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Chain and ring motifs in bis(creatininium) sulfate

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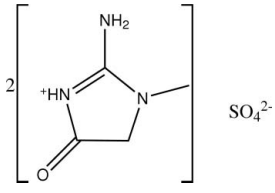
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.085; data-to-parameter ratio = 10.9.

The title compound, $2C_4H_8N_3O^+\cdot SO_4^{2-}$, crystallizes with two creatininium cations and one sulfate anion in the asymmetric unit. Cations and anions dimerize through N—H···O hydrogen bonds forming $R_2^2(8)$ ring motifs. Furthermore, these rings are connected *via* N—H···O hydrogen bonds, leading to $C_2^2(6)$ and $C_2^2(8)$ chain motifs. These interactions lead to a parallel set of hydrogen-bonded lamellar aggregations propagating along the *c* axis of the unit cell. Another cation is situated above these sheets, leading to a grid-like structure.

Related literature

For related structures, see Bahadur, Kannan *et al.* (2007); Bahadur, Sivapragasam *et al.* (2007). For the notation of hydrogen-bonding motifs, see Bernstein *et al.* (1995). For information on the biological importance of creatinine, refer to Madaras & Buck (1996); Narayanan & Appleton (1980).



Experimental

Crystal data

$2C_4H_8N_3O^+\cdot SO_4^{2-}$
M_r = 324.33
Monoclinic, $P2_1/c$
a = 12.469 (6) Å
b = 7.560 (3) Å
c = 14.382 (9) Å
β = 97.347 (11)°
V = 1344.6 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 293 (2) K
0.23 × 0.20 × 0.17 mm

Data collection

Nonius MACH3 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.948, T_{max} = 0.960
2856 measured reflections
2343 independent reflections
2073 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.085
S = 1.06
2343 reflections
214 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N14—H14···O13^{i}	0.90 (3)	1.74 (3)	2.639 (2)	176 (2)
N15—H15A···O12^{ii}	0.92 (3)	1.99 (3)	2.879 (2)	163 (2)
N15—H15B···O11^{i}	0.81 (3)	2.42 (3)	3.171 (3)	154 (3)
N24—H24···O12	0.87 (3)	1.83 (3)	2.693 (2)	173 (2)
N25—H25A···O14^{iii}	0.87 (2)	2.01 (3)	2.882 (3)	174 (2)
N25—H25B···O11	0.86 (3)	2.08 (3)	2.928 (3)	169 (2)

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEP-3* (Farrugia, 1997), *Mercury* (Macrae *et al.*, 2006) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2364).

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supplementary materials

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Chain and ring motifs in bis(creatininium) sulfate

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Comment

Creatine, a nitrogenous organic acid, is found in the muscle tissue of vertebrates mainly in the form of phosphocreatine and supplies energy for muscle contraction. It is a derivative of the amino acids glycine and arginine, important in muscle as a store of phosphate for resynthesis of ATP during muscle contraction and work. In renal physiology, creatinine clearance (Madaras & Buck, 1996) is the volume of blood plasma that is cleared of creatinine per unit time. Clinically, creatinine clearance is a useful measure for estimating the Glomerular Filtration Rate (GFR) of the kidneys. An abnormal level of creatinine in biological fluids is an indicator of various disease states (Narayanan & Appleton, 1980).

The asymmetric unit of the title compound, (I), $2(C_4H_8N_3O^+)\cdot SO_4^{2-}$, consists of two crystallographically independent protonated creatine residues and one sulfate anion (Fig. 1). Two protons of the sulfuric acid have migrated to protonate two creatine molecules forming creatinium cations. The protonation on this site is evident from the C—N bond distances and the values are comparable with creatinium hydrogen oxalate monohydrate (Bahadur, Kannan *et al.*, 2007) and creatinium benzoate (Bahadur, Sivapragasam *et al.*, 2007). Both the cations are oriented nearly perpendicular to each other with a dihedral angle of 86.45 (6)° between them.

