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Phenothiazine–picric acid (1/1)

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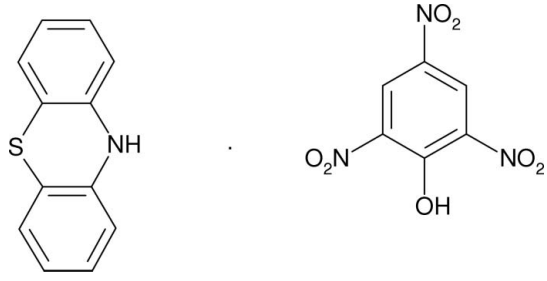
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.047; wR factor = 0.097; data-to-parameter ratio = 13.9.

The title compound, $C_{12}H_9NS{\cdot}C_6H_3N_3O_7$, is a 1:1 adduct of neutral phenothiazine (pz) and picric acid (pa). A weak bifurcated N—H···(O,O) hydrogen bond links the pa and pz species and an intramolecular O—H···O bond occurs within the pa molecule. The O atoms of one of the pa nitro groups are disordered over two positions of almost equal [0.54 (2): 0.46 (2)] occupancy. The dihedral angle between the pz aromatic ring planes is 11.81 (10)°.

Related literature

For background, see: Bell *et al.* (1968); McDowell (1976); van de Waal & Feil (1977); Sun *et al.* (2004); Feinberg & Snyder (1975); Amaral *et al.* (2001). For related literature, see: Herbstein & Kaftory (1976).



Experimental

Crystal data

$C_{12}H_9NS{\cdot}C_6H_3N_3O_7$
M_r = 428.38
Orthorhombic, $P2_12_12_1$
a = 7.2723 (7) Å
b = 8.9800 (9) Å
c = 27.549 (3) Å
V = 1799.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 295 (2) K
0.30 × 0.10 × 0.10 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: none
11121 measured reflections
4124 independent reflections
2300 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.097
S = 0.89
4124 reflections
296 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Absolute structure: Flack (1983), 1716 Friedel pairs
Flack parameter: 0.12 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O6A	0.81 (3)	2.74 (4)	3.520 (7)	162 (3)
N1—H1···O6B	0.81 (3)	2.77 (3)	3.533 (8)	157 (3)
N1—H1···O7A	0.81 (3)	2.60 (3)	3.339 (10)	151 (3)
N1—H1···O7B	0.81 (3)	2.56 (3)	3.311 (11)	156 (3)
O1—H2···O2	0.95 (3)	1.69 (3)	2.550 (3)	148 (3)

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2440).

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supplementary materials

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Comment

Phenothiazine, $C_{12}H_9NS$, has a number of interesting features. It is a potent antibacterial agent (Feinberg & Snyder, 1975; Amaral *et al.*, 2001) and shows remarkable redox properties, easily generating a stable $C_{12}H_9NS^+$ radical cation that can be crystallized (Sun *et al.*, 2004). Phenothiazine is polymorphic: as well as a $P2_1$ monoclinic form (Bell *et al.*, 1968), a second modification shows unusual twinning, with the true $P2_1/c$ monoclinic structure (van de Waal & Feil, 1977) masquerading as orthorhombic (McDowell, 1976).

Here we describe the synthesis and structure of the title compound a 1:1 adduct of neutral phenothiazine and picric acid (Fig. 1).

The phenothiazine molecule shows a rather small deviation from planarity [dihedral angle between the C1—C6 and C7—C12 rings = 11.81 (10)°] and the C—S distances [C1—S1 = 1.762 (3) Å, C12—S1 = 1.747 (3) Å] are consistent with the presence of the neutral molecule, rather than the radical cation (Sun *et al.*, 2004), in (I). With respect to the mean plane of the C1—C6 ring, N1 and S1 deviate by 0.034 (5) and 0.122 (4) Å, respectively. For the C7—C12 ring, the equivalent deviations are 0.038 (5) and 0.028 (4) Å.

The significant variation of the C—C bond lengths around the picric acid aromatic ring can be related to the contributions of various resonance forms involving the nitro groups (Herbstein & Kaftory, 1976). The N4/O6/O7 nitro group is disordered over two orientations, with almost equal occupancies of 0.54 (2):0.46 (2). The dihedral angle between the disorder components is 78 (1)°. The other two nitro groups are almost co-planar with the benzene ring.

