Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dipotassium disulfanilamidate trihydrate

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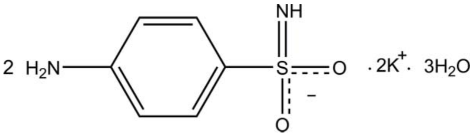
Received 3 July 2011; accepted 5 July 2011

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.015; wR factor = 0.042; data-to-parameter ratio = 14.9.

The asymmetric unit of the title compound, $2K^+\cdot 2C_6H_7N_2O_2S^-\cdot 3H_2O$, consists of two potassium cations located on mirror planes, one sulfanilamidate anion in a general position and one and a half molecules of water, one of which is also located on a mirror plane. One potassium cation is seven-coordinated by six sulfonyl O atoms and one water molecule, whereas the other is surrounded by six water O atoms and two sulfonyl O atoms. In the crystal structure, the components are connected into polymeric sheets in the *bc* plane. The two-dimensional structure is consolidated by N—H⋯O, O—H⋯O, O—H⋯N and C—H⋯π interactions. The layers are further linked into a three-dimensional network *via* N—H⋯O, N—H⋯N and O—H⋯N hydrogen bonds.

Related literature

For the structures of similar potassium salts, see: Gowda *et al.* (2011) and references cited therein; Moers *et al.* (2001). For the structure of sodium sulfanilamide monohydrate, see: Moreno & Alleaume (1968).



Experimental

Crystal data

$2K^+\cdot 2C_6H_7N_2O_2S^-\cdot 3H_2O$
M_r = 474.64
Orthorhombic, $Cmc2_1$
a = 23.8174 (4) Å
b = 10.9141 (2) Å
c = 7.4645 (1) Å
V = 1940.36 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.75 mm^{-1}
T = 100 K
0.33 × 0.27 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) $T_{\min}$ = 0.791, $T_{\max}$ = 0.929
8594 measured reflections
2157 independent reflections
2149 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.015
$wR(F^2)$ = 0.042
S = 1.11
2157 reflections
145 parameters
7 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$ = 0.26 e Å^{-3}
$\Delta\rho_{\min}$ = −0.23 e Å^{-3}
Absolute structure: Flack (1983), 985 Friedel pairs
Flack parameter: 0.04 (3)

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

Cg1 is the centroid of the C1–C6 ring.

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1⋯O1$^{\rm i}$	0.88 (1)	2.17 (1)	2.9854 (15)	154 (2)
N2—H2A⋯N1$^{\rm ii}$	0.90 (1)	2.13 (1)	3.0109 (16)	166 (1)
N2—H2B⋯O3$^{\rm iii}$	0.91 (1)	2.12 (1)	3.0183 (15)	171 (1)
O3—H3A⋯N2$^{\rm iv}$	0.85 (2)	1.99 (2)	2.8366 (15)	172 (2)
O3—H3B⋯O2$^{\rm v}$	0.83 (2)	1.95 (2)	2.7561 (13)	164 (2)
O4—H4⋯N1$^{\rm vi}$	0.79 (1)	2.05 (1)	2.8291 (14)	175 (2)
C2—H2⋯Cg1$^{\rm i}$	0.95	2.98	3.5872 (14)	123
C5—H5⋯Cg1$^{\rm ii}$	0.95	2.66	3.4531 (14)	141

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97* and *publCIF* (Westrip, 2010).

IIUM is acknowledged for funding this study (Endowment fund A No: EDW A10–150-0697).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2446).

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supporting information

Acta Cryst. (2011). E**67**, m1071 [doi:10.1107/S1600536811026791]

Dipotassium disulfanilamidate trihydrate

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S1. Comment

The title potassium salt (Fig. 1) was obtained through the deprotonation of sulfanilamide by KOH. The structure contains two types of potassium cation, one of which, K1, is hepta-coordinated by six sulfonyl O atoms and one water molecule while the other one, K2, is octa-coordinated by six water O atoms and two sulfonyl O atoms. Both potassium atoms and one water oxygen atom, O4, are placed on a mirror plane.

The bond distance of S—N [1.5410 (12) Å] implies its double bond character and is slightly shorter than the observed values (~ 1.58 Å) in similar potassium salts (Gowda *et al.*, 2011; Moers *et al.*, 2001), but comparable with the bond length reported for sodium sulfanilamide (Moreno & Alleaume, 1968). The S1—O1 and S1—O2 distances of 1.4686 (9) and 1.4705 (9) Å attest to delocalization of the negative charge over the O—S—O fragment. These values are similar to the corresponding values in sodium sulfanilamide (1.45–1.46 Å).

