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## Crystal structure of 2,4-diamino-6-oxo-3,6-dihydropyrimidin-1-ium *p*-toluenesulfonate

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In the title salt,  $C_4H_7N_4O^+\cdot C_7H_7O_3S^-$ , the 2,6-diamino-4-oxo-1,3-dihydropyrimidin-1-ium cation interacts with the sulfonate group of the *p*-toluenesulfonate anion *via* a pair of  $N-H\cdots O$  hydrogen bonds, forming a heterosynthon  $R_2^2(8)$  that mimics the role of a carboxylate. The self-assembled cations form a homo-synthon  $R_2^1(6)$  motif which is further linked with the sulfonate anion *via*  $N-H\cdots O$  hydrogen bonds to generate an  $R_3^2(10)$  ring motif. The three motifs are fused together and extended as supramolecular ribbons along the *b*axis direction. Adjacent ribbons are further linked *via*  $N-H\cdots O$  hydrogen bonds to form an annulus, with an  $R_4^4(20)$  ring motif, resulting in a tunnel-like arrangement propagating along [010]. There are slipped parallel  $\pi-\pi$  stacking interactions [inter-centroid distance = 3.6539 (7) Å], between the tunnel-like polymer chains, forming slabs parallel to (100).

### 1. Chemical context

Di- and tri-aminopyrimidines show various biological and pharmacological properties like tyrosine kinase (Thomas, 1995*a*,*b*), dihydrofolate reductase inhibitors (Ayer, 1991) and are used as antiviral and antiprotozoan agents. 2,6-Diamino-4hydroxy pyrimidine (DAHP), an inhibitor of guanosine triphosphate cyclohydrolase I, blocks the synthesis of tetrahydrobiopterin which is a known cofactor of inducible nitric oxide synthesis (iNOS) (Bogdan *et al.*, 1995). The study of hydrogen-bonding patterns involving sulfonate groups in biological systems and metal complexes are of current interest (Gomathi & Muthiah, 2011; Wang, 2006). The present report deals with the supramolecular interactions exhibited by the title salt.



2. Structural commentary

The asymmetric unit of the title salt contains one 2,6-diamino-4-oxo-1,3-dihydropyrimidin-1-ium cation and one *p*-toluene



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Figure 1

A view of the molecular structure of the title molecular salt, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

sulfonate anion (Fig. 1). The cation is protonated at the N3 position, which is reflected by the slight increase in the C2–N3–C4 bond angle to 123.2 (1)°. The dihedral angle between the cation and anion ring mean planes is 54.04 (6)°.

The three C–S–O angles, C7–S1–O3 [106.83 (7)°], C7–S1–O2 [105.89 (7)°] and C7–S1–O4 [106.91 (7)°], and the O–S–O angles, O3–S1–O2 [110.84 (7)°], O2–S1–O4 [111.93 (7)°] and O3–S1–O4 [113.91 (8)°], indicate that the geometry of the sulfonate group is slightly distorted from an ideal tetrahedral geometry.

#### 3. Supramolecular features

The primary interaction between the cation and anion takes place *via* a pair of  $N-H\cdots O$  hydrogen bonds, forming a robust six-membered hetero-synthon,  $R_2^2(8)$ , and here the sulfonate group mimics the role of a carboxylate. This motif links the protonated ring N atom, N3, and the 2-amino N



#### Figure 2

A view of the supramolecular tunnel-like architecture built by  $N-H \cdots O$  hydrogen bonds [dashed lines; see Table 1 for details; symmetry codes: (i) x, y + 1, z; (ii) -x + 1, -y + 1, -z + 1], in the crystal structure of the title molecular salt.

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

		-		
$D - H \cdots A$	$D-\mathrm{H}$	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$N1-H1\cdotsO1^{i}$	0.86	1.86	2.6515 (14)	152
$N2-H2A\cdots O3$	0.86	1.95	2.7935 (17)	166
$N2 - H2B \cdot \cdot \cdot O2^{i}$	0.86	2.01	2.8669 (16)	175
N3−H3···O2	0.86	1.92	2.7689 (14)	169
$N6-H6A\cdots O4^{ii}$	0.86	2.25	2.9498 (18)	139
$N6-H6B\cdotsO1^{i}$	0.86	2.08	2.8201 (15)	143

Symmetry codes: (i) x, y + 1, z; (ii) -x + 1, -y + 1, -z + 1.

atom, N2, of the cation with the sulfonate atoms O2 and O3 of the anion. Adjacent  $R_2^2(8)$  ring motifs are connected via an N-H···O hydrogen bond by linking the 2-amino N atom, N2 with atom O3<sup>i</sup> [symmetry code: x, y + 1, z]. The cation undergoes self-association via a pair of bifurcated N-H···(O,O) hydrogen bonds, forming a homo-synthon,  $R_2^1(6)$ . This motif involves ring N1 and the 6-amino N atoms and carbonyl atom O1<sup>i</sup> of the cation (Table 1). The self-assembled cations extend as a supramolecular chain propagating along [010]. The homo- and hetero-synthons  $[R_2^2(8)]$  and  $R_2^1(6)$ ] are linked by an  $R_3^2(10)$  ring motif. The three motifs are fused together continuously, forming supramolecular ribbons along [010]. Two such ribbons in adjacent planes are connected via N-H···O hydrogen bonds by linking the 6-amino N of the cation and the sulfonate atom O4<sup>ii</sup> [symmetry code: -x + 1, -y + 1, -z + 1 of the anion, generating an annulus (Su *et al.*, 2007) with an  $R_4^4(20)$  graph-set motif (Fig. 2). This motif extends in the direction of the supramolecular ribbons and generates a tunnel-like architecture along the *b*-axis direction (Figs. 2 and 3).

Adjacent tunnels interact by off-set aromatic  $\pi$ - $\pi$  stacking interactions which are observed between symmetry-related pyrimidine rings of the cations with a centroid-centroid distance  $Cg \cdots Cg^{\text{iii}}$  of 3.6539 (7) Å [Cg is the centroid of ring N1/C2/N3/C4-C6; the dihedral angle between the ring planes = 1.86 (6)°; perpendicular separation = 3.2501 (5) Å; symmetry code: (iii) -x + 1, y,  $-z + \frac{3}{2}$ ]. These interactions result in the formation of slabs parallel to (100); as shown in Fig. 3.



#### Figure 3

A view along the *b* axis of the crystal packing of the title molecular salt. Hydrogen bonds (see Table 1 for details) and  $\pi$ - $\pi$  interactions are shown as dashed lines.

### 4. Database survey

A search of the Cambridge Structural Database (Version 5.36; Groom & Allen, 2014) revealed the presence of over 700 compounds involving *p*-toluene sulfonate but only three hits for the 2,6-diamino-4-oxo-1,3-dihydropyrimidin-1-ium cation. These include the sulfate monohydrate (ACEYUD; Muthiah *et al.*, 2004), the di(methanesulfanyl)amide (ESAQOE; Wijaya *et al.*, 2004) and the chloride dihydrate (SUZFOJ; Suleiman Gwaram *et al.*, 2010). In ACEYUD the cation is protonated at the N atom adjacent to the carbonyl group, as in the title compound, while in compounds ESAQOE and SUZFOJ it is the N atom *para* to the carbonyl group that is protonated. Otherwise, the bond distances in these three compounds are very similar and close to those observed for the title compound.

### 5. Synthesis and crystallization

A hot methanolic solution (20 ml) of 2,6-diamino-4-hydroxy pyrimidine (31.5 mg, Aldrich) and *p*-toluene sulfonic acid (43 mg, Loba chemie) was warmed at 323 K for 30 min over a water bath. The mixture was cooled slowly and kept at room temperature and after three weeks light-yellow needle-shaped crystals were obtained.

### 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were positioned geometrically and refined using a riding model: N-H =0.86 Å, C-H = 0.93-0.96 Å with  $U_{iso}(H) = 1.5U_{eq}(C)$  for methyl H atoms and  $1.2U_{eq}(N,C)$  for other H atoms.

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### References

- Ayer, D. E. (1991). Chem Abstr. 115, 114546.
- Bogdan, C., Werner, E., Stenger, S., Wachter, H., Röllinghoff, M. & Werner-Felmayer, G. (1995). FEBS Lett. 363, 69–74.
- Bruker (2004). APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.

Table	2	
Experi	mental	details.

Crystal data	
Chemical formula	$C_4H_7N_4O^+ \cdot C_7H_7O_3S^-$
M <sub>r</sub>	298.33
Crystal system, space group	Monoclinic, C2/c
Temperature (K)	296
a, b, c (Å)	30.8628 (7), 6.5559 (2), 13.1565 (3)
$\beta$ (°)	96.428 (1)
$V(Å^3)$	2645.27 (12)
Ζ	8
Radiation type	Μο Κα
$\mu (\text{mm}^{-1})$	0.27
Crystal size (mm)	$0.30 \times 0.20 \times 0.20$
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2004)
$T_{\min}, T_{\max}$	0.925, 0.949
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	14972, 3580, 2986
R <sub>int</sub>	0.022
$(\sin \theta / \lambda)_{\max} (\text{\AA}^{-1})$	0.687
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.037, 0.109, 1.06
No. of reflections	3580
No. of parameters	182
H-atom treatment	H-atom parameters constrained
$\Delta \rho_{\rm max},  \Delta \rho_{\rm min}  ({\rm e}  {\rm \AA}^{-3})$	0.31, -0.25

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *PLATON* (Spek, 2009), *Mercury* (Macrae *et al.*, 2008) and *publCIF* (Westrip, 2010).

- Gomathi, S. & Muthiah, P. T. (2011). Acta Cryst. E67, o2679–o2680.
   Groom, C. R. & Allen, F. H. (2014). Angew. Chem. Int. Ed. 53, 662–671.
- Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). J. Appl. Cryst. 41, 466–470.
- Muthiah, P. T., Hemamalini, M., Bocelli, G. & Cantoni, A. (2004). *Acta Cryst.* E60, o2038–o2040.
- Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
- Spek, A. L. (2009). Acta Cryst. D65, 148-155.
- Su, X.-Y., Wang, W.-H., Lan, J.-B., Mao, Z.-H. & Xie, R.-G. (2007). *Acta Cryst.* E63, 04513–04514.
- Suleiman Gwaram, N., Khaledi, H. & Mohd Ali, H. (2010). Acta Cryst. E66, o2294.
- Thomas, A. P. (1995a). World Patent WO 9515952.
- Thomas, A. P. (1995b). Chem Abstr. 123, 286077.
- Wang, K.-W. (2006). Acta Cryst. E62, o5136-o5137.
- Westrip, S. P. (2010). J. Appl. Cryst. 43, 920-925.
- Wijaya, K., Moers, O., Blaschette, A. & Jones, P. G. (2004). Z. Naturforsch. Teil B, 59, 17–26.