The two constituents of the title adduct interact by a weak, bifurcated N—H···(O,*O*) bond from phenothiazine to the disordered nitro group of the picric acid, with both disorder components resulting in similar H bond geometries. A typical (Herbstein & Kaftory, 1976) intramolecular O—H···O hydrogen bond occurs within the picric acid molecule. The disorder of the nitro group appears to be correlated with close intermolecular O···O contacts involving the picric acid molecules in the a unit-cell direction.

Experimental

Phenothiazine (0.9970 g, 0.05 mol) and picric acid (1.1468 g, 0.05 mol) were dissolved in chloroform separately and the solutions were mixed and stirred in a beaker. After one week, black needle shaped crystals were harvested and washed well with carbon tetrachloride and dried in a vacuum desiccator over P_2O_5. Dark, very soft, rods of the title compound were recrystallized from $CHCl_3$. When the rods are crushed and smeared on a glass slide, a dark orange colour is apparent. They melt with decomposition at 393 K.

Refinement

The N4 nitro group is disordered over two orientations with populations 0.54 (2):0.46 (2) (sum constraind to unity).

The O– and N-bound H atoms were located in difference maps and their positions were freely refined with U_{iso}(H) = 1.2U_{eq}(carrier).

The C-bound H atoms were geometrically placed (C—H = 0.93 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier).

Figures

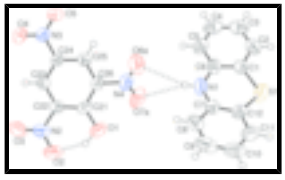


Fig. 1. View of the molecular structure showing 50% displacement ellipsoids (arbitrary sphere for the H atom). The hydrogen bonds are shown as double-dashed lines. Only one orientation of the disordered N4/O6/O7 nitro group is shown.

Phenothiazine–picric acid (1/1)

Crystal data

$C_{12}H_9NS·C_6H_3N_3O_7$	$Z = 4$
$M_r = 428.38$	$F_{000} = 880$
Orthorhombic, $P2_12_12_1$	$D_x = 1.582$ Mg m^{-3}
Hall symbol: P 2ac 2ab	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.2723$ (7) Å	$\mu = 0.23$ mm^{-1}
$b = 8.9800$ (9) Å	$T = 295$ (2) K
$c = 27.549$ (3) Å	Rod, very dark orange
$V = 1799.1$ (3) Å^3	0.30 × 0.10 × 0.10 mm

Data collection

Bruker SMART1000 CCD diffractometer	2300 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.044$
Monochromator: graphite	$\theta_{max} = 27.6°$
$T = 295(2)$ K	$\theta_{min} = 4.3°$
ω scans	$h = -9\rightarrow9$
Absorption correction: none	$k = -7\rightarrow11$
11121 measured reflections	$l = -35\rightarrow35$
4124 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: difmap (O-H and N-H) and geom (C-H)
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.047$	$w = 1/[\sigma^2(F_o^2) + (0.0411P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.097$	$(\Delta/\sigma)_{max} = 0.001$
$S = 0.89$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
4124 reflections	$\Delta\rho_{min} = -0.16$ e Å^{-3}
296 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1716 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.12 (10)

Special details

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.

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 $F^2 > 2$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}	Occ. (<1)
C1	0.6577 (3)	0.5800 (3)	0.33533 (10)	0.0512 (7)	
C2	0.6216 (4)	0.6559 (4)	0.29269 (11)	0.0675 (9)	
H2A	0.6261	0.6059	0.2632	0.081*	
C3	0.5791 (5)	0.8049 (5)	0.29381 (15)	0.0800 (10)	
H3	0.5542	0.8554	0.2651	0.096*	
C4	0.5735 (4)	0.8792 (4)	0.33742 (15)	0.0767 (9)	
H4	0.5426	0.9797	0.3382	0.092*	
C5	0.6135 (4)	0.8054 (3)	0.37971 (12)	0.0664 (9)	
H5	0.6124	0.8572	0.4089	0.080*	
C6	0.6555 (4)	0.6544 (3)	0.37959 (10)	0.0530 (7)	
C7	0.7653 (4)	0.4400 (3)	0.42768 (10)	0.0531 (7)	
C8	0.8347 (4)	0.3950 (4)	0.47242 (11)	0.0662 (8)	
H8	0.8314	0.4601	0.4987	0.079*	
C9	0.9084 (5)	0.2543 (5)	0.47808 (14)	0.0859 (11)	
H9	0.9551	0.2256	0.5081	0.103*	
C10	0.9133 (5)	0.1569 (4)	0.43996 (18)	0.0901 (12)	

