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Proton-transfer compounds with 4-amino-*N*-(4,6-dimethylpyrimidin-2-yl)benzenesulfonamide (sulfamethazine): the structures and hydrogen bonding in the salts with 5-nitrosalicylic acid and picric acid

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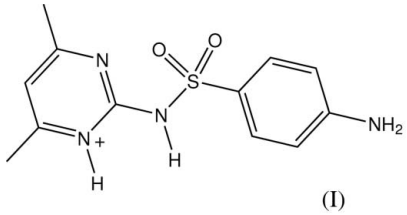
The structures of the anhydrous proton-transfer compounds of the sulfa drug sulfamethazine with 5-nitrosalicylic acid and picric acid, namely 2-(4-aminobenzenesulfonamido)-4,6-dimethylpyrimidinium 2-hydroxy-5-nitrobenzoate, $C_{12}H_{15}N_4O_2S^+\cdot C_7H_4NO_4^-$, (I), and 2-(4-aminobenzenesulfonamido)-4,6-dimethylpyrimidinium 2,4,6-trinitrophenolate, $C_{12}H_{15}N_4O_2S^+\cdot C_6H_2N_3O_7^-$, (II), respectively, have been determined. In the asymmetric unit of (I), there are two independent but conformationally similar cation–anion heterodimer pairs which are formed through duplex intermolecular $N^+—H\cdots O_{carboxylate}$ and $N—H\cdots O_{carboxylate}$ hydrogen-bond pairs, giving a cyclic motif [graph set $R_2^2(8)$]. These heterodimers form separate and different non-associated substructures through aniline $N—H\cdots O$ hydrogen bonds, one one-dimensional, involving carboxylate O-atom acceptors, the other two-dimensional, involving both carboxylate and hydroxy O-atom acceptors. The overall two-dimensional structure is stabilized by π–π interactions between the pyrimidinium ring and the 5-nitrosalicylate ring in both heterodimers [minimum ring-centroid separation = 3.4580 (8) Å]. For picrate (II), the cation–anion interaction involves a slightly asymmetric chelating $N—H\cdots O$ $R_2^1(6)$ hydrogen-bonding association with the phenolate O atom, together with peripheral conjoint $R_1^2(6)$ interactions between the same N—H groups and O atoms of the *ortho*-related nitro groups. An inter-unit amine $N—H\cdots O_{sulfone}$ hydrogen bond gives one-dimensional chains which extend along *a* and inter-associate through π–π interactions between the pyrimidinium rings [centroid–centroid separation = 3.4752 (9) Å]. The two structures reported here now bring to a total of four the crystallographically characterized examples of proton-transfer salts of sulfamethazine with strong organic acids.

Comment

The drug sulfamethazine [or sulfadimidine; systematic name: 4-amino-*N*-(4,6-dimethylpyrimidin-2-yl)benzenesulfonamide] (O'Neil, 2001) has been used as a model for cocrystal formation (Caira, 2007; Ghosh *et al.*, 2011), commonly forming 1:1 adducts with carboxylic acids, predominantly the benzoic acid analogues. The structures of a significant number of these have been reported, *e.g.* with benzoic acid (Arman *et al.*, 2010), salicylic acid (Patel *et al.*, 1988), anthranilic and 4-aminobenzoic acids (Caira, 1991), 4-aminosalicylic and acetylsalicylic acids (Caira, 1992), 2-nitrobenzoic acid (Smith & Wermuth, 2013*a*), 4-nitrobenzoic acid (Smith & Wermuth, 2012), 2,4-dinitrobenzoic and indole-2-carboxylic acids (Lynch *et al.*, 2000), 4-chlorobenzoic acid (Lucaciu *et al.*, 2008), and 4-hydroxybenzoic, 2,4-dihydroxybenzoic, 3,4-dichlorobenzoic, 1-hydroxy-2-naphthoic and 3-hydroxy-2-naphthoic acids (Ghosh *et al.*, 2011). Only two aliphatic examples are known, *viz.* with fumaric and sorbic acids. The structures of the cocrystals with the amides benzamide, 4-hydroxybenzamide and picolinamide (Ghosh *et al.*, 2011) are also known. The structures of the adducts with trimethoprim, *viz.* a 1:1 methanol monosolvate (Bettinetti & Sardone, 1997) and a 2:1 monohydrate (Sardone *et al.*, 1997), represent a small number of solvated examples.



In the previously mentioned cocrystals of sulfamethazine, heterodimers are usually formed through a cyclic hydrogen-bonding motif [graph set $R_2^2(8)$; Etter *et al.*, 1990], involving amide $N—H\cdots O_{carboxy}$ and carboxylic acid $O—H\cdots N_{pyrimidine}$ pairs. Other structures not involving carboxylic acids are the 1:1 complex with saccharin (Lu *et al.*, 2008), where a protonated sulfamethazine cation is present, and the 2:1 complex with theophylline (Lu *et al.*, 2011), in which two tautomeric forms of sulfamethazine are found, *viz.* the amidine and the imidine forms, similar to those found in the benzamide cocrystal (Ghosh *et al.*, 2011). The structures of the parent compound sulfamethazine (Tiwari *et al.*, 1984) and its methanol monosolvate (Rambaud *et al.*, 1985) are also known.

However, no examples of proton-transfer salts of sulfamethazine with strong 'conventional' organic acids were present in the crystallographic literature before that of the

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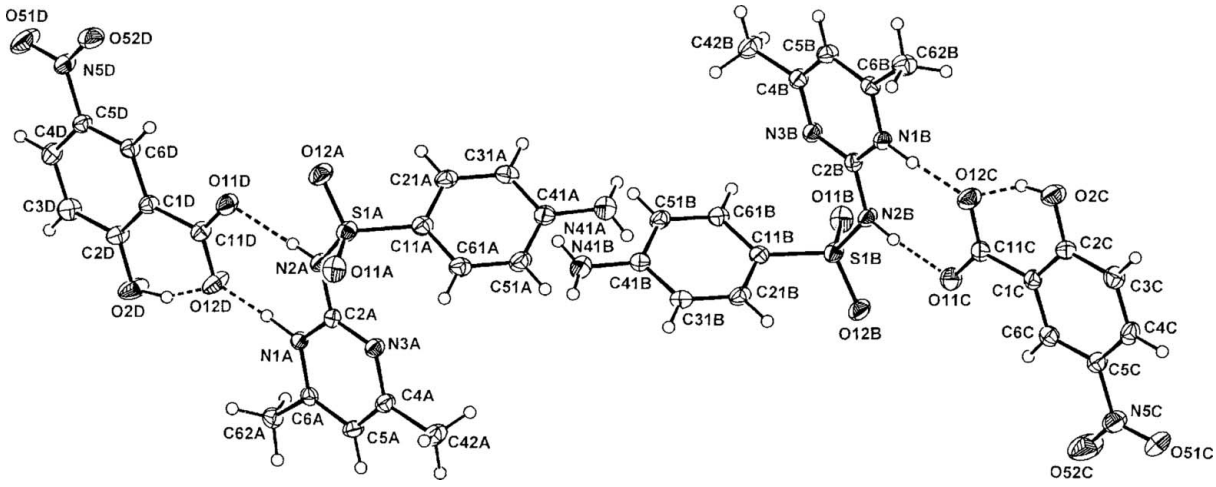


Figure 1
The molecular conformation and atom-numbering scheme for the two independent hydrogen-bonded heteromolecular pairs (*A*–*D* and *B*–*C*) in the asymmetric unit of (I), with inter-species hydrogen bonds shown as dashed lines. Displacement ellipsoids are drawn at the 40% probability level.

structure of the anhydrous picrate salt with 3,5-dinitrosalicylic acid (DNSA) (Smith & Wermuth, 2013*b*). In this salt, a hydrogen-bonded heterodimer analogous to those in the non-proton-transfer cocrystals is present, the subtle variation being that, with proton transfer, one $N^+—H\cdots O_{carboxy}$ and one $N—H\cdots O_{carboxy}$ interaction are involved in the $R_2^2(8)$ motif. The phenolate group is only involved in the intramolecular cyclic carboxylic acid $O—H\cdots O$ hydrogen bond, similar to that found in the majority of the proton-transfer salts of DNSA (Smith *et al.*, 2007). We therefore carried out the reaction of sulfamethazine with other strong organic acids under similar conditions to those used in the DNSA preparation (1:1 stoichiomety in 50% ethanol–water). Suitable crystalline products were obtained with 5-nitrosalicylic acid (5-NSA) and picric acid, namely the title salts 2-(4-aminobenzenesulfonamido)-4,6-dimethylpyrimidinium 2-hydroxy-5-nitrobenzoate, (I) (Fig. 1), and 2-(4-aminobenzenesulfonamido)-4,6-dimethylpyrimidinium 2,4,6-trinitrophenolate, (II) (Fig. 2), and the structures are reported herein. Although not as effective as picric acid for producing crystalline proton-transfer salts with amines, 5-NSA ($pK_a \simeq 2.2$) has proved relatively useful in this respect, particularly with the aromatic amines (Smith *et al.*, 1996, 2005, 2006; Kumar *et al.*, 2003).

In the 5-NSA salt of sulfamethazine, (I), the asymmetric unit (Fig. 1) contains two independent cation–anion pairs (cations labelled *A* and *B*, and anions labelled *C* and *D*, respectively), which interact through $N—H\cdots O_{carboxylate}$ hydrogen-bonding pairs (Table 1), giving cyclic $R_2^2(8)$ heterodimers (*A*–*D* and *B*–*C*). These differ from the heterodimer adduct only in the presence in (I) of the transferred H atom on the pyrimidine N atom of the sulfamethazine cation. Asymmetry is found in the $N^+—H\cdots O$ [$N^+\cdots O$ = 2.5847 (17) (*A*) and 2.6162 (18) Å (*B*)] and $N—H\cdots O$ distances [$N\cdots O$ = 2.7810 (18) (*A*) and 2.7221 (18) Å (*B*)] within the cyclic association. This asymmetry is comparable with that found in the cocrystal examples [$O—H\cdots N$ and $N—H\cdots O$ ranges for eight examples (Lynch *et al.*, 2000) are $O\cdots N$ = 2.526 (4)–2.724 (4) Å and $N\cdots O$ = 2.719 (4)–2.840 (4) Å]. The corresponding values in the DNSA proton-transfer salt (Smith & Wermuth, 2013*b*) are 2.617 (4) and 2.729 (4) Å.

