Table 3. *Interatomic distances*

Caesium–oxygen distances (standard deviation ± 0.02 Å)

Cs–O(1), Cs–O(1')	3·40 Å
Cs–O(2), Cs–O(2')	3·36
Cs–O(3), Cs–O(3'')	3·38
Cs–O(4'), Cs–O(4'')	3·24
Cs–O(5'), Cs–O(5'')	3·14

Boron–oxygen bond lengths (standard deviation $\pm$ 0·05Å)
in triangles

B(1)–O(1)	1·43 Å	B(3)–O(2)	1·32 Å
B(1)–O(4)	1·35	B(3)–O(5)	1·42
B(1)–O(5)	1·35	B(3)–O(6)	1·41
B(2)–O(3)	1·31	B(4)–O(1)	1·33
B(2)–O(4)	1·44	B(4)–O(6)	1·28
B(2)–O(8')	1·23	B(4)–O(7)	1·37

Boron–oxygen bond lengths in the tetrahedron

B(5')–O(2), B(5')–O(2')	1·46 Å
B(5')–O(3), B(5')–O(3')	1·43

with the average values 3·27 and 3·37 Å reported in *International Tables for X-ray Crystallography* (1962) for caesium coordinated by 8 and 12 oxygen atoms respectively.

The presence of boroxol groups in caesium enneaborate is interesting. It has been suggested from spectroscopic data (Krogh-Moe, 1965) that boron oxide glass consists largely of boroxol groups. This would seem to be supported by the here established tendency to form such groups in borates of very low alkali content.

References

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The Crystal Structure of *cis*-2-Butene Episulfone

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The crystal structure of *cis*-2-butene episulfone has been determined by X-ray diffraction techniques. The crystals are orthorhombic, space group $Pna2_1$ (C^9_{2v}), with four molecules per unit cell. The unit cell constants are $a = 9.790 \pm 0.006$, $b = 11.04 \pm 0.005$ and $c = 5.53 \pm 0.01$ Å. Atomic and thermal coordinates were refined by isotropic least-squares methods. A unique feature of this molecule is the unusually long observed ring carbon–carbon bond length of 1·60 Å.

Introduction

We have determined the crystal structure of *cis*-2-butene episulfone as part of a program of research on the effect of the sulfone group on the geometry of small ring systems.

Experimental

Crystals of *cis*-2-butene episulfone prepared by the method of Hesse, Reichold & Majmudar (1957) were obtained from Dr S. Hastings of the Humble Oil Company Research Laboratories, Baytown, Texas. These crystals were long, white needles averaging about 0·2–0·3 mm in diameter. Several crystals were mounted along the needle axis and a series of rotation, precession and Weissenberg photographs were taken. Because the compound slowly decomposed at room temperature, all X-ray data were obtained with the crystals enclosed in glass capillaries under an equilibrium pressure of SO_2 and butene.

On the basis of Weissenberg (Cu $K\alpha$ radiation, $\lambda = 1.5418$ Å) and precession (Mo $K\alpha$ radiation, $\lambda = 0.707$ Å) photographs, the Laue symmetry was found to be orthorhombic. The observed systematic absences are

$0kl$ absent when $k + l = 2n + 1$
$h0l$ absent when $h = 2n + 1$.

The two space groups corresponding to this set of absences are $Pnam$ (D^{16}_{2h}) and $Pna2_1$ (C^9_{2v}). The unit-cell constants, determined from sodium chloride calibrated rotation and zero layer Weissenberg photographs, are

$$a = 9.790 \pm 0.006 \text{ Å}$$
$$b = 11.040 \pm 0.005$$
$$c = 5.53 \pm 0.01$$
$$[a_0(\text{NaCl}) = 5.637 \text{ Å}]$$

Density measurements showed that the unit cell contains four molecules. If the centric space group $Pnam$ (D^{16}_{2h}) were the correct one, the molecules must lie on the mirror planes located at $z = \pm \frac{1}{4}$. However, this type of structure was considered highly unlikely because the short repeat distance in the **c** direction would place successive molecules too close together. For this reason, $Pnam$ was discarded and $Pna2_1$ was assumed to be the correct space group. This assumption was later proven to be correct.

