

1-(4-Methoxybenzyl)pyridinium *p*-toluenesulfonate

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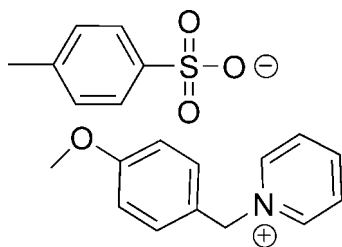
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å;
 R factor = 0.036; wR factor = 0.092; data-to-parameter ratio = 18.8.

In the title compound, $\text{C}_{13}\text{H}_{14}\text{NO}^+\cdot\text{C}_7\text{H}_7\text{O}_3\text{S}^-$, intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds in the range 3.26–3.45 Å are observed. The *p*-toluenesulfonate anions stack in a tail-to-tail (*i.e.* methyl-to-methyl) fashion, with an interplanar toluene-toluene distance of 3.472 Å.

Related literature

For similar benzylpyridinium compounds, see: Ren *et al.* (2002). For reference bond-length data, see: Allen (2002).



Experimental

Crystal data

$\text{C}_{13}\text{H}_{14}\text{NO}^+\cdot\text{C}_7\text{H}_7\text{O}_3\text{S}^-$	$V = 1791.3$ (14) Å ³
$M_r = 371.44$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 9.668$ (5) Å	$\mu = 0.21$ mm ⁻¹
$b = 20.096$ (5) Å	$T = 100$ (2) K
$c = 9.852$ (5) Å	$0.4 \times 0.2 \times 0.1$ mm
$\beta = 110.639$ (5)°	

Data collection

Bruker X8 APEXII diffractometer	32879 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2004)	4447 independent reflections
$T_{\min} = 0.922$, $T_{\max} = 0.979$	3789 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.043$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$	237 parameters
$wR(F^2) = 0.092$	H-atom parameters constrained
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.32$ e Å ⁻³
4447 reflections	$\Delta\rho_{\text{min}} = -0.59$ e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C1}-\text{H1B}\cdots\text{O1}$	0.97	2.49	3.450 (2)	172
$\text{C32}-\text{H32}\cdots\text{O3}$	0.93	2.38	3.265 (2)	159

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT-Plus (Bruker, 2004); data reduction: SAINT-Plus and XPREP (Bruker, 2004); program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: DIAMOND (Brandenburg & Putz, 2005); software used to prepare material for publication: WinGX (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2098).

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1-(4-Methoxybenzyl)pyridinium *p*-toluenesulfonate

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Comment

Tosylation of *p*-methoxybenzylalcohol with tosylchloride in dry pyridine yielded *N*-(4-methoxybenzyl)-pyridinium toluene-4-sulfonate, (I), as a crystalline product in almost quantitative yield. This product exhibited not only NMR signals corresponding to the initially anticipated benzylic tosylate, but also peaks from a pyridine moiety, in a 1:1 ratio. Electro spray mass spectrometry showed a $m/e = 200$ base peak in positive mode corresponding to a *N*-(4-methoxybenzyl)-pyridinium cation and a $m/e = 171$ base peak in negative mode corresponding to a toluene-4-sulfonic acid anion. The unexpected nature of this product and the reaction responsible for it prompted us to prove its structure unequivocally with crystallography. Benzylpyridinium derivatives are described as structurally and magnetically 1-D molecular solids. This is in part due to the cation being nonplanar. The stacking structure of benzylpyridinium molecules can be fine-tuned by varying substituents on the aromatic rings, creating a more conductive solid (Ren *et al.*, 2002).

The title compound, (I), crystallizes with anionic [*p*-Ts][−] (*p*-Ts = *p*-toluenesulfonate) and cationic moieties [MeOBzPy]⁺ (MeOBzPy = 4-methoxy-benzylpyridinium) respectively. In the [MeOBzPy]⁺ cation packing of the pyridinium and 4-methoxybenzyl rings induces a slight distortion from ideal tetrahedral geometry at C1 (C21—C1—N angle of 111.25 (3)°). The methoxy moiety itself is almost in plane with the benzene ring as shown by the torsion angle of 178.23 (3)° through atoms C25—C24—O4—C27. In comparing the rotation of the pyridinium and 4-methoxyphenyl ring systems with respect to the plane formed by atoms C21—C1—N, dihedral angles of 77.6 (1)° and 73.7 (1)°, respectively, are observed. Other bond distances and angles for (I) fall well within the range of similar compounds reported to date [Cambridge Structural Database (CSD), Version 5.27, August 2006 update; Allen, 2002]. In this structure no significant π – π stacking is observed between the [MeOBzPy]⁺ moieties, as typically found in other similar compounds (Ren *et al.*, 2002).