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Crystal structure of 2,4-diamino-6-oxo-3,6-dihydropyrimidin-1-ium *p*-toluene-sulfonate

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### **Computing details**

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

2,4-Diamino-6-oxo-3,6-dihydropyrimidin-1-ium p-toluenesulfonate

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Crystal data
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C<sub>4</sub>H<sub>7</sub>N<sub>4</sub>O<sup>+</sup>·C<sub>7</sub>H<sub>7</sub>O<sub>3</sub>S<sup>-</sup>  $M_r = 298.33$ Monoclinic, C2/c Hall symbol: -C 2yc a = 30.8628 (7) Å b = 6.5559 (2) Å c = 13.1565 (3) Å  $\beta = 96.428$  (1)° V = 2645.27 (12) Å<sup>3</sup> Z = 8

### Data collection

Bruker Kappa APEXII CCD diffractometer Radiation source: fine-focus sealed tube Graphite monochromator  $\omega$  and  $\varphi$  scan Absorption correction: multi-scan (SADABS; Bruker, 2004)  $T_{\min} = 0.925, T_{\max} = 0.949$ 

### Refinement

Refinement on  $F^2$ Least-squares matrix: full  $R[F^2 > 2\sigma(F^2)] = 0.037$  $wR(F^2) = 0.109$ S = 1.063580 reflections 182 parameters 0 restraints F(000) = 1248  $D_x = 1.498 \text{ Mg m}^{-3}$ Mo K $\alpha$  radiation,  $\lambda = 0.71073 \text{ Å}$ Cell parameters from 3580 reflections  $\theta = 2.7-29.3^{\circ}$   $\mu = 0.27 \text{ mm}^{-1}$  T = 296 KPrism, colourless  $0.30 \times 0.20 \times 0.20 \text{ mm}$ 

14972 measured reflections 3580 independent reflections 2986 reflections with  $I > 2\sigma(I)$  $R_{int} = 0.022$  $\theta_{max} = 29.2^\circ, \theta_{min} = 2.7^\circ$  $h = -40 \rightarrow 42$  $k = -9 \rightarrow 7$  $l = -18 \rightarrow 16$ 

Primary atom site location: structure-invariant direct methods Secondary atom site location: difference Fourier map Hydrogen site location: inferred from neighbouring sites H-atom parameters constrained  $w = 1/[\sigma^2(F_o^2) + (0.0552P)^2 + 1.4509P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\rm max} = 0.001$ 

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are

 $\Delta \rho_{\text{max}} = 0.31 \text{ e } \text{\AA}^{-3}$  $\Delta \rho_{\text{min}} = -0.25 \text{ e } \text{\AA}^{-3}$ 

estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**Refinement**. Refinement on  $F^2$  for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of  $F^2 > \sigma(F^2)$  is used only for calculating -*R*-factor-obs *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 param	eters (Ų)
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	x	У	Ζ	$U_{ m iso}$ */ $U_{ m eq}$
<b>S</b> 1	0.37258(1)	0.33503 (6)	0.60709 (3)	0.0395 (1)
O2	0.41787 (3)	0.26937 (17)	0.63677 (10)	0.0469 (4)
O3	0.36871 (4)	0.55423 (17)	0.61453 (11)	0.0559 (4)
O4	0.35526 (4)	0.2530 (2)	0.50899 (10)	0.0594 (4)
C7	0.34167 (4)	0.2292 (2)	0.69886 (12)	0.0379 (4)
C8	0.33328 (5)	0.3414 (3)	0.78333 (14)	0.0508 (5)
C9	0.30882 (6)	0.2558 (4)	0.85489 (15)	0.0631 (7)
C10	0.29210 (5)	0.0608 (4)	0.84233 (15)	0.0611 (7)
C11	0.30171 (6)	-0.0499 (3)	0.75883 (16)	0.0595 (6)
C12	0.32634 (5)	0.0315 (3)	0.68668 (14)	0.0477 (5)
C13	0.26346 (7)	-0.0295 (5)	0.9167 (2)	0.0946 (12)
01	0.52384 (3)	0.28686 (15)	0.61202 (10)	0.0461 (4)
N1	0.50945 (3)	0.88937 (16)	0.62432 (8)	0.0306 (3)
N2	0.43613 (4)	0.84071 (18)	0.63472 (10)	0.0382 (3)
N3	0.48173 (3)	0.56345 (16)	0.62787 (9)	0.0314 (3)
N6	0.58157 (4)	0.95420 (18)	0.60830 (11)	0.0424 (4)
C2	0.47500 (4)	0.76549 (19)	0.62867 (9)	0.0289 (3)
C4	0.52230 (4)	0.4758 (2)	0.61702 (10)	0.0321 (3)
C5	0.55713 (4)	0.6088 (2)	0.61103 (11)	0.0343 (4)
C6	0.55075 (4)	0.8158 (2)	0.61406 (10)	0.0308 (3)
H8	0.34390	0.47360	0.79230	0.0610*
H9	0.30360	0.33110	0.91220	0.0760*
H11	0.29140	-0.18290	0.75060	0.0710*
H12	0.33250	-0.04600	0.63080	0.0570*
H13A	0.23360	0.00590	0.89590	0.1420*
H13B	0.27210	0.02330	0.98400	0.1420*
H13C	0.26650	-0.17530	0.91740	0.1420*
H1	0.50570	1.01900	0.62810	0.0370*
H2A	0.41430	0.76020	0.63830	0.0460*
H2B	0.43230	0.97070	0.63510	0.0460*
Н3	0.46010	0.48390	0.63430	0.0380*
H5	0.58480	0.55720	0.60500	0.0410*

H6A	0.60780	0.91650	0.60220	0.0510*
H6B	0.57530	1.08180	0.61070	0.0510*

Atomic displacement parameters  $(Å^2)$ 

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0285 (2)	0.0340 (2)	0.0570 (2)	-0.0021 (1)	0.0095 (1)	-0.0001 (2)
O2	0.0284 (5)	0.0346 (5)	0.0788 (8)	-0.0014 (4)	0.0105 (5)	0.0016 (5)
O3	0.0434 (6)	0.0332 (6)	0.0928 (10)	0.0018 (5)	0.0154 (6)	0.0087 (6)
O4	0.0459 (6)	0.0783 (9)	0.0554 (7)	-0.0116 (6)	0.0117 (5)	-0.0091 (6)
C7	0.0265 (6)	0.0356 (7)	0.0519 (8)	-0.0021 (5)	0.0053 (5)	0.0004 (6)
C8	0.0409 (8)	0.0524 (10)	0.0600 (10)	-0.0048 (7)	0.0094 (7)	-0.0104 (8)
C9	0.0469 (9)	0.0889 (15)	0.0554 (10)	-0.0014 (10)	0.0140 (8)	-0.0057 (10)
C10	0.0336 (7)	0.0877 (15)	0.0618 (11)	-0.0043 (8)	0.0039 (7)	0.0239 (10)
C11	0.0458 (9)	0.0518 (11)	0.0791 (13)	-0.0138 (8)	-0.0004 (8)	0.0191 (9)
C12	0.0411 (7)	0.0379 (8)	0.0638 (10)	-0.0056 (6)	0.0047 (7)	-0.0005 (7)
C13	0.0533 (11)	0.149 (3)	0.0824 (15)	-0.0176 (14)	0.0114 (10)	0.0509 (16)
01	0.0415 (5)	0.0209 (5)	0.0767 (8)	0.0010 (4)	0.0104 (5)	0.0001 (5)
N1	0.0338 (5)	0.0190 (5)	0.0395 (6)	-0.0006 (4)	0.0066 (4)	0.0008 (4)
N2	0.0333 (5)	0.0271 (6)	0.0552 (7)	0.0018 (4)	0.0092 (5)	0.0027 (5)
N3	0.0307 (5)	0.0221 (5)	0.0417 (6)	-0.0022 (4)	0.0061 (4)	0.0018 (4)
N6	0.0353 (6)	0.0269 (6)	0.0665 (8)	-0.0041 (5)	0.0126 (6)	-0.0005 (5)
C2	0.0332 (6)	0.0244 (6)	0.0293 (6)	-0.0003 (5)	0.0042 (4)	0.0014 (4)
C4	0.0346 (6)	0.0230 (6)	0.0388 (6)	0.0009 (5)	0.0040 (5)	0.0010 (5)
C5	0.0316 (6)	0.0256 (6)	0.0462 (7)	0.0008 (5)	0.0068 (5)	0.0001 (5)
C6	0.0328 (6)	0.0261 (6)	0.0338 (6)	-0.0020 (5)	0.0055 (5)	0.0008 (5)

Geometric parameters (Å, °)

S1—O2	1.4728 (10)	C7—C12	1.383 (2)
S1—O3	1.4462 (12)	С7—С8	1.381 (2)
S1—O4	1.4444 (14)	C8—C9	1.389 (3)
S1—C7	1.7628 (15)	C9—C10	1.382 (4)
O1—C4	1.2416 (16)	C10—C13	1.511 (3)
N1-C6	1.3835 (16)	C10—C11	1.376 (3)
N1-C2	1.3442 (16)	C11—C12	1.388 (3)
N2-C2	1.3077 (18)	C8—H8	0.9300
N3—C2	1.3410 (16)	С9—Н9	0.9300
N3—C4	1.3994 (16)	C11—H11	0.9300
N6C6	1.3228 (18)	C12—H12	0.9300
N1—H1	0.8600	C13—H13C	0.9600
N2—H2A	0.8600	C13—H13A	0.9600
N2—H2B	0.8600	C13—H13B	0.9600
N3—H3	0.8600	C4—C5	1.3932 (18)
N6—H6B	0.8600	C5—C6	1.3725 (19)
N6—H6A	0.8600	С5—Н5	0.9300
S1…H2A	3.0800	C5…O4 <sup>ii</sup>	3.4031 (18)

