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Benzotriazolium 4-methylbenzenesulfonate

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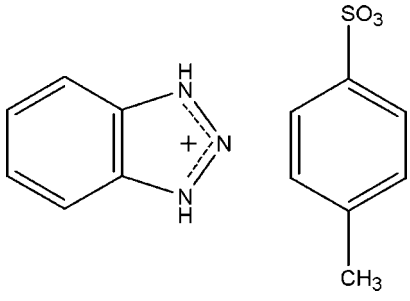
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.108; data-to-parameter ratio = 20.4.

In the title molecular salt, $C_6H_6N_3^+\cdot C_7H_7O_3S^-$, the components are linked by N—H···O hydrogen bonds into zigzag chains along [100]. These chains are further connected by weak C—H···O, C—H···π and π–π (centroid-to-centroid distances = 3.510, 3.701 and 3.754 Å) interactions into a three-dimensional network.

Related literature

For biological activities of benzotriazole derivates, see: Dubey *et al.* (2011); Gaikwad *et al.* (2012). For related structures, see: Sudhahar *et al.* (2013); Yang *et al.* (2010).



Experimental

Crystal data

$C_6H_6N_3^+\cdot C_7H_7O_3S^-$
M_r = 291.32
Orthorhombic, *Pbca*
a = 12.2330 (5) Å
b = 13.4144 (6) Å
c = 16.3320 (9) Å
V = 2680.1 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 295 K
0.26 × 0.24 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.937, T_{max} = 0.951
45507 measured reflections
3889 independent reflections
2766 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.108
S = 1.08
3889 reflections
191 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2^{i}	0.87 (1)	1.82 (1)	2.661 (2)	161 (2)
N3—H3A···O3^{ii}	0.87 (1)	1.77 (1)	2.6326 (19)	176 (2)
C3—H3···O2^{iii}	0.93	2.48	3.359 (2)	158
C12—H12···$Cg1^{iv}$	0.93	2.66	3.500 (2)	150

Symmetry codes: (i) $-x+2, -y, -z$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, z$; (iii) $x-\frac{1}{2}, y, -z+\frac{1}{2}$; (iv) $x-\frac{3}{2}, y, -z-\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

The authors thank SAIF, IIT, Madras, for data collection.

Supporting information for this paper is available from the IUCr electronic archives (Reference: BT6963).

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supporting information

Acta Cryst. (2014). E**70**, o350 [doi:10.1107/S1600536814003857]

Benzotriazolium 4-methylbenzenesulfonate

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S1. Comment

Benzotriazole derivates exhibit antitubercular and antimicrobial (Dubey *et al.*, 2011; Gaikwad *et al.*, 2012) bio-activities. We herewith report the crystal structure of the title compound (Fig. 1). In the title compound, the geometric parameters are comparable with reported structures (Sudhahar *et al.*, 2013; Yang *et al.*, 2010).

The crystal structure exhibits intermolecular N-H···O, C-H···O, C-H···π (Table 1; Fig. 2) and π···π interactions [Cg1···Cg2^{i}: 3.510Å; Cg2···Cg3^{ii}: 3.754Å; Cg3···Cg3^{ii}: 3.701Å; symmetry operators: (i) x,y,z; (ii) 1-x,-y,-z; Cg1, Cg2 and Cg3 are the centroids of the rings (C1-C6), (N1/N2/C8/C13/N3) and (C8-C13), respectively].

S2. Experimental

Benzotriazole ($C_6H_5N_3$, 1.1913 g) and p-toluenesulfonic acid ($CH_3C_6H_4S0_3H$, 1.90 g) were taken in an equimolar ratio and dissolved in methanol and water. The solution was allowed for slow evaporation at room temperature. The crystals were collected after a the period of 45 days.

S3. Refinement

All H atoms were located in a difference Fourier map. N-bound H atoms were refined with an N-H distance restraint of 0.86 (1)Å. The C-bound H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 and U_{iso}(H) = 1.2U_{eq}(C) for CH and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for CH_3.

