Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Amino-4,6-dimethylpyridinium benzoate

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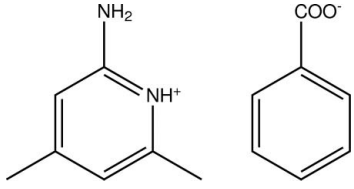
Received 17 August 2010; accepted 29 August 2010

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.127; data-to-parameter ratio = 11.7.

In the title compound, $C_7H_{11}N_2^+\cdot C_7H_5O_2^-$, the 2-amino-4,6-dimethylpyridinium cation and the benzoate anion are linked by two N—H···O hydrogen bonds, forming an $R_2^2(8)$ ring motif. The H atoms in both the methyl groups are rotationally disordered, with fixed site occupancies of 0.50. In the crystal structure, the molecules are stabilized by intermolecular N—H···O hydrogen bonds. A π–π interaction, with a centroid–centroid distance of 3.661 (2) Å, is also observed.

Related literature

For the biological activity of Schiff bases with azomethine linkages, see Dhar & Taploo (1982). For hydrogen bonding, see: Jeffrey (1997); Jeffrey & Saenger (1991). For graph-set descriptions of hydrogen-bond ring motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_7H_{11}N_2^+\cdot C_7H_5O_2^-$ M_r = 244.29
Monoclinic, $P2_1/c$
a = 7.5362 (16) Å
b = 22.937 (4) Å
c = 8.2124 (14) Å
β = 109.820 (2)°
V = 1335.5 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
0.57 × 0.23 × 0.05 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*;p Bruker, 2009)
T_{min} = 0.954, T_{max} = 0.996
7639 measured reflections
2336 independent reflections
1527 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.127
S = 1.02
2336 reflections
199 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.10 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*1···O2	1.04	1.65	2.683 (2)	172
N2—H1*N*2···O1	1.01	1.78	2.779 (2)	171
N2—H2*N*2···O1^{i}	0.90	1.97	2.853 (2)	168

Symmetry code: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

This research was supported by Universiti Sains Malaysia (USM) under the University Research grant (No. 1001/PFARMASI/815004) and the Ministry of Science, Technology and Innovation through an R&D Initiative Grant (09-05-IFN-MEB 004). HKF and MMR also thank USM for the Research University Grant (No. 1001/PFIZIK/811160). MRA gratefully acknowledges a PhD scholarship from Universiti Malaysia Sarawak.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2327).

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