The crystal structure is stabilized by an intricate three dimensional N—H···O hydrogen bonding network (Fig. 2; Table 2). Cations are linked to anions forming ion pairs through N—H···O hydrogen bonds that produce $R_2^2(8)$ ring motifs (Bernstein *et al.*, 1995). Further these rings are connected *via* N—H···O hydrogen bonds leading to chain $C_2^2(6)$ and $C_2^2(8)$ motifs (Fig. 3). These ring and chain motifs result in lamellar aggreation or parallel sheets along the *c* axis of the unit cell in opposing directions. Another cation is situated just above these sheets through another $R_2^2(8)$ motif forming a grid-like structure.

Experimental

The title compound was crystallized from an aqueous mixture containing creatinine and sulfuric acid in the stoichiometric ratio of 2:1 at room temperature by the slow evaporation technique.

Refinement

H atoms involved in the H-bonding interactions were located from a difference Fourier map and refined isotropically. All other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2–1.5 U_{eq} (parent atom).

Figures

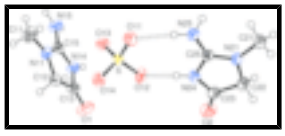

Fig. 1. The molecular structure of the title compound (I) with the numbering scheme for the atoms and 50% probability displacement ellipsoids. H bonds are drawn as double dashed lines.

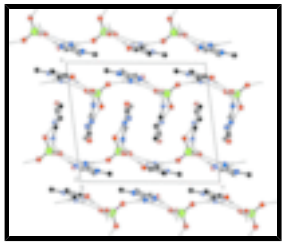

Fig. 2. Packing diagram of the molecules viewed down the *b*-axis. H atoms not involved in the H-bonds (dashed lines) are omitted for clarity.

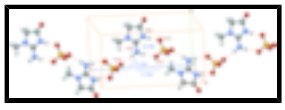

Fig. 3. A view of $R_2^2(8)$ ring and $C_2^2(6)$ and $C_2^2(8)$ chain motifs formed through one of the cations and the anion. H bonds are drawn as dashed lines.

bis(creatininium) sulfate

Crystal data

$2C_4H_8N_3O^+·SO_4^{2-}$	F_{000} = 680
M_r = 324.33	D_x = 1.602 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71069 Å
Hall symbol: -P 2ybc	Cell parameters from 25 reflections
a = 12.469 (6) Å	θ = 9.6–14.1°
b = 7.560 (3) Å	μ = 0.28 mm^{-1}
c = 14.382 (9) Å	T = 293 (2) K
β = 97.347 (11)°	Block, colourless
V = 1344.6 (12) Å^3	0.23 × 0.20 × 0.17 mm
Z = 4	

Data collection

Nonius MACH3 diffractometer	R_{int} = 0.013
Radiation source: fine-focus sealed tube	θ_{max} = 25.0°
Monochromator: graphite	θ_{min} = 2.9°
T = 293(2) K	h = 0→14
ω–2θ scans	k = −1→8
Absorption correction: ψ scan (North *et al.*, 1968)	l = −17→16
T_{min} = 0.948, T_{max} = 0.960	3 standard reflections
2856 measured reflections	every 60 min
2343 independent reflections	intensity decay: none
2073 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.031$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.085$	$w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 0.7548P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
2343 reflections	$\Delta\rho_{max} = 0.22$ e Å^{-3}
214 parameters	$\Delta\rho_{min} = -0.35$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2$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}
C11	0.4691 (2)	0.1587 (3)	0.09121 (18)	0.0539 (6)
H11A	0.5429	0.1199	0.1028	0.081*
H11B	0.4385	0.1225	0.0295	0.081*
H11C	0.4286	0.1071	0.1368	0.081*
N11	0.46512 (12)	0.3494 (2)	0.09796 (11)	0.0328 (4)
C12	0.36537 (14)	0.4484 (3)	0.07720 (13)	0.0329 (4)
H12A	0.3110	0.4072	0.1147	0.039*
H12B	0.3371	0.4399	0.0113	0.039*
C13	0.40016 (15)	0.6342 (3)	0.10316 (13)	0.0351 (4)
O1	0.34592 (12)	0.7661 (2)	0.09920 (13)	0.0581 (5)
N14	0.50903 (13)	0.6252 (2)	0.13392 (12)	0.0340 (4)
N15	0.64548 (15)	0.4119 (3)	0.16074 (14)	0.0446 (4)
C15	0.54436 (15)	0.4556 (3)	0.13264 (12)	0.0310 (4)
H14	0.5512 (19)	0.714 (3)	0.1593 (17)	0.053 (7)*
H15A	0.668 (2)	0.297 (4)	0.1600 (18)	0.063*
H15B	0.687 (2)	0.495 (4)	0.1682 (19)	0.063*
C21	0.06709 (18)	0.5279 (3)	0.71596 (14)	0.0439 (5)

