Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,3,5,6-Tetrafluoro-1,4-bis(2-pyridylmethyleneaminomethyl)benzene

Ming-Yang He,[a,b]* Chao Li,[b] Xu-Jie Yang,[a] Lu-De Lu[a] and Xin Wang[a]

[a]School of Chemistry and Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210093, People's Republic of China, and [b]Key Laboratory of Fine Petro-chemical Technology, Jiangsu Polytechnic University, Changzhou 213164, People's Republic of China
Correspondence e-mail: hemingyangjpu@yahoo.com

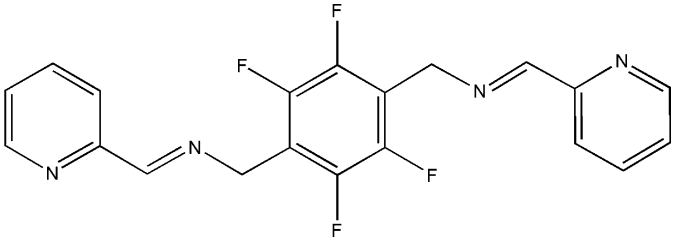
Received 1 December 2008; accepted 10 January 2009

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.151; data-to-parameter ratio = 15.9.

The title compound, $C_{20}H_{14}F_4N_4$, is a flexible bis-pyridine-type ligand with an extended fluorinated spacer group between the two pyridyl functions. The centroid of the central aromatic ring is situated on a crystallographic center of inversion. The dihedral angle between the pyridine ring and the central benzene ring is 63.85 (9)°. The crystal structure exhibits intermolecular C—H···F hydrogen-bonding interactions.

Related literature

For background information on bis-pyridine-type Schiff base ligands see: Barboiu *et al.* (2006); Keegan *et al.* (2002); Yue *et al.* (2004). Haga *et al.* (1985) describe the synthesis of the title compound.



Experimental

Crystal data

$C_{20}H_{14}F_4N_4$
M_r = 386.35
Monoclinic, $P2_1/c$
a = 9.637 (3) Å
b = 7.783 (3) Å
c = 12.070 (4) Å
β = 105.940 (4)°
V = 870.5 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 296 (2) K
0.26 × 0.24 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.963, T_{max} = 0.974
7194 measured reflections
2014 independent reflections
1341 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.151
S = 1.05
2014 reflections
127 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···F2^{i}	0.93	2.53	3.370 (3)	151

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank the Center for Testing and Analysis at Yangzhou University for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2091).

References

Barboiu, M., Petit, E., Van d Lee, A. & Vaughan, G. (2006). *Inorg. Chem.* **45**, 484–486.
Bruker (2000). *SADABS*, *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Haga, M. & Koizumi, K. (1985). *Inorg. Chim. Acta*, **104**, 47–50.
Keegan, J., Kruger, P. E., Nieuwenhuyzen, M. & Martin, N. (2002). *Cryst. Growth Des.* **2**, 329–332.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Yue, Y. F., Gao, E. Q., Bai, S. Q., He, Z. & Yan, C. H. (2004). *CrystEngComm*, **6**, 549–555.

supplementary materials

Acta Cryst. (2009). E**65**, o331 [**doi:10.1107/S1600536809001172**]

2,3,5,6-Tetrafluoro-1,4-bis(2-pyridylmethyleneaminomethyl)benzene

M.-Y. He, C. Li, X.-J. Yang, L.-D. Lu and X. Wang

Comment

Bis-pyridine type bidentate Schiff base ligands have been utilized intensively to assemble various coordination polymers with interesting topologies and fascinating structural diversities (Barboiu *et al.*, 2006; Keegan *et al.*, 2002; Yue *et al.*, 2004). We report here the crystal structure of the title compound, (I).

A perspective view of (I), including the atomic numbering scheme, is shown in Fig. 1. (I) crystallizes around a crystallographic center of inversion with a half molecule in the asymmetric unit. The bond lengths and angles are within normal ranges. The terminal pyridyl groups are coplanar, and they form a dihedral angle of 63.85 (9)° with the central benzene ring.

