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(*E*)-3-[4-(Benzo[*d*]oxazol-2-yl)styryl]-1-methylpyridin-1-ium hexafluoridophosphate

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Keywords: crystal structure; benzoxazole derivative; hexafluoridophosphate; C—H···F hydrogen bond.

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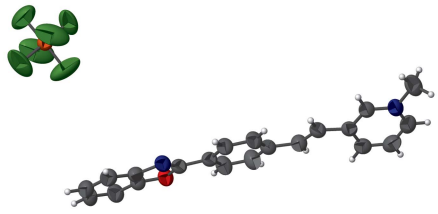
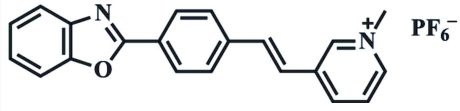
Structural data: full structural data are available from iucrdata.iucr.org

In the cation of the title molecular salt, $C_{21}H_{17}N_2O^+\cdot PF_6^-$, the pyridine ring and benzoxazole ring system are twisted with respect to the central benzene ring at dihedral angles of 23.75 (18) and 5.53 (16)°. In the crystal, the hexafluoridophosphate anion accepts a weak C—H···F hydrogen bond from the cation to form an ion-pair.

3D view



Chemical scheme



Structure description

In this study, we report the crystal structure of title salt (Fig. 1). In the cation, the benzoxazole ring system and the pyridine ring are twisted by 23.75 (18) and 5.53 (16)°, respectively, to the central benzene ring, similar to the values found in a related structure (Qu *et al.*, 2008). In the crystal, the hexafluoridophosphate anion accepts a weak C—H···F hydrogen bond from the cation to form an ion-pair (Table 1).

Synthesis and crystallization

To a solution of silver hexafluoridophosphate (0.17 g, 0.68 mmol) in acetonitrile was added (*E*)-3-[4-(benzo[*d*]oxazol-2-yl)styryl]-1-methylpyridin-1-ium iodide (0.3 g, 0.68 mmol). The mixture was refluxed for 4 h, then filtered and evaporated, and concentrated *in vacuo* to give a solid product. Yellow single crystals were obtained in a 15% yield by recrystallization from acetonitrile solution.

Refinement

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C18—H18A···F6^{i}	0.96	2.51	3.228 (7)	132

Symmetry code: (i) $-x+2, -y, -z+1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{17}N_2O^+\cdot PF_6^-$
M_r	458.33
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	6.717 (2), 8.155 (3), 19.936 (6)
α, β, γ (°)	85.032 (3), 85.188 (3), 65.893 (3)
V (Å^3)	991.6 (5)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.21
Crystal size (mm)	0.25 × 0.2 × 0.18
Data collection	
Diffractometer	Bruker SMART 1000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7021, 3442, 3035
R_{int}	0.023
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.080, 0.246, 1.08
No. of reflections	3442
No. of parameters	281
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.69, −0.59

Computer programs: *SMART* and *SAINT* (Bruker, 2001), *SHELXTL* (Sheldrick, 2008) and *SHELXL2014* (Sheldrick, 2015).

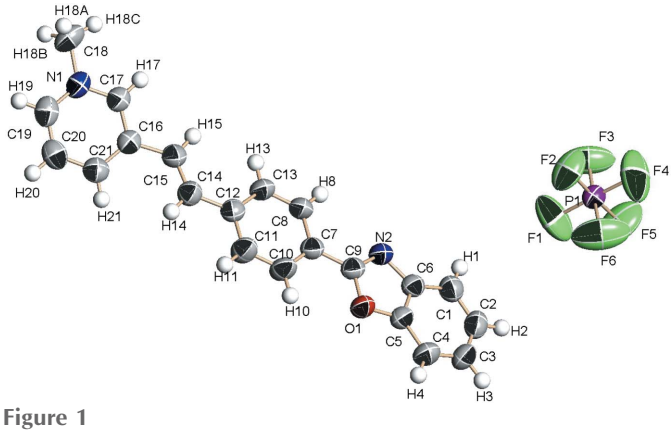

Figure 1
The molecular structure of the title salt with displacement ellipsoids drawn at the 50% probability level.

Funding information

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full crystallographic data

IUCrData (2017). **2**, x171735 [https://doi.org/10.1107/S2414314617017357]

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Crystal data

$C_{21}H_{17}N_2O^+\cdot PF_6^-$
M_r = 458.33
Triclinic, $P\overline{1}$
a = 6.717 (2) Å
b = 8.155 (3) Å
c = 19.936 (6) Å
α = 85.032 (3)°
β = 85.188 (3)°
γ = 65.893 (3)°
V = 991.6 (5) Å^3
Z = 2
F(000) = 468
D_x = 1.535 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4838 reflections
θ = 2.7–27.0°
μ = 0.21 mm^{-1}
T = 296 K
Block, yellow
0.25 × 0.2 × 0.18 mm

Data collection

Bruker SMART 1000 diffractometer
phi and ω scans
7021 measured reflections
3442 independent reflections
3035 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 25.0°, θ_{min} = 2.1°
h = −7→7
k = −9→9
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.080
$wR(F^2)$ = 0.246
S = 1.08
3442 reflections
281 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1562P)^2 + 0.6275P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

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.