$SI^{+}H2B^{+}$ $SO100^{+}$ $C6^{+}O1^{+}$ $S12880$ (19) $O1^{-}C6^{i}$ $3.1973$ (16) $C6^{-}O1^{+}$ $3.1973$ (16) $O1^{-}N6^{i}$ $2.8600$ $C6^{-}O2^{+}$ $3.5776$ (18) $O1^{-}N6^{i}$ $2.2501$ (15) $C4^{-}H1^{i}$ $3.0400$ $O1^{-}C2^{ii}$ $3.1894$ (18) $C4^{-}H6B^{i}$ $3.0600$ $O2^{-}N3$ $2.7689$ (14) $C7^{-}H13A^{iij}$ $3.1000$ $O3^{-}N2$ $2.8669$ (16) $C12^{-}H13B^{iij}$ $3.0100$ $O3^{-}N2$ $2.7935$ (17) $H1^{-}H2B$ $2.3000$ $O4^{-}C5^{ii}$ $3.4031$ (18) $H1^{-}C4^{iv}$ $3.0400$ $O4^{-}C5^{ii}$ $3.4031$ (18) $H1^{-}C4^{iv}$ $3.0400$ $O4^{-}C13^{iii}$ $3.298$ (3) $H1^{-}O1^{iv}$ $1.8600$ $O1^{-}H1^{ii}$ $1.8600$ $H2A^{-N}3$ $1.9500$ $O2^{-}H2B^{ii}$ $2.0100$ $H2B^{-}H1$ $2.3000$ $O3^{-}H12^{-}$ $2.8400$ $H2B^{-}O2^{iv}$ $2.0100$ $O3^{-}H2A$ $1.9500$ $H3^{-}G2A^{-}$ $2.3000$ $O3^{-}H2A^{-}$ $1.9500$		2 0100		2,2000((10))
S1 <sup>-+</sup> R5       2.6800 $C6^{-0}C1^{-0}$ 3.1973 (16)         O1C6 <sup>i</sup> 3.1973 (16)       C6 <sup></sup> C2 <sup>-</sup> 3.5776 (18)         O1Nf <sup>i</sup> 2.6515 (14)       C13O4 <sup>xi</sup> 3.298 (3)         O1Nf <sup>i</sup> 2.8201 (15)       C4H1 <sup>i</sup> 3.0400         O1C2 <sup>ii</sup> 3.1894 (18)       C4H1 <sup>ii</sup> 3.0400         O2N3       2.7689 (14)       C7H13A <sup>viii</sup> 3.1000         O3N2       2.7935 (17)       H1H6B       2.2000         O4C5 <sup>ii</sup> 3.4031 (18)       H1H6B       2.2000         O4C5 <sup>iii</sup> 3.4031 (18)       H1C4 <sup>ix</sup> 3.0400         O4C5 <sup>iii</sup> 3.498 (18)       H1C4 <sup>ix</sup> 3.0400         O1H1 <sup>i</sup> 1.8600       H2AH3       2.3000         O1H1 <sup>ii</sup> 1.8600       H2AH3       3.0800         O2H2B <sup>i</sup> 2.0100       H2BS1 <sup>iv</sup> 3.0100         O3H12 <sup>ix</sup> 2.8700       H2BS1 <sup>iv</sup> 3.0100         O3H12 <sup>ix</sup> 2.8400       H2BS1 <sup>iv</sup> 2.0100         O3H12 <sup>ix</sup> 2.8000       H3Q2       1.9200         O4H5 <sup>iii</sup> 2.8000       H3Q2       1.9200         O4H5 <sup>iii</sup>	S1 H2	3.0100		3.2880 (19)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	SIH3	2.8000		3.19/3 (10)
O1-*Ni <sup>+</sup> 2.65 15 (14)         C13-*O4 <sup>**</sup> 3.298 (3)           O1-*Ni <sup>+</sup> 2.8201 (15)         C4-*H1 <sup>i</sup> 3.0400           O1-*C2 <sup>ii</sup> 3.1894 (18)         C4-*H6B <sup>i</sup> 3.0600           O2-*N3         2.7689 (14)         C7-*H13A <sup>*ii</sup> 3.1000           O3-*N2         2.7935 (17)         H1-*H2B         2.3000           O4-*C5 <sup>ii</sup> 3.4031 (18)         H1-*C4 <sup>ii</sup> 3.0400           O4-*C5 <sup>ii</sup> 3.4031 (18)         H1-*C4 <sup>ii</sup> 3.0400           O4-*C13 <sup>iii</sup> 2.9498 (18)         H1-*C4 <sup>iii</sup> 3.0400           O4-*C13 <sup>iii</sup> 3.298 (3)         H1-*O1 <sup>iii</sup> 1.8600           O1-*H6B <sup>ii</sup> 2.0800         H2A-*H3         2.3000           O2-*H3         1.9200         H2A-*S1         3.0800           O2-*H3         1.9200         H2B-*G2 <sup>iii</sup> 3.0100           O3-*H3         2.8700         H2B-*S1 <sup>iii</sup> 3.0100           O3-*H3         2.8400         H2B-*O2 <sup>iii</sup> 2.8600           O3-*H4         2.9500         H3-*O2         1.9200           O4-*H5 <sup>ii</sup> 2.9100         H3-*O2         1.9200           O4-*H6 <sup>iii</sup> 2.500 <td></td> <td>3.1973 (16)</td> <td></td> <td>3.5776(18)</td>		3.1973 (16)		3.5776(18)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		2.6515 (14)		3.298 (3)
$O1 - C2^{\mu}$ 3.1894 (18) $C4^{\mu}$ -H6B <sup>3</sup> 3.0600 $O2 - N3$ 2.7689 (14) $C7 - H13A^{\mu \mu}$ 3.1000 $O2 - N2^{\lambda}$ 2.8669 (16) $C12 - H13B^{\mu \mu}$ 3.0100 $O3 - N2$ 2.7935 (17) $H1 - H2B$ 2.3000 $O4 - C5^{\mu}$ 3.4031 (18) $H1 - H4B$ 2.2000 $O4 - N6^{\mu}$ 2.9498 (18) $H1 - C4^{\nu}$ 3.0400 $O4 - C13^{\mu \mu}$ 3.298 (3) $H1 - O1^{\nu}$ 1.8600 $O1 - H6B^{i}$ 2.0800 $H2A - H3$ 2.3000 $O1 - H1^{i}$ 1.8600 $H2A - S1$ 3.0800 $O2 - H3$ 1.9200 $H2A - S1$ 3.0800 $O2 - H2B^{i}$ 2.0100 $H2B - H1$ 2.3000 $O3 - H12^{\nu}$ 2.8700 $H2B - S1^{\nu}$ 3.0100 $O3 - H3$ 2.8400 $H2B - O2^{\mu}$ 2.0100 $O3 - H4$ 1.9500 $H3 - S1$ 2.8600 $O3 - H4$ 2.8000 $H3 - C2$ 1.9200 $O4 - H5^{\mu}$ 2.8000 $H3 - C2$ 1.9200 $O4 - H6A^{\mu}$ 2.8000 $H3 - C2$ 1.9200 $O4 - H6A^{\mu}$ 2.8000 $H3 - C2$ 1.9200 $O4 - H6A^{\mu}$ 2.5100 $H3 - C2$ 1.9200 $O4 - H6A^{\mu}$ 2.5100 $H3 - C2^{\mu}$ 2.5100 $N1 - O1^{\mu}$ 2.6515 (14) $H5 - H8^{\mu}$ 2.5100 $N1 - O1^{\mu}$ 2.6515 (14) $H5 - H8^{\mu}$ 2.5100 $N1 - O2^{\nu}$ 3.3319 (16) $H6A - C4^{\mu}$ 3.0600 $N2 - C2^{\nu}$ 3.2846 (19) $H6B - H1$ 2.2200 $N3 - C2^{\mu}$ 3.2846		2.8201 (15)		3.0400
$O2 \cdots N3$ $2.7689$ $(14)$ $C7 \cdots H13A^{rn}$ $3.0100$ $O2 \cdots N2^i$ $2.8669$ $(16)$ $C12 \cdots H13B^{rn}$ $3.0100$ $O3 \cdots N2$ $2.7935$ $(17)$ $H1 \cdots H2B$ $2.3000$ $O4 \cdots K6^i$ $3.4031$ $(18)$ $H1 \cdots H2B$ $2.3000$ $O4 \cdots K6^i$ $2.9498$ $(18)$ $H1 \cdots C1^{rv}$ $3.6400$ $O4 \cdots C13^{rni}$ $3.298$ $(3)$ $H1 \cdots C1^{rv}$ $3.6600$ $O4 \cdots C13^{rni}$ $3.298$ $(3)$ $H1 \cdots C1^{rv}$ $3.6600$ $O1 \cdots H6B^i$ $2.0800$ $H2A \cdots H3$ $2.3000$ $O1 \cdots H1^i$ $1.8600$ $H2A \cdots G3$ $1.9500$ $O2 \cdots H2B^i$ $2.0100$ $H2B \cdots S1^{rv}$ $3.0100$ $O3 \cdots H12^{rv}$ $2.8700$ $H2B \cdots S1^{rv}$ $3.0100$ $O3 \cdots H12^{rv}$ $2.8700$ $H2B \cdots S1^{rv}$ $2.0100$ $O3 \cdots H2A$ $1.9500$ $H3 \cdots H2A$ $2.3000$ $O3 \cdots H2A$ $1.9500$ $H3 \cdots H2A$ $2.3000$ $O4 \cdots H5^{ri}$ $2.8000$ $H3 \cdots O2^{rv}$ $2.8400$ $O4 \cdots H64^{ri}$ $2.2500$ $H3 \cdots O3$ $2.8400$ $O4 \cdots H64^{ri}$ $2.2500$ $H3 \cdots O3$ $2.8400$ $O4 \cdots H64^{ri}$ $2.2500$ $H3 \cdots H5$ $2.4600$ $N1 \cdots O1^{rv}$ $2.6515$ $H4$ $H5 \cdots H4^{rv}$ $2.5100$ $N1 \cdots O1^{rv}$ $2.6515$ $H4$ $H5 \cdots H4^{rv}$ $2.6000$ $N1 \cdots O1^{rv}$ $2.6515$ $H4$ $H5 \cdots H5^{rv}$ $2.5100$ $N1 \cdots O1^{rv}$ $2.850(16)$ $H6B \cdots O1^{rv}$ $2.8600$ <	O1…C2 <sup>n</sup>	3.1894 (18)		3.0600
$02 \cdots N2^i$ $2.8669 (16)$ $C12 \cdots H13B^{m}$ $3.0100$ $03 \cdots N2$ $2.7935 (17)$ $H1 \cdots H2B$ $2.3000$ $04 \cdots C5^{ii}$ $3.0401 (18)$ $H1 \cdots H2^{iv}$ $3.0400$ $04 \cdots C5^{ii}$ $2.9498 (18)$ $H1 \cdots C4^{iv}$ $3.0400$ $04 \cdots C13^{iii}$ $3.298 (3)$ $H1 \cdots O1^{iv}$ $1.8600$ $01 \cdots H6B^i$ $2.0800$ $H2A \cdots H3$ $2.3000$ $01 \cdots H6B^i$ $2.0800$ $H2A \cdots H3$ $2.3000$ $01 \cdots H1^i$ $1.8600$ $H2A \cdots O3$ $1.9500$ $02 \cdots H3$ $1.9200$ $H2A \cdots O3$ $1.9500$ $02 \cdots H3$ $1.9200$ $H2B \cdots O1^{iv}$ $2.0100$ $03 \cdots H1^{iv}$ $2.8700$ $H2B \cdots S1^{iv}$ $3.0100$ $03 \cdots H3$ $2.8400$ $H3 \cdots S1$ $2.8600$ $03 \cdots H48$ $2.6000$ $H3 \cdots S1$ $2.8600$ $03 \cdots H48$ $2.6000$ $H3 \cdots O2$ $1.9200$ $04 \cdots H5^{ii}$ $2.2500$ $H5 \cdots H8^{iv}$ $2.5100$ $04 \cdots H6A^{ii}$ $2.2500$ $H5 \cdots H8^{iv}$ $2.5100$ $04 \cdots H12$ $2.6800$ $H5 \cdots H8^{iv}$ $2.5100$ $01 \cdots O1^{iv}$ $2.6515 (14)$ $H5 \cdots H4^{iv}$ $3.0600$ $02 \cdots O3$ $2.7935 (17)$ $H6A \cdots H5^{iv}$ $2.4600$ $03 \cdots C5^{iv}$ $3.2866 (16)$ $H6B \cdots O1^{iv}$ $2.0800$ $03 \cdots C5^{iv}$ $3.2844 (17)$ $H8 \cdots O3$ $2.5000$ $03 \cdots C4^{iv}$ $3.4276 (18)$ $H6B \cdots O1^{iv}$ $2.6800$ $03 \cdots C4^{iv}$ $3.4276 (18)$ $H9 \cdots H13B$ $2.4700$ $03 \cdots C4^$	O2…N3	2.7689 (14)	С7…Н13А <sup>vn</sup>	3.1000