Multiple-film equi-inclination Weissenberg photographs of the $l = 0$, 1, 2 and 3 layers were taken with filtered Cu $K\alpha$ radiation. The intensities of the various reflections were estimated visually by comparison with a standard intensity strip. Interlayer correlation of intensities was made with data from $h0l$ and $0kl$ per-

cession photographs. The intensities were corrected by the appropriate Lorentz, polarization and Tunell factors; absorption was neglected.

Structure determination

A sharpened Patterson projection, $P(uv)$, was synthesized with the use of the 95 observed $hk0$ reflections. A set of peaks attributed to sulfur–sulfur interactions was consistent with a sulfur atom located at $x=0\cdot167$ and $y=0$. Using these trial parameters, a fourfold superposition function was synthesized. The resulting map, although clearly resolved, contained a set of false symmetry elements which necessarily arose because the y parameter of the sulfur atom was zero. Nevertheless, a straightforward treatment of the observed peaks gave a consistent set of trial coordinates for the molecule. A total of 124 observed and unobserved reflections were then used in a full-matrix, isotropic, two-dimensional least-squares refinement of this trial structure. Form factors were obtained from *International Tables for X-ray Crystallography* (1962), using a table look-up and linear interpolation. During early stages of refinement, all reflections were given equal weights. For the

