organic compounds

1-(4-Nitrobenzoyl)-3-(4-nitrophenyl)-thiourea acetone hemisolvate

Liang Xian,* Lujuan Cui and Ming Cheng

Chemical Engineering Institute, Northwest University for Nationalities, Lanzhou 730124, People's Republic of China
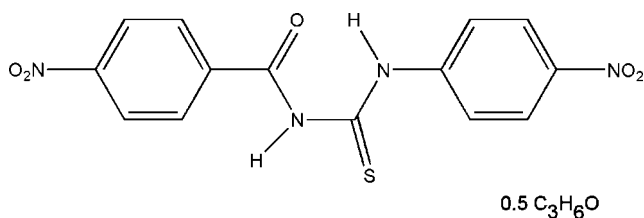
Correspondence e-mail: xianliangchina@yahoo.com.cn

In the title compound, $C_{14}H_{10}N_4O_5S\cdot0.5C_3H_6O$, the nitro-benzoyl and nitrophenyl groups have *trans* and *cis* configurations, respectively, with respect to the thiourea S atom. The molecular conformation is stabilized by intramolecular N—H$\cdots$O and C—H$\cdots$S hydrogen bonds. The acetone solvent molecule possesses a crystallographically imposed twofold axis. In the crystal packing, thiourea molecules are linked by intermolecular C—H$\cdots$O hydrogen-bond interactions to form chains running parallel to the *c* axis. The chains are further bridged *via* N—H$\cdots$O and C—H$\cdots$O hydrogen bonds involving the acetone molecules.

Related literature

For general background on the chemistry of thiourea derivatives, see: Choi *et al.* (2008); Jones *et al.* (2008); Kushwaha *et al.* (2008); Su *et al.* (2006). For related structures, see: Su (2005, 2007). For graph-set notation, see: Bernstein *et al.* (1995).

Experimental

Crystal data

$C_{14}H_{10}N_4O_5S\cdot0.5C_3H_6O$	c = 15.224 (7) Å
M_r = 375.36	β = 107.262 (12)°
Monoclinic, $C2/c$	V = 3377 (3) Å^3
a = 30.828 (14) Å	Z = 8
b = 7.534 (3) Å	Mo $K\alpha$ radiation

μ = 0.23 mm^{-1}	0.34 × 0.31 × 0.27 mm
T = 296 (2) K	

Data collection

Bruker SMART CCD area-detector diffractometer	9659 measured reflections
	3926 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2804 reflections with $I > 2\sigma(I)$
T_{min} = 0.924, T_{max} = 0.941	R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.133	
S = 1.05	
3926 reflections	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
245 parameters	$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C1—H1$\cdots$S1	0.93	2.79	3.235 (2)	111
N2—H2A$\cdots$O3	0.90 (3)	1.88 (3)	2.659 (3)	144 (2)
C2—H2$\cdots$O4^i	0.93	2.48	3.394 (3)	167
C12—H12$\cdots$O5^{ii}	0.93	2.54	3.318 (3)	141
N3—H3A$\cdots$O6	0.86 (2)	2.442 (19)	3.300 (2)	175 (2)
C13—H13$\cdots$O6	0.93	2.59	3.207 (3)	124
C14—H14B$\cdots$O5^{iii}	0.96	2.56	3.446 (3)	154
C14—H14C$\cdots$O4^{iv}	0.96	2.52	3.476 (3)	175

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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supporting information

1-(4-Nitrobenzoyl)-3-(4-nitrophenyl)thiourea acetone hemisolvate

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S1. Comment

Thiourea and its derivatives are broadly applied in anion recognition, nonlinear optics and catalysis, and display also high bioactivity and good coordination ability (Choi *et al.*, 2008; Kushwaha *et al.*, 2008; Jones *et al.* 2008; Su *et al.*, 2006). As part of our research on thiourea coordination chemistry, we are interested in the study of the influence of noncovalent interactions, especially hydrogen bonds and π-π stacking interactions, on the coordination modes of benzoylthiourea with transition metal ions. In the present paper, the crystal structure of the title compound is reported.

