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N,*N*,*N*-Trimethyl-1-[4-(pyridin-2-yl)phenyl]methanaminium hexafluoridophosphate

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Keywords: crystal structure; 2-phenylpyridine; quaternary ammonium salt.

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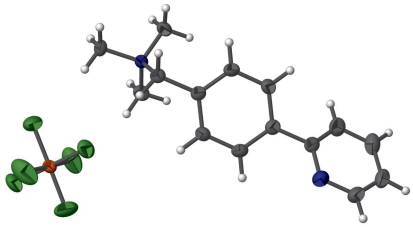
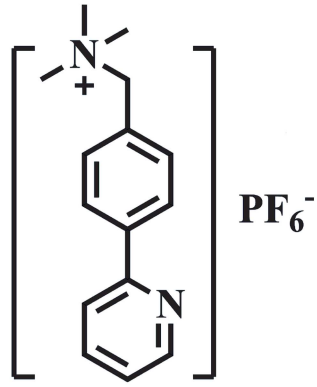
Structural data: full structural data are available from iucrdata.iucr.org

In the cation of the title molecular salt, $C_{15}H_{19}N_2^+\cdot PF_6^-$, the dihedral angle between the benzene and pyridine rings is 38.21 (10)°. In the crystal, weak C—H···F interactions arising from methyl and methylene groups adjacent to the quaternary N atom generate (001) sheets.

3D view



Chemical scheme



Structure description

Quaternary ammonium derivatives have been investigated as fluorescent probes for biological applications (Choi *et al.*, 2014) because of their favourable water solubility (Du *et al.*, 2017).

As part of our studies in this area, we now describe the synthesis and structure of the title molecular salt (Fig. 1). The dihedral angle between the C6–C11 benzene ring and its attached C1–C5/N1 pyridine ring is 37.86 (10)° and the C11—C12—N2—C13 torsion angle is 175.60 (15)°. In the crystal, weak C—H···F interactions (Table 1) link the components into (001) sheets.

Synthesis and crystallization

Phenylpyridine benzylbromide (2.48 g, 0.1 mol) was dissolved in 20 ml of tetrahydrofuran and 60 ml of trimethylamine (40%) were added and the mixture stirred at 363 K for 12 h. Then, excess NH_4PF_6 was added after the reaction had cooled to room temperature, and the solid product recovered by filtration (1.2 g, 80%). Yellow blocks were recrystallized from ethanol solution.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

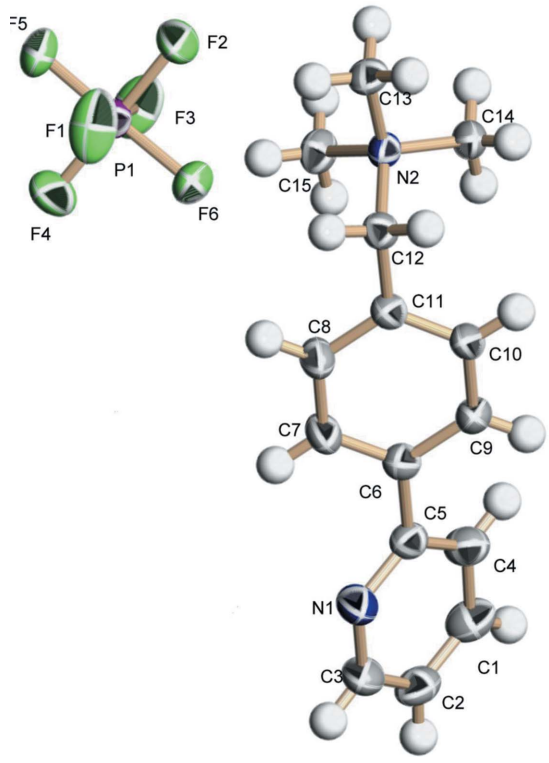


Figure 1
The molecular structure of the title compound showing 50% displacement ellipsoids.

Funding information

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12A···F4^{i}	0.97	2.50	3.441 (2)	163
C14—H14A···F5^{ii}	0.96	2.55	3.070 (3)	114
C15—H15C···F3	0.96	2.54	3.414 (2)	151

Symmetry codes: (i) $x, y-1, z$; (ii) $x-1, y-1, z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{19}N_2^+\cdot F_6P^-$
M_r	372.29
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	5.9107 (14), 8.5110 (19), 33.155 (8)
β (°)	90.726 (3)
V (Å^3)	1667.7 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.23
Crystal size (mm)	0.19 × 0.18 × 0.17
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.615, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9197, 2929, 2642
R_{int}	0.024
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.109, 1.04
No. of reflections	2929
No. of parameters	221
No. of restraints	3
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.50, −0.32

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

full crystallographic data

IUCrData (2019). **4**, x191206 [https://doi.org/10.1107/S2414314619012069]

