C1—N1—C4	108.8 (5)	111.4 (5)	109.9 (5)	109.8 (5)
O1—C1—N1	123.6 (5)	126.1 (6)	125.3 (6)	124.9 (6)
O1—C1—C2	129.3 (6)	127.9 (6)	128.4 (6)	129.5 (6)
N1—C1—C2	107.1 (5)	106.1 (5)	106.4 (5)	105.6 (5)
C3—C2—C1	109.1 (6)	107.3 (6)	108.0 (6)	108.6 (6)
C2—C3—C4	109.6 (6)	110.1 (6)	109.5 (6)	110.2 (6)
O2—C4—N1	123.0 (6)	124.9 (6)	123.3 (6)	123.3 (6)
O2—C4—C3	131.7 (6)	129.9 (6)	130.5 (6)	130.9 (6)
N1—C4—C3	105.4 (5)	105.2 (5)	106.2 (6)	105.8 (5)

The unit-cell and intensity data were collected on a Delft Instruments FAST diffractometer using the routines *ENDEX*, *REFINE* and *MADONL* in the *MADNES* software (Pflugrath & Messerschmidt, 1989) and processed using *ABSMAD* (Karaulov, 1992); detailed procedures are described by Darr, Drake, Hursthouse & Malik (1993). Owing to the small number of observed reflections, only the O atoms were refined with anisotropic displacement parameters. The absence of crystal decay in the X-ray beam was confirmed by checking equivalent reflections at the beginning and end of data collection which lasted about 8 h. Refinement was on F^2 for all reflections except for three which had very negative F^2 or were flagged by the user for potential systematic errors.

The H atoms were initially placed in calculated positions and thereafter allowed to ride on their attached C atoms with a common isotropic displacement parameter of 0.044 (5) Å^2.

Program(s) used to solve structure: *SIR92* (Altomare et al., 1994). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *ZORTEP* (Zsolnai, 1995). Software used to prepare material for publication: *SHELXL93*.

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Trimethylsulfonium Bromide

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Abstract

The reaction of dimethyl sulfoxide and ethyl bromoacetate at room temperature gives the title compound $(CH_3)_3S.Br$, which consists of layers of pyramidal trimethylsulfonium ions and bromide ions.

Comment

Vibrational spectra of $(CH_3)_3S.3I$ (*I*) and $(C_2H_5)_3S.3I$ (*I*) have been shown (Bengtsson, Oskarsson, Stegemann & Redeker, 1994; Bengtsson, Stegemann, Holmberg & Füllbier, 1991) to have extra spectral features in the region of 130–170 cm^{-1} which are unexpected since the triiodide ions in these compounds have D_{ih} symmetry. An ion of C_{iv} symmetry could provide essential information for the further elucidation of the reasons for the breakdown of selection rules. This is not possible in the liquid state if only iodine is present in the linear triatomic ion but if one of the terminal I atoms is replaced by another halogen atom, C_{iv} symmetry is obtained. The title compound was found to be a suitable starting material to form linear I_2Br^- (Svensson & Kloo, 1996). The structure of the title compound has been determined in order to obtain data for future comparisons.
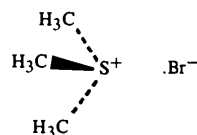
(I)

The $(CH_3)_3S^+$ cation is pyramidal and its angles indicate sp^3 hybridization of the S atom (Table 2). The bond distances in the cation are normal (Jannin, Puget, De Brauer & Perret, 1991). $(CH_3)_3S.I$ (Jannin et al., 1991) crystallizes in the same space group as and has similar cell parameters to $(CH_3)_3S.Br$. A comparison of the positional parameters of $(CH_3)_3S.I$ and $(CH_3)_3S.Br$ shows them to be almost identical if the sign of the z coordinates in the title compound is changed and the a and c axes are interchanged.
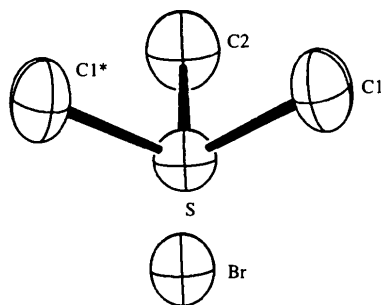

Fig. 1. Molecular structure showing 50% probability displacement ellipsoids. H atoms are omitted for clarity. (* indicates that the atom is generated by the mirror plane through S—C2.)

