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4,4′-Bipyridine–3-(thiophen-3-yl)acrylic acid (1/2)

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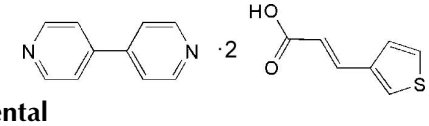
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.132; data-to-parameter ratio = 14.9.

In the title 1/2 adduct, $C_{10}H_8N_2\cdot 2C_7H_6O_2S$, the dihedral angle between the pyridine rings is 18.41 (11)°. In the thiopheneacrylic acid molecules, the dihedral angles between the respective thiophene and acrylic acid units are 5.52 (17)° and 23.92 (9)°. In the crystal, the components are linked *via* O—H···N hydrogen-bonding interactions, forming units of two 3-thiopheneacrylic acid molecules and one 4,4′-bipyridine molecule.

Related literature

For the synthesis and *in vitro* antibacterial activity of oxazolidines, see: Srivastava *et al.* (2008). For crystal engineering cocrystal and polymorph architectures, see: Friščić & MacGillivray (2009); Eccles *et al.* (2010). For the supramolecular construction of molecular ladders, see: Gao *et al.* (2004); MacGillivray *et al.* (2008); Friščić & MacGillivray (2005). For C—H···O hydrogen bonds in supramolecular design, see: Desiraju (1996) and for C—H···π interactions in crystal engineering, see: Desiraju (2002).



Experimental

Crystal data

$C_{10}H_8N_2\cdot 2C_7H_6O_2S$
M_r = 464.54
Triclinic, $P\overline{1}$
a = 7.3454 (5) Å
b = 10.7319 (8) Å
c = 15.0196 (11) Å
α = 102.518 (6)°
β = 103.648 (6)°
γ = 94.892 (6)°
V = 1111.54 (14) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 2.46 mm^{-1}
T = 293 K
0.37 × 0.15 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min} = 0.692, T_{max} = 1.000
9038 measured reflections
4344 independent reflections
3498 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.132
S = 1.05
4344 reflections
291 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N1^{i}	0.82	1.86	2.668 (2)	168
O4—H4A···N2^{ii}	0.82	1.87	2.684 (2)	174

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

Data collection: *CrysAlis PRO* (Oxford Diffraction 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *publCIF* (Westrip, 2010) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2368).

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supporting information

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4,4′-Bipyridine–3-(thiophen-3-yl)acrylic acid (1/2)

Palanisamy Rajakannu, Firasat Hussain and Malaichamy Sathiyendiran

S1. Comment

Supramolecular synthons that are based upon hydrogen bonds represent a prototypal tool for crystal engineering (Desiraju, 1996; 2002). Supramolecular heterosynthons formed from pyridine/amide and carboxylic acids have previously been exploited for liquid crystalline materials, two-dimensional beta networks, two-dimensional corrugated sheets and ternary supramolecules (MacGillivray *et al.*, 2008; Gao *et al.*, 2004; Friščić & MacGillivray, 2005; 2009). Recently, pharmaceutical molecules such as aspirin, *rac*-ibuprofen, and *rac*-flurbiprofen form heterosynthons with ditopic pyridine donors. Herein, we report co-crystal **1** synthesized and characterized by FT—IR, UV-Vis, ^{1}H-NMR spectroscopy, EA, DSC, and TGA.

The co-crystal **1** of the 2:1 adduct of 3-thiopheneacrylic acid with 4,4′-bipyridine was obtained by layering methanolic solution of 4,4′-bipyridyl to the methanolic solution of 3-thiopheneacrylic acid at room temperature. Each 3-thiopheneacrylic acid molecule forms a moderate intermolecular O—H···N bond with pyridine (Table 1). The 4,4′-bipyridine molecule in the adduct is non-planar with the two pyridine rings forming a dihedral angle of 18.41 (11)°. The two thiophene and the bipyridine are not coplanar and the dihedral angles between the S1 thiophene/N1 pyridine and S2 thiophene/ N2 pyridine are 30.14 (11)° and 47.64 (7)°, respectively. The heterosynthon extends to one-dimensional latterane like sheets held together by moderate π-π stacking interactions (Fig. 2). The *Cg*1–*Cg*2^{ii} distance (between the N1,C8-C12 and N2,C13-C17 4,4′-bipyridine moieties) and the dihedral angle between pyridine planes α are 4.1411 (13)Å and 18.4 (1)°, respectively. [Symmetry code ii: (-1+*x*,y,*z*).