In (I), the cyclic motifs result in near-coplanarity of the pyrimidinium and 5-NSA ring systems, with inter-ring dihedral angles of 3.74 (7) and 7.84 (7)° for dimers *A*–*D* and *B*–*C*, respectively. The heterodimers form separate and different non-associated substructures through aniline $N—H\cdots O$ hydrogen bonds (Table 1), the first system being one-dimensional (*A*–*D*), involving carboxylate O-atom acceptors (O11*D*) and extending parallel to [010] (Fig. 3*a*). The second system (*B*–*C*) is two-dimensional, involving both carboxylate and hydroxy O-atom acceptors (O12*B* and O2*C*, respectively), and extends parallel to the (011) plane (Fig. 3*b*). The composite structure of (I) is two-dimensional (Fig. 3*c*), lying in the $(10\bar{1})$ plane. Unlike the structure of the sulfamethazine salt with 3,5-dinitrosalicylic acid, no intermolecular aniline $N—H\cdots O_{sulfone}$ hydrogen-bonding interactions are present. However, π–π interactions are present between the pyrimi-

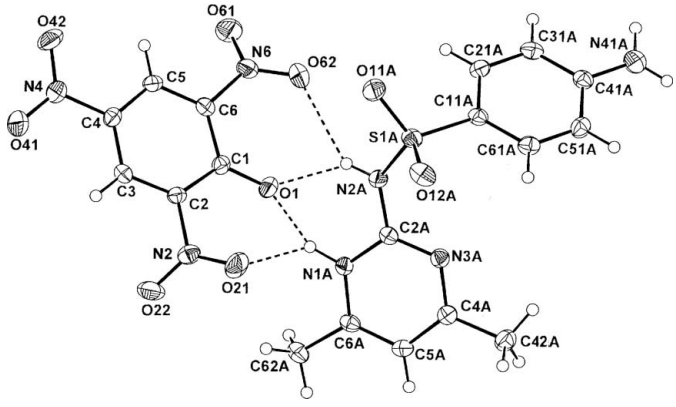
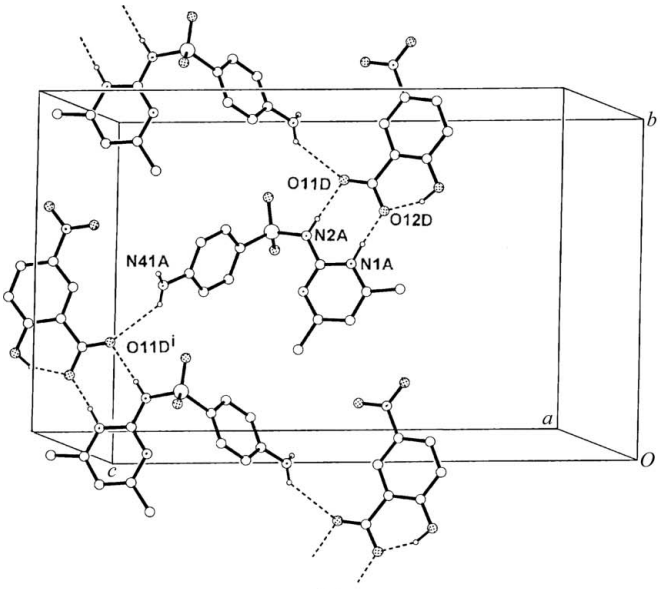
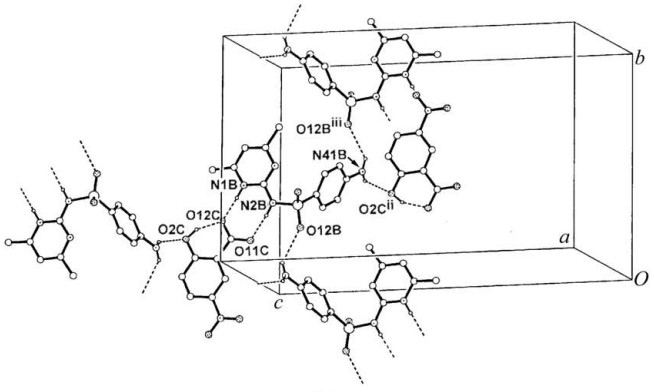


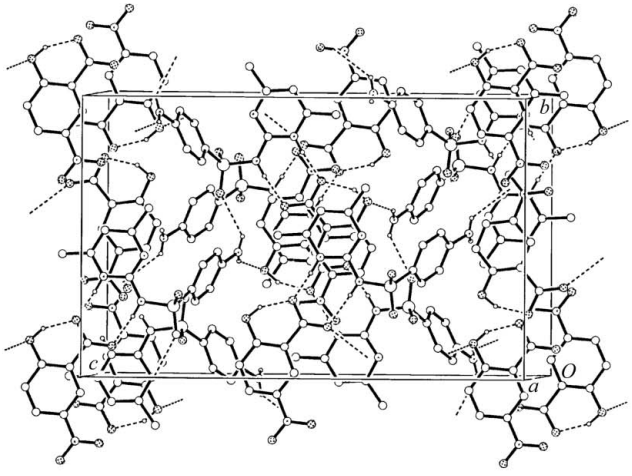
Figure 2
The molecular conformation and atom-numbering scheme for (II), with inter-species hydrogen bonds shown as dashed lines. Displacement ellipsoids are drawn at the 40% probability level.



(*a*)



(*b*)



(*c*)

Figure 3
(*a*) The one-dimensional hydrogen-bonded chain structure formed by the *A*–*D* heterodimer units in (I), extending down *b*. Hydrogen-bonding associations are shown as dashed lines and non-associative H atoms have been omitted. (*b*) The two-dimensional hydrogen-bonded structure formed by the *B*–*C* heterodimer units in (I). (*c*) The composite two-dimensional hydrogen-bonded structure of (I), viewed down *a*. Symmetry codes are as in Table 1.

dine rings of both cations and both anions [$A\cdots C(x-\frac{1}{2},-y+\frac{1}{2},z-\frac{1}{2})$ and $B\cdots D(x+\frac{1}{2},-y+\frac{3}{2},z+\frac{1}{2})$; ring-centroid separations ($Cg\cdots Cg$) = 3.4580 (8) and 3.6815 (9) Å, respectively].

For picrate salt (II) (Fig. 2), the pyrimidine ring of the sulfamethazine molecule (*A*) is protonated at N1*A* and this group, together with the adjacent amide N2*A*—H group, gives a slighly asymmetric chelating hydrogen-bonding association with the picrate anion through a cyclic $R_2^1(6)$ motif. Conjoint lateral $R_1^2(6)$ cyclic associations are also formed between the N1*A*—H donor group and the O-atom acceptors of adjacent *ortho*-related picrate nitro groups (Table 2). A single intermolecular amine N41*A*—H$\cdots$O$_{\rm sulfone}$ hydrogen-bonding interaction between the cation–anion units gives one-dimensional chains which extend along the [100] direction (Fig. 4). Also present in the structure are π–π interactions between the pyrimidine rings of centosymmetrically related sulfamethazine cations [$Cg\cdots Cg^{\rm ii}$ = 3.4752 (9) Å; symmetry code: (ii) $-x+2,-y+1,-z+1$] (Fig. 5). As found in the two structures reported here and in many of the sulfamethazine adduct structures, the 4-amino substituent is often only weakly or partially involved in hydrogen-bonding associations in the crystal structures. The planes of the nitro groups of the picrate anion are variously rotated out of the plane of the benzene ring [torsion angles C1—C2—N2—O22, C3—C4—N4—O42 and C5—C6—N6—O62 of −137.67 (15), 170.19 (15) and 146.91 (16)°, respectively].

In the sulfamethazine cations, the conformation differs significantly between carboxylate (I) and picrate (II). For (I), the dihedral angles between the planes of the pyrimidinium and benzene rings of the sulfamethazine cations are 70.60 (7) (*A*) and 84.78 (7)° (*B*), compared with 78.77 (8) and 82.33 (9)° for those in the two independent heterodimers in the 4-nitrobenzoic acid adduct (Smith & Wermuth, 2012). The value for the equivalent pyrimidinium–benzene dihedral angle in the cation of (II) [58.18 (7)°] is similar to that in the picrate salt with DNSA [59.70 (17)°], but is significantly smaller than commonly found in the other adduct structures and in (I), and probably in the case of (II) is attributable to the markedly different hydrogen-bonding pattern present in that structure. In (I), the two interacting pyrimidine–5-NSA dimers are essentially planar, with inter-ring dihedral angles of 3.74 (7) and 7.84 (7)°, compared with a value of 12.2 (2)° in the structure of the DNSA salt (Smith & Wermuth, 2013*b*).

The two structures presented here now give a small total of four crystallographically characterized examples of proton-transfer salts of sulfamethazine with strong organic acids.

Experimental

The title salts, (I) and (II), were prepared by the reaction of 4-amino-*N*-(4,6-dimethylpyrimidin-2-yl)benzenesulfonamide (sulfamethazine; 1 mmol, 280 mg) with, respectively, 5-nitrosalicylic acid (1 mmol, 180 mg) or picric acid (1 mmol, 230 mg) in 50% ethanol–water (50 ml) under reflux for 10 min. Partial evaporation of the solvent gave colourless plates of (I) (m.p. 478–479 K) or yellow blocks of (II) (m.p. 469–471 K), from which specimens were cleaved for the X-ray analyses.

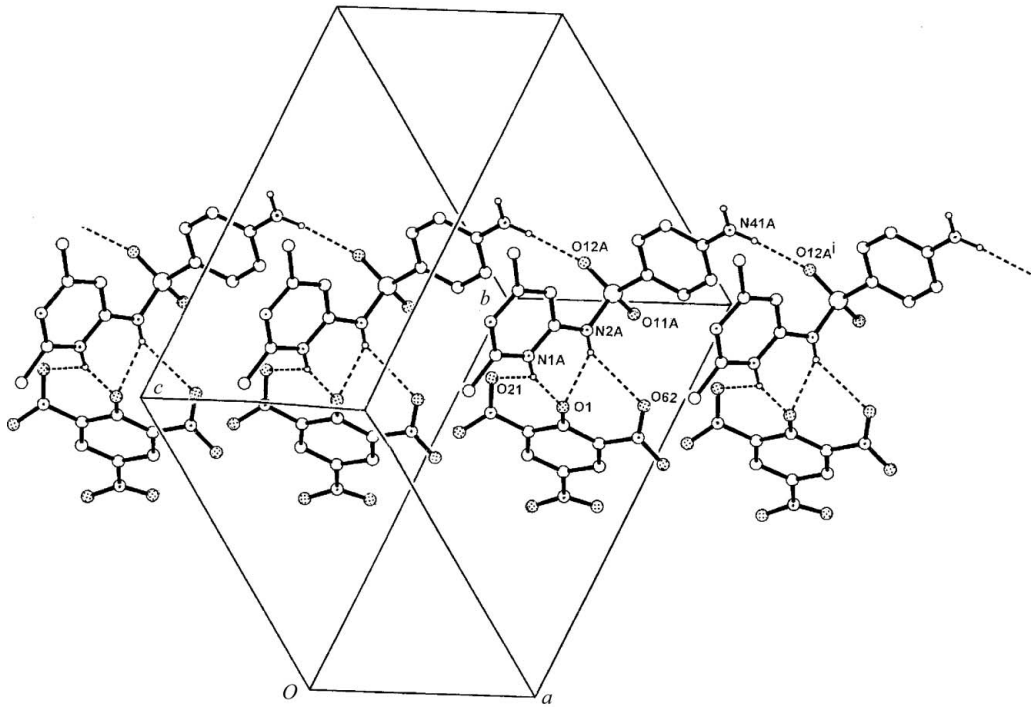


Figure 4
A perspective view of the two-dimensional chain structure of (II), which extends along *a*, showing the hydrogen-bonding associations as dashed lines. [Symmetry code: (i) $x + 1, y, z$.]

