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Creatininium phosphite

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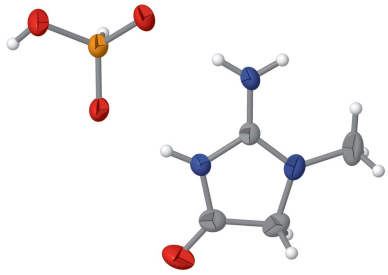
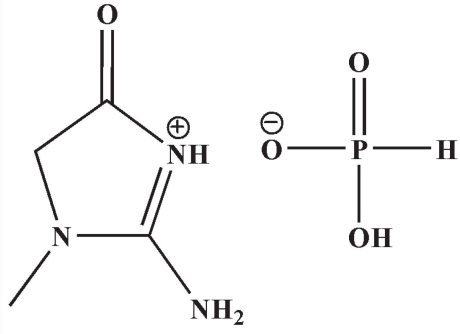
Structural data: full structural data are available from iucrdata.iucr.org

The title salt, $C_4H_8N_3O^+\cdot H_2PO_3^-$, contains a creatininium cation (2-amino-1-methyl-4-oxo-4,5-dihydro-1*H*-imidazol-3-ium) and a phosphite anion. The crystal packing shows layers of hydrogen-bonded ions lying parallel to the $(\bar{1}14)$ and $(11\bar{4})$ planes.

3D view



Chemical scheme



Structure description

Creatinine as one such material is more valuable for the detection of renal dysfunction than urea (Sharma *et al.*, 2004).

The title compound comprises a protonated creatininium cation and a deprotonated phosphite anion (Fig. 1). The geometric parameters of the title ion-pair agree well with those reported for a similar structure (Thayanithi *et al.*, 2016). The crystal packing (Fig. 2) shows planes of hydrogen-bonded ions parallel to the $(\bar{1}14)$ and $(11\bar{4})$ planes (Table 1).

Synthesis and crystallization

The title compound was synthesized by dissolving creatinine (1.1312 g, 0.01 mol) in 30 ml of deionized water. Phosphorus acid (0.82 g, 0.01 mol) was then added slowly. The solution was stirred for 4 h, filtered into a beaker and kept dust-free. Colourless crystals were obtained from the mother solution in 93% yield.

Refinement

Crystal data, data collection and structure refinement details are presented in Table 2.

Acknowledgements

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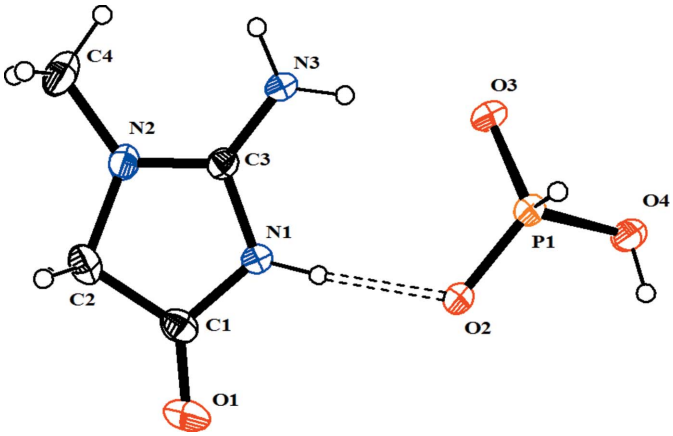

Figure 1
The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids for the non-H atoms.

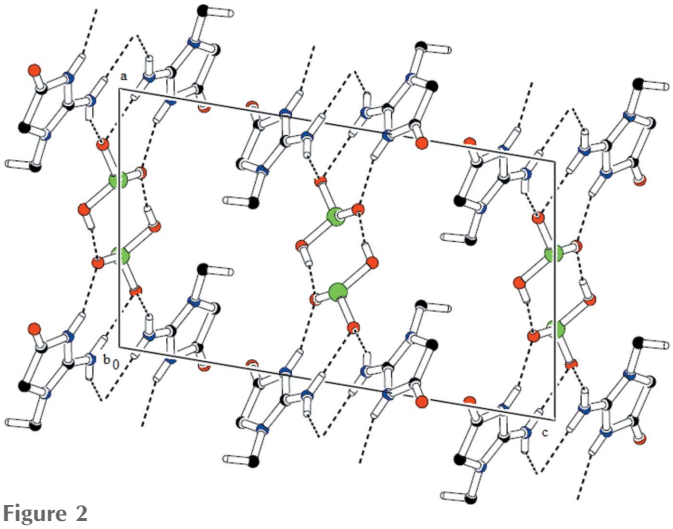

Figure 2
The packing of the title compound, viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2B···O1^{i}	0.97	2.58	2.997 (4)	106
C4—H4A···O4^{ii}	0.96	2.61	3.470 (3)	150
N1—H1···O2	0.86	1.94	2.754 (2)	157
N3—H3A···O3^{iii}	0.86	1.98	2.800 (2)	158
N3—H3B···O3	0.86	1.96	2.821 (2)	178
O4—H4···O2^{iv}	0.82	1.77	2.585 (2)	170