In the crystal, coordination polymeric layers are formed in the *bc* plane (Fig. 2). The two dimensional structure is supplemented by N—H···O, O—H···O, O—H···N and C—H···π interactions (Table 1). The layers are further linked into a three dimensional network *via* N—H···O, N—H···N and O—H···N hydrogen bonds (Fig. 3)

S2. Experimental

Sulfanilamide (2 g) in ethanol (30 ml) was mixed with an equimolar amount of KOH in 90% ethanol (10 ml). The solution was then refluxed for 2 hr and left to cool down at room temperature. The colorless crystals of the the potassium salt were obtained within a day.

S3. Refinement

The C-bound H atoms were placed at calculated positions and were treated as riding on their parent C atoms with C—H = 0.95 Å. The N– and O-bound H atoms were located in a difference Fourier map, and refined with distance restraints of O—H = 0.84 (2) Å and N—H = 0.91 (2) Å. For all H atoms, U_{iso}(H) was set to 1.2(1.5 for hydroxyl)U_{eq}(carrier atom). An absolute structure was established using anomalous dispersion effects; 985 Friedel pairs were not merged.

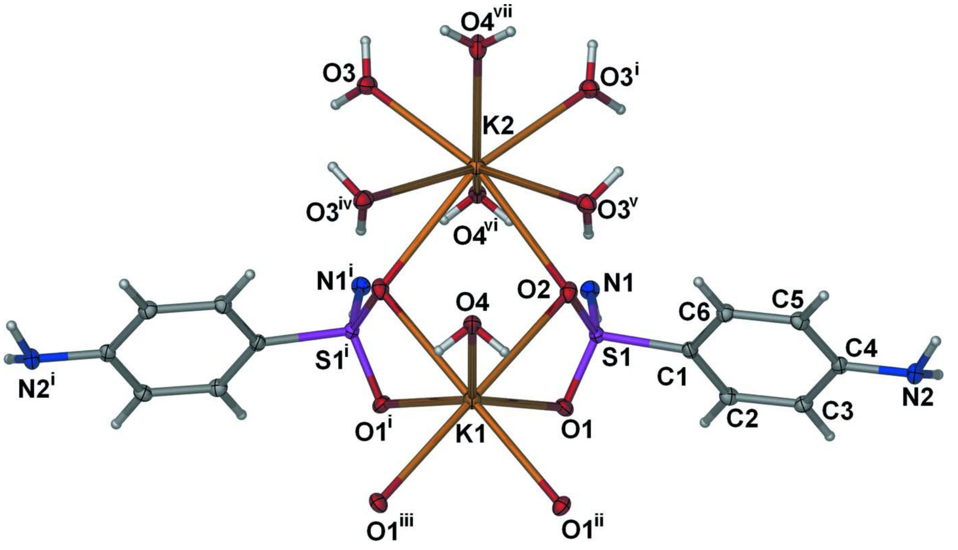

Figure 1

Thermal ellipsoid plot of the title compound at the 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius. Symmetry code: i = -*x* + 1, *y*, *z*; ii = *x*, -*y* + 1, *z* + 1/2; iii = -*x* + 1, -*y* + 1, *z* + 1/2; iv = *x*, -*y*, *z* + 1/2; v = -*x* + 1, -*y*, *z* + 1/2; vi = *x*, *y*, *z* - 1; vii = -*x* + 1, -*y*, *z* - 1/2.