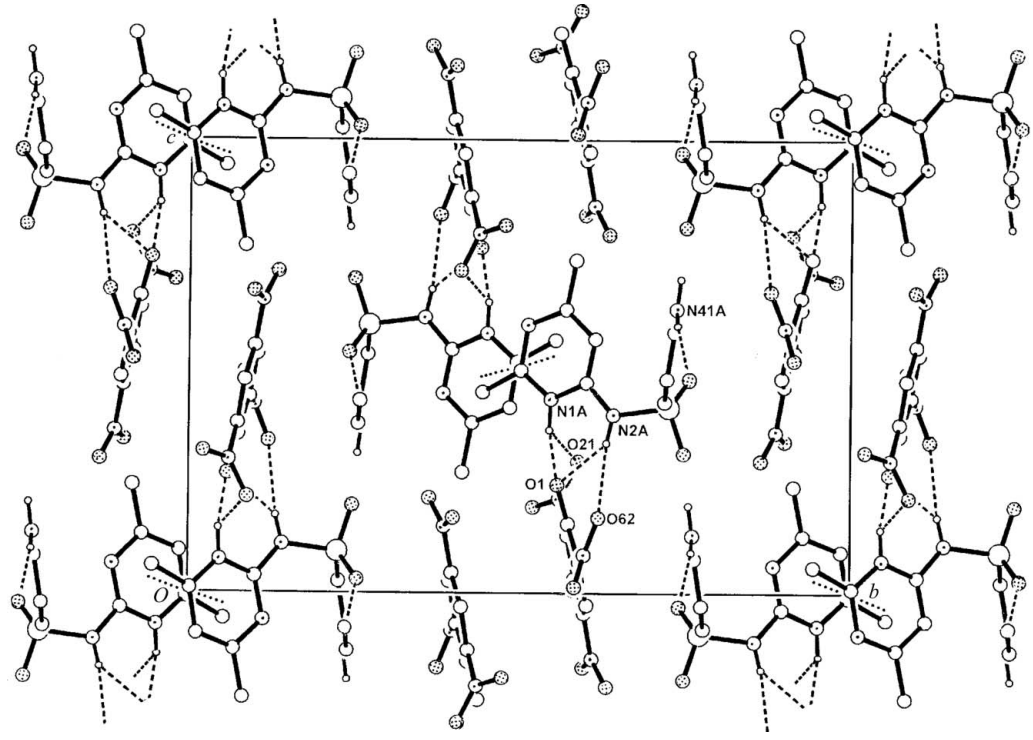


Figure 5
A view of (II) down the *a* axis of the unit cell, showing the π–π interactions of the centrosymmetrically related pyrimidinium rings of the sulfamethazine cations as dotted lines. Hydrogen bonds are shown as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1A—H1A···O12D	0.939 (18)	1.647 (18)	2.5847 (17)	176 (2)
N1B—H1B···O12C	0.91 (2)	1.71 (2)	2.6162 (18)	176.4 (18)
N2A—H2A···O11D	0.85 (2)	1.94 (2)	2.7810 (18)	177 (2)
N2B—H2B···O11C	0.889 (19)	1.836 (19)	2.7221 (18)	174.3 (18)
N41A—H41A···O11D^{i}	0.82 (3)	2.57 (2)	3.217 (2)	138 (2)
N41B—H41B···O2C^{ii}	0.89 (2)	2.49 (2)	3.269 (2)	147 (2)
N41B—H42B···O12B^{iii}	0.83 (2)	2.45 (2)	3.106 (2)	136.6 (18)
O2C—H2C···O12C	0.89 (3)	1.70 (3)	2.5223 (17)	152 (2)
O2D—H2D···O12D	0.90 (2)	1.70 (2)	2.5215 (17)	151 (2)

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

Compound (I)

Crystal data

$C_{12}H_{15}N_4O_2S^+\cdot C_7H_4NO_5^-$
M_r = 461.46
Monoclinic, $P2_1/n$
a = 13.1611 (2) Å
b = 14.0977 (2) Å
c = 22.1219 (3) Å
β = 90.094 (2)°
V = 4104.52 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 200 K
0.35 × 0.35 × 0.15 mm

Data collection

Oxford Gemini-S Ultra CCD area-detector diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.960, T_{max} = 0.980
30179 measured reflections
8057 independent reflections
5991 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.090
S = 0.95
8057 reflections
621 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Compound (II)

Crystal data

$C_{12}H_{15}N_4O_2S^+\cdot C_6H_2N_3O_7^-$
M_r = 507.45
Monoclinic, $P2_1/c$
a = 8.3131 (2) Å
b = 19.2779 (5) Å
c = 13.4483 (4) Å
β = 99.158 (3)°
V = 2127.74 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 200 K
0.35 × 0.35 × 0.26 mm

Data collection

Oxford Gemini-S CCD area-detector diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.970, T_{max} = 0.981
14211 measured reflections
4171 independent reflections
3318 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.091
S = 1.04
4171 reflections
334 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 2
Hydrogen-bond geometry (Å, °) for (II).

D—H···A	D—H	H···A	D···A	D—H···A
N1A—H1A···O1	0.91 (2)	1.70 (2)	2.5545 (19)	154 (2)
N1A—H1A···O21	0.91 (2)	2.46 (2)	2.974 (2)	116.2 (18)
N2A—H2A···O1	0.85 (2)	2.07 (2)	2.7661 (19)	139.2 (17)
N2A—H2A···O62	0.85 (2)	2.59 (2)	3.319 (2)	145.0 (15)
N41A—H41A···O12A^{i}	0.90 (2)	2.16 (2)	3.035 (2)	163 (2)

Symmetry code: (i) $x+1, y, z$.

H atoms potentially involved in hydrogen-bonding interactions were located by difference methods, and their positional and isotropic displacement parameters were refined. In (I), the N1A—H1A distance was restrained to 0.88 (2) Å. All other H atoms were included at calculated positions (aromatic C—H = 0.95 Å or methyl C—H = 0.98 Å) and treated as riding, with U_{iso}(H) = 1.2U_{eq}(C) for aromatic or 1.5U_{eq}(C) for methyl H atoms. For (I), in the absence of any indication of twinning ['no twin law detected', TwinRotMat (*PLATON*, Spek, 2009)], the pseudo-orthorhombic $P2_1/n$ unit cell was accepted. For (II), the H atoms of one of the methyl groups (C42A) were rotationally disordered over six half-occupancy sites and were treated accordingly in the refinement.

For both compounds, data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008) within *WinGX* (Farrugia, 2012); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON* (Spek, 2009).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: KY3031). Services for accessing these data are described at the back of the journal.

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supplementary materials

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Proton-transfer compounds with 4-amino-*N*-(4,6-dimethylpyrimidin-2-yl)benzenesulfonamide (sulfamethazine): the structures and hydrogen bonding in the salts with 5-nitrosalicylic acid and picric acid

Graham Smith and Urs D. Wermuth

(I) 2-(4-Aminobenzenesulfonamido)-4,6-dimethylpyrimidinium 2-hydroxy-5-nitrobenzoate

Crystal data

$C_{12}H_{15}N_4O_2S^+\cdot C_7H_4NO_5^-$
M_r = 461.46
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 13.1611 (2) Å
b = 14.0977 (2) Å
c = 22.1219 (3) Å
β = 90.094 (2)°
V = 4104.52 (10) Å^3
Z = 8
$F(000)$ = 1920
D_x = 1.493 Mg m^{-3}
Melting point = 478–479 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 13808 reflections
θ = 3.2–28.7°
μ = 0.21 mm^{-1}
T = 200 K
Plate, colourless
0.35 × 0.35 × 0.15 mm

Data collection

Oxford Gemini-S Ultra CCD area-detector diffractometer
Radiation source: Enhance (Mo) X-ray source
Graphite monochromator
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.960, T_{max} = 0.980
30179 measured reflections
8057 independent reflections
5991 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 26.0°, θ_{min} = 3.3°
h = −16→16
k = −17→17
l = −27→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.090
S = 0.95
8057 reflections
621 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are 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 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}
S1A	0.07153 (3)	0.67064 (3)	0.69347 (2)	0.0288 (1)
O11A	−0.02458 (8)	0.62533 (8)	0.70202 (5)	0.0372 (4)
O12A	0.08020 (9)	0.77122 (8)	0.70003 (5)	0.0387 (4)
N1A	0.12334 (9)	0.56980 (9)	0.53296 (6)	0.0223 (4)
N2A	0.10773 (10)	0.65526 (10)	0.62149 (6)	0.0268 (4)
N3A	0.10208 (9)	0.49098 (9)	0.62605 (6)	0.0261 (4)
N41A	0.37418 (14)	0.48612 (14)	0.85115 (8)	0.0476 (7)
C2A	0.11060 (11)	0.56942 (10)	0.59352 (7)	0.0219 (4)
C4A	0.10701 (11)	0.40782 (10)	0.59619 (7)	0.0269 (5)
C5A	0.11914 (11)	0.40380 (11)	0.53373 (7)	0.0265 (5)
C6A	0.12785 (10)	0.48715 (10)	0.50191 (7)	0.0231 (4)
C11A	0.16171 (12)	0.61476 (11)	0.73886 (7)	0.0273 (5)
C21A	0.25203 (13)	0.66125 (11)	0.75263 (7)	0.0301 (5)
C31A	0.32363 (13)	0.61707 (12)	0.78855 (7)	0.0320 (5)
C41A	0.30519 (13)	0.52674 (11)	0.81264 (7)	0.0315 (5)
C42A	0.09958 (15)	0.32077 (12)	0.63395 (8)	0.0409 (6)
C51A	0.21385 (13)	0.48115 (11)	0.79852 (7)	0.0331 (6)
C61A	0.14306 (12)	0.52406 (11)	0.76199 (7)	0.0295 (5)
C62A	0.14456 (12)	0.49267 (11)	0.43539 (7)	0.0293 (5)
S1B	0.92340 (3)	0.25241 (3)	0.79543 (2)	0.0281 (1)
O11B	1.01786 (8)	0.29519 (8)	0.77910 (5)	0.0375 (4)
O12B	0.91201 (9)	0.15187 (8)	0.78933 (5)	0.0381 (4)
N1B	0.87859 (9)	0.35527 (10)	0.95621 (6)	0.0241 (4)
N2B	0.90467 (10)	0.26742 (10)	0.86958 (6)	0.0283 (4)
N3B	0.91195 (10)	0.43170 (9)	0.86353 (6)	0.0266 (4)
N41B	0.58517 (14)	0.44107 (13)	0.66992 (9)	0.0504 (7)
C2B	0.89904 (11)	0.35379 (10)	0.89624 (7)	0.0233 (5)
C4B	0.90126 (11)	0.51537 (11)	0.89198 (7)	0.0270 (5)
C5B	0.88147 (12)	0.52088 (11)	0.95369 (7)	0.0286 (5)
C6B	0.86996 (11)	0.43832 (11)	0.98618 (7)	0.0251 (5)
C11B	0.82365 (11)	0.31070 (11)	0.75987 (7)	0.0245 (5)
C21B	0.72877 (12)	0.26729 (11)	0.75756 (7)	0.0283 (5)
C31B	0.65008 (12)	0.31123 (11)	0.72858 (7)	0.0299 (5)
C41B	0.66316 (12)	0.39982 (11)	0.70119 (7)	0.0299 (5)
C42B	0.91208 (14)	0.60161 (11)	0.85326 (8)	0.0369 (6)
C51B	0.75855 (12)	0.44401 (11)	0.70520 (7)	0.0299 (5)
C61B	0.83785 (12)	0.39970 (11)	0.73375 (7)	0.0272 (5)
C62B	0.84715 (13)	0.43421 (12)	1.05216 (8)	0.0346 (6)