In the crystal packing, C1 of the [MeOBzPy]⁺ molecule acts as a hydrogen-bond donor, *via* H1B, to the sulfonate atom O1. Likewise, C32 acts as a donor, *via* H32, to atom O3, resulting in an intermolecular link and the preferred conformation of the sulfonate O-atoms (Fig. 1). The *p*-toluenesulfonate anions stack in a "tail to tail" fashion with an interplanar toluene–phenyl distance of 3.472 Å (Fig. 2).

Experimental

p-Toluenesulfonyl chloride (3.0 g, 15.7 mmol) and 4-methoxybenzyl alcohol (2.0 g, 14.7 mmol) were dissolved in dry pyridine (3.5 ml). The reaction was left for 5 days at room temperature with a CaCl₂ tube fitted for protection against atmospheric moisture. The resulting solidified reaction mixture was washed with hexane. Recrystallization of the product from dichloromethane yielded 1-(4-methoxybenzyl)-pyridinium *p*-toluene-4-sulfonate (4.91 g, 90%) as colourless cuboid crystals; mp 128–131°; δ_{H} (300 MHz; CDCl₃; Me₄Si) 9.30 (2H, dd, $J = 1.0$ Hz and 8.0 Hz, H-36, H-32); 8.73 (2H, t, $J = 8.0$ Hz, H-35, H-33); 8.22 (1H, t, $J = 8.0$ Hz, H-34); 7.50 (2H, d, $J = 9.0$ Hz, H-25, H-23); 6.75 (2H, d, $J = 9.0$ Hz, H-26, H-22); 7.10 (2H, d, $J = 8.0$ Hz, H-15, H-13); 7.77 (2H, d, $J = 8.0$ Hz, H-16, H-12); 5.91 (2H, s, –CH₂–, H-1); 3.74 (3H,

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s, Ar-OCH₃, H-27); 2.34 (3H, s, Ar—CH₃, H-17); $\delta^{13}\text{C}_{\{\text{H}\}}$ (75 MHz; CDCl₃) 160.9 (C-24), 145.4 (C-32 and C-36), 144.2 (C-34), 142.6 (C-11'), 139.8 (C-14), 131.6 (C-22 and C-26), 129.2 (C-13 and C-15), 128.6 (C-33 and C-35), 126.3 (C-12 and C-16), 125.7 (C-21), 115.1 (C-23 and C-25), 64.5 (—CH₂—, C-1), 55.7 (Ar-OCH₃, C-27), and 21.7 (Ar—CH₃, C-17); *m/z*: (positive mode) 201.3 ($[M+1]^+$, 10%), 200.3 (M^+ , 60%), 122.2 (24%), 121.2 (100%); *m/z* (negative mode) 172.2 ($[M-1]^-$, 8%), 171.2 (M^+ , 100%).

Refinement

The H atoms were positioned geometrically and refined using a riding model with fixed C—H distances of 0.93 Å (CH) [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$], 0.97 Å (CH₂) [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$] and 0.96 Å (CH₃) [$U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}$] respectively.

The highest density peak is 0.32, located 0.78 Å from C11, and the deepest hole is -0.59, located at 0.56 Å from S.

Figures

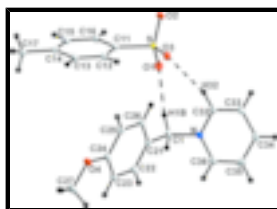


Fig. 1. A view of (I) showing the atom-numbering scheme with displacement ellipsoids at the 30% probability level.

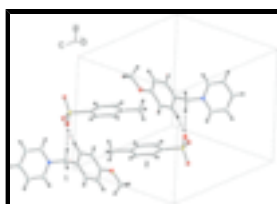


Fig. 2. Partly occupied unit-cell indicating the packing fashion. Symmetry operators for molecules 1 and 2: 1) $1 - x, 1 - y, 2 - z$. 2) x, y, z .

