Electronic structures of the S_2O and S_3 isomers: an *ab initio* CI study*,**

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The electronic structures of the S_2O and S_3 isomers have been dealt with by the multireference double-excitation (MRD) configuration-interaction (CI) calculations, using contracted $[5s3p1d]$ and $[4s2p1d]$ basis functions for the S and O atoms, respectively. The ground-state geometries for the SOS (symmetric chain), S_2O (symmetric ring) and SSO (unsymmetric chain) are optimized, and their vertical singlet excitation energies are calculated. It is found that SSO is the most stable of the three isomers and that the ground state ($^1A_1$) of the S_2O (ring) is correlated with the excited states of SOS (2^1A_1) and SSO ($3^1A'$). The chain and ring isomers of S_3 have been treated in a similar manner. Energetics for the ring closure of the O_3, SO_2, SSO and S_3 chain molecules are discussed on a unified ground.

Key words: Disulfur oxide (S_2O)—Thiozone (S_3)—Vertical excitation—Ring closure—CI calculations

1. Introduction

The electronic structures of S_2O and S_3 are intriguing in comparison with those of SO_2 and O_3, their isovalent homologs. It is known that the ground state of S_2O is in an unsymmetric SSO chain structure [1], but its stability relative to the

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symmetric SOS chain and the symmetric S_2O ring isomers remains to be examined. In the case of S_3 also, the chain structure appears to be slightly more stable than the ring form [2, 3], but the exact energy difference between them is still a matter of debate [4, 5].

In this work, we deal with the various isomers of S_2O and S_3 by the multireference double-excitation (MRD) CI calculations [6], using the $[5s3p1d]$ and $[4s2p1d]$ basis sets for the S and O atoms, respectively [7, 8]. the ground state geometries for the various isomers were optimized by locating the positions of the CI energy minima. The vertical singlet excitation energies were then computed, to understand the essential modes of the state correlations between the isomers. Variations in energy for the ground as well as the excited singlet states of chain S_2O and S_3 molecules undergoing ring closure are examined in detail in order to establish the state correlations. Similarities and dissimilarities in the electronic-structural properties of the S_nO_{3-n} [$n = 0, 1, 2$ and 3] are discussed in the light of the calculated ground state geometries and the singlet vertical excitation energies.

2. Method of calculations

All calculations were carried out by the multireference double-excitation (MRD) configuration-interaction (CI) method. The table MRD-CI program [9–11] was used throughout. The basis functions adopted for calculations are the contracted $[5s3p]/(12s9p)$ and $[4s2p]/(9s5p)$ sets for the S and O atoms, respectively [7, 8], both augmented with a set of d functions. The exponents adopted for the d orbitals are $\zeta_d(S) = 0.6$ and $\zeta_d(O) = 0.8$. The electronic configurations whose contributions $|C_i|^2$ to any given state exceed 0.5 % are all regarded as the main (reference) configurations. The number of the main configurations used for one state was typically 3 or 4.

In all calculations, the $1s$ orbitals (K shell) for both the S and O atoms were frozen as the core. The corresponding top-most molecular orbitals were also left out of the CI treatments. In addition, the low-lying molecular orbitals ascribable primarily to the $2s$ and $2p$ orbitals (L shell) for S were also treated as frozen orbitals, since they exert little influence on the resulting CI energies. The problems to be handled in the present CI procedure are thus those of the isoelectronic systems involving 18 valence electrons.

The lowest configuration selection threshold T was set to be a certain value between 5 and 30 μhartrees, depending on the size of the systems treated, so that the maximal dimension of the CI space could be kept close enough to, and yet below, 10 000. Four successive T values increasing stepwise by 5 μhartree each were then used to permit evaluation of the CI energy $E_{CI,T\to0}$ extrapolated to $T = 0$ μhartree. The generalized Langhoff–Davidson approximation [12] was adopted to estimate possible correlation errors that might arise from the use of a limited number of reference configurations. This last procedure can provide sufficiently reliable estimates of the full CI energies [11, 13]. The estimated full CI energies thus obtained will here be denoted as E_{CI}.

