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4-[(2′-Cyanobiphenyl-4-yl)methyl]-morpholin-4-ium tetrafluoridoborate

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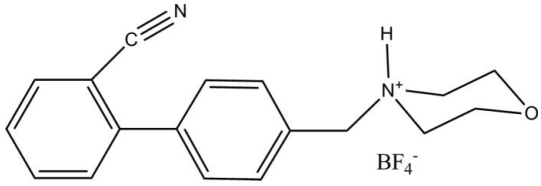
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.067; wR factor = 0.202; data-to-parameter ratio = 17.1.

In the crystal structure of the title compound, $C_{18}H_{19}N_2O^+\cdot BF_4^-$, bifurcated N—H···(F,F) hydrogen bonds link the protonated 4′-morpholinemethylbiphenyl-2-carbonitrile cations and slightly distorted tetrafluoroborate anions. π–π interactions [centroid–centroid distance = 3.805 (3) Å] help to consolidate the packing. The dihedral angle between the benzene rings in the cation is 57.24 (11)°.

Related literature

For a related structure, see: SiMa (2010).



Experimental

Crystal data

$C_{18}H_{19}N_2O^+\cdot BF_4^-$
M_r = 366.16
Triclinic, $P\overline{1}$
a = 9.059 (6) Å
b = 9.859 (8) Å
c = 10.597 (8) Å
α = 76.324 (14)°
β = 83.71 (2)°
γ = 86.50 (3)°
V = 913.5 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 298 K
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.978, T_{max} = 0.978
9817 measured reflections
4098 independent reflections
3039 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.202
S = 1.06
4098 reflections
239 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···F1	0.90 (2)	2.14 (2)	2.902 (3)	141 (2)
N2—H2···F3	0.90 (2)	2.35 (2)	3.219 (3)	161 (2)

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to RiZhao Polytechnic for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2276).

References

Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
SiMa, W. (2010). *Acta Cryst.* E**66**, o2042.

supplementary materials

Acta Cryst. (2011). E**67**, o1061 [**doi:10.1107/S160053681101186X**]

4-[(2'-Cyanobiphenyl-4-yl)methyl]morpholin-4-ium tetrafluoridoborate

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Comment

The crystal structure of 4'-morpholinemethylbiphenyl-2-carbonitrile with nitrate is known (SiMa, 2010).

The asymmetric unit of the title compound is built up of one 4'-morpholinemethylbiphenyl-2-carbonitrile cation with the dihedral angle of 57.24 (11)° between two benzene rings and one tetrafluoroborate anion (Fig 1). The intermolecular N—H···F hydrogen bonds link the cations and anions to chains (Table 1). The π–π stacking interactions of adjacent cyanobenzene rings with a centroid–centroid distance of 3.805 (3)Å stabilize the crystal structure (Fig 2).

Experimental

Tetrafluoroboric acid(10 mmol) was added dropwise under stirring to a solution of 4'-morpholinemethylbiphenyl-2-carbonitrile (10 mmol) ethanol solution. Water was added until all suspended substrates disappeared. Colorless single crystals of the title compound suitable for X-ray analysis were obtained by slow evaporation from the solution at room temperature after 5 d, giving a yield of *ca* 78%.

Refinement

Positional parameters of all the H atoms for C atoms were calculated geometrically and were allowed to ride on the C atoms to which they are bonded, with U_{iso}(H) = 1.2Ueq(C). The H atoms bonded to N atoms were found in a difference Fourier map and refined with restraints for N—H distances of 0.87 (2).

Figures

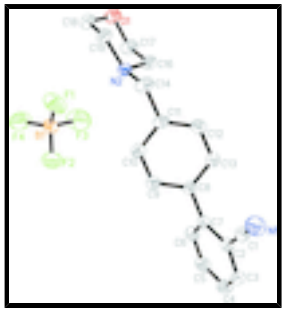

Fig. 1. The molecular structure of the title compound, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

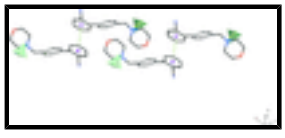

Fig. 2. A view of the packing of the title compound. Dashed lines indicate hydrogen bonds and π-π interactions.