H10	0.9614	0.0618	0.4440	0.108*	
C11	0.8468 (5)	0.2008 (3)	0.39565 (13)	0.0718 (9)	
H11	0.8508	0.1347	0.3697	0.086*	
C12	0.7738 (4)	0.3412 (3)	0.38875 (10)	0.0543 (7)	
N1	0.6881 (5)	0.5818 (3)	0.42300 (9)	0.0762 (9)	
H1	0.697 (5)	0.631 (4)	0.4475 (12)	0.091*	
S1	0.69464 (12)	0.38660 (9)	0.33075 (3)	0.0718 (3)	
C21	0.6419 (4)	0.7960 (3)	0.63036 (10)	0.0486 (7)	
C22	0.6397 (3)	0.8755 (3)	0.67412 (9)	0.0457 (6)	
C23	0.6772 (3)	1.0262 (3)	0.67629 (9)	0.0458 (6)	
H23	0.6704	1.0772	0.7056	0.055*	
C24	0.7245 (3)	1.0987 (3)	0.63455 (8)	0.0427 (6)	
C25	0.7296 (4)	1.0264 (3)	0.59049 (9)	0.0480 (7)	
H25	0.7613	1.0774	0.5623	0.058*	
C26	0.6870 (4)	0.8776 (3)	0.58903 (9)	0.0478 (6)	
N2	0.5977 (4)	0.8011 (3)	0.71962 (10)	0.0636 (7)	
N3	0.7712 (3)	1.2571 (3)	0.63615 (9)	0.0562 (6)	
N4	0.6920 (5)	0.8059 (3)	0.54120 (10)	0.0714 (7)	
O1	0.6062 (3)	0.6509 (2)	0.62691 (9)	0.0744 (7)	
H2	0.572 (5)	0.623 (4)	0.6589 (12)	0.089*	
O2	0.5599 (4)	0.6672 (3)	0.71851 (9)	0.0902 (8)	
O3	0.6021 (4)	0.8721 (3)	0.75672 (9)	0.0945 (8)	
O4	0.7424 (3)	1.3233 (2)	0.67420 (8)	0.0773 (6)	
O5	0.8380 (3)	1.3140 (2)	0.59996 (7)	0.0734 (6)	
O6A	0.803 (3)	0.8473 (16)	0.5120 (4)	0.118 (5)	0.54 (2)
O7A	0.576 (2)	0.7138 (16)	0.5324 (2)	0.116 (5)	0.54 (2)
O6B	0.672 (3)	0.8824 (10)	0.5057 (3)	0.109 (5)	0.46 (2)
O7B	0.717 (4)	0.6743 (8)	0.5391 (4)	0.126 (7)	0.46 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0421 (15)	0.0557 (17)	0.0559 (18)	−0.0024 (13)	0.0034 (14)	−0.0001 (14)
C2	0.066 (2)	0.083 (3)	0.0535 (19)	−0.0080 (19)	−0.0008 (16)	0.0050 (17)
C3	0.080 (2)	0.079 (3)	0.081 (3)	−0.004 (2)	−0.008 (2)	0.026 (2)
C4	0.068 (2)	0.0543 (19)	0.108 (3)	0.0069 (17)	−0.001 (2)	0.013 (2)
C5	0.070 (2)	0.055 (2)	0.074 (2)	0.0141 (17)	0.0044 (17)	−0.0071 (16)
C6	0.0517 (18)	0.0544 (19)	0.0529 (17)	0.0086 (14)	−0.0027 (14)	−0.0038 (13)
C7	0.0487 (17)	0.0538 (18)	0.0568 (18)	0.0030 (14)	0.0045 (14)	0.0016 (14)
C8	0.0632 (19)	0.076 (2)	0.0595 (18)	0.0041 (18)	0.0086 (16)	0.0085 (16)
C9	0.076 (2)	0.097 (3)	0.085 (3)	0.020 (2)	0.018 (2)	0.044 (3)
C10	0.091 (3)	0.063 (2)	0.116 (3)	0.021 (2)	0.029 (3)	0.031 (2)
C11	0.073 (2)	0.050 (2)	0.092 (3)	−0.0019 (17)	0.0130 (19)	0.0046 (17)
C12	0.0458 (16)	0.0477 (17)	0.0694 (19)	−0.0047 (14)	0.0077 (14)	−0.0011 (14)
N1	0.117 (2)	0.0646 (19)	0.0475 (16)	0.0315 (19)	−0.0094 (16)	−0.0129 (12)
S1	0.0836 (5)	0.0639 (5)	0.0680 (5)	0.0109 (5)	−0.0123 (5)	−0.0211 (4)
C21	0.0466 (17)	0.0352 (16)	0.0639 (19)	−0.0031 (13)	−0.0079 (13)	0.0002 (13)
C22	0.0460 (15)	0.0444 (15)	0.0465 (15)	0.0011 (12)	−0.0011 (12)	0.0046 (14)