The optimal geometry for the ground state of each isomer was searched for by requiring that the calculated $E_{CI,T\to 0}$ be minimal. The E_{CI} values obtained at such geometries were adopted as the total energy for the ground state of given isomers.

The vertical singlet excitation energies were evaluated by multi-root CI calculations; the total number of the main configurations needed for such calculations ranged from 6 to 13, depending on the structure as well as the symmetry of the molecule considered. No attempt was made to locate the optimal geometries for excited states except for some special cases of particular interest.

3. Results

3.1. Singlet-triplet separation energy for O_2, SO and S_2

For the purpose of preliminary tests, the singlet–triplet spearation energies for the O_2, SO, and S_2 molecules as the diatomic homologs were examined. The $E_{CI,T\to 0}$ energies for the lowest singlet and triplet states of each diatomic molecule were calculated as the function of the interatomic distance. The theoretically optimal distance R which gives a minimal value of $E_{CI,T\to 0}$ was determined. The E_{CI} values for both the singlet and triplet states were obtained at their respective optimal distances R, to evaluate the singlet-triplet energy separations. The results of calculations are summarized in Table 1, together with the relevant experimental data [14].

Table 1 shows that the optimal bond distances R predicted for the singlet state are somewhat (by 0.01–0.02 Å) longer than those for the triplet state, in harmony with the experimental results. All these calculated distances are, however, uniformly too long (by 0.02–0.04 Å) as compared with the observed distances. The distances obtained in previous CI calculations for the triplet states all show a similar trend [15-18].

Table 1. The lowest singlet ($^1\Delta$) and triplet ($^3\Sigma^-$) states of O_2, SO and S_2

Molecule	State	Calcd[a]			Obsd[b]	
		R^c (Å)	ΔE_{SCF} (eV)	ΔE_{CI} (eV)	R (Å)	ΔE (eV)
O_2	$^3\Sigma_g^-$	1.228	(0)	(0)	1.2075	(0)
	$^1\Delta_g$	1.240	1.356	1.072	1.2156	0.981
SO	$^3\Sigma^-$	1.520	(0)	(0)	1.4811	(0)
	$^1\Delta$	1.531	1.057	0.818	1.4920	0.79
S_2	$^3\Sigma_g^-$	1.918	(0)	(0)	1.8892	(0)
	$^1\Delta_g$	1.929	0.852	0.596	1.8983	0.58

[a] Open-shell calculations with two-reference ($2M$) configurations
[b] See [14]
[c] Determined by minimizing the $E_{CI,T\to 0}$ values obtained. The minimal threshold values adopted for configuration selections are $T = 5$, 10 and 10 μhartrees for O_2, SO and S_2, respectively

For the singlet-triplet energy gap in question, the theoretically obtained data ΔE_{CI} agree reasonably well with the experimental results. The deviation of ΔE_{CI} from the experimental energy gap ΔE is largest (0.091 eV) in the case of O_2. The gap tends to decrease in the order $O_2 > SO > S_2$, and so does the deviation of ΔE_{CI} from ΔE. The open-shell SCF energy gaps ΔE_{SCF} are too large compared with the experimental data and hence cannot be regarded as a useful criterion for quantitative considerations.

As a whole, the present CI procedure appears to be reliable enough in at least semi-quantitative considerations of the electronic structures of small compounds comprising the S and O atoms. Dependences of the results on the size of the basis functions were not examined, but the basis sets employed in this work are believed to be sufficient in quality for comparative studies of the S_2O as well as S_3 isomers.

3.2. S_2O isomers

Three isomers are conceivable for S_2O. They are SOS (symmetric chain), S_2O (ring) and SSO (unsymmetric chain). Of these three isomers, SSO is the only observed entity ($r_{SS} = 1.884$ Å, $r_{SO} = 1.465$ Å and $\theta_{SSO} = 118.0°$) [1].