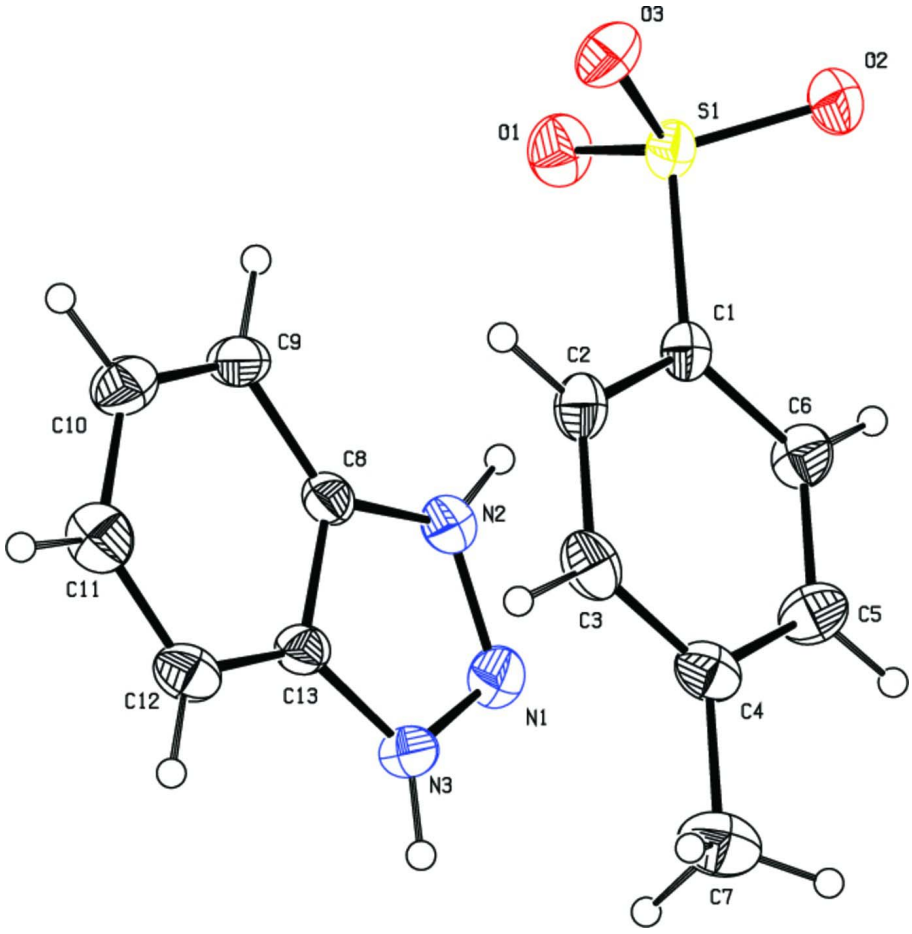

Figure 1

The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids for non-H atoms.