Refinement. All hydrogen atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for the methyl H atoms and 1.2U_{eq}(C) for the others.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
P1	0.69074 (14)	0.22595 (11)	0.11548 (4)	0.0542 (4)
F2	0.7984 (6)	0.0467 (4)	0.15891 (17)	0.1251 (13)
F6	0.4733 (6)	0.1997 (5)	0.1158 (3)	0.181 (2)
F1	0.6114 (8)	0.3458 (6)	0.1756 (2)	0.1692 (19)
F3	0.9069 (5)	0.2535 (4)	0.1129 (3)	0.1514 (17)
F4	0.7680 (10)	0.1089 (6)	0.05329 (19)	0.179 (2)
F5	0.5907 (7)	0.4022 (5)	0.0697 (2)	0.1567 (17)
O1	0.2734 (4)	0.8061 (3)	0.46644 (12)	0.0638 (7)
C9	0.4846 (5)	0.7808 (4)	0.47330 (17)	0.0572 (8)
C17	1.3454 (6)	0.2823 (4)	0.82449 (18)	0.0585 (8)
H17	1.4452	0.2606	0.7876	0.070*
C7	0.5824 (5)	0.6955 (4)	0.53677 (17)	0.0556 (8)
N1	1.4199 (5)	0.2301 (4)	0.88659 (15)	0.0620 (8)
N2	0.5754 (4)	0.8382 (4)	0.42255 (14)	0.0596 (7)
C5	0.2272 (5)	0.8911 (5)	0.40320 (17)	0.0582 (8)
C16	1.1258 (5)	0.3669 (4)	0.81385 (17)	0.0560 (8)
C6	0.4113 (5)	0.9123 (5)	0.37623 (17)	0.0577 (8)
C14	0.8545 (6)	0.4733 (5)	0.72631 (19)	0.0648 (9)
H14	0.7538	0.4660	0.7601	0.078*
C12	0.7684 (5)	0.5421 (5)	0.65957 (18)	0.0594 (8)
C15	1.0544 (6)	0.4212 (5)	0.74411 (18)	0.0622 (9)
H15	1.1603	0.4179	0.7104	0.075*
C13	0.8911 (5)	0.5823 (5)	0.60598 (19)	0.0657 (9)
H13	1.0376	0.5565	0.6109	0.079*
C21	0.9837 (6)	0.3997 (5)	0.87051 (19)	0.0660 (9)
H21	0.8341	0.4599	0.8658	0.079*
C19	1.2841 (7)	0.2591 (5)	0.9406 (2)	0.0721 (10)
H19	1.3389	0.2221	0.9832	0.086*
C8	0.7991 (5)	0.6594 (5)	0.54604 (18)	0.0632 (9)
H8	0.8829	0.6877	0.5112	0.076*
C10	0.4596 (6)	0.6525 (6)	0.5896 (2)	0.0704 (10)
H10	0.3148	0.6738	0.5841	0.084*
C18	1.6587 (7)	0.1359 (7)	0.8941 (3)	0.0868 (13)
H18A	1.6944	0.0118	0.9079	0.130*
H18B	1.7015	0.1913	0.9275	0.130*
H18C	1.7347	0.1435	0.8518	0.130*
C1	0.4092 (7)	0.9970 (5)	0.31239 (19)	0.0694 (9)
H1	0.5319	1.0120	0.2929	0.083*
C11	0.5524 (6)	0.5786 (6)	0.6501 (2)	0.0739 (11)
H11	0.4679	0.5526	0.6853	0.089*
C2	0.2198 (7)	1.0570 (5)	0.2796 (2)	0.0743 (10)
H2	0.2129	1.1162	0.2372	0.089*
C20	1.0635 (7)	0.3432 (5)	0.9341 (2)	0.0751 (10)
H20	0.9680	0.3623	0.9720	0.090*
C3	0.0344 (7)	1.0318 (6)	0.3080 (2)	0.0779 (11)