To begin with, geometries for the ground electronic state of these isomers were optimized by requiring that the calculated $E_{CI,T \to 0}$ be minimal. The optimized structures are given in Table 2. SOS is bent ($\theta_{SOS} = 120.6°$) and symmetric (C_{2v}). The ring isomer, which will hereafter be denoted as $S_2O(R)$, is also structurally symmetric (C_{2v}) with the bond angle $\theta_{SOS} = 74.5°$, and SSO is a bent chain (C_s symmetry) with an optimized structure ($r_{SS} = 1.884$ Å, $r_{SO} = 1.500$ Å and $\theta_{SSO} = 117.5°$) that is in good agreement with the experimentally determined one [1].

Table 2. Optimized geometries and the relative stabilities of the S_2O isomers

		SOS	$S_2O(R)$	SSO
Geometry[a]	r_{SO} (Å)	1.65	1.71	1.500
	r_{SS} (Å)	—	2.07	1.884
	θ_{SOS} (°)	120.6	74.5	—
	θ_{SSO} (°)	—	52.75	117.5
Symmetry		$^1A_1(C_{2v})$	$^1A_1(C_{2v})$	$^1A'(C_s)$
Principal configuration		$...(9a_1)^2(2a_2)^2$ $(2b_1)^2(7b_2)^2$	$...(9a_1)^2(2a_2)^2$ $(3b_1)^2(6b_2)^2$	$...(16a')^2(4a'')^2$
Energy, $E + 870$ (hartree)				
SCF		0.28234	0.22109	0.17897
$CI, T \to 0$		-0.16609	-0.17620	-0.23622
CI		-0.20968	-0.22145	-0.27953
Relative energy (eV)				
ΔE_{CI}^G		1.90	1.58	(0)

[a] Based on the minimum of $E_{CI,T \to 0}$

Both SOS and $S_2O(R)$ in the ground state belong to the irreducible representation A_1. Clearly, the ground state ($\tilde{X}\,^1A_1$) of $S_2O(R)$, which is a 6π-valence-electron system, has an electronic structure that is correlated with an excited singlet state of SOS which would result from the two-electron transition $(7b_2)^2 \to (3b_1)^2$. SSO in its ground state ($\tilde{X}\,^1A'$) is a 4π-valence-electron system, and so is the symmetric chain molecule SOS($\tilde{X}\,^1A_1$).

Table 2 also lists the total energies calculated for the optimized geometries. The SCF and CI energies obtained unanimously indicate that SSO is the most stable of the three isomers. Their relative ground-state energies, expressed by taking SSO as standard, are $\Delta E_{CI}^G = 1.90$ (SOS), 1.58 ($S_2O(R)$) and 0 (SSO) eV. The pattern of the relative stabilities found for these isomeric molecules is in contrast to that reported for a similar isomeric family of SO_2; 0 (OSO), 4.1 ($SO_2(R)$) and 4.3 (SOO) eV [19].

Next, singlet excited states of the S_2O isomers were examined. The vertical excitation energies ΔE_{CI}^{vert} obtained by muti-root CI calculations for each irreducible representation of the isomers are shown in Table 3. For the sake of easier comparison of the results, the level heights of all the singlet ground and excited states examined here are diagrammatically illustrated in Fig. 1, taking the $\tilde{X}\,^1A_1$ state of SSO as the common standard. The state energies shown in Fig. 1 are, therefore,

$$\Delta E_{CI} = \Delta E_{CI}^{vert} + \Delta E_{CI}^G. \tag{1}$$

As is shown in Fig. 1, the ground state of $S_2O(R)$ is correlated with the $3^1A'$ state (the lowest 6π-valence-electron system) of SSO, which results from the two-electron transition $(15a')(16a') \to (5a'')^2$. Also, it is the $2^1A_1(6\pi)$ state of SOS that the ground-state $S_2O(R)$ approaches as the S–S bond is broken. Note that the $2^1A'$ state of SSO is the so-called $\pi-\pi^*$ excited state, which is ascribable primarily to the one-electron transition $(4a'') \to (5a'')$.

