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1-Methyl-4-(1-methyl-1*H*-benzimidazol-2-yl)pyridinium iodide

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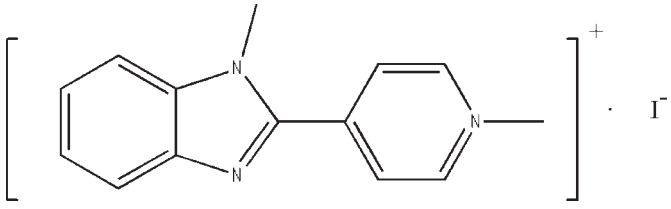
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.009 Å; R factor = 0.043; wR factor = 0.092; data-to-parameter ratio = 14.2.

The cation of the title compound, $C_{14}H_{14}N_3^+\cdot I^-$, is non-planar, the dihedral angle between the benzimidazole and the 1-methylpyridinium planes being 37.4 (2)°. The crystal structure is stabilized by weak π–π stacking interactions, the centroid–centroid distances between 1-methylimidazole and benzimidazole planes being 3.678 (4) Å.

Related literature

For background to imidazole and its derivatives, see: Huang *et al.* (2004). For the biological activity of benzimidazole, see: Demirayak *et al.* (2002); Pawar *et al.* (2004).



Experimental

Crystal data

$C_{14}H_{14}N_3^+\cdot I^-$
M_r = 351.18
Triclinic, $P\overline{1}$
a = 7.7048 (15) Å
b = 9.9264 (18) Å
c = 10.1772 (19) Å
α = 64.888 (3)°
β = 72.933 (3)°
γ = 76.394 (4)°
V = 668.2 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.38 mm^{-1}
T = 291 K
0.35 × 0.25 × 0.05 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.493, T_{max} = 0.887
3353 measured reflections
2307 independent reflections
1840 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.092
S = 1.00
2307 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.94 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2252).

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supporting information

Acta Cryst. (2010). E**66**, o198 [doi:10.1107/S1600536809053938]

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S1. Comment

Imidazole and its derivatives are a very important kind of heterocyclic compounds with N-donor atoms, therefore they can be excellent organic ligands to generate various complexes (Huang *et al.*, 2004). Owing to its biological activities such as antimicrobial, antifungal (Pawar *et al.*, 2004), anticancer (Demirayak *et al.*, 2002), and so on, benzimidazoles have also received much attention. The construction of new member of this family is an important direction in the development of modern coordination chemistry and biological chemistry. We report here the synthesis and crystal structure of the title compound. The molecular structure is shown in Fig. 1. The cation of (I) is non-planar, the dihedral angle between the benzimidazolyl plane and the *N*-methylpyridinium plane is 37.4 (2)°. The crystal structure is stabilized by *π*–*π* [Cg1: N2-C7-N3-C13-C8; Cg2(i): C8/C13, code symmetry: (i) -x+2, -y+1, -z] stacking interaction, the distance centroid-centroid between these planes is 3.678 (4) Å. The crystal packing also exhibits a weak intermolecular C—H···I interaction.

S2. Experimental

Metallic sodium (0.25 g, 10.8 mmol) was dissolved in the stirred anhydrous ethanol(10 ml) under an atmosphere of nitrogen. Then added 2-(4-pyridinyl)-1*H*-benzimidazole (1.95 g, 10 mmol), dry actone (150 ml) and methyl iodide(1.24 ml, 20 mmol) in the above solution. The reaction mixture was refluxed for 24 h. When the reaction stopped and the mixture were cooled to room temperature, the solution were removed under decompression. Then the residue recrystallized from water twice to obtain the single crystals (3.0 g, 8.66 mmol).

S3. Refinement

All H atoms were fixed geometrically and were treated as riding on their parent C atoms, with C—H distances in the range of 0.93—0.96 Å, and with U_{iso}(H) = 1.2U_{eq}(parent atom), or U_{iso}(H) = 1.5U_{eq}(C_{methyl}).

