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The Crystal and Molecular Structure of 2-Chloro-4-*tert*-butylthiacyclohexane Sulphoxide

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$C_9H_{17}SOCl$ is monoclinic, space group $P2_1/c$, with a = 10·987 (3), b = 20·202 (6), c = 10·193 (3) Å, β = 92·01 (8)°, Z = 8. The structure was refined to a final R of 0·048 for 2783 counter reflexions. The O atom is in the unusual equatorial position, and the thiacyclohexane ring is not distorted. The *tert*-butyl group is slightly twisted away from the staggered position.

Introduction

The O atom of a thiacyclohexane sulphoxide prefers the axial to the equatorial position. It has been shown that the oxidation of 4-substituted thianes (Johnson & McCants, 1964, 1965) gives an equilibrium mixture. The compound present in the larger amount always has its O atom in the axial position. This is attributed to steric interaction between the O atom and the ring. The energy difference between the axial and the equatorial position was estimated to be about $-1{\cdot}3$ kcal mol^{-1}. Further, electrophilic substitution on C_α (Durst & Fraser, 1970; Lett, Bory, Moreau & Marquet, 1971; Nishihata & Nishio, 1971; Bory, Lett, Moreau & Marquet, 1972, 1973) was found to be very stereoselective. Sulphoxides with an equatorial O atom were then prepared. Configurational assignment by systematic NMR studies of the products of methylation and halogenation of *tert*-butylthiacyclohexane sulphoxides (Lett, Bory, Moreau & Marquet, 1973) showed anomalous chemical shifts which have been related to additional interactions introduced by the O atom in the equatorial position. It was therefore of interest to apply X-ray analysis to this 4-*tert*-butylthiacyclohexane series. A preliminary account of 2-chloro-4-*tert*-butylthiacyclohexane sulphoxide has appeared (Robert, 1974).

Experimental section

The crystals are colourless needles. Cell constants were determined from oscillation and Weissenberg photographs. The systematic absences correspond to the space group $P2_1/c$. Least-squares refinement of the Bragg angles of 64 reflexions led to a = 10·987 (3), b = 20·202 (6), c = 10·193 (3) Å, β = 92·01 (8)°, V = 2267 Å^3. The density (d_o = 1·21, d_c = 1·24 g cm^{-3}) is in agreement with two independent molecules per asymmetric unit (referred to as A and B). Data were collected at room temperature with a 0·22 × 0·25 × 0·35 mm crystal mounted parallel to **c** on a Siemens AED diffractometer. 4700 reflexions were collected in the θ–2θ scan mode up to θ_{max} = 66° with Cu $K\alpha$ (λ =

Table 1. *Fractional atomic coordinates* (× 10⁴)

Estimated standard deviations (× 10⁴) are in parentheses.

Molecule *A*

	x	*y*	*z*
Cl_x	6036 (1)	7725 (1)	4325 (1)
Cl_{1-x}	3153 (6)	2246 (4)	2372 (8)
S	4499 (1)	6659 (1)	3134 (1)
O	5938 (3)	2215 (1)	2722 (3)
C(2)	4938 (4)	2010 (2)	323 (4)
C(3)	4260 (4)	1486 (2)	−507 (4)
C(4)	3135 (3)	1222 (2)	113 (4)
C(5)	3454 (4)	913 (2)	1448 (4)
C(6)	4038 (6)	1411 (3)	2414 (4)
C(7)	2361 (4)	757 (2)	−796 (4)
C(8)	2993 (6)	95 (2)	−1017 (5)
C(9)	1136 (8)	630 (5)	−167 (8)
C(10)	2129 (7)	1080 (3)	−2132 (6)

Molecule *B*

	x	*y*	*z*
Cl′	2407 (1)	8920 (1)	2005 (1)
S′	4061 (1)	9233 (1)	4278 (1)
O′	5249 (1)	4609 (2)	1709 (4)
C′(2)	6855 (4)	3610 (2)	1541 (4)
C′(3)	7742 (4)	3299 (2)	599 (4)
C′(4)	8686 (3)	3779 (1)	83 (4)
C′(5)	8028 (4)	4352 (2)	--623 (5)
C′(6)	7178 (4)	4740 (2)	252 (5)
C′(7)	9640 (3)	3440 (2)	- 764 (4)
C′(8)	9116 (9)	3202 (5)	-2077 (9)
C′(9)	654 (5)	3938 (3)	- 1039 (7)
C′(10)	244 (5)	2864 (3)	- 19 (7)