O2C	0.86063 (10)	0.12638 (9)	1.12344 (6)	0.0409 (4)
O11C	0.87460 (9)	0.10804 (8)	0.93667 (5)	0.0349 (4)
O12C	0.86850 (10)	0.19851 (8)	1.01921 (5)	0.0407 (4)
O51C	0.88240 (11)	−0.29921 (9)	1.05247 (7)	0.0568 (5)
O52C	0.88819 (14)	−0.23713 (10)	0.96357 (7)	0.0721 (7)
N5C	0.88198 (11)	−0.23014 (10)	1.01871 (8)	0.0408 (6)
C1C	0.87128 (11)	0.03235 (11)	1.03253 (7)	0.0249 (5)
C2C	0.86472 (11)	0.04133 (11)	1.09589 (7)	0.0273 (5)
C3C	0.86229 (12)	−0.03944 (12)	1.13268 (8)	0.0330 (5)
C4C	0.86768 (12)	−0.12790 (12)	1.10761 (8)	0.0321 (5)
C5C	0.87478 (11)	−0.13593 (11)	1.04502 (8)	0.0285 (5)
C6C	0.87714 (11)	−0.05767 (11)	1.00755 (7)	0.0271 (5)
C11C	0.87166 (11)	0.11811 (11)	0.99236 (7)	0.0274 (5)
O2D	0.14667 (11)	0.79122 (9)	0.36510 (6)	0.0483 (5)
O11D	0.11640 (9)	0.81801 (8)	0.55065 (5)	0.0357 (4)
O12D	0.13518 (10)	0.72445 (8)	0.47061 (5)	0.0425 (4)
O51D	0.12968 (12)	1.22050 (9)	0.42635 (7)	0.0572 (5)
O52D	0.11007 (10)	1.16310 (8)	0.51618 (6)	0.0442 (5)
N5D	0.12073 (10)	1.15325 (10)	0.46110 (7)	0.0348 (5)
C1D	0.12832 (11)	0.88941 (11)	0.45319 (7)	0.0246 (5)
C2D	0.13815 (12)	0.87685 (11)	0.39024 (7)	0.0293 (5)
C3D	0.14014 (13)	0.95564 (12)	0.35148 (8)	0.0358 (6)
C4D	0.13393 (12)	1.04569 (12)	0.37452 (8)	0.0322 (5)
C5D	0.12471 (11)	1.05756 (11)	0.43673 (7)	0.0261 (5)
C6D	0.12100 (11)	0.98103 (10)	0.47596 (7)	0.0248 (5)
C11D	0.12604 (12)	0.80620 (11)	0.49551 (7)	0.0272 (5)
H1A	0.1296 (15)	0.6270 (12)	0.5115 (9)	0.066 (7)*
H2A	0.1125 (14)	0.7051 (14)	0.6004 (9)	0.050 (6)*
H5A	0.12140	0.34440	0.51340	0.0320*
H21A	0.26440	0.72320	0.73740	0.0360*
H31A	0.38610	0.64820	0.79700	0.0380*
H41A	0.3718 (17)	0.4292 (18)	0.8578 (11)	0.076 (9)*
H42A	0.4348 (18)	0.5140 (15)	0.8518 (10)	0.066 (7)*
H43A	0.10930	0.26470	0.60840	0.0610*
H44A	0.03240	0.31800	0.65290	0.0610*
H45A	0.15210	0.32230	0.66540	0.0610*
H51A	0.20060	0.41980	0.81440	0.0400*
H61A	0.08150	0.49220	0.75240	0.0350*
H63A	0.21500	0.51120	0.42740	0.0440*
H64A	0.09840	0.53990	0.41790	0.0440*
H65A	0.13120	0.43060	0.41710	0.0440*
H1B	0.8742 (14)	0.2998 (14)	0.9766 (9)	0.050 (6)*
H2B	0.8939 (13)	0.2133 (13)	0.8892 (9)	0.041 (5)*
H5B	0.87600	0.58080	0.97310	0.0340*
H21B	0.71870	0.20720	0.77610	0.0340*
H31B	0.58550	0.28120	0.72700	0.0360*
H41B	0.5276 (18)	0.4084 (16)	0.6715 (11)	0.076 (8)*
H42B	0.5908 (15)	0.4978 (15)	0.6598 (9)	0.052 (6)*
H43B	0.86600	0.59680	0.81850	0.0550*

H44B	0.98230	0.60640	0.83890	0.0550*
H45B	0.89500	0.65820	0.87690	0.0550*
H51B	0.76820	0.50510	0.68800	0.0360*
H61B	0.90250	0.42960	0.73580	0.0330*
H63B	0.85550	0.49740	1.06990	0.0520*
H64B	0.89390	0.38980	1.07190	0.0520*
H65B	0.77700	0.41270	1.05810	0.0520*
H2C	0.8596 (18)	0.1687 (18)	1.0934 (12)	0.088 (9)*
H3C	0.85690	−0.03270	1.17530	0.0400*
H4C	0.86660	−0.18290	1.13240	0.0380*
H6C	0.88270	−0.06540	0.96500	0.0320*
H2D	0.1502 (17)	0.7500 (15)	0.3961 (11)	0.069 (7)*
H3D	0.14580	0.94650	0.30910	0.0430*
H4D	0.13590	1.09920	0.34840	0.0390*
H6D	0.11350	0.99110	0.51820	0.0300*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0366 (2)	0.0253 (2)	0.0246 (2)	0.0057 (2)	0.0043 (2)	−0.0012 (2)
O11A	0.0326 (6)	0.0433 (7)	0.0358 (7)	0.0063 (5)	0.0071 (5)	0.0024 (6)
O12A	0.0566 (8)	0.0255 (6)	0.0340 (7)	0.0101 (5)	0.0032 (6)	−0.0046 (5)
N1A	0.0231 (7)	0.0198 (7)	0.0239 (7)	0.0007 (5)	−0.0004 (5)	0.0017 (6)
N2A	0.0393 (8)	0.0188 (7)	0.0222 (7)	0.0012 (6)	0.0028 (6)	0.0017 (6)
N3A	0.0305 (7)	0.0219 (7)	0.0258 (7)	−0.0005 (5)	0.0009 (6)	0.0015 (6)
N41A	0.0518 (11)	0.0364 (11)	0.0544 (12)	−0.0002 (9)	−0.0185 (9)	0.0039 (8)
C2A	0.0210 (7)	0.0223 (8)	0.0225 (8)	0.0016 (6)	0.0000 (6)	0.0016 (6)
C4A	0.0271 (8)	0.0218 (8)	0.0318 (9)	−0.0009 (6)	−0.0002 (7)	0.0009 (7)
C5A	0.0279 (8)	0.0195 (8)	0.0322 (9)	−0.0002 (6)	−0.0006 (7)	−0.0047 (7)
C6A	0.0192 (7)	0.0243 (8)	0.0257 (8)	0.0014 (6)	−0.0023 (6)	−0.0016 (7)
C11A	0.0359 (9)	0.0255 (9)	0.0204 (8)	0.0006 (7)	0.0038 (7)	−0.0027 (7)
C21A	0.0445 (10)	0.0230 (8)	0.0227 (8)	−0.0031 (7)	0.0033 (7)	−0.0025 (7)
C31A	0.0370 (9)	0.0297 (9)	0.0293 (9)	−0.0040 (7)	−0.0007 (7)	−0.0073 (7)
C41A	0.0412 (10)	0.0273 (9)	0.0259 (9)	0.0047 (7)	−0.0015 (7)	−0.0054 (7)
C42A	0.0611 (12)	0.0245 (9)	0.0370 (10)	−0.0028 (8)	0.0039 (9)	0.0050 (8)
C51A	0.0459 (10)	0.0230 (9)	0.0304 (10)	−0.0024 (7)	0.0004 (8)	0.0026 (7)
C61A	0.0353 (9)	0.0266 (9)	0.0265 (9)	−0.0050 (7)	0.0022 (7)	−0.0009 (7)
C62A	0.0324 (9)	0.0300 (9)	0.0255 (9)	0.0030 (7)	−0.0019 (7)	−0.0026 (7)
S1B	0.0368 (2)	0.0250 (2)	0.0224 (2)	0.0059 (2)	0.0015 (2)	−0.0006 (2)
O11B	0.0336 (6)	0.0452 (7)	0.0338 (7)	0.0075 (5)	0.0063 (5)	0.0026 (6)
O12B	0.0594 (8)	0.0246 (6)	0.0304 (7)	0.0115 (5)	−0.0033 (6)	−0.0038 (5)
N1B	0.0285 (7)	0.0221 (7)	0.0218 (7)	0.0000 (5)	−0.0007 (5)	0.0017 (6)
N2B	0.0444 (8)	0.0196 (7)	0.0209 (7)	0.0023 (6)	−0.0004 (6)	0.0021 (6)
N3B	0.0318 (7)	0.0234 (7)	0.0247 (7)	0.0012 (5)	0.0000 (6)	0.0013 (6)
N41B	0.0495 (11)	0.0296 (10)	0.0719 (13)	−0.0001 (8)	−0.0258 (9)	0.0056 (9)
C2B	0.0251 (8)	0.0232 (8)	0.0215 (8)	0.0013 (6)	−0.0016 (6)	0.0013 (6)
C4B	0.0270 (8)	0.0239 (9)	0.0302 (9)	0.0001 (6)	−0.0010 (7)	0.0023 (7)
C5B	0.0335 (9)	0.0245 (9)	0.0278 (9)	−0.0005 (7)	0.0016 (7)	−0.0040 (7)
C6B	0.0228 (8)	0.0272 (9)	0.0252 (9)	−0.0010 (6)	−0.0011 (6)	−0.0016 (7)
C11B	0.0330 (9)	0.0236 (8)	0.0168 (8)	0.0008 (6)	0.0013 (6)	−0.0018 (6)