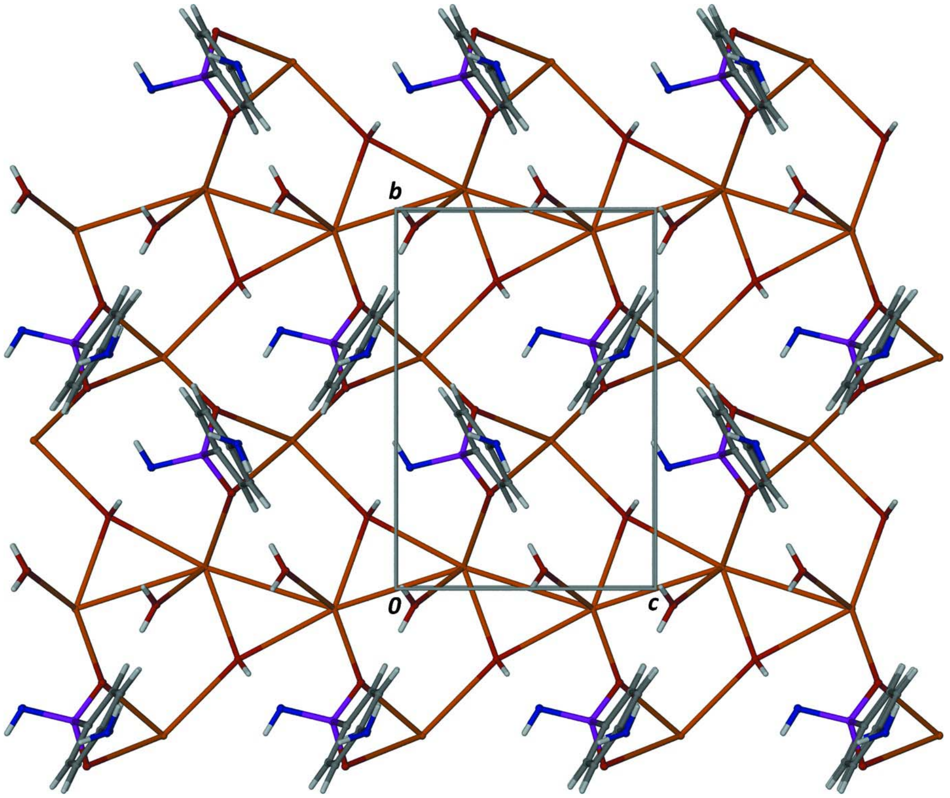

Figure 2

Packing view looking down the crystallographic *α* axis showing the two dimensional coordination polymer netwrok.

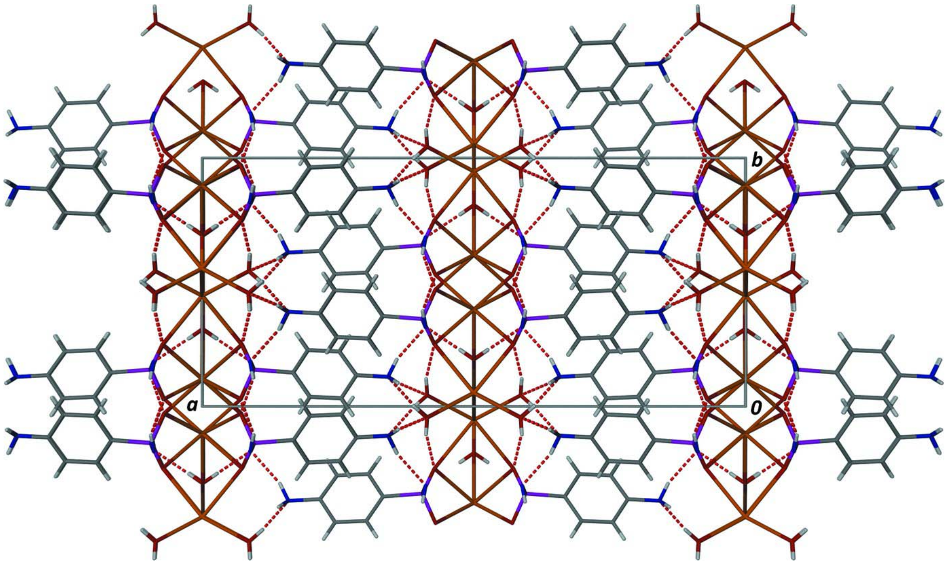

Figure 3

Packing view looking down the crystallographic *c* axis. H-bonds are shown as red dashed lines.

Dipotassium disulfanilamidate trihydrate

Crystal data

$2K^+\cdot 2C_6H_7N_2O_2S^-\cdot 3H_2O$
$M_r = 474.64$
Orthorhombic, *Cmc*2₁
Hall symbol: C 2c -2
$a = 23.8174\ (4)$ Å
$b = 10.9141\ (2)$ Å
$c = 7.4645\ (1)$ Å
$V = 1940.36\ (5)$ Å^3
$Z = 4$
$F(000) = 984$
$D_x = 1.625$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9001 reflections
$\theta = 2.7$–$30.5°$
$\mu = 0.75$ mm^{-1}
$T = 100$ K
Blade, colorless
0.33 × 0.27 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.791$, $T_{\max} = 0.929$
8594 measured reflections
2157 independent reflections
2149 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.015$
$\theta_{\max} = 27.0°$, $\theta_{\min} = 2.1°$
$h = -30 \rightarrow 30$
$k = -13 \rightarrow 13$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.015$
$wR(F^2) = 0.042$
$S = 1.11$
2157 reflections
145 parameters
7 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