N,*N*,*N*-Trimethyl-1-[4-(pyridin-2-yl)phenyl]methanaminium hexafluoridophosphate

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Crystal data

$C_{15}H_{19}N_2^+ \cdot F_6P^-$
M_r = 372.29
Monoclinic, $P2_1/n$
a = 5.9107 (14) Å
b = 8.5110 (19) Å
c = 33.155 (8) Å
β = 90.726 (3)°
V = 1667.7 (7) Å^3
Z = 4
$F(000)$ = 768
D_x = 1.483 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5626 reflections
θ = 2.4–27.5°
μ = 0.23 mm^{-1}
T = 296 K
Block, yellow
0.19 × 0.18 × 0.17 mm

Data collection

Bruker APEXII CCD diffractometer
Graphite monochromator
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.615, T_{max} = 0.746
9197 measured reflections
2929 independent reflections
2642 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 25.0°, θ_{min} = 2.5°
h = −7→5
k = −10→10
l = −39→39

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.109
S = 1.04
2929 reflections
221 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0518P)^2 + 1.2216P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Extinction correction: SHELXL2016 (Sheldrick, 2015), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0052 (9)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
P1	0.90293 (8)	0.73732 (5)	0.07069 (2)	0.02656 (17)
F1	1.1645 (2)	0.72985 (18)	0.07985 (6)	0.0716 (5)
F2	0.9394 (3)	0.63740 (16)	0.03048 (4)	0.0637 (5)
F3	0.6414 (2)	0.74621 (18)	0.05956 (5)	0.0631 (5)
F4	0.8649 (3)	0.83845 (17)	0.10989 (4)	0.0653 (5)
F5	0.9381 (2)	0.89666 (14)	0.04538 (4)	0.0480 (4)
F6	0.8645 (2)	0.57788 (14)	0.09500 (4)	0.0446 (3)
N1	0.0843 (3)	0.2266 (2)	0.26972 (5)	0.0409 (4)
N2	0.5066 (3)	0.24358 (17)	0.05910 (5)	0.0260 (4)
C1	−0.3375 (4)	0.0822 (3)	0.26267 (7)	0.0453 (5)
H1	−0.478424	0.034325	0.260160	0.054*
C2	−0.2701 (4)	0.1496 (3)	0.29865 (7)	0.0421 (5)
H2	−0.364510	0.148830	0.320881	0.051*
C3	−0.0590 (4)	0.2184 (3)	0.30082 (7)	0.0451 (6)
H3	−0.012898	0.261769	0.325324	0.054*
C4	−0.1916 (4)	0.0870 (3)	0.23029 (6)	0.0404 (5)
H4	−0.232793	0.041313	0.205797	0.048*
C5	0.0170 (3)	0.1608 (2)	0.23482 (6)	0.0318 (4)
C6	0.1751 (3)	0.1712 (2)	0.20039 (6)	0.0310 (4)
C7	0.3061 (4)	0.3046 (2)	0.19437 (6)	0.0371 (5)
H7	0.299121	0.387348	0.212637	0.045*
C8	0.4471 (4)	0.3154 (2)	0.16140 (6)	0.0357 (5)
H8	0.529710	0.406868	0.157265	0.043*
C9	0.1968 (4)	0.0460 (2)	0.17366 (6)	0.0344 (5)
H9	0.111937	−0.044679	0.177472	0.041*
C10	0.3437 (4)	0.0551 (2)	0.14138 (6)	0.0333 (5)
H10	0.359911	−0.030722	0.124292	0.040*
C11	0.4664 (3)	0.1911 (2)	0.13441 (6)	0.0292 (4)
C12	0.6243 (3)	0.2045 (2)	0.09932 (5)	0.0282 (4)
H12A	0.704960	0.105971	0.096452	0.034*
H12B	0.735173	0.285529	0.105267	0.034*
C13	0.6872 (4)	0.2653 (2)	0.02812 (6)	0.0336 (5)
H13A	0.617977	0.286957	0.002369	0.050*
H13B	0.776180	0.171279	0.026361	0.050*
H13C	0.782871	0.351684	0.035842	0.050*
C14	0.3537 (4)	0.1130 (2)	0.04599 (6)	0.0336 (5)
H14A	0.232047	0.102903	0.064740	0.050*
H14B	0.437619	0.016475	0.045190	0.050*
H14C	0.293017	0.135565	0.019630	0.050*