$03 \cdots N2$ $2.7935 (17)$ $H1 \cdots H2B$ $2.3000$ $04 \cdots C5^{ii}$ $3.4031 (18)$ $H1 \cdots H6B$ $2.2200$ $04 \cdots K6^{ii}$ $2.9498 (18)$ $H1 \cdots C4^{1v}$ $3.0400$ $04 \cdots C1^{iii}$ $3.298 (3)$ $H1 \cdots C4^{1v}$ $1.6600$ $01 \cdots H6B^{ii}$ $2.0800$ $H2A \cdots H3$ $2.3000$ $01 \cdots H1^{ii}$ $1.8600$ $H2A \cdots S1$ $3.0800$ $02 \cdots H2B^{i}$ $2.0100$ $H2B \cdots H1$ $2.3000$ $02 \cdots H2B^{i}$ $2.0100$ $H2B \cdots S1^{iv}$ $3.0100$ $03 \cdots H1^{iv}$ $2.8700$ $H2B \cdots S1^{iv}$ $3.0100$ $03 \cdots H3$ $2.8400$ $H2B \cdots O2^{iv}$ $2.0100$ $03 \cdots H48$ $2.6000$ $H3 \cdots S1$ $2.8600$ $03 \cdots H2A$ $1.9500$ $H3 \cdots O2$ $1.9200$ $04 \cdots H5^{iv}$ $2.8000$ $H3 \cdots O2$ $1.9200$ $04 \cdots H5^{iv}$ $2.8000$ $H3 \cdots O2$ $1.9200$ $04 \cdots H1^{iv}$ $2.6510$ $H5 \cdots O4^{ii}$ $2.8000$ $04 \cdots H12$ $2.6800$ $H5 \cdots H8^{v}$ $2.5100$ $01 \cdots O1^{iv}$ $2.6515 (14)$ $H5 \cdots O4^{ii}$ $2.2500$ $02 \cdots O2^{iv}$ $2.8669 (16)$ $H6B \cdots O1^{iv}$ $2.0800$ $02 \cdots O2^{iv}$ $2.8669 (16)$ $H6B \cdots O1^{iv}$ $2.0800$ $02 \cdots O2^{iv}$ $2.8669 (16)$ $H6B \cdots O1^{iv}$ $2.0800$ $03 \cdots C4^{v}$ $3.4276 (18)$ $H9 \cdots H13B$ $2.4700$ $03 \cdots C4^{iv}$ $3.2207 (18)$ $H1 \cdots H13C^{iii}$ $2.5100$ $03 \cdots C4^{iv}$ $3.2864 (17)$ $H13 \cdots H13B^{iii}$ $2.5300$	O2…N2 <sup>i</sup>	2.8669 (16)	C12…H13B <sup>iii</sup>	3.0100
$04 \dots CS^{ii}$ $3.4031 (18)$ $H1 \dots H6B$ $2.2200$ $04 \dots K6^{ii}$ $2.9498 (18)$ $H1 \dots C4^{iv}$ $3.0400$ $04 \dots C13^{iii}$ $3.298 (3)$ $H1 \dots C1^{iv}$ $1.8600$ $01 \dots H6B^{ii}$ $2.0800$ $H2A \dots H3$ $2.3000$ $01 \dots H6B^{ii}$ $2.0800$ $H2A \dots G3$ $1.9500$ $02 \dots H2B$ $1.9200$ $H2A \dots O3$ $1.9500$ $02 \dots H2B^{ii}$ $2.0100$ $H2B \dots S1^{iv}$ $3.0100$ $03 \dots H1^{2iv}$ $2.8700$ $H2B \dots S1^{iv}$ $3.0100$ $03 \dots H3$ $2.8400$ $H2B \dots O2^{iv}$ $2.0100$ $03 \dots H3$ $2.8400$ $H3 \dots S1$ $2.8600$ $03 \dots H3$ $2.8000$ $H3 \dots O2$ $1.9200$ $04 \dots H5^{iv}$ $2.9100$ $H3 \dots O2$ $1.9200$ $04 \dots H5^{iv}$ $2.8000$ $H5 \dots 04^{ii}$ $2.8000$ $04 \dots H12$ $2.6800$ $H5 \dots H8^{v}$ $2.5100$ $04 \dots H6A^{ii}$ $2.2500$ $H5 \dots 04^{ii}$ $2.8000$ $04 \dots H12$ $2.6800$ $H5 \dots H8^{v}$ $2.5100$ $01^{iu} \dots C2^{v}$ $3.319 (16)$ $H6A \dots O4^{ii}$ $2.2500$ $02^{iu} \dots O3^{iv}$ $2.8669 (16)$ $H6B \dots C4^{iv}$ $3.0600$ $02^{iu} \dots O3^{v}$ $2.8669 (16)$ $H6B \dots O1^{iv}$ $2.0800$ $02^{iu} \dots O3^{v}$ $2.8669 (16)$ $H6B \dots O1^{iv}$ $2.0800$ $03^{iu} \dots O3^{iv}$ $2.844 (17)$ $H8 \dots O1^{iv}$ $2.6000$ $03^{iu} \dots O3^{iu}$ $2.844 (17)$ $H8 \dots O1^{iv}$ $2.6000$ $03^{iu} \dots O3^{iv}$ $2.8207 (18)$	O3…N2	2.7935 (17)	H1…H2B	2.3000
$04 \cdots K6^{ii}$ $2.9498 (18)$ $H1 \cdots C4^{iv}$ $3.0400$ $04 \cdots C13^{iii}$ $3.298 (3)$ $H1 \cdots O1^{iv}$ $1.8600$ $01 \cdots H6B^{i}$ $2.0800$ $H2A \cdots H3$ $2.3000$ $01 \cdots H1^{i}$ $1.8600$ $H2A \cdots G3$ $1.9500$ $02 \cdots H3$ $1.9200$ $H2A \cdots O3$ $1.9500$ $02 \cdots H2B^{i}$ $2.0100$ $H2B \cdots H1$ $2.3000$ $03 \cdots H12^{iv}$ $2.8700$ $H2B \cdots S1^{iv}$ $3.0100$ $03 \cdots H3$ $2.8400$ $H2B \cdots O2^{iv}$ $2.0100$ $03 \cdots H3$ $2.6000$ $H3 \cdots S1$ $2.8600$ $03 \cdots H48$ $2.6000$ $H3 \cdots S1$ $2.8600$ $03 \cdots H2A$ $1.9500$ $H3 \cdots H2A$ $2.3000$ $04 \cdots H5^{ii}$ $2.8000$ $H3 \cdots O2$ $1.9200$ $04 \cdots H6A^{ii}$ $2.2500$ $H5 \cdots O4^{ii}$ $2.8000$ $04 \cdots H6A^{ii}$ $2.2500$ $H5 \cdots O4^{ii}$ $2.8000$ $04 \cdots H6A^{ii}$ $2.2500$ $H5 \cdots H6A$ $2.4600$ $N1 \cdots C2^{v}$ $3.3319$ $16$ $H6B \cdots C4^{iv}$ $3.0600$ $N2 \cdots O3$ $2.7935$ $17$ $H6A \cdots H5$ $2.4600$ $N2 \cdots O2^{iv}$ $2.8669$ $16$ $H6B \cdots C4^{iv}$ $3.0600$ $N2 \cdots C5^{v}$ $3.2886$ $19$ $H6B \cdots H1$ $2.2200$ $N3 \cdots C2^{iv}$ $3.2886$ $19$ $H6B \cdots O1^{iv}$ $2.6800$ $N3 \cdots C2^{iv}$ $3.2844$ $17$ $H8 \cdots H5^{v}$ $2.5100$ $N3 \cdots C4^{iv}$ $3.2207$ $H1B \cdots H13B^{ii}$ $2.5300$ $O2 \cdots O1^{iv}$ $2.8201$ $H12 \cdots O3^$	O4····C5 <sup>ii</sup>	3.4031 (18)	H1…H6B	2.2200
$O4 \cdots C13^{iii}$ $3.298 (3)$ $H1 \cdots O1^{iv}$ $1.8600$ $O1 \cdots H6B^{1}$ $2.0800$ $H2A \cdots H3$ $2.3000$ $O1 \cdots H1^{1}$ $1.8600$ $H2A \cdots O3$ $1.9500$ $O2 \cdots H3$ $1.9200$ $H2A \cdots O3$ $1.9500$ $O2 \cdots H2B^{1}$ $2.0100$ $H2B \cdots H1$ $2.3000$ $O3 \cdots H12^{iv}$ $2.8700$ $H2B \cdots O2^{iv}$ $2.0100$ $O3 \cdots H3$ $2.8400$ $H2B \cdots O2^{iv}$ $2.0100$ $O3 \cdots H3$ $2.8400$ $H3 \cdots S1$ $2.8600$ $O3 \cdots H2A$ $1.9500$ $H3 \cdots H2A$ $2.3000$ $O4 \cdots H5^{ii}$ $2.8000$ $H3 \cdots O2$ $1.9200$ $O4 \cdots H5^{ii}$ $2.8000$ $H3 \cdots O2$ $1.9200$ $O4 \cdots H5^{ii}$ $2.2500$ $H5 \cdots O4^{ii}$ $2.8000$ $O4 \cdots H6A^{ii}$ $2.2500$ $H5 \cdots O4^{ii}$ $2.25100$ $N1 \cdots O1^{iv}$ $2.6515 (14)$ $H5 \cdots H6A$ $2.4600$ $N1 \cdots C2^{v}$ $3.319 (16)$ $H6A \cdots O4^{ii}$ $2.2500$ $N2 \cdots O3$ $2.7935 (17)$ $H6A \cdots H5$ $2.4600$ $N2 \cdots C5^{ii}$ $3.2886 (19)$ $H6B \cdots O1^{iv}$ $2.0800$ $N3 \cdots C5^{ii}$ $3.4276 (18)$ $H6B \cdots O1^{iv}$ $2.6800$ $N3 \cdots C4^{ii}$ $3.2207 (18)$ $H11 \cdots H13C$ $2.4100$ $N3 \cdots C4^{ii}$ $3.2207 (18)$ $H11 \cdots H13B^{ii}$ $2.5300$ $O2 \cdots N1^{iv}$ $3.319 (16)$ $H12 \cdots O3^{ii}$ $2.8700$ $C2 \cdots C4^{iv}$ $3.3207 (18)$ $H13B \cdots H1 2^{iv}$ $3.1000$ $C2 \cdots C4^{iv}$ $3.3868 (17)$ $H13B \cdots H12^{iv}$ $3.1000$	O4…N6 <sup>ii</sup>	2.9498 (18)	H1····C4 <sup>iv</sup>	3.0400
$O1 \cdots H6B^i$ 2.0800 $H2A \cdots H3$ 2.3000 $O1 \cdots H1^i$ 1.8600 $H2A \cdots S1$ 3.0800 $O2 \cdots H3$ 1.9200 $H2A \cdots O3$ 1.9500 $O2 \cdots H2B^i$ 2.0100 $H2B \cdots H1$ 2.3000 $O3 \cdots H12^{iv}$ 2.8700 $H2B \cdots S1^{iv}$ 3.0100 $O3 \cdots H3$ 2.8400 $H2B \cdots O2^{iv}$ 2.0100 $O3 \cdots H3$ 2.8400 $H2B \cdots O2^{iv}$ 2.0100 $O3 \cdots H3$ 2.8400 $H3 \cdots S1$ 2.8600 $O3 \cdots H48$ 2.6000 $H3 \cdots H2A$ 2.3000 $O4 \cdots H5^{ii}$ 2.8000 $H3 \cdots O2$ 1.9200 $O4 \cdots H5^{ii}$ 2.9100 $H3 \cdots O3$ 2.8400 $O4 \cdots H5^{ii}$ 2.500 $H5 \cdots O4^{ii}$ 2.8000 $O4 \cdots H12$ 2.6800 $H5 \cdots H4^{ii}$ 2.5100 $N1 \cdots O1^{iv}$ 2.6515 (14) $H5 \cdots H4^{ii}$ 2.2500 $N2 \cdots O3$ 2.7935 (17) $H6A \cdots H5$ 2.4600 $N2 \cdots O2^{iv}$ 2.8669 (16) $H6B \cdots C1^{iv}$ 3.0600 $N2 \cdots C5^{ii}$ 3.2886 (19) $H6B \cdots H1$ 2.2200 $N3 \cdots C5^{ii}$ 3.4276 (18) $H6B \cdots O1^{iv}$ 2.0800 $N3 \cdots C4^{ii}$ 3.2207 (18) $H11 \cdots H13C$ 2.4100 $N6 \cdots O1^{iv}$ 2.8201 (15) $H12 \cdots O3^{i}$ 2.8700 $C2 \cdots C1^{iv}$ 3.3319 (16) $H12 \cdots O3^{i}$ 2.8700 $C2 \cdots C1^{iv}$ 3.3319 (16) $H12 \cdots O3^{i}$ 2.8700 $C2 \cdots C1^{iv}$ 3.3319 (16) $H12 \cdots O3^{i}$ 2.8700 $C2 \cdots C1^{iv}$ 3.3319 (16) $H12 \cdots O3^{i}$ 2.8700 $C2 \cdots C1^{iv}$	O4…C13 <sup>iii</sup>	3.298 (3)	H1…O1 <sup>iv</sup>	1.8600
$O1 \cdots H1^i$ 1.8600 $H2A \cdots S1$ 3.0800 $O2 \cdots H3$ 1.9200 $H2A \cdots O3$ 1.9500 $O2 \cdots H2B^i$ 2.0100 $H2B \cdots H1$ 2.3000 $O3 \cdots H12^{iv}$ 2.8700 $H2B \cdots S1^{iv}$ 3.0100 $O3 \cdots H3$ 2.8400 $H2B \cdots O2^{iv}$ 2.0100 $O3 \cdots H3$ 2.8400 $H2B \cdots O2^{iv}$ 2.0100 $O3 \cdots H3$ 2.8400 $H3 \cdots S1$ 2.8600 $O3 \cdots H4$ 1.9500 $H3 \cdots H2A$ 2.3000 $O4 \cdots H5^{ii}$ 2.8000 $H3 \cdots O2$ 1.9200 $O4 \cdots H5^{ii}$ 2.9100 $H3 \cdots O3$ 2.8400 $O4 \cdots H6A^{ii}$ 2.2500 $H5 \cdots O4^{ii}$ 2.8000 $O4 \cdots H12$ 2.6800 $H5 \cdots H8^v$ 2.5100 $N1 \cdots O1^{iv}$ 2.6515 (14) $H5 \cdots H6A$ 2.4600 $N1 \cdots O1^{iv}$ 2.6515 (14) $H5 \cdots H6A$ 2.4600 $N2 \cdots O3$ 2.7935 (17) $H6A \cdots H5$ 2.4600 $N2 \cdots O2^{iv}$ 2.8669 (16) $H6B \cdots C4^{iv}$ 3.0600 $N2 \cdots C5^v$ 3.2886 (19) $H6B \cdots H1$ 2.2200 $N3 \cdots C5^{ii}$ 3.4276 (18) $H6B \cdots O1^{iv}$ 2.0800 $N3 \cdots O2$ 2.7689 (14) $H8 \cdots H5^v$ 2.5100 $N3 \cdots N3^v$ 3.2844 (17) $H8 \cdots O3$ 2.6000 $N3 \cdots C4^u$ 3.2207 (18) $H11 \cdots H13C$ 2.4100 $N6 \cdots O1^{iv}$ 2.8201 (15) $H12 \cdots O4$ 2.6800 $N6 \cdots O1^{iv}$ 2.8210 (15) $H12 \cdots O4$ 2.6800 $N6 \cdots O1^{iv}$ 3.3319 (16) $H12 \cdots O3^i$ 2.8700 $C2 \cdots C4^v$ 3.3868 (17) $H13A$	O1…H6B <sup>i</sup>	2.0800	Н2А…Н3	2.3000