   In the molecule of the title compound (Fig. 1), the nitrobenzoyl and nitrophenyl groups have *trans* and *cis* configurations, respectively, with respect of the thiourea S atom. The dihedral angle formed by the two aromatic rings is 7.68 (6)°. The molecular conformation is stabilized by intramolecular N—H···O and C—H···S hydrogen bonds (Table 1) forming six-membered rings of graph set *S*(6) (Bernstein *et al.*, 1995). This conformation is similar to that reported for N-(4-chlorophenyl)-N′-(4-nitrobenzoyl)urea (Su, 2005) and for N-(p-nitrobenzoyl)-N′-(p-chlorophenyl)thiourea (Su, 2007). The acetone solvent molecule has a crystallographically imposed twofold symmetry. In the crystal packing (Fig. 2), thiourea molecules are linked into chains running parallel to the *c* axis by intermolecular C—H···O hydrogen bonds (Table 1). These chains are further bridged *via* N—H···O and C—H···O hydrogen bonds (Table 1) involving the acetone molecules.

S2. Experimental

All reagents and organic solvents were of analytical reagent grade and commercially available. p-Nitrobenzoyl chloride (1.86 g) was treated with ammonium thiocyanate (1.20 g) in CH_2Cl_2 under solid-liquid phase transfer catalysis conditions, using 3% polyethylene glycol-400 as catalyst, to give the corresponding benzoyl isothiocyanate, which was reacted with p-nitroaniline (1.38 g) to give the title compound. The solid was separated from the liquid phase by filtration, washed with CH_2Cl_2 and then dried in air. Yellow single crystals suitable for X-ray analysis were obtained after one week by slow evaporation of an acetone solution. The infrared spectrum was recorded in the range of 4000–400 cm^{-1} on a Nicolet NEXUS 670 F T—IR spectrometer, using KBr pellets. ^{1}H NMR spectrum was obtained on an INOVA-400 MHz superconduction spectrometer, DMSO-$_{d6}$ was used as solvent and TMS as internal standard, and the chemical shifts are expressed as delta. Elemental analyses were carried out on a PE-2400 elemental analysis instrument. Melting point determination was performed in YRT-3 melting point instrument (Tianjin) and was uncorrected. Melting Point: 201–204°C. Elemental analysis (%) found (calcd.): C, 50.25(49.6); H, 3.55(3.47); N, 11.30(14.93); S, 8.50(8.53). IR (KBr, cm[-1]): 3385 (N—H), 3064, 1680 (C=O), 1571(C=C), 1318, 1259(C=S), 1137, 1106. ^{1}H NMR(delta, p.p.m.): 2.50 (s, 6H, 2CH₃); 8.07–8.38 (m, 8H, 2C₆H₄); 12.15 (s, 1H, NH); 12.61 (s, 1H, NH).

S3. Refinement

All H atoms bound to C atoms were placed in calculated positions and refined using the riding model approximation, with C—H = 0.93-0.96 Å and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5 U_{eq}(C) for methyl H atoms. The H atoms bound to N atoms were located in a difference Fourier map and refined freely.
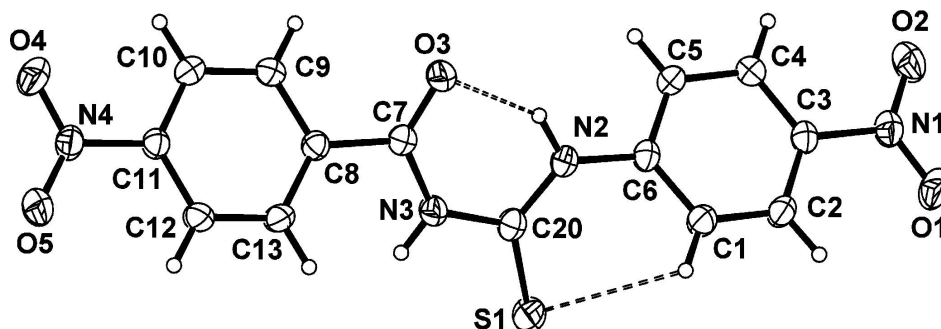
Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. Intramolecular hydrogen bonds are shown as dashed lines.
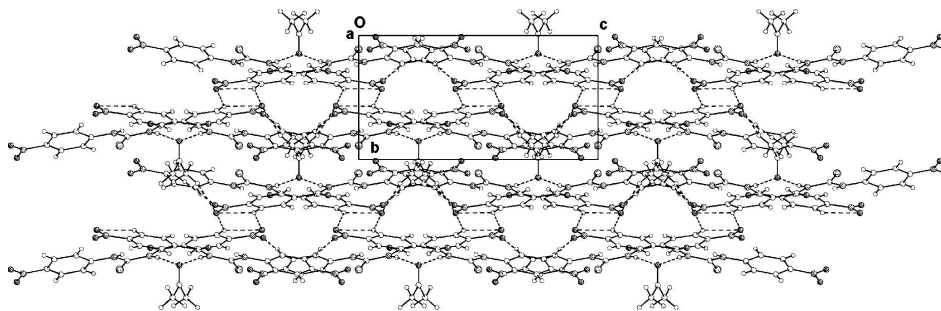
Figure 2

