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L-Argininium bis(dihydrogen phosphate)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.044
wR factor = 0.132
Data-to-parameter ratio = 7.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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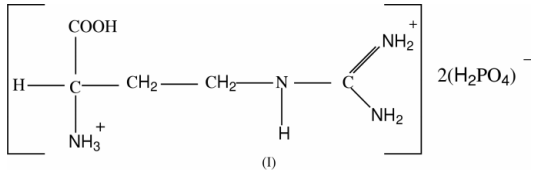
In the crystal structure of the title compound, $C_6H_{16}N_4O_2^{2+}\cdot 2H_2PO_4^-$, the argininium residue has a *gauche* II-*trans-trans-trans* conformation. The argininium residue forms N—H···O and O—H···O hydrogen bonds with the phosphate anions; the latter form O—H···O hydrogen bonds with each other. Three-centered hydrogen bonding is also observed.

Comment

Arginine is known to possess non-linear optical properties (Jiang *et al.*, 1983). The crystal structure of L-arginine dihydrate (Karle & Karle, 1964), L-arginine chloride (Mazumdar *et al.*, 1969), L-arginine hydrochloride monohydrate (Dow *et al.*, 1970), L-arginine phosphate monohydrate (Aoki *et al.*, 1971), L-arginine perchlorate (Monaco *et al.*, 1987; Srinivasan & Rajaram, 1997) and L-arginine diarsenate (Zalkin *et al.*, 1989), L-argininium dinitrate (Ramaswamy *et al.*, 2001) and a triclinic polymorph of L-argininium chloride (Sridhar *et al.*, 2002) have been reported. In the present study, the crystal structure of L-argininum bis(dihydrogen phosphate), (I), has been determined.



(I)

The asymmetric unit of (I) contains one argininium residue and two dihydrogen phosphate anions. The C—O distances and O—C—C bond angles clearly show the presence of the COOH group. Futhermore, the guanidyl group is protonated to form a guanidinium ion. The backbone conformation angles, χ^1 and χ^2, are in *cis* and *trans* forms, respectively. The side-chain angle ψ^1 has the most favoured *gauche* II conformation, while the other three conformation angles ψ^2, ψ^3 and ψ^4 have the *trans-trans-trans* form. The P—O distances agree well with the values for normal single- and double-bond distances (Table 1).

The phosphate anions play a vital role in forming hydrogen bonds with the argininium residue and with each other (Table 2). All the phosphate O atoms are involved in hydrogen bonding. Interestingly, three-centered hydrogen bonding is observed, involving the η^1 N atom (N3) and phosphate O atoms.

Experimental

The title compound was crystallized by slow evaporation of an aqueous solution of L-arginine and orthophosphoric acid in a stoichiometric ratio of 1:2.

Crystal data

$C_6H_{16}N_4O_2^{2+}\cdot 2H_2PO_4^-$
$M_r = 370.20$
Orthorhombic, $P2_12_12_1$
$a = 6.9910\ (2)$ Å
$b = 9.6760\ (5)$ Å
$c = 21.735\ (2)$ Å
$V = 1470.26\ (16)$ Å^3
$Z = 4$
$D_x = 1.672$ Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 15.2$–$23.8°$
$\mu = 3.28$ mm^{-1}
$T = 293\ (2)$ K
Plate, colorless
0.3 × 0.2 × 0.2 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.367$, $T_{max} = 0.519$
1567 measured reflections
1567 independent reflections
1548 reflections with $I > 2\sigma(I)$
$\theta_{max} = 67.9°$
$h = -8 \rightarrow 0$
$k = -11 \rightarrow 0$
$l = -26 \rightarrow 0$
2 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.132$
$S = 1.27$
1567 reflections
216 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1002P)^2 + 0.2388P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.57$ e Å^{-3}
$\Delta\rho_{min} = -0.82$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.047 (3)
Absolute structure: Flack (1983)
Flack parameter = 0.03 (4)

Table 1
Selected geometric parameters (Å, °).

P1—O3	1.504 (3)	P2—O8	1.508 (2)
P1—O4	1.515 (3)	P2—O9	1.564 (3)
P1—O5	1.561 (3)	P2—O10	1.573 (3)
P1—O6	1.565 (3)	O1—C1	1.307 (5)
P2—O7	1.503 (3)	O2—C1	1.208 (5)
O2—C1—C2—N1	−2.8 (5)	C3—C4—C5—N2	−174.3 (3)
N1—C2—C3—C4	−61.3 (4)	C4—C5—N2—C6	149.0 (4)
C2—C3—C4—C5	−171.2 (3)	C5—N2—C6—N4	−170.2 (4)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5···O8^{i}	0.79 (5)	1.85 (5)	2.637 (4)	172 (5)
O6—H6···O4^{ii}	0.91 (6)	1.69 (5)	2.564 (4)	159 (5)
O9—H9···O3^{iii}	1.18 (5)	1.39 (5)	2.518 (4)	157 (5)
O10—H10···O4^{i}	0.77 (7)	1.94 (8)	2.610 (4)	145 (7)
O1—H1···O7^{iv}	0.82	1.76	2.566 (4)	169
N1—H1*A*···O4^{v}	0.89	2.01	2.732 (4)	137
N1—H1*B*···O8^{v}	0.89	2.05	2.895 (4)	159
N1—H1*C*···O8^{vi}	0.89	2.04	2.911 (4)	165
N2—H2*A*···O10^{iii}	0.86	2.35	3.077 (5)	142
N3—H3*C*···O9^{vii}	0.86	2.16	2.981 (4)	158
N3—H3*D*···O7^{viii}	0.86	2.41	3.158 (5)	146
N3—H3*D*···O10^{viii}	0.86	2.47	3.237 (5)	150
N4—H4*C*···O3	0.86	2.13	2.914 (5)	152
N4—H4*D*···O7^{viii}	0.86	2.17	2.977 (5)	155