Table 1. *Observed and calculated structure factors*

h	k	Y(obs)	Y(calc)		h	k	Y(obs)	Y(calc)		h	k	Y(obs)	Y(calc)		h	k	Y(obs)	Y(calc)		h	k	Y(obs)	Y(calc)
		l = 0			7	7	10.29	11.69		4	8	15.86	15.15		2	5	17.20	18.15		1	2	3.77	3.69
0	2	73.91	80.11		7	8	3.57	.66		4	9	·2.29	.63		2	6	19.47	19.59		1	3	13.29	12.22
0	4	24.12	23.19		7	9	3.32	1.73		4	10	5.61	5.13		2	7	6.03	7.86		1	4	9.06	8.60
0	6	4.34	3.50		8	0	5.13	3.79		4	11	4.34	2.82		2	8	11.09	11.31		1	5	13.82	13.12
0	8	20.39	19.94		8	1	<2.29	1.50		4	12	5.39	4.28			9	<2.74	1.79		1	6	4.56	4.55
0	10	9.97	11.31		8	2	5.00	4.38		5	1	14.54	15.01		2	10	5.39	4.08		1	7	16.73	16.08
0	12	9.55	8.81		8	3	<2.29	4.19		5	2	9.20	8.38		2	11	4.30	3.21		1	8	<2.65	3.31
0	14	2.21	3.97		8	4	9.94	9.50		5	3	16.35	14.85		2	12	<2.38	1.75		1	9	9.06	9.47
1	1	45.33	45.66		8	5	6.95	7.57		5	4	5.18	5.14		2	13	3.68	3.77		1	10	<2.65	2.50
1	2	23.67	24.59		8	6	<2.29	2.52		5	5	23.96	22.37		3	1	34.50	34.52		1	11	4.43	6.25
1	3	13.28	12.09		8	7	<2.29	3.10		5	6	4.59	3.93		3	2	10.60	10.27		2	0	30.36	31.88
1	4	18.78	16.69		8	8	4.63	3.83		5	7	20.26	19.24		3	3	21.91	21.91		2	1	3.44	2.94
1	5	6.81	9.62		8	9	<2.19	1.41		5	8	6.77	6.21		3	4	15.49	15.78		2	2	26.37	24.82
1	6	18.96	19.98		8	10	4.32	3.93		5	9	8.39	7.72		3	5	23.15	22.64		2	3	8.47	7.47
1	7	8.93	7.39		9	1	15.99	16.76		5	10	<2.29	2.84		3	6	4.00	3.63		2	4	17.59	17.57
1	8	14.66	14.43		9	2	<2.19	3.55		5	11	4.75	4.09		3	7	23.55	22.12		2	5	4.59	5.55
1	9	7.44	6.92		9	3	10.92	11.93		6	0	14.33	12.86		3	8	<2.65	1.24		2	6	16.89	15.85
1	10	6.18	7.13		9	4	<2.10	.72		6	1	7.44	6.30		3	9	12.41	11.84		2	7	<2.56	2.17
1	11	5.45	5.45		9	5	7.10	8.21		6	2	7.83	9.24		3	10	5.24	2.42		2	8	9.67	10.85
1	12	7.58	6.89		9	6	<2.10	3.37		6	3	6.34	5.76		3	11	5.86	5.24		2	9	<2.56	1.35
1	13	4.16	4.64		9	7	6.60	7.58		6	4	6.45	5.98		3	12	3.95	2.69		2	10	4.85	6.34
2	0	64.71	70.82		9	8	<2.01	.48		6	5	9.07	6.69		3	13	3.50	3.65		3	1	17.31	15.91
2	1	5.26	6.29		9	9	5.87	6.50		6	6	7.48	7.90		4	0	27.17	29.14		3	2	7.52	7.77
2	2	28.94	31.74		10	0	7.76	8.73		6	7	6.61	5.87		4	1	4.52	3.41		3	3	<2.47	3.36
2	3	29.64	34.19		10	1	<2.01	2.51		6	8	<2.19	1.51		4	2	21.34	20.84		3	4	4.81	5.22
2	4	40.58	41.65		10	2	6.55	7.50		6	9	4.67	3.86		4	3	10.22	11.24		3	5	7.00	5.72
2	5	6.50	7.33		10	3	4.16	4.53		6	10	3.80	3.12		4	4	12.41	12.68		3	6	8.95	8.85
2	6	12.33	12.24		11	1	<2.01	2.19		6	11	3.80	3.60		4	5	8.73	7.57		3	7	5.18	4.15
2	7	<2.29	1.19		11	2	<2.01	3.16		7	1	17.70	16.21		4	6	11.36	10.23		3	8	<2.74	3.98
2	8	7.95	7.07		11	3	4.00	5.45		7	2	7.39	6.75		4	7	7.50	7.43		3	9	<2.74	1.01
2	9	<2.29	1.57		11	4	<2.01	2.52		7	3	15.89	14.51		4	8	5.43	3.66		3	10	4.43	4.26
2	10	<2.29	.69		11	5	4.40	5.08		7	4	2.47	1.37		4	9	6.03	5.72		4	0	22.16	20.93
2	11	7.79	8.03		12	0	3.34	4.55		7	5	11.57	11.84		5	1	4.64	4.95		4	1	5.06	4.07
2	12	<1.83	2.96		12	1	<1.83	.58		7	6	6.21	5.78		5	2	8.04	8.12		4	2	21.37	20.19
2	13	4.16	5.23		12	2	4.32	6.36		7	7	7.52	7.78		5	3	17.20	15.82		4	3	5.06	4.25
3	1	36.56	38.95		12	3	<1.83	1.37		7	8	<2.29	2.91		5	4	<2.65	2.71		4	4	16.73	15.64
3	2	2.76	3.56		12	4	3.71	6.24		7	9	6.93	7.79		5	5	16.82	15.59		4	5	8.17	7.68
3	3	29.54	29.89				*l = 1*			7	10	<2.19	2.32		5	6	9.07	9.45		4	6	17.43	17.33
3	4	5.05	5.19		0	3	50.90	66.25		7	11	5.13	5.17		5	7	8.16	7.54		4	7	4.85	5.55
3	5	32.12	33.78		0	5	22.79	22.66		8	0	17.34	16.26		5	8	7.62	7.36		4	8	7.75	8.55
3	6	3.71	2.83		0	7	11.92	10.08		8	1	6.83	6.77		5	9	<2.47	3.64		4	9	<2.56	2.45
3	7	23.67	22.22		0	9	<2.10	.65		8	2	14.27	14.23		5	10	6.33	6.11		4	10	4.70	5.12
3	8	14.66	13.17		0	11	7.72	7.88		8	3	8.74	9.07		5	11	<2.38	2.13		5	1	23.71	21.42
3	9	12.74	11.03		0	13	6.21	5.73		8	4	10.44	9.42		5	12	3.60	3.89		5	2	5.65	5.24