Packing diagram of the title compound viewed along the a axis. Intermolecular hydrogen bonds are shown as dashed lines.

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Crystal data

$C_{14}H_{10}N_4O_5S \cdot 0.5C_3H_6O$	$F(000) = 1552$
$M_r = 375.36$	$D_x = 1.477$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 3344 reflections
$a = 30.828$ (14) Å	$\theta = 2.7–28.3°$
$b = 7.534$ (3) Å	$\mu = 0.23$ mm^{-1}
$c = 15.224$ (7) Å	$T = 296$ K
$\beta = 107.262$ (12)°	Block, yellow
$V = 3377$ (3) Å^3	$0.34 \times 0.31 \times 0.27$ mm
$Z = 8$	

Data collection

Bruker SMART CCD area-detector diffractometer	Graphite monochromator
	φ and ω scans
Radiation source: fine-focus sealed tube	

Absorption correction: multi-scan
  (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.924$, $T_{max} = 0.941$
9659 measured reflections
3926 independent reflections
2804 reflections with $I > 2\sigma(I)$

$R_{int} = 0.023$
$\theta_{max} = 28.0°$, $\theta_{min} = 1.4°$
$h = -39 \rightarrow 32$
$k = -9 \rightarrow 9$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.133$
$S = 1.05$
3926 reflections
245 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.063P)^2 + 1.6044P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.06837 (2)	0.61209 (9)	0.99931 (4)	0.0607 (2)
N2	0.15507 (6)	0.7121 (2)	1.02255 (11)	0.0464 (4)
C8	0.11880 (6)	0.8073 (2)	0.72951 (12)	0.0378 (4)
O3	0.17768 (5)	0.7877 (2)	0.87122 (9)	0.0576 (4)
C7	0.13716 (6)	0.7739 (3)	0.83134 (12)	0.0418 (4)
C11	0.09121 (6)	0.8598 (2)	0.54287 (12)	0.0393 (4)
C3	0.21046 (6)	0.6165 (2)	1.30383 (12)	0.0406 (4)
N4	0.07617 (6)	0.8875 (2)	0.44189 (11)	0.0494 (4)
N1	0.22987 (6)	0.5784 (2)	1.40277 (11)	0.0501 (4)
N3	0.10573 (6)	0.7234 (2)	0.87465 (11)	0.0443 (4)
C6	0.17262 (6)	0.6799 (2)	1.11874 (12)	0.0402 (4)
O4	0.10416 (6)	0.8676 (3)	0.39985 (10)	0.0737 (5)
C12	0.06084 (7)	0.8910 (3)	0.59207 (13)	0.0473 (5)
H12	0.0315	0.9292	0.5624	0.057*
O1	0.20702 (6)	0.6125 (2)	1.45421 (11)	0.0714 (5)
C10	0.13499 (7)	0.8041 (3)	0.58343 (13)	0.0450 (5)
H10	0.1548	0.7844	0.5487	0.054*
C5	0.21595 (7)	0.6070 (3)	1.15057 (13)	0.0440 (5)