H21A	0.0873	0.4054	0.7183	0.066*
H21B	−0.0090	0.5382	0.7197	0.066*
H21C	0.1069	0.5895	0.7677	0.066*
N21	0.09134 (12)	0.60459 (19)	0.62860 (10)	0.0302 (3)
C22	0.07541 (16)	0.7917 (2)	0.60682 (13)	0.0344 (4)
H22A	0.1194	0.8653	0.6520	0.041*
H22B	0.0001	0.8252	0.6053	0.041*
C23	0.11147 (15)	0.8053 (2)	0.51119 (13)	0.0337 (4)
O2	0.12097 (13)	0.93682 (19)	0.46507 (11)	0.0522 (4)
N24	0.13415 (12)	0.6355 (2)	0.48531 (11)	0.0291 (3)
N25	0.15128 (14)	0.3535 (2)	0.55284 (13)	0.0351 (4)
C25	0.12714 (13)	0.5222 (2)	0.55775 (11)	0.0253 (4)
H24	0.1656 (19)	0.609 (3)	0.4365 (17)	0.050 (7)*
H25A	0.1556 (18)	0.286 (3)	0.6023 (17)	0.046 (6)*
H25B	0.1728 (19)	0.316 (3)	0.5017 (17)	0.047 (6)*
S	0.25681 (3)	0.39808 (5)	0.30401 (3)	0.02599 (14)
O11	0.23687 (12)	0.27155 (18)	0.37745 (10)	0.0429 (4)
O12	0.24043 (12)	0.58043 (16)	0.33621 (10)	0.0388 (3)
O13	0.36978 (10)	0.38111 (19)	0.28408 (9)	0.0400 (3)
O14	0.18331 (10)	0.36562 (18)	0.21808 (9)	0.0370 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0665 (15)	0.0276 (11)	0.0668 (15)	−0.0012 (10)	0.0050 (12)	−0.0057 (10)
N11	0.0348 (8)	0.0283 (8)	0.0361 (8)	−0.0017 (7)	0.0074 (7)	−0.0032 (6)
C12	0.0307 (9)	0.0368 (10)	0.0316 (9)	−0.0045 (8)	0.0054 (7)	−0.0020 (8)
C13	0.0319 (9)	0.0339 (10)	0.0388 (10)	−0.0005 (8)	0.0019 (8)	0.0007 (8)
O1	0.0420 (8)	0.0379 (9)	0.0906 (13)	0.0094 (7)	−0.0067 (8)	−0.0055 (8)
N14	0.0305 (8)	0.0272 (8)	0.0432 (9)	−0.0018 (7)	0.0010 (7)	−0.0036 (7)
N15	0.0357 (10)	0.0387 (10)	0.0572 (11)	0.0060 (8)	−0.0025 (8)	−0.0039 (9)
C15	0.0345 (10)	0.0325 (10)	0.0264 (8)	0.0010 (8)	0.0061 (7)	0.0000 (7)
C21	0.0497 (12)	0.0510 (13)	0.0340 (10)	0.0146 (10)	0.0171 (9)	0.0072 (9)
N21	0.0358 (8)	0.0272 (8)	0.0290 (8)	0.0026 (6)	0.0095 (6)	−0.0005 (6)
C22	0.0384 (10)	0.0266 (9)	0.0386 (10)	0.0013 (8)	0.0059 (8)	−0.0052 (8)
C23	0.0332 (10)	0.0285 (10)	0.0390 (10)	0.0001 (8)	0.0032 (8)	0.0024 (8)
O2	0.0641 (10)	0.0334 (8)	0.0613 (10)	0.0050 (7)	0.0166 (8)	0.0154 (7)
N24	0.0298 (8)	0.0303 (8)	0.0280 (8)	0.0016 (6)	0.0064 (6)	0.0014 (6)
N25	0.0435 (9)	0.0289 (9)	0.0348 (9)	0.0083 (7)	0.0126 (7)	0.0024 (7)
C25	0.0203 (8)	0.0277 (9)	0.0275 (8)	−0.0001 (7)	0.0019 (6)	−0.0008 (7)
S	0.0302 (2)	0.0229 (2)	0.0256 (2)	0.00194 (17)	0.00626 (17)	0.00078 (16)
O11	0.0582 (9)	0.0341 (7)	0.0387 (7)	0.0008 (6)	0.0154 (6)	0.0096 (6)
O12	0.0516 (8)	0.0265 (7)	0.0417 (7)	−0.0028 (6)	0.0196 (6)	−0.0054 (6)
O13	0.0306 (7)	0.0489 (8)	0.0411 (7)	0.0093 (6)	0.0073 (6)	0.0091 (6)
O14	0.0359 (7)	0.0405 (8)	0.0340 (7)	−0.0020 (6)	0.0021 (5)	−0.0045 (6)