H3	−0.0908	1.0731	0.2837	0.093*
C4	0.0342 (6)	0.9480 (6)	0.3705 (2)	0.0753 (11)
H4	−0.0871	0.9305	0.3898	0.090*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0594 (6)	0.0470 (5)	0.0577 (6)	−0.0233 (4)	−0.0063 (4)	0.0006 (4)
F2	0.175 (3)	0.086 (2)	0.124 (2)	−0.062 (2)	−0.068 (2)	0.0443 (18)
F6	0.094 (2)	0.118 (3)	0.355 (7)	−0.066 (2)	−0.030 (3)	−0.001 (4)
F1	0.225 (5)	0.161 (4)	0.140 (3)	−0.095 (3)	0.068 (3)	−0.092 (3)
F3	0.0738 (19)	0.096 (2)	0.289 (5)	−0.0416 (16)	−0.003 (2)	−0.006 (3)
F4	0.309 (6)	0.121 (3)	0.097 (2)	−0.070 (3)	−0.006 (3)	−0.041 (2)
F5	0.183 (4)	0.086 (2)	0.201 (4)	−0.054 (2)	−0.087 (3)	0.070 (3)
O1	0.0502 (12)	0.0778 (16)	0.0629 (14)	−0.0259 (11)	−0.0069 (10)	0.0024 (12)
C9	0.0510 (17)	0.0540 (18)	0.063 (2)	−0.0165 (14)	−0.0066 (14)	−0.0074 (15)
C17	0.064 (2)	0.0539 (18)	0.0607 (19)	−0.0261 (15)	−0.0076 (15)	−0.0032 (14)
C7	0.0501 (17)	0.0540 (17)	0.0595 (18)	−0.0172 (14)	−0.0041 (14)	−0.0053 (14)
N1	0.0731 (18)	0.0532 (15)	0.0662 (18)	−0.0300 (14)	−0.0190 (14)	0.0016 (13)
N2	0.0476 (14)	0.0661 (17)	0.0614 (16)	−0.0193 (12)	−0.0034 (12)	−0.0017 (13)
C5	0.0534 (18)	0.0600 (19)	0.0589 (18)	−0.0199 (14)	−0.0078 (14)	−0.0027 (15)
C16	0.0625 (19)	0.0443 (16)	0.0629 (19)	−0.0225 (14)	−0.0075 (15)	−0.0032 (13)
C6	0.0541 (18)	0.0572 (18)	0.0595 (18)	−0.0186 (14)	−0.0042 (14)	−0.0103 (14)
C14	0.064 (2)	0.067 (2)	0.063 (2)	−0.0269 (17)	−0.0055 (16)	−0.0005 (16)
C12	0.0570 (19)	0.0549 (18)	0.0617 (19)	−0.0178 (15)	−0.0045 (15)	−0.0024 (15)
C15	0.0570 (19)	0.0601 (19)	0.064 (2)	−0.0180 (15)	−0.0034 (15)	−0.0024 (16)
C13	0.0455 (17)	0.079 (2)	0.068 (2)	−0.0208 (16)	−0.0079 (15)	0.0000 (18)
C21	0.068 (2)	0.0565 (19)	0.073 (2)	−0.0241 (16)	−0.0030 (17)	−0.0057 (16)
C19	0.099 (3)	0.065 (2)	0.062 (2)	−0.042 (2)	−0.011 (2)	−0.0015 (17)
C8	0.0476 (17)	0.076 (2)	0.0596 (19)	−0.0200 (16)	0.0023 (14)	−0.0029 (16)
C10	0.0505 (18)	0.088 (3)	0.076 (2)	−0.0326 (18)	−0.0084 (16)	0.011 (2)
C18	0.073 (3)	0.091 (3)	0.100 (3)	−0.034 (2)	−0.035 (2)	0.008 (2)
C1	0.073 (2)	0.071 (2)	0.062 (2)	−0.0281 (18)	−0.0005 (17)	−0.0038 (17)
C11	0.062 (2)	0.093 (3)	0.072 (2)	−0.040 (2)	−0.0065 (17)	0.015 (2)
C2	0.087 (3)	0.070 (2)	0.059 (2)	−0.023 (2)	−0.0120 (18)	−0.0027 (17)
C20	0.093 (3)	0.069 (2)	0.068 (2)	−0.039 (2)	0.009 (2)	−0.0106 (18)
C3	0.070 (2)	0.089 (3)	0.069 (2)	−0.023 (2)	−0.0232 (19)	−0.003 (2)
C4	0.055 (2)	0.090 (3)	0.079 (3)	−0.0261 (19)	−0.0131 (17)	−0.002 (2)

Geometric parameters (Å, º)

P1—F1	1.532 (3)	C14—H14	0.9300
P1—F4	1.552 (3)	C12—C11	1.383 (5)
P1—F3	1.553 (3)	C12—C13	1.393 (5)
P1—F6	1.559 (3)	C15—H15	0.9300
P1—F2	1.559 (3)	C13—C8	1.372 (5)
P1—F5	1.561 (3)	C13—H13	0.9300
O1—C9	1.364 (4)	C21—C20	1.385 (6)