The state correlations between $S_2O(R)$ and SSO were examined in more detail. Thus, the variations in ΔE_{CI} of the four low-lying $^1A'$ states of SSO with the decrease in the SSO bond angle θ were traced. θ was allowed to diminish from

Table 3. Vertical excitation energies ΔE_{CI}^{vert} (eV) of the S_2O isomers

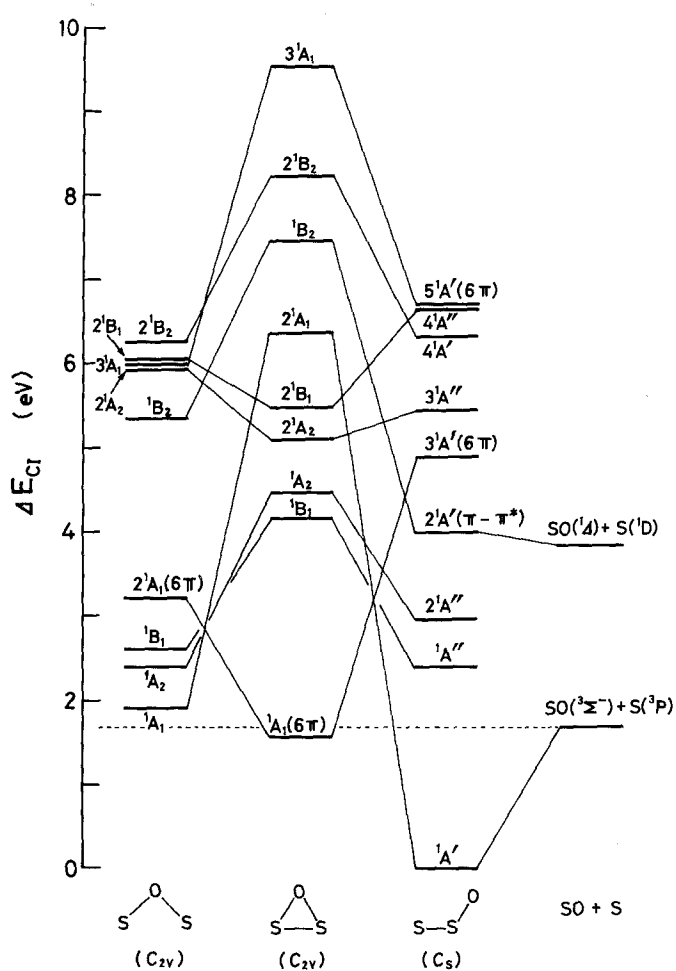| State	SOS (C_{2v})	$S_2O(R)$ (C_{2v})	SSO (C_s)
$^1A_1(^1A')$	(0)	(0)	(0)
$^1B_1(^1A'')$	0.63	2.60	2.39
$^1A_2(2^1A'')$	0.49	2.91	2.97
$^1B_2(2^1A')$	3.45	5.90	4.00
$2^1A_1(3^1A')$	1.31	4.82	4.92
$2^1B_1(3^1A'')$	4.15	3.92	5.49
$2^1A_2(4^1A'')$	4.04	3.54	6.66
$2^1B_2(4^1A')$	4.36	6.64	6.37
$3^1A_1(5^1A')$	4.12	7.98	6.97

Fig. 1. Vertical singlet excitations of the S_2O isomers. The state energy levels are given, taking the ground state ($^1A'$) of SSO as the common origin

117.5°, the optimal bond angle for SSO($\tilde{X}\,^1A'$), down to 52.75°, where the ring closure giving rise to $S_2O(R)(\tilde{X}\,^1A_1)$ may be considered to have been completed. The bond lengths r_{SS} and r_{SO} were varied linearly with the change in θ:

$$r_{SS} = 1.884 + (117.5 - \theta)(2.07 - 1.884)/(117.5 - 52.75) \tag{2}$$

and

$$r_{SO} = 1.500 + (117.5 - \theta)(1.71 - 1.50)/(117.5 - 52.75) \tag{3}$$

The results of calculations are shown in Fig. 2.