4-[(2'-Cyanobiphenyl-4-yl)methyl]morpholin-4-ium tetrafluoridoborate

Crystal data

$C_{18}H_{19}N_2O^+ \cdot BF_4^-$	$Z = 2$
$M_r = 366.16$	$F(000) = 380$
Triclinic, $P\overline{1}$	$D_x = 1.331$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 9.059$ (6) Å	Cell parameters from 2199 reflections
$b = 9.859$ (8) Å	$\theta = 2.6$–$27.4°$
$c = 10.597$ (8) Å	$\mu = 0.11$ mm^{-1}
$\alpha = 76.324$ (14)°	$T = 298$ K
$\beta = 83.71$ (2)°	Prism, colourless
$\gamma = 86.50$ (3)°	0.20 × 0.20 × 0.20 mm
$V = 913.5$ (12) Å^3	

Data collection

Rigaku SCXmini diffractometer	4098 independent reflections
Radiation source: fine-focus sealed tube	3039 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.028$
Detector resolution: 13.6612 pixels mm^{-1}	$\theta_{max} = 27.4°$, $\theta_{min} = 2.6°$
ω scans	$h = -11 \rightarrow 11$
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)	$k = -12 \rightarrow 12$
$T_{min} = 0.978$, $T_{max} = 0.978$	$l = -13 \rightarrow 13$
9817 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.067$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.202$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.1049P)^2 + 0.2107P]$ where $P = (F_o^2 + 2F_c^2)/3$
4098 reflections	$(\Delta/\sigma)_{max} < 0.001$
239 parameters	$\Delta\rho_{max} = 0.49$ e Å^{-3}
1 restraint	$\Delta\rho_{min} = -0.30$ e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.9918 (2)	0.3886 (3)	0.3969 (2)	0.0559 (5)
C2	1.0478 (2)	0.2599 (2)	0.47565 (19)	0.0472 (5)
C3	1.1901 (2)	0.2084 (3)	0.4395 (2)	0.0613 (6)
H3A	1.2463	0.2570	0.3658	0.074*
C4	1.2460 (3)	0.0863 (3)	0.5129 (3)	0.0662 (7)
H4A	1.3404	0.0522	0.4890	0.079*
C5	1.1631 (3)	0.0144 (3)	0.6214 (2)	0.0644 (6)
H5A	1.2009	−0.0692	0.6700	0.077*
C6	1.0234 (2)	0.0653 (2)	0.6593 (2)	0.0533 (5)
H6A	0.9695	0.0162	0.7341	0.064*
C7	0.9623 (2)	0.1888 (2)	0.58744 (18)	0.0436 (4)
C8	0.8154 (2)	0.24449 (19)	0.63377 (18)	0.0424 (4)
C9	0.7937 (2)	0.2673 (2)	0.75930 (19)	0.0521 (5)
H9A	0.8707	0.2464	0.8128	0.062*
C10	0.6601 (2)	0.3203 (3)	0.8053 (2)	0.0564 (5)
H10A	0.6487	0.3376	0.8885	0.068*
C11	0.5416 (2)	0.3483 (2)	0.7281 (2)	0.0475 (5)
C12	0.5617 (2)	0.3237 (2)	0.6039 (2)	0.0513 (5)
H12A	0.4831	0.3409	0.5519	0.062*
C13	0.6973 (2)	0.2736 (2)	0.55624 (19)	0.0480 (5)
H13A	0.7098	0.2594	0.4720	0.058*
C14	0.3952 (2)	0.4050 (2)	0.7809 (2)	0.0570 (6)
H14A	0.4119	0.4897	0.8081	0.068*
H14B	0.3293	0.4291	0.7120	0.068*
C16	0.2802 (2)	0.1734 (2)	0.8569 (2)	0.0523 (5)
H16A	0.3689	0.1267	0.8251	0.063*
H16B	0.2158	0.1995	0.7870	0.063*
C17	0.2012 (3)	0.0752 (2)	0.9722 (3)	0.0633 (6)
H17A	0.1733	−0.0066	0.9457	0.076*
H17B	0.2678	0.0446	1.0400	0.076*
C18	0.1109 (3)	0.2580 (3)	1.0663 (2)	0.0645 (6)
H18A	0.1768	0.2267	1.1345	0.077*
H18B	0.0222	0.3002	1.1034	0.077*