1-(4-Methoxybenzyl)pyridinium *p*-toluenesulfonate

Crystal data

C₁₃H₁₄NO⁺·C₇H₇O₃S⁻

$M_r = 371.44$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 9.668$ (5) Å

$b = 20.096$ (5) Å

$c = 9.852$ (5) Å

$\beta = 110.639$ (5)°

$V = 1791.3$ (14) Å³

$Z = 4$

$F_{000} = 784$

$D_x = 1.377$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71069$ Å

Cell parameters from 9909 reflections

$\theta = 2.4$ – 28.3°

$\mu = 0.21$ mm⁻¹

$T = 100$ (2) K

Cuboid, colourless

$0.4 \times 0.2 \times 0.1$ mm

Data collection

Bruker X8 APEXII 4K KappaCCD diffractometer	3789 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.043$
$T = 100(2)$ K	$\theta_{\text{max}} = 28.3^\circ$
ω and φ scans	$\theta_{\text{min}} = 2.4^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$h = -12 \rightarrow 12$
$T_{\text{min}} = 0.922$, $T_{\text{max}} = 0.979$	$k = -25 \rightarrow 26$
32879 measured reflections	$l = -13 \rightarrow 13$
4447 independent reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0394P)^2 + 0.9825P]$
$R[F^2 > 2\sigma(F^2)] = 0.036$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.092$	$(\Delta/\sigma)_{\text{max}} = 0.002$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.32 \text{ e } \text{\AA}^{-3}$
4447 reflections	$\Delta\rho_{\text{min}} = -0.59 \text{ e } \text{\AA}^{-3}$
237 parameters	Extinction correction: none

Special details

Experimental. The intensity data was collected on a Bruker X8 Apex II 4 K Kappa CCD diffractometer using an exposure time of 20 s/frame. A total of 1896 frames were collected with a frame width of 0.5° covering up to $\theta = 28.3^\circ$ with 100° completeness accomplished.

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.60595 (14)	0.59526 (7)	0.48918 (14)	0.0132 (3)
H1A	0.6495	0.5553	0.4661	0.016*
H1B	0.5078	0.5841	0.4876	0.016*
C11	0.24154 (13)	0.57692 (7)	0.70133 (14)	0.0109 (3)
C12	0.33487 (14)	0.61530 (7)	0.81413 (15)	0.0127 (3)
H12	0.3693	0.6561	0.7947	0.015*
C13	0.37633 (14)	0.59236 (7)	0.95594 (15)	0.0137 (3)
H13	0.4392	0.6181	1.0308	0.016*
C14	0.32567 (14)	0.53154 (7)	0.98852 (14)	0.0131 (3)

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C15	0.23085 (14)	0.49412 (7)	0.87397 (15)	0.0138 (3)
H15	0.1953	0.4536	0.8934	0.017*
C16	0.18852 (14)	0.51633 (7)	0.73120 (14)	0.0127 (3)
H16	0.1252	0.4908	0.6562	0.015*
C17	0.37284 (15)	0.50757 (8)	1.14311 (15)	0.0174 (3)
H17A	0.4769	0.515	1.1905	0.026*
H17B	0.3522	0.4609	1.1442	0.026*
H17C	0.3194	0.5315	1.1932	0.026*
C21	0.69908 (14)	0.61896 (7)	0.63891 (14)	0.0116 (3)
C22	0.83990 (14)	0.59323 (7)	0.70717 (14)	0.0131 (3)
H22	0.8782	0.5631	0.658	0.016*
C23	0.92469 (14)	0.61195 (7)	0.84837 (15)	0.0134 (3)
H23	1.0187	0.5943	0.8935	0.016*
C24	0.86712 (14)	0.65725 (7)	0.92094 (14)	0.0118 (3)
C25	0.72601 (14)	0.68448 (7)	0.85261 (14)	0.0129 (3)
H25	0.6884	0.7153	0.901	0.015*
C26	0.64303 (14)	0.66515 (7)	0.71257 (14)	0.0123 (3)
H26	0.5493	0.683	0.6671	0.015*
C27	1.08315 (15)	0.65152 (8)	1.13428 (15)	0.0194 (3)
H27A	1.0742	0.6042	1.1423	0.029*
H27B	1.1233	0.6707	1.2295	0.029*
H27C	1.1476	0.6609	1.0816	0.029*
C32	0.47083 (14)	0.68464 (7)	0.32476 (14)	0.0122 (3)
H32	0.393	0.6777	0.3579	0.015*
C33	0.45966 (15)	0.73291 (7)	0.22225 (14)	0.0145 (3)
H33	0.374	0.7582	0.1853	0.017*
C34	0.57662 (15)	0.74365 (7)	0.17419 (15)	0.0164 (3)
H34	0.5701	0.776	0.1048	0.02*
C35	0.70346 (15)	0.70537 (8)	0.23123 (15)	0.0174 (3)
H35	0.7832	0.7121	0.2009	0.021*
C36	0.71029 (14)	0.65740 (7)	0.33293 (15)	0.0148 (3)
H36	0.7951	0.6316	0.3715	0.018*
N	0.59458 (11)	0.64748 (6)	0.37720 (12)	0.0108 (2)
O1	0.24697 (11)	0.55275 (5)	0.44539 (11)	0.0182 (2)
O2	0.03159 (10)	0.60938 (5)	0.46323 (11)	0.0174 (2)
O3	0.26504 (10)	0.66785 (5)	0.52365 (10)	0.0145 (2)
O4	0.94071 (10)	0.67943 (5)	1.05911 (10)	0.0161 (2)
S	0.19217 (3)	0.603727 (16)	0.51832 (3)	0.01009 (9)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0142 (6)	0.0113 (7)	0.0119 (6)	-0.0007 (5)	0.0018 (5)	0.0025 (5)
C11	0.0092 (5)	0.0124 (7)	0.0117 (6)	0.0022 (5)	0.0042 (5)	0.0011 (5)
C12	0.0128 (6)	0.0109 (6)	0.0151 (6)	-0.0008 (5)	0.0057 (5)	0.0000 (5)
C13	0.0135 (6)	0.0150 (7)	0.0121 (6)	-0.0011 (5)	0.0039 (5)	-0.0025 (5)
C14	0.0132 (6)	0.0144 (7)	0.0130 (6)	0.0035 (5)	0.0063 (5)	0.0020 (5)
C15	0.0141 (6)	0.0111 (7)	0.0176 (7)	-0.0003 (5)	0.0073 (5)	0.0019 (5)

