



Figure 1. Molecular structure of the compound (ellipsoids are drawn with 50% probability).

The structure determination and the report are by Oksana O. Gerlits.

Experimental Part.

X-ray diffraction data on **1** were collected at 90(1)K using a Bruker SMART1000 CCD diffractometer installed at a rotating anode source (MoK α radiation, $\lambda=0.71073\text{\AA}$), and equipped with an Oxford Cryosystems nitrogen gas-flow apparatus. The data were collected by the rotation method with 0.3° frame-width (ω scan) and 20 sec exposure time per frame. Four sets of data (600 frames in each set) were collected, nominally covering half of reciprocal space. The data were integrated, scaled, sorted and averaged

using the SMART software package.¹ The structure was solved by Direct methods using SHELXTL NT Version 5.10.² The structure was refined by full-matrix least squares against F^2 .

Non-hydrogen atoms were refined anisotropically. Positions of hydrogen atoms were found by difference electron density Fourier synthesis. The CH₃ hydrogens were treated as part of idealized CH₃ groups with $U_{\text{iso}}=1.5U_{\text{eq}}$, while the remainder of the hydrogen atoms were refined with the “riding” model with $U_{\text{iso}}=1.2U_{\text{eq}}$.

Atomic coordinates, anisotropic displacement parameters, bond lengths and angles are given in Tables 2, 3, 4 respectively.

Table 1. Crystallographic data.

Compound	1
Formula	C17 H18 Br N O2 S
M_r [g·mol ⁻¹]	380.29
Crystal shape/color	parallelepipeds/colorless
Crystal system	Monoclinic
Space group	P2 ₁ /n
a [Å]	11.5532(4)
b [Å]	11.4494(4)
c [Å]	12.2883(4)
α [°]	90
β [°]	96.685(1)
γ [°]	90
V [Å ³]	1614.4(1)
Z	4
ρ_{calc} [g/cm ³]	1.565
μ [mm ⁻¹]	2.682
T [K]	90(1)
Max. 2θ [°]	56.62
Absorption correction method	SADABS 2.05
Reflections measured	19441
Unique reflections (R_{int})	4016 (0.0332)
Reflections $I > 4\sigma(I)$	3458
Parameters refined	201
R [$I > 2\sigma(I)$]	0.0310
wR_2	0.0816
G.O.F.	1.075

Table 2. Atomic coordinates (10^4) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$).

Atom	x	y	z	U(eq)
Br(1)	1704(1)	4058(1)	995(1)	
29(1)				
S(1)	5172(1)	3182(1)	1806(1)	
13(1)				
O(1)	4974(1)	1951(1)	1908(1)	
18(1)				
O(2)	5090(1)	3702(1)	738(1)	
19(1)				
N(1)	4206(2)	3845(1)	2463(1)	
13(1)				
C(1)	3779(2)	5079(2)	2216(2)	
15(1)				
C(2)	3099(2)	5371(2)	3200(2)	
20(1)				
C(3)	3318(2)	4367(2)	3977(2)	
16(1)				
C(4)	2955(2)	4217(2)	5002(2)	
20(1)				
C(5)	3221(2)	3181(2)	5572(2)	
22(1)				
C(6)	3855(2)	2316(2)	5113(2)	
19(1)				
C(7)	4222(2)	2453(2)	4080(2)	
15(1)				
C(8)	3951(2)	3496(2)	3524(2)	
13(1)				
C(9)	6584(2)	3472(2)	2468(2)	
14(1)				
C(10)	7047(2)	2789(2)	3352(2)	
15(1)				
C(11)	8187(2)	2974(2)	3814(2)	
16(1)				
C(12)	8888(2)	3823(2)	3404(2)	
15(1)				
C(13)	8400(2)	4510(2)	2526(2)	
16(1)				
C(14)	7263(2)	4340(2)	2055(2)	
16(1)				
C(15)	10137(2)	4004(2)	3877(2)	
19(1)				
C(16)	4777(2)	5954(2)	2166(2)	
26(1)				
C(17)	3021(2)	5137(2)	1121(2)	
21(1)				

Table 3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$).