1·5418 Å) Ni-filtered radiation. During data collection standard reflexions decreased by 20%. This was attributed to sublimation, a common feature of sulphoxides at room temperature. After correction, 2783 reflexions with $I > 3\sigma(I)$, where $\sigma(I)$ is the standard deviation based on counting statistics, were considered as observed. Lorentz and polarization but no absorption corrections were applied (μ = 41·6 cm^{-1}). The scale and overall thermal parameters (B = 4·4 Å^2) were deduced from a Wilson plot.

Structure solution

Cl and S coordinates were deduced from a Patterson function. A Fourier synthesis led to the coordinates of all non-hydrogen atoms. After full-matrix least-squares refinement with isotropic and then anisotropic thermal parameters, $R = \Sigma(||F_o| - |F_c||)/\Sigma|F_o|$ was 0·110, somewhat high. A difference synthesis computed with all non-hydrogen atoms revealed a 3 e Å^{-3} peak at 1·95 Å from the non-substituted C_α of A. This was interpreted as a statistical distribution of the Cl atom over both C_α atoms. Refinement of the occupancy factor x with equal isotropic thermal parameters for both atoms led to 0·82 and 0·18 for x and $1-x$. These two atoms were then refined anisotropically to an R of 0·079. The Hamilton (1965) test showed this decrease to be significant. There is no statistical distribution on B. All H atoms were then located on a difference synthesis. Their coordinates were refined independently with isotropic thermal parameters equal to that of the C atom to which they are bound.

The final R was 0·048 and R_w was 0·047 with $R_w = [\Sigma w(|F_o| - |F_c|)^2/\Sigma wF_o^2]^{1/2}$ (here w = 1·0). The atomic coordinates are listed in Tables 1 and 2.*

Table 2. *Hydrogen atom coordinates* (× 10^3) *and their e.s.d.'s* (× 10^3) *in parentheses*

	x	y	z
Molecule A			
H(21)	569 (4)	210 (2)	−9 (4)
H(31)	391 (4)	171 (2)	−142 (4)
H(32)	485 (4)	113 (2)	−62 (4)
H(41)	262 (3)	159 (2)	31 (4)
H(51)	262 (4)	75 (2)	187 (4)
H(52)	405 (4)	58 (2)	134 (4)
H(61)	418 (5)	102 (2)	297 (4)
H(81)	370 (4)	18 (2)	−152 (5)
H(82)	323 (4)	−12 (2)	−25 (5)
H(83)	238 (4)	−19 (2)	−158 (5)
H(91)	163 (7)	46 (3)	−31 (8)
H(92)	63 (5)	40 (3)	−88 (5)
H(93)	84 (5)	99 (3)	3 (6)
H(101)	165 (5)	151 (3)	−200 (5)
H(102)	147 (5)	85 (3)	−251 (5)
H(103)	279 (5)	118 (3)	−265 (5)
Molecule B			
H'(21)	639 (4)	332 (2)	182 (4)
H'(31)	725 (4)	312 (2)	−9 (4)
H'(32)	820 (3)	296 (2)	107 (4)
H'(41)	916 (3)	395 (2)	91 (4)
H'(51)	769 (4)	414 (2)	−135 (4)
H'(52)	861 (4)	465 (2)	−91 (4)
H'(61)	757 (4)	491 (2)	114 (5)
H'(62)	677 (4)	507 (2)	−17 (4)
H'(81)	982 (5)	302 (2)	−263 (5)
H'(82)	861 (7)	348 (4)	−140 (8)
H'(83)	850 (5)	282 (3)	−169 (5)
H'(101)	1061 (5)	304 (2)	75 (5)
H'(102)	1091 (5)	271 (2)	−49 (5)
H'(103)	955 (5)	252 (2)	1 (5)
H'(91)	1024 (4)	433 (3)	−173 (5)
H'(92)	1116 (5)	374 (3)	−155 (5)
H'(93)	1094 (5)	413 (3)	−35 (5)