$O2 \cdots H3$ 1.9200 $H2A \cdots O3$ 1.9500 $O2 \cdots H2B^i$ 2.0100 $H2B \cdots H1$ 2.3000 $O3 \cdots H12^{iv}$ 2.8700 $H2B \cdots S1^{iv}$ 3.0100 $O3 \cdots H3$ 2.8400 $H2B \cdots O2^{iv}$ 2.0100 $O3 \cdots H3$ 2.8400 $H3 \cdots S1$ 2.8600 $O3 \cdots H2A$ 1.9500 $H3 \cdots H2A$ 2.3000 $O4 \cdots H5^{ii}$ 2.8000 $H3 \cdots O2$ 1.9200 $O4 \cdots H5^{ii}$ 2.9100 $H3 \cdots O3$ 2.8400 $O4 \cdots H6A^{ii}$ 2.2500 $H5 \cdots O4^{ii}$ 2.8000 $O4 \cdots H12$ 2.6800 $H5 \cdots H8^{v}$ 2.5100 $N1 \cdots O1^{iv}$ 2.6515 (14) $H5 \cdots H6A$ 2.4600 $N1 \cdots C2^{v}$ 3.319 (16) $H6A \cdots O4^{ii}$ 2.2500 $N2 \cdots O2^{iv}$ 2.8669 (16) $H6B \cdots C4^{iv}$ 3.0600 $N2 \cdots C2^{iv}$ 3.2886 (19) $H6B \cdots H1$ 2.2200 $N3 \cdots O2$ 2.7689 (14) $H8 \cdots H5^{v}$ 2.5100 $N3 \cdots O2$ 2.7689 (14) $H8 \cdots H5^{v}$ 2.5100 $N3 \cdots O4^{ii}$ 3.2207 (18) $H11 \cdots H13C$ 2.4400 $N3 \cdots C4^{ii}$ 3.2207 (18) $H11 \cdots H13C$ 2.4100 $N6 \cdots O1^{iv}$ 2.8201 (15) $H12 \cdots O4$ 2.6800 $N6 \cdots O4^{ii}$ 2.9498 (18) $H12 \cdots H13B^{iii}$ 2.5300 $C2 \cdots C1^{ii}$ 3.3319 (16) $H12 \cdots O3^{i}$ 2.8700 $C2 \cdots C1^{ii}$ 3.319 (16) $H12 \cdots O3^{ii}$ 2.8700 $C2 \cdots C1^{ii}$ 3.319 (16) $H12 \cdots H13B^{iii}$ 3.1000 $C2 \cdots C1^{ii}$ 3.319 (16) $H13 \cdots H12^{vi}$ 3.0100<	O1…H1 <sub>i</sub>	1.8600	H2A…S1	3.0800
$O2 \cdots H2B^i$ 2.0100 $H2B \cdots H1$ 2.3000 $O3 \cdots H12^{iv}$ 2.8700 $H2B \cdots S1^{iv}$ 3.0100 $O3 \cdots H3$ 2.8400 $H2B \cdots O2^{iv}$ 2.0100 $O3 \cdots H8$ 2.6000 $H3 \cdots S1$ 2.8600 $O3 \cdots H5^{ii}$ 2.8000 $H3 \cdots H2A$ 2.3000 $O4 \cdots H5^{ii}$ 2.8000 $H3 \cdots O2$ 1.9200 $O4 \cdots H5^{ii}$ 2.9100 $H3 \cdots O2$ 1.9200 $O4 \cdots H13C^{iii}$ 2.9100 $H3 \cdots O3$ 2.8400 $O4 \cdots H6A^{ii}$ 2.2500 $H5 \cdots O4^{ii}$ 2.8000 $O4 \cdots H6A^{ii}$ 2.2500 $H5 \cdots H8^v$ 2.5100 $N1 \cdots O1^{iv}$ 2.6515 (14) $H5 \cdots H6A$ 2.4600 $N1 \cdots C2^v$ 3.3319 (16) $H6A \cdots O4^{ii}$ 2.2500 $N2 \cdots C6^v$ 3.2866 (16) $H6B \cdots C4^{iv}$ 3.0600 $N2 \cdots C6^v$ 3.2886 (19) $H6B \cdots O1^{iv}$ 2.0800 $N3 \cdots C5^{ii}$ 3.4276 (18) $H6B \cdots O1^{iv}$ 2.0800 $N3 \cdots C2^i$ 3.4212 (18) $H9 \cdots H13B$ 2.4700 $N3 \cdots C4^{ii}$ 3.2207 (18) $H11 \cdots H13C$ 2.4100 $N6 \cdots O1^{iv}$ 2.8201 (15) $H12 \cdots O4$ 2.6800 $N3 \cdots C4^{ii}$ 3.3319 (16) $H12 \cdots O3^i$ 2.8700 $C2 \cdots C1^{iv}$ 3.3868 (17) $H13B \cdots C1^{vii}$ 3.1000 $C2 \cdots C1^{ii}$ 3.1894 (18) $H13B \cdots H12^{vii}$ 2.5300 $C2 \cdots C1^{ii}$ 3.1894 (18) $H13B \cdots H12^{vii}$ 3.0100	O2…H3	1.9200	H2A…O3	1.9500
$O3 \cdots H12^{1\nu}$ $2.8700$ $H2B \cdots S1^{1\nu}$ $3.0100$ $O3 \cdots H3$ $2.8400$ $H2B \cdots O2^{1\nu}$ $2.0100$ $O3 \cdots H8$ $2.6000$ $H3 \cdots S1$ $2.8600$ $O3 \cdots H2A$ $1.9500$ $H3 \cdots H2A$ $2.3000$ $O4 \cdots H5^{1i}$ $2.8000$ $H3 \cdots O2$ $1.9200$ $O4 \cdots H13C^{1ii}$ $2.9100$ $H3 \cdots O3$ $2.8400$ $O4 \cdots H6A^{1i}$ $2.2500$ $H5 \cdots O4^{1i}$ $2.8000$ $O4 \cdots H12$ $2.6800$ $H5 \cdots H8^{v}$ $2.5100$ $N1 \cdots O1^{1v}$ $2.6515$ (14) $H5 \cdots H6A$ $2.4600$ $N1 \cdots C2^{v}$ $3.3319$ (16) $H6A \cdots O4^{1i}$ $2.2500$ $N2 \cdots O3$ $2.7935$ (17) $H6A \cdots H5$ $2.4600$ $N2 \cdots C6^{v}$ $3.2886$ (19) $H6B \cdots C4^{1v}$ $3.0600$ $N3 \cdots C5^{1i}$ $3.4276$ (18) $H6B \cdots O1^{1v}$ $2.0800$ $N3 \cdots O2$ $2.7689$ (14) $H8 \cdots H5^{v}$ $2.5100$ $N3 \cdots C4^{v}$ $3.2244$ (17) $H8 \cdots O3$ $2.6000$ $N3 \cdots C4^{v}$ $3.2207$ (18) $H11 \cdots H13C$ $2.4100$ $N6 \cdots O1^{1v}$ $2.8201$ (15) $H12 \cdots O4$ $2.6800$ $N6 \cdots O4^{1i}$ $2.9498$ (18) $H12 \cdots H13B^{1ii}$ $2.5300$ $C2 \cdots C1^{v}$ $3.3319$ (16) $H12 \cdots O3^{3}$ $2.8700$ $C2 \cdots C1^{v}$ $3.3868$ (17) $H13A \cdots C7^{viii}$ $3.1000$ $C2 \cdots C1^{v}$ $3.3868$ (17) $H13B \cdots H12^{vi}$ $2.5300$ $C2 \cdots C1^{v}$ $3.3864$ (18) $H13B \cdots H12^{vi}$ $2.7700$ $C2 \cdots C1^{v}$ $3.3864$ (17) $H13B \cdots C$	O2…H2B <sup>i</sup>	2.0100	H2B…H1	2.3000
$O3 \cdots H3$ $2.8400$ $H2B \cdots O2^{iv}$ $2.0100$ $O3 \cdots H8$ $2.6000$ $H3 \cdots S1$ $2.8600$ $O3 \cdots H2A$ $1.9500$ $H3 \cdots H2A$ $2.3000$ $O4 \cdots H5^{ii}$ $2.8000$ $H3 \cdots O2$ $1.9200$ $O4 \cdots H13C^{iii}$ $2.9100$ $H3 \cdots O3$ $2.8400$ $O4 \cdots H6A^{ii}$ $2.2500$ $H5 \cdots O4^{ii}$ $2.8000$ $O4 \cdots H12$ $2.6800$ $H5 \cdots H8^{v}$ $2.5100$ $N \cdots O1^{iv}$ $2.6515$ (14) $H5 \cdots H6A$ $2.4600$ $N \cdots C2^{v}$ $3.3319$ (16) $H6A \cdots O4^{ii}$ $2.2500$ $N \cdots C2^{v}$ $3.3319$ (16) $H6A \cdots O4^{ii}$ $2.2500$ $N \cdots C2^{v}$ $3.28669$ (16) $H6B \cdots C4^{iv}$ $3.0600$ $N2 \cdots C2^{iv}$ $2.8669$ (16) $H6B \cdots O1^{iv}$ $2.0800$ $N3 \cdots C5^{ii}$ $3.4276$ (18) $H6B \cdots O1^{iv}$ $2.0800$ $N3 \cdots C5^{ii}$ $3.4276$ (18) $H6B \cdots O1^{iv}$ $2.6000$ $N3 \cdots C4^{iv}$ $3.2207$ (18) $H11 \cdots H13C$ $2.4100$ $N6 \cdots O1^{iv}$ $2.8201$ (15) $H12 \cdots O4$ $2.6800$ $N6 \cdots O1^{iv}$ $2.8201$ (15) $H12 \cdots O4$ $2.6800$ $N6 \cdots O1^{iv}$ $2.8201$ (15) $H12 \cdots O4$ $2.6800$ $N6 \cdots O4^{ii}$ $2.9498$ (18) $H12 \cdots H13B^{iii}$ $2.5300$ $C2 \cdots C1^{v}$ $3.3868$ (17) $H13A \cdots C7^{viiii}$ $3.1000$ $C2 \cdots C1^{ii}$ $3.1894$ (18) $H13B \cdots H12^{vii}$ $2.5100$ $N6 \cdots O1^{iv}$ $3.2207$ (18) $H13B \cdots C12^{vii}$ $3.0100$ $C2 \cdots C1^{ii}$ $3.1894$	O3…H12 <sup>iv</sup>	2.8700	H2B····S1 <sup>iv</sup>	3.0100
$O3 \cdots H8$ $2.6000$ $H3 \cdots S1$ $2.8600$ $O3 \cdots H2A$ $1.9500$ $H3 \cdots H2A$ $2.3000$ $O4 \cdots H5^{ii}$ $2.8000$ $H3 \cdots O2$ $1.9200$ $O4 \cdots H13C^{iii}$ $2.9100$ $H3 \cdots O3$ $2.8400$ $O4 \cdots H6A^{ii}$ $2.2500$ $H5 \cdots O4^{ii}$ $2.8000$ $O4 \cdots H12$ $2.6800$ $H5 \cdots H8^{v}$ $2.5100$ $N1 \cdots O1^{iv}$ $2.6515$ (14) $H5 \cdots H6A$ $2.4600$ $N1 \cdots C2^{v}$ $3.3319$ (16) $H6A \cdots O4^{ii}$ $2.2500$ $N2 \cdots O3$ $2.7935$ (17) $H6A \cdots H5$ $2.4600$ $N2 \cdots O2^{iv}$ $2.8669$ (16) $H6B \cdots C4^{iv}$ $3.0600$ $N2 \cdots C6^{v}$ $3.2886$ (19) $H6B \cdots H1$ $2.2200$ $N3 \cdots C5^{ii}$ $3.4276$ (18) $H6B \cdots O1^{iv}$ $2.0800$ $N3 \cdots O2$ $2.7689$ (14) $H8 \cdots H5^{v}$ $2.5100$ $N3 \cdots C4^{ii}$ $3.2207$ (18) $H11 \cdots H13B$ $2.4700$ $N3 \cdots C4^{ii}$ $3.2207$ (18) $H11 \cdots H13C$ $2.4100$ $N6 \cdots O1^{iv}$ $2.8201$ (15) $H12 \cdots O4$ $2.6800$ $N6 \cdots O1^{iv}$ $3.319$ (16) $H12 \cdots O3^{i}$ $2.8700$ $C2 \cdots N1^{v}$ $3.3319$ (16) $H12 \cdots O3^{i}$ $2.8700$ $C2 \cdots C2^{v}$ $3.3868$ (17) $H13A \cdots C7^{viii}$ $3.1000$ $C2 \cdots C1^{ii}$ $3.1894$ (18) $H13B \cdots H19$ $2.4700$ $C2 \cdots O1^{ii}$ $3.1894$ (18) $H13B \cdots H12^{vi}$ $2.500$	O3…H3	2.8400	H2B····O2 <sup>iv</sup>	2.0100