Experimental

The title compound was synthesized and purified according to the method described by by Haga *et al.* (1985) performing a condensation of pyridine-2-carboxaldehyde and 2,3,5,6-tetrafluoro-1,4-benzenedimethanamine (yield 83%). Colorless block single crystals (m.p. 465.1–465.3 K) suitable for X-ray analysis were obtained by slow evaporation of a methanolic solution at room temperature. Analysis calculated for $C_{20}H_{18}F_4N_4$: C 61.54, H 4.62, N 14.36%; found: C 62.26, H 3.64, N 14.45%. IR (KBr pellet, cm^{-1}): 3445 (*b*), 3087 (*m*), 3018 (*m*), 2922 (*m*), 2868 (*m*), 1639 (*s*), 1586 (*s*), 1568 (*s*), 1489 (*s*), 1470 (*s*), 1436 (*m*), 1372 (*m*), 1335 (*m*), 1275 (*m*), 1211 (*m*), 1148 (*w*), 1063 (*s*), 1013 (*m*), 987 (*s*), 892 (*s*), 776 (*s*), 742 (*m*), 697 (*m*), 621 (*w*), 590 (*m*), 509 (*m*), 413 (*w*).

Refinement

H atoms were assigned to calculated positions, with C—H = 0.97 (methylene) and 0.93 Å (aromatic), and refined using a riding model, with U_{iso}(H) = 1.2 U_{eq}(C).

Figures

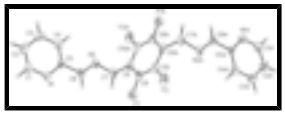


Fig. 1. The molecular structure of the title compound showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code: (A) 2 - *x*, - *y*, - *z*].

Fig. 2. A packing diagram of the title molecule (Dashed lines indicate hydrogen bonds).

2,3,5,6-Tetrafluoro-1,4-bis(2-pyridylmethyleneaminomethyl)benzene

Crystal data

$C_{20}H_{14}F_4N_4$	F_{000} = 396
M_r = 386.35	D_x = 1.474 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3894 reflections
a = 9.637 (3) Å	θ = 2.6–27.2º
b = 7.783 (3) Å	μ = 0.12 mm^{-1}
c = 12.070 (4) Å	T = 296 (2) K
β = 105.940 (4)º	Block, colorless
V = 870.5 (5) Å^3	0.26 × 0.24 × 0.22 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	2014 independent reflections
Radiation source: fine-focus sealed tube	1341 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.037
T = 296(2) K	θ_{max} = 27.6º
φ and ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −12→12
T_{min} = 0.963, T_{max} = 0.974	k = −10→10
7194 measured reflections	l = −15→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.045	H-atom parameters constrained
$wR(F^2)$ = 0.151	$w = 1/[\sigma^2(F_o^2) + (0.0739P)^2 + 0.1642P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
2014 reflections	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
127 parameters	$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	0.6996 (3)	0.1926 (3)	0.52870 (19)	0.0733 (6)
H1	0.7326	0.2286	0.6049	0.088*
C2	0.5633 (3)	0.2358 (3)	0.4693 (2)	0.0781 (7)
H2	0.5047	0.2981	0.5044	0.094*
C3	0.5132 (2)	0.1855 (3)	0.3558 (2)	0.0761 (7)
H3	0.4201	0.2127	0.3128	0.091*
C4	0.6041 (2)	0.0941 (3)	0.30767 (18)	0.0624 (5)
H4	0.5734	0.0591	0.2311	0.075*
C5	0.74130 (19)	0.0548 (2)	0.37431 (15)	0.0482 (4)
C6	0.8435 (2)	−0.0426 (2)	0.32794 (16)	0.0507 (4)
H6	0.9325	−0.0738	0.3770	0.061*
C7	0.9207 (2)	−0.1847 (3)	0.18519 (18)	0.0643 (6)
H7A	0.8812	−0.2964	0.1577	0.077*
H7B	1.0053	−0.2024	0.2496	0.077*
C8	0.9627 (2)	−0.0904 (2)	0.08987 (16)	0.0538 (5)
C9	1.0951 (2)	−0.0132 (3)	0.10554 (16)	0.0547 (5)
C10	1.1317 (2)	0.0740 (2)	0.01844 (18)	0.0556 (5)
F1	1.19419 (14)	−0.02363 (18)	0.20914 (11)	0.0756 (4)
F2	1.26344 (13)	0.14574 (17)	0.04184 (11)	0.0762 (4)
N1	0.79039 (18)	0.1014 (2)	0.48488 (14)	0.0622 (5)
N2	0.81318 (17)	−0.0848 (2)	0.22290 (14)	0.0567 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0789 (15)	0.0860 (16)	0.0611 (12)	0.0097 (13)	0.0293 (11)	−0.0086 (11)
C2	0.0766 (15)	0.0762 (16)	0.0951 (18)	0.0164 (12)	0.0465 (13)	−0.0028 (13)
C3	0.0537 (11)	0.0797 (16)	0.0951 (18)	0.0162 (11)	0.0207 (11)	0.0089 (13)
C4	0.0584 (11)	0.0667 (13)	0.0620 (12)	0.0040 (10)	0.0161 (9)	−0.0002 (10)
C5	0.0519 (10)	0.0463 (10)	0.0503 (10)	−0.0013 (8)	0.0206 (8)	0.0049 (8)
C6	0.0498 (10)	0.0523 (11)	0.0539 (10)	−0.0006 (8)	0.0207 (8)	0.0059 (8)
C7	0.0798 (13)	0.0555 (12)	0.0732 (13)	0.0025 (10)	0.0472 (11)	0.0011 (10)

