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1,2-Dimethyl-3-(2-nitrophenyl)-4,5-dihydroimidazolium iodide

Dong-Hong Li,[a] Jun-Sheng Hao,[a] Fang-Jun Huo,[a] Shu-Ping Huang,[b]* Yong-Bin Zhang[a] and Chi-Zhong Xia[a]*

[a]School of Chemistry and Chemical Engineering, University of Shanxi, Taiyuan, Shanxi 030006, People's Republic of China, and [b]Institute of Modern Chemistry, University of Shanxi, Taiyuan, Shanxi 030006, People's Republic of China

Correspondence e-mail: sphuang@sxu.edu.cn, xiac@public.ty.sx.cn

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In the crystal structure of the title compound, $C_{11}H_{14}N_3O_2^+ \cdot I^-$, intermolecular C—H···O and C—H···I hydrogen bonds link the ions into a three-dimensional structure. The imidazolinium ring is planar within 0.0502 (2) Å. The dihedral angle of the imidazolinium plane and the benzene ring plane is 78.45 (7)°.

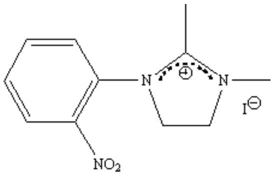
Key indicators

Single-crystal X-ray study
T = 183 K
Mean σ(C–C) = 0.004 Å
R factor = 0.021
wR factor = 0.054
Data-to-parameter ratio = 14.8

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

Comment

Tetrahydrofolate (THFo) co-enzymes are involved in the biological transfer of a one-carbon fragment at different oxidation levels (Xia *et al.*, 2000, 2002). The title compound, (I), is a THFo co-enzyme model. The study of THFo co-enzyme models can provide information on a valuable class of reagents for transfer reactions of practical significance.



(I)

Selected geometric parameters for (I) are listed in Table 1. The molecular structure is illustrated in Fig. 1. The imidazolinium ring is planar to within 0.0502 (2) Å. The dihedral angle between the imidazolinium and benzene rings is 78.45 (7)°. In the imidazolium ring, the bond lengths N2—C9 and N3—C9 are 1.325 (3) and 1.307 (4) Å, respectively. These values indicate that there is delocalization of the π-electron density over N2—C9—N3, with an angle of 111.4 (2)°. Hydrogen-bonding information is given in Table 2 and a crystal packing diagram is shown in Fig. 2. Three weak intermolecular hydrogen bonds, *viz*. C—H···O and C—H···I interactions, are mainly responsible for stabilizing the crystal structure, together with normal ionic interactions. One of the intermolecular contacts [C11—H11*A*···O2^{ii}; symmetry code: (ii) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$] involves the O atom of the nitro group as an acceptor and links the molecules into pairs. Other weak interactions [C7—H7···I1^{i}; symmetry code: (i) $-x, \frac{1}{2} + y, \frac{1}{2} - z$] occur between the iodide anion and two CH_3 groups from two neighboring molecules and play a stabilizing role in the molecular stacking. Additional van der Waals attractions also play an important in the crystal.

Experimental

1-Methyl-2-(2-nitrophenyl)imidazoline (2.05 g, 10 mmol) and iodomethane (1.9 ml, 30 mmol) were refluxed in 20 ml dry ether for 1 h. A large quantity of yellow solid separated out. The solution was cooled to room temperature and the precipitate collected by filtration and

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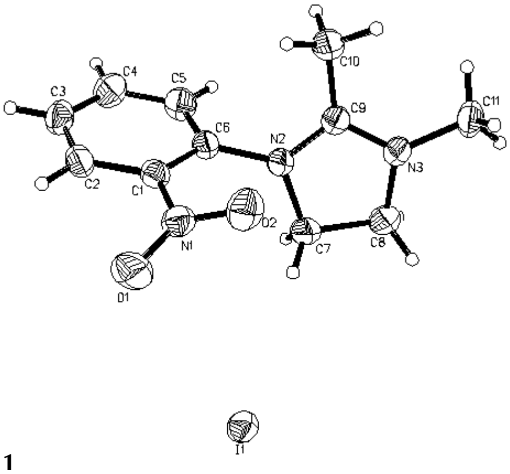