S2. Experimental

All starting materials and products were found to be stable towards moisture and air. Starting materials such as 4,4′-bipyridyl (bpy) and 3-thiopheneacrylic acid (taa) were procured from commercial sources and used as received. Commercial grade solvents *e.g.* methanol was used as received further purification. The mixture of 1:2 ratio of 4,4′-bipyridyl (100.1 mg, 0.6409 mmol) and 3-thiopheneacrylic acid (197.8 mg, 1.2828 mmol) in methanol was stirred for 3 h at room temperature. The clear solution was obtained by filtration and that solution was kept at room temperature for several days. The white colored crystals were obtained. Yield: 83% (248.3 mg, 0.5344 mmol). Anal. Calcd for $C_{24}H_{20}N_2O_4S_2$: C, 62.05; H, 4.34; N, 6.03; S, 13.8. Found: C, 60.93; H, 4.13; N, 5.87; S, 12.93. ^{1}H NMR ($CDCl_3$,): 8.72 (dd, J = 4.7 Hz, 4H, H$^{\alpha}$, bpy), 7.71 (d, J = 1.54 Hz, 2H, H^4, taa), 7.53 (dd, J = 4.7 Hz, 4H, H$^{\beta}$, bpy), 7.47 (dd, J = 1.32 Hz, 2H, H^1, taa), 7.29 (m, 4H, H^{2,3}, taa), 6.20 (d, J = 15.44 Hz, 2H, H^5, taa).

S3. Refinement

All H atoms were placed in geometrically calculated positions and refined using a riding model, with C—H = 0.95–1.00 Å and U_{iso}(H) = 1.2Ueq(C).

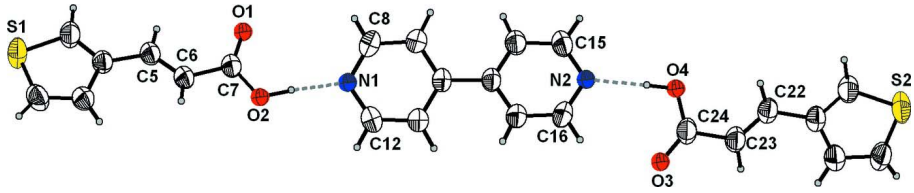

Figure 1

ORTEP view of the molecule with thermal ellipsoids drawn at 50% probability level Color code: White: C; red: O; blue: N; grey: H; yellow:*S*;

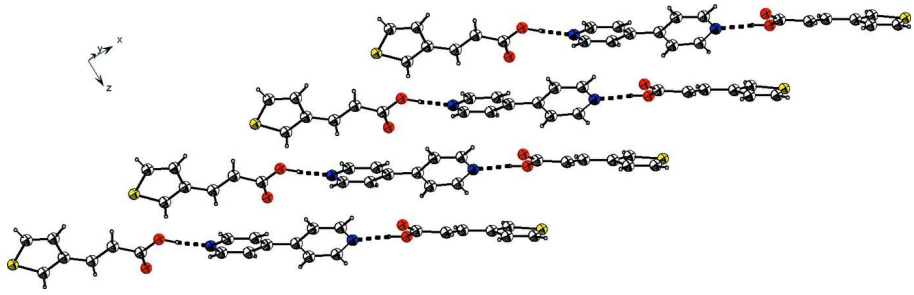

Figure 2

One-dimensional latterane like sheet formed though π-π stacking interactions between the two neighboring heterosynthons.

