating the wave functions, using Eq. (1), their eigenvalues are determined. These coupled single-center equations describing the scattering in the outer region are integrated to identify the $K$-matrix elements. Consequently the resonance positions, widths, and various cross sections can be evaluated using the $T$ matrix obtained from the $S$ matrix, which is in turn obtained from the $K$-matrix element.

C. High-energy formalism (15–2000 eV)

In the intermediate- and high-energy regime a conventional close-coupled theory [32] of an electron-molecule system is a complex and arduous task even with present day supercomputers. Hence many groups [17,19,24,25] employ spherical complex optical potential formalism in this region as it is consistent and simple and provides computationally fast solutions. The SCOP formalism [35,36] employs a partial wave analysis to solve the Schrödinger equation with various model potentials as its input. The interaction of incoming electrons with the target molecule can be represented by a local complex potential comprised of real and imaginary parts as

$$
V_{\text{pp}}(E_i,r) = V_R(E_i,r) + i V_I(E_i,r),
$$

(2)

such that

$$
V_R(r,E_i) = V_{st}(r) + V_{eq}(r,E_i) + V_p(r,E_i),
$$

(3)

where $E_i$ is the incident energy. Equation (3) corresponds to various real potentials to account for the electron-target interaction, namely, static, exchange, and the polarization potentials, respectively. These potentials are obtained using the
molecular charge density of the target, the ionization potential, and the polarizability as inputs. We describe the scattering process within the confines of the fixed-nuclei approximation which neglects any dynamics involving the nuclear motion (rotational and vibrational), with the bound electrons being assumed to be in the ground electronic state of the target at its optimized equilibrium geometry. The molecular charge density may be derived from the atomic charge density by expanding it from the center of mass of the system. Thus, the single-center molecular charge density is obtained by a linear combination of constituent atomic charge densities, renormalized to account for covalent molecular bonding.

The atomic charge densities and static potentials \( V_a \) are formulated from the parametrized Hartree-Fock wave functions given by Cox and Bonham [37]. The parameter-free Hara’s “free electron gas exchange model” [38] is used to generate the exchange potential \( V_{\text{ex}} \). The polarization potential \( V_p \) is constructed from the parameter-free model of correlation-polarization potential given by Zhang et al. [39]. Here, various multipole nonadiabatic corrections are incorporated in the intermediate region which will approach the correct asymptotic form at large \( r \) smoothly. In the low-energy region, the small \( r \) region is not important due to the fact that higher-order partial waves are unable to penetrate the scattering region. However, in the present energy region, a large number of partial waves contributes to the scattering parameters such that a correct short-range behavior of the potential is essential.

The imaginary part in \( V_{\text{opt}} \) is called the absorption potential \( V_{\text{abs}} \) and accounts for the total loss of flux scattered into the allowed electronic excitation or ionization channels. \( V_{\text{abs}} \) is not a long-range effect and its penetration towards the origin increases with increasing \( e \) energy. This implies that at high energies, the absorption potential accounts for the inner-shell excitations and ionization processes that may be neglected at low energies.

The well-known quasi-free-model form of Staszeweska et al. [40] is employed for the absorption part and is given by

\[
V_{\text{abs}}(r, E_i) = \Delta + \rho(r) - \delta_{\text{loc}} \left( \frac{8\pi}{10k_F^2 E_i} \right) \frac{1}{4} \left( p^2 - k_F^2 - 2\Delta \right) \left( A_1 + A_2 + A_3 \right),
\]

where the local kinetic energy of the incident electron is

\[
\delta_{\text{loc}} = E_i - (V_a + V_{\text{ex}} + V_p),
\]