Figure 1
A view of the molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

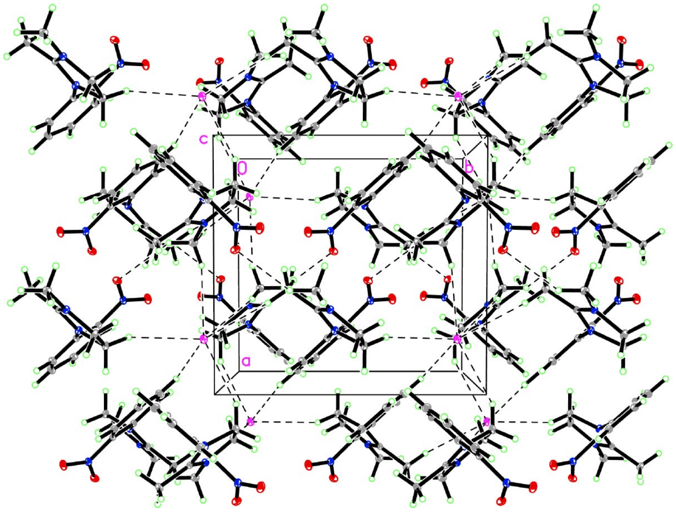

Figure 2
A packing diagram of the title compound, viewed down the *c* axis. Hydrogen bonds are indicated by dashed lines.

crystallized from ethyl alcohol, giving 3.123 g (90%) of the title compound as yellow crystals.

Crystal data

$C_{11}H_{14}N_3O_2^+ \cdot I^-$
$M_r = 347.15$
Monoclinic, $P2_1/c$
$a = 9.597$ (2) Å
$b = 10.090$ (2) Å
$c = 13.577$ (3) Å
$\beta = 94.187$ (2)°
$V = 1311.3$ (5) Å^3
$Z = 4$

$D_x = 1.758$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3981 reflections
$\theta = 2.5$–27.3°
$\mu = 2.44$ mm^{-1}
$T = 183$ (2) K
Block, yellow
0.40 × 0.40 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.403$, $T_{\max} = 0.481$
4370 measured reflections

2304 independent reflections
2123 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.014$
$\theta_{\max} = 25.0$°
$h = -11 \rightarrow 7$
$k = -5 \rightarrow 12$
$l = -16 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.021$
$wR(F^2) = 0.054$
$S = 1.06$
2304 reflections
156 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0289P)^2 + 0.5719P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.47$ e Å^{-3}
$\Delta\rho_{\min} = -0.42$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N2—C9	1.325 (3)	N3—C11	1.464 (3)
N2—C6	1.431 (3)	N3—C8	1.473 (3)
N2—C7	1.485 (3)	C7—C8	1.525 (4)
N3—C9	1.307 (3)	C9—C10	1.480 (3)
C9—N2—C6	127.0 (2)	C1—C6—N2	122.8 (2)
C9—N2—C7	111.2 (2)	N2—C7—C8	101.9 (2)
C6—N2—C7	121.8 (2)	N3—C8—C7	103.1 (2)
C9—N3—C11	126.6 (2)	N3—C9—N2	111.4 (2)
C9—N3—C8	111.6 (2)	N3—C9—C10	124.9 (2)
C11—N3—C8	121.5 (2)	N2—C9—C10	123.6 (2)
C5—C6—N2	118.5 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···I1$^{\rm i}$	0.99	2.95	3.833 (3)	148
C11—H11A···O2$^{\rm ii}$	0.98	2.58	3.416 (4)	143
C7—H7B···I1	0.99	3.01	3.940 (3)	157

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

H atoms were placed in calculated positions and allowed to ride on their parent atoms, with $U_{\rm iso}$(H) values set to $1.5U_{\rm eq}$(parent atom) for Csp^3 H atoms and $1.2U_{\rm eq}$(parent atom) for Csp^2 H atoms. The C—H distances were fixed in the range 0.95–0.98 Å.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT* and *SHELXTL* (Bruker, 2000); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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