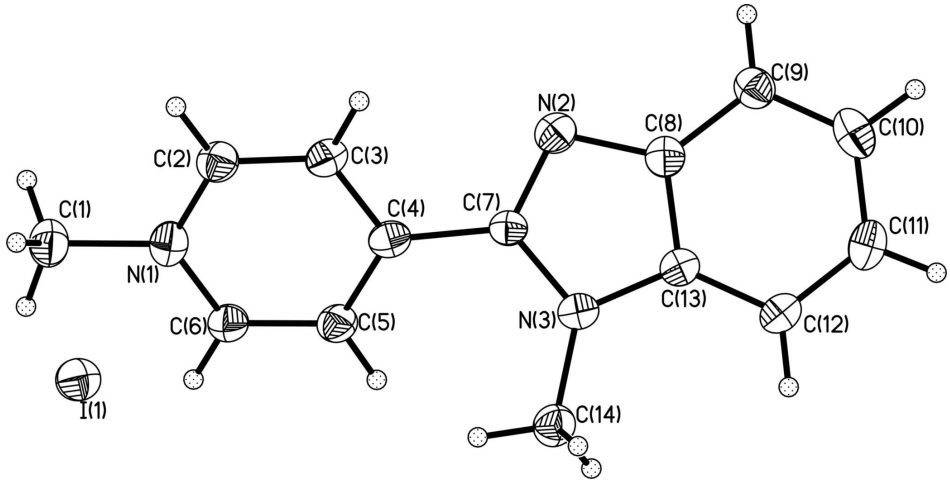

Figure 1

The asymmetric unit of the title compound with atom labels. Displacement ellipsoids were drawn at the 30% probability level.

1-Methyl-4-(1-methyl-1*H*-benzimidazol-2-yl)pyridinium iodide

Crystal data

$C_{14}H_{14}N_3^+ \cdot I^-$
$M_r = 351.18$
Triclinic, $P\overline{1}$
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$a = 7.7048$ (15) Å
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$c = 10.1772$ (19) Å
$\alpha = 64.888$ (3)°
$\beta = 72.933$ (3)°
$\gamma = 76.394$ (4)°
$V = 668.2$ (2) Å^3
$Z = 2$
$F(000) = 344$
$D_x = 1.745$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1236 reflections
$\theta = 3.1$–22.1°
$\mu = 2.38$ mm^{-1}
$T = 291$ K
Piece, colorless
0.35 × 0.25 × 0.05 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.493$, $T_{max} = 0.887$
3353 measured reflections
2307 independent reflections
1840 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.3°$
$h = -9 \rightarrow 7$
$k = -10 \rightarrow 11$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.092$
$S = 1.00$
2307 reflections
163 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

$w = 1/[\sigma^2(F_o^2) + (0.0301P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.94$ e Å^{-3}
$\Delta\rho_{min} = -0.48$ e Å^{-3}

Special details

Geometry. Least-squares planes (*x*,*y*,*z* in crystal coordinates) and deviations from them (* indicates atom used to define plane)
7.5483 (0.0040) *x* + 0.9256 (0.0225) *y* + 1.1206 (0.0247) *z* = 6.5511 (0.0171)
* 0.0017 (0.0039) N1 * 0.0018 (0.0041) C2 * -0.0063 (0.0040) C3 * 0.0074 (0.0040) C4 * -0.0041 (0.0042) C5 * -0.0004 (0.0041) C6
Rms deviation of fitted atoms = 0.0044
6.8822 (0.0088) *x* + 3.4760 (0.0239) *y* + 7.0324 (0.0184) *z* = 8.6547 (0.0229)
Angle to previous plane (with approximate e.s.d.) = 37.43 (0.15)
* -0.0020 (0.0031) C7 * -0.0067 (0.0031) N2 * 0.0128 (0.0031) C8 * -0.0138 (0.0030) C13 * 0.0098 (0.0030) N3
Rms deviation of fitted atoms = 0.0100

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.7976 (9)	0.1720 (7)	0.3724 (7)	0.0574 (18)
H1A	0.7850	0.1418	0.4774	0.086*
H1B	0.9149	0.1293	0.3311	0.086*
H1C	0.7027	0.1374	0.3557	0.086*
C2	0.7960 (8)	0.4044 (7)	0.1519 (7)	0.0443 (15)
H2A	0.8121	0.3452	0.0977	0.053*
C3	0.7870 (8)	0.5551 (6)	0.0807 (7)	0.0422 (15)
H3A	0.7948	0.5992	−0.0214	0.051*
C4	0.7660 (8)	0.6442 (6)	0.1610 (6)	0.0387 (14)
C5	0.7505 (8)	0.5736 (6)	0.3135 (6)	0.0422 (15)
H5A	0.7337	0.6297	0.3707	0.051*
C6	0.7598 (8)	0.4226 (7)	0.3784 (7)	0.0445 (15)
H6A	0.7506	0.3759	0.4806	0.053*
C7	0.7700 (8)	0.8070 (6)	0.0779 (6)	0.0339 (13)
C8	0.8426 (8)	1.0150 (6)	−0.0938 (6)	0.0395 (14)
C9	0.9152 (8)	1.1306 (7)	−0.2232 (7)	0.0443 (15)
H9A	1.0063	1.1104	−0.2983	0.053*
C10	0.8473 (9)	1.2748 (7)	−0.2354 (7)	0.0498 (17)
H10A	0.8941	1.3536	−0.3202	0.060*
C11	0.7082 (9)	1.3076 (7)	−0.1230 (7)	0.0482 (16)
H11A	0.6644	1.4071	−0.1361	0.058*
C12	0.6369 (8)	1.1955 (6)	0.0047 (7)	0.0423 (15)
H12A	0.5454	1.2161	0.0793	0.051*
C13	0.7076 (7)	1.0494 (6)	0.0175 (6)	0.0344 (13)
C14	0.5260 (8)	0.8957 (7)	0.2645 (7)	0.0478 (16)
H14A	0.5225	0.7909	0.3245	0.072*
H14B	0.4090	0.9405	0.2400	0.072*