Geometric parameters (Å, °)

C11—N11	1.447 (3)	C21—H21B	0.9600

C11—H11A	0.9600	C21—H21C	0.9600
C11—H11B	0.9600	N21—C25	1.320 (2)
C11—H11C	0.9600	N21—C22	1.457 (2)
N11—C15	1.320 (2)	C22—C23	1.504 (3)
N11—C12	1.450 (2)	C22—H22A	0.9700
C12—C13	1.503 (3)	C22—H22B	0.9700
C12—H12A	0.9700	C23—O2	1.209 (2)
C12—H12B	0.9700	C23—N24	1.376 (2)
C13—O1	1.203 (2)	N24—C25	1.360 (2)
C13—N14	1.375 (3)	N24—H24	0.87 (3)
N14—C15	1.357 (2)	N25—C25	1.315 (2)
N14—H14	0.90 (3)	N25—H25A	0.87 (2)
N15—C15	1.316 (3)	N25—H25B	0.86 (3)
N15—H15A	0.92 (3)	S—O14	1.4621 (15)
N15—H15B	0.81 (3)	S—O11	1.4695 (15)
C21—N21	1.450 (2)	S—O12	1.4768 (14)
C21—H21A	0.9600	S—O13	1.4785 (15)
N11—C11—H11A	109.5	N21—C21—H21C	109.5
N11—C11—H11B	109.5	H21A—C21—H21C	109.5
H11A—C11—H11B	109.5	H21B—C21—H21C	109.5
N11—C11—H11C	109.5	C25—N21—C21	127.52 (16)
H11A—C11—H11C	109.5	C25—N21—C22	110.03 (15)
H11B—C11—H11C	109.5	C21—N21—C22	122.44 (15)
C15—N11—C11	126.92 (18)	N21—C22—C23	102.39 (15)
C15—N11—C12	110.18 (16)	N21—C22—H22A	111.3
C11—N11—C12	122.48 (17)	C23—C22—H22A	111.3
N11—C12—C13	102.61 (14)	N21—C22—H22B	111.3
N11—C12—H12A	111.2	C23—C22—H22B	111.3
C13—C12—H12A	111.2	H22A—C22—H22B	109.2
N11—C12—H12B	111.2	O2—C23—N24	125.49 (18)
C13—C12—H12B	111.2	O2—C23—C22	128.28 (18)
H12A—C12—H12B	109.2	N24—C23—C22	106.23 (15)
O1—C13—N14	125.63 (19)	C25—N24—C23	110.17 (15)
O1—C13—C12	128.37 (18)	C25—N24—H24	123.5 (15)
N14—C13—C12	106.00 (16)	C23—N24—H24	124.3 (15)
C15—N14—C13	110.57 (16)	C25—N25—H25A	121.0 (15)
C15—N14—H14	122.4 (15)	C25—N25—H25B	117.6 (16)
C13—N14—H14	126.6 (15)	H25A—N25—H25B	121 (2)
C15—N15—H15A	121.2 (16)	N25—C25—N21	127.00 (17)
C15—N15—H15B	114.4 (19)	N25—C25—N24	122.17 (17)
H15A—N15—H15B	123 (3)	N21—C25—N24	110.81 (16)
N15—C15—N11	127.21 (19)	O14—S—O11	110.66 (9)
N15—C15—N14	122.22 (18)	O14—S—O12	108.96 (8)
N11—C15—N14	110.55 (16)	O11—S—O12	109.84 (9)
N21—C21—H21A	109.5	O14—S—O13	109.35 (8)
N21—C21—H21B	109.5	O11—S—O13	109.62 (8)
H21A—C21—H21B	109.5	O12—S—O13	108.37 (8)
C15—N11—C12—C13	1.60 (19)	C25—N21—C22—C23	−1.55 (19)