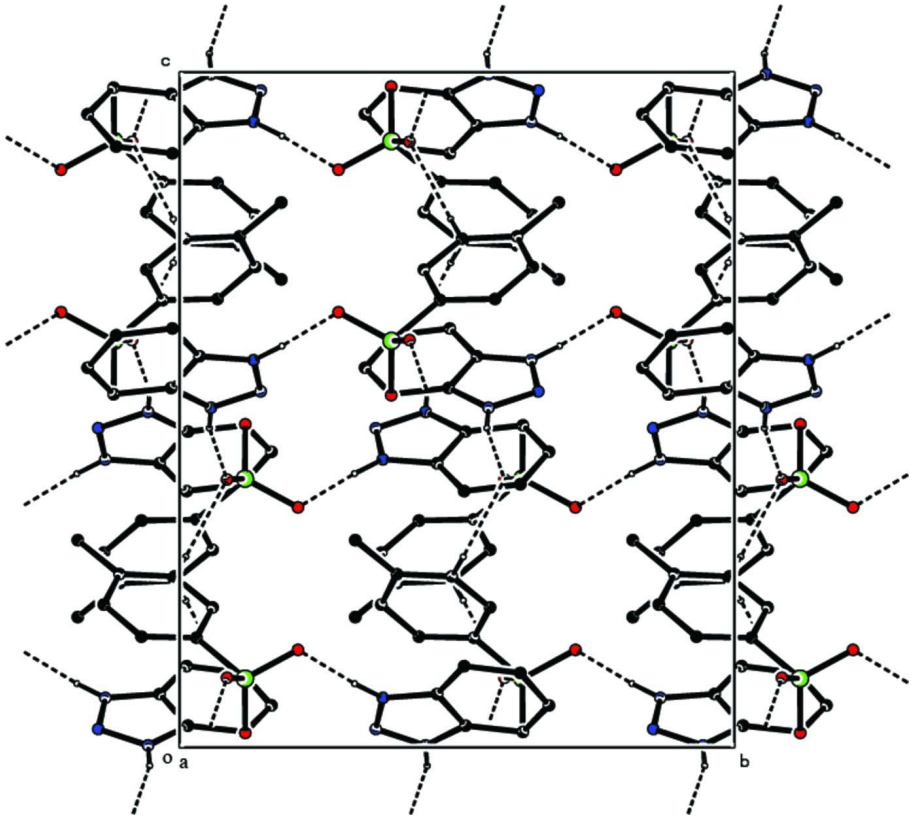

Figure 2

The packing of the title compound, viewed down *a* axis. Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

Benzotriazolium 4-methylbenzenesulfonate

Crystal data

$C_6H_6N_3^+·C_7H_7O_3S^-$
M_r = 291.32
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 12.2330 (5) Å
b = 13.4144 (6) Å
c = 16.3320 (9) Å
V = 2680.1 (2) Å^3
Z = 8
F(000) = 1216
D_x = 1.444 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9880 reflections
θ = 2.5–29.4°
μ = 0.25 mm^{-1}
T = 295 K
Block, colourless
0.26 × 0.24 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and *φ* scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.937, T_{max} = 0.951
45507 measured reflections
3889 independent reflections
2766 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 30.5°, θ_{min} = 2.5°
h = −17→17
k = −18→18
l = −22→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.108$
$S = 1.08$
3889 reflections
191 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0359P)^2 + 1.3937P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0071 (5)

Special details

Geometry. 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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.90878 (12)	0.03041 (12)	0.16244 (9)	0.0333 (3)
C2	0.81836 (14)	0.05952 (13)	0.20733 (11)	0.0418 (4)
H2	0.7961	0.1258	0.2066	0.050*
C3	0.76102 (15)	−0.00918 (15)	0.25324 (11)	0.0460 (4)
H3	0.6998	0.0114	0.2824	0.055*
C4	0.79293 (15)	−0.10826 (14)	0.25669 (11)	0.0432 (4)
C5	0.88410 (16)	−0.13637 (13)	0.21152 (12)	0.0475 (4)
H5	0.9074	−0.2023	0.2132	0.057*
C6	0.94106 (15)	−0.06856 (13)	0.16406 (11)	0.0429 (4)
H6	1.0009	−0.0894	0.1333	0.051*
C7	0.73032 (19)	−0.18330 (17)	0.30695 (13)	0.0633 (6)
H7A	0.6711	−0.2097	0.2750	0.095*
H7B	0.7017	−0.1515	0.3550	0.095*
H7C	0.7783	−0.2366	0.3228	0.095*
C8	0.67586 (12)	0.01515 (12)	0.03229 (10)	0.0344 (3)
C9	0.67158 (15)	0.11875 (12)	0.02304 (11)	0.0414 (4)
H9	0.7228	0.1535	−0.0079	0.050*
C10	0.58772 (16)	0.16563 (14)	0.06224 (12)	0.0486 (4)
H10	0.5809	0.2344	0.0569	0.058*
C11	0.51133 (16)	0.11404 (15)	0.11036 (12)	0.0504 (5)
H11	0.4563	0.1499	0.1363	0.061*
C12	0.51505 (15)	0.01289 (14)	0.12041 (11)	0.0448 (4)
H12	0.4647	−0.0211	0.1526	0.054*