As can be seen in Fig. 2, the curve connecting the $^1A_1(6\pi)$ state of $S_2O(R)$ and the $3^1A'(6\pi)$ state of SSO crosses the $^1B_2-2^1A'$ curve as well as the $2^1A_1-{}^1A'$ (ground state) curve, corroborating the state correlations shown in Fig. 1. Apparently, the avoided crossings associated with the $3^1A'(6\pi)$ state are too
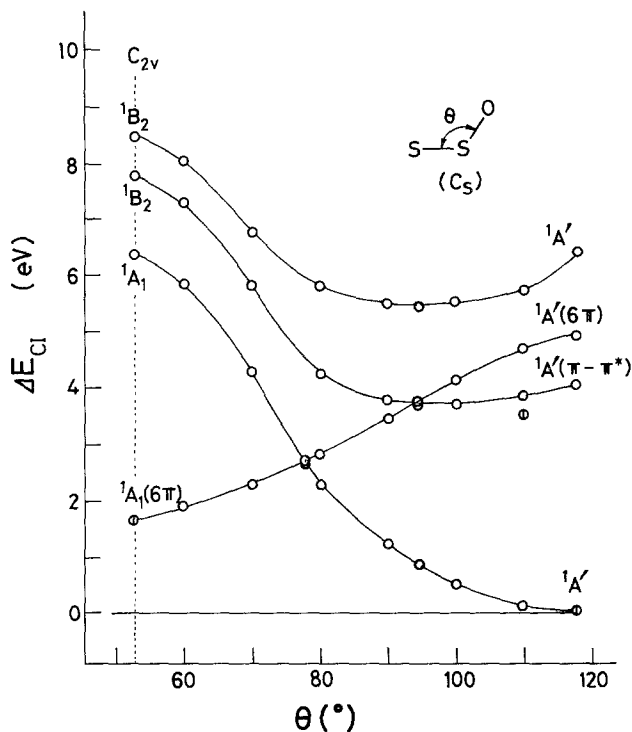
Fig. 2. Variations in the CI energies for low-lying $^1A'(C_s)$ states of SSO with the change in the bond angle θ. ⊕ indicates the plots for the CI-optimized geometries. The bond distances are varied in proportion to the change in θ

sharp to be discernible. The $\tilde{X}\,^1A'$ curve intersects the $3\,^1A'(6\pi)$ curve at the bond angle $\theta = 77.8°$; the crossing point lies 2.63 eV above the ground state of SSO. It can also be seen in Fig. 2 that both the $2\,^1A'$ and $4\,^1A'$ states appear to take on an energy minimum at a structure where θ is somewhat smaller than the optimal bond angle of $117.5°$ for the ground state.

For the $2\,^1A'(\pi - \pi^*)$ and the lowest $^3A''$ states of SSO, geometry optimizations based on $E_{CI,T\to0}$ have been carried out separately. The equilibrium geometry for the former has proved to be such that $r_{SS} = 2.15$ Å, $r_{SO} = 1.50$ Å and $\theta_{SSO} = 110°$. The predicted bond angle agrees well with the value $109°$ deduced from the results of the fluorescence spectroscopy [20]. The adiabatic excitation energy obtained in the present CI treatment is 3.51 eV, which compares well with the experimental value of 3.68 eV [21]. The lowest $^3A''$ state has been found to have essentially the same geometry as the $2\,^1A'$ state. The calculated adiabatic excitation energy is as low as 1.81 eV, in reasonable agreement with the value of 1.7 eV estimated from the phosphorescence excitation spectrum [21].

3.3. S_3 isomers

The relative stabilities of the open chain structure (C_{2v}) and the ring isomer (D_{3h}) of S_3 have been a matter of debate. Thus, the Hartree-Fock SCF calculations [2, 4] predict that the ring isomer is more stable, whereas CI calculations [2]

tend to favor the chain form. A local spin density (LSD) treatment [3] of the exchange-correlation energy concludes that the open chain is more stable by 0.61 eV. A more recent LSD approximation [5], however, predicts a near-degeneracy between the two forms, with a marginal preference (<0.1 eV) for the ring structure.