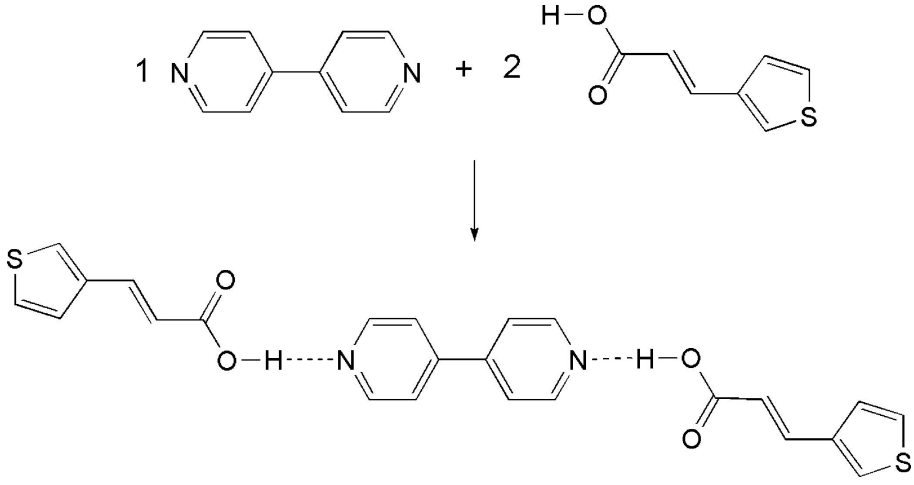

Figure 3

Synthesis of co-crystal of 4,4′-bipyridine and di(3-thiopheneacrylic acid)

4,4′-bipyridine–3-(thiophen-3-yl)acrylic acid (1/2)

Crystal data

$C_{10}H_8N_2{\cdot}2C_7H_6O_2S$
$M_r = 464.54$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.3454\ (5)$ Å
$b = 10.7319\ (8)$ Å
$c = 15.0196\ (11)$ Å
$\alpha = 102.518\ (6)°$
$\beta = 103.648\ (6)°$
$\gamma = 94.892\ (6)°$
$V = 1111.54\ (14)$ Å^3
$Z = 2$
$F(000) = 484$
$D_x = 1.388$ Mg m^{-3}

Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 3251 reflections
θ = 3.1–72.9°
μ = 2.46 mm^{-1}
T = 293 K
Plate, white
0.37 × 0.15 × 0.10 mm

Data collection

Xcalibur, Sapphire3 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 15.9853 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min} = 0.692, T_{max} = 1.000
9038 measured reflections
4344 independent reflections
3498 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 72.1°, θ_{min} = 3.1°
h = −8→9
k = −13→12
l = −18→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.132
S = 1.05
4344 reflections
291 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0658P)^2 + 0.2003P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.0548 (3)	0.0002 (2)	−0.17354 (15)	0.0547 (5)
H1	0.0689	−0.0528	−0.1316	0.066*
C2	0.1988 (3)	0.08388 (19)	−0.17968 (13)	0.0439 (4)
C3	0.1338 (3)	0.1521 (2)	−0.25031 (15)	0.0542 (5)
H3	0.2120	0.2136	−0.2645	0.065*
C4	−0.0525 (3)	0.1183 (2)	−0.29432 (16)	0.0611 (6)
H4	−0.1172	0.1531	−0.3420	0.073*
C5	0.3899 (3)	0.09887 (19)	−0.12014 (13)	0.0447 (4)
H5	0.4097	0.0504	−0.0753	0.054*
C6	0.5392 (3)	0.1746 (2)	−0.12320 (14)	0.0479 (4)
H6	0.5262	0.2230	−0.1681	0.058*
C7	0.7262 (3)	0.18356 (19)	−0.05652 (14)	0.0467 (4)