C21B	0.0412 (10)	0.0213 (8)	0.0224 (8)	−0.0014 (7)	0.0038 (7)	0.0004 (7)
C31B	0.0322 (9)	0.0254 (9)	0.0322 (9)	−0.0033 (7)	−0.0001 (7)	−0.0048 (7)
C41B	0.0374 (9)	0.0250 (9)	0.0274 (9)	0.0033 (7)	−0.0054 (7)	−0.0043 (7)
C42B	0.0520 (11)	0.0261 (9)	0.0327 (10)	0.0004 (8)	0.0047 (8)	0.0043 (8)
C51B	0.0443 (10)	0.0217 (8)	0.0236 (9)	−0.0025 (7)	−0.0012 (7)	0.0027 (7)
C61B	0.0325 (9)	0.0260 (9)	0.0232 (8)	−0.0030 (7)	0.0018 (7)	−0.0001 (7)
C62B	0.0421 (10)	0.0339 (10)	0.0279 (9)	−0.0030 (8)	0.0045 (8)	−0.0037 (8)
O2C	0.0644 (9)	0.0274 (7)	0.0310 (7)	−0.0040 (6)	0.0002 (6)	0.0009 (6)
O11C	0.0451 (7)	0.0326 (7)	0.0269 (7)	−0.0026 (5)	−0.0013 (5)	0.0059 (5)
O12C	0.0668 (9)	0.0249 (7)	0.0304 (7)	−0.0046 (6)	−0.0010 (6)	0.0051 (5)
O51C	0.0772 (10)	0.0245 (7)	0.0686 (10)	0.0024 (6)	−0.0139 (8)	0.0057 (7)
O52C	0.1214 (15)	0.0410 (9)	0.0538 (10)	0.0047 (8)	0.0094 (10)	−0.0133 (8)
N5C	0.0386 (9)	0.0293 (9)	0.0545 (11)	0.0021 (7)	−0.0038 (7)	−0.0036 (8)
C1C	0.0192 (7)	0.0252 (8)	0.0303 (9)	−0.0020 (6)	−0.0025 (6)	0.0049 (7)
C2C	0.0273 (8)	0.0243 (9)	0.0303 (9)	−0.0034 (7)	−0.0013 (7)	0.0002 (7)
C3C	0.0374 (9)	0.0339 (10)	0.0277 (9)	−0.0038 (8)	−0.0007 (7)	0.0058 (8)
C4C	0.0267 (9)	0.0280 (9)	0.0415 (10)	−0.0022 (7)	−0.0015 (7)	0.0101 (8)
C5C	0.0203 (8)	0.0248 (9)	0.0404 (10)	0.0005 (6)	−0.0012 (7)	0.0011 (7)
C6C	0.0210 (8)	0.0312 (9)	0.0290 (9)	0.0002 (6)	−0.0004 (6)	−0.0013 (7)
C11C	0.0239 (8)	0.0279 (9)	0.0303 (9)	−0.0033 (7)	−0.0020 (7)	0.0051 (7)
O2D	0.0902 (11)	0.0265 (7)	0.0283 (7)	−0.0028 (7)	0.0147 (7)	−0.0059 (6)
O11D	0.0570 (8)	0.0265 (6)	0.0235 (6)	0.0013 (5)	0.0009 (5)	0.0034 (5)
O12D	0.0757 (9)	0.0197 (6)	0.0320 (7)	0.0045 (6)	0.0147 (6)	0.0019 (5)
O51D	0.0918 (11)	0.0228 (7)	0.0570 (9)	−0.0029 (7)	0.0057 (8)	0.0089 (7)
O52D	0.0656 (9)	0.0297 (7)	0.0373 (8)	0.0035 (6)	−0.0029 (6)	−0.0090 (6)
N5D	0.0378 (8)	0.0219 (8)	0.0448 (10)	−0.0005 (6)	−0.0030 (7)	0.0012 (7)
C1D	0.0268 (8)	0.0224 (8)	0.0246 (8)	−0.0019 (6)	0.0023 (6)	0.0013 (7)
C2D	0.0374 (9)	0.0232 (9)	0.0272 (9)	−0.0029 (7)	0.0065 (7)	−0.0016 (7)
C3D	0.0490 (11)	0.0353 (10)	0.0230 (9)	−0.0057 (8)	0.0060 (8)	0.0024 (7)
C4D	0.0377 (9)	0.0270 (9)	0.0318 (10)	−0.0042 (7)	0.0011 (7)	0.0084 (7)
C5D	0.0261 (8)	0.0211 (8)	0.0311 (9)	−0.0018 (6)	−0.0009 (7)	0.0011 (7)
C6D	0.0260 (8)	0.0253 (8)	0.0232 (8)	0.0000 (6)	0.0013 (6)	−0.0008 (7)
C11D	0.0302 (9)	0.0237 (9)	0.0278 (9)	0.0009 (7)	0.0032 (7)	0.0019 (7)

Geometric parameters (Å, º)

S1A—O11A	1.4299 (11)	C5A—H5A	0.9500
S1A—O12A	1.4299 (12)	C21A—H21A	0.9500
S1A—N2A	1.6770 (14)	C31A—H31A	0.9500
S1A—C11A	1.7417 (16)	C42A—H45A	0.9800
S1B—O11B	1.4287 (11)	C42A—H43A	0.9800
S1B—O12B	1.4316 (12)	C42A—H44A	0.9800
S1B—N2B	1.6726 (14)	C51A—H51A	0.9500
S1B—C11B	1.7362 (15)	C61A—H61A	0.9500
O2C—C2C	1.346 (2)	C62A—H65A	0.9800
O11C—C11C	1.2408 (19)	C62A—H63A	0.9800
O12C—C11C	1.2804 (19)	C62A—H64A	0.9800
O51C—N5C	1.227 (2)	C4B—C5B	1.392 (2)
O52C—N5C	1.227 (2)	C4B—C42B	1.494 (2)
O2C—H2C	0.89 (3)	C5B—C6B	1.376 (2)

O2D—C2D	1.334 (2)	C6B—C62B	1.492 (2)
O11D—C11D	1.2378 (19)	C11B—C21B	1.392 (2)
O12D—C11D	1.2831 (19)	C11B—C61B	1.394 (2)
O51D—N5D	1.226 (2)	C21B—C31B	1.366 (2)
O52D—N5D	1.235 (2)	C31B—C41B	1.399 (2)
O2D—H2D	0.90 (2)	C41B—C51B	1.404 (2)
N1A—C2A	1.350 (2)	C51B—C61B	1.370 (2)
N1A—C6A	1.3539 (19)	C5B—H5B	0.9500
N2A—C2A	1.360 (2)	C21B—H21B	0.9500
N3A—C4A	1.3473 (19)	C31B—H31B	0.9500
N3A—C2A	1.3242 (19)	C42B—H45B	0.9800
N41A—C41A	1.370 (2)	C42B—H44B	0.9800
N1A—H1A	0.939 (18)	C42B—H43B	0.9800
N2A—H2A	0.85 (2)	C51B—H51B	0.9500
N41A—H41A	0.82 (3)	C61B—H61B	0.9500
N41A—H42A	0.89 (2)	C62B—H65B	0.9800
N1B—C6B	1.350 (2)	C62B—H63B	0.9800
N1B—C2B	1.354 (2)	C62B—H64B	0.9800
N2B—C2B	1.355 (2)	C1C—C11C	1.501 (2)
N3B—C2B	1.3264 (19)	C1C—C6C	1.386 (2)
N3B—C4B	1.344 (2)	C1C—C2C	1.410 (2)
N41B—C41B	1.367 (2)	C2C—C3C	1.400 (2)
N1B—H1B	0.91 (2)	C3C—C4C	1.367 (2)
N2B—H2B	0.889 (19)	C4C—C5C	1.393 (3)
N41B—H41B	0.89 (2)	C5C—C6C	1.380 (2)
N41B—H42B	0.83 (2)	C3C—H3C	0.9500
N5C—C5C	1.453 (2)	C4C—H4C	0.9500
N5D—C5D	1.454 (2)	C6C—H6C	0.9500
C4A—C5A	1.392 (2)	C1D—C6D	1.390 (2)
C4A—C42A	1.488 (2)	C1D—C11D	1.501 (2)
C5A—C6A	1.375 (2)	C1D—C2D	1.410 (2)
C6A—C62A	1.490 (2)	C2D—C3D	1.404 (2)
C11A—C21A	1.391 (2)	C3D—C4D	1.371 (2)
C11A—C61A	1.399 (2)	C4D—C5D	1.392 (2)
C21A—C31A	1.380 (2)	C5D—C6D	1.386 (2)
C31A—C41A	1.402 (2)	C3D—H3D	0.9500
C41A—C51A	1.398 (2)	C4D—H4D	0.9500
C51A—C61A	1.373 (2)	C6D—H6D	0.9500

O11A—S1A—O12A	120.00 (7)	N1B—C2B—N2B	116.83 (13)
O11A—S1A—N2A	108.70 (7)	N1B—C2B—N3B	123.20 (14)
O11A—S1A—C11A	108.90 (7)	N3B—C4B—C42B	115.81 (14)
O12A—S1A—N2A	101.64 (7)	C5B—C4B—C42B	122.33 (14)
O12A—S1A—C11A	109.63 (7)	N3B—C4B—C5B	121.86 (14)
N2A—S1A—C11A	107.13 (7)	C4B—C5B—C6B	119.06 (14)
O11B—S1B—N2B	108.92 (7)	N1B—C6B—C5B	117.86 (14)
O11B—S1B—C11B	110.08 (7)	C5B—C6B—C62B	124.49 (14)
O12B—S1B—N2B	101.66 (7)	N1B—C6B—C62B	117.64 (14)
O12B—S1B—C11B	110.30 (7)	S1B—C11B—C21B	119.10 (12)

N2B—S1B—C11B	105.78 (7)	S1B—C11B—C61B	120.80 (12)
O11B—S1B—O12B	119.02 (7)	C21B—C11B—C61B	120.10 (14)
C2C—O2C—H2C	105.0 (17)	C11B—C21B—C31B	119.84 (14)
C2D—O2D—H2D	105.7 (14)	C21B—C31B—C41B	120.97 (15)
C2A—N1A—C6A	120.37 (13)	C31B—C41B—C51B	118.65 (14)
S1A—N2A—C2A	123.73 (11)	N41B—C41B—C51B	120.92 (15)
C2A—N3A—C4A	117.13 (13)	N41B—C41B—C31B	120.41 (15)
C6A—N1A—H1A	118.6 (12)	C41B—C51B—C61B	120.48 (14)
C2A—N1A—H1A	121.1 (12)	C11B—C61B—C51B	119.93 (14)
S1A—N2A—H2A	116.0 (13)	C4B—C5B—H5B	120.00
C2A—N2A—H2A	119.1 (14)	C6B—C5B—H5B	120.00
C41A—N41A—H41A	119.8 (16)	C31B—C21B—H21B	120.00
H41A—N41A—H42A	118 (2)	C11B—C21B—H21B	120.00
C41A—N41A—H42A	114.8 (14)	C21B—C31B—H31B	120.00
C2B—N1B—C6B	120.75 (14)	C41B—C31B—H31B	120.00
S1B—N2B—C2B	123.29 (11)	C4B—C42B—H43B	109.00
C2B—N3B—C4B	117.23 (13)	C4B—C42B—H44B	109.00
C6B—N1B—H1B	120.0 (13)	H43B—C42B—H44B	109.00
C2B—N1B—H1B	119.2 (13)	C4B—C42B—H45B	110.00
C2B—N2B—H2B	123.3 (13)	H44B—C42B—H45B	110.00
S1B—N2B—H2B	113.2 (13)	H43B—C42B—H45B	109.00
C41B—N41B—H42B	118.5 (14)	C61B—C51B—H51B	120.00
C41B—N41B—H41B	113.6 (15)	C41B—C51B—H51B	120.00
H41B—N41B—H42B	126 (2)	C11B—C61B—H61B	120.00
O51C—N5C—C5C	118.80 (16)	C51B—C61B—H61B	120.00
O52C—N5C—C5C	118.44 (15)	H63B—C62B—H65B	109.00
O51C—N5C—O52C	122.77 (15)	H64B—C62B—H65B	109.00
O51D—N5D—O52D	122.88 (14)	C6B—C62B—H64B	109.00
O51D—N5D—C5D	118.78 (15)	H63B—C62B—H64B	109.00
O52D—N5D—C5D	118.33 (13)	C6B—C62B—H65B	110.00
N2A—C2A—N3A	119.57 (14)	C6B—C62B—H63B	110.00
N1A—C2A—N2A	116.84 (13)	C2C—C1C—C11C	121.10 (14)
N1A—C2A—N3A	123.59 (13)	C6C—C1C—C11C	120.09 (14)
N3A—C4A—C5A	121.85 (14)	C2C—C1C—C6C	118.81 (14)
N3A—C4A—C42A	116.05 (14)	O2C—C2C—C3C	117.41 (14)
C5A—C4A—C42A	122.10 (14)	C1C—C2C—C3C	120.42 (15)
C4A—C5A—C6A	118.89 (14)	O2C—C2C—C1C	122.18 (14)
N1A—C6A—C62A	117.56 (13)	C2C—C3C—C4C	120.33 (16)
N1A—C6A—C5A	118.17 (14)	C3C—C4C—C5C	118.77 (16)
C5A—C6A—C62A	124.25 (14)	N5C—C5C—C6C	119.24 (15)
S1A—C11A—C61A	120.29 (12)	C4C—C5C—C6C	122.26 (15)
S1A—C11A—C21A	119.64 (12)	N5C—C5C—C4C	118.49 (15)
C21A—C11A—C61A	120.07 (14)	C1C—C6C—C5C	119.41 (15)
C11A—C21A—C31A	119.73 (15)	O12C—C11C—C1C	116.00 (13)
C21A—C31A—C41A	120.69 (16)	O11C—C11C—O12C	124.26 (14)
N41A—C41A—C51A	121.05 (15)	O11C—C11C—C1C	119.73 (14)
N41A—C41A—C31A	120.09 (16)	C2C—C3C—H3C	120.00
C31A—C41A—C51A	118.82 (15)	C4C—C3C—H3C	120.00
C41A—C51A—C61A	120.76 (14)	C5C—C4C—H4C	121.00