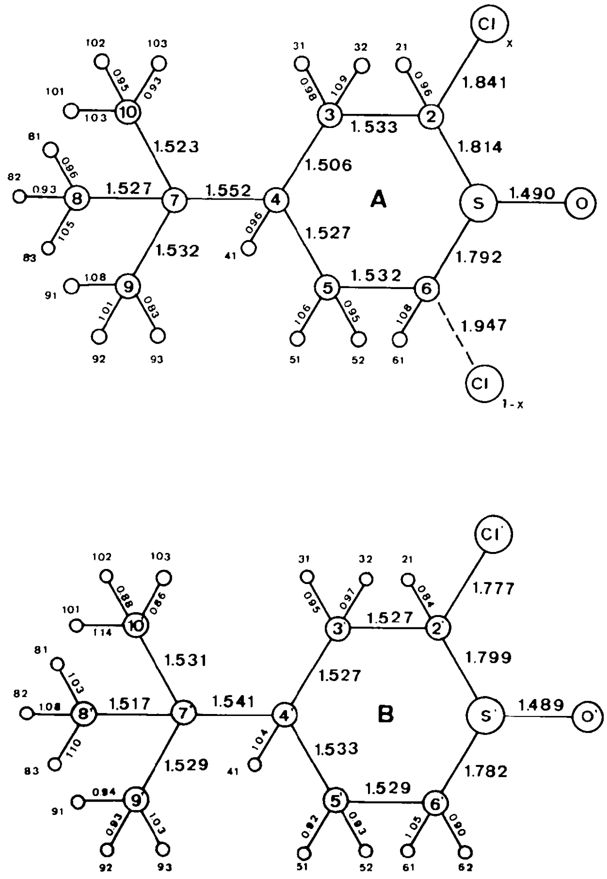

Fig. 1. Atomic numbering and bond distances (Å). The estimated standard deviations are less than 0·009 Å for C–C, C–Cl, C–S, S–O bonds and 0·06 Å for C–H bonds.

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32740 (22 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

All calculations were performed on an IBM 370-168 computer with local versions of *ORFLS* (Busing, Martin & Levy, 1962) for least-squares refinement, *GEST* (De Rango, Tsoucaris, Zelwer & Baudour, 1964) for Fourier syntheses and NRC programs (Ahmed, Hall, Pippy & Huber, 1966) for geometrical calculations. Scattering factors were taken from *International Tables for X-ray Crystallography* (1962) [$F(000) = 896$]. The anomalous dispersion of the Cl atom was ignored.

Structure description

Atomic numbering and interatomic distances are shown in Fig. 1. Bond angles are listed in Table 3. The geometrical parameters will be compared with those of 4-*tert*-butylcyclohexane [force-field calculations (Altona & Sundaralingam, 1970, hereinafter AS, 1970)] and to different substituted 4-*tert*-butylcyclohexane X-ray structure investigations, *e.g.* *cis*-4-*tert*-butylcyclohexane-1-carboxylic acid (referred to as BCA) (van Koningsveld, 1972) and 2b-*seq*-*cis*-1-phenyl-4-*tert*-butylcyclohexanecarboxylic acid (referred to as PBCA) (Mallissard, Sicsic, Welvart, Chiaroni, Riche & Pascard-Billy, 1974).

Thiacyclohexane ring

The ring is anchored in the chair conformation by the *tert*-butyl group in the equatorial position. Planes *P*1 defined by C(2), C(3), C(5), C(6) and *P*2 defined by C′(2), C′(3), C′(5), C′(6) (Table 4) show that the mean distances of these atoms to their planes ($d_{\text{mean}} = 0{\cdot}009$ Å) is about twice the corresponding standard deviation (e.s.d.$_{\text{mean}} = 0{\cdot}005$ Å). Thus the expected distortion of the ring consistent with the twist of the *tert*-butyl group cannot be firmly established.

C(4) and C′(4) are respectively +0·68 and +0·69 Å out of *P*1 and *P*2 while S and S′ are −0·98 and −0·96 Å out of the same planes. This can be related to the C(3)–C(4)–C(5) angles (110·6 and 109·1°): the angles reported for BCA and PBCA are respectively 107·9 and 108·4°. The C(2)–S–C(6) angles (95·6 and 96·1°) are similar to those chosen in sulphoxide conformational analysis (95·8°) by Allinger, Hirsch, Miller & Tyminski (1969) and to the values tabulated by Chu (1975) for three-coordinate S in thioxanthene derivatives (98·58°). The mean C–C length of 1·527

Table 3. *Bond angles* (°)

The e.s.d.'s in parentheses refer to the last decimal place; those for the hydrogen bond angles range from 2·5° for C–C–H to 5·0° for H–C–H.