C19	0.1868 (2)	0.3662 (2)	0.9572 (2)	0.0550 (5)
H19A	0.1184	0.4039	0.8922	0.066*
H19B	0.2162	0.4423	0.9914	0.066*
N1	0.9501 (3)	0.4903 (3)	0.3325 (2)	0.0805 (7)
N2	0.32178 (17)	0.30144 (17)	0.89484 (16)	0.0432 (4)
H2	0.384 (2)	0.273 (3)	0.958 (2)	0.064 (7)*
O1	0.07139 (17)	0.14212 (18)	1.02265 (16)	0.0638 (4)
B1	0.5558 (3)	0.2295 (3)	1.1710 (3)	0.0583 (6)
F1	0.4631 (2)	0.33813 (19)	1.1168 (2)	0.1044 (7)
F2	0.70030 (18)	0.2643 (2)	1.13544 (18)	0.0962 (6)
F3	0.5250 (3)	0.1264 (2)	1.1129 (3)	0.1298 (9)
F4	0.5317 (2)	0.2022 (4)	1.29990 (17)	0.1466 (12)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0508 (12)	0.0678 (14)	0.0446 (11)	−0.0121 (10)	−0.0021 (9)	−0.0030 (10)
C2	0.0432 (10)	0.0557 (11)	0.0435 (10)	−0.0053 (8)	−0.0042 (8)	−0.0122 (8)
C3	0.0464 (12)	0.0853 (16)	0.0557 (12)	−0.0068 (11)	0.0029 (9)	−0.0257 (12)
C4	0.0478 (12)	0.0833 (17)	0.0756 (16)	0.0131 (11)	−0.0107 (11)	−0.0360 (14)
C5	0.0664 (14)	0.0620 (13)	0.0698 (15)	0.0143 (11)	−0.0248 (12)	−0.0215 (12)
C6	0.0572 (12)	0.0519 (11)	0.0503 (11)	0.0005 (9)	−0.0105 (9)	−0.0090 (9)
C7	0.0411 (10)	0.0486 (10)	0.0421 (10)	−0.0043 (8)	−0.0064 (7)	−0.0107 (8)
C8	0.0398 (9)	0.0442 (10)	0.0409 (9)	−0.0062 (7)	−0.0018 (7)	−0.0049 (8)
C9	0.0424 (10)	0.0708 (13)	0.0423 (10)	−0.0109 (9)	−0.0033 (8)	−0.0099 (9)
C10	0.0463 (11)	0.0756 (15)	0.0490 (11)	−0.0132 (10)	0.0053 (8)	−0.0196 (10)
C11	0.0411 (10)	0.0427 (10)	0.0556 (11)	−0.0074 (8)	0.0039 (8)	−0.0077 (8)
C12	0.0441 (10)	0.0528 (11)	0.0541 (11)	−0.0020 (8)	−0.0094 (8)	−0.0047 (9)
C13	0.0476 (11)	0.0542 (11)	0.0423 (10)	−0.0019 (8)	−0.0062 (8)	−0.0106 (8)
C14	0.0495 (11)	0.0417 (10)	0.0723 (14)	−0.0059 (8)	0.0111 (10)	−0.0054 (10)
C16	0.0475 (11)	0.0501 (11)	0.0614 (12)	−0.0106 (8)	0.0070 (9)	−0.0208 (10)
C17	0.0554 (13)	0.0523 (12)	0.0777 (15)	−0.0121 (10)	0.0077 (11)	−0.0101 (11)
C18	0.0563 (13)	0.0836 (16)	0.0521 (12)	−0.0033 (11)	0.0075 (10)	−0.0183 (12)
C19	0.0485 (11)	0.0586 (12)	0.0594 (12)	0.0031 (9)	0.0049 (9)	−0.0224 (10)
N1	0.0768 (15)	0.0817 (15)	0.0685 (13)	−0.0147 (12)	−0.0147 (11)	0.0177 (12)
N2	0.0370 (8)	0.0448 (8)	0.0486 (9)	−0.0033 (6)	−0.0026 (7)	−0.0125 (7)
O1	0.0457 (8)	0.0748 (11)	0.0671 (10)	−0.0151 (7)	0.0091 (7)	−0.0123 (8)
B1	0.0525 (14)	0.0645 (15)	0.0594 (15)	0.0077 (11)	−0.0145 (11)	−0.0158 (12)
F1	0.1023 (14)	0.0844 (12)	0.1375 (16)	0.0327 (10)	−0.0665 (12)	−0.0316 (11)
F2	0.0606 (10)	0.1263 (15)	0.0970 (12)	−0.0091 (9)	−0.0087 (8)	−0.0145 (11)
F3	0.1141 (16)	0.0880 (13)	0.211 (3)	−0.0028 (11)	−0.0255 (16)	−0.0766 (16)
F4	0.0801 (13)	0.281 (3)	0.0580 (10)	0.0229 (16)	−0.0057 (8)	−0.0060 (14)