$03 \cdots H2A$ $19500$ $H3 \cdots H2A$ $2.3000$ $04 \cdots H5^{ii}$ $2.8000$ $H3 \cdots O2$ $1.9200$ $04 \cdots H13C^{iii}$ $2.9100$ $H3 \cdots O3$ $2.8400$ $04 \cdots H6A^{ii}$ $2.2500$ $H5 \cdots O4^{ii}$ $2.8000$ $04 \cdots H12$ $2.6800$ $H5 \cdots H8^{v}$ $2.5100$ $N1 \cdots O1^{iv}$ $2.6515(14)$ $H5 \cdots H6A$ $2.4600$ $N1 \cdots C2^{v}$ $3.3319(16)$ $H6A \cdots O4^{ii}$ $2.2500$ $N2 \cdots O3$ $2.7935(17)$ $H6A \cdots H5$ $2.4600$ $N2 \cdots O2^{iv}$ $2.8669(16)$ $H6B \cdots C4^{iv}$ $3.0600$ $N2 \cdots C6^{v}$ $3.2886(19)$ $H6B \cdots H1$ $2.2200$ $N3 \cdots C5^{ii}$ $3.4276(18)$ $H6B \cdots O1^{iv}$ $2.0800$ $N3 \cdots O2$ $2.7689(14)$ $H8 \cdots H5^{v}$ $2.5100$ $N3 \cdots C4^{v}$ $3.2207(18)$ $H11 \cdots H13B$ $2.4700$ $N3 \cdots C4^{ii}$ $3.2207(18)$ $H11 \cdots H13B^{iii}$ $2.5300$ $N6 \cdots O1^{iv}$ $2.8201(15)$ $H12 \cdots O3^{i}$ $2.8700$ $C2 \cdots N1^{v}$ $3.3319(16)$ $H12 \cdots O3^{i}$ $2.8700$ $C2 \cdots C1^{v}$ $3.368(17)$ $H13A \cdots C7^{viii}$ $3.1000$ $C2 \cdots C1^{ii}$ $3.1894(18)$ $H13B \cdots H12^{vi}$ $2.5300$ $C2 \cdots O1^{ii}$ $3.1894(18)$ $H13B \cdots H12^{vi}$ $2.5300$	O3…H8	2.6000	H3…S1	2.8600
OorHar1000H31000 $O4 \cdots H5^{ii}$ 2.8000H31.9200 $O4 \cdots H13C^{iii}$ 2.9100H32.8400 $O4 \cdots H6A^{ii}$ 2.2500H52.8000 $O4 \cdots H12$ 2.6800H52.8000 $O4 \cdots H12$ 2.6515 (14)H54.600 $N1 \cdots O1^{iv}$ 2.6515 (14)H54.600 $N1 \cdots C2^{v}$ 3.3319 (16)H6AH6A $N2 \cdots O3$ 2.7935 (17)H6A4.600 $N2 \cdots O3$ 2.7935 (17)H6AH6B $N2 \cdots O2^{iv}$ 2.8669 (16)H6BH6B $N2 \cdots C6^{v}$ 3.2886 (19)H6BH1 $N3 \cdots C5^{ii}$ 3.4276 (18)H6B2.5100 $N3 \cdots C2$ 2.7689 (14)H8H1 $N3 \cdots O2$ 2.7689 (14)H8H001 $N3 \cdots O2$ 2.7689 (14)H8H001 $N3 \cdots C4^{ii}$ 3.2207 (18)H11H100 $N3 \cdots C4^{ii}$ 2.8201 (15)H122.6800 $N6 \cdots O1^{iv}$ 2.8201 (15)H124.600 $N6 \cdots O1^{iv}$ 2.8201 (15)H122.6800 $N6 \cdots O1^{iv}$ 3.319 (16)H122.8700 $C2 \cdots N1^{v}$ 3.319 (16)H122.8700 $C2 \cdots C2^{v}$ 3.3868 (17)H13B2.4700 $C2 \cdots C1^{ii}$ 3.1894 (18)H13B2.4700 $C2 \cdots O1^{ii}$ 3.1894 (18)H13B2.4700 $C2 \cdots O1^{ii}$ 3.2207 (18)H13B2.5300	03…H2A	1 9500	H3···H2A	2 3000
O4H13C <sup>iiii</sup> 2.000H3O32.8400O4H6A <sup>ii</sup> 2.2500H5O4 <sup>ii</sup> 2.8000O4H6A <sup>ii</sup> 2.2500H5O4 <sup>ii</sup> 2.8000O4H122.6800H5H8 <sup>v</sup> 2.5100N1O1 <sup>iv</sup> 2.6515 (14)H5H6A2.4600N1C2 <sup>v</sup> 3.3319 (16)H6AO4 <sup>ii</sup> 2.2500N2O32.7935 (17)H6AH52.4600N2O2 <sup>iv</sup> 2.8669 (16)H6BC4 <sup>iv</sup> 3.0600N2C6 <sup>v</sup> 3.2886 (19)H6BH12.2200N3C5 <sup>ii</sup> 3.4276 (18)H6BO1 <sup>iv</sup> 2.0800N3O22.7689 (14)H8H5 <sup>v</sup> 2.5100N3C4 <sup>ii</sup> 3.2207 (18)H11H13C2.4700N3C4 <sup>ii</sup> 3.2207 (18)H11H13C2.4100N6O1 <sup>iv</sup> 2.8201 (15)H12O42.6800N6O4 <sup>ii</sup> 2.9498 (18)H12H13B <sup>iii</sup> 2.5300C2C2 <sup>v</sup> 3.3868 (17)H13AC7 <sup>viii</sup> 3.1000C2C2 <sup>v</sup> 3.868 (17)H13BH92.4700C2C1 <sup>ii</sup> 3.1894 (18)H13BH92.4700C2O1 <sup>ii</sup> 3.1894 (18)H13BH12 <sup>vii</sup> 2.5300	04···H5 <sup>ii</sup>	2 8000	H3····O2	1 9200
OA: HEAD.1 HOD.1 HOD.1 HOOA: HEA2.2500H5···OA <sup>ii</sup> 2.8000OA: H122.6800H5···H8 <sup>v</sup> 2.5100N1···O1 <sup>iv</sup> 2.6515 (14)H5···H6A2.4600N1···C2 <sup>v</sup> 3.3319 (16)H6A···O4 <sup>ii</sup> 2.2500N2···O32.7935 (17)H6A···H52.4600N2···O2 <sup>iv</sup> 2.8669 (16)H6B···C4 <sup>iv</sup> 3.0600N2···C6 <sup>v</sup> 3.2886 (19)H6B···H12.2200N3···C5 <sup>ii</sup> 3.4276 (18)H6B···O1 <sup>iv</sup> 2.0800N3···O22.7689 (14)H8···H5 <sup>v</sup> 2.5100N3···C4 <sup>v</sup> 3.2207 (18)H11···H13B2.4700N3···C4 <sup>ii</sup> 3.2207 (18)H11···H13C2.4100N6···O1 <sup>iv</sup> 2.8201 (15)H12···O42.6800N6···O4 <sup>ii</sup> 2.9498 (18)H12···H13B <sup>iii</sup> 2.5300C2···C2 <sup>v</sup> 3.3868 (17)H13A···C7 <sup>viii</sup> 3.1000C2···C1 <sup>ii</sup> 3.1894 (18)H13B···H12 <sup>vi</sup> 3.0100C2···O1 <sup>ii</sup> 3.1894 (18)H13B···H12 <sup>vi</sup> 2.5300	04…H13C <sup>iii</sup>	2 9100	H3····O3	2 8400
O4H122.6800H5H82.5100 $N1O1^{iv}$ 2.6515 (14)H5H8v2.5100 $N1O1^{iv}$ 2.6515 (14)H5H6A2.4600 $N1C2^{v}$ 3.3319 (16)H6AO4"2.2500 $N2O3$ 2.7935 (17)H6AH52.4600 $N2O2^{iv}$ 2.8669 (16)H6BC4iv3.0600 $N2C6^{v}$ 3.2886 (19)H6BH12.2200 $N3C5^{ii}$ 3.4276 (18)H6BO1'v2.0800 $N3O2$ 2.7689 (14)H8H5v2.5100 $N3O2$ 2.7689 (14)H8H5v2.5100 $N3O4^{v}$ 3.2244 (17)H8O32.6000 $N3C4^{v}$ 3.2207 (18)H11H13C2.4100 $N6O1^{iv}$ 2.8201 (15)H12O42.6800 $N6O4^{ii}$ 2.9498 (18)H12O42.6800 $N6O4^{ii}$ 2.9498 (17)H13AC7'iii3.1000 $C2C2^{v}$ 3.3868 (17)H13BH122.4700 $C2C1^{ii}$ 3.1894 (18)H13BH123.0100 $C2O1^{ii}$ 3.1894 (18)H13BH122.5300	O4···H6A <sup>ii</sup>	2 2500	H5…O4 <sup>ii</sup>	2.8100
N1···O1 <sup>iv</sup> 2.6500H5 H62.5100N1···O1 <sup>iv</sup> 2.6515 (14)H5···H6A2.4600N1···C2 <sup>v</sup> 3.3319 (16)H6A···O4 <sup>ii</sup> 2.2500N2···O32.7935 (17)H6A···H52.4600N2···O2 <sup>iv</sup> 2.8669 (16)H6B···C4 <sup>iv</sup> 3.0600N2···C6 <sup>v</sup> 3.2886 (19)H6B···H12.2200N3···C5 <sup>ii</sup> 3.4276 (18)H6B···O1 <sup>iv</sup> 2.0800N3···C22.7689 (14)H8···H5 <sup>v</sup> 2.5100N3···C4 <sup>ii</sup> 3.2207 (18)H9···H13B2.4700N3···C4 <sup>ii</sup> 3.2207 (18)H11···H13C2.4100N6···O1 <sup>iv</sup> 2.8201 (15)H12···O42.6800N6···O4 <sup>ii</sup> 2.9498 (18)H12···H13B <sup>iii</sup> 2.5300C2···C2 <sup>v</sup> 3.3868 (17)H13A···C7 <sup>viii</sup> 3.1000C2···C6 <sup>v</sup> 3.5776 (18)H13B···H92.4700C2···O1 <sup>ii</sup> 3.1894 (18)H13B···H12 <sup>vii</sup> 3.0100C4···N3 <sup>ii</sup> 3.2207 (18)H13B···H12 <sup>vii</sup> 2.5300	04H12	2.6800	H5H8 <sup>v</sup>	2.5000
N1 ···C2v $2.0515(14)$ H5 ··IOA $2.4000$ N1···C2v $3.3319(16)$ H6A···O4ii $2.2500$ N2···O3 $2.7935(17)$ H6A···H5 $2.4600$ N2···O2iv $2.8669(16)$ H6B···C4iv $3.0600$ N2···C6v $3.2886(19)$ H6B···H1 $2.2200$ N3···C5ii $3.4276(18)$ H6B···O1iv $2.0800$ N3···C2 $2.7689(14)$ H8···H5v $2.5100$ N3···C4v $3.2844(17)$ H8···O3 $2.6000$ N3···C4ii $3.2207(18)$ H11···H13C $2.4100$ N6···O1iv $2.8201(15)$ H12···O4 $2.6800$ N6···O4ii $2.9498(18)$ H12···H13Biii $2.5300$ C2···N1v $3.3319(16)$ H12···O3i $2.8700$ C2···C2v $3.3868(17)$ H13A···C7viii $3.1000$ C2···C1ii $3.1894(18)$ H13B···H12vii $3.0100$ C4···N3ii $3.2207(18)$ H13B···H12vii $3.0100$	N1Oliv	2.0000	Н5 Н6	2.5100
N1 $^{11}$ C23.3319 (10)H0A $^{11}$ O42.2500N2 $^{}$ O32.7935 (17)H6A $^{}$ H52.4600N2 $^{}$ O22.8669 (16)H6B $^{}$ C4 $^{iv}$ 3.0600N2 $^{}$ C6 $^{v}$ 3.2886 (19)H6B $^{}$ H12.2200N3 $^{}$ C5 $^{ii}$ 3.4276 (18)H6B $^{}$ O1 $^{iv}$ 2.0800N3 $^{}$ O22.7689 (14)H8 $^{}$ H5 $^{v}$ 2.5100N3 $^{}$ O22.7689 (14)H8 $^{}$ H5 $^{v}$ 2.6000N3 $^{}$ C4 $^{v}$ 3.2844 (17)H8 $^{}$ O32.6000N3 $^{}$ C4 $^{v}$ 3.4212 (18)H9 $^{}$ H13B2.4700N3 $^{}$ C4 $^{ii}$ 3.2207 (18)H11 $^{}$ H13C2.4100N6 $^{}$ O1 $^{iv}$ 2.8201 (15)H12 $^{}$ O42.6800N6 $^{}$ O4 $^{ii}$ 2.9498 (18)H12 $^{}$ O32.5300C2 $^{}$ N1 $^{v}$ 3.3319 (16)H12 $^{}$ O3 $^{i}$ 2.8700C2 $^{}$ C2 $^{v}$ 3.3868 (17)H13A $^{}$ C7 $^{viii}$ 3.1000C2 $^{}$ C6 $^{v}$ 3.5776 (18)H13B $^{}$ H192.4700C2 $^{}$ O1 $^{ii}$ 3.1894 (18)H13B $^{}$ H12 $^{.vi}$ 3.0100C4 $^{}$ N3 $^{ii}$ 3.2207 (18)H13B $^{}$ H12 $^{.vi}$ 2.5300	N1C2v	2.0313(14) 2.3310(16)		2.4000
$N2\cdots O3$ $2.7933 (17)$ $H0A^{4}H3$ $2.4000$ $N2\cdots O2^{iv}$ $2.8669 (16)$ $H6B\cdots C4^{iv}$ $3.0600$ $N2\cdots C6^v$ $3.2886 (19)$ $H6B\cdots H1$ $2.2200$ $N3\cdots C5^{ii}$ $3.4276 (18)$ $H6B\cdots O1^{iv}$ $2.0800$ $N3\cdots O2$ $2.7689 (14)$ $H8\cdots H5^v$ $2.5100$ $N3\cdots N3^v$ $3.2844 (17)$ $H8\cdots O3$ $2.6000$ $N3\cdots C4^v$ $3.4212 (18)$ $H9\cdots H13B$ $2.4700$ $N3\cdots C4^{ii}$ $3.2207 (18)$ $H11\cdots H13C$ $2.4100$ $N6\cdots O1^{iv}$ $2.8201 (15)$ $H12\cdots O4$ $2.6800$ $N6\cdots O4^{ii}$ $2.9498 (18)$ $H12\cdots H13B^{iii}$ $2.5300$ $C2\cdots N1^v$ $3.3319 (16)$ $H12\cdots O3^i$ $3.1000$ $C2\cdots C2^v$ $3.3868 (17)$ $H13B\cdots H9$ $2.4700$ $C2\cdots O1^{ii}$ $3.1894 (18)$ $H13B\cdots H12^{vi}$ $3.0100$ $C4\cdots N3^{ii}$ $3.2207 (18)$ $H13B\cdots H12^{vi}$ $2.5300$	N202	2.7025(17)	H6A	2.2500