$w = 1/[\sigma^2(F_o^2) + (0.0201P)^2 + 1.0371P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}
Absolute structure: Flack (1983), 985 Friedel pairs
Absolute structure parameter: 0.04 (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*	$U_{iso}*/U_{eq}$
K1	0.5000	0.39021 (4)	0.59975 (5)	0.01535 (8)
K2	0.5000	0.05477 (3)	0.26065 (6)	0.01442 (8)
S1	0.404982 (11)	0.35192 (2)	0.25404 (4)	0.01158 (7)
O1	0.42926 (4)	0.47094 (8)	0.30427 (12)	0.01535 (19)
O2	0.42708 (4)	0.25122 (8)	0.36386 (12)	0.01634 (19)
N1	0.41122 (4)	0.31915 (11)	0.05418 (15)	0.0147 (2)
H1	0.4057 (7)	0.3869 (13)	−0.007 (2)	0.018*
N2	0.15806 (5)	0.38097 (11)	0.38621 (15)	0.0148 (2)
H2A	0.1423 (6)	0.3121 (13)	0.430 (2)	0.018*
H2B	0.1402 (6)	0.4057 (14)	0.285 (2)	0.018*
C1	0.33256 (5)	0.36379 (11)	0.30816 (17)	0.0124 (2)
C2	0.30175 (5)	0.46150 (10)	0.23864 (18)	0.0138 (2)
H2	0.3202	0.5243	0.1732	0.017*
C3	0.24417 (5)	0.46705 (10)	0.26498 (19)	0.0134 (2)
H3	0.2234	0.5342	0.2183	0.016*
C4	0.21636 (5)	0.37450 (11)	0.35982 (16)	0.0126 (2)
C5	0.24773 (5)	0.27905 (12)	0.43346 (18)	0.0144 (2)
H5	0.2295	0.2175	0.5023	0.017*
C6	0.30546 (5)	0.27342 (11)	0.40674 (17)	0.0138 (2)
H6	0.3265	0.2075	0.4561	0.017*
O3	0.58605 (4)	−0.04452 (9)	0.07181 (13)	0.0173 (2)
H3A	0.6103 (6)	0.0020 (18)	0.023 (3)	0.026*
H3B	0.5880 (8)	−0.1110 (15)	0.019 (3)	0.026*
O4	0.5000	0.18900 (13)	0.8893 (2)	0.0207 (3)
H4	0.4747 (6)	0.2267 (16)	0.929 (3)	0.031*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1	0.01301 (16)	0.01830 (18)	0.01474 (17)	0.000	0.000	−0.00331 (15)
K2	0.01360 (16)	0.01577 (17)	0.01391 (16)	0.000	0.000	−0.00172 (17)

S1	0.01032 (12)	0.01235 (13)	0.01206 (13)	−0.00085 (9)	0.00042 (13)	0.00013 (13)
O1	0.0144 (4)	0.0149 (4)	0.0168 (5)	−0.0035 (3)	0.0009 (3)	−0.0022 (3)
O2	0.0134 (4)	0.0169 (4)	0.0188 (5)	0.0009 (3)	−0.0002 (4)	0.0048 (4)
N1	0.0158 (5)	0.0161 (5)	0.0123 (5)	−0.0002 (4)	0.0024 (4)	−0.0005 (4)
N2	0.0118 (5)	0.0178 (5)	0.0148 (5)	0.0007 (4)	0.0004 (4)	0.0019 (4)
C1	0.0113 (6)	0.0142 (5)	0.0118 (5)	−0.0010 (5)	0.0009 (4)	−0.0027 (4)
C2	0.0163 (5)	0.0129 (5)	0.0120 (6)	−0.0015 (4)	0.0019 (5)	0.0017 (5)
C3	0.0157 (5)	0.0123 (5)	0.0121 (5)	0.0017 (4)	−0.0004 (5)	0.0008 (5)
C4	0.0121 (6)	0.0156 (6)	0.0102 (6)	−0.0001 (5)	0.0009 (4)	−0.0028 (5)
C5	0.0161 (6)	0.0136 (5)	0.0136 (5)	−0.0019 (5)	0.0017 (5)	0.0016 (5)
C6	0.0139 (6)	0.0134 (5)	0.0142 (6)	0.0010 (4)	−0.0007 (5)	0.0016 (5)
O3	0.0177 (4)	0.0155 (4)	0.0187 (5)	−0.0009 (3)	0.0033 (4)	−0.0010 (4)
O4	0.0135 (7)	0.0205 (7)	0.0280 (8)	0.000	0.000	−0.0097 (6)