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_4H_8N_3O^+\cdot H_2O_3P^-$
M_r	195.12
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	8.8083 (11), 6.6316 (9), 15.068 (2)
β (°)	99.539 (4)
V (Å^3)	868.0 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.30
Crystal size (mm)	0.20 × 0.20 × 0.15
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 1996)
T_{min}, T_{max}	0.942, 0.956
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17033, 2806, 1735
R_{int}	0.058
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.732
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.056, 0.152, 1.10
No. of reflections	2806
No. of parameters	112
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.41, −0.48

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97*and *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

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full crystallographic data

IUCrData (2017). **2**, x171043 [https://doi.org/10.1107/S2414314617010434]

Creatininium phosphite

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2-Amino-1-methyl-4-oxo-4,5-dihydro-1*H*-imidazol-3-ium phosphite

Crystal data

$C_4H_8N_3O^+·H_2O_3P^-$
M_r = 195.12
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 8.8083 (11) Å
b = 6.6316 (9) Å
c = 15.068 (2) Å
β = 99.539 (4)°
V = 868.0 (2) Å^3
Z = 4
$F(000)$ = 408
D_x = 1.493 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2806 reflections
θ = 2.7–31.3°
μ = 0.30 mm^{-1}
T = 296 K
Block, colourless
0.20 × 0.20 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.942, T_{max} = 0.956
17033 measured reflections
2806 independent reflections
1735 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 31.3°, θ_{min} = 2.7°
h = −12→12
k = −9→9
l = −21→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.152
S = 1.10
2806 reflections
112 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
$w = 1/[\sigma^2(F_o^2) + (0.0518P)^2 + 0.7395P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}
Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.016 (3)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	0.9486 (3)	0.6568 (4)	0.82130 (17)	0.0371 (6)

C2	0.7886 (3)	0.5893 (4)	0.78225 (18)	0.0411 (6)
H2A	0.7124	0.6864	0.7945	0.049*
H2B	0.7781	0.5690	0.7178	0.049*
C3	0.9043 (3)	0.3583 (4)	0.88290 (15)	0.0288 (5)
C4	0.6448 (4)	0.2661 (5)	0.8068 (2)	0.0604 (9)
H4A	0.6381	0.2209	0.7458	0.091*
H4B	0.5519	0.3359	0.8135	0.091*
H4C	0.6582	0.1519	0.8465	0.091*
N1	1.0075 (2)	0.5102 (3)	0.88175 (14)	0.0311 (4)
H1	1.0973	0.5141	0.9144	0.037*
N2	0.7741 (2)	0.4002 (3)	0.82874 (14)	0.0369 (5)
N3	0.9339 (2)	0.1983 (3)	0.93186 (15)	0.0394 (5)
H3A	0.8651	0.1060	0.9311	0.047*
H3B	1.0225	0.1842	0.9652	0.047*
O1	1.0143 (3)	0.8075 (3)	0.80485 (15)	0.0575 (6)
O2	1.3127 (2)	0.4455 (3)	0.95142 (14)	0.0501 (6)
O3	1.2272 (2)	0.1521 (3)	1.03801 (13)	0.0435 (5)
O4	1.4909 (2)	0.2863 (3)	1.08076 (14)	0.0506 (6)
H4	1.5505	0.3698	1.0658	0.076*
P1	1.35438 (7)	0.25366 (10)	1.00218 (5)	0.0336 (2)
H1A	1.3903	0.1593	0.9601	0.040*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0422 (14)	0.0362 (14)	0.0346 (13)	0.0032 (11)	0.0109 (11)	0.0059 (11)
C2	0.0395 (14)	0.0473 (15)	0.0351 (13)	0.0085 (12)	0.0024 (11)	0.0080 (12)
C3	0.0269 (11)	0.0309 (12)	0.0283 (11)	−0.0017 (9)	0.0037 (9)	−0.0001 (9)
C4	0.0389 (16)	0.074 (2)	0.061 (2)	−0.0176 (16)	−0.0118 (14)	0.0016 (17)
N1	0.0279 (10)	0.0288 (10)	0.0354 (10)	−0.0039 (8)	0.0018 (8)	0.0028 (8)
N2	0.0279 (10)	0.0444 (12)	0.0366 (11)	−0.0025 (9)	−0.0001 (8)	0.0037 (9)
N3	0.0307 (11)	0.0323 (11)	0.0511 (13)	−0.0109 (9)	−0.0055 (10)	0.0085 (10)
O1	0.0677 (15)	0.0442 (12)	0.0624 (14)	−0.0077 (10)	0.0158 (11)	0.0210 (10)
O2	0.0263 (9)	0.0522 (12)	0.0668 (14)	−0.0108 (8)	−0.0071 (9)	0.0278 (10)
O3	0.0318 (10)	0.0419 (11)	0.0554 (11)	−0.0127 (8)	0.0033 (8)	0.0104 (9)
O4	0.0342 (10)	0.0585 (14)	0.0536 (12)	−0.0164 (9)	−0.0090 (9)	0.0230 (10)
P1	0.0249 (3)	0.0355 (3)	0.0398 (4)	−0.0038 (3)	0.0034 (2)	0.0050 (3)