C8	0.2956 (3)	0.2219 (2)	0.08555 (15)	0.0559 (5)
H8	0.2325	0.1394	0.0762	0.067*
C9	0.4852 (3)	0.2485 (2)	0.13424 (15)	0.0508 (5)
H9	0.5459	0.1850	0.1574	0.061*
C10	0.5840 (3)	0.36980 (18)	0.14838 (13)	0.0429 (4)
C11	0.4821 (3)	0.4604 (2)	0.11311 (16)	0.0571 (5)
H11	0.5412	0.5437	0.1213	0.069*
C12	0.2929 (3)	0.4253 (2)	0.06605 (17)	0.0610 (6)
H12	0.2273	0.4872	0.0432	0.073*
C13	0.7889 (3)	0.40367 (18)	0.19703 (13)	0.0430 (4)
C14	0.8822 (3)	0.3308 (2)	0.25474 (15)	0.0537 (5)
H14	0.8163	0.2593	0.2646	0.064*
C15	1.0737 (3)	0.3656 (2)	0.29725 (16)	0.0575 (5)
H15	1.1340	0.3149	0.3347	0.069*
C16	1.0874 (3)	0.5381 (2)	0.23340 (17)	0.0595 (6)
H16	1.1565	0.6104	0.2263	0.071*
C17	0.8972 (3)	0.5096 (2)	0.18718 (16)	0.0556 (5)
H17	0.8417	0.5614	0.1494	0.067*
C18	1.2549 (3)	0.6734 (2)	0.52895 (16)	0.0584 (5)
H18	1.2472	0.5856	0.5026	0.070*
C19	1.1052 (3)	0.7401 (2)	0.51574 (13)	0.0475 (4)
C20	1.1585 (3)	0.8722 (2)	0.56515 (17)	0.0614 (6)
H20	1.0746	0.9324	0.5652	0.074*
C21	1.3461 (3)	0.9011 (2)	0.61250 (18)	0.0660 (6)
H21	1.4053	0.9830	0.6477	0.079*
C22	0.9150 (3)	0.6807 (2)	0.46025 (13)	0.0490 (5)
H22	0.8956	0.5918	0.4362	0.059*
C23	0.7683 (3)	0.7418 (2)	0.44109 (15)	0.0548 (5)
H23	0.7857	0.8303	0.4668	0.066*
C24	0.5778 (3)	0.6803 (2)	0.38173 (15)	0.0549 (5)
O1	0.7640 (2)	0.11251 (16)	−0.00462 (11)	0.0637 (4)
O2	0.8489 (2)	0.27837 (16)	−0.05983 (12)	0.0645 (4)
H2	0.9510	0.2794	−0.0227	0.097*
O3	0.4670 (2)	0.74129 (19)	0.34314 (14)	0.0809 (6)
O4	0.5423 (2)	0.55602 (16)	0.37539 (13)	0.0650 (4)
H4A	0.4325	0.5289	0.3450	0.098*
S1	−0.15372 (8)	0.00362 (7)	−0.25123 (4)	0.0671 (2)
S2	1.45740 (8)	0.76787 (7)	0.59882 (5)	0.0697 (2)
N1	0.1992 (2)	0.30804 (19)	0.05151 (13)	0.0568 (5)
N2	1.1767 (2)	0.46765 (18)	0.28753 (13)	0.0552 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0390 (10)	0.0657 (13)	0.0557 (12)	0.0000 (9)	0.0023 (8)	0.0207 (10)
C2	0.0382 (10)	0.0472 (10)	0.0429 (9)	0.0050 (8)	0.0058 (7)	0.0098 (8)
C3	0.0474 (11)	0.0583 (12)	0.0553 (12)	0.0055 (9)	0.0045 (9)	0.0213 (10)
C4	0.0512 (12)	0.0715 (14)	0.0548 (12)	0.0142 (11)	−0.0025 (9)	0.0193 (11)