C11—N11—C12—C13	174.59 (18)	C21—N21—C22—C23	179.86 (17)
N11—C12—C13—O1	−179.4 (2)	N21—C22—C23—O2	−174.3 (2)
N11—C12—C13—N14	0.18 (19)	N21—C22—C23—N24	4.73 (19)
O1—C13—N14—C15	177.7 (2)	O2—C23—N24—C25	172.70 (18)
C12—C13—N14—C15	−1.9 (2)	C22—C23—N24—C25	−6.4 (2)
C11—N11—C15—N15	6.3 (3)	C21—N21—C25—N25	−2.1 (3)
C12—N11—C15—N15	178.89 (19)	C22—N21—C25—N25	179.40 (17)
C11—N11—C15—N14	−175.47 (19)	C21—N21—C25—N24	176.20 (18)
C12—N11—C15—N14	−2.9 (2)	C22—N21—C25—N24	−2.3 (2)
C13—N14—C15—N15	−178.63 (18)	C23—N24—C25—N25	−175.95 (16)
C13—N14—C15—N11	3.0 (2)	C23—N24—C25—N21	5.7 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N14—H14···O13^{i}	0.90 (3)	1.74 (3)	2.639 (2)	176 (2)
N15—H15A···O12^{ii}	0.92 (3)	1.99 (3)	2.879 (2)	163 (2)
N15—H15B···O11^{i}	0.81 (3)	2.42 (3)	3.171 (3)	154 (3)
N24—H24···O12	0.87 (3)	1.83 (3)	2.693 (2)	173 (2)
N25—H25A···O14^{iii}	0.87 (2)	2.01 (3)	2.882 (3)	174 (2)
N25—H25B···O11	0.86 (3)	2.08 (3)	2.928 (3)	169 (2)

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

Fig. 1

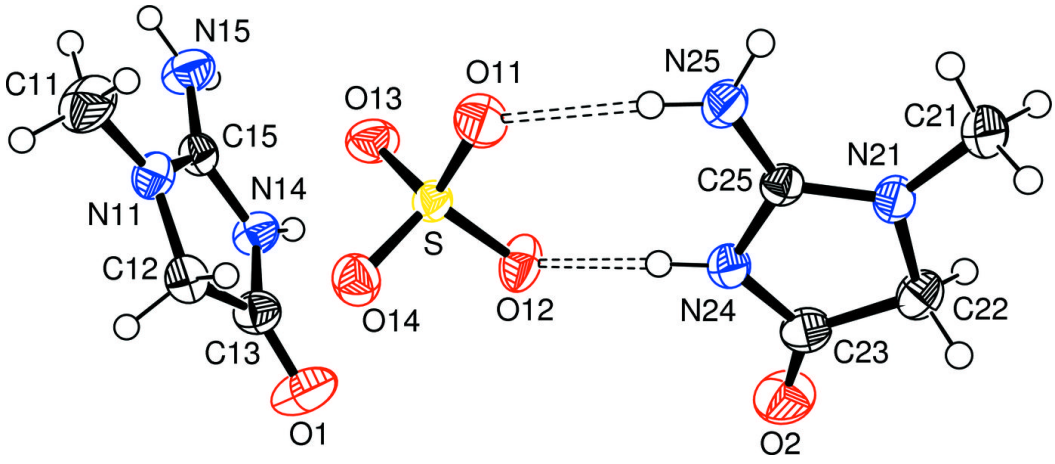
N15
C11
C15
N14
N11
C12
C13
O1
O13
O11
S
O14
O12
N25
C25
N21
C21
N24
C22
C23
O2