C13	0.59940 (13)	−0.03593 (12)	0.07916 (10)	0.0349 (3)
N1	0.71524 (13)	−0.14630 (11)	0.02730 (11)	0.0486 (4)
N2	0.74412 (12)	−0.05667 (11)	0.00306 (10)	0.0430 (3)
N3	0.62856 (13)	−0.13358 (11)	0.07344 (10)	0.0425 (3)
O1	0.93251 (11)	0.11850 (10)	0.02148 (8)	0.0524 (3)
O2	1.09402 (10)	0.08554 (10)	0.10320 (9)	0.0507 (3)
O3	0.96735 (11)	0.21352 (9)	0.14451 (8)	0.0507 (3)
S1	0.98089 (3)	0.11794 (3)	0.10202 (3)	0.03644 (12)
H2A	0.8027 (13)	−0.0538 (18)	−0.0271 (13)	0.075 (8)*
H3A	0.5961 (17)	−0.1848 (12)	0.0946 (13)	0.068 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0331 (8)	0.0359 (8)	0.0310 (8)	0.0049 (6)	−0.0028 (6)	−0.0038 (6)
C2	0.0387 (8)	0.0433 (9)	0.0434 (9)	0.0115 (7)	−0.0001 (7)	−0.0048 (7)
C3	0.0345 (8)	0.0616 (11)	0.0419 (9)	0.0035 (8)	0.0046 (7)	−0.0070 (9)
C4	0.0439 (9)	0.0508 (10)	0.0349 (9)	−0.0100 (8)	−0.0045 (7)	−0.0063 (7)
C5	0.0605 (12)	0.0349 (8)	0.0471 (10)	0.0004 (8)	0.0034 (9)	−0.0053 (7)
C6	0.0455 (9)	0.0392 (9)	0.0440 (9)	0.0079 (7)	0.0083 (8)	−0.0063 (7)
C7	0.0662 (14)	0.0698 (14)	0.0539 (12)	−0.0192 (11)	0.0060 (10)	0.0002 (11)
C8	0.0292 (7)	0.0383 (8)	0.0356 (8)	−0.0036 (6)	−0.0033 (6)	0.0015 (6)
C9	0.0429 (9)	0.0369 (8)	0.0443 (9)	−0.0090 (7)	0.0000 (7)	0.0052 (7)
C10	0.0580 (11)	0.0344 (8)	0.0534 (11)	−0.0022 (8)	−0.0013 (9)	−0.0022 (8)
C11	0.0490 (10)	0.0524 (11)	0.0499 (11)	0.0039 (9)	0.0062 (9)	−0.0123 (9)
C12	0.0415 (9)	0.0531 (10)	0.0399 (9)	−0.0085 (8)	0.0070 (7)	−0.0001 (8)
C13	0.0349 (8)	0.0343 (8)	0.0356 (8)	−0.0063 (6)	−0.0049 (6)	0.0023 (6)
N1	0.0438 (8)	0.0392 (8)	0.0628 (10)	0.0038 (7)	−0.0060 (8)	0.0024 (7)
N2	0.0329 (7)	0.0426 (8)	0.0536 (9)	0.0011 (6)	0.0020 (7)	0.0027 (7)
N3	0.0429 (8)	0.0352 (7)	0.0496 (9)	−0.0059 (6)	−0.0045 (7)	0.0072 (6)
O1	0.0532 (8)	0.0656 (9)	0.0383 (7)	0.0041 (7)	−0.0027 (6)	0.0063 (6)
O2	0.0346 (6)	0.0543 (7)	0.0631 (9)	0.0069 (6)	0.0037 (6)	0.0067 (6)
O3	0.0629 (8)	0.0335 (6)	0.0558 (8)	0.0072 (6)	−0.0009 (7)	0.0004 (5)
S1	0.0347 (2)	0.0360 (2)	0.0387 (2)	0.00720 (16)	−0.00031 (16)	0.00142 (16)

Geometric parameters (Å, º)

C1—C2	1.383 (2)	C8—C9	1.399 (2)
C1—C6	1.385 (2)	C9—C10	1.363 (3)
C1—S1	1.7694 (17)	C9—H9	0.9300
C2—C3	1.380 (3)	C10—C11	1.404 (3)
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.386 (3)	C11—C12	1.368 (3)
C3—H3	0.9300	C11—H11	0.9300
C4—C5	1.389 (3)	C12—C13	1.395 (2)
C4—C7	1.508 (3)	C12—H12	0.9300
C5—C6	1.383 (3)	C13—N3	1.361 (2)
C5—H5	0.9300	N1—N3	1.312 (2)

C6—H6	0.9300	N1—N2	1.314 (2)
C7—H7A	0.9600	N2—H2A	0.871 (9)
C7—H7B	0.9600	N3—H3A	0.866 (9)
C7—H7C	0.9600	O1—S1	1.4423 (14)
C8—N2	1.361 (2)	O2—S1	1.4507 (13)
C8—C13	1.389 (2)	O3—S1	1.4673 (13)