C23	0.0501 (15)	0.0424 (15)	0.0450 (15)	0.0047 (13)	−0.0031 (13)	0.0005 (12)
C24	0.0480 (15)	0.0330 (14)	0.0469 (15)	0.0007 (13)	−0.0051 (12)	−0.0012 (12)
C25	0.0550 (17)	0.0450 (16)	0.0440 (15)	0.0011 (14)	0.0012 (13)	0.0027 (12)
C26	0.0520 (15)	0.0441 (15)	0.0473 (15)	0.0047 (15)	−0.0048 (13)	−0.0096 (12)
N2	0.0690 (16)	0.0524 (18)	0.0694 (18)	0.0041 (14)	0.0053 (14)	0.0146 (14)
N3	0.0658 (17)	0.0432 (14)	0.0597 (16)	−0.0010 (13)	−0.0043 (13)	−0.0022 (13)
N4	0.095 (2)	0.0576 (19)	0.0618 (18)	0.003 (2)	−0.004 (2)	−0.0163 (15)
O1	0.0936 (16)	0.0415 (13)	0.0881 (15)	−0.0134 (12)	−0.0104 (13)	−0.0010 (11)
O2	0.118 (2)	0.0613 (16)	0.0916 (17)	−0.0266 (14)	−0.0041 (15)	0.0236 (13)
O3	0.153 (2)	0.0712 (15)	0.0594 (14)	0.0167 (17)	0.0229 (15)	0.0142 (13)
O4	0.1124 (18)	0.0496 (11)	0.0700 (14)	−0.0081 (12)	0.0071 (13)	−0.0163 (10)
O5	0.1043 (18)	0.0492 (12)	0.0668 (13)	−0.0180 (12)	0.0052 (13)	0.0078 (10)
O6A	0.161 (11)	0.120 (7)	0.072 (4)	−0.036 (7)	0.029 (6)	−0.025 (4)
O7A	0.160 (10)	0.086 (7)	0.100 (4)	−0.034 (7)	−0.029 (4)	−0.035 (4)
O6B	0.176 (13)	0.101 (5)	0.049 (4)	0.027 (6)	−0.005 (5)	−0.011 (4)
O7B	0.235 (19)	0.054 (4)	0.088 (5)	0.030 (5)	0.002 (7)	−0.034 (3)

Geometric parameters (Å, °)

C1—C2	1.383 (4)	C12—S1	1.747 (3)
C1—C6	1.390 (3)	N1—H1	0.81 (3)
C1—S1	1.762 (3)	C21—O1	1.332 (3)
C2—C3	1.373 (5)	C21—C26	1.393 (4)
C2—H2A	0.9300	C21—C22	1.401 (3)
C3—C4	1.375 (5)	C22—C23	1.381 (3)
C3—H3	0.9300	C22—N2	1.453 (3)
C4—C5	1.372 (4)	C23—C24	1.365 (3)
C4—H4	0.9300	C23—H23	0.9300
C5—C6	1.390 (4)	C24—C25	1.377 (3)
C5—H5	0.9300	C24—N3	1.463 (3)
C6—N1	1.382 (3)	C25—C26	1.373 (4)
C7—C8	1.392 (4)	C25—H25	0.9300
C7—C12	1.393 (4)	C26—N4	1.467 (3)
C7—N1	1.398 (4)	N2—O3	1.205 (3)
C8—C9	1.382 (5)	N2—O2	1.234 (3)
C8—H8	0.9300	N3—O5	1.221 (3)
C9—C10	1.367 (5)	N3—O4	1.223 (3)
C9—H9	0.9300	N4—O7B	1.197 (8)
C10—C11	1.371 (5)	N4—O6B	1.205 (9)
C10—H10	0.9300	N4—O6A	1.197 (9)
C11—C12	1.381 (4)	N4—O7A	1.207 (7)
C11—H11	0.9300	O1—H2	0.95 (3)
C2—C1—C6	120.4 (3)	C7—N1—H1	113 (2)
C2—C1—S1	117.0 (2)	C12—S1—C1	102.40 (14)
C6—C1—S1	122.6 (2)	O1—C21—C26	120.1 (3)
C3—C2—C1	120.3 (3)	O1—C21—C22	123.9 (3)
C3—C2—H2A	119.9	C26—C21—C22	116.0 (2)
C1—C2—H2A	119.9	C23—C22—C21	122.3 (2)
C2—C3—C4	120.0 (3)	C23—C22—N2	117.1 (2)