C8	0.0672 (12)	0.0464 (11)	0.0597 (11)	−0.0007 (9)	0.0373 (10)	−0.0084 (8)
C9	0.0618 (11)	0.0549 (11)	0.0537 (10)	−0.0018 (9)	0.0267 (9)	−0.0124 (8)
C10	0.0577 (11)	0.0512 (11)	0.0688 (12)	−0.0102 (9)	0.0354 (10)	−0.0153 (9)
F1	0.0769 (8)	0.0893 (10)	0.0619 (8)	−0.0030 (7)	0.0213 (6)	−0.0061 (6)
F2	0.0663 (7)	0.0819 (9)	0.0898 (9)	−0.0222 (6)	0.0376 (7)	−0.0141 (7)
N1	0.0599 (10)	0.0747 (11)	0.0535 (9)	0.0079 (8)	0.0179 (7)	−0.0038 (8)
N2	0.0602 (9)	0.0624 (10)	0.0566 (9)	−0.0033 (8)	0.0316 (7)	0.0011 (7)

Geometric parameters (Å, °)

C1—N1	1.343 (3)	C6—H6	0.9300
C1—C2	1.355 (3)	C7—N2	1.464 (2)
C1—H1	0.9300	C7—C8	1.511 (3)
C2—C3	1.378 (3)	C7—H7A	0.9700
C2—H2	0.9300	C7—H7B	0.9700
C3—C4	1.375 (3)	C8—C9	1.375 (3)
C3—H3	0.9300	C8—C10^{i}	1.379 (3)
C4—C5	1.380 (3)	C9—F1	1.351 (2)
C4—H4	0.9300	C9—C10	1.376 (3)
C5—N1	1.338 (2)	C10—F2	1.344 (2)
C5—C6	1.470 (3)	C10—C8^{i}	1.379 (3)
C6—N2	1.264 (2)		
N1—C1—C2	124.4 (2)	N2—C7—C8	109.82 (16)
N1—C1—H1	117.8	N2—C7—H7A	109.7
C2—C1—H1	117.8	C8—C7—H7A	109.7
C1—C2—C3	118.6 (2)	N2—C7—H7B	109.7
C1—C2—H2	120.7	C8—C7—H7B	109.7
C3—C2—H2	120.7	H7A—C7—H7B	108.2
C4—C3—C2	118.5 (2)	C9—C8—C10^{i}	115.87 (17)
C4—C3—H3	120.7	C9—C8—C7	122.69 (19)
