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Fragmentation dynamics of SO_2^{2+}

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Abstract

Photoelectron–photoion coincidence measurements have been performed on SO_2 at energies up to 40.8 eV, and analysed using a new method of data analysis to determine the energy balance in the main dissociation pathways. In $SO^+ + O^+$ formation, ground state products are formed near threshold, but excited products are formed with higher energy transfer. (Int J Mass Spectrom 192 (1999) 281–288) © 1999 Elsevier Science B.V.

Keywords: Ion spectroscopy; Photoionization; Doubly charged ions; Fragmentation dynamics

1. Introduction

Significant advances have been made over the past five years in the spectroscopy of dications, particularly the measurement of vibrational structure in spectra of diatomic and triatomic dications by threshold photoelectrons coincidence spectroscopy (TPEsCO) [1,2]. Vibrational resolution has also been achieved recently in experiments where kinetic energy releases in the fragmentation of diatomic dications are measured very accurately [3]. The rates of dication fragmentation can sometimes be deduced from details of the kinetic energy release spectra, or by combination of the TPEsCO technique with detection of fragment ions in coincidence [4]. For polyatomic dications, however, where there can be several competing reaction pathways, another method is required to determine the fragmentation dynamics.

In the ideal experiment the energies of the polyatomic dication and fragment ions would be determined. The energy of a dication, $E_{m^{++}}$, formed in double photoionization is given by

$$E_{m^{++}} = h\nu - E_{e_1^-} - E_{e_2^-} \tag{1}$$

where $h\nu$ is the energy of the photon and $E_{e_1^-}$ and $E_{e_2^-}$ are the energies of the two electrons ejected. Thus, to determine the dication energy it is necessary to energy analyse and detect both electrons. If we take the mean of Eq. (1) for all events observed where a certain product is formed, e.g. $SO^+ + O^+$, we obtain

$$\overline{E_{m^{++}}} = h\nu - \overline{E_{e_1^-}} - \overline{E_{e_2^-}} \tag{2}$$

where $\bar{E}_{m^{++}}$ represents the mean energy of the dication and $\bar{E}_{e_1^-}$ and $\bar{E}_{e_2^-}$ represent the mean energies of the two different electrons ejected in double photoionization. The electrons, however, are indistinguishable so we may write

$$\overline{E_{m^{++}}} = h\nu - 2\overline{E_{e^-}} \tag{3}$$

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where $\bar{E}_{e^-}$ represents the mean energy of all electrons observed in coincidence with a specific double photoionization process. In the present experiment a single energy-analysed electron is detected in coincidence with doubly charged products, and the energy deposition is estimated using Eq. (3).

Direct experimental observation of a metastable SO_2^{2+} ion has not been reported. The only experimental evidence for its existence is the observation of the slow $SO_2^{2+} \rightarrow SO^+ + O^+$ reaction (on a time scale of $\approx 10^{-5}$ s) [5]. Experimental observation of metastable SO_2^{2+} is not easy as it has a mass to charge ratio of 32, identical to that of S^+ and O_2^+, which may account for the lack of direct observations.

Winkoun *et al.* [6] have calculated the energies of low lying electronic states of SO_2^{2+} in the ground state equilibrium geometries of neutral SO_2 (bond angle 119.5 °), SO_2^+ (bond angle 136.5 °) and SO_2^{2+} (linear). Double charge transfer spectra have not been reported for sulphur dioxide, though the lowest singlet state of SO_2^{2+} was reported to lie at 33.8 ± 0.4 eV from an unpublished double charge transfer spectrum [7]. The TPEsCO spectrum of SO_2^{2+} has been measured [8] and indicates a double photoionization energy of 34.0 ± 0.2 eV. The energies of electronic states are not clearly visible from the TPEsCO spectrum which shows no sharp structure.