In view of the above-mentioned controversies, we felt it worthwhile to extend the present study to the S_3 isomers. Geometries of both the ring (D_{3h}) and chain (C_{2v}) isomers of S_3 were optimized on the basis of the $E_{CI,T\to 0}$ values calculated. The results are given in Table 4. The optimal S–S bond distance for the ring isomer is 2.100 Å, a value which agrees well with 2.1 Å obtained by an early SCF calculation [4]. The structure ($r_{SS} = 1.914$ Å and $\theta = 119.0°$) obtained here for the S_3 chain is also in accord with that ($r_{SS} = 1.92$ Å and $\theta = 117.5°$) deduced by the SCF calculations [4]. However, the structural parameters obtained by the present CI procedure differ somewhat from those that have recently been deduced by Jones from the LSD calculation results: $r_{SS} = 2.16$ Å for the D_{3h} ring, and $r_{SS} = 2.00$ Å and $\theta = 114°$ for the C_{2v} chain [5].

As for the relative stabilities of the isomers, the present CI study predicts that the chain form is more stable than the ring isomer. The energy difference based on the E_{CI} values is 0.32 eV, which is noticeably smaller than the value 0.73 eV reported in a previous CI study [2]. Again, our prediction, which favors the chain isomer, contradicts the conclusion reached by Jones on the basis of the LSD approximation [5]. The energy difference obtained in this work for the S_3 isomers is, however, much smaller than the difference (1.2 eV) reported for the case of O_3 [21]. We will give a more detailed and unified discussion of the chain-ring problem for S_nO_{3-n} [$n = 0, 1, 2$ and 3] later.

Clearly, the ring isomer of S_3 is essentially a 6π-valence-electron system; hence

Table 4. Optimized geometries and the relative stabilities of the chain and ring isomers of S_3

		S_3 (ring)	S_3 (chain)
Geometry[a]	r_{SS} (Å)	2.100	1.914
	θ_{SSS} (°)	60.0	119.0
Symmetry		$^1A_1'(D_{3h})$	$^1A_1(C_{2v})$
Principal configuration (C_{2v})		$\ldots(4b_1)^2(7b_2)^2$ $(11a_1)^2(2a_2)^2$	$\ldots(3b_1)^2(8b_2)^2$ $(11a_1)^2(2a_2)^2$
Energies, $E + 1192$ (hartree)			
	SCF	−0.47675	−0.46531
	CI, $T \to 0$	−0.82745	−0.84225
	CI	−0.87139	−0.88333
Relative energy (eV)			
	ΔE_{CI}^G	0.32	(0)

[a] Based on the minimum of $E_{CI,T\to 0}$

the ground state ($\tilde{X}\,^1A_1'$) of the S_3 ring (D_{3h}) should correlate with the $2^1A_1(6\pi)$ state of the S_3 bent chain (C_{2v}), exactly as in the case of O_3 [22]. Our CI calculations have indicated, however, that the $2^1A_1(6\pi)$ states of S_3 (chain) at the geometry of the ground state is primarily a mixture of two two-electron transition configurations, $(8b_2)^2 \to (4b_1)^2$ and $(11a_1)^2 \to (4b_1)^2$, with the contribution of the latter component ($|C_i|^2 = 0.703$) outweighing that of the former ($|C_i|^2 = 0.168$). The vertical excitation energy is calculated to be 3.14 eV. As the ring closure proceeds, the contribution of the former configuration increases progressively until it reaches a maximum ($|C_i|^2 = 0.874$). The state energy is lowered monotonically, finally attaining the energy for the ground state S_3 ring.

