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Bis(isopropylamino)methylcarbenium tetrakis(pentafluorophenyl)gallate

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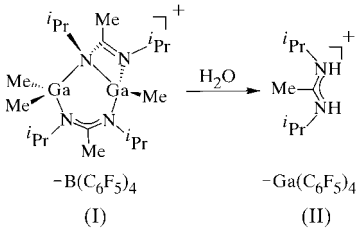
The title compound, $[MeC(NH^iPr)_2][Ga(C_6F_5)_4]$ crystallizes as discrete ions forming interionic hydrogen bonds of the type N—H···F.

Comment

As part of our reactivity studies of cationic Group 13 metal complexes (Coles & Jordan, 1997; Ihara *et al.*, 1998; Radzewich *et al.*, 1998, 1999), the reaction of the Ga amidinate salt $[\{MeC(N^iPr)_2\}_2Ga_2Me_3][B(C_6F_5)_4]$, (I), with H_2O was investigated. Compound (I) reacts readily with H_2O to yield the title compound, (II).



(I) (II)

Complex (II) crystallizes as discrete acetamidinium cations $\{MeC(NH^iPr)_2\}^+$ and $Ga(C_6F_5)_4^-$ anions that form interionic hydrogen bonds. There are two likely hydrogen-bonding interactions N1—H1···F21($\frac{1}{2}-x$, $\frac{1}{2}+y$, z) and N2—H2···F16($\frac{1}{2}+x$, y, $\frac{1}{2}-z$), with N···F separations of 3.121 (4) and 3.135 (3) Å, and N—H···F angles of 162 and 167°, respectively.

The bond distances and angles in the cation (Table 1) are very similar to those in the closely related acetamidinium cations in $[MeC(NH_2)_2]Cl$ (Cannon *et al.*, 1976) and $[\{MeC(NH_2)_2\}_2]CO_3$ (Norrestam, 1984). The bond angles about the central C28 atom [average 120.0 (6)°] are very similar and their sum is *ca* 360°, as expected for an sp^2-carbon. The bond distances C28—N1 [1.306 (4) Å] and C28—N2 [1.311 (4) Å] are statistically equivalent. These bond distances are intermediate between normal Csp^2—N single (1.458 Å; Sutton, 1965) and C=N double [1.271 (2) Å; Levine, 1963] bond distances and are similar to those in $[\{MeC(NH_2)_2\}_2]CO_3$ (Norrestam, 1984). Thus, the π electrons are delocalized over the NCN unit. The N^{i}Pr units are normal and the C27 and C30 ^{i}Pr groups are oriented *syn* and *anti* with respect to the C29 Me group [torsion angles: C30—N2—C28—C20 −176.8 (3)°; C27—N1—C28—C29 0.3 (5)°].

The $Ga(C_6F_5)_4^-$ anion adopts a nearly ideal tetrahedral structure. The angles about Ga range between 105.0 (1) and 112.8 (1)°, and thus remain close to the ideal tetrahedral angle of 109.47°. The Ga—C bond lengths [average 2.009 (13) Å] are in excellent agreement with the Ga—C distances in $[(Ph_3P)_2N][Ga(C_6F_5)_4]$ [average 2.01 (2) Å; Tebbe *et al.*, 1996] and are slightly longer than those in $GaPh_3$ [average 1.957 (16) Å; Malone & McDonald, 1970], probably due to a less electrophilic Ga center in $Ga(C_6F_5)_4^-$.

Experimental

Analytically pure (II) (70 mg, 0.35 mmol) was dissolved in wet C_6H_5Cl (*ca* 0.5 ml) and layered with pentane (*ca* 3 ml). Colorless crystals of (II) formed after 3 d at 296 K.

Crystal data

$(C_8H_{19}N_2)[Ga(C_6F_5)_4]$
M_r = 881.21
Orthorhombic, *Pbca*
a = 21.4651 (12) Å
b = 13.3773 (8) Å
c = 23.3868 (14) Å
V = 6715.4 (7) Å^3
Z = 8
D_x = 1.743 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5204 reflections
θ = 2–27°
μ = 0.959 mm^{-1}
T = 193 (2) K
Block, yellow
0.35 × 0.32 × 0.10 mm

Data collection

Bruker CCD area-detector diffractometer
φ scans
Absorption correction: empirical (*SADABS*; Blessing, 1995)
T_{min} = 0.730, T_{max} = 0.910
31 325 measured reflections
6850 independent reflections
3685 reflections with $I > 2\sigma(I)$
R_{int} = 0.084
θ_{max} = 26.37°
$h = 0 \rightarrow 26$
$k = 0 \rightarrow 16$
$l = 0 \rightarrow 29$
Intensity decay: <1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.075
S = 1.014
6850 reflections
501 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0180P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ga—C1	1.993 (3)	N1—C28	1.306 (4)
Ga—C13	2.005 (3)	N1—C27	1.454 (4)
Ga—C7	2.019 (3)	N2—C28	1.311 (4)
Ga—C19	2.020 (3)	N2—C30	1.472 (4)
C1—Ga—C13	105.03 (12)	C13—Ga—C19	110.62 (13)
C1—Ga—C7	111.78 (13)	C7—Ga—C19	105.18 (13)
C13—Ga—C7	111.54 (13)	C28—N1—C27	127.3 (3)
C1—Ga—C19	112.84 (13)	C28—N2—C30	126.9 (3)

Data collection: *SMART* (Bruker, 1996); cell refinement: *SMART*; data reduction: *SHELXTL* (Sheldrick, 1997); 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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