H14C	0.5541	0.9438	0.3187	0.072*
I1	0.26309 (6)	0.26836 (5)	0.37099 (4)	0.05037 (19)
N1	0.7821 (6)	0.3387 (5)	0.2996 (6)	0.0432 (12)
N2	0.8779 (7)	0.8606 (5)	−0.0548 (5)	0.0426 (12)
N3	0.6668 (6)	0.9141 (5)	0.1277 (5)	0.0367 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.062 (5)	0.042 (4)	0.064 (5)	−0.010 (3)	−0.008 (4)	−0.019 (3)
C2	0.047 (4)	0.049 (4)	0.045 (4)	−0.011 (3)	−0.011 (3)	−0.023 (3)
C3	0.043 (4)	0.046 (4)	0.042 (4)	0.001 (3)	−0.011 (3)	−0.022 (3)
C4	0.030 (3)	0.047 (4)	0.042 (4)	−0.001 (3)	−0.008 (3)	−0.021 (3)
C5	0.046 (4)	0.045 (4)	0.042 (4)	−0.010 (3)	−0.007 (3)	−0.022 (3)
C6	0.053 (4)	0.044 (4)	0.037 (3)	−0.004 (3)	−0.008 (3)	−0.018 (3)
C7	0.032 (3)	0.039 (3)	0.033 (3)	−0.005 (3)	−0.008 (3)	−0.016 (3)
C8	0.043 (4)	0.042 (4)	0.039 (3)	−0.006 (3)	−0.016 (3)	−0.016 (3)
C9	0.045 (4)	0.046 (4)	0.043 (4)	−0.011 (3)	−0.010 (3)	−0.016 (3)
C10	0.052 (4)	0.051 (4)	0.046 (4)	−0.020 (3)	−0.021 (3)	−0.005 (3)
C11	0.048 (4)	0.038 (4)	0.065 (5)	−0.001 (3)	−0.024 (4)	−0.021 (3)
C12	0.041 (4)	0.044 (4)	0.048 (4)	0.001 (3)	−0.013 (3)	−0.024 (3)
C13	0.032 (3)	0.041 (4)	0.036 (3)	−0.003 (3)	−0.014 (3)	−0.017 (3)
C14	0.042 (4)	0.047 (4)	0.053 (4)	−0.004 (3)	−0.008 (3)	−0.021 (3)
I1	0.0493 (3)	0.0535 (3)	0.0478 (3)	−0.0021 (2)	−0.0128 (2)	−0.0197 (2)
N1	0.034 (3)	0.039 (3)	0.057 (3)	−0.003 (2)	−0.013 (3)	−0.017 (3)
N2	0.045 (3)	0.046 (3)	0.044 (3)	−0.006 (2)	−0.014 (3)	−0.021 (2)
N3	0.031 (3)	0.045 (3)	0.038 (3)	−0.004 (2)	−0.009 (2)	−0.020 (3)

Geometric parameters (Å, º)

C1—N1	1.490 (8)	C8—N2	1.389 (7)
C1—H1A	0.9600	C8—C13	1.397 (8)
C1—H1B	0.9600	C8—C9	1.397 (8)
C1—H1C	0.9600	C9—C10	1.368 (8)
C2—N1	1.343 (7)	C9—H9A	0.9300
C2—C3	1.353 (8)	C10—C11	1.412 (9)
C2—H2A	0.9300	C10—H10A	0.9300
C3—C4	1.395 (7)	C11—C12	1.368 (8)
C3—H3A	0.9300	C11—H11A	0.9300
C4—C5	1.386 (7)	C12—C13	1.388 (7)
C4—C7	1.475 (8)	C12—H12A	0.9300
C5—C6	1.350 (7)	C13—N3	1.369 (7)
C5—H5A	0.9300	C14—N3	1.462 (7)
C6—N1	1.336 (7)	C14—H14A	0.9600
C6—H6A	0.9300	C14—H14B	0.9600
C7—N2	1.318 (7)	C14—H14C	0.9600
C7—N3	1.357 (7)		