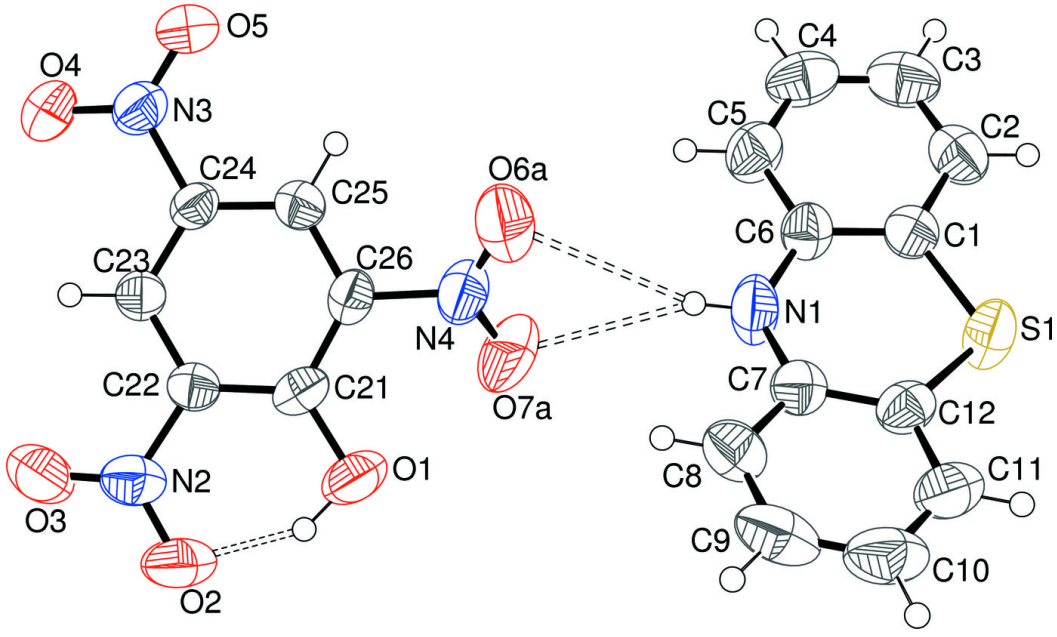
C2—C3—H3	120.0	C21—C22—N2	120.7 (2)
C4—C3—H3	120.0	C24—C23—C22	118.7 (2)
C5—C4—C3	120.1 (3)	C24—C23—H23	120.6
C5—C4—H4	120.0	C22—C23—H23	120.6
C3—C4—H4	120.0	C23—C24—C25	121.6 (2)
C4—C5—C6	121.1 (3)	C23—C24—N3	119.8 (2)
C4—C5—H5	119.5	C25—C24—N3	118.6 (2)
C6—C5—H5	119.5	C26—C25—C24	118.6 (2)
N1—C6—C5	119.7 (3)	C26—C25—H25	120.7
N1—C6—C1	122.0 (3)	C24—C25—H25	120.7
C5—C6—C1	118.2 (3)	C25—C26—C21	122.8 (2)
C8—C7—C12	118.7 (3)	C25—C26—N4	116.6 (3)
C8—C7—N1	119.5 (3)	C21—C26—N4	120.6 (3)
C12—C7—N1	121.8 (3)	O3—N2—O2	122.9 (3)
C9—C8—C7	120.4 (3)	O3—N2—C22	118.8 (3)
C9—C8—H8	119.8	O2—N2—C22	118.3 (3)
C7—C8—H8	119.8	O5—N3—O4	124.4 (2)
C10—C9—C8	120.6 (3)	O5—N3—C24	118.3 (2)
C10—C9—H9	119.7	O4—N3—C24	117.3 (2)
C8—C9—H9	119.7	O7B—N4—O6B	122.8 (7)
C9—C10—C11	119.4 (3)	O7B—N4—O6A	99.9 (7)
C9—C10—H10	120.3	O6B—N4—O6A	50.1 (4)
C11—C10—H10	120.3	O7B—N4—O7A	54.6 (6)
C10—C11—C12	121.4 (3)	O6B—N4—O7A	98.1 (7)
C10—C11—H11	119.3	O6A—N4—O7A	123.2 (7)
C12—C11—H11	119.3	O7B—N4—C26	118.7 (6)
C11—C12—C7	119.5 (3)	O6B—N4—C26	118.5 (5)
C11—C12—S1	117.8 (2)	O6A—N4—C26	119.0 (5)
C7—C12—S1	122.8 (2)	O7A—N4—C26	117.7 (6)
C6—N1—C7	125.3 (2)	C21—O1—H2	104 (2)
C6—N1—H1	119 (2)		
C6—C1—C2—C3	−1.5 (5)	C26—C21—C22—C23	0.9 (4)
S1—C1—C2—C3	175.6 (3)	O1—C21—C22—N2	0.3 (4)
C1—C2—C3—C4	0.4 (5)	C26—C21—C22—N2	−178.9 (2)
C2—C3—C4—C5	1.2 (5)	C21—C22—C23—C24	−2.4 (4)
C3—C4—C5—C6	−1.7 (5)	N2—C22—C23—C24	177.4 (2)
C4—C5—C6—N1	−177.5 (3)	C22—C23—C24—C25	2.2 (4)
C4—C5—C6—C1	0.6 (5)	C22—C23—C24—N3	−177.8 (2)
C2—C1—C6—N1	179.0 (3)	C23—C24—C25—C26	−0.4 (4)
S1—C1—C6—N1	2.1 (4)	N3—C24—C25—C26	179.6 (2)
C2—C1—C6—C5	1.0 (4)	C24—C25—C26—C21	−1.1 (4)
S1—C1—C6—C5	−175.9 (2)	C24—C25—C26—N4	179.2 (3)
C12—C7—C8—C9	−0.8 (4)	O1—C21—C26—C25	−178.3 (3)
N1—C7—C8—C9	178.8 (3)	C22—C21—C26—C25	0.9 (4)
C7—C8—C9—C10	−0.4 (5)	O1—C21—C26—N4	1.3 (4)
C8—C9—C10—C11	1.0 (6)	C22—C21—C26—N4	−179.5 (3)
C9—C10—C11—C12	−0.4 (6)	C23—C22—N2—O3	−1.9 (4)
C10—C11—C12—C7	−0.8 (5)	C21—C22—N2—O3	177.9 (3)
C10—C11—C12—S1	179.4 (3)	C23—C22—N2—O2	178.5 (3)