Geometric parameters (Å, °)

C1—N1	1.140 (3)	C13—H13A	0.9300
C1—C2	1.441 (3)	C14—N2	1.506 (3)
C2—C7	1.403 (3)	C14—H14A	0.9700
C2—C3	1.403 (3)	C14—H14B	0.9700

C3—C4	1.372 (4)	C16—N2	1.493 (3)
C3—H3A	0.9300	C16—C17	1.509 (3)
C4—C5	1.371 (4)	C16—H16A	0.9700
C4—H4A	0.9300	C16—H16B	0.9700
C5—C6	1.386 (3)	C17—O1	1.428 (3)
C5—H5A	0.9300	C17—H17A	0.9700
C6—C7	1.393 (3)	C17—H17B	0.9700
C6—H6A	0.9300	C18—O1	1.408 (3)
C7—C8	1.486 (3)	C18—C19	1.510 (3)
C8—C9	1.392 (3)	C18—H18A	0.9700
C8—C13	1.395 (3)	C18—H18B	0.9700
C9—C10	1.374 (3)	C19—N2	1.505 (3)
C9—H9A	0.9300	C19—H19A	0.9700
C10—C11	1.396 (3)	C19—H19B	0.9700
C10—H10A	0.9300	N2—H2	0.904 (16)
C11—C12	1.386 (3)	B1—F4	1.324 (3)
C11—C14	1.509 (3)	B1—F3	1.363 (3)
C12—C13	1.384 (3)	B1—F2	1.363 (3)
C12—H12A	0.9300	B1—F1	1.374 (3)
N1—C1—C2	178.5 (3)	N2—C14—H14B	109.2
C7—C2—C3	120.7 (2)	C11—C14—H14B	109.2
C7—C2—C1	120.47 (18)	H14A—C14—H14B	107.9
C3—C2—C1	118.78 (19)	N2—C16—C17	110.42 (18)
C4—C3—C2	120.0 (2)	N2—C16—H16A	109.6
C4—C3—H3A	120.0	C17—C16—H16A	109.6
C2—C3—H3A	120.0	N2—C16—H16B	109.6
C5—C4—C3	120.1 (2)	C17—C16—H16B	109.6
C5—C4—H4A	120.0	H16A—C16—H16B	108.1
C3—C4—H4A	120.0	O1—C17—C16	110.81 (19)
C4—C5—C6	120.5 (2)	O1—C17—H17A	109.5
C4—C5—H5A	119.8	C16—C17—H17A	109.5
C6—C5—H5A	119.8	O1—C17—H17B	109.5
C5—C6—C7	121.3 (2)	C16—C17—H17B	109.5
C5—C6—H6A	119.4	H17A—C17—H17B	108.1
C7—C6—H6A	119.4	O1—C18—C19	111.95 (18)
C6—C7—C2	117.45 (19)	O1—C18—H18A	109.2
C6—C7—C8	120.07 (17)	C19—C18—H18A	109.2
C2—C7—C8	122.40 (18)	O1—C18—H18B	109.2
C9—C8—C13	118.51 (18)	C19—C18—H18B	109.2
C9—C8—C7	119.17 (17)	H18A—C18—H18B	107.9
C13—C8—C7	122.31 (18)	N2—C19—C18	110.08 (18)
C10—C9—C8	121.01 (19)	N2—C19—H19A	109.6
C10—C9—H9A	119.5	C18—C19—H19A	109.6
C8—C9—H9A	119.5	N2—C19—H19B	109.6
C9—C10—C11	120.4 (2)	C18—C19—H19B	109.6
C9—C10—H10A	119.8	H19A—C19—H19B	108.2
C11—C10—H10A	119.8	C16—N2—C19	109.84 (16)
C12—C11—C10	118.88 (19)	C16—N2—C14	112.09 (17)
C12—C11—C14	121.43 (19)	C19—N2—C14	111.26 (16)

