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Substituted Imidazonaphthyridine Derivatives. I. $C_{19}H_{14}F_3N_3$, $C_{18}H_{10}F_5N_3$, $C_{18}H_{11}ClF_3N_3$ and $C_{18}H_{11}BrF_3N_3$

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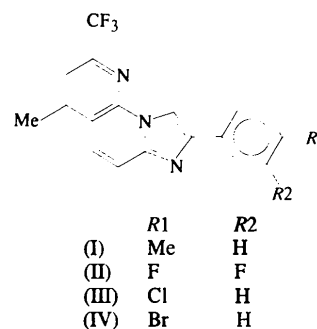
Abstract

The structures of four 2,6,8-trisubstituted imidazonaphthyridine derivatives, 6-methyl-2-(4-methylphenyl)-8-trifluoromethylimidazo[1,2-*a*][1,8]naphthyridine, (I), 2-(3,4-difluorophenyl)-6-methyl-8-trifluoromethylimidazo[1,2-*a*][1,8]naphthyridine, (II), 2-(4-chlorophenyl)-6-methyl-8-trifluoromethylimidazo[1,2-*a*][1,8]naphthyridine, (III), and 2-(4-bromophenyl)-6-methyl-8-trifluoromethylimidazo[1,2-*a*][1,8]naphthyridine, (IV), are reported. The molecules are planar and exist as dimers, formed through intermolecular C—H···N hydrogen bonds in all four cases. The trifluoromethyl group

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undergoes rotational disorder in (II)–(IV). The molecules are laid in two-dimensional planes in the crystal lattice with possible intermoleculear π–π interactions.

Comment

Imidazo[1,2-*a*]pyridine derivatives have been found to have potential biological activities and photophysical properties (Kaminski *et al.*, 1989; Knolker & Boese, 1988). Recently, imidazo[1,2-*a*]1,8-naphthyridine derivatives were reported to possess potential antibacterial activity (Kondo, Taguchi, Inoue, Sakamoto & Tsukamoto, 1990). This prompted us to synthesize a series of imidazonaphthyridine compounds, characterize them, and study their biological and photophysical properties. Like their pyridine analogues, these compounds also show fluorescence in the visible region. We have obtained the compounds *via* facile condensation of 2-amino-1,8-naphthyridine with appropriate 1,3-dicarbonyl compounds (Chua & Jackson, 1995; Anwair, 1995). Although 1- and 2-substituted isomers are possible, only the 2-substituted isomer has been isolated consistently. We have determined the crystal structures and hereby report the structures of four of them. We believe that this is the first report on the crystal structures of imidazonaphthyridines. Compounds (III) and (IV) are isomorphous.

	R1	R2
(I)	Me	H
(II)	F	F
(III)	Cl	H
(IV)	Br	H

All four structures confirm the double bonds N1=C1, C2=C3 and C9=C10 and the other bond lengths and angles are normal. The imidazonaphthyridine moiety is planar in each case, with maximum deviations of 0.044 (2) (C5), 0.036 (5) (C5), 0.024 (2) (C5) and 0.023 (6) Å (C6), and dihedral angles between the planes of the imidazonaphthyridine moiety and the phenyl ring of 6.6 (1), 1.5 (1), 6.9 (1) and 7.8 (1)° in (I), (II), (III) and (IV), respectively. Hence each molecule is almost planar.