2. Experimental

The apparatus used for the present work has been described elsewhere [9], so only a brief description will be given here. A schematic diagram of the apparatus is shown in Fig. 1. Ultraviolet light from a helium discharge is energy selected with a toroidal grating and focused in the common source region of a small time-of-flight mass spectrometer and a photoelectron spectrometer. Sample gas is introduced to the source region through an effusive needle perpendicular to both the axis of the light beam and the shared axis of the mass spectrometer and the electron lens of the photoelectron spectrometer. During coincidence measurements the source region is pulsed for optimum mass and electron energy resolution; electrons are detected during field free periods, on detection of an electron a large voltage pulse is used to extract ions into the time-of-flight mass spectrometer. The resolution of the mass spectrometer ($M/\Delta M$) is greater than 200 (FWHM definition) and that of the photoelectron spectrometer is 300 meV under the conditions employed for studying double photoionization. Photoelectron, PEPICO, and PEPIPICO spectra are all recorded simultaneously. The two different methods used to distinguish true and false coincidences in these PEPICO and PEPIPICO spectra have already been described [9], briefly background spectra of false coincidences are subtracted from the PEPICO data to obtain spectra that represent only true coincidences, whereas true coincidences in PEPIPICO spectra can be identified due to the correlation of the momenta of the two ions formed in the same event (see sec. 3 for $SO^+ + O^+$). Great care has been taken to calibrate the variation in transmission efficiency of the photoelectron spectrometer with photoelectron energy [10]. This is essential for the determination of the mean dication energies described below, all photoelectron spectra presented are normalized to compensate for this variation. The transmission efficiency varies by a factor of 1.5 over the range of photoelectron energies in the present data.

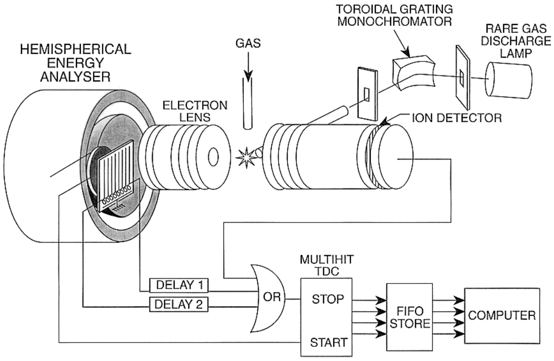

Fig. 1. Schematic diagram of the coincidence spectrometer.

The present data were recorded photoionizing sulphur dioxide with HeIIα (30.4 nm, 40.8 eV) radiation for over 70 h.

3. Data analysis

Complete spectra of photoelectrons ejected in specific double photoionization process, such as the formation of $SO^+ + O^+$, are obtained in this experiment. The quantitative analysis of these photoelectron spectra to give mean dication energies and maximum dication energies follows.

The mean energy of dication states which form a certain product, $\bar{E}_{m^{++}}$, can be determined from the mean energy of electrons detected in coincidence with that product, $\bar{E}_{e^-}$, and the photon energy, $h\nu$, with Eq. (3) above. The mean energy of electrons detected in coincidence with specific ionic products can be determined from the photoelectron spectrum coincident with these products, provided that the variation in the transmission efficiency of the photoelectron spectrometer is understood. Furthermore, the mean energy of the fragments formed in dissociation is equal to the mean energy of dication states which fragment to give these fragments less the mean kinetic energy released in fragmentation.

If in fragmentation an indirect mechanism is responsible for double photoionization and the second photoelectron is ejected following molecular dissociation then no true dication state is formed in the Franck-Condon region and the calculated value of $\bar{E}_{m^{++}}$ cannot be interpreted as the energy of a state of the molecular ion, but relates only to the fragments.

Knowledge of the energy of one of the two photoelectrons sets an upper limit on the internal energy of the dication. Rearranging Eq. (1) and labelling the electron with known energy as e_1^- and the electron with unknown energy as e_2^- we obtain

$$E_{m^{++}} + E_{e_2^-} = h\nu - E_{e_1^-} \tag{4}$$

from which we may assert that

$$E_{m^{++}} \leq h\nu - E_{e_1^-} \tag{5}$$

thus, if the energy of one electron is known (E_{e^-}) then the energy the doubly charged state is limited to a maximum value of $h\nu - E_{e^-}$.