C2—C1—C6	119.24 (16)	C10—C9—H9	122.1
C2—C1—S1	120.46 (13)	C8—C9—H9	122.1
C6—C1—S1	120.29 (13)	C9—C10—C11	122.46 (17)
C3—C2—C1	120.40 (16)	C9—C10—H10	118.8
C3—C2—H2	119.8	C11—C10—H10	118.8
C1—C2—H2	119.8	C12—C11—C10	122.29 (18)
C2—C3—C4	121.28 (16)	C12—C11—H11	118.9
C2—C3—H3	119.4	C10—C11—H11	118.9
C4—C3—H3	119.4	C11—C12—C13	115.62 (16)
C3—C4—C5	117.69 (17)	C11—C12—H12	122.2
C3—C4—C7	121.27 (18)	C13—C12—H12	122.2
C5—C4—C7	121.04 (18)	N3—C13—C8	105.09 (15)
C6—C5—C4	121.57 (17)	N3—C13—C12	132.75 (16)
C6—C5—H5	119.2	C8—C13—C12	122.16 (15)
C4—C5—H5	119.2	N3—N1—N2	105.75 (14)
C5—C6—C1	119.81 (16)	N1—N2—C8	112.14 (15)
C5—C6—H6	120.1	N1—N2—H2A	115.6 (16)
C1—C6—H6	120.1	C8—N2—H2A	132.3 (16)
C4—C7—H7A	109.5	N1—N3—C13	112.12 (14)
C4—C7—H7B	109.5	N1—N3—H3A	119.8 (16)
H7A—C7—H7B	109.5	C13—N3—H3A	128.1 (16)
C4—C7—H7C	109.5	O1—S1—O2	113.90 (8)
H7A—C7—H7C	109.5	O1—S1—O3	112.36 (8)
H7B—C7—H7C	109.5	O2—S1—O3	111.30 (8)
N2—C8—C13	104.90 (14)	O1—S1—C1	107.91 (8)
N2—C8—C9	133.48 (16)	O2—S1—C1	105.62 (7)
C13—C8—C9	121.62 (15)	O3—S1—C1	105.06 (8)
C10—C9—C8	115.83 (16)		

C6—C1—C2—C3	0.1 (3)	N2—C8—C13—C12	179.46 (15)
S1—C1—C2—C3	178.81 (13)	C9—C8—C13—C12	−0.8 (3)
C1—C2—C3—C4	0.9 (3)	C11—C12—C13—N3	−179.15 (18)
C2—C3—C4—C5	−0.7 (3)	C11—C12—C13—C8	1.2 (3)
C2—C3—C4—C7	179.93 (18)	N3—N1—N2—C8	−0.8 (2)
C3—C4—C5—C6	−0.5 (3)	C13—C8—N2—N1	0.63 (19)
C7—C4—C5—C6	178.86 (18)	C9—C8—N2—N1	−179.05 (18)
C4—C5—C6—C1	1.5 (3)	N2—N1—N3—C13	0.6 (2)
C2—C1—C6—C5	−1.2 (3)	C8—C13—N3—N1	−0.21 (19)
S1—C1—C6—C5	180.00 (14)	C12—C13—N3—N1	−179.87 (18)
N2—C8—C9—C10	179.18 (18)	C2—C1—S1—O1	−89.85 (15)
C13—C8—C9—C10	−0.4 (3)	C6—C1—S1—O1	88.90 (15)

C8—C9—C10—C11	1.2 (3)	C2—C1—S1—O2	147.97 (14)
C9—C10—C11—C12	−0.8 (3)	C6—C1—S1—O2	−33.28 (16)
C10—C11—C12—C13	−0.5 (3)	C2—C1—S1—O3	30.22 (15)
N2—C8—C13—N3	−0.24 (17)	C6—C1—S1—O3	−151.04 (14)
C9—C8—C13—N3	179.48 (15)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O2^{i}	0.87 (1)	1.82 (1)	2.661 (2)	161 (2)
N3—H3*A*···O3^{ii}	0.87 (1)	1.77 (1)	2.6326 (19)	176 (2)
C3—H3···O2^{iii}	0.93	2.48	3.359 (2)	158
C12—H12···*Cg*1^{iv}	0.93	2.66	3.500 (2)	150

Symmetry codes: (i) −*x*+2, −*y*, −*z*; (ii) −*x*+3/2, *y*−1/2, *z*; (iii) *x*−1/2, *y*, −*z*+1/2; (iv) *x*−3/2, *y*, −*z*−1/2.