All four compounds crystallize in the triclinic space group $P\bar{1}$ and form dimeric pairs through intermolecular C2—H2···N1 hydrogen bonds around the inversion centres. The C2···N1 distance is found to increase with heavier halogen substitution at C14 (in the order F, Cl, Br). The halogen atoms in (II), (III) and (IV) have interactions with the F atoms of the trifluoromethyl group
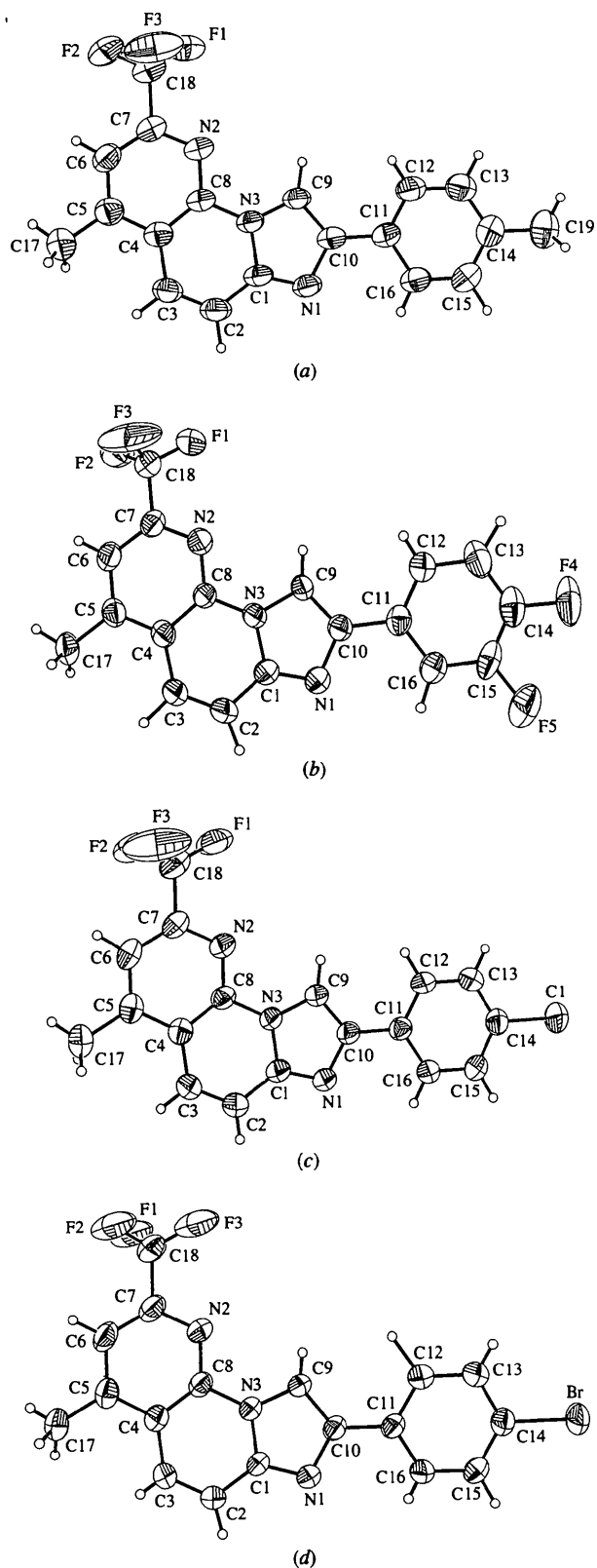
(a)

(b)

(c)

(d)

Fig. 1. Views of (a) (I), (b) (II), (c) (III) and (d) (IV) showing numbering schemes; displacement ellipsoids are drawn at the 50% probability level. For clarity, the CF_3 disorder in (II)–(IV) is not shown.

and this may be the reason for the rotational disorder observed in this group in these compounds. Notably short intermolecular contacts observed are: in (II) F4$\cdots$F2^i 2.863 (5), F4$\cdots$F2$^{\prime i}$ 2.88 (3), F5$\cdots$F3^{ii} 3.022 (6) Å; in (III) Cl$\cdots$F2$^{\prime iii}$ 3.05 (1); in (IV) Br$\cdots$F1$^{\prime\prime iv}$ 3.01 (1) Å [symmetry codes: (i) $1 + x$, y, $z-1$; (ii) $1-x$, $1-y$, $1-z$; (iii) $x-1$, y, $z-1$; (iv) $x-1$, $y-1$, $z + 1$]. Other intermolecular hydrogen bonds are given in Table 3.

In all four cases the molecules form two-dimensional layers in the solid state and these layers are found parallel to the (12$\bar{1}$), (212), (21$\bar{2}$) and (213) planes in (I), (II), (III) and (IV), respectively. The planarity of these molecules, the interlayer distances of 3.426 (I), 3.429 (II), 3.414 (III) and 3.444 Å (IV), and their packing modes suggest that intermolecular π–π interactions may also play a role in the crystal packing (see Fig. 2). Such π–π interactions were also observed in the imidazopyridine derivatives (Knolker, Boese & Hitzemann, 1990).
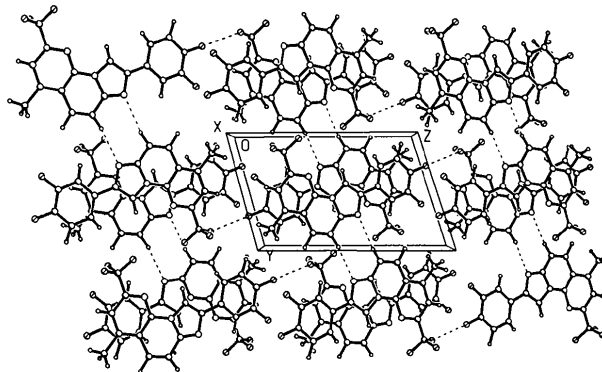