H5	0.2322	0.5810	1.1095	0.053*
C4	0.23498 (6)	0.5731 (3)	1.24383 (13)	0.0433 (4)
H4	0.2637	0.5222	1.2656	0.052*
C13	0.07482 (6)	0.8645 (3)	0.68621 (13)	0.0455 (5)
H13	0.0548	0.8850	0.7204	0.055*
C9	0.14873 (6)	0.7782 (3)	0.67771 (13)	0.0434 (4)
H9	0.1783	0.7409	0.7069	0.052*
C2	0.16818 (7)	0.6953 (3)	1.27367 (13)	0.0467 (5)
H2	0.1527	0.7270	1.3153	0.056*
C20	0.11244 (7)	0.6852 (3)	0.96836 (13)	0.0420 (4)
C1	0.14910 (7)	0.7265 (3)	1.18041 (13)	0.0479 (5)
H1	0.1206	0.7787	1.1591	0.057*
O2	0.26788 (6)	0.5125 (3)	1.42899 (10)	0.0722 (5)
O5	0.03714 (6)	0.9316 (3)	0.40451 (10)	0.0722 (5)
O6	0.0000	0.6468 (3)	0.7500	0.0792 (8)
C15	0.0000	0.4863 (4)	0.7500	0.0500 (7)
C14	−0.03535 (9)	0.3861 (3)	0.7781 (2)	0.0754 (7)
H14A	−0.0541	0.4678	0.7990	0.113*
H14B	−0.0210	0.3057	0.8270	0.113*
H14C	−0.0538	0.3203	0.7265	0.113*
H3A	0.0780 (7)	0.711 (3)	0.8413 (14)	0.049 (6)*
H2A	0.1744 (9)	0.733 (4)	0.9897 (18)	0.081 (8)*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0563 (4)	0.0823 (4)	0.0462 (3)	−0.0144 (3)	0.0194 (3)	0.0088 (3)
N2	0.0452 (10)	0.0642 (11)	0.0310 (8)	−0.0001 (8)	0.0131 (7)	0.0046 (7)
C8	0.0392 (10)	0.0399 (10)	0.0344 (9)	−0.0020 (7)	0.0112 (7)	0.0026 (7)
O3	0.0408 (8)	0.0929 (12)	0.0379 (7)	−0.0029 (7)	0.0096 (6)	0.0058 (7)
C7	0.0420 (10)	0.0464 (11)	0.0371 (10)	−0.0002 (8)	0.0122 (8)	0.0013 (8)
C11	0.0419 (10)	0.0420 (10)	0.0339 (9)	−0.0017 (8)	0.0111 (8)	0.0008 (7)
C3	0.0459 (11)	0.0421 (10)	0.0321 (9)	−0.0038 (8)	0.0091 (8)	0.0008 (7)
N4	0.0564 (11)	0.0560 (11)	0.0353 (9)	0.0027 (8)	0.0126 (8)	−0.0015 (7)
N1	0.0566 (11)	0.0545 (10)	0.0368 (9)	−0.0028 (8)	0.0099 (8)	0.0020 (7)
N3	0.0400 (9)	0.0574 (10)	0.0340 (8)	−0.0039 (8)	0.0089 (7)	0.0049 (7)
C6	0.0458 (10)	0.0433 (10)	0.0317 (9)	−0.0013 (8)	0.0119 (8)	0.0012 (8)
O4	0.0754 (12)	0.1094 (15)	0.0437 (9)	0.0136 (10)	0.0289 (8)	0.0056 (9)
C12	0.0370 (10)	0.0629 (13)	0.0415 (10)	0.0084 (9)	0.0108 (8)	0.0091 (9)
O1	0.0845 (12)	0.0950 (13)	0.0394 (8)	0.0095 (10)	0.0257 (8)	0.0075 (8)
C10	0.0427 (11)	0.0536 (12)	0.0426 (10)	0.0032 (9)	0.0189 (8)	−0.0015 (9)
C5	0.0419 (10)	0.0553 (12)	0.0379 (10)	−0.0018 (8)	0.0164 (8)	−0.0049 (8)
C4	0.0382 (10)	0.0493 (11)	0.0411 (10)	0.0002 (8)	0.0096 (8)	−0.0024 (8)
C13	0.0395 (10)	0.0596 (12)	0.0415 (10)	0.0052 (9)	0.0184 (8)	0.0060 (9)
C9	0.0351 (10)	0.0529 (12)	0.0415 (10)	0.0047 (8)	0.0101 (8)	0.0021 (8)
C2	0.0505 (12)	0.0576 (12)	0.0359 (10)	0.0067 (9)	0.0187 (8)	0.0008 (9)
C20	0.0487 (11)	0.0420 (10)	0.0363 (10)	0.0010 (8)	0.0138 (8)	0.0027 (8)
C1	0.0477 (11)	0.0570 (12)	0.0390 (10)	0.0132 (9)	0.0130 (8)	0.0037 (9)