N1—C1—H1A	109.5	C10—C9—H9A	121.3
N1—C1—H1B	109.5	C8—C9—H9A	121.3
H1A—C1—H1B	109.5	C9—C10—C11	122.1 (6)
N1—C1—H1C	109.5	C9—C10—H10A	119.0
H1A—C1—H1C	109.5	C11—C10—H10A	119.0
H1B—C1—H1C	109.5	C12—C11—C10	121.1 (6)
N1—C2—C3	121.1 (5)	C12—C11—H11A	119.5
N1—C2—H2A	119.5	C10—C11—H11A	119.5
C3—C2—H2A	119.5	C11—C12—C13	116.7 (6)
C2—C3—C4	119.7 (6)	C11—C12—H12A	121.6
C2—C3—H3A	120.1	C13—C12—H12A	121.6
C4—C3—H3A	120.1	N3—C13—C12	131.6 (5)
C5—C4—C3	118.0 (5)	N3—C13—C8	105.5 (5)
C5—C4—C7	123.9 (5)	C12—C13—C8	122.9 (6)
C3—C4—C7	118.1 (5)	N3—C14—H14A	109.5
C6—C5—C4	119.6 (5)	N3—C14—H14B	109.5
C6—C5—H5A	120.2	H14A—C14—H14B	109.5
C4—C5—H5A	120.2	N3—C14—H14C	109.5
N1—C6—C5	121.8 (6)	H14A—C14—H14C	109.5
N1—C6—H6A	119.1	H14B—C14—H14C	109.5
C5—C6—H6A	119.1	C6—N1—C2	119.9 (5)
N2—C7—N3	114.0 (5)	C6—N1—C1	121.0 (5)
N2—C7—C4	121.4 (5)	C2—N1—C1	119.1 (5)
N3—C7—C4	124.6 (5)	C7—N2—C8	103.7 (5)
N2—C8—C13	110.2 (5)	C7—N3—C13	106.5 (5)
N2—C8—C9	130.0 (6)	C7—N3—C14	128.7 (5)
C13—C8—C9	119.8 (5)	C13—N3—C14	124.6 (5)
C10—C9—C8	117.4 (6)		

N1—C2—C3—C4	1.1 (9)	N2—C8—C13—C12	−176.0 (5)
C2—C3—C4—C5	−1.6 (9)	C9—C8—C13—C12	1.7 (8)
C2—C3—C4—C7	175.7 (5)	C5—C6—N1—C2	0.1 (9)
C3—C4—C5—C6	1.3 (9)	C5—C6—N1—C1	178.2 (6)
C7—C4—C5—C6	−175.7 (5)	C3—C2—N1—C6	−0.3 (9)
C4—C5—C6—N1	−0.6 (9)	C3—C2—N1—C1	−178.5 (6)
C5—C4—C7—N2	141.4 (6)	N3—C7—N2—C8	0.4 (6)
C3—C4—C7—N2	−35.7 (8)	C4—C7—N2—C8	−179.7 (5)
C5—C4—C7—N3	−38.7 (8)	C13—C8—N2—C7	−1.9 (6)
C3—C4—C7—N3	144.2 (5)	C9—C8—N2—C7	−179.3 (6)
N2—C8—C9—C10	176.4 (5)	N2—C7—N3—C13	1.2 (6)
C13—C8—C9—C10	−0.8 (8)	C4—C7—N3—C13	−178.7 (5)
C8—C9—C10—C11	−0.4 (8)	N2—C7—N3—C14	176.0 (5)
C9—C10—C11—C12	0.9 (9)	C4—C7—N3—C14	−3.8 (8)
C10—C11—C12—C13	−0.1 (8)	C12—C13—N3—C7	176.2 (5)
C11—C12—C13—N3	−179.4 (5)	C8—C13—N3—C7	−2.2 (5)
C11—C12—C13—C8	−1.2 (8)	C12—C13—N3—C14	1.1 (9)
N2—C8—C13—N3	2.6 (6)	C8—C13—N3—C14	−177.3 (5)
C9—C8—C13—N3	−179.7 (5)		