Fig. 2

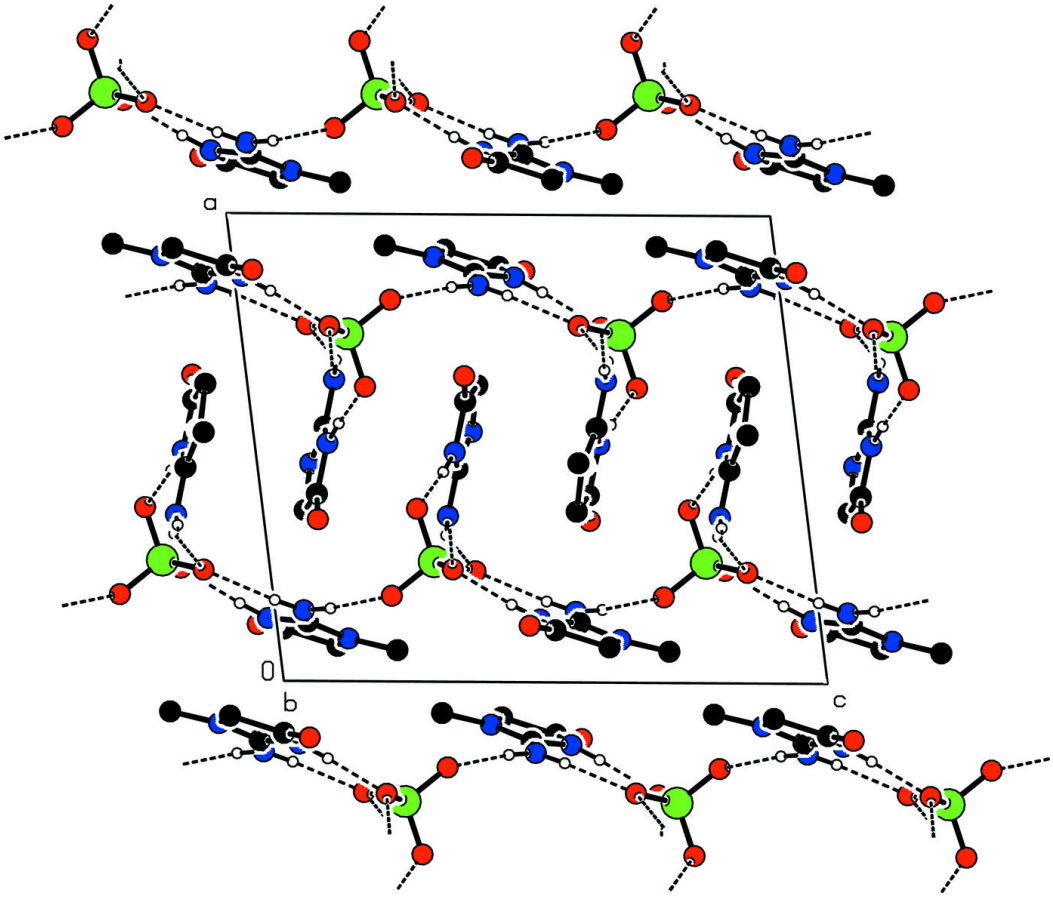

Fig. 3