$N2\cdots C6^{\vee}$ $2.8009 (10)$ $H0B\cdots C4$ $3.0000$ $N2\cdots C6^{\vee}$ $3.2886 (19)$ $H6B\cdots H1$ $2.2200$ $N3\cdots C5^{ii}$ $3.4276 (18)$ $H6B\cdots O1^{iv}$ $2.0800$ $N3\cdots O2$ $2.7689 (14)$ $H8\cdots H5^{\vee}$ $2.5100$ $N3\cdots N3^{\vee}$ $3.2844 (17)$ $H8\cdots O3$ $2.6000$ $N3\cdots C4^{\vee}$ $3.4212 (18)$ $H9\cdots H13B$ $2.4700$ $N3\cdots C4^{ii}$ $3.2207 (18)$ $H11\cdots H13C$ $2.4100$ $N6\cdots O1^{iv}$ $2.8201 (15)$ $H12\cdots O4$ $2.6800$ $N6\cdots O4^{ii}$ $2.9498 (18)$ $H12\cdots O3^{i}$ $2.8700$ $C2\cdots C1^{\vee}$ $3.3319 (16)$ $H13A\cdots C7^{\nu iii}$ $3.1000$ $C2\cdots C6^{\vee}$ $3.5776 (18)$ $H13B\cdots H9$ $2.4700$ $C2\cdots O1^{ii}$ $3.1894 (18)$ $H13B\cdots H12^{\nu i}$ $3.0100$ $C4\cdots N3^{ii}$ $3.2207 (18)$ $H13B\cdots H12^{\nu i}$ $2.5300$	N2O2iv	2.7933(17) 2.8660(16)		2.4000
N2···C6' $3.2886 (19)$ H0B···H1 $2.2200$ N3···C5 <sup>ii</sup> $3.4276 (18)$ H6B···O1 <sup>iv</sup> $2.0800$ N3···O2 $2.7689 (14)$ H8···H5 <sup>v</sup> $2.5100$ N3···N3 <sup>v</sup> $3.2844 (17)$ H8···O3 $2.6000$ N3···C4 <sup>v</sup> $3.4212 (18)$ H9···H13B $2.4700$ N3···C4 <sup>ii</sup> $3.2207 (18)$ H11···H13C $2.4100$ N6···O1 <sup>iv</sup> $2.8201 (15)$ H12···O4 $2.6800$ N6···O4 <sup>ii</sup> $2.9498 (18)$ H12···H13B <sup>iii</sup> $2.5300$ C2···N1 <sup>v</sup> $3.3319 (16)$ H12···O3 <sup>i</sup> $2.8700$ C2···C6 <sup>v</sup> $3.5776 (18)$ H13B···H9 $2.4700$ C2···O1 <sup>ii</sup> $3.1894 (18)$ H13B···C12 <sup>vi</sup> $3.0100$ C4···N3 <sup>ii</sup> $3.2207 (18)$ H13B···H12 <sup>vi</sup> $2.5300$		2.8009(10)		3.0000
N3···C3 <sup>ar</sup> $3.4276 (18)$ H6B···C1 <sup>ar</sup> $2.0800$ N3···C4 <sup>ar</sup> $2.7689 (14)$ H8···H5 <sup>v</sup> $2.5100$ N3···N3 <sup>v</sup> $3.2844 (17)$ H8···O3 $2.6000$ N3···C4 <sup>ar</sup> $3.4212 (18)$ H9···H13B $2.4700$ N3···C4 <sup>ari</sup> $3.2207 (18)$ H11···H13C $2.4100$ N6···O1 <sup>iv</sup> $2.8201 (15)$ H12···O4 $2.6800$ N6···O4 <sup>ari</sup> $2.9498 (18)$ H12···H13B <sup>arii</sup> $2.5300$ C2···N1 <sup>v</sup> $3.3319 (16)$ H12···O3 <sup>i</sup> $2.8700$ C2···C2 <sup>v</sup> $3.3868 (17)$ H13A···C7 <sup>viii</sup> $3.1000$ C2···C6 <sup>v</sup> $3.5776 (18)$ H13B···H9 $2.4700$ C2···O1 <sup>ii</sup> $3.1894 (18)$ H13B···H12 <sup>vi</sup> $3.0100$ C4···N3 <sup>ii</sup> $3.2207 (18)$ H13B···H12 <sup>vii</sup> $2.5300$		5.2880 (19) 2.427( (19)		2.2200
N3···O2 $2.7689 (14)$ $H8···H5^{v}$ $2.5100$ N3···N3v $3.2844 (17)$ $H8···H5^{v}$ $2.6000$ N3···C4v $3.4212 (18)$ $H9···H13B$ $2.4700$ N3···C4ii $3.2207 (18)$ $H11···H13C$ $2.4100$ N6···O1iv $2.8201 (15)$ $H12···O4$ $2.6800$ N6···O4ii $2.9498 (18)$ $H12···H13B^{iii}$ $2.5300$ C2···N1v $3.3319 (16)$ $H12···O3^{i}$ $2.8700$ C2···C2v $3.3868 (17)$ $H13A···C7^{viii}$ $3.1000$ C2···C6v $3.5776 (18)$ $H13B···H9$ $2.4700$ C2···O1ii $3.1894 (18)$ $H13B···H12^{vi}$ $3.0100$ C4···N3ii $3.2207 (18)$ $H13B···H12^{vi}$ $2.5300$	N3C5"	3.4276 (18)		2.0800
N3···N3 <sup>v</sup> $3.2844 (17)$ H8···O3 $2.6000$ N3···C4 <sup>v</sup> $3.4212 (18)$ H9···H13B $2.4700$ N3···C4 <sup>ii</sup> $3.2207 (18)$ H11···H13C $2.4100$ N6···O1 <sup>iv</sup> $2.8201 (15)$ H12···O4 $2.6800$ N6···O4 <sup>ii</sup> $2.9498 (18)$ H12···H13B <sup>iii</sup> $2.5300$ C2···N1 <sup>v</sup> $3.3319 (16)$ H12···O3 <sup>i</sup> $2.8700$ C2···C2 <sup>v</sup> $3.3868 (17)$ H13A···C7 <sup>viii</sup> $3.1000$ C2···C6 <sup>v</sup> $3.5776 (18)$ H13B···H9 $2.4700$ C2···O1 <sup>ii</sup> $3.1894 (18)$ H13B···H12 <sup>vi</sup> $3.0100$ C4···N3 <sup>ii</sup> $3.2207 (18)$ H13B···H12 <sup>vi</sup> $2.5300$	N302	2.7689 (14)		2.5100
N3···C4 $^{v}$ 3.4212 (18)H9···H13B2.4700N3···C4 $^{ii}$ 3.2207 (18)H11···H13C2.4100N6···O1 $^{iv}$ 2.8201 (15)H12···O42.6800N6···O4 $^{ii}$ 2.9498 (18)H12···H13B $^{iii}$ 2.5300C2···N1 $^{v}$ 3.3319 (16)H12···O3 $^{i}$ 2.8700C2···C2 $^{v}$ 3.3868 (17)H13A···C7 $^{viii}$ 3.1000C2···C6 $^{v}$ 3.5776 (18)H13B···H92.4700C2···O1 $^{ii}$ 3.1894 (18)H13B···C12 $^{vi}$ 3.0100C4···N3 $^{ii}$ 3.2207 (18)H13B···H12 $^{vi}$ 2.5300	N3N3 <sup>v</sup>	3.2844 (17)	H803	2.6000
N3···C4 <sup>ii</sup> $3.2207 (18)$ H11···H13C $2.4100$ N6···O1 <sup>iv</sup> $2.8201 (15)$ H12···O4 $2.6800$ N6···O4 <sup>ii</sup> $2.9498 (18)$ H12···H13B <sup>iii</sup> $2.5300$ C2···N1 <sup>v</sup> $3.3319 (16)$ H12···O3 <sup>i</sup> $2.8700$ C2···C2 <sup>v</sup> $3.3868 (17)$ H13A···C7 <sup>viii</sup> $3.1000$ C2···C6 <sup>v</sup> $3.5776 (18)$ H13B···H9 $2.4700$ C2···O1 <sup>ii</sup> $3.1894 (18)$ H13B···C12 <sup>vi</sup> $3.0100$ C4···N3 <sup>ii</sup> $3.2207 (18)$ H13B···H12 <sup>vi</sup> $2.5300$	N3…C4 <sup>v</sup>	3.4212 (18)	H9…H13B	2.4700
N6···O1 <sup>iv</sup> 2.8201 (15)H12···O42.6800N6···O4 <sup>ii</sup> 2.9498 (18)H12···H13B <sup>iii</sup> 2.5300C2···N1 <sup>v</sup> 3.3319 (16)H12···O3 <sup>i</sup> 2.8700C2···C2 <sup>v</sup> 3.3868 (17)H13A···C7 <sup>viii</sup> 3.1000C2···C6 <sup>v</sup> 3.5776 (18)H13B···H92.4700C2···O1 <sup>ii</sup> 3.1894 (18)H13B···C12 <sup>vi</sup> 3.0100C4···N3 <sup>ii</sup> 3.2207 (18)H13B···H12 <sup>vi</sup> 2.5300	N3···C4 <sup>n</sup>	3.2207 (18)	H11···H13C	2.4100
N6···O4 <sup>ii</sup> 2.9498 (18)H12···H13B <sup>iii</sup> 2.5300C2···N1 <sup>v</sup> $3.3319 (16)$ H12···O3 <sup>i</sup> 2.8700C2···C2 <sup>v</sup> $3.3868 (17)$ H13A···C7 <sup>viii</sup> $3.1000$ C2···C6 <sup>v</sup> $3.5776 (18)$ H13B···H9 $2.4700$ C2···O1 <sup>ii</sup> $3.1894 (18)$ H13B···C12 <sup>vi</sup> $3.0100$ C4···N3 <sup>ii</sup> $3.2207 (18)$ H13B···H12 <sup>vi</sup> $2.5300$	N6…O1 <sup>iv</sup>	2.8201 (15)	H12…O4	2.6800
C2···N1v $3.3319 (16)$ $H12\cdots O3^{i}$ $2.8700$ C2···C2v $3.3868 (17)$ $H13A\cdots C7^{viii}$ $3.1000$ C2···C6v $3.5776 (18)$ $H13B\cdots H9$ $2.4700$ C2···O1ii $3.1894 (18)$ $H13B\cdots C12^{vi}$ $3.0100$ C4···N3ii $3.2207 (18)$ $H13B\cdots H12^{vi}$ $2.5300$	N6…O4 <sup>ii</sup>	2.9498 (18)	H12···H13B <sup>iii</sup>	2.5300
$C2\cdots C2^v$ $3.3868 (17)$ $H13A\cdots C7^{viii}$ $3.1000$ $C2\cdots C6^v$ $3.5776 (18)$ $H13B\cdots H9$ $2.4700$ $C2\cdots O1^{ii}$ $3.1894 (18)$ $H13B\cdots C12^{vi}$ $3.0100$ $C4\cdots N3^{ii}$ $3.2207 (18)$ $H13B\cdots H12^{vi}$ $2.5300$	C2···N1 <sup>v</sup>	3.3319 (16)	H12…O3 <sup>i</sup>	2.8700
C2···C6 $^{v}$ 3.5776 (18)H13B···H92.4700C2···O1 $^{ii}$ 3.1894 (18)H13B···C12 $^{vi}$ 3.0100C4···N3 $^{ii}$ 3.2207 (18)H13B···H12 $^{vi}$ 2.5300	$C2\cdots C2^{v}$	3.3868 (17)	H13A…C7 <sup>viii</sup>	3.1000
C2···O1 <sup>ii</sup> $3.1894 (18)$ H13B···C12 <sup>vi</sup> $3.0100$ C4···N3 <sup>ii</sup> $3.2207 (18)$ H13B···H12 <sup>vi</sup> $2.5300$	C2…C6 <sup>v</sup>	3.5776 (18)	H13B…H9	2.4700
C4···N3 <sup>ii</sup> 3.2207 (18) H13B···H12 <sup>vi</sup> 2 5300	C2…O1 <sup>ii</sup>	3.1894 (18)	H13B····C12 <sup>vi</sup>	3.0100
	C4…N3 <sup>ii</sup>	3.2207 (18)	H13B…H12 <sup>vi</sup>	2.5300
C4···C4 <sup>ii</sup> 3.2446 (18) H13C···H11 2.4100	C4···C4 <sup>ii</sup>	3.2446 (18)	H13C…H11	2.4100
C4…N3 <sup>v</sup> 3.4212 (18) H13C…O4 <sup>vi</sup> 2.9100	C4…N3 <sup>v</sup>	3.4212 (18)	H13C····O4 <sup>vi</sup>	2.9100
C5…N3 <sup>ii</sup> 3.4276 (18)	C5…N3 <sup>ii</sup>	3.4276 (18)		
O2—S1—O3 110.84 (7) C7—C12—C11 119.19 (17)	O2—S1—O3	110.84 (7)	C7—C12—C11	119.19 (17)
O2—S1—O4 111.93 (7) C9—C8—H8 120.00	O2—S1—O4	111.93 (7)	С9—С8—Н8	120.00
O2—S1—C7 105.89 (7) C7—C8—H8 120.00	O2—S1—C7	105.89 (7)	С7—С8—Н8	120.00