C11A—C61A—C51A	119.92 (15)	C3C—C4C—H4C	121.00
C6A—C5A—H5A	121.00	C1C—C6C—H6C	120.00
C4A—C5A—H5A	121.00	C5C—C6C—H6C	120.00
C31A—C21A—H21A	120.00	C2D—C1D—C11D	121.32 (14)
C11A—C21A—H21A	120.00	C6D—C1D—C11D	119.92 (14)
C41A—C31A—H31A	120.00	C2D—C1D—C6D	118.77 (14)
C21A—C31A—H31A	120.00	O2D—C2D—C1D	122.23 (14)
H43A—C42A—H45A	110.00	O2D—C2D—C3D	117.38 (14)
C4A—C42A—H44A	109.00	C1D—C2D—C3D	120.39 (15)
H44A—C42A—H45A	109.00	C2D—C3D—C4D	120.31 (16)
C4A—C42A—H43A	109.00	C3D—C4D—C5D	118.98 (16)
C4A—C42A—H45A	109.00	N5D—C5D—C6D	119.27 (14)
H43A—C42A—H44A	109.00	C4D—C5D—C6D	121.93 (15)
C61A—C51A—H51A	120.00	N5D—C5D—C4D	118.78 (14)
C41A—C51A—H51A	120.00	C1D—C6D—C5D	119.61 (14)
C51A—C61A—H61A	120.00	O11D—C11D—C1D	120.77 (14)
C11A—C61A—H61A	120.00	O12D—C11D—C1D	115.61 (13)
C6A—C62A—H63A	109.00	O11D—C11D—O12D	123.62 (14)
C6A—C62A—H64A	109.00	C2D—C3D—H3D	120.00
H63A—C62A—H64A	109.00	C4D—C3D—H3D	120.00
H64A—C62A—H65A	109.00	C3D—C4D—H4D	120.00
C6A—C62A—H65A	110.00	C5D—C4D—H4D	121.00
H63A—C62A—H65A	109.00	C1D—C6D—H6D	120.00
N2B—C2B—N3B	119.97 (14)	C5D—C6D—H6D	120.00

O11A—S1A—N2A—C2A	−51.52 (14)	C11A—C21A—C31A—C41A	−1.7 (2)
O12A—S1A—N2A—C2A	−179.01 (12)	C21A—C31A—C41A—C51A	1.4 (2)
C11A—S1A—N2A—C2A	66.00 (14)	C21A—C31A—C41A—N41A	−176.06 (16)
O11A—S1A—C11A—C21A	−160.97 (12)	N41A—C41A—C51A—C61A	177.13 (16)
O11A—S1A—C11A—C61A	18.27 (15)	C31A—C41A—C51A—C61A	−0.3 (2)
O12A—S1A—C11A—C21A	−27.88 (15)	C41A—C51A—C61A—C11A	−0.5 (2)
O12A—S1A—C11A—C61A	151.36 (13)	C42B—C4B—C5B—C6B	178.39 (15)
N2A—S1A—C11A—C21A	81.64 (14)	N3B—C4B—C5B—C6B	−1.7 (2)
N2A—S1A—C11A—C61A	−99.12 (14)	C4B—C5B—C6B—C62B	−179.08 (15)
N2B—S1B—C11B—C21B	−78.04 (14)	C4B—C5B—C6B—N1B	0.0 (2)
N2B—S1B—C11B—C61B	102.11 (14)	C21B—C11B—C61B—C51B	−0.7 (2)
O11B—S1B—N2B—C2B	59.70 (14)	S1B—C11B—C21B—C31B	−178.54 (12)
O12B—S1B—N2B—C2B	−173.83 (12)	C61B—C11B—C21B—C31B	1.3 (2)
C11B—S1B—N2B—C2B	−58.59 (14)	S1B—C11B—C61B—C51B	179.14 (12)
O11B—S1B—C11B—C21B	164.44 (12)	C11B—C21B—C31B—C41B	−0.2 (2)
O11B—S1B—C11B—C61B	−15.41 (15)	C21B—C31B—C41B—C51B	−1.4 (2)
O12B—S1B—C11B—C21B	31.14 (15)	C21B—C31B—C41B—N41B	176.95 (16)
O12B—S1B—C11B—C61B	−148.71 (13)	C31B—C41B—C51B—C61B	2.0 (2)
C2A—N1A—C6A—C5A	0.00 (19)	N41B—C41B—C51B—C61B	−176.33 (16)
C2A—N1A—C6A—C62A	−178.53 (13)	C41B—C51B—C61B—C11B	−1.0 (2)
C6A—N1A—C2A—N3A	0.2 (2)	C6C—C1C—C2C—O2C	178.79 (14)
C6A—N1A—C2A—N2A	179.44 (13)	C6C—C1C—C2C—C3C	−1.2 (2)
S1A—N2A—C2A—N3A	−12.4 (2)	C2C—C1C—C11C—O11C	−177.96 (14)
S1A—N2A—C2A—N1A	168.33 (11)	C2C—C1C—C11C—O12C	1.8 (2)

C2A—N3A—C4A—C5A	−0.9 (2)	C6C—C1C—C11C—O11C	1.9 (2)
C4A—N3A—C2A—N1A	0.3 (2)	C6C—C1C—C11C—O12C	−178.37 (14)
C4A—N3A—C2A—N2A	−178.99 (13)	C11C—C1C—C2C—O2C	−1.4 (2)
C2A—N3A—C4A—C42A	178.67 (14)	C11C—C1C—C2C—C3C	178.65 (14)
C6B—N1B—C2B—N3B	0.2 (2)	C2C—C1C—C6C—C5C	1.0 (2)
C2B—N1B—C6B—C5B	0.7 (2)	C11C—C1C—C6C—C5C	−178.79 (13)
C6B—N1B—C2B—N2B	−178.90 (13)	O2C—C2C—C3C—C4C	−179.05 (14)
C2B—N1B—C6B—C62B	179.89 (13)	C1C—C2C—C3C—C4C	0.9 (2)
S1B—N2B—C2B—N1B	176.82 (10)	C2C—C3C—C4C—C5C	−0.5 (2)
S1B—N2B—C2B—N3B	−2.3 (2)	C3C—C4C—C5C—C6C	0.4 (2)
C2B—N3B—C4B—C5B	2.5 (2)	C3C—C4C—C5C—N5C	179.12 (14)
C2B—N3B—C4B—C42B	−177.57 (14)	N5C—C5C—C6C—C1C	−179.38 (13)
C4B—N3B—C2B—N2B	177.27 (13)	C4C—C5C—C6C—C1C	−0.7 (2)
C4B—N3B—C2B—N1B	−1.8 (2)	C6D—C1D—C2D—O2D	179.26 (15)
O51C—N5C—C5C—C6C	178.18 (15)	C6D—C1D—C2D—C3D	−0.2 (2)
O51C—N5C—C5C—C4C	−0.6 (2)	C11D—C1D—C2D—O2D	−0.5 (2)
O52C—N5C—C5C—C4C	179.97 (16)	C11D—C1D—C2D—C3D	−180.00 (15)
O52C—N5C—C5C—C6C	−1.3 (2)	C2D—C1D—C6D—C5D	−0.8 (2)
O51D—N5D—C5D—C6D	176.04 (15)	C11D—C1D—C6D—C5D	179.02 (14)
O52D—N5D—C5D—C6D	−2.8 (2)	C2D—C1D—C11D—O11D	−179.30 (15)
O51D—N5D—C5D—C4D	−2.9 (2)	C2D—C1D—C11D—O12D	1.1 (2)
O52D—N5D—C5D—C4D	178.27 (14)	C6D—C1D—C11D—O11D	0.9 (2)
N3A—C4A—C5A—C6A	1.0 (2)	C6D—C1D—C11D—O12D	−178.73 (14)
C42A—C4A—C5A—C6A	−178.48 (15)	O2D—C2D—C3D—C4D	−178.60 (15)
C4A—C5A—C6A—C62A	177.87 (14)	C1D—C2D—C3D—C4D	0.9 (2)
C4A—C5A—C6A—N1A	−0.6 (2)	C2D—C3D—C4D—C5D	−0.6 (2)
C21A—C11A—C61A—C51A	0.3 (2)	C3D—C4D—C5D—N5D	178.47 (14)
S1A—C11A—C61A—C51A	−178.96 (12)	C3D—C4D—C5D—C6D	−0.4 (2)
S1A—C11A—C21A—C31A	−179.96 (13)	N5D—C5D—C6D—C1D	−177.77 (13)
C61A—C11A—C21A—C31A	0.8 (2)	C4D—C5D—C6D—C1D	1.1 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···O12*D*	0.939 (18)	1.647 (18)	2.5847 (17)	176 (2)
N1*B*—H1*B*···O12*C*	0.91 (2)	1.71 (2)	2.6162 (18)	176.4 (18)
N2*A*—H2*A*···O11*D*	0.85 (2)	1.94 (2)	2.7810 (18)	177 (2)
N2*B*—H2*B*···O11*C*	0.889 (19)	1.836 (19)	2.7221 (18)	174.3 (18)
N41*A*—H41*A*···O11*D*^{i}	0.82 (3)	2.57 (2)	3.217 (2)	138 (2)
N41*B*—H41*B*···O2*C*^{ii}	0.89 (2)	2.49 (2)	3.269 (2)	147 (2)
N41*B*—H42*B*···O12*B*^{iii}	0.83 (2)	2.45 (2)	3.106 (2)	136.6 (18)
O2*C*—H2*C*···O12*C*	0.89 (3)	1.70 (3)	2.5223 (17)	152 (2)
O2*D*—H2*D*···O12*D*	0.90 (2)	1.70 (2)	2.5215 (17)	151 (2)
C5*A*—H5*A*···O52*D*^{iv}	0.95	2.56	3.4175 (19)	150
C5*B*—H5*B*···O51*C*^{v}	0.95	2.44	3.348 (2)	160
C5*B*—H5*B*···O52*C*^{v}	0.95	2.58	3.420 (2)	147
C42*A*—H43*A*···O52*D*^{iv}	0.98	2.49	3.428 (2)	159