C10—C11—C14	119.7 (2)	C16—N2—H2	107.1 (16)
C13—C12—C11	120.69 (19)	C19—N2—H2	105.8 (16)
C13—C12—H12A	119.7	C14—N2—H2	110.5 (16)
C11—C12—H12A	119.7	C18—O1—C17	110.10 (17)
C12—C13—C8	120.45 (19)	F4—B1—F3	116.5 (3)
C12—C13—H13A	119.8	F4—B1—F2	108.7 (2)
C8—C13—H13A	119.8	F3—B1—F2	109.0 (2)
N2—C14—C11	112.09 (17)	F4—B1—F1	109.9 (2)
N2—C14—H14A	109.2	F3—B1—F1	102.7 (2)
C11—C14—H14A	109.2	F2—B1—F1	109.9 (2)
C7—C2—C3—C4	0.8 (3)	C9—C10—C11—C14	179.33 (19)
C1—C2—C3—C4	179.9 (2)	C10—C11—C12—C13	−0.8 (3)
C2—C3—C4—C5	0.1 (3)	C14—C11—C12—C13	179.01 (18)
C3—C4—C5—C6	−1.1 (4)	C11—C12—C13—C8	1.3 (3)
C4—C5—C6—C7	1.2 (3)	C9—C8—C13—C12	−0.2 (3)
C5—C6—C7—C2	−0.3 (3)	C7—C8—C13—C12	179.14 (18)
C5—C6—C7—C8	−177.10 (19)	C12—C11—C14—N2	114.6 (2)
C3—C2—C7—C6	−0.7 (3)	C10—C11—C14—N2	−65.7 (3)
C1—C2—C7—C6	−179.81 (19)	N2—C16—C17—O1	58.1 (3)
C3—C2—C7—C8	176.01 (18)	O1—C18—C19—N2	−56.8 (3)
C1—C2—C7—C8	−3.1 (3)	C17—C16—N2—C19	−53.4 (2)
C6—C7—C8—C9	54.6 (3)	C17—C16—N2—C14	−177.59 (18)
C2—C7—C8—C9	−122.0 (2)	C18—C19—N2—C16	52.3 (2)
C6—C7—C8—C13	−124.7 (2)	C18—C19—N2—C14	176.95 (18)
C2—C7—C8—C13	58.6 (3)	C11—C14—N2—C16	−64.1 (2)
C13—C8—C9—C10	−1.5 (3)	C11—C14—N2—C19	172.46 (17)
C7—C8—C9—C10	179.17 (19)	C19—C18—O1—C17	61.2 (2)
C8—C9—C10—C11	2.0 (3)	C16—C17—O1—C18	−61.4 (3)
C9—C10—C11—C12	−0.9 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···F1	0.90 (2)	2.14 (2)	2.902 (3)	141 (2)
N2—H2···F3	0.90 (2)	2.35 (2)	3.219 (3)	161 (2)