C16	0.0112 (5)	0.0123 (7)	0.0140 (6)	-0.0004 (5)	0.0037 (5)	-0.0015 (5)
C17	0.0198 (6)	0.0185 (7)	0.0146 (7)	0.0014 (6)	0.0070 (5)	0.0028 (6)
C21	0.0122 (6)	0.0113 (6)	0.0103 (6)	-0.0018 (5)	0.0028 (5)	0.0020 (5)
C22	0.0138 (6)	0.0124 (7)	0.0130 (6)	0.0015 (5)	0.0045 (5)	-0.0004 (5)
C23	0.0107 (5)	0.0150 (7)	0.0130 (6)	0.0028 (5)	0.0023 (5)	0.0018 (5)
C24	0.0121 (6)	0.0136 (7)	0.0095 (6)	-0.0009 (5)	0.0035 (5)	0.0014 (5)
C25	0.0138 (6)	0.0137 (7)	0.0129 (6)	0.0013 (5)	0.0068 (5)	0.0007 (5)
C26	0.0098 (5)	0.0134 (7)	0.0131 (6)	0.0006 (5)	0.0034 (5)	0.0028 (5)
C27	0.0139 (6)	0.0265 (8)	0.0138 (7)	0.0028 (6)	-0.0001 (5)	-0.0015 (6)
C32	0.0101 (5)	0.0151 (7)	0.0118 (6)	0.0006 (5)	0.0045 (5)	-0.0021 (5)
C33	0.0161 (6)	0.0126 (7)	0.0139 (6)	0.0032 (5)	0.0042 (5)	-0.0007 (5)
C34	0.0234 (7)	0.0127 (7)	0.0141 (6)	-0.0045 (5)	0.0077 (5)	-0.0011 (5)
C35	0.0152 (6)	0.0224 (8)	0.0175 (7)	-0.0060 (5)	0.0092 (5)	-0.0049 (6)
C36	0.0092 (5)	0.0181 (7)	0.0165 (7)	-0.0001 (5)	0.0039 (5)	-0.0038 (5)
N	0.0105 (5)	0.0115 (6)	0.0097 (5)	-0.0004 (4)	0.0027 (4)	-0.0014 (4)
O1	0.0246 (5)	0.0158 (5)	0.0153 (5)	0.0057 (4)	0.0084 (4)	-0.0011 (4)
O2	0.0093 (4)	0.0252 (6)	0.0158 (5)	0.0009 (4)	0.0019 (4)	0.0039 (4)
O3	0.0160 (4)	0.0141 (5)	0.0137 (5)	-0.0020 (4)	0.0055 (4)	0.0016 (4)
O4	0.0137 (4)	0.0223 (6)	0.0099 (5)	0.0032 (4)	0.0011 (4)	-0.0027 (4)
S	0.00905 (14)	0.01113 (17)	0.00985 (15)	0.00089 (11)	0.00302 (11)	0.00019 (12)