3	10	5.39	6.44		1	1	58.98	72.99		8	5	<2.47	3.01		6	0	26.72	26.67		5	3	15.02	15.97
3	11	5.71	5.61		1	2	19.96	19.92		8	6	8.90	9.82		6	1	12.01	11.45		5	4	<2.65	1.58
3	12	<1.83	.53		1	3	36.69	34.70		8	7	<2.38	1.55		6	2	23.67	22.98		5	5	14.01	14.51
3	13	7.10	6.59		1	4	21.23	21.50		8	8	6.15	6.89		6	3	11.91	12.61		5	6	<2.65	3.18
4	0	12.71	10.24		1	5	33.18	31.83		9	1	<2.19	1.58		6	4	19.38	17.41		5	7	9.66	11.04
4	1	24.68	26.73		1	6	4.10	4.53		9	2	4.40	4.60		6	5	<2.65	2.14		5	8	<2.56	3.09
4	2	3.34	1.58		1	7	19.45	18.76		9	3	<2.10	2.75		6	6	13.60	13.77		5	9	5.43	5.39
4	3	13.92	13.98		1	8	6.39	5.83		9	4	4.34	4.41		6	7	<2.56	3.33		6	0	6.87	6.38
4	4	5.21	4.76		1	9	12.68	12.54		10	0	8.82	8.99		6	8	8.96	9.14		6	1	<2.56	3.30
4	5	6.39	5.88		1	10	<2.29	1.02		10	1	<2.10	1.27		6	9	<2.47	1.23		6	2	4.32	4.17
4	6	15.39	14.37		1	11	6.75	7.13		10	2	8.69	9.36		6	10	5.66	5.49		6	3	7.09	7.18
4	7	13.34	12.73		1	12	5.05	4.47		10	3	<1.83	1.48		7	1	10.09	10.43		6	4	<2.56	1.66
4	8	15.33	14.38		1	13	6.50	5.44		10	4	8.15	8.31		7	2	4.56	3.97		6	5	6.83	5.95
4	9	7.58	6.65		2	0	69.48	77.59		10	5	<1.74	3.22		7	3	4.56	4.59		6	6	<2.65	.83
4	10	5.26	5.05		2	1	17.08	16.53		10	6	4.34	4.52		7	4	4.64	3.95		6	7	5.94	5.37
4	11	5.45	5.26		2	2	11.30	33.24		10	7	<1.74	.89		7	5	6.08	4.92		6	8	<2.65	1.70
5	1	18.41	18.75		2	3	36.69	35.43		10	8	3.72	3.94		7	6	6.08	4.92		6	9	5.18	4.52
5	2	17.39	18.57		2	4	17.54	17.81		11	1	6.67	7.68		7	7	6.92	6.17		7	1	15.02	15.58
5	3	12.15	10.88		2	5	15.38	12.89		11	2	<1.83	1.32		7	8	6.92	5.35		7	2	8.80	8.03
5	4	3.71	3.77		2	6	19.69	16.56		11	3	4.96	6.06		7	9	<2.47	3.29		7	3	14.69	13.44
5	5	7.71	7.02		2	7	14.54	13.75		11	4	<1.83	.12		7	10	4.52	3.29		7	4	<2.56	2.68
5	6	6.55	6.65		2	8	20.77	17.64		11	5	3.07	4.02		8	0	13.87	13.97		7	5	10.86	9.96
5	7	<2.29	4.04		2	9	6.56	6.43				*l = 2*			8	1	<2.56	1.71		7	6	<2.56	2.41
5	8	<2.29	2.47		2	10	8.37	8.52		0	2	19.85	22.33		8	2	11.52	11.93		7	7	6.58	6.43
5	9	7.20	7.66		2	11	4.67	3.82		0	4	29.16	31.63		8	3	<2.56	1.06		8	0	9.62	11.04
5	10	<2.29	1.14		2	12	6.67	6.67		0	6	26.26	26.90		8	4	6.08	5.17		8	1	<2.65	3.47
5	11	3.71	4.35		3	1	26.43	25.33		0	8	17.37	17.81		8	5	<2.38	1.41		8	2	9.00	8.25
6	0	8.80	7.16		3	2	13.76	12.76		0	10	10.60	9.37		8	6	<2.38	.95		8	3	<2.65	2.72
6	1	<2.29	2.64		3	3	13.36	14.44		0	12	6.56	6.77		9	1	11.94	12.20		8	4	8.09	6.94
6	2	9.81	8.68		3	4	4.76	5.82		1	1	38.71	40.41		9	2	<2.38	2.48		8	5	<2.56	1.86
6	3	<2.29	1.86		3	5	13.70	11.86		1	2	12.94	13.19		9	3	10.22	10.44		8	6	7.18	6.24
6	4	22.25	21.83		3	6	9.12	10.28		1	3	8.16	7.79		9	4	<2.38	.79		8	7	<2.56	1.55
6	5	3.76	7.77		3	7	<2.74	2.53		1	4	12.41	12.77		9	5	7.09	6.99		8	8	5.18	5.07
6	6	20.21	20.66		3	8	6.66	6.87		1	5	7.15	7.08		9	6	<2.38	.54		10	0	5.81	5.45
6	7	<2.29	.74		3	9	<2.29	2.39		1	6	4.21	3.12		9	7	4.96	4.41		10	1	<2.65	.64
6	8	15.15	14.47		3	10	6.15	5.36		1	7	9.45	9.64		10	0	5.49	5.54		10	2	5.43	6.22
6	9	<2.29	.37		3	11	4.10	2.38		1	8	8.83	7.83		11	1	4.00	3.18		10	3	<2.56	1.60
6	10	5.00	5.99		3	12	6.10	5.39		1	9	8.90	8.73		11	2	<2.38	.60		10	4	<2.65	5.26
6	11	<2.01	.54		4	0	21.12	22.38		1	10	<2.56	1.30		11	3	4.07	4.14		11	1	3.70	4.49
6	12	3.81	4.06		4	1	6.26	6.32		1	11	5.66	4.71				*l = 3*					*l = 4*	
7	1	6.50	5.57		4	2	17.48	17.62		1	12	4.96	4.64		0	1	12.92	13.12		0	0	31.23	32.16
7	2	9.76	9.40		4	3	9.12	9.31		2	0	31.27	32.55		0	3	16.13	17.29		0	2	25.12	24.71
7	3	8.76	8.42		4	4	31.02	30.37		2	1	8.79	7.97		0	5	14.54	12.87		0	6	7.59	11.05
7	4	6.71	5.44		4	5	14.56	13.77		2	2	5.49	5.49		0	7	7.00	8.07					
7	5	13.62	13.89		4	6	22.93	21.84		2	3	<2.29	4.49		1	1	14.69	16.64					
7	6	<2.19	2.60		4	7	6.85	7.45		2	4	16.08	16.37										