C5	0.0378 (10)	0.0497 (10)	0.0448 (10)	0.0062 (8)	0.0048 (8)	0.0147 (8)
C6	0.0390 (10)	0.0518 (11)	0.0511 (11)	0.0052 (8)	0.0018 (8)	0.0200 (9)
C7	0.0358 (9)	0.0512 (11)	0.0511 (10)	0.0048 (8)	0.0049 (8)	0.0163 (9)
C8	0.0430 (11)	0.0567 (12)	0.0597 (12)	−0.0069 (9)	0.0073 (9)	0.0086 (10)
C9	0.0421 (10)	0.0491 (11)	0.0569 (11)	0.0014 (8)	0.0065 (9)	0.0130 (9)
C10	0.0351 (9)	0.0489 (10)	0.0400 (9)	0.0028 (8)	0.0049 (7)	0.0074 (8)
C11	0.0437 (11)	0.0502 (11)	0.0701 (13)	0.0020 (9)	−0.0004 (10)	0.0178 (10)
C12	0.0426 (11)	0.0653 (14)	0.0701 (14)	0.0101 (10)	0.0000 (10)	0.0208 (11)
C13	0.0338 (9)	0.0472 (10)	0.0422 (9)	0.0030 (7)	0.0039 (7)	0.0065 (8)
C14	0.0396 (10)	0.0610 (12)	0.0590 (12)	0.0026 (9)	0.0047 (9)	0.0224 (10)
C15	0.0415 (11)	0.0663 (14)	0.0609 (13)	0.0078 (10)	0.0005 (9)	0.0220 (11)
C16	0.0406 (11)	0.0591 (13)	0.0695 (14)	−0.0079 (9)	0.0010 (10)	0.0165 (11)
C17	0.0422 (11)	0.0544 (12)	0.0629 (13)	−0.0014 (9)	−0.0013 (9)	0.0186 (10)
C18	0.0406 (11)	0.0641 (13)	0.0612 (13)	0.0030 (9)	0.0058 (9)	0.0059 (10)
C19	0.0372 (10)	0.0588 (12)	0.0421 (9)	0.0004 (8)	0.0040 (7)	0.0121 (9)
C20	0.0439 (12)	0.0593 (13)	0.0700 (14)	0.0058 (10)	−0.0008 (10)	0.0101 (11)
C21	0.0461 (12)	0.0624 (14)	0.0716 (15)	−0.0046 (10)	−0.0014 (10)	0.0021 (11)
C22	0.0390 (10)	0.0576 (12)	0.0453 (10)	−0.0037 (9)	0.0036 (8)	0.0140 (9)
C23	0.0406 (11)	0.0612 (13)	0.0559 (12)	−0.0025 (9)	0.0000 (9)	0.0182 (10)
C24	0.0371 (10)	0.0682 (14)	0.0571 (12)	−0.0024 (9)	0.0027 (9)	0.0248 (10)
O1	0.0460 (8)	0.0779 (11)	0.0686 (10)	0.0059 (7)	−0.0012 (7)	0.0399 (9)
O2	0.0389 (8)	0.0669 (10)	0.0806 (11)	−0.0046 (7)	−0.0068 (7)	0.0324 (8)
O3	0.0477 (9)	0.0871 (12)	0.0997 (13)	−0.0059 (9)	−0.0160 (9)	0.0502 (11)
O4	0.0359 (8)	0.0668 (10)	0.0792 (11)	−0.0008 (7)	−0.0064 (7)	0.0169 (8)
S1	0.0359 (3)	0.0853 (4)	0.0685 (4)	−0.0024 (3)	−0.0014 (2)	0.0156 (3)
S2	0.0343 (3)	0.0880 (5)	0.0729 (4)	0.0059 (3)	−0.0003 (2)	0.0073 (3)
N1	0.0350 (9)	0.0705 (12)	0.0563 (10)	−0.0002 (8)	0.0024 (7)	0.0110 (9)
N2	0.0359 (9)	0.0640 (11)	0.0558 (10)	0.0012 (8)	0.0006 (7)	0.0089 (8)

Geometric parameters (Å, º)

C1—C2	1.361 (3)	C13—C14	1.392 (3)
C1—S1	1.701 (2)	C14—C15	1.382 (3)
C1—H1	0.9300	C14—H14	0.9300
C2—C3	1.430 (3)	C15—N2	1.332 (3)
C2—C5	1.451 (3)	C15—H15	0.9300
C3—C4	1.351 (3)	C16—N2	1.328 (3)
C3—H3	0.9300	C16—C17	1.380 (3)
C4—S1	1.703 (3)	C16—H16	0.9300
C4—H4	0.9300	C17—H17	0.9300
C5—C6	1.324 (3)	C18—C19	1.362 (3)
C5—H5	0.9300	C18—S2	1.699 (2)
C6—C7	1.478 (3)	C18—H18	0.9300
C6—H6	0.9300	C19—C20	1.423 (3)
C7—O1	1.207 (2)	C19—C22	1.456 (3)
C7—O2	1.318 (2)	C20—C21	1.367 (3)
C8—N1	1.328 (3)	C20—H20	0.9300
C8—C9	1.385 (3)	C21—S2	1.705 (3)