C2—C3—H3	120.7	C10^{i}—C8—C7	121.43 (18)
C3—C4—C5	119.2 (2)	F1—C9—C8	119.61 (17)
C3—C4—H4	120.4	F1—C9—C10	118.19 (18)
C5—C4—H4	120.4	C8—C9—C10	122.21 (19)
N1—C5—C4	122.76 (18)	F2—C10—C9	118.03 (19)
N1—C5—C6	115.41 (16)	F2—C10—C8^{i}	120.04 (17)
C4—C5—C6	121.82 (18)	C9—C10—C8^{i}	121.93 (18)
N2—C6—C5	121.41 (17)	C5—N1—C1	116.50 (17)
N2—C6—H6	119.3	C6—N2—C7	117.46 (17)
C5—C6—H6	119.3		
N1—C1—C2—C3	−0.8 (4)	C10^{i}—C8—C9—C10	−0.5 (3)
C1—C2—C3—C4	−0.2 (4)	C7—C8—C9—C10	−179.29 (17)
C2—C3—C4—C5	0.5 (4)	F1—C9—C10—F2	−0.8 (3)
C3—C4—C5—N1	0.3 (3)	C8—C9—C10—F2	179.80 (16)
C3—C4—C5—C6	179.96 (19)	F1—C9—C10—C8^{i}	179.86 (16)
N1—C5—C6—N2	−175.63 (17)	C8—C9—C10—C8^{i}	0.5 (3)
C4—C5—C6—N2	4.7 (3)	C4—C5—N1—C1	−1.2 (3)

N2—C7—C8—C9	108.5 (2)	C6—C5—N1—C1	179.09 (18)
N2—C7—C8—C10^{i}	−70.3 (2)	C2—C1—N1—C5	1.5 (4)
C10^{i}—C8—C9—F1	−179.83 (16)	C5—C6—N2—C7	−178.80 (16)
C7—C8—C9—F1	1.3 (3)	C8—C7—N2—C6	−122.2 (2)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···F2^{ii}	0.93	2.53	3.370 (3)	151

Symmetry codes: (ii) *x*−1, −*y*+1/2, *z*+1/2.

Fig. 1

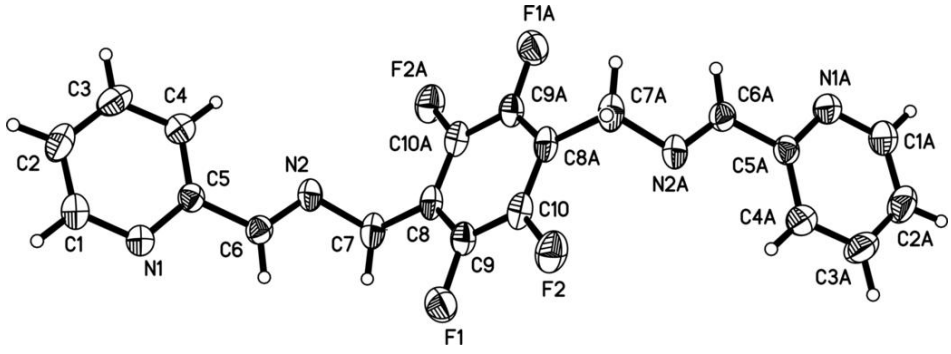

F1A
F2A
C9A
C7A
C6A
N1A
C3
C4
C10A
C8A
C1A
C2
C5
N2
N2A
C5A
C10
C4A
C1
C6
C7
C8
C9
C2A
N1
F2
C3A
F1

Fig. 2