O2	0.0641 (10)	0.0925 (13)	0.0481 (9)	0.0169 (9)	−0.0016 (7)	0.0059 (9)
O5	0.0597 (10)	0.1078 (14)	0.0417 (8)	0.0188 (9)	0.0038 (7)	0.0013 (9)
O6	0.0867 (19)	0.0590 (15)	0.111 (2)	0.000	0.0586 (17)	0.000
C15	0.0476 (16)	0.060 (2)	0.0417 (15)	0.000	0.0121 (12)	0.000
C14	0.0655 (16)	0.0731 (17)	0.096 (2)	−0.0050 (13)	0.0367 (15)	0.0070 (14)

Geometric parameters (Å, º)

S1—C20	1.659 (2)	N3—H3A	0.86 (2)
N2—C20	1.344 (3)	C6—C1	1.391 (3)
N2—C6	1.423 (2)	C6—C5	1.392 (3)
N2—H2A	0.90 (3)	C12—C13	1.383 (3)
C8—C13	1.389 (3)	C12—H12	0.9300
C8—C9	1.397 (3)	C10—C9	1.385 (3)
C8—C7	1.505 (3)	C10—H10	0.9300
O3—C7	1.221 (2)	C5—C4	1.389 (3)
C7—N3	1.378 (2)	C5—H5	0.9300
C11—C10	1.373 (3)	C4—H4	0.9300
C11—C12	1.382 (3)	C13—H13	0.9300
C11—N4	1.483 (2)	C9—H9	0.9300
C3—C2	1.381 (3)	C2—C1	1.386 (3)
C3—C4	1.387 (3)	C2—H2	0.9300
C3—N1	1.475 (2)	C1—H1	0.9300
N4—O5	1.215 (2)	O6—C15	1.209 (4)
N4—O4	1.227 (2)	C15—C14	1.489 (3)
N1—O2	1.225 (2)	C14—H14A	0.9600
N1—O1	1.226 (2)	C14—H14B	0.9600
N3—C20	1.409 (2)	C14—H14C	0.9600
C20—N2—C6	127.59 (17)	C11—C10—H10	121.1
C20—N2—H2A	112.0 (17)	C9—C10—H10	121.1
C6—N2—H2A	119.4 (17)	C4—C5—C6	119.93 (17)
C13—C8—C9	119.73 (17)	C4—C5—H5	120.0
C13—C8—C7	123.80 (16)	C6—C5—H5	120.0
C9—C8—C7	116.46 (16)	C3—C4—C5	118.84 (18)
O3—C7—N3	123.16 (17)	C3—C4—H4	120.6
O3—C7—C8	120.96 (16)	C5—C4—H4	120.6
N3—C7—C8	115.86 (16)	C12—C13—C8	119.79 (17)
C10—C11—C12	122.83 (17)	C12—C13—H13	120.1
C10—C11—N4	118.20 (16)	C8—C13—H13	120.1
C12—C11—N4	118.96 (17)	C10—C9—C8	120.85 (17)
C2—C3—C4	121.85 (17)	C10—C9—H9	119.6
C2—C3—N1	118.69 (17)	C8—C9—H9	119.6
C4—C3—N1	119.46 (18)	C3—C2—C1	119.02 (18)
O5—N4—O4	122.79 (18)	C3—C2—H2	120.5
O5—N4—C11	119.06 (17)	C1—C2—H2	120.5
O4—N4—C11	118.14 (17)	N2—C20—N3	114.45 (16)
O2—N1—O1	123.50 (18)	N2—C20—S1	127.59 (15)