Atom	U11	U22	U33	U23	U13
Br(1)	18(1)	30(1)	37(1)	-9(1)	-7(1)
-2(1)					
S(1)	15(1)	12(1)	11(1)	-1(1)	1(1)
0(1)					
O(1)	21(1)	12(1)	21(1)	-4(1)	2(1)
-1(1)					
O(2)	21(1)	23(1)	11(1)	0(1)	0(1)
0(1)					
N(1)	15(1)	10(1)	13(1)	2(1)	2(1)
2(1)					
C(1)	16(1)	10(1)	18(1)	2(1)	-1(1)
1(1)					
C(2)	25(1)	15(1)	20(1)	-2(1)	3(1)
6(1)					
C(3)	15(1)	16(1)	17(1)	-2(1)	0(1)
-2(1)					
C(4)	17(1)	25(1)	19(1)	-8(1)	4(1)
-2(1)					
C(5)	20(1)	33(1)	13(1)	0(1)	2(1)
-10(1)					
C(6)	17(1)	23(1)	17(1)	7(1)	-1(1)
-7(1)					
C(7)	14(1)	16(1)	17(1)	3(1)	1(1)
-1(1)					
C(8)	12(1)	14(1)	12(1)	0(1)	0(1)
-2(1)					
C(9)	15(1)	14(1)	13(1)	-2(1)	2(1)
2(1)					
C(10)	17(1)	13(1)	17(1)	1(1)	4(1)
2(1)					
C(11)	17(1)	15(1)	17(1)	1(1)	2(1)
3(1)					
C(12)	16(1)	13(1)	17(1)	-4(1)	3(1)
2(1)					
C(13)	19(1)	13(1)	18(1)	0(1)	6(1)
-1(1)					
C(14)	20(1)	15(1)	15(1)	2(1)	3(1)
1(1)					
C(15)	16(1)	17(1)	25(1)	-1(1)	1(1)
-1(1)					
C(16)	17(1)	17(1)	43(1)	9(1)	2(1)
1(1)					
C(17)	16(1)	25(1)	20(1)	6(1)	-4(1)
1(1)					

Table 4. Bond lengths [Å] and angles [°].

Br(1)-C(17)	1.953(2)	C(3)-C(8)	1.391(3)
S(1)-O(2)	1.434(2)	C(4)-C(5)	1.394(3)
S(1)-O(1)	1.436(2)	C(5)-C(6)	1.390(3)
S(1)-N(1)	1.639(2)	C(6)-C(7)	1.393(3)
S(1)-C(9)	1.768(2)	C(7)-C(8)	1.393(3)
N(1)-C(8)	1.427(2)	C(9)-C(10)	1.394(3)
N(1)-C(1)	1.515(2)	C(9)-C(14)	1.397(3)
C(1)-C(17)	1.519(3)	C(10)-C(11)	1.388(3)
C(1)-C(16)	1.534(3)	C(11)-C(12)	1.396(3)
C(1)-C(2)	1.553(3)	C(12)-C(13)	1.399(3)
C(2)-C(3)	1.498(3)	C(12)-C(15)	1.507(3)
C(3)-C(4)	1.384(3)	C(13)-C(14)	1.386(3)
O(2)-S(1)-O(1)		C(4)-C(3)-C(8)	120.3(2)
119.57(9)		C(4)-C(3)-C(2)	129.0(2)
O(2)-S(1)-N(1)		C(8)-C(3)-C(2)	110.7(2)
106.39(9)		C(3)-C(4)-C(5)	119.4(2)
O(1)-S(1)-N(1)		C(6)-C(5)-C(4)	119.9(2)
106.69(9)		C(5)-C(6)-C(7)	121.3(2)
O(2)-S(1)-C(9)		C(6)-C(7)-C(8)	117.9(2)
107.60(9)		C(3)-C(8)-C(7)	121.2(2)
O(1)-S(1)-C(9)		C(3)-C(8)-N(1)	109.8(2)
107.01(9)		C(7)-C(8)-N(1)	129.0(2)
N(1)-S(1)-C(9)		C(10)-C(9)-C(14)	120.1(2)
109.33(9)		C(10)-C(9)-S(1)	120.2(2)
C(8)-N(1)-C(1)	110.3(2)	C(14)-C(9)-S(1)	119.6(2)
C(8)-N(1)-S(1)	123.1(1)	C(11)-C(10)-C(9)	119.5(2)
C(1)-N(1)-S(1)	123.9(1)	C(10)-C(11)-C(12)	121.4(2)
N(1)-C(1)-C(17)	111.1(2)	C(11)-C(12)-C(13)	118.1(2)
N(1)-C(1)-C(16)	112.8(2)	C(11)-C(12)-C(15)	121.8(2)
C(17)-C(1)-C(16)	107.1(2)	C(13)-C(12)-C(15)	120.1(2)
N(1)-C(1)-C(2)	103.2(2)	C(14)-C(13)-C(12)	121.3(2)
C(17)-C(1)-C(2)	112.9(2)	C(13)-C(14)-C(9)	119.5(2)
C(16)-C(1)-C(2)	109.9(2)	C(1)-C(17)-Br(1)	114.0(2)
C(3)-C(2)-C(1)	105.5(2)		