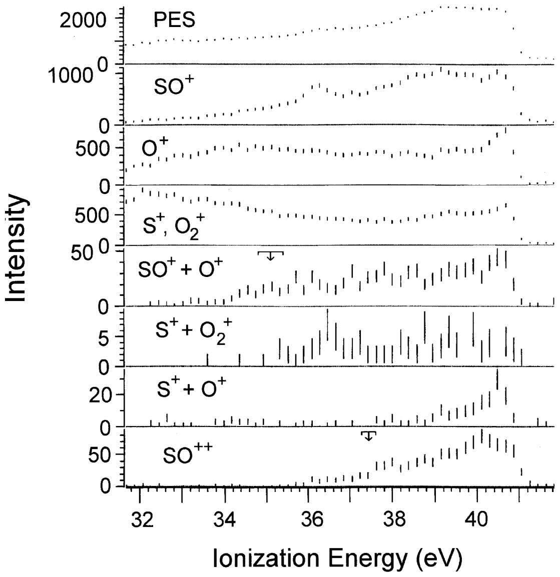

Fig. 2. The total photoelectron spectrum and spectra of photoelectrons detected in coincidence with different ionic products.

4. Results and discussion

The total photoelectron spectrum recorded and spectra of the photoelectrons detected in coincidence with ions, extracted from PEPICO and PEPIPICO spectra, are shown in Fig. 2. There is a common abscissa labelled with ionization energy, *viz.* the photon energy less the energy of the photoelectron detected. The ordinates show the number of experimental counts corrected for the variation in the photoelectron transmission with kinetic energy. The error bars indicate an uncertainty of plus or minus one standard deviation. Two vertical arrows with error bars are shown which indicate mean dication energies. It should be remembered that the mass to charge ratios (*m/z*) of both S^+ and O_2^+ are 32 and hence these ions are indistinguishable in the mass spectrum.

The thresholds for double photoionization processes determined from these photoelectron spectra are presented in Table 1 along with limits calculated from thermodynamic data [11] and literature values.

Table 1
Dissociative double ionization thresholds (eV); PIPICO—photoion photoion coincidence, PIMS—photoionization mass spectroscopy

	$SO^+ + O^+$	$S^+ + O_2^+$	$S^+ + O^+ + O$	$SO^{2+} + O$
Thermodynamic limit	29.7	28.3	35.1	35.2
This work	34.0 ± 0.5	≤36.0	≤39.0	35.8 ± 0.2
E.I. Mass Sp. [5]	33.8[a]	. . .	. . .	. . .
PIPICO [7]	34.5 ± 0.4	. . .	44 ± 2	. . .
PIPICO [12]	34.3 ± 0.5	. . .	37.7 ± 0.5	. . .
EPIC [16][b]	34–38[b]	33–35[b]	>38[b]	. . .
(e,e + ion) [17]	. . .	. . .	. . .	41
PIMS [17]	. . .	. . .	. . .	32.62
PIMS [18]	. . .	. . .	. . .	35 ± 1

[a] This is the threshold for the slow metastable dissociation $SO_2^{2+} \rightarrow SO^+ + O^+$.

[b] Electron pairs were detected with some kinetic energy analysis in coincidence with ions (EPIC), the energy ranges indicate the ionization energies at which ion pairs are observed.

4.1. $SO^+ + O^+$

A clear threshold is observed in the spectrum of photoelectrons detected in coincidence with $SO^+ + O^+$ ions at 34.0 ± 0.5 eV. The weak signal observed in the coincident photoelectron spectrum below this threshold is due to false coincidences (see below). This value is in agreement with the double ionization potential of sulphur dioxide measured by double charge transfer and the TPEsCO technique, 33.8 [7] and 34.0 eV [8], respectively. It is also consistent with thresholds reported for $SO^+ + O^+$ production in PIPICO experiments with variable wavelength excitation; 34.5 ± 0.4 eV [7] and 34.3 ± 0.5 eV [12].