and where \( p^2 = 2E_i, \) \( k_F = \left[ 3\pi^2 \rho(r) \right]^{1/3} \) is the Fermi wave vector and \( \theta(\alpha) \) is the Heaviside unit step function such that \( \theta(\alpha) = 1 \) for \( x \geq 0 \), and is zero elsewhere. \( A_1, A_2, \) and \( A_3 \) are dynamic functions that depend differently on \( \theta(\alpha), I, \Delta, \) and \( E_i \). Here, \( \Delta \) is the principal factor which decides the values of total inelastic cross section, since below this value ionization or excitation is not permissible. This is one of the main characteristics of the Staszewka model [40,41]. In the original Staszewsa model [40,41] \( \Delta = I \) is considered and hence ignores the contributions coming from discrete excitations at lower incident energies. This was recognized by Garcia and Manero [42] who discussed the need to modify \( \Delta \) value. In the present calculation we consider \( \Delta \) as a slowly varying function of \( E_i \) around \( I \). Such an approximation is meaningful since \( \Delta \) fixed at \( I \) would not allow excitation at energies \( E_i < I \). Alternatively, if \( \Delta \) is much less than the ionization threshold, then \( V_{\text{abs}} \) becomes unexpectedly high near the peak position. The amendment we introduced gives a reasonable minimum value 0.8\( I \) to \( \Delta \) [43] and expresses the parameter as a function of \( E_i \) around \( I \), i.e.,

\[
\Delta(E_i) = 0.8I + \beta(E_i - 1).
\]

Here the value of the parameter \( \beta \) is obtained by requiring that \( \Delta = I \) (eV) at \( E_i = E_p \), the value of incident energy at which \( Q_{\text{inel}} \) reaches its peak. \( E_p \) can be found by calculating \( Q_{\text{inel}} \) by keeping \( \Delta = I \). Beyond \( E_p, \Delta \) is kept constant and is equal to \( I \). The theoretical basis for having a variable \( \Delta \) is discussed in more detail by Vinodkumar et al. [43]. The expression (6) is meaningful since if \( \Delta \) is fixed at the ionization potential it would not allow any inelastic channel to open below \( I \), and if it is very much less than \( I \), then \( V_{\text{abs}} \) become significantly high close to the peak position of \( Q_{\text{inel}} \).

The complex potential formulated in this way is used to solve the Schrödinger equation numerically through a partial wave analysis. This calculation will produce complex phase shifts for each partial wave which carries the signature of interaction of the incoming projectile with the target. At low impact energies only a few partial waves are significant, but as the incident energy increases more partial waves are needed for convergence. The phase shifts (\( \delta_i \)) thus obtained are employed to find the relevant cross sections, total elastic (\( Q_{\text{el}} \)), and the total inelastic cross sections (\( Q_{\text{inel}} \)) using the scattering matrix \( S(k) = \exp(2i\delta) \) [44]. Total cross sections such as the total elastic (\( Q_{\text{el}} \)) and the total inelastic cross sections (\( Q_{\text{inel}} \)) can then be derived from the scattering matrix [34]. The sum of these cross sections then gives the total scattering cross section (TCS) \( Q_T \) [35].

III. RESULTS AND DISCUSSION

We have carried out a comprehensive set of calculations on electron scattering from SO\(_2\) between \(-0.1\) and 2000 eV. The results are represented graphically in Figs. 1–4 along with the available comparisons and numerical values which are tabulated in Table III.

Let us consider Figs. 1(a), 1(b), and 2, which show the total scattering cross-section curves. For clarity we have separated comparisons between the present results with experiments [Figs. 1(a) and 1(b)] and theory (Fig. 2). Below the ionization threshold calculations were performed using the R-matrix code and above it the SCOP formalism was employed. As evident from Figs. 1(b) and 2 the data produced by these two formalisms are consistent at the transition energy (\(-15\) eV), and it validates the use of the two formalisms to provide a self-consistent TCS over such an extensive energy range. We have employed two models for our low-energy calculations, one employing the Born correction and other without the Born correction.