References.

1. SMART and SAINTPLUS, Area detector control and integration software, Ver. 6.01. Bruker Analytical X-ray Systems, Madison, Wisconsin, U.S.A, **1999**.
2. SHELXTL, An integrated system for solving, refining and displaying crystal structures from diffraction data, Ver. 5.10. Bruker Analytical X-ray Systems, Madison, Wisconsin, U.S.A, **1997**.

CIF File

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C10 0.0174(10) 0.0125(9) 0.0167(9) 0.0012(8) 0.0036(8) 0.0015(8)
C11 0.0168(9) 0.0147(9) 0.0167(9) 0.0013(7) 0.0018(8) 0.0027(8)
C12 0.0157(9) 0.0130(9) 0.0165(9) -0.0042(7) 0.0032(8) 0.0023(7)
C13 0.0186(10) 0.0130(9) 0.0183(10) -0.0004(8) 0.0056(8) -0.0012(8)
C14 0.0198(10) 0.0149(9) 0.0146(9) 0.0021(7) 0.0030(8) 0.0010(8)
C15 0.0161(10) 0.0170(10) 0.0245(11) -0.0009(8) 0.0011(8) -0.0006(8)
C16 0.0174(10) 0.0169(11) 0.0425(14) 0.0091(10) 0.0019(10) 0.0007(8)
C17 0.0161(10) 0.0247(11) 0.0203(10) 0.0058(9) -0.0038(8) 0.0005(8)

_geom_special_details

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All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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loop_

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_geom_bond_atom_site_label_2

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_geom_bond_site_symmetry_2

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Br1 C17 1.953(2) . ?

S1 O2 1.4339(15) . ?

S1 O1 1.4355(15) . ?

S1 N1 1.6385(17) . ?

S1 C9 1.768(2) . ?

N1 C8 1.427(2) . ?

N1 C1 1.515(2) . ?

C1 C17 1.519(3) . ?

C1 C16 1.534(3) . ?

C1 C2 1.553(3) . ?

C2 C3 1.498(3) . ?

C3 C4 1.384(3) . ?

C3 C8 1.391(3) . ?

C4 C5 1.394(3) . ?

C5 C6 1.390(3) . ?

C6 C7 1.393(3) . ?

C7 C8 1.393(3) . ?

C9 C10 1.394(3) . ?

C9 C14 1.397(3) . ?

C10 C11 1.388(3) . ?

C11 C12 1.396(3) . ?

C12 C13 1.399(3) . ?

C12 C15 1.507(3) . ?

C13 C14 1.386(3) . ?