Geometric parameters (Å, º)

K1—O1$^{\mathrm{i}}$	2.7325 (9)	N1—H1	0.878 (14)
K1—O1$^{\mathrm{ii}}$	2.7325 (9)	N2—C4	1.4044 (16)
K1—O2$^{\mathrm{iii}}$	2.9014 (10)	N2—H2A	0.903 (13)
K1—O2	2.9014 (10)	N2—H2B	0.906 (14)
K1—O1	2.9121 (10)	C1—C6	1.3895 (17)
K1—O1$^{\mathrm{iii}}$	2.9121 (10)	C1—C2	1.3947 (17)
K1—O4	3.0810 (16)	C2—C3	1.3868 (17)
K2—O3	2.7133 (10)	C2—H2	0.9500
K2—O3$^{\mathrm{iii}}$	2.7133 (10)	C3—C4	1.4000 (17)
K2—O4$^{\mathrm{iv}}$	2.8285 (15)	C3—H3	0.9500
K2—O2$^{\mathrm{iii}}$	2.8648 (10)	C4—C5	1.3948 (18)
K2—O2	2.8648 (10)	C5—C6	1.3908 (17)
K2—O3$^{\mathrm{v}}$	3.0996 (10)	C5—H5	0.9500
K2—O3$^{\mathrm{vi}}$	3.0996 (10)	C6—H6	0.9500
K2—O4$^{\mathrm{vii}}$	3.1355 (17)	O3—K2$^{\mathrm{iv}}$	3.0996 (10)
S1—O2	1.4686 (9)	O3—H3A	0.852 (15)
S1—O1	1.4705 (9)	O3—H3B	0.828 (15)
S1—N1	1.5413 (12)	O4—K2$^{\mathrm{vi}}$	2.8284 (15)
S1—C1	1.7763 (13)	O4—K2$^{\mathrm{ix}}$	3.1355 (17)
O1—K1$^{\mathrm{viii}}$	2.7324 (9)	O4—H4	0.787 (13)
O1$^{\mathrm{i}}$—K1—O1$^{\mathrm{ii}}$	76.15 (4)	O3$^{\mathrm{vi}}$—K2—O4$^{\mathrm{vii}}$	132.79 (2)
O1$^{\mathrm{i}}$—K1—O2$^{\mathrm{iii}}$	105.06 (3)	O2—S1—O1	112.21 (6)
O1$^{\mathrm{ii}}$—K1—O2$^{\mathrm{iii}}$	176.54 (3)	O2—S1—N1	109.40 (6)
O1$^{\mathrm{i}}$—K1—O2	176.54 (3)	O1—S1—N1	114.44 (6)
O1$^{\mathrm{ii}}$—K1—O2	105.06 (3)	O2—S1—C1	106.00 (6)
O2$^{\mathrm{iii}}$—K1—O2	73.54 (4)	O1—S1—C1	105.03 (6)
O1$^{\mathrm{i}}$—K1—O1	127.75 (2)	N1—S1—C1	109.31 (6)
O1$^{\mathrm{ii}}$—K1—O1	84.18 (2)	S1—O1—K1$^{\mathrm{viii}}$	126.15 (5)
O2$^{\mathrm{iii}}$—K1—O1	92.57 (3)	S1—O1—K1	98.82 (4)
O2—K1—O1	49.62 (3)	K1$^{\mathrm{viii}}$—O1—K1	103.54 (3)
O1$^{\mathrm{i}}$—K1—O1$^{\mathrm{iii}}$	84.18 (2)	S1—O2—K2	128.84 (5)