C42*B*—H45*B*···O52*C*^{v}	0.98	2.42	3.350 (2)	158
C61*A*—H61*A*···O11*A*	0.95	2.59	2.9422 (19)	102

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

(II) 2-(4-Aminobenzenesulfonamido)-4,6-dimethylpyrimidinium 2,4,6-trinitrophenolate

Crystal data

$C_{12}H_{15}N_4O_2S^+·C_6H_2N_3O_7^-$
M_r = 507.45
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 8.3131 (2) Å
b = 19.2779 (5) Å
c = 13.4483 (4) Å
β = 99.158 (3)°
V = 2127.74 (10) Å^3
Z = 4
$F(000)$ = 1048
D_x = 1.584 Mg m^{-3}
Melting point = 469–471 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7676 reflections
θ = 3.2–28.8°
μ = 0.22 mm^{-1}
T = 200 K
Block, yellow
0.35 × 0.35 × 0.26 mm

Data collection

Oxford Gemini-S CCD area-detector diffractometer
Radiation source: Enhance (Mo) X-ray source
Graphite monochromator
Detector resolution: 16.077 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.970, T_{max} = 0.981
14211 measured reflections
4171 independent reflections
3318 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 26.0°, θ_{min} = 3.3°
h = −8→10
k = −23→23
l = −15→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.091
S = 1.04
4171 reflections
334 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
$w = 1/[\sigma^2(F_o^2) + (0.0541P)^2 + 0.1041P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are 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 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}	Occ. (<1)
S1A	1.01736 (5)	0.72633 (2)	0.40874 (3)	0.0286 (1)	
O11A	1.01403 (16)	0.74900 (6)	0.30725 (10)	0.0411 (4)	
O12A	0.91002 (15)	0.75680 (6)	0.46966 (11)	0.0381 (4)	
N1A	0.81196 (16)	0.54828 (6)	0.42730 (11)	0.0240 (4)	
N2A	0.96357 (18)	0.64262 (7)	0.39275 (12)	0.0289 (5)	
N3A	0.95185 (16)	0.61463 (7)	0.56049 (10)	0.0254 (4)	
N41A	1.6891 (2)	0.73736 (9)	0.62678 (16)	0.0419 (6)	
C2A	0.90857 (19)	0.60189 (8)	0.46347 (13)	0.0232 (5)	
C4A	0.89632 (19)	0.57061 (8)	0.62539 (13)	0.0247 (5)	
C5A	0.79877 (19)	0.51355 (8)	0.59168 (13)	0.0267 (5)	
C6A	0.75510 (18)	0.50281 (8)	0.49024 (13)	0.0244 (5)	
C11A	1.2145 (2)	0.72872 (8)	0.47392 (13)	0.0250 (5)	
C21A	1.3454 (2)	0.72025 (8)	0.42106 (13)	0.0300 (6)	
C31A	1.5022 (2)	0.72321 (9)	0.47158 (14)	0.0317 (6)	
C41A	1.5335 (2)	0.73431 (8)	0.57572 (13)	0.0275 (5)	
C42A	0.9460 (2)	0.58500 (9)	0.73449 (13)	0.0337 (6)	
C51A	1.4001 (2)	0.74275 (8)	0.62754 (14)	0.0299 (6)	
C61A	1.2436 (2)	0.73988 (8)	0.57729 (13)	0.0280 (5)	
C62A	0.6501 (2)	0.44540 (9)	0.44236 (15)	0.0326 (6)	
O1	0.81506 (14)	0.55856 (6)	0.23824 (9)	0.0327 (4)	
O21	0.51094 (17)	0.58897 (8)	0.28921 (10)	0.0483 (5)	
O22	0.35141 (16)	0.52229 (7)	0.18893 (11)	0.0455 (5)	
O41	0.33961 (17)	0.59866 (9)	−0.16549 (11)	0.0573 (6)	
O42	0.56354 (17)	0.63473 (7)	−0.20899 (10)	0.0476 (5)	
O61	1.06573 (16)	0.58522 (8)	0.01325 (11)	0.0492 (5)	
O62	1.06389 (16)	0.62078 (8)	0.16560 (11)	0.0482 (5)	
N2	0.46886 (17)	0.56092 (7)	0.20714 (11)	0.0301 (5)	
N4	0.48456 (19)	0.61225 (8)	−0.14630 (12)	0.0343 (5)	
N6	0.99501 (17)	0.59915 (8)	0.08397 (12)	0.0333 (5)	
C1	0.7383 (2)	0.57497 (8)	0.15227 (12)	0.0248 (5)	
C2	0.56423 (19)	0.57448 (8)	0.12657 (12)	0.0236 (5)	
C3	0.4795 (2)	0.58495 (8)	0.03122 (13)	0.0251 (5)	
C4	0.5685 (2)	0.60005 (8)	−0.04467 (13)	0.0256 (5)	
C5	0.7370 (2)	0.60378 (8)	−0.02677 (13)	0.0253 (5)	
C6	0.81761 (19)	0.59217 (8)	0.06853 (13)	0.0259 (5)	
H42A	1.706 (3)	0.7434 (12)	0.693 (2)	0.061 (8)*	
H1A	0.784 (3)	0.5461 (10)	0.3591 (17)	0.048 (6)*	
H2A	0.943 (2)	0.6323 (10)	0.3307 (16)	0.037 (6)*	
H5A	0.76320	0.48260	0.63860	0.0320*	
H21A	1.32560	0.71250	0.35040	0.0360*	
H31A	1.59070	0.71770	0.43540	0.0380*	
H41A	1.771 (3)	0.7388 (10)	0.5900 (16)	0.039 (6)*	
H48A	1.06370	0.57810	0.75290	0.0510*	0.500
H43A	0.88850	0.55330	0.77380	0.0510*	0.500
H44A	0.91840	0.63300	0.74880	0.0510*	0.500
H45A	0.85000	0.59820	0.76410	0.0510*	0.500
H46A	1.02530	0.62300	0.74320	0.0510*	0.500

H47A	0.99530	0.54330	0.76820	0.0510*	0.500
H51A	1.41910	0.75050	0.69820	0.0360*	
H61A	1.15470	0.74550	0.61310	0.0340*	
H62A	0.61050	0.41780	0.49470	0.0490*	
H63A	0.71360	0.41570	0.40390	0.0490*	
H64A	0.55710	0.46490	0.39700	0.0490*	
H3	0.36400	0.58190	0.01800	0.0300*	
H5	0.79580	0.61430	−0.08000	0.0300*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0292 (2)	0.0220 (2)	0.0337 (3)	−0.0017 (2)	0.0023 (2)	0.0062 (2)
O11A	0.0486 (8)	0.0353 (7)	0.0360 (8)	−0.0070 (6)	−0.0037 (6)	0.0162 (6)
O12A	0.0287 (7)	0.0291 (7)	0.0572 (9)	0.0035 (5)	0.0089 (6)	0.0007 (6)
N1A	0.0241 (7)	0.0244 (7)	0.0228 (8)	−0.0015 (5)	0.0016 (6)	0.0012 (6)
N2A	0.0349 (8)	0.0273 (8)	0.0241 (9)	−0.0086 (6)	0.0034 (7)	0.0022 (6)
N3A	0.0256 (7)	0.0250 (7)	0.0253 (8)	−0.0006 (6)	0.0036 (6)	−0.0002 (6)
N41A	0.0290 (9)	0.0555 (11)	0.0403 (11)	−0.0033 (7)	0.0029 (8)	0.0042 (8)
C2A	0.0207 (8)	0.0210 (8)	0.0280 (9)	0.0009 (6)	0.0045 (7)	0.0006 (6)
C4A	0.0212 (8)	0.0267 (8)	0.0265 (9)	0.0051 (6)	0.0050 (7)	0.0011 (7)
C5A	0.0256 (9)	0.0267 (9)	0.0292 (10)	0.0008 (6)	0.0089 (7)	0.0049 (7)
C6A	0.0194 (8)	0.0221 (8)	0.0323 (10)	0.0012 (6)	0.0061 (7)	0.0031 (7)
C11A	0.0264 (9)	0.0203 (8)	0.0286 (10)	−0.0028 (6)	0.0054 (7)	0.0032 (7)
C21A	0.0348 (10)	0.0327 (9)	0.0236 (10)	−0.0052 (7)	0.0084 (7)	0.0015 (7)
C31A	0.0284 (9)	0.0350 (10)	0.0347 (11)	−0.0029 (7)	0.0138 (8)	0.0017 (8)
C41A	0.0274 (9)	0.0221 (8)	0.0330 (10)	−0.0024 (6)	0.0045 (7)	0.0032 (7)
C42A	0.0379 (10)	0.0370 (10)	0.0266 (10)	−0.0003 (8)	0.0064 (8)	−0.0009 (8)
C51A	0.0354 (10)	0.0295 (9)	0.0250 (10)	0.0003 (7)	0.0051 (8)	−0.0021 (7)
C61A	0.0297 (9)	0.0255 (9)	0.0309 (10)	0.0010 (7)	0.0114 (8)	−0.0023 (7)
C62A	0.0301 (9)	0.0283 (9)	0.0390 (11)	−0.0059 (7)	0.0041 (8)	−0.0008 (8)
O1	0.0325 (7)	0.0420 (7)	0.0225 (7)	−0.0006 (5)	0.0009 (5)	0.0029 (5)
O21	0.0460 (8)	0.0731 (10)	0.0279 (8)	0.0014 (7)	0.0127 (6)	−0.0108 (7)
O22	0.0446 (8)	0.0470 (8)	0.0493 (9)	−0.0146 (6)	0.0213 (7)	0.0014 (6)
O41	0.0370 (9)	0.0912 (12)	0.0393 (9)	−0.0111 (8)	−0.0076 (7)	0.0123 (8)
O42	0.0496 (8)	0.0635 (9)	0.0298 (8)	0.0009 (7)	0.0071 (7)	0.0190 (7)
O61	0.0303 (7)	0.0740 (10)	0.0462 (9)	0.0036 (6)	0.0153 (7)	0.0032 (7)
O62	0.0344 (8)	0.0657 (9)	0.0420 (9)	−0.0154 (6)	−0.0012 (6)	−0.0027 (7)
N2	0.0314 (8)	0.0318 (8)	0.0288 (9)	0.0044 (6)	0.0097 (7)	0.0029 (6)
N4	0.0355 (9)	0.0371 (8)	0.0288 (9)	0.0012 (7)	0.0008 (7)	0.0043 (7)
N6	0.0261 (8)	0.0386 (8)	0.0353 (9)	−0.0043 (6)	0.0050 (7)	0.0052 (7)
C1	0.0303 (9)	0.0217 (8)	0.0224 (9)	−0.0014 (6)	0.0042 (7)	−0.0030 (6)
C2	0.0262 (9)	0.0225 (8)	0.0232 (9)	−0.0015 (6)	0.0075 (7)	−0.0004 (6)
C3	0.0227 (8)	0.0225 (8)	0.0298 (10)	−0.0015 (6)	0.0030 (7)	−0.0005 (7)
C4	0.0317 (10)	0.0227 (8)	0.0220 (9)	−0.0001 (7)	0.0027 (7)	0.0003 (7)
C5	0.0301 (9)	0.0234 (8)	0.0240 (9)	−0.0030 (6)	0.0090 (7)	0.0010 (7)
C6	0.0239 (9)	0.0248 (8)	0.0291 (10)	−0.0034 (6)	0.0046 (7)	−0.0011 (7)