Molecule *A*		Molecule *B*		Molecule *A*		Molecule *B*	
O–S–C(2)	107·8 (2)	O′–S′–C′(2)	109·4 (2)	H(4)–C(4)–C(7)	106	H′(4)–C′(4)–C′(7)	106
O–S–C(6)	107·6 (2)	O′–S′–C′(6)	107·5 (2)	H(51)–C(5)–C(6)	107	H′(51)–C′(5)–C′(6)	118
C(2)–S–C(6)	95·6 (2)	C′(2)–S′–C′(6)	96·1 (2)	H(51)–C(5)–C(4)	109	H′(51)–C′(5)–C′(4)	102
S–C(2)–Cl$_x$	108·7 (3)	S′–C′(2)–Cl′	111·9 (2)	H(51)–C(5)–H(52)	116	H′(51)–C′(5)–H′(52)	108
S–C(2)–C(3)	110·6 (3)	S′–C′(2)–C′(3)	110·8 (3)	H(52)–C(5)–C(4)	109	H′(52)–C′(5)–C′(4)	108
C(3)–C(2)–Cl$_x$	112·1 (3)	C′(3)–C′(2)–Cl′	112·8 (3)	H(52)–C(5)–C(6)	105	H′(52)–C′(5)–C′(6)	107
C(2)–C(3)–C(4)	113·8 (4)	C′(2)–C′(3)–C′(4)	114·3 (3)	H(81)–C(8)–C(7)	107	H′(81)–C′(8)–C′(7)	109
C(3)–C(4)–C(5)	110·6 (4)	C′(3)–C′(4)–C′(5)	109·1 (3)	H(81)–C(8)–H(82)	109	H′(81)–C′(8)–H′(82)	120
C(3)–C(4)–C(7)	113·9 (4)	C′(3)–C′(4)–C′(7)	113·3 (3)	H(81)–C(8)–H(83)	109	H′(81)–C′(8)–H′(83)	115
C(5)–C(4)–C(7)	112·9 (4)	C′(5)–C′(4)–C′(7)	113·0 (3)	H(82)–C(8)–C(7)	114	H′(82)–C′(8)–C′(7)	118
C(4)–C(5)–C(6)	112·6 (4)	C′(4)–C′(5)–C′(6)	113·7 (4)	H(82)–C(8)–H(83)	111	H′(82)–C′(8)–H′(83)	95
C(5)–C(6)–S	110·1 (4)	C′(5)–C′(6)–S′	110·5 (3)	H(83)–C(8)–C(7)	107	H′(83)–C′(8)–C′(7)	97
C(4)–C(7)–C(8)	112·0 (4)	C′(4)–C′(7)–C′(8)	113·0 (4)	H(91)–C(9)–C(7)	109	H′(91)–C′(9)–C′(7)	107
C(4)–C(7)–C(9)	108·8 (4)	C′(4)–C′(7)–C′(9)	108·9 (4)	H(91)–C(9)–H(92)	113	H′(91)–C′(9)–CH′(92)	101
C(4)–C(7)–C(10)	110·2 (4)	C′(4)–C′(7)–C′(10)	110·6 (4)	H(91)–C(9)–H(93)	111	H′(91)–C′(9)–H′(93)	109
C(8)–C(7)–C(9)	109·0 (5)	C′(8)–C′(7)–C′(9)	107·5 (5)	H(92)–C(9)–C(7)	104	H′(92)–C′(9)–C′(7)	107
C(8)–C(7)–C(10)	107·9 (4)	C′(8)–C′(7)–C′(10)	109·9 (5)	H(92)–C(9)–H(93)	111	H′(92)–C′(9)–H′(93)	118
C(9)–C(7)–C(10)	108·9 (5)	C′(9)–C′(7)–C′(10)	106·6 (4)	H(93)–C(9)–C(7)	108	H′(93)–C′(9)–C′(7)	114
C(5)–C(6)–Cl$_{1,x}$	110·9 (4)			H(101)–C(10)–C(7)	108	H′(101)–C′(10)–C′(7)	106
S–C(6)–Cl$_{1,x}$	101·7 (4)			H(101)–C(10)–H(102)	94	H′(101)–C′(10)–H′(102)	103
H(2)–C(2)–S	100	H′(2)–C′(2)–S′	108	H(101)–C(10)–H(103)	108	H′(101)–C′(10)–H′(103)	122
H(2)–C(2)–Cl$_x$	117	H′(2)–C′(2)–Cl′	104	H(102)–C(10)–C(7)	105	H′(102)–C′(10)–C′(7)	109
H(2)–C(2)–C(3)	108	H′(2)–C′(2)–C′(3)	109	H(102)–C(10)–H(103)	119	H′(102)–C′(10)–H′(103)	113
H(31)–C(3)–C(2)	109	H′(31)–C′(3)–C′(2)	106	H(103)–C(10)–C(7)	119	H′(103)–C′(10)–C′(7)	103
H(31)–C(3)–C(4)	103	H′(31)–C′(3)–C′(4)	111	H(6)–C(6)–C(5)	114	H′(6)–C′(6)–C′(5)	116
H(31)–C(3)–H(32)	115	H′(31)–C′(3)–H′(32)	111	H(6)–C(6)–S	101	H′(61)–C′(6)–S′	105
H(32)–C(3)–C(2)	105	H′(32)–C′(3)–C′(2)	108	H(6)–C(6)–Cl$_{1,x}$	118	H′(61)–C′(6)–H′(62)	111
H(32)–C(3)–C(4)	110	H′(32)–C′(3)–C′(4)	106			H′(62)–C′(6)–S′	100
H(4)–C(4)–C(3)	108	H′(4)–C′(4)–C′(3)	106			H′(62)–C′(6)–C′(5)	113
H(4)–C(4)–C(5)	104	H′(4)–C′(4)–C′(5)	109				