O2—N1—C3	118.07 (17)	N3—C20—S1	117.96 (15)
O1—N1—C3	118.43 (18)	C2—C1—C6	120.06 (18)
C7—N3—C20	128.92 (17)	C2—C1—H1	120.0
C7—N3—H3A	117.7 (14)	C6—C1—H1	120.0
C20—N3—H3A	113.4 (14)	O6—C15—C14	120.45 (15)
C1—C6—C5	120.22 (17)	C15—C14—H14A	109.5
C1—C6—N2	122.44 (18)	C15—C14—H14B	109.5
C5—C6—N2	117.26 (16)	H14A—C14—H14B	109.5
C11—C12—C13	118.96 (17)	C15—C14—H14C	109.5
C11—C12—H12	120.5	H14A—C14—H14C	109.5
C13—C12—H12	120.5	H14B—C14—H14C	109.5
C11—C10—C9	117.83 (17)		
C13—C8—C7—O3	−152.9 (2)	C1—C6—C5—C4	2.9 (3)
C9—C8—C7—O3	26.9 (3)	N2—C6—C5—C4	179.80 (17)
C13—C8—C7—N3	28.7 (3)	C2—C3—C4—C5	−1.2 (3)
C9—C8—C7—N3	−151.55 (18)	N1—C3—C4—C5	178.93 (17)
C10—C11—N4—O5	177.8 (2)	C6—C5—C4—C3	−1.3 (3)
C12—C11—N4—O5	−2.3 (3)	C11—C12—C13—C8	0.0 (3)
C10—C11—N4—O4	−3.4 (3)	C9—C8—C13—C12	0.5 (3)
C12—C11—N4—O4	176.51 (19)	C7—C8—C13—C12	−179.73 (18)
C2—C3—N1—O2	−178.25 (19)	C11—C10—C9—C8	0.3 (3)
C4—C3—N1—O2	1.6 (3)	C13—C8—C9—C10	−0.6 (3)
C2—C3—N1—O1	2.5 (3)	C7—C8—C9—C10	179.60 (18)
C4—C3—N1—O1	−177.63 (19)	C4—C3—C2—C1	2.1 (3)
O3—C7—N3—C20	2.4 (3)	N1—C3—C2—C1	−178.03 (18)
C8—C7—N3—C20	−179.26 (18)	C6—N2—C20—N3	−177.66 (18)
C20—N2—C6—C1	−43.5 (3)	C6—N2—C20—S1	1.7 (3)
C20—N2—C6—C5	139.8 (2)	C7—N3—C20—N2	4.1 (3)
C10—C11—C12—C13	−0.3 (3)	C7—N3—C20—S1	−175.35 (17)
N4—C11—C12—C13	179.78 (18)	C3—C2—C1—C6	−0.5 (3)
C12—C11—C10—C9	0.2 (3)	C5—C6—C1—C2	−2.0 (3)
N4—C11—C10—C9	−179.88 (17)	N2—C6—C1—C2	−178.72 (18)

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C1—H1⋯S1	0.93	2.79	3.235 (2)	111
N2—H2A⋯O3	0.90 (3)	1.88 (3)	2.659 (3)	144 (2)
C2—H2⋯O4ⁱ	0.93	2.48	3.394 (3)	167
C12—H12⋯O5ⁱⁱ	0.93	2.54	3.318 (3)	141
N3—H3A⋯O6	0.86 (2)	2.442 (19)	3.300 (2)	175 (2)
C13—H13⋯O6	0.93	2.59	3.207 (3)	124
C14—H14B⋯O5ⁱⁱⁱ	0.96	2.56	3.446 (3)	154
C14—H14C⋯O4^{iv}	0.96	2.52	3.476 (3)	175

Symmetry codes: (i) $x, y, z+1$; (ii) $-x, -y+2, -z+1$; (iii) $x, -y+1, z+1/2$; (iv) $-x, -y+1, -z+1$.