Illustrated in Fig. 3 are the variations in ΔE_{CI} for the three lowest-lying $^1A_1$ states of S_3 (chain) with the change in the bond angle. In calculating E_{CI}, the C_{2v} symmetry has been assumed and the S–S bond distances r_{SS} have been altered linearly with the change in θ:

$$r_{SS} = 1.914 + (119 - \theta)(2.100 - 1.914)/(119 - 60) \qquad (4)$$

It can be seen in Fig. 3 that the curve associated with the $2^1A_1(6\pi)$ state intersects that for the ground state ($\tilde{X}\,^1A_1$) of S_3 (chain). Here again, the avoided crossing is so sharp that it is practically indiscernible. The crossing point lies at an angle $\theta = 87°$ with the energy height of 1.50 eV. It is noteworthy that this energy barrier (1.50 eV) for the ring closure of S_3 (chain) in the ground state is as low as the lowest singlet ($^1B_1$) vertical excitation energy (1.53 eV).
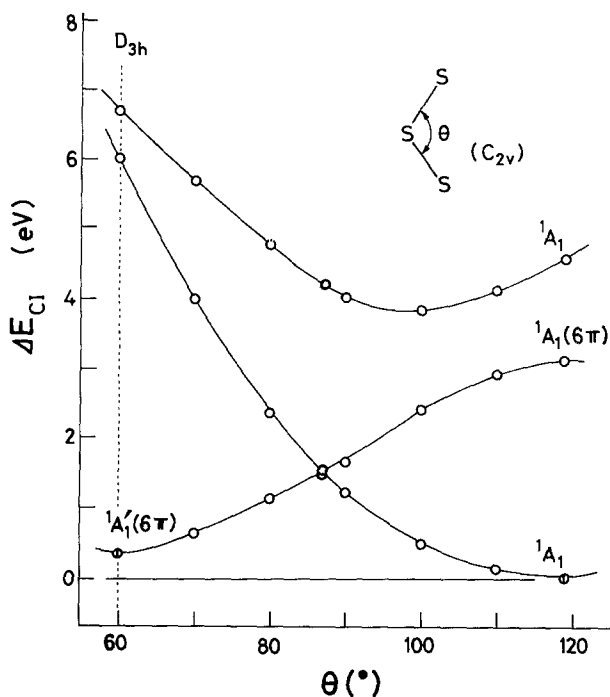

Fig. 3. Variations in the CI energies for the three lowest $^1A_1(C_{2v})$ states of the bent chain S_3 molecule with the change in the bond angle θ. $\oplus$ indicates the plots for the CI-optimized geometries. The bond distances are varied in proportion to the change in θ

4. Discussion

Of the triatomic molecules O_3, SO_2, S_2O and S_3, which are isoelectronic homologs, S_2O is unique in that its most stable form is structurally unsymmetric. The symmetric isomer SOS, which has hitherto never been identified experimentally, should be much less stable than SSO.

The ground states for the ring isomers of all these triatomic molecules have electronic structures that are related to the lowest 6π-electron excited states of the chain isomers. The vertical excitation energies ΔE_{CI}^{vert} for the 2^1A_1 ($3^1A''$) states of these chain molecules decrease in the order:

$$SO_2 > SSO > O_3 > S_3$$

as is shown in Fig. 4. The ground-state energies ΔE_{CI}^{G} of the ring isomers relative to the bent chain molecules in their ground state decrease in exactly the same order (Table 5). As a natural consequence, the energy barrier height which the
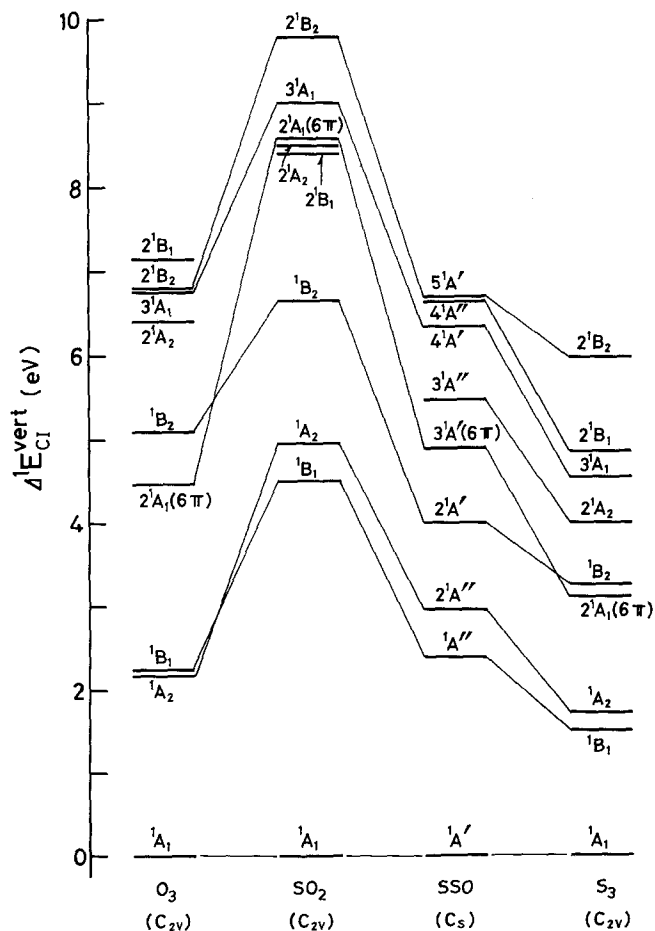

Fig. 4. Comparisons of the vertical singlet excitation energies for the bent chain O_3, SO_2, SSO and S_3 molecules. For O_3 and SO_2, the experimental geometries [1] are used. For the geometries of SSO and S_3, see Tables 2 and 4, respectively

Table 5. Comparisons of the chain-ring energetics for O_3, SO_2, SSO and S_3

Energy	O_3	SO_2	SSO	S_3
ΔE_{CI}^{vert}(eV) chain $2^1A_1(3^1A')^a$	4.48	8.7	4.92	3.14
ΔE_{CI}(eV) barrier height[b]	2.1[e]	~6	2.63	1.50
ΔE_{CI}^G(eV) ring isomer[c]	1.2[f]	4.1[g]	1.58	0.32
λ^{LUMO}(eV) chain $^1A_1(^1A')^d$	−1.263 ($2b_1$)	0.408 ($3b_1$)	−0.797 ($5a''$)	−1.420 ($4b_1$)

[a] Vertical excitation energy for the lowest 6π-valence-electron state of the chain isomer. For O_3 and SO_2, the experimental geometries [1] are used
[b] Energy barrier height against the ring closure of the chain isomer in the ground state (see Figs. 2 and 3 for SSO and S_3, respectively)
[c] Total energy for the ring isomer relative to the chain isomer (see Tables 2 and 4 for SSO and S_3, respectively)
[d] Orbital energy of the lowest unoccupied MO for the chain isomer in the ground state
[e] See [23]
[f] See [22]
[g] See [19]

chain molecules will have to overcome in effecting the ring closure also decreases in this order. In simple language, all these parallel features are a reflection of the relative heights λ^{LUMO} of the lowest unoccupied $b_1(a'')$ molecular orbitals in the ground-state bent chain molecules, as can be seen from Table 5. The bond angles for the chain isomers, 116.8° (O_3), 119.5° (SO_2), 117.5° (SSO) and 119° (S_3), have no bearing on the relative stabilities of the ring isomers.

The present study predicts that $SSO(\tilde{X}\,^1A')$ should dissociate thermally according to

$$SSO(\tilde{X}\,^1A') \to S(^3P) + SO(^3\Sigma^-) \tag{5}$$

However, the calculated dissociation energy is 1.77 eV, which is too small compared with the thermochemical value of 3.45 ± 0.01 eV [24]. The energetics predicted for the dissociation process

$$SOS(\tilde{X}\,^1A_1) \to S(^3P) + SO(^3\Sigma^-) \tag{6}$$

will likewise involve an error amounting to approximately 1.7 eV. Correcting for this error, the dissociation energy for process (6) is estimated to be approximately 1.6 eV. It is thus likely that $SOS(\tilde{X}\,^1A_1)$ is a species capable of existing in the gas phase under ordinary conditions, once it is formed.

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