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O2 S1 O1 119.57(9) . . ?
O2 S1 N1 106.39(9) . . ?
O1 S1 N1 106.69(9) . . ?
O2 S1 C9 107.60(9) . . ?
O1 S1 C9 107.01(9) . . ?
N1 S1 C9 109.33(9) . . ?
C8 N1 C1 110.33(16) . . ?
C8 N1 S1 123.07(14) . . ?
C1 N1 S1 123.92(13) . . ?
N1 C1 C17 111.09(17) . . ?
N1 C1 C16 112.81(17) . . ?
C17 C1 C16 107.10(18) . . ?
N1 C1 C2 103.16(16) . . ?
C17 C1 C2 112.86(18) . . ?
C16 C1 C2 109.92(18) . . ?
C3 C2 C1 105.51(17) . . ?
C4 C3 C8 120.3(2) . . ?
C4 C3 C2 129.0(2) . . ?
C8 C3 C2 110.71(18) . . ?
C3 C4 C5 119.4(2) . . ?
C6 C5 C4 119.9(2) . . ?
C5 C6 C7 121.3(2) . . ?
C6 C7 C8 117.9(2) . . ?
C3 C8 C7 121.15(19) . . ?
C3 C8 N1 109.79(17) . . ?
C7 C8 N1 129.04(18) . . ?
C10 C9 C14 120.10(19) . . ?
C10 C9 S1 120.22(16) . . ?
C14 C9 S1 119.55(16) . . ?
C11 C10 C9 119.52(19) . . ?
C10 C11 C12 121.39(19) . . ?
C11 C12 C13 118.13(19) . . ?
C11 C12 C15 121.76(19) . . ?

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C13 C12 C15 120.11(19) . . ?
C14 C13 C12 121.32(19) . . ?
C13 C14 C9 119.52(19) . . ?
C1 C17 Br1 113.95(15) . . ?

loop_

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O2 S1 N1 C8 174.05(15) ?
O1 S1 N1 C8 45.36(18) ?
C9 S1 N1 C8 -70.03(18) ?
O2 S1 N1 C1 -26.32(18) ?
O1 S1 N1 C1 -155.01(15) ?
C9 S1 N1 C1 89.60(17) ?
C8 N1 C1 C17 -127.88(18) ?
S1 N1 C1 C17 70.2(2) ?
C8 N1 C1 C16 111.8(2) ?
S1 N1 C1 C16 -50.0(2) ?
C8 N1 C1 C2 -6.7(2) ?
S1 N1 C1 C2 -168.58(14) ?
N1 C1 C2 C3 6.8(2) ?
C17 C1 C2 C3 126.79(19) ?
C16 C1 C2 C3 -113.72(19) ?
C1 C2 C3 C4 176.8(2) ?
C1 C2 C3 C8 -5.0(2) ?
C8 C3 C4 C5 -0.6(3) ?
C2 C3 C4 C5 177.4(2) ?
C3 C4 C5 C6 0.7(3) ?
C4 C5 C6 C7 -0.9(3) ?
C5 C6 C7 C8 1.1(3) ?
C4 C3 C8 C7 0.8(3) ?
C2 C3 C8 C7 -177.56(19) ?
C4 C3 C8 N1 179.17(18) ?

C2 C3 C8 N1 0.8(2) ?
 C6 C7 C8 C3 -1.0(3) ?
 C6 C7 C8 N1 -179.05(19) ?
 C1 N1 C8 C3 3.9(2) ?
 S1 N1 C8 C3 166.00(15) ?
 C1 N1 C8 C7 -177.85(19) ?
 S1 N1 C8 C7 -15.8(3) ?
 O2 S1 C9 C10 -159.74(16) ?
 O1 S1 C9 C10 -30.07(19) ?
 N1 S1 C9 C10 85.12(18) ?
 O2 S1 C9 C14 16.12(19) ?
 O1 S1 C9 C14 145.79(16) ?
 N1 S1 C9 C14 -99.02(17) ?
 C14 C9 C10 C11 -0.4(3) ?
 S1 C9 C10 C11 175.48(16) ?
 C9 C10 C11 C12 -0.7(3) ?
 C10 C11 C12 C13 1.6(3) ?
 C10 C11 C12 C15 -178.03(19) ?
 C11 C12 C13 C14 -1.4(3) ?
 C15 C12 C13 C14 178.21(19) ?
 C12 C13 C14 C9 0.4(3) ?
 C10 C9 C14 C13 0.5(3) ?
 S1 C9 C14 C13 -175.34(16) ?
 N1 C1 C17 Br1 55.1(2) ?
 C16 C1 C17 Br1 178.75(15) ?
 C2 C1 C17 Br1 -60.1(2) ?

<u>_diffn_measured_fraction_theta_max</u>	0.997
<u>_diffn_reflns_theta_full</u>	28.31
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<u>_refine_diff_density_max</u>	1.499
<u>_refine_diff_density_min</u>	-0.615
<u>_refine_diff_density_rms</u>	0.092