Figure 1(a) shows a comparison of present total cross sections with the experiments for low impact energies up to 10 eV. There are two important features to be observed in the low-energy regime; first, there is clear evidence for the presence of structure at 3.4 eV in the TCS curve.
which coincides with the observation of a resonance. Such a resonance was first observed by Sanche and Schulz [11] and subsequently confirmed by the measurements of Simon et al. [12] and Andric et al. [13] who showed the temporary formation of the SO$_2^-$ state which decays into vibrational excitation of the neutral. Andric et al. [13] further confirmed that the symmetry of this state was most likely $^2B_2$ with the additional electron being in the $^6B_2$ orbital. This resonance is reproduced exactly at 3.4 eV in our ab initio calculations using the $R$ matrix shown by the arrow but it was not observed in the earlier calculations of Gupta and Baluja [14], Gianturco et al. [15], Natalense et al. [16], and Machado et al. [17]. The second feature observed in the present TCS is a weak structure at 5.1 eV which was also observed as a broad minimum by Gulley and Buckman [6] in their Differential Cross Section (DCS) measurement at 5 eV between 20° and 50°.

Figure 1(b) shows a comparison of electron-impact total cross sections for $e$-SO$_2$ scattering with experimental results from 0.1 to 2000 eV. Electron interactions with SO$_2$ have
been extensively studied, interestingly with more experimental investigations \[6–10,17,18\] being reported than theoretical study \[14–20\]. The present results are in good agreement with most measured total cross sections if Born corrections are not included, suggesting that the Born corrected data overestimate the total cross section.

The overestimation in the Born corrected data is attributed to a larger value (30% higher compared to experimental value) of the dipole moment. Experimental values for integral cross sections are basically obtained by visual extrapolation of measured differential cross section over those angles which are not accessible experimentally. This introduces a large error in the low-energy regime below 2 eV \[17\]. The data of Szymtowski \textit{et al.} \[9\], Zubek \textit{et al.} \[7\], and Sokolov and Sokolova \[10\] are considerably higher than all other data sets, perhaps an overestimation of the effects of forward scattering as discussed above and should therefore be considered as outliers.

Table III. Total cross sections of e-SO$_2$.  

<table>
<thead>
<tr>
<th>$E_i$ (eV)</th>
<th>TCS ($\text{Å}^2$) (with Born correction)</th>
<th>TCS ($\text{Å}^2$) (without Born correction)</th>
<th>TCS ($\text{Å}^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>1581.51</td>
<td>384.02</td>
<td>20</td>
</tr>
<tr>
<td>0.2</td>
<td>891.79</td>
<td>192.40</td>
<td>25</td>
</tr>
<tr>
<td>0.3</td>
<td>633.19</td>
<td>128.20</td>
<td>30</td>
</tr>
<tr>
<td>0.4</td>
<td>493.03</td>
<td>96.60</td>
<td>36</td>
</tr>
<tr>
<td>0.5</td>
<td>406.72</td>
<td>78.01</td>
<td>40</td>
</tr>
<tr>
<td>1.0</td>
<td>224.39</td>
<td>42.57</td>
<td>50</td>
</tr>
<tr>
<td>2.0</td>
<td>126.78</td>
<td>27.41</td>
<td>60</td>
</tr>
<tr>
<td>3.0</td>
<td>94.66</td>
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<td>3.4</td>
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<td>67.40</td>
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<td>9.0</td>
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<td>10</td>
<td>44.44</td>
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</tr>
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<tr>
<td>15</td>
<td>37.47</td>
<td>20.14</td>
<td>500</td>
</tr>
</tbody>
</table>

Figure 2 depicts the comparison of present total cross sections for e-SO$_2$ scattering with other theoretical data over a wide range of impact energies from 0.1 to 2000 eV. Low-energy electron scattering calculations have been reported by four groups, Gupta and Baluja \[14\], Gianturco \textit{et al.} \[15\], Natalense \textit{et al.} \[16\], and Machado \textit{et al.} \[17\]. SO$_2$ has a strong permanent dipole moment, 1.63 D, which is clearly reflected in the TCS curve as a steep fall in the elastic cross sections at low energies. The data of Gianturco \textit{et al.} \[15\] and Natalense \textit{et al.} \[16\] appear to overestimate the cross section while the two \textit{R}-matrix-based results, present and that of Gupta and Baluja \[14\], appear to provide data that match the experimental results at least to energies as low as 2–3 eV. It is also clearly seen that inclusion of additional partial waves, through the Born correction, results in a much higher low-energy cross section which is greatly in excess of the majority of the experimental data and theoretical calculations. This overestimation in the Born corrected data is due to the strong dipole moment of 1.63 D of the SO$_2$ molecule. It is to be noted that above the ionization threshold the results obtained using SCOP formalism are in excellent agreement with all three \[17,19,20\] theoretical results, which reflects the consistency of SCOP formalism.