C8—H8	0.9300	C21—H21	0.9300
C9—C10	1.383 (3)	C22—C23	1.315 (3)
C9—H9	0.9300	C22—H22	0.9300
C10—C11	1.395 (3)	C23—C24	1.479 (3)
C10—C13	1.485 (2)	C23—H23	0.9300
C11—C12	1.380 (3)	C24—O3	1.208 (3)
C11—H11	0.9300	C24—O4	1.315 (3)
C12—N1	1.330 (3)	O2—H2	0.8200
C12—H12	0.9300	O4—H4A	0.8200
C13—C17	1.386 (3)		

C2—C1—S1	112.31 (16)	C15—C14—C13	119.4 (2)
C2—C1—H1	123.8	C15—C14—H14	120.3
S1—C1—H1	123.8	C13—C14—H14	120.3
C1—C2—C3	110.97 (18)	N2—C15—C14	123.6 (2)
C1—C2—C5	122.51 (18)	N2—C15—H15	118.2
C3—C2—C5	126.52 (18)	C14—C15—H15	118.2
C4—C3—C2	113.3 (2)	N2—C16—C17	123.3 (2)
C4—C3—H3	123.4	N2—C16—H16	118.3
C2—C3—H3	123.4	C17—C16—H16	118.3
C3—C4—S1	111.33 (17)	C16—C17—C13	120.1 (2)
C3—C4—H4	124.3	C16—C17—H17	120.0
S1—C4—H4	124.3	C13—C17—H17	120.0
C6—C5—C2	126.60 (18)	C19—C18—S2	112.62 (18)
C6—C5—H5	116.7	C19—C18—H18	123.7
C2—C5—H5	116.7	S2—C18—H18	123.7
C5—C6—C7	121.21 (18)	C18—C19—C20	111.27 (19)
C5—C6—H6	119.4	C18—C19—C22	123.4 (2)
C7—C6—H6	119.4	C20—C19—C22	125.35 (19)
O1—C7—O2	123.23 (18)	C21—C20—C19	112.8 (2)
O1—C7—C6	124.35 (18)	C21—C20—H20	123.6
O2—C7—C6	112.42 (17)	C19—C20—H20	123.6
N1—C8—C9	123.5 (2)	C20—C21—S2	111.29 (18)
N1—C8—H8	118.3	C20—C21—H21	124.4
C9—C8—H8	118.3	S2—C21—H21	124.4
C10—C9—C8	119.7 (2)	C23—C22—C19	125.7 (2)
C10—C9—H9	120.1	C23—C22—H22	117.1
C8—C9—H9	120.1	C19—C22—H22	117.1
C9—C10—C11	116.67 (18)	C22—C23—C24	124.9 (2)
C9—C10—C13	122.63 (18)	C22—C23—H23	117.6
C11—C10—C13	120.69 (18)	C24—C23—H23	117.6
C12—C11—C10	119.5 (2)	O3—C24—O4	124.2 (2)
C12—C11—H11	120.3	O3—C24—C23	121.6 (2)
C10—C11—H11	120.2	O4—C24—C23	114.25 (18)
N1—C12—C11	123.6 (2)	C7—O2—H2	109.5
N1—C12—H12	118.2	C24—O4—H4A	109.5
C11—C12—H12	118.2	C1—S1—C4	92.12 (11)
C17—C13—C14	116.54 (18)	C18—S2—C21	91.96 (11)

C17—C13—C10	121.64 (18)	C8—N1—C12	117.01 (18)
C14—C13—C10	121.82 (18)	C16—N2—C15	117.01 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···N1^{i}	0.82	1.86	2.668 (2)	168
O4—H4*A*···N2^{ii}	0.82	1.87	2.684 (2)	174

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