Geometric parameters (Å, °)

C1—N	1.4983 (17)	C23—H23	0.93
C1—C21	1.5091 (19)	C24—O4	1.3693 (17)
C1—H1A	0.97	C24—C25	1.4022 (18)
C1—H1B	0.97	C25—C26	1.3849 (19)
C11—C12	1.3918 (19)	C25—H25	0.93
C11—C16	1.3921 (19)	C26—H26	0.93
C11—S	1.7783 (16)	C27—O4	1.4285 (17)
C12—C13	1.389 (2)	C27—H27A	0.96
C12—H12	0.93	C27—H27B	0.96
C13—C14	1.3954 (19)	C27—H27C	0.96
C13—H13	0.93	C32—N	1.3492 (17)
C14—C15	1.397 (2)	C32—C33	1.377 (2)
C14—C17	1.507 (2)	C32—H32	0.93
C15—C16	1.393 (2)	C33—C34	1.3881 (19)
C15—H15	0.93	C33—H33	0.93
C16—H16	0.93	C34—C35	1.388 (2)
C17—H17A	0.96	C34—H34	0.93
C17—H17B	0.96	C35—C36	1.375 (2)
C17—H17C	0.96	C35—H35	0.93
C21—C22	1.3884 (19)	C36—N	1.3511 (17)
C21—C26	1.3996 (19)	C36—H36	0.93
C22—C23	1.3945 (19)	O1—S	1.4542 (11)
C22—H22	0.93	O2—S	1.4573 (12)
C23—C24	1.3895 (19)	O3—S	1.4606 (11)
N—C1—C21	111.25 (11)	O4—C24—C25	115.27 (12)
N—C1—H1A	109.4	C23—C24—C25	120.47 (12)

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C21—C1—H1A	109.4	C26—C25—C24	119.52 (12)
N—C1—H1B	109.4	C26—C25—H25	120.2
C21—C1—H1B	109.4	C24—C25—H25	120.2
H1A—C1—H1B	108	C25—C26—C21	120.55 (12)
C12—C11—C16	119.96 (12)	C25—C26—H26	119.7
C12—C11—S	120.55 (11)	C21—C26—H26	119.7
C16—C11—S	119.48 (10)	O4—C27—H27A	109.5
C13—C12—C11	119.67 (13)	O4—C27—H27B	109.5
C13—C12—H12	120.2	H27A—C27—H27B	109.5
C11—C12—H12	120.2	O4—C27—H27C	109.5
C12—C13—C14	121.44 (13)	H27A—C27—H27C	109.5
C12—C13—H13	119.3	H27B—C27—H27C	109.5
C14—C13—H13	119.3	N—C32—C33	120.03 (12)
C13—C14—C15	118.00 (12)	N—C32—H32	120
C13—C14—C17	120.45 (12)	C33—C32—H32	120
C15—C14—C17	121.55 (13)	C32—C33—C34	119.81 (13)
C16—C15—C14	121.27 (13)	C32—C33—H33	120.1
C16—C15—H15	119.4	C34—C33—H33	120.1
C14—C15—H15	119.4	C35—C34—C33	119.04 (13)
C11—C16—C15	119.66 (12)	C35—C34—H34	120.5
C11—C16—H16	120.2	C33—C34—H34	120.5
C15—C16—H16	120.2	C36—C35—C34	119.49 (13)
C14—C17—H17A	109.5	C36—C35—H35	120.3
C14—C17—H17B	109.5	C34—C35—H35	120.3
H17A—C17—H17B	109.5	N—C36—C35	120.41 (13)
C14—C17—H17C	109.5	N—C36—H36	119.8
H17A—C17—H17C	109.5	C35—C36—H36	119.8
H17B—C17—H17C	109.5	C32—N—C36	121.20 (12)
C22—C21—C26	119.25 (12)	C32—N—C1	119.65 (11)
C22—C21—C1	120.08 (12)	C36—N—C1	119.13 (11)
C26—C21—C1	120.63 (12)	C24—O4—C27	117.11 (11)
C21—C22—C23	120.93 (13)	O1—S—O2	113.37 (6)
C21—C22—H22	119.5	O1—S—O3	112.59 (6)
C23—C22—H22	119.5	O2—S—O3	112.43 (6)
C24—C23—C22	119.26 (12)	O1—S—C11	105.86 (7)
C24—C23—H23	120.4	O2—S—C11	105.74 (6)
C22—C23—H23	120.4	O3—S—C11	106.09 (6)
O4—C24—C23	124.25 (12)		
C16—C11—C12—C13	0.95 (19)	C22—C21—C26—C25	-0.8 (2)
S—C11—C12—C13	-177.72 (10)	C1—C21—C26—C25	176.94 (12)
C11—C12—C13—C14	-0.4 (2)	N—C32—C33—C34	-0.7 (2)
C12—C13—C14—C15	-0.28 (19)	C32—C33—C34—C35	-0.2 (2)
C12—C13—C14—C17	179.68 (12)	C33—C34—C35—C36	0.5 (2)
C13—C14—C15—C16	0.43 (19)	C34—C35—C36—N	0.0 (2)
C17—C14—C15—C16	-179.53 (12)	C33—C32—N—C36	1.2 (2)
C12—C11—C16—C15	-0.80 (19)	C33—C32—N—C1	179.75 (12)
S—C11—C16—C15	177.88 (10)	C35—C36—N—C32	-0.9 (2)
C14—C15—C16—C11	0.11 (19)	C35—C36—N—C1	-179.44 (12)
N—C1—C21—C22	-107.37 (14)	C21—C1—N—C32	-101.63 (14)