Experimental

$(CH_3)_3SBr$ was prepared by the reaction between dimethyl sulfoxide and ethyl bromoacetate (1.4:1). The reaction mixture was kept in darkness and at room temperature. After 6 d the crystals were separated from the orange viscous solution and treated with acetone. They were recrystallized from an ether/methanol (1:1) solution.

Crystal data

$C_3H_9S^+.Br^-$	Mo $K\alpha$ radiation
$M_r = 157.07$	$\lambda = 0.71069$ Å
Monoclinic	Cell parameters from 25
$P2_1/m$	reflections
$a = 5.766\,(1)$ Å	$\theta = 2.15–20.60°$
$b = 7.460\,(1)$ Å	$\mu = 6.789$ mm^{-1}
$c = 7.267\,(3)$ Å	$T = 293$ K
$\beta = 92.45\,(3)°$	Prismatic
$V = 312.3\,(1)$ Å^3	$0.20 \times 0.18 \times 0.15$ mm
$Z = 2$	White
$D_x = 1.670$ Mg m^{-3}	
D_m not measured	

Data collection

CAD-4 diffractometer	499 observed reflections
$\omega–2\theta$ scans	$[I > 3\sigma(I)]$
Absorption correction:	$R_{int} = 0.031$
empirical via ψ scans	$\theta_{max} = 26.29°$
(CAD-4 EXPRESS; Enraf–	$h = 0 \rightarrow 7$
Nonius, 1992)	$k = -9 \rightarrow 0$
$T_{min} = 0.22$, $T_{max} =$	$l = -9 \rightarrow 9$
0.36	3 standard reflections
751 measured reflections	monitored every 120 min
686 independent reflections	reflections
	intensity decay: -1.8%

Refinement

Refinement on F	$(\Delta/\sigma)_{max} < 0.001$
$R = 0.0250$	$\Delta\rho_{max} = 0.36$ e Å^{-3}
$wR = 0.0260$	$\Delta\rho_{min} = -0.33$ e Å^{-3}
$S = 1.540$	Extinction correction: none
499 reflections	Atomic scattering factors
28 parameters	from International Tables
H-atom parameters not	for X-ray Crystallography
refined	(1974, Vol. IV)
$w = 4F_o^2/\sigma^2(F_o^2)$, $\sigma^2(F_o^2)$	
based on counting	
statistics	

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Br	0.6686 (1)	1/4	0.22742 (8)	0.0448 (2)
S	0.9898 (2)	1/4	0.6731 (2)	0.0404 (4)
C1	0.8018 (7)	0.0648 (6)	0.7089 (6)	0.0536 (10)
C2	1.166 (1)	1/4	0.8812 (8)	0.052 (2)

Table 2. Selected geometric parameters $(\text{Å}, °)$

Br—S	3.662 (2)	S—C2	1.786 (6)
S—C1	1.782 (4)		
C1—S—C2	101.8 (2)	C1—S—C1^i	101.6 (3)

Symmetry code: (i) $x, \frac{1}{2} - y, z$.

H atoms were fixed at calculated positions and included in the structure-factor calculations.

Data collection: CAD-4 EXPRESS (Enraf–Nonius, 1992). Cell refinement: CELDIM (CAD-4 Version). Data reduction: TEXSAN: PROCESS (Molecular Structure Corporation, 1993). Program(s) used to solve structure: SAPI91 (Fan, 1991). Program(s) used to refine structure: TEXSAN: LS. Software used to prepare material for publication: TEXSAN.

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