C15	0.3718 (3)	0.3917 (2)	0.06230 (6)	0.0344 (5)
H15A	0.254210	0.377693	0.081684	0.052*
H15B	0.305506	0.416454	0.036489	0.052*
H15C	0.469121	0.476111	0.070778	0.052*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0267 (3)	0.0212 (3)	0.0319 (3)	−0.00140 (19)	0.0044 (2)	−0.00271 (19)
F1	0.0331 (8)	0.0500 (9)	0.1314 (16)	−0.0012 (6)	−0.0107 (9)	0.0026 (9)
F2	0.1072 (13)	0.0403 (8)	0.0442 (8)	−0.0088 (8)	0.0261 (8)	−0.0127 (6)
F3	0.0327 (8)	0.0586 (9)	0.0977 (12)	−0.0065 (6)	−0.0076 (7)	0.0213 (8)
F4	0.1109 (14)	0.0430 (8)	0.0423 (8)	0.0112 (8)	0.0106 (8)	−0.0130 (6)
F5	0.0593 (9)	0.0290 (7)	0.0557 (8)	−0.0117 (6)	0.0046 (6)	0.0070 (6)
F6	0.0606 (9)	0.0323 (7)	0.0410 (7)	−0.0053 (6)	0.0017 (6)	0.0085 (5)
N1	0.0478 (11)	0.0399 (10)	0.0352 (9)	−0.0055 (8)	0.0093 (7)	−0.0068 (8)
N2	0.0297 (9)	0.0213 (8)	0.0272 (8)	−0.0011 (6)	0.0044 (6)	−0.0004 (6)
C1	0.0378 (12)	0.0524 (14)	0.0458 (12)	−0.0019 (10)	0.0056 (8)	0.0123 (11)
C2	0.0489 (13)	0.0387 (12)	0.0391 (11)	0.0057 (10)	0.0164 (10)	0.0081 (9)
C3	0.0623 (15)	0.0405 (12)	0.0330 (11)	−0.0039 (11)	0.0133 (9)	−0.0059 (9)
C4	0.0416 (11)	0.0472 (13)	0.0323 (10)	−0.0045 (9)	−0.0005 (8)	0.0042 (9)
C5	0.0384 (10)	0.0278 (10)	0.0293 (9)	0.0026 (8)	0.0039 (8)	0.0024 (8)
C6	0.0349 (11)	0.0301 (10)	0.0281 (9)	0.0001 (8)	0.0022 (8)	−0.0001 (8)
C7	0.0453 (13)	0.0309 (11)	0.0354 (11)	−0.0041 (9)	0.0082 (9)	−0.0105 (9)
C8	0.0405 (12)	0.0292 (10)	0.0375 (11)	−0.0090 (9)	0.0087 (9)	−0.0069 (9)
C9	0.0465 (12)	0.0274 (10)	0.0294 (10)	−0.0065 (9)	0.0040 (8)	0.0018 (8)
C10	0.0484 (12)	0.0243 (10)	0.0272 (9)	−0.0001 (9)	0.0040 (8)	−0.0027 (7)
C11	0.0338 (11)	0.0270 (10)	0.0270 (9)	0.0006 (8)	0.0018 (8)	−0.0015 (8)
C12	0.0291 (10)	0.0267 (9)	0.0287 (9)	0.0017 (8)	0.0005 (8)	−0.0012 (7)
C13	0.0364 (11)	0.0338 (11)	0.0308 (10)	−0.0031 (9)	0.0109 (8)	0.0022 (8)
C14	0.0405 (12)	0.0288 (10)	0.0315 (10)	−0.0092 (9)	−0.0006 (8)	−0.0015 (8)
C15	0.0335 (11)	0.0248 (10)	0.0451 (11)	0.0054 (8)	0.0030 (9)	0.0022 (8)

Geometric parameters (Å, º)

P1—F1	1.5729 (15)	C6—C9	1.392 (3)
P1—F2	1.5982 (14)	C7—H7	0.9300
P1—F3	1.5865 (15)	C7—C8	1.386 (3)
P1—F4	1.5774 (14)	C8—H8	0.9300
P1—F5	1.6096 (13)	C8—C11	1.391 (3)
P1—F6	1.5960 (13)	C9—H9	0.9300
N1—C3	1.345 (3)	C9—C10	1.389 (3)
N1—C5	1.341 (3)	C10—H10	0.9300
N2—C12	1.532 (2)	C10—C11	1.387 (3)
N2—C13	1.502 (2)	C11—C12	1.505 (3)
N2—C14	1.494 (2)	C12—H12A	0.9700
N2—C15	1.496 (2)	C12—H12B	0.9700
C1—H1	0.9300	C13—H13A	0.9600

C1—C2	1.378 (3)	C13—H13B	0.9600
C1—C4	1.386 (3)	C13—H13C	0.9600
C2—H2	0.9300	C14—H14A	0.9600
C2—C3	1.379 (3)	C14—H14B	0.9600
C3—H3	0.9300	C14—H14C	0.9600
C4—H4	0.9300	C15—H15A	0.9600
C4—C5	1.390 (3)	C15—H15B	0.9600
C5—C6	1.487 (3)	C15—H15C	0.9600
C6—C7	1.391 (3)		