Having observed the clear evidence of resonant structures (at 3.4 and 5.1 eV) in the total cross-section curve it was necessary to study the eigenphase diagrams for the e-SO$_2$ system to confirm the presence of resonance structures. Figure 3 shows the eigenphase diagram for four doublet scattering states ($^2A_1$, $^2B_1$, $^2B_2$, $^2A_2$) of the e-SO$_2$ system. The $^2A_1$ state shows a prominent structure at 3.4, 8.17, and 13.05 eV. The prominent structure leads to the resonance peak
at 3.4 eV in the TCS curve as observed in earlier experiments [11–13]. The doublet $A_2$ state also shows a distinct structure at 5.1 eV which matches the broad minima observed by Gulley and Buckman [6] in their DCS measurement at 5 eV between 20° and 50°.

Figures 4(a) and 4(b) represent electron-impact excitation cross sections for ground state $1A_1$ to the first eight excited states $3B_1, 3B_2, 1A_2, 3A_2, 3B_2, 1A_1,$ and $3A_2$. For clarity we have shown the excitation cross-section curves for excited states $3B_1, 3B_2, 1B_1,$ and $1B_2$ in Fig. 4(a) and $3A_2, 3A_1, 3A_1,$ and $3A_2$ in Fig. 4(b). Transitions to excited states $3B_1$ and $3B_2$ symmetry are in accordance with the dipole selection rule and show a strong peak in the cross section. The excitation cross section due to transition from ground state $X\ ^1A_1$ to $3B_2$ rises as a strong peak at 5.1 eV and corresponds to the shape resonance in $2\ A_1$ symmetry due to its higher transition moment [14]. The excitation cross-section curve then flattens and shows a small peak at 8.1 eV. The same structure is also observed in the transition from $X\ ^1A_1$ to $1B_1$. The excitation cross section arising due to the transition from $X\ ^1A_1$ to $1B_1$ rises slowly, attains a broad peak around 8 eV, and then slowly decreases. Finally the excitation cross section arising due to the $X\ ^1A_1$ to $1B_2$ transition starts at 8 eV and reaches a broad maximum around 14 eV before gradually decreasing.

The excitation cross sections for the remaining four states of $A$-type symmetries are shown in Fig. 4(b). It is evident from the figure that transition from ground state $X\ ^1A_1$ to $3A_2$ is more prominent compared to $A_2$, and the excitation cross sections due to both transitions show strong peaks at 5.1 and 8.1 eV.

IV. CONCLUSION

In this paper we report results of theoretical calculations of electron scattering from sulfur dioxide over a wide energy range from 0.1 to 2000 eV. We have used the \textit{ab initio} $R$-matrix formalism at low impact energies (below the ionization threshold of the target) and the spherical complex optical potential (SCOP) methodology above the ionization threshold; the two methods are shown to produce comparable cross sections at 15 eV. Both the eigenphase diagram and total cross section indicate a structure at 3.4 eV which is ascribed to a shape resonance which has been reported in earlier experimental studies. There is also detection of a second weaker resonance at 5.1 eV for which there is also some experimental evidence. We also report estimates of electronic state excitation cross sections.

The paper reviews all previous experimental and theoretical data and therefore provides a survey, that with the present consistent set of data, may be used to recommend a self-consistent set of total scattering cross sections from SO$_2$ that may be used in plasma and other applied studies. Indeed we would recommend the data in Table III be used as a preferred data set for the extensive energy range (0.1–2000 eV) with a 30% uncertainty, particularly at low energy below ionization threshold.

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[27] [http://www.nist.gov/chemistry-portal.cfm].