The mean energy of dications which fragment to give $SO^+ + O^+$ is calculated to be 35.1 ± 0.3 eV from the coincident photoelectron spectrum. The error in the mean energy, determined with a standard propagation of errors calculation, represents plus or minus one standard deviation. The small gap between this mean energy and the threshold for double ionization (~1 eV) indicates that dication states which fragment to give $SO^+ + O^+$ are mostly within two electronvolts of the double ionization threshold. Subtracting the mean kinetic energy release in the formation of $SO^+ + O^+$, 4.8 eV, from the mean dication energy gives a mean fragment energy of 30.3 ± 0.3 eV. Comparing this mean energy with the thermodynamic limit for $SO_2 \rightarrow SO^+ + O^+ + 2e^-$, 29.7 eV, indicates that the fragments have a mean internal energy of ~0.6 eV following dissociation. From this low mean internal energy it is concluded that only a small fraction of fragment ions can be formed in electronically excited states because the first excited electronic states of the fragment ions are SO^+ (a $^4\Pi$) + O^+ ($^4S^0$) and SO^+ (X $^2\Pi$) + O^+ ($^2D^0$), which lie 3.24 and 3.32 eV above the ground state fragments SO^+ (X $^2\Pi$) + O^+ ($^4S^0$) respectively [13,14].

Kinetic energy releases (KERs) have been determined from the present data; PEPIPICO coincidences have been grouped by maximum dication energy (from electron energies) in blocks of 1 eV. KERs determined from these groups are shown in Table 2 and two-dimensional mass spectra showing $SO^+ + O^+$ mass peaks for certain groups are shown in Fig. 3. The KERs have been determined from the length of the peaks in the two-dimensional mass spectrum to give maximum KERs; the statistics are insufficient for determination of KERs from the full width half maxima (FWHM) of these peaks. The characteristic peak shapes with gradients of −1 are seen in all spectra in Fig. 3 except for the first where no correlation is observed between the flight times of the two ions. The lack of correlation is characteristic of false coincidences, hence with maximum dication energies of 33–34 eV no true $SO^+ + O^+$ production is observed. The kinetic energy release remains remarkably constant over the range of maximum dication energies observed. The highest and lowest kinetic

Table 2
Kinetic energy releases of SO_2^{2+} dications with selected maximum energies

Maximum dication energy (eV)	Kinetic energy release (KER) (eV)		
	Maximum KER		FWHM KER
	$SO_2^{2+} \rightarrow SO^+ + O^+$	$SO_2^{2+} \rightarrow SO^{2+} + O$	$SO_2^{2+} \rightarrow SO^{2+} + O$
32–33	[a]	. . .	. . .
33–34	[a]	. . .	. . .
34–35	4.3 ± 0.5	. . .	. . .
35–36	4.7 ± 0.5	(Trace)[b]	(Trace)[b]
36–37	4.3 ± 0.5	0.36 ± 0.09	0.14 ± 0.06
37–38	4.7 ± 0.5	0.82 ± 0.14	0.46 ± 0.14
38–39	5.0 ± 0.5	1.8 ± 0.2	0.63 ± 0.12
39–40	5.0 ± 0.5	1.8 ± 0.2	1.12 ± 0.16
40–41	5.2 ± 0.5	2.3 ± 0.3	1.12 ± 0.16

[a] No true coincidence peak observed.
[b] Signal too weak for kinetic energy release determination.

energy releases lie within their uncertainties. For the group of coincidences with maximum dication energies between 34 and 35 eV we can be confident that the initial energy of the dication formed prior to dissociation lies between 34 and 35 eV because the threshold for $SO^+ + O^+$ production is 34 eV. Now, subtracting the kinetic energy release observed for this group, 4.3 ± 0.5 eV, from the initial dication energy, 34–35 eV, we find that the fragments $SO^+ + O^+$ can have an energy of between 29.7 and 31.2 eV (*N.B.* the thermodynamic limit for $SO^+ + O^+$ is 29.7 eV). This analysis demonstrates that the fragments are produced in the ground electronic state from the dissociation of dications produced close to threshold in agreement with the mean energy calculations above. The slow change in kinetic energy release with increasing maximum dication energy rules out the charge separation of dication states above 36 eV to give $SO^+ + O^+$ fragment ions in the ground electronic state, which would show higher kinetic energy releases.