F1—P1—F2	89.82 (10)	C6—C7—H7	119.7
F1—P1—F3	177.64 (10)	C8—C7—C6	120.58 (18)
F1—P1—F4	90.74 (10)	C8—C7—H7	119.7
F1—P1—F5	90.10 (8)	C7—C8—H8	119.6
F1—P1—F6	90.81 (8)	C7—C8—C11	120.80 (19)
F2—P1—F5	89.64 (8)	C11—C8—H8	119.6
F3—P1—F2	88.43 (10)	C6—C9—H9	119.6
F3—P1—F5	88.30 (8)	C10—C9—C6	120.75 (18)
F3—P1—F6	90.77 (8)	C10—C9—H9	119.6
F4—P1—F2	178.94 (9)	C9—C10—H10	119.7
F4—P1—F3	90.98 (10)	C11—C10—C9	120.55 (18)
F4—P1—F5	89.46 (8)	C11—C10—H10	119.7
F4—P1—F6	91.44 (8)	C8—C11—C12	119.77 (18)
F6—P1—F2	89.45 (7)	C10—C11—C8	118.68 (18)
F6—P1—F5	178.71 (7)	C10—C11—C12	121.51 (17)
C5—N1—C3	117.2 (2)	N2—C12—H12A	108.7
C13—N2—C12	107.65 (15)	N2—C12—H12B	108.7
C14—N2—C12	110.97 (14)	C11—C12—N2	114.22 (15)
C14—N2—C13	108.99 (14)	C11—C12—H12A	108.7
C14—N2—C15	109.06 (15)	C11—C12—H12B	108.7
C15—N2—C12	110.95 (14)	H12A—C12—H12B	107.6
C15—N2—C13	109.17 (14)	N2—C13—H13A	109.5
C2—C1—H1	120.6	N2—C13—H13B	109.5
C2—C1—C4	118.8 (2)	N2—C13—H13C	109.5
C4—C1—H1	120.6	H13A—C13—H13B	109.5
C1—C2—H2	120.9	H13A—C13—H13C	109.5
C1—C2—C3	118.2 (2)	H13B—C13—H13C	109.5
C3—C2—H2	120.9	N2—C14—H14A	109.5
N1—C3—C2	124.1 (2)	N2—C14—H14B	109.5
N1—C3—H3	118.0	N2—C14—H14C	109.5
C2—C3—H3	118.0	H14A—C14—H14B	109.5
C1—C4—H4	120.4	H14A—C14—H14C	109.5
C1—C4—C5	119.3 (2)	H14B—C14—H14C	109.5
C5—C4—H4	120.4	N2—C15—H15A	109.5
N1—C5—C4	122.33 (19)	N2—C15—H15B	109.5
N1—C5—C6	117.06 (18)	N2—C15—H15C	109.5
C4—C5—C6	120.60 (18)	H15A—C15—H15B	109.5
C7—C6—C5	121.02 (18)	H15A—C15—H15C	109.5

C7—C6—C9	118.53 (18)	H15B—C15—H15C	109.5
C9—C6—C5	120.44 (18)		
N1—C5—C6—C7	−36.7 (3)	C6—C7—C8—C11	−2.2 (3)
N1—C5—C6—C9	142.5 (2)	C6—C9—C10—C11	−2.0 (3)
C1—C2—C3—N1	1.4 (4)	C7—C6—C9—C10	−0.9 (3)
C1—C4—C5—N1	0.7 (3)	C7—C8—C11—C10	−0.7 (3)
C1—C4—C5—C6	−178.6 (2)	C7—C8—C11—C12	−178.75 (19)
C2—C1—C4—C5	−0.7 (3)	C8—C11—C12—N2	−101.0 (2)
C3—N1—C5—C4	0.2 (3)	C9—C6—C7—C8	3.0 (3)
C3—N1—C5—C6	179.52 (19)	C9—C10—C11—C8	2.8 (3)
C4—C1—C2—C3	−0.3 (3)	C9—C10—C11—C12	−179.17 (18)
C4—C5—C6—C7	142.6 (2)	C10—C11—C12—N2	81.1 (2)
C4—C5—C6—C9	−38.2 (3)	C13—N2—C12—C11	175.60 (15)
C5—N1—C3—C2	−1.3 (3)	C14—N2—C12—C11	−65.2 (2)
C5—C6—C7—C8	−177.7 (2)	C15—N2—C12—C11	56.2 (2)
C5—C6—C9—C10	179.84 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12*A*···F4^{i}	0.97	2.50	3.441 (2)	163
C14—H14*A*···F5^{ii}	0.96	2.55	3.070 (3)	114
C15—H15*C*···F3	0.96	2.54	3.414 (2)	151

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) *x*−1, *y*−1, *z*.