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3-(4-Methoxyphenyl)-1,2-dimethyl-4,5-dihydroimidazolium iodide

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Key indicators

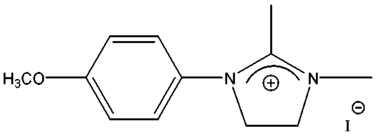
Single-crystal X-ray study
T = 183 K
Mean σ(C–C) = 0.005 Å
R factor = 0.026
wR factor = 0.063
Data-to-parameter ratio = 15.7

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

The title compound, $C_{12}H_{17}N_2O^+\cdot I^-$, is a new example of a tetrahydrofolate (THF) co-enzyme model. The N—C—N moiety of the imidazoline ring shows C—N bond lengths of 1.306 (4) and 1.326 (4) Å, suggesting that the positive charge is delocalized.

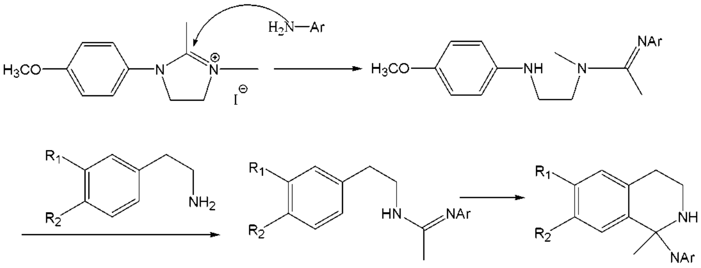
Comment

Tetrahydrofolate (THF) co-enzymes are involved in the biological transfer of a one-carbon fragment at different oxidation levels (Xia *et al.*, 2000, 2002). Though transfer reactions of practical significant models of 5,10-methylene–THF have been reported (Bieraügel *et al.*, 1983), the study of THF co-enzyme models can provide a valuable class of reagents.



(I)

As a new example of this co-enzyme model, the title compound, (I), has been synthesized. The mechanism of the tetrahydrofurate co-enzymes model for (I) is presented in the scheme below.



The molecular structure of (I) is shown in Fig. 1. The dihedral angle between the benzene and imidazolium rings is 50.4 (3)°. The C5—N1 bond length is 1.419 (4) Å, which is shorter than the standard single C—N bond, indicating some degree of π-electron overlap. Meanwhile, in the imidazolium ring, the lengths of N2—C10 and N1—C10 are 1.306 (4) and 1.326 (4) Å, respectively. These values indicate that the π-electron density is delocalized aver the N2—C10—N1 moiety. Thus, atom C10 is expected to be the reaction point of nucleophilic reagents.

Experimental

1-Methyl-2-(4-methoxyphenyl)imidazoline (1.90 g, 10 mmol) and iodomethane (1.9 ml, 30 mmol) were refluxed in 20 ml dry ether for

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1 h. A large amount of white solid separated out. The solution was cooled to room temperature and the precipitate was collected by filtration and crystallized from ethyl alcohol, giving 3.04 g (80%) of the title compound, (I). Crystals were grown from $CHCl_3$ solution by slow evaporation (m.p. 383–387 K). ^{1}H NMR ($CDCl_3$): 2.07 (*s*, 3H), 3.11 (*d*, 3H), 3.75 (*t*, 2H), 4.16 (*t*, 2H), 7.02 (*d*, 2H), 7.36; ^{13}C NMR ($CDCl_3$): 166.50, 160.24, 128.55, 128.35, 115.23, 55.68, 52.32, 50.75, 35.16, 13.16.

Crystal data

$C_{12}H_{17}N_2O^+\cdot I^-$
$M_r = 332.18$
Monoclinic, $P2_1/n$
$a = 11.4580$ (17) Å
$b = 7.5134$ (12) Å
$c = 16.307$ (3) Å
$\beta = 110.014$ (2)°
$V = 1319.0$ (4) Å^3
$Z = 4$
$D_x = 1.673$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3377 reflections
$\theta = 2.7$–26.9°
$\mu = 2.41$ mm^{-1}
$T = 183$ (2) K
Block, colorless
0.40 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.446$, $T_{\max} = 0.795$
5195 measured reflections
2324 independent reflections
2083 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.019$
$\theta_{\max} = 25.0°$
$h = -13 \rightarrow 13$
$k = -8 \rightarrow 8$
$l = -19 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.063$
$S = 1.04$
2324 reflections
148 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0347P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.92$ e Å^{-3}
$\Delta\rho_{\min} = -0.29$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C10	1.326 (4)	N2—C10	1.306 (4)
N1—C5	1.419 (4)	N2—C12	1.456 (4)
N1—C8	1.491 (4)	N2—C9	1.460 (4)
N2—C10—N1	112.3 (3)		
C1—O1—C2—C7	5.2 (4)	C8—N1—C5—C4	−46.2 (4)
C10—N1—C5—C6	−50.2 (4)		

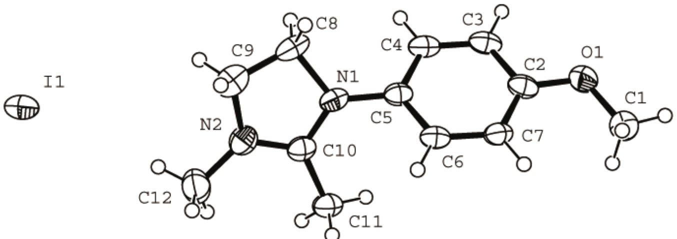

Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

All H atoms were initially located in difference Fourier maps. The methyl H atoms were then constrained to an ideal geometry, with C—H distances of 0.98 Å and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$, but each group was allowed to rotate freely about its C—C bond. Other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.95–1.00 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

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