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Benzyl(1,1-dimethyl-3-oxobutyl)ammonium iodide

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The crystal structure of benzyl(1,1-dimethyl-3-oxobutyl)ammonium iodide, $C_{13}H_{20}INO$, has been determined at 120 K. An intramolecular N—H···O hydrogen bond is present that influences the geometry of the cation. In the crystal structure, intermolecular N—H···O hydrogen bonds connect pairs of molecules and N—H···I hydrogen-bonding interactions are also present.

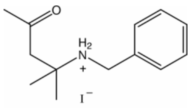
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.025
wR factor = 0.059
Data-to-parameter ratio = 30.7

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

Comment

Compounds containing ammonium and carbonyl groups are likely to exhibit crystal structures involving classical hydrogen bonding. When halide ions are also present, interesting hydrogen-bonding networks may be formed. As part of an ongoing study of the structural and hydrogen-bonding characteristics of organic–inorganic hybrid solids, the title compound, (I), a derivative of benzylammonium iodide, was crystallized and the structure determined by X-ray diffraction analysis.



(I)

Fig. 1 shows the molecular structure of (I) and the atomic numbering scheme. All bond distances and angles are within the ranges of accepted values. In the cation, the aromatic ring and atom C7 are coplanar, with an r.m.s. deviation of 0.013 Å. An interesting feature of the molecular geometry is that the chain comprising atoms C7, N1, C8, C11, C12 and C13 is not in the all-*trans* conformation, but is bent at atom C8, the atom to which the two methyl groups are bonded. The N1—C8—C11 angle is 110.88 (13)°. The adoption of this geometry is

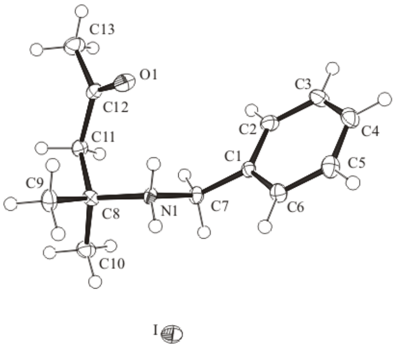


Figure 1
The molecular structure of (I), showing the atomic numbering scheme and displacement ellipsoids at the 50% probability level (*ORTEP*-3; Farrugia, 1997).

explained by the formation of an intramolecular N—H···O hydrogen bond (see below). The sets of atoms C11/C12/C13/O1 and C7/N1/C8/C9 are each coplanar with r.m.s deviations of 0.002 and 0.003 Å, respectively. The angle between the two planes is 88.22 (8)°.

Intermolecular and intramolecular hydrogen bonds occur in the crystal structure. These interactions involve the N and O atoms and the iodide anion. One H atom (H1) on the N atom forms a bifurcated hydrogen bond to two O atoms at donor–acceptor distances of 2.746 (2) (intramolecular) and 2.9444 (19) Å (intermolecular; symmetry code: $-x$, y, z), respectively. The second H atom (H2) on the N atom is hydrogen bonded to an iodide ion at an N···I distance of 3.532 (2) Å. Additional hydrogen-bonding parameters are given in Table 1.

The molecular packing and hydrogen-bonding interactions are illustrated in Fig. 2. The ion pairs pack in layers of hydrogen-bonded dimers parallel to the c axis.

Experimental

Benzylammonium iodide was prepared by the dropwise addition of HI (47%, Acros Organics) to a solution of benzylamine (99%, Saarchem) in chloroform (99%, Merck). The resulting precipitate was filtered and allowed to dry. Good-quality single crystals of the title compound were crystallized at room temperature from a solution of benzylammonium iodide in acetone (99%, Rochelle Chemicals).

Crystal data

$C_{13}H_{20}NO^+\cdot I^-$
$M_r = 333.20$
Monoclinic, $P2_1/n$
$a = 8.008\ (4)$ Å
$b = 18.046\ (3)$ Å
$c = 9.8377\ (16)$ Å
$\beta = 96.04\ (2)°$
$V = 1413.8\ (8)$ Å^3
$Z = 4$
$D_x = 1.565$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 54 reflections
$\theta = 2$–$31°$
$\mu = 2.25$ mm^{-1}
$T = 293\ (2)$ K
Block, light brown
0.40 × 0.30 × 0.30 mm

Data collection

Oxford Excalibur2 diffractometer
ω–2θ scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{\min} = 0.429$, $T_{\max} = 0.508$
12724 measured reflections
4475 independent reflections
4097 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.024$
$\theta_{\max} = 31.9°$
$h = -11 \rightarrow 7$
$k = -26 \rightarrow 26$
$l = -13 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.059$
$S = 1.07$
4475 reflections
146 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0277P)^2 + 0.8647P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.003$
$\Delta\rho_{\max} = 0.80$ e Å^{-3}
$\Delta\rho_{\min} = -0.92$ e Å^{-3}

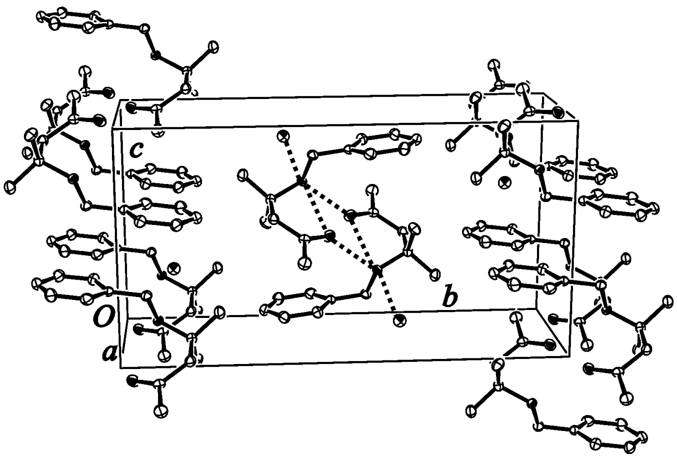


Figure 2
Packing diagram for (I), showing some of the hydrogen-bonding interactions as dashed lines (*ORTEP*-3; Farrugia, 1997).

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H0A···O1	0.90	2.09	2.746 (2)	128
N1—H0A···O1$^{\rm i}$	0.90	2.19	2.9444 (19)	141
N1—H0B···I	0.90	2.65	3.532 (2)	166

Symmetry code: (i) $-x$, $-y$, $-z$.

All H atoms were included in the riding-model approximation, with C—H = 0.93–0.97 and N—H = 0.90 Å and $U_{\rm iso}({\rm H}) = 1.5U_{\rm iso}({\rm C})$ for methyl H atoms and $1.2U_{\rm iso}$(C/N) for the remaining H atoms.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2003); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2000).

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References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Oxford Diffraction (2003). *CrysAlis CCD* and *CrysAlis RED*. Version 1.170. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.