N—C1—C21—C26	74.91 (15)	C21—C1—N—C36	76.93 (15)
C26—C21—C22—C23	1.1 (2)	C23—C24—O4—C27	-2.85 (19)
C1—C21—C22—C23	-176.69 (12)	C25—C24—O4—C27	178.23 (12)
C21—C22—C23—C24	-0.3 (2)	C12—C11—S—O1	118.83 (11)
C22—C23—C24—O4	-179.58 (12)	C16—C11—S—O1	-59.85 (12)
C22—C23—C24—C25	-0.7 (2)	C12—C11—S—O2	-120.61 (11)
O4—C24—C25—C26	179.93 (12)	C16—C11—S—O2	60.72 (12)
C23—C24—C25—C26	1.0 (2)	C12—C11—S—O3	-1.01 (12)
C24—C25—C26—C21	-0.2 (2)	C16—C11—S—O3	-179.68 (10)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C1—H1B \cdots O1	0.97	2.49	3.450 (2)	172
C32—H32 \cdots O3	0.93	2.38	3.265 (2)	159

Fig. 1

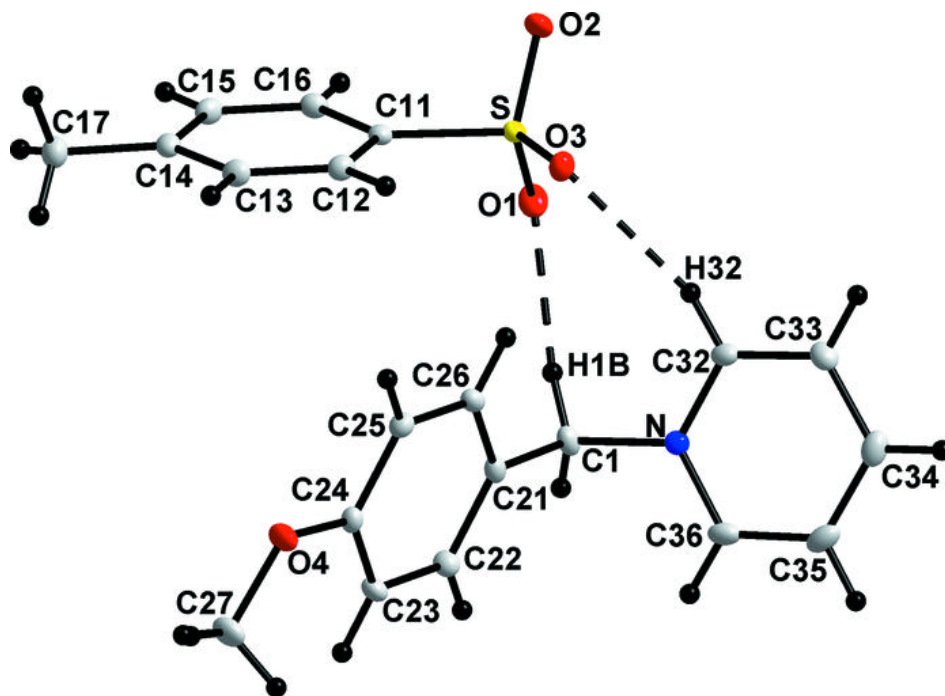


Fig. 2