final iterations, the data were divided into five equal ranges according to intensity. Integral weights from one to five were given to each group such that those reflections of highest intensity were given a weight of one and those of lowest intensity a weight of five. The 'reliability factor', R, was reduced from 0·41 to 0·13 during refinement.

An electron density projection, $\varrho(xy)$, was synthesized with phases based on the above refinement. The atomic peaks were well resolved and no spurious peaks were in evidence. Trial z parameters for all of the atoms were assigned based on the expected structure. In $Pna2_1$, molecules are symmetrically related along the c axis solely by twofold screw axes. Therefore, the choice for positioning a molecule in the z direction was arbitrary. The fractional z parameter for sulfur was arbitrarily set at 0·341, in order to place the entire trial molecule in a single unit cell. This parameter was then fixed in all subsequent refinements.

A total of 354 observed and 86 unobserved reflections were used in a full matrix three-dimensional least-squares refinement using the Busing–Levy program. The Hughes weighting scheme was employed using an $|F_{min}|$ of 3·0. The quantity minimized was $\Sigma\ w(k|F_{obs}| - |F_{calc}|)^2$. After four cycles of isotropic refinement the reliability index (omitting unobserved reflections) was reduced to 0·089. A difference Fourier map* indicated the positions of the eight hydrogen atoms. The structure was refined further with the positional and thermal parameters for the hydrogen atoms fixed. An isotropic B of 5·0 was assumed for all hydrogen atoms. The reliability index was reduced from 0·089 to 0·081 (omitting unobserved reflections). The observed and final calculated structure factors are shown in Table 1. The final atomic parameters and estimated standard deviations are listed in Table 2.