O1—C5	1.380 (4)	C21—H21	0.9300
C9—N2	1.289 (4)	C19—C20	1.367 (6)
C9—C7	1.460 (5)	C19—H19	0.9300
C17—N1	1.343 (4)	C8—H8	0.9300
C17—C16	1.376 (5)	C10—C11	1.378 (5)
C17—H17	0.9300	C10—H10	0.9300
C7—C8	1.388 (5)	C18—H18A	0.9600
C7—C10	1.393 (5)	C18—H18B	0.9600
N1—C19	1.323 (5)	C18—H18C	0.9600
N1—C18	1.483 (5)	C1—C2	1.365 (6)
N2—C6	1.401 (4)	C1—H1	0.9300
C5—C6	1.376 (5)	C11—H11	0.9300
C5—C4	1.385 (5)	C2—C3	1.408 (6)
C16—C21	1.386 (5)	C2—H2	0.9300
C16—C15	1.480 (5)	C20—H20	0.9300
C6—C1	1.393 (5)	C3—C4	1.370 (6)
C14—C15	1.303 (5)	C3—H3	0.9300
C14—C12	1.468 (5)	C4—H4	0.9300

F1—P1—F4	178.5 (3)	C13—C12—C14	122.9 (3)
F1—P1—F3	88.0 (3)	C14—C15—C16	125.0 (3)
F4—P1—F3	92.1 (3)	C14—C15—H15	117.5
F1—P1—F6	93.1 (3)	C16—C15—H15	117.5
F4—P1—F6	86.8 (3)	C8—C13—C12	121.0 (3)
F3—P1—F6	178.3 (3)	C8—C13—H13	119.5
F1—P1—F2	95.1 (3)	C12—C13—H13	119.5
F4—P1—F2	86.4 (2)	C20—C21—C16	120.3 (4)
F3—P1—F2	90.0 (2)	C20—C21—H21	119.8
F6—P1—F2	91.2 (2)	C16—C21—H21	119.8
F1—P1—F5	86.8 (3)	N1—C19—C20	120.3 (4)
F4—P1—F5	91.7 (3)	N1—C19—H19	119.9
F3—P1—F5	88.7 (2)	C20—C19—H19	119.9
F6—P1—F5	90.1 (2)	C13—C8—C7	120.7 (3)
F2—P1—F5	177.6 (2)	C13—C8—H8	119.6
C9—O1—C5	103.8 (3)	C7—C8—H8	119.6
N2—C9—O1	115.6 (3)	C11—C10—C7	120.1 (3)
N2—C9—C7	127.0 (3)	C11—C10—H10	120.0
O1—C9—C7	117.4 (3)	C7—C10—H10	120.0
N1—C17—C16	121.9 (3)	N1—C18—H18A	109.5
N1—C17—H17	119.0	N1—C18—H18B	109.5
C16—C17—H17	119.0	H18A—C18—H18B	109.5
C8—C7—C10	118.7 (3)	N1—C18—H18C	109.5
C8—C7—C9	120.4 (3)	H18A—C18—H18C	109.5
C10—C7—C9	120.9 (3)	H18B—C18—H18C	109.5
C19—N1—C17	121.2 (3)	C2—C1—C6	117.2 (4)
C19—N1—C18	119.9 (3)	C2—C1—H1	121.4
C17—N1—C18	119.0 (3)	C6—C1—H1	121.4
C9—N2—C6	104.1 (3)	C10—C11—C12	121.4 (3)

C6—C5—O1	107.6 (3)	C10—C11—H11	119.3
C6—C5—C4	124.1 (4)	C12—C11—H11	119.3
O1—C5—C4	128.3 (3)	C1—C2—C3	121.9 (4)
C17—C16—C21	116.9 (3)	C1—C2—H2	119.1
C17—C16—C15	119.3 (3)	C3—C2—H2	119.1
C21—C16—C15	123.8 (3)	C19—C20—C21	119.4 (4)
C5—C6—C1	119.8 (3)	C19—C20—H20	120.3
C5—C6—N2	108.8 (3)	C21—C20—H20	120.3
C1—C6—N2	131.4 (3)	C4—C3—C2	121.6 (4)
C15—C14—C12	128.1 (4)	C4—C3—H3	119.2
C15—C14—H14	115.9	C2—C3—H3	119.2
C12—C14—H14	115.9	C3—C4—C5	115.4 (4)
C11—C12—C13	118.1 (3)	C3—C4—H4	122.3
C11—C12—C14	118.9 (3)	C5—C4—H4	122.3

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18*A*···F6^{i}	0.96	2.51	3.228 (7)	132

Symmetry code: (i) −*x*+2, −*y*, −*z*+1.