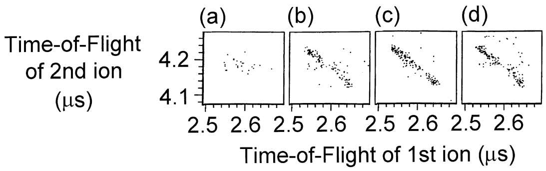

Fig. 3. Two dimensional mass spectra of $SO^+ + O^+$ ions formed in the fragmentation of dications with maximum energies of (a) 33–34 eV, (b) 35–36 eV, (c) 37–38 eV, (d) 39–40 eV. *N.B.* in (a) only false coincidences are observed (see text).

No potential energy surfaces have been reported for SO_2^{2+} to our knowledge and so an adiabatic correlation diagram, Fig. 4, has been constructed to aid the interpretation of the present data. The correlation diagram has been built up by standard methods

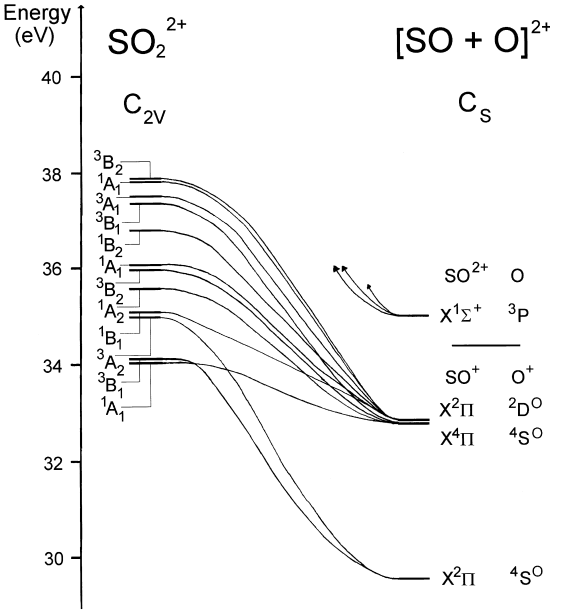

Fig. 4. Correlation diagram show adiabatic correlations between SO_2^{2+} and $[SO + O]^{2+}$.

[15] using the energies and symmetries of dicationic states of SO_2^{2+} in the Franck-Condon region calculated by Winkoun *et al*. [6]. The validity of this correlation diagram depends on the formation of SO_2^{2+} in the Franck-Condon region and its relevance to actual dissociation depends on dissociation proceeding over adiabatic surfaces with no curve crossing, neither of which are certain. The present conclusion from the mean energy analysis, that formation of $SO^+ + O^+$ is due mostly to dication states within 2 eV of threshold dissociating to give ground state products, is consistent with the correlation diagram, which shows that two dication triplet states $^3B_1$ and $^3A_2$ within 1 eV of threshold correlate to the ground state products. The observation from examining kinetic energy releases that ground state products are not formed in the dissociation of dication states above 36 eV is also consistent with the correlation diagram, which predicts that these states correlate to electronically excited products. Despite these successes, the correlation diagram does not correctly predict the dynamics of $SO_2^{2+} \rightarrow SO^{2+} + O$.