Symmetry codes: (i) $x-\frac{1}{2},\frac{3}{2}-y,1-z$; (ii) $x-\frac{1}{2},\frac{1}{2}-y,1-z$; (iii) $\frac{1}{2}+x,\frac{3}{2}-y,1-z$; (iv) $\frac{3}{2}+x,\frac{1}{2}-y,1-z$; (v) $\frac{1}{2}+x,\frac{1}{2}-y,1-z$; (vi) $1+x,y-1,z$; (vii) $\frac{5}{2}-x,1-y,\frac{1}{2}+z$; (viii) $\frac{3}{2}-x,1-y,\frac{1}{2}+z$.

The H atoms of the phosphate anions were located in difference Fourier maps and refined isotropically. All other H atoms were placed in geometrically calculated positions and included in the refinement in the riding-model approximation, with U_{iso} values set at $1.2U_{eq}$ of the carrier atom.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *CAD*-4 *Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1999); software used to prepare material for publication: *SHELXL*97.

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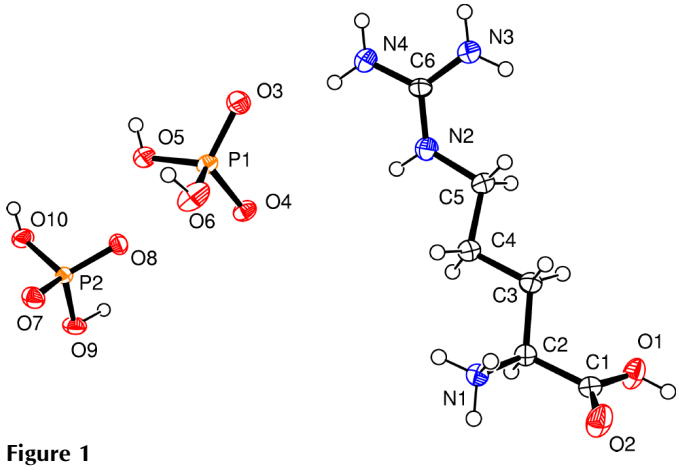

Figure 1
A view of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

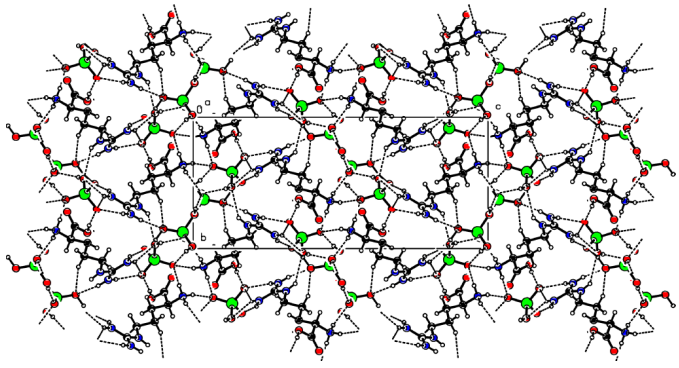

Figure 2
A packing diagram of the title compound, viewed down the *b* axis.

References

Aoki, K., Nagano, K. & Iitaka, Y. (1971). *Acta Cryst.* B**27**, 11–23.
Dow, J., Jensen, L. H., Mazumdar, S. K., Srinivasan, R. & Ramachandran, G. N. (1970). *Acta Cryst.* B**26**, 1662–1671.
Enraf–Nonius (1989). *CAD*-4 *Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Jiang, M., Xu, D. & Tan, Z. (1983). Abstracts of the VIIth International Conference on Crystal Growth, p. 2.67, Stuttgart, Germany.
Karle, I. L. & Karle, J. (1964). *Acta Cryst.* **17**, 835–841.
Mazumdar, S. K., Venkatesan, K., Mez, H. C. & Donohue, J. (1969). *Z. Kristallogr.* **130**, 328–339.
Monaco, S. B., Davis, L. E., Velsko, S. P., Wang, F. T., Eimerl, D. & Zalkin, A. (1987). *J. Cryst. Growth*, **85**, 252–255.

North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Ramaswamy, S., Sridhar, B., Ramakrishnan, V. & Rajaram, R. K. (2001). *Acta Cryst.* E**57**, o872–o874.
Sheldrick, G. M. (1997). *SHELXL*97 and *SHELXS*97. University of Göttingen, Germany.
Spek, A. L. (1999). *PLATON for Windows*. Utretcht University, The Netherlands.
Sridhar, B., Srinivasan, R. & Rajaram, R. K. (2002). *Acta Cryst.* E**5**8, o747–o749.
Srinivasan, N. & Rajaram, R. K. (1997). *Z. Kristallogr.* **212**, 311–312.
Zalkin, A., Eimeral, D. & Velsko, S. P. (1989). *Acta Cryst.* C**45**, 812–813.