Fig. 2. Packing of the molecules in (II) viewed down the a axis. C—H$\cdots$N hydrogen bonds and F$\cdots$F short contacts are shown as dashed lines.

Experimental

Single crystals of (I), (II), (III) and (IV) were obtained from slow evaporation of ethanol solution, ethyl acetate solution, ethanol/ethyl acetate solution, and ethanol solution, respectively.

Compound (I)

Crystal data

$C_{19}H_{14}F_3N_3$	Mo $K\alpha$ radiation
$M_r = 341.33$	$\lambda = 0.71073$ Å
Triclinic	Cell parameters from 36
$P\bar{1}$	reflections
$a = 9.092$ (1) Å	$\theta = 10$–$25°$
$b = 9.849$ (1) Å	$\mu = 0.110$ mm^{-1}
$c = 10.428$ (1) Å	$T = 293$ (2) K
$\alpha = 68.90$ (1)$°$	Thick plate
$\beta = 69.39$ (1)$°$	$0.58 \times 0.48 \times 0.22$ mm
$\gamma = 72.67$ (1)$°$	Yellow
$V = 799.62$ (14) Å^3	
$Z = 2$	
$D_x = 1.418$ Mg m^{-3}	
D_m not measured	

Data collection

Siemens *P*4 diffractometer
$\theta/2\theta$ scans
Absorption correction:
 none
3324 measured reflections
2760 independent reflections
1981 observed reflections
 $[I > 2\sigma(I)]$
$R_{int} = 0.0123$

$\theta_{max} = 24.99°$
$h = -1 \rightarrow 10$
$k = -10 \rightarrow 11$
$l = -11 \rightarrow 12$
3 standard reflections
 monitored every 97
 reflections
 intensity decay: $<2\%$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0457$
$wR(F^2) = 0.1446$
$S = 1.045$
2760 reflections
283 parameters
All H-atom parameters
 refined
$w = 1/[\sigma^2(F_o^2) + (0.0922P)^2 + 0.0191P]$
 where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}
Extinction correction:
 *SHELXL*93 (Sheldrick,
 1993)
Extinction coefficient:
 0.011 (4)
Atomic scattering factors
 from *International Tables*
 for Crystallography (1992,
 Vol. C, Tables 4.2.6.8 and
 6.1.1.4)

Compound (II)

Crystal data

$C_{18}H_{10}F_5N_3$
$M_r = 363.29$
Triclinic
$P\bar{1}$
$a = 7.916$ (7) Å
$b = 8.454$ (6) Å
$c = 12.838$ (9) Å
$\alpha = 73.64$ (2)°
$\beta = 87.62$ (6)°
$\gamma = 70.08$ (7)°
$V = 773.6$ (10) Å^3
$Z = 2$
$D_x = 1.560$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25
 reflections
$\theta = 8-25°$
$\mu = 0.137$ mm^{-1}
$T = 293$ (2) K
Plate
$0.66 \times 0.52 \times 0.14$ mm
Light brown

Data collection

Siemens *P*4 diffractometer
$\theta/2\theta$ scans
Absorption correction:
 none
3308 measured reflections
2706 independent reflections
1949 observed reflections
 $[I > 2\sigma(I)]$
$R_{int} = 0.0247$

$\theta_{max} = 25.00°$
$h = -9 \rightarrow 9$
$k = -10 \rightarrow 1$
$l = -15 \rightarrow 15$
3 standard reflections
 monitored every 97
 reflections
 intensity decay: $<3\%$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.1027$
$wR(F^2) = 0.3248$
$S = 1.077$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.59$ e Å^{-3}
Extinction correction: none

2706 reflections
282 parameters
All H-atom parameters
 refined
$w = 1/[\sigma^2(F_o^2) + (0.2583P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$

Atomic scattering factors
 from *International Tables*
 for Crystallography (1992,