C8—C7—C12—C11	1.4 (4)	C21—C22—N2—O2	−1.7 (4)
N1—C7—C12—C11	−178.2 (3)	C23—C24—N3—O5	169.7 (2)
C8—C7—C12—S1	−178.9 (2)	C25—C24—N3—O5	−10.3 (4)
N1—C7—C12—S1	1.5 (4)	C23—C24—N3—O4	−9.4 (4)
C5—C6—N1—C7	−167.0 (3)	C25—C24—N3—O4	170.6 (2)
C1—C6—N1—C7	15.1 (5)	C25—C26—N4—O7B	155.5 (15)
C8—C7—N1—C6	163.4 (3)	C21—C26—N4—O7B	−24.2 (16)
C12—C7—N1—C6	−17.0 (5)	C25—C26—N4—O6B	−24.1 (14)
C11—C12—S1—C1	−169.1 (2)	C21—C26—N4—O6B	156.2 (14)
C7—C12—S1—C1	11.2 (3)	C25—C26—N4—O6A	33.6 (14)
C2—C1—S1—C12	169.9 (2)	C21—C26—N4—O6A	−146.0 (13)
C6—C1—S1—C12	−13.0 (3)	C25—C26—N4—O7A	−141.9 (11)
O1—C21—C22—C23	−179.9 (3)	C21—C26—N4—O7A	38.5 (12)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O6A	0.81 (3)	2.74 (4)	3.520 (7)	162 (3)
N1—H1···O6B	0.81 (3)	2.77 (3)	3.533 (8)	157 (3)
N1—H1···O7A	0.81 (3)	2.60 (3)	3.339 (10)	151 (3)
N1—H1···O7B	0.81 (3)	2.56 (3)	3.311 (11)	156 (3)
O1—H2···O2	0.95 (3)	1.69 (3)	2.550 (3)	148 (3)

Fig. 1


O5
O4
N3
C24
C25
O6a
C23
C26
N4
C22
C21
O7a
N2
O1
O3
O2
C4
C3
C5
C2
C6
C1
N1
S1
C7
C12
C8
C11
C9
C10