Geometric parameters (Å, º)

C1—O1	1.201 (3)	C4—H4B	0.9600
C1—N1	1.374 (3)	C4—H4C	0.9600
C1—C2	1.502 (4)	N1—H1	0.8600
C2—N2	1.452 (4)	N3—H3A	0.8600
C2—H2A	0.9700	N3—H3B	0.8600
C2—H2B	0.9700	O2—P1	1.4983 (19)
C3—N3	1.294 (3)	O3—P1	1.4833 (18)
C3—N2	1.322 (3)	O4—P1	1.5566 (19)

C3—N1	1.359 (3)	O4—H4	0.8200
C4—N2	1.440 (4)	P1—H1A	0.9800
C4—H4A	0.9600		
O1—C1—N1	125.7 (3)	H4B—C4—H4C	109.5
O1—C1—C2	128.3 (2)	C3—N1—C1	110.7 (2)
N1—C1—C2	106.0 (2)	C3—N1—H1	124.7
N2—C2—C1	102.7 (2)	C1—N1—H1	124.7
N2—C2—H2A	111.2	C3—N2—C4	125.7 (2)
C1—C2—H2A	111.2	C3—N2—C2	110.0 (2)
N2—C2—H2B	111.2	C4—N2—C2	123.5 (2)
C1—C2—H2B	111.2	C3—N3—H3A	120.0
H2A—C2—H2B	109.1	C3—N3—H3B	120.0
N3—C3—N2	126.6 (2)	H3A—N3—H3B	120.0
N3—C3—N1	122.9 (2)	P1—O4—H4	109.5
N2—C3—N1	110.5 (2)	O3—P1—O2	115.80 (11)
N2—C4—H4A	109.5	O3—P1—O4	108.73 (11)
N2—C4—H4B	109.5	O2—P1—O4	111.31 (11)
H4A—C4—H4B	109.5	O3—P1—H1A	106.8
N2—C4—H4C	109.5	O2—P1—H1A	106.8
H4A—C4—H4C	109.5	O4—P1—H1A	106.8
O1—C1—C2—N2	−179.2 (3)	N3—C3—N2—C4	−6.6 (4)
N1—C1—C2—N2	0.4 (3)	N1—C3—N2—C4	173.9 (3)
N3—C3—N1—C1	177.4 (2)	N3—C3—N2—C2	−177.2 (2)
N2—C3—N1—C1	−3.1 (3)	N1—C3—N2—C2	3.4 (3)
O1—C1—N1—C3	−178.9 (3)	C1—C2—N2—C3	−2.3 (3)
C2—C1—N1—C3	1.5 (3)	C1—C2—N2—C4	−173.1 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*B*···O1^{i}	0.97	2.58	2.997 (4)	106
C4—H4*C*···N3	0.96	2.57	2.941 (4)	103
C4—H4*A*···O4^{ii}	0.96	2.61	3.470 (3)	150
N1—H1···O2	0.86	1.94	2.754 (2)	157
N3—H3*A*···O3^{iii}	0.86	1.98	2.800 (2)	158
N3—H3*B*···O3	0.86	1.96	2.821 (2)	178
O4—H4···O2^{iv}	0.82	1.77	2.585 (2)	170

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