O1^{ii}—K1—O1^{iii}	127.75 (2)
O2^{iii}—K1—O1^{iii}	49.62 (3)
O2—K1—O1^{iii}	92.58 (3)
O1—K1—O1^{iii}	70.71 (4)
O1^{i}—K1—O4	90.20 (3)
O1^{ii}—K1—O4	90.20 (3)
O2^{iii}—K1—O4	93.04 (3)
O2—K1—O4	93.04 (3)
O1—K1—O4	138.32 (2)
O1^{iii}—K1—O4	138.32 (2)
O3—K2—O3^{iii}	98.12 (4)
O3—K2—O4^{iv}	78.50 (3)
O3^{iii}—K2—O4^{iv}	78.50 (3)
O3—K2—O2^{iii}	88.89 (3)
O3^{iii}—K2—O2^{iii}	153.71 (3)
O4^{iv}—K2—O2^{iii}	127.79 (3)
O3—K2—O2	153.71 (3)
O3^{iii}—K2—O2	88.89 (3)
O4^{iv}—K2—O2	127.78 (3)
O2^{iii}—K2—O2	74.64 (4)
O3—K2—O3^{v}	82.84 (3)
O3^{iii}—K2—O3^{v}	150.97 (2)
O4^{iv}—K2—O3^{v}	73.24 (3)
O2^{iii}—K2—O3^{v}	54.88 (3)
O2—K2—O3^{v}	103.08 (3)
O3—K2—O3^{vi}	150.97 (2)
O3^{iii}—K2—O3^{vi}	82.84 (3)
O4^{iv}—K2—O3^{vi}	73.24 (3)
O2^{iii}—K2—O3^{vi}	103.08 (3)
O2—K2—O3^{vi}	54.87 (3)
O3^{v}—K2—O3^{vi}	82.79 (4)
O3—K2—O4^{vii}	74.17 (3)
O3^{iii}—K2—O4^{vii}	74.17 (3)
O4^{iv}—K2—O4^{vii}	137.70 (5)
O2^{iii}—K2—O4^{vii}	83.57 (3)
O2—K2—O4^{vii}	83.57 (3)
O3^{v}—K2—O4^{vii}	132.79 (2)
S1—O2—K1	99.32 (5)
K2—O2—K1	101.04 (3)
S1—N1—H1	106.9 (11)
C4—N2—H2A	114.8 (10)
C4—N2—H2B	111.3 (10)
H2A—N2—H2B	110.9 (15)
C6—C1—C2	119.69 (11)
C6—C1—S1	121.31 (10)
C2—C1—S1	118.83 (10)
C3—C2—C1	120.07 (11)
C3—C2—H2	120.0
C1—C2—H2	120.0
C2—C3—C4	120.53 (11)
C2—C3—H3	119.7
C4—C3—H3	119.7
C5—C4—C3	119.00 (11)
C5—C4—N2	120.79 (11)
C3—C4—N2	120.15 (11)
C6—C5—C4	120.40 (12)
C6—C5—H5	119.8
C4—C5—H5	119.8
C1—C6—C5	120.25 (11)
C1—C6—H6	119.9
C5—C6—H6	119.9
K2—O3—K2^{iv}	84.51 (3)
K2—O3—H3A	119.9 (14)
K2^{iv}—O3—H3A	98.5 (13)
K2—O3—H3B	129.9 (13)
K2^{iv}—O3—H3B	69.3 (13)
H3A—O3—H3B	106 (2)
K2^{vi}—O4—K1	115.62 (5)
K2^{vi}—O4—K2^{ix}	81.99 (4)
K1—O4—K2^{ix}	162.39 (5)
K2^{vi}—O4—H4	128.2 (13)
K1—O4—H4	83.7 (15)
K2^{ix}—O4—H4	85.1 (16)

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

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{x}	0.88 (1)	2.17 (1)	2.9854 (15)	154 (2)
N2—H2*A*···N1^{xi}	0.90 (1)	2.13 (1)	3.0109 (16)	166 (1)
N2—H2*B*···O3^{xii}	0.91 (1)	2.12 (1)	3.0183 (15)	171 (1)
O3—H3*A*···N2^{xiii}	0.85 (2)	1.99 (2)	2.8366 (15)	172 (2)

O3—H3*B*···O2^{iv}	0.83 (2)	1.95 (2)	2.7561 (13)	164 (2)
O4—H4···N1^{ix}	0.79 (1)	2.05 (1)	2.8291 (14)	175 (2)
C2—H2···*Cg*1^{x}	0.95	2.98	3.5872 (14)	123
C5—H5···*Cg*1^{xi}	0.95	2.66	3.4531 (14)	141

Symmetry codes: (iv) −*x*+1, −*y*, *z*−1/2; (ix) *x*, *y*, *z*+1; (x) *x*, −*y*+1, *z*−1/2; (xi) −*x*+1/2, −*y*+1/2, *z*+1/2; (xii) *x*−1/2, *y*+1/2, *z*; (xiii) *x*+1/2, −*y*+1/2, *z*−1/2.