Table 4. *Equations of mean least-squares planes and deviations from these planes in* Å

The asterisk denotes atoms not included in the calculation of the plane. E.s.d.'s in parentheses refer to the last decimal place.

Molecule *A*

$P1$: $-0{\cdot}8124X + 0{\cdot}5796Y - 0{\cdot}0641Z + 2{\cdot}0559 = 0$

Molecule *B*

$P2$: $-0{\cdot}7474X - 0{\cdot}2325Y - 0{\cdot}6223Z + 8{\cdot}2665 = 0$

Molecule *A*		Molecule *B*	
C(2)	−0·009 (5)	C′(2)	−0·005 (4)
C(3)	0·011 (5)	C′(3)	0·005 (4)
C(5)	−0·010 (5)	C′(5)	−0·007 (5)
C(6)	0·016 (6)	C′(6)	0·007 (5)
S*	−0·979 (1)	S′*	−0·962 (1)
O*	−0·749 (3)	O′*	−0·753 (4)
C(4)*	0·692 (4)	C′(4)*	0·685 (4)

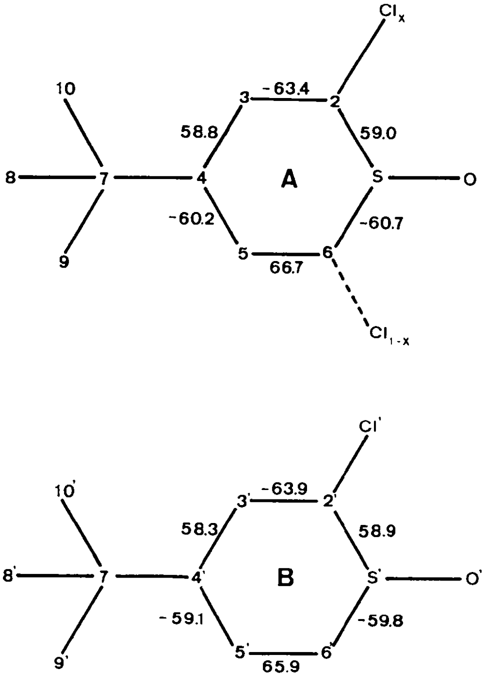

Fig. 2. Ring torsion angles (°) for both molecules.