Fig. 1

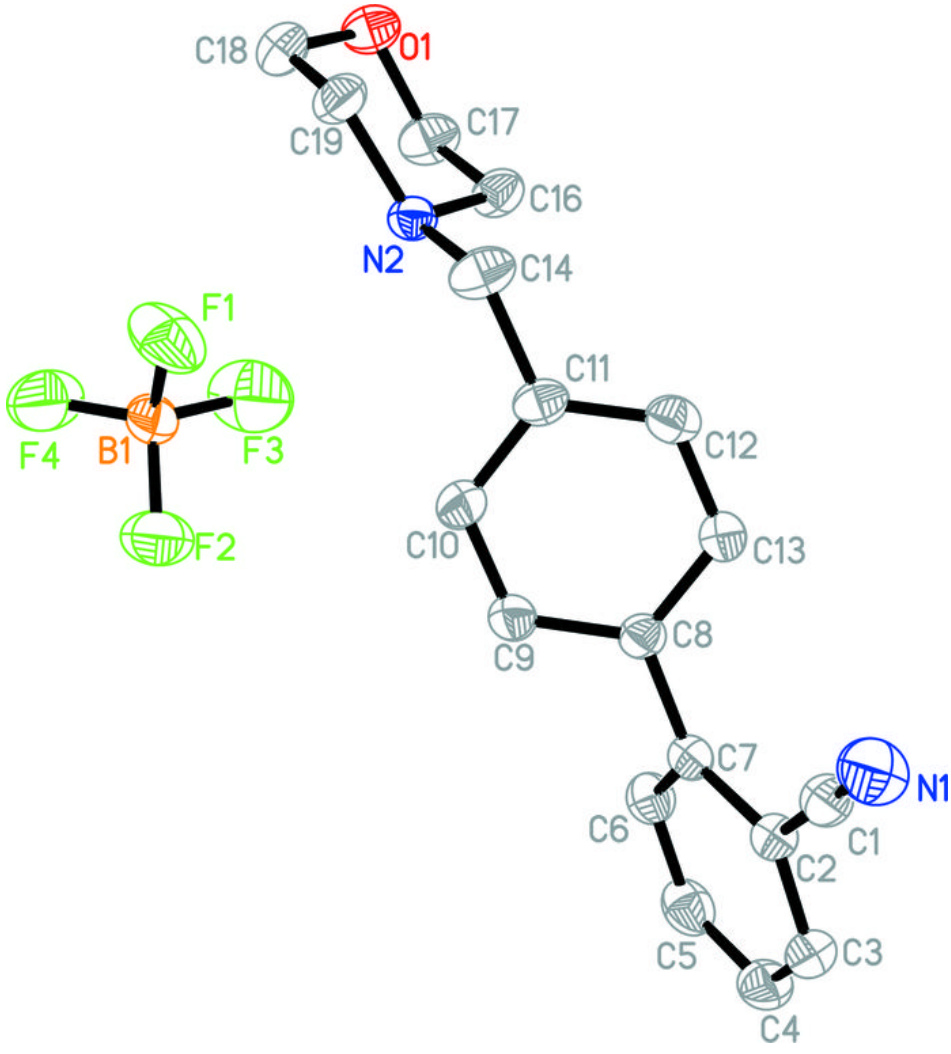
C18
O1
C19
C17
C16
N2
C14
F1
C11
F4
B1
F3
C12
C10
C13
F2
C9
C8
C7
N1
C6
C1
C2
C5
C3
C4

Fig. 2