The kinetic energy release in $SO_2^{2+} \rightarrow SO^+ + O^+$ fragmentation has been measured by Masuoka [12] using the PIPICO technique with photon energies between 37 and 130 eV. He observed that the minimum (2.4 eV), mean (4.8 eV), and maximum (7.6 eV) kinetic energy releases did not vary but remained constant across this broad range of excitation energies and concluded that this dissociation process only proceeds from low-lying states of SO_2^{2+}, in agreement with the analysis of the present data. Eland and Mathur have also investigated this fragmentation process recording coincidences between ions and electron pairs with some energy analysis of the electrons [16]. They concluded that $SO^+ + O^+$ fragments were formed from fragmentation of SO_2^{2+} states between 34 and 38 eV.

4.2. $SO^{2+} + O$

There has been some uncertainty in the threshold for the formation of SO^{2+} from SO_2; experimental values of 32.62, 35, and 41 eV have been reported [17,18]. Here we obtain a value of 35.8 ± 0.2 eV, which is consistent with the most recently reported threshold, 35 ± 1 eV determined by photoionization mass spectroscopy [18]. The thermodynamic limit for this process can be calculated by summing the energy for neutral dissociation $SO_2 \rightarrow SO + O$, 5.71 eV, and the first and second ionization energies of SO, 10.3 and 19.2 eV determined by experiment [19] and theory [20], respectively, which gives 35.2 eV.

The mean energy of dications which fragment to give SO^{2+} is 37.4 ± 0.2 eV. The mean kinetic energy release calculated from the SO^{2+} peak shape in the present data is 1.0 ± 0.1 eV which indicates that the fragments $SO^{2+} + O$ are formed at a mean energy of 36.4 ± 0.3 eV. Comparing this value with the theoretical threshold for the formation of these products, 35.2 eV, it is deduced that $SO^{2+} + O$ have a mean internal energy of ~1 eV following dissociation. The low-lying electronic states of SO^{2+} have been calculated by Basch *et al*. [21]. These calculations indicate that the first excited state of SO^{2+} ($^3\Sigma^+$) lies 2.2 eV above the ground state ($^1\Sigma^+$). It is also known that the first excited state of the O atom (^1D) lies 2.0 eV above the ground state (^3P) [14]. Therefore, the products $SO^{2+} + O$, with ~1 eV mean internal energy, will mostly be formed in the ground electronic state.

The coincidences observed between SO^{2+} ions and electrons have been binned into groups of 1 eV maximum dication energy and peaks in the mass spectrum are shown in Fig. 5. The kinetic energy releases calculated from the base widths (maximum KERs) and the FWHM of these peaks are shown in Table 2. The range of kinetic energy releases observed, from 0 to 2.3 eV indicate that SO^{2+} is produced from the dissociation of a band of states at least 2 eV wide. This hypothetical band would therefore run from the threshold at 35.8 ± 0.2 eV to ~37.8 eV which is close to the experimental thresholds for formation of $O^+ + S^+ + O$ shown in Table 1. Thus it appears that the formation of SO^{2+} is concentrated below the threshold for formation of $O^+ + S^+ + O$. This conclusion supports the result of Hsieh and Eland [22], obtained by analysing the kinematics of

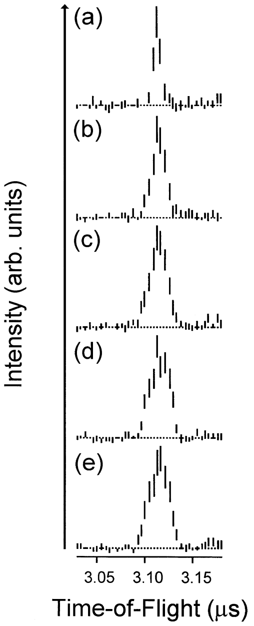

Fig. 5. Mass peaks of SO^{2+} formed in the fragmentation of dications with maximum energies of (a) 36–37 eV, (b) 37–38 eV, (c) 38–39 eV, (d) 39–40 eV, (e) 40–40.8 eV.

dissociation, that $S^+ + O^+ + O$ is formed from SO_2^{2+} by a sequential mechanism in which $SO_2^{2+} \rightarrow SO^{2+} + O \rightarrow O^+ + S^+ + O$. Their result suggests that above the threshold for formation of $O^+ + S^+ + O$ any SO^{2+} formed would dissociate to give $O^+ + S^+$ in agreement with the present observations. Further evidence for this mechanism is found in the calculations of Basch *et al*. [21]. They calculate a 1.5 eV barrier to dissociation for SO^{2+} in the ground state potential energy surface; this value is close to the 2 eV difference between the threshold for $SO^{2+} + O$ and the threshold for $O^+ + S^+ + O$.