Å is in agreement with that of the semi-empirical force-field model of AS (1970) (1·533 Å) and those reported for cyclohexane derivatives; 1·529 Å has been found for *trans*-1,4-aminomethylcyclohexanecarboxylic acid (Groth, 1968). Fig. 2 shows the ring torsion angles for *A* and *B*. The average value (61·2°) is far above that found for cyclohexane (54·5°) by Bucourt & Hainaut (1965) but is in agreement with the AS (1970) prediction for heterocyclic compounds, which allows for a decreased C—S—C angle.

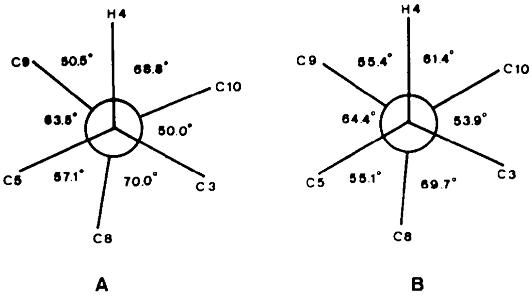

Fig. 3. Newman projections through the C(4)—C(7) bond.

Sulphoxide group

The O atom, as predicted, is bound in the energetically unfavourable equatorial position. The S—O distances (1·490 in *A* and 1·489 Å in *B*) are slightly longer than those found in 1,4-dithiane 1,4-dioxide (*α* form) (Shearer, 1959) but agree with those reported by Chu (1975) for thioxanthene derivatives (1·497 Å), and by Palmer & Lee (1966), De la Camp & Hope (1970) and Hine (1962) for other cyclic sulphoxides.

tert-Butyl group

The *tert*-butyl group is twisted away from the staggered position (mean value of twist 8° for *A* and 6° for *B*). These values agree with 8° for BCA and 6° for PBCA, but are far from the calculated value (17°) of AS (1970). Fig. 3 is the Newman projection through C(4)—C(7). The mean C(4)—C(7) length is less (1·546 Å) than other values (1·561 for PBCA and 1·550 Å for BCA). AS (1970) calculated 1·570 Å but suggested that the probable true value would be 1·564 Å.

The 1·777 Å C—Cl distance of *B* agrees with 1·767 Å (Sutton, 1965). On the other hand, both C—Cl distances in *A* are too long (1·841 and 1·947 Å). This may be due to the disorder. A 1·92 Å C—Cl distance has been reported in the disordered structure of 3-chloro-3-iodopropyltrimethylammonium iodide (Mallard, Vaughan & Hamor, 1974). The packing is governed by van der Waals contacts; no particular short distances were found.

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The Crystal and Molecular Structure of 2-Chloro-4-*tert*-butyl-6-methylthiacyclohexane Sulphoxide

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$C_{10}H_{19}SOCl$ is orthorhombic, space group *Pbcn*, with $a = 20{\cdot}124$ (5), $b = 12{\cdot}921$ (3), $c = 9{\cdot}238$ (2) Å, $Z = 8$. The structure was refined to a final R of 0·078 for 1274 counter reflexions. The O atom is in the axial position. The weak ring distortion is related to the twist of the *tert*-butyl group.

Introduction

Having solved the structure of 2-chloro-4-*tert*-butylthiacyclohexane sulphoxide (CTTH, Robert, 1977) we report the structure of 2-chloro-4-*tert*-butyl-6-methylthiacyclohexane sulphoxide. Our goal is to obtain information on conformational differences, if any, of the thiacyclohexane ring. Since the O atom in CTTH is equatorial and because NMR shows an axial O atom in the title compound it is interesting to look for distortion differences in the ring.

During this work we will refer to force-field calculations of 4-*tert*-butylcyclohexane (Altona & Sundaralingam, 1970, hereinafter AS, 1970) and to two X-ray investigations: *cis*-4-*tert*-butylcyclohexane-1-carboxylic acid (van Koningsveld, 1972) and 2b *seq cis*-1-phenyl-4-*tert*-butylcyclohexanecarboxylic acid (Mallissard, Sicsic, Welvart, Chiaroni, Riche & Pascard-Billy, 1974) referred to respectively as BCA and PBCA.

Experimental

The description by Bory, Lett, Moreau & Marquet (1973) of halogenation of sulphoxides shows the high stereoselectivity of these reactions. This stereoselectivity has been used to isolate the title compound.