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* In the original manuscript, there was no attempt made to locate the hydrogen atoms of the methyl groups. The referee not only suggested that this be done but had also synthesized a difference Fourier map and obtained coordinates for the hydrogen atoms. Following his suggestion, we calculated a difference Fourier synthesis and found that our values for the positional parameters of the hydrogen atoms were in substantial agreement with his.

Discussion

A view of the cell projected down the c axis is shown in Fig. 1. The overall packing within the cell appears reasonable. There are no intermolecular distances which fall below normally accepted van der Waals distances.

Calculated intermolecular bond distances and angles are listed in Table 3 along with standard deviations calculated from the least-squares results. The molecule exhibits m (C_s) symmetry to within experimental error. The terminal C–C bond lengths of 1·52 and 1·50 Å are quite normal. The S–O distances of 1·44 and 1·41 Å and the O–S–O angle of 120° agree with values reported for a variety of sulfones (Abrahams, 1956). There has been a considerable amount of discussion in the literature on the length of sulfur–carbon single bonds in a variety of substances. A value between 1·78 and 1·82 Å would seem reasonable to expect in this present structure (Abrahams, 1956). However, Jeffrey (1951) observed S–C bond distances similar to those found in *cis*-2-butene episulfone in the compound β-isoprene
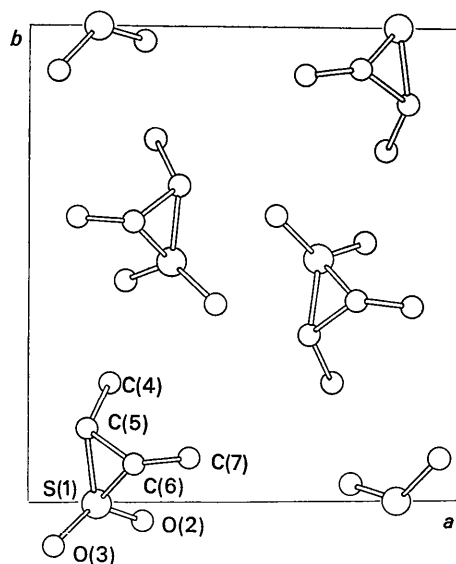

Fig. 1. (001) Projection of *cis*-2-butene episulfone.

Table 2. *Final atomic parameters and estimated standard deviations*

	x	y	z	B
S(1)	0·1672 (3)	−0·0080 (2)	0·3410	3·90 (7)
O(2)	0·2607 (10)	0·9634 (8)	0·1543 (32)	5·83 (23)
O(3)	0·0590 (8)	0·9090 (6)	0·4020 (30)	5·06 (20)
C(4)	0·1956 (16)	0·2395 (16)	0·2230 (48)	6·85 (43)
C(5)	0·1357 (12)	0·1436 (11)	0·3864 (45)	4·55 (29)
C(6)	0·2300 (13)	0·0783 (11)	0·5804 (42)	4·43 (29)
C(7)	0·3815 (16)	0·1086 (13)	0·5915 (48)	5·47 (33)
H(5)	0·035	0·190	0·450	5·00
H(6)	0·180	0·045	0·690	5·00
H(4a)	0·130	0·250	0·075	5·00
H(4b)	0·280	0·210	0·140	5·00
H(4c)	0·200	0·320	0·310	5·00
H(7a)	0·420	0·080	0·410	5·00
H(7b)	0·400	0·200	0·640	5·00
H(7c)	0·430	0·060	0·730	5·00