It is interesting that the mean kinetic energy release in the formation of $SO^{2+} + O$ is significantly smaller than in charge separation dissociations such as $SO_2^{2+} \rightarrow SO^+ + O^+$, perhaps because there is no coulombic repulsion between the SO^{2+} and O fragments. The formation of $SO^{2+} + O$ is not predicted adiabatically from the correlation diagram (Fig. 4), although diabatically the ground state of $SO^{2+} + O$ correlates with the triplet states of SO_2^{2+}. It is concluded, therefore, that the $SO^{2+} + O$ products are formed either by diabatic dissociation of the parent dication or by dissociation of super excited singly charged states followed by autoionization.

4.3. $S^+ + O_2^+$, $O^+ + S^+ + O$

The weak signal in the photoelectron spectrum coincident with $S^+ + O_2^+$ and the presence of false coincidences in the photoelectron spectrum coincident with $O^+ + S^+ + O$ impede the determination of thresholds for these processes. It is possible, however, to determine upper limits of these thresholds from the present data; 36.0 eV for $S^+ + O_2^+$ and 39.0 eV for $O^+ + S^+ + O$. If the threshold for $O^+ + S^+ + O$ is taken to be 37.7 eV, as determined by Masuoka [12], then approximate mean energies can be determined from the present data. This analysis indicates that the fragments $O^+ + S^+ + O$ are formed predominantly in the ground state with less than 1 eV internal energy [23].

4.4. SO^+, O^+, and S^+/O_2^+

The peak in the photoelectron spectrum coincident with SO^+ at 36.2 eV is due to the photoionization of valence electrons by HeIα impurity in the light. The shape of the SO^+ coincident photoelectron spectrum, apart from this peak, is similar to that of the photoelectron spectrum in coincidence with $SO^+ + O^+$ ion pairs. Comparing the intensities of the SO^+ signal and the $SO^+ + O^+$ signal in Fig. 2 it is found that the SO^+ signal is approximately double that expected if all SO^+ ions observed were formed in dissociative double photoionization, bearing in mind that the ion pair signal is expected to be lower by a factor of 0.14, the ion collection efficiency.

The shapes of the photoelectron spectra coincident with O^+ and S^+/O_2^+ ions are quite different to that coincident with SO^+. Below the double ionization threshold at 34 eV there are strong signals due to the formation of O^+, S^+, and possibly O_2^+ in the fragmentation of satellite states of SO_2^+ below the double ionization threshold. These signal levels are maintained above the double ionization threshold; close to the 34 eV the signal levels in both spectra are at least five times greater than that expected due to double photoionization. With increasing photoionization energy this effect is less pronounced, e.g. above 40 eV ionization energy the O^+ signal is less than twice the level which would be expected from double photoionization.

5. Conclusions

One conclusion which must be drawn from these observations is that a major process above the double ionization threshold is the excitation and dissociation of super excited states of SO_2^+. These processes are dominant close to the double photoionization threshold. Similar processes have also been observed in the photoionization of CS_2 [10]. More generally the importance of superexcited negative ion states and neutral states above ionization threshold is well known in dissociative attachment [24] and dissociative recombination [25], respectively; the equivalent involvement of superexcited monocation states, therefore, should not be unexpected.

The present measurements support the view that in SO_2^{2+} dissociation both the charge separation products and the products of homolytic bond cleavage are formed in ground electronic states when dissociation occurs from the lowest states of the parent dication capable of undergoing such processes. When higher states of the dication are populated, however, it seems that electronically excited products are formed; further experiments are needed to test this.

Acknowledgement

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