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N^9,N^7-Dimethylhypoxanthinium iodide

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.009 Å
R factor = 0.042
wR factor = 0.108
Data-to-parameter ratio = 15.6

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

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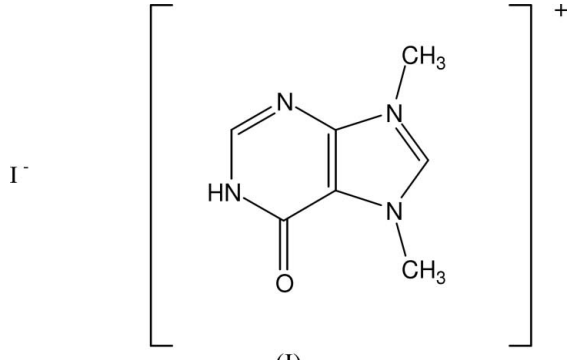
The structure of the title compound, $C_4H_9N_4O^+\cdot I^-$, consists of discrete N^9,N^7-dimethylhypoxanthinium cations and iodide anions which are connected through hydrogen bonds.

Comment

Methylation of DNA nucleic acid bases is an important and not well understood process. This reaction is catalysed by the enzyme DNA methyl transferase, which requires the co-factor *S*-adenosylmethionine. The methylated DNA-bases exert structural and functional effects on the DNA. For instance, 5-methylcytosine favours the formation of left-handed DNA double helices (*Z*-DNA). In addition, N^6-methyladenine exists in two rotameric states with only one of these forms able to establish base pairing. Methylation of DNA is used by bacteria to distinguish between their own and foreign DNA. Methylation starts immediately after replication. Each new strand is methylated; non-methylated DNA is recognized and digested by restriction enzymes. In natural DNA, the following methylated bases have been discovered: 5-methylcytosine, N^6-methyladenine, N^4-methylcytosine and 5-hydroxymethyluracil (Bloomfield *et al.*, 2000). The methylation of O^6-methylguanine with methyliodide in dimethylformamide gives a mixture of O^6,N^3-dimethylguanine, N^3-methylguanine and N^3,N^7-dimethylguanine in a ratio of 1:1.3:1.3 (Kohda *et al.*, 1987). With O^6-methylhypoxanthine as the starting material, we obtained the title product, (I).



(I)

A perspective view of the title compound is shown in Fig. 1. The structure is composed of discrete N^9,N^7-dimethylhypoxanthinium cations and I^- anions. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 1.6 plus three updates; *MOGUL* Version 1.0; Allen, 2002), except that the bond between N2 and C1 is rather long (Table 1). The crystal structure shows N—H···I hydrogen bonds and C—H···N, C—H···O and C—H···I contacts (Table 2).

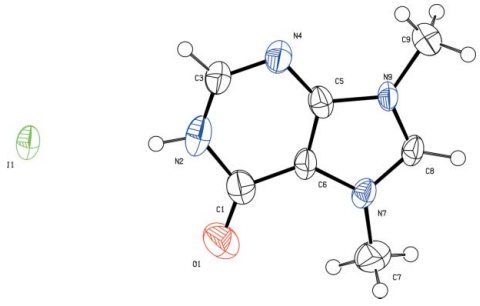


Figure 1
Perspective view of the title compound, showing the atom numbering, with displacement ellipsoids drawn at the 50% probability level.

Experimental

O^6-Methylhypoxanthine (0.5 g, 3.3 mmol) and methyl iodide (0.4 ml, 6.6 mmol, 2 equivalents) were refluxed in dimethylformamide (DMF, 100 ml) overnight. After removal of DMF under vacuum, single crystals of (I) were obtained.

Crystal data

$C_7H_9N_4O^+\cdot I^-$
M_r = 292.08
Monoclinic, $P2_1/n$
a = 7.5961 (13) Å
b = 11.6988 (12) Å
c = 11.8222 (15) Å
β = 90.063 (12)°
V = 1050.6 (2) Å^3
Z = 4
D_x = 1.847 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10175 reflections
θ = 3.5–25.7°
μ = 3.02 mm^{-1}
T = 173 (2) K
Plate, light red
0.25 × 0.19 × 0.03 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.519, T_{max} = 0.915
6468 measured reflections
1866 independent reflections
1496 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 25.6°
$h = -9 \rightarrow 8$
$k = -14 \rightarrow 14$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.108
S = 1.02
1866 reflections
120 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0735P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.41 e Å^{-3}
$\Delta\rho_{min}$ = −1.45 e Å^{-3}

Table 1
Selected bond lengths (Å).

O1—C1	1.214 (8)	C5—C6	1.399 (10)
C1—N2	1.453 (9)	C6—N7	1.386 (7)
N2—C3	1.334 (9)	N7—C8	1.353 (9)
C3—N4	1.308 (8)	N7—C7	1.463 (9)
N4—C5	1.360 (8)	C8—N9	1.328 (9)
C5—N9	1.375 (7)	N9—C9	1.475 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···I1	0.88	2.64	3.502 (7)	166
C3—H3···N4^{i}	0.95	2.58	3.420 (9)	148
C7—H7A···O1^{ii}	0.98	2.39	3.203 (10)	140
C8—H8···I1^{iii}	0.95	2.91	3.807 (6)	159

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

All H atoms were located in a difference electron-density map, but were positioned with idealized geometry and refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C,N) or 1.5U_{eq}(methyl C)] using a riding model with N—H = 0.88 Å, and C—H = 0.95 and 0.98 Å for aromatic and methyl H atoms, respectively. The methyl groups were allowed to rotate but not to tip. The highest peak in the final difference map is located 0.93 Å from I1. The deepest hole is located 0.83 Å from I1.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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