Geometric parameters (Å, º)

S1A—O11A	1.4292 (14)	C11A—C61A	1.389 (2)
S1A—O12A	1.4301 (14)	C11A—C21A	1.401 (2)
S1A—N2A	1.6792 (14)	C21A—C31A	1.372 (2)
S1A—C11A	1.7318 (17)	C31A—C41A	1.400 (3)
O1—C1	1.269 (2)	C41A—C51A	1.410 (2)
O21—N2	1.229 (2)	C51A—C61A	1.368 (2)
O22—N2	1.221 (2)	C5A—H5A	0.9500
O41—N4	1.220 (2)	C21A—H21A	0.9500
O42—N4	1.227 (2)	C31A—H31A	0.9500
O61—N6	1.225 (2)	C42A—H44A	0.9800
O62—N6	1.228 (2)	C42A—H48A	0.9800
N1A—C2A	1.351 (2)	C42A—H43A	0.9800
N1A—C6A	1.355 (2)	C42A—H47A	0.9800
N2A—C2A	1.367 (2)	C42A—H45A	0.9800
N3A—C4A	1.350 (2)	C42A—H46A	0.9800
N3A—C2A	1.320 (2)	C51A—H51A	0.9500
N41A—C41A	1.366 (2)	C61A—H61A	0.9500
N1A—H1A	0.91 (2)	C62A—H62A	0.9800
N2A—H2A	0.85 (2)	C62A—H63A	0.9800
N41A—H42A	0.89 (3)	C62A—H64A	0.9800
N41A—H41A	0.90 (2)	C1—C2	1.433 (2)
N2—C2	1.464 (2)	C1—C6	1.432 (2)
N4—C4	1.451 (2)	C2—C3	1.376 (2)
N6—C6	1.462 (2)	C3—C4	1.384 (2)
C4A—C5A	1.399 (2)	C4—C5	1.385 (2)
C4A—C42A	1.486 (2)	C5—C6	1.367 (2)
C5A—C6A	1.370 (2)	C3—H3	0.9500
C6A—C62A	1.491 (2)	C5—H5	0.9500
O11A—S1A—O12A	120.16 (8)	C4A—C5A—H5A	120.00
O11A—S1A—N2A	101.96 (8)	C11A—C21A—H21A	120.00
O11A—S1A—C11A	110.38 (8)	C31A—C21A—H21A	120.00
O12A—S1A—N2A	106.88 (7)	C41A—C31A—H31A	120.00
O12A—S1A—C11A	109.00 (8)	C21A—C31A—H31A	120.00
N2A—S1A—C11A	107.56 (8)	H43A—C42A—H44A	109.00
C2A—N1A—C6A	121.10 (15)	H45A—C42A—H46A	109.00
S1A—N2A—C2A	125.08 (13)	H45A—C42A—H47A	109.00
C2A—N3A—C4A	117.03 (14)	H46A—C42A—H47A	110.00
C6A—N1A—H1A	122.8 (14)	C4A—C42A—H47A	109.00
C2A—N1A—H1A	116.1 (14)	H48A—C42A—H43A	109.00
C2A—N2A—H2A	120.8 (13)	H48A—C42A—H44A	110.00
S1A—N2A—H2A	111.1 (13)	C4A—C42A—H43A	109.00
H42A—N41A—H41A	122 (2)	C4A—C42A—H44A	109.00
C41A—N41A—H42A	119.8 (16)	C4A—C42A—H45A	109.00
C41A—N41A—H41A	117.5 (14)	C4A—C42A—H46A	109.00
O22—N2—C2	118.04 (14)	C4A—C42A—H48A	109.00
O21—N2—O22	123.55 (15)	C41A—C51A—H51A	120.00
O21—N2—C2	118.41 (14)	C61A—C51A—H51A	120.00

O42—N4—C4	118.33 (15)	C51A—C61A—H61A	120.00
O41—N4—O42	123.30 (16)	C11A—C61A—H61A	120.00
O41—N4—C4	118.36 (15)	C6A—C62A—H63A	110.00
O61—N6—O62	123.76 (15)	C6A—C62A—H64A	109.00
O62—N6—C6	118.33 (15)	H62A—C62A—H64A	109.00
O61—N6—C6	117.87 (15)	H63A—C62A—H64A	109.00
N2A—C2A—N3A	120.80 (15)	H62A—C62A—H63A	109.00
N1A—C2A—N2A	115.75 (15)	C6A—C62A—H62A	109.00
N1A—C2A—N3A	123.44 (15)	O1—C1—C2	124.07 (15)
N3A—C4A—C42A	116.81 (14)	O1—C1—C6	123.16 (15)
C5A—C4A—C42A	121.51 (15)	C2—C1—C6	112.68 (14)
N3A—C4A—C5A	121.67 (15)	N2—C2—C1	117.87 (14)
C4A—C5A—C6A	119.31 (15)	N2—C2—C3	117.30 (14)
N1A—C6A—C62A	116.68 (15)	C1—C2—C3	124.83 (15)
N1A—C6A—C5A	117.43 (14)	C2—C3—C4	117.63 (15)
C5A—C6A—C62A	125.89 (15)	N4—C4—C3	119.69 (15)
S1A—C11A—C21A	119.28 (13)	N4—C4—C5	118.47 (15)
S1A—C11A—C61A	120.71 (13)	C3—C4—C5	121.84 (16)
C21A—C11A—C61A	120.01 (16)	C4—C5—C6	119.07 (16)
C11A—C21A—C31A	119.83 (16)	N6—C6—C1	119.34 (15)
C21A—C31A—C41A	120.84 (16)	N6—C6—C5	116.80 (15)
C31A—C41A—C51A	118.47 (16)	C1—C6—C5	123.86 (15)
N41A—C41A—C31A	121.33 (16)	C2—C3—H3	121.00
N41A—C41A—C51A	120.20 (17)	C4—C3—H3	121.00
C41A—C51A—C61A	120.80 (17)	C4—C5—H5	120.00
C11A—C61A—C51A	120.06 (16)	C6—C5—H5	120.00
C6A—C5A—H5A	120.00		

O11A—S1A—N2A—C2A	−162.41 (14)	N3A—C4A—C5A—C6A	−1.5 (2)
O12A—S1A—N2A—C2A	−35.47 (17)	C42A—C4A—C5A—C6A	179.47 (15)
C11A—S1A—N2A—C2A	81.46 (16)	C4A—C5A—C6A—C62A	−178.97 (15)
O11A—S1A—C11A—C21A	−28.19 (15)	C4A—C5A—C6A—N1A	1.0 (2)
O11A—S1A—C11A—C61A	150.90 (13)	S1A—C11A—C21A—C31A	178.90 (13)
O12A—S1A—C11A—C21A	−162.20 (12)	C61A—C11A—C21A—C31A	−0.2 (2)
O12A—S1A—C11A—C61A	16.88 (15)	S1A—C11A—C61A—C51A	−178.95 (12)
N2A—S1A—C11A—C21A	82.26 (14)	C21A—C11A—C61A—C51A	0.1 (2)
N2A—S1A—C11A—C61A	−98.65 (14)	C11A—C21A—C31A—C41A	0.3 (2)
C6A—N1A—C2A—N2A	177.49 (14)	C21A—C31A—C41A—C51A	−0.3 (2)
C6A—N1A—C2A—N3A	−1.2 (2)	C21A—C31A—C41A—N41A	−180.00 (16)
C2A—N1A—C6A—C5A	0.3 (2)	C31A—C41A—C51A—C61A	0.3 (2)
C2A—N1A—C6A—C62A	−179.73 (14)	N41A—C41A—C51A—C61A	179.94 (16)
S1A—N2A—C2A—N1A	154.00 (12)	C41A—C51A—C61A—C11A	−0.2 (2)
S1A—N2A—C2A—N3A	−27.3 (2)	O1—C1—C2—N2	6.3 (2)
C4A—N3A—C2A—N1A	0.7 (2)	O1—C1—C2—C3	−172.77 (15)
C4A—N3A—C2A—N2A	−177.96 (15)	C6—C1—C2—N2	−177.07 (13)
C2A—N3A—C4A—C5A	0.7 (2)	C6—C1—C2—C3	3.8 (2)
C2A—N3A—C4A—C42A	179.73 (14)	O1—C1—C6—N6	−7.2 (2)
O21—N2—C2—C3	−138.41 (16)	O1—C1—C6—C5	173.80 (15)
O22—N2—C2—C1	−137.67 (15)	C2—C1—C6—N6	176.16 (14)

O22—N2—C2—C3	41.5 (2)	C2—C1—C6—C5	−2.8 (2)
O21—N2—C2—C1	42.4 (2)	N2—C2—C3—C4	177.92 (14)
O41—N4—C4—C3	−10.9 (2)	C1—C2—C3—C4	−3.0 (2)
O42—N4—C4—C3	170.19 (15)	C2—C3—C4—N4	−179.35 (14)
O42—N4—C4—C5	−10.0 (2)	C2—C3—C4—C5	0.8 (2)
O41—N4—C4—C5	168.93 (16)	N4—C4—C5—C6	−179.78 (14)
O61—N6—C6—C5	−30.7 (2)	C3—C4—C5—C6	0.0 (2)
O62—N6—C6—C1	−32.2 (2)	C4—C5—C6—N6	−177.92 (14)
O62—N6—C6—C5	146.91 (16)	C4—C5—C6—C1	1.1 (2)
O61—N6—C6—C1	150.26 (16)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···O1	0.91 (2)	1.70 (2)	2.5545 (19)	154 (2)
N1*A*—H1*A*···O21	0.91 (2)	2.46 (2)	2.974 (2)	116.2 (18)
N2*A*—H2*A*···O1	0.85 (2)	2.07 (2)	2.7661 (19)	139.2 (17)
N2*A*—H2*A*···O62	0.85 (2)	2.59 (2)	3.319 (2)	145.0 (15)
N41*A*—H41*A*···O12*A*^{i}	0.90 (2)	2.16 (2)	3.035 (2)	163 (2)

Symmetry code: (i) *x*+1, *y*, *z*.