sulfone; namely, 1·74 and 1·76 Å. He explains these distances by postulating a considerable amount of hyperconjugation in the molecule. His argument is supported by a rather long C–C ring double bond of 1·38 Å and somewhat short ring single bonds of 1·47 Å. Use of similar resonance forms would predict a rather long ring C–C single bond in cis-2-butene episulfone. Our observed value of 1·60 Å is considerably longer than the expected value of 1·47–1·49 Å indicated in Table 4. Another interesting point is contained in the similarity between the chemistry of carbonyl and sulfone compounds. Both groups give acid character to α hydrogen atoms. Neurieter & Bordwell (1963) report the episulfone as an intermediate in the formation of alkenes from α-chlorosulfones in the presence of base. This reaction is analogous to the Favorskii rearrangements of α-haloketones. Several investigators (Cram, 1965) have suggested that the postulated intermediates in this reaction are substituted cyclopropanones in which charge and/or bonds are highly delocalized as in the resonance hybrid,
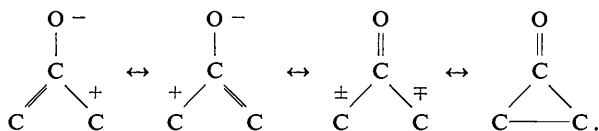
Analogous structures would explain not only the long C–C bond in this episulfone but also the observed shortening of the S–C bond. Unfortunately there exists no stable solid cyclopropanone against which to test these arguments. We are, however, presently investigating the structure of trans-2-butene episulfone, in order to test if the ring dimensions observed in the cis-2-butene episulfone persist in a situation of comparable molecular structure but of different crystal geometry.

Table 3. Intramolecular distances and angles

Distances		Angles	
S(1)–O(2)	1·41 (1) Å	O(2)—S(1)–O(3)	120·4 (7)°
S(1)–O(3)	1·44 (1)	O(2)—S(1)–C(5)	115·7 (8)
S(1)–C(5)	1·72 (1)	O(2)—S(1)–C(6)	116·4 (7)
S(1)–C(6)	1·74 (2)	O(3)—S(1)–C(5)	117·2 (6)
C(4)–C(5)	1·50 (2)	O(3)—S(1)–C(6)	115·5 (9)
C(6)–C(7)	1·52 (2)	C(5)—S(1)–C(6)	55·4 (8)
C(5)–C(6)	1·60 (2)	S(1) —C(6)–C(5)	61·6 (9)
C(4)–H(4a)	1·04	S(1) —C(5)–C(6)	63·3 (8)
C(4)–H(4b)	1·08	C(4)—C(5)–S(1)	123·0 (14)
C(4)–H(4c)	1·12	C(4)—C(5)–C(6)	119·6 (11)
C(7)–H(7a)	1·06	C(7)—C(6)–S(1)	119·7 (14)
C(7)–H(7b)	1·01	C(7)—C(6)–C(5)	119·4 (14)
C(7)–H(7c)	1·07	H(4a)–C(4)–H(4b)	113
C(5)–H(5)	1·17	H(4a)–C(4)–H(4c)	105
C(6)–H(6)	0·86	H(4b)–C(4)–H(4c)	107

Table 3 (cont.)

Angles

C(5)—C(4)–H(4a)	112
C(5)—C(4)–H(4b)	111
C(5)—C(4)–H(4c)	109
C(7a)–C(7)–H(7b)	101
H(7a)–C(7)–H(7c)	110
H(7b)–C(7)–H(7c)	112
C(6)—C(7)–H(7a)	110
C(6)—C(7)–H(7b)	113
C(6)—C(7)–H(7c)	111

Table 4. Dimensions of selected three-membered ring and chain compounds*

	C–X–C	C–X	C–C
Ethylene oxide	61°40′	1·436 Å	1·472 Å
Dimethyl ether	111°	1·42	
Ethylene-imine	59°40′	1·488	1·480
Dimethylamine	111°	1·47	
Ethylene sulfide	48°20′	1·819	1·492
Dimethyl sulfide	98°52′	1·802	
cis-2-Butene episulfone	55·4°	1·73	1·60
Dimethyl sulfone	103°	1·78	
Dimethyl sulfoxide	100°	1·82	

* These data are taken from Sutton (1958) with the exception of the values for dimethyl sulfide (Dreizler & Rudolph, 1962), dimethyl sulfone (Sanders, 1963) and cis-2-butene episulfone (this paper). The value of 58·8° for the C–S–C bond angle of ethylene sulfide reported in Sutton reproduces an error in the original paper. The correct value is given above.

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