O3—S1—O4	113.91 (8)	С10—С9—Н9	119.00
O3—S1—C7	106.83 (7)	С8—С9—Н9	119.00
O4—S1—C7	106.91 (7)	C10-C11-H11	119.00
C2—N1—C6	122.36 (11)	C12—C11—H11	119.00
C2—N3—C4	123.20 (10)	C11—C12—H12	120.00
C6—N1—H1	119.00	C7—C12—H12	120.00
C2—N1—H1	119.00	C10-C13-H13C	109.00
C2—N2—H2B	120.00	H13B—C13—H13C	109.00
H2A—N2—H2B	120.00	C10-C13-H13A	109.00
C2—N2—H2A	120.00	C10-C13-H13B	109.00
C4—N3—H3	118.00	H13A—C13—H13C	109.00
C2—N3—H3	118.00	H13A—C13—H13B	110.00
C6—N6—H6A	120.00	N1—C2—N3	118.20 (11)
H6A—N6—H6B	120.00	N1—C2—N2	120.67 (12)
C6—N6—H6B	120.00	N2—C2—N3	121.13 (11)
S1—C7—C12	119.60 (12)	N3—C4—C5	116.98 (11)
C8—C7—C12	119.99 (15)	O1—C4—C5	125.95 (12)
S1—C7—C8	120.41 (11)	O1—C4—N3	117.07 (11)
C7—C8—C9	119.68 (18)	C4—C5—C6	120.20 (12)
C8—C9—C10	121.11 (19)	N1—C6—N6	116.28 (12)
C11—C10—C13	120.3 (2)	N1—C6—C5	118.97 (11)
C9—C10—C13	121.5 (2)	N6—C6—C5	124.76 (12)
C9—C10—C11	118.19 (18)	C4—C5—H5	120.00
C10-C11-C12	121.79 (19)	С6—С5—Н5	120.00
	. ,		
O2—S1—C7—C8	94.26 (13)	S1—C7—C12—C11	-179.44 (13)
O2—S1—C7—C12	-84.77 (13)	S1—C7—C8—C9	179.93 (13)
O3—S1—C7—C8	-23.93 (14)	C12—C7—C8—C9	-1.0 (2)
O3—S1—C7—C12	157.04 (12)	C8—C7—C12—C11	1.5 (2)
O4—S1—C7—C8	-146.24 (13)	C7—C8—C9—C10	-1.0(3)
O4—S1—C7—C12	34.72 (14)	C8—C9—C10—C13	-176.68 (19)
C6—N1—C2—N2	-177.54 (12)	C8—C9—C10—C11	2.4 (3)
C6—N1—C2—N3	3.24 (18)	C13—C10—C11—C12	177.18 (19)
C2—N1—C6—N6	178.45 (12)	C9-C10-C11-C12	-2.0 (3)
C2—N1—C6—C5	-1.84 (19)	C10-C11-C12-C7	0.0 (3)
C2—N3—C4—O1	-176.29 (13)	O1—C4—C5—C6	177.72 (14)
C2—N3—C4—C5	2.62 (19)	N3—C4—C5—C6	-1.1 (2)
C4—N3—C2—N2	177.12 (12)	C4—C5—C6—N6	-179.57 (14)
C4—N3—C2—N1	-3.67 (18)	C4—C5—C6—N1	0.8 (2)

Symmetry codes: (i) *x*, *y*-1, *z*; (ii) -*x*+1, -*y*+1, -*z*+1; (iii) *x*, -*y*, *z*-1/2; (iv) *x*, *y*+1, *z*; (v) -*x*+1, *y*, -*z*+3/2; (vi) *x*, -*y*, *z*+1/2; (vii) -*x*+1/2, *y*+1/2, -*z*+3/2; (viii) -*x*+1/2, *y*-1/2, -*z*+3/2.

### Hydrogen-bond geometry (Å, °)

D—H···A	D—H	Н…А	D····A	<i>D</i> —H… <i>A</i>
N1—H1···O1 <sup>iv</sup>	0.86	1.86	2.6515 (14)	152
N2—H2A···O3	0.86	1.95	2.7935 (17)	166
N2—H2 $B$ ····O2 <sup>iv</sup>	0.86	2.01	2.8669 (16)	175

N3—H3…O2	0.86	1.92	2.7689 (14)	169
N6—H6A····O4 <sup>ii</sup>	0.86	2.25	2.9498 (18)	139
N6—H6B····O1 <sup>iv</sup>	0.86	2.08	2.8201 (15)	143

Symmetry codes: (ii) -x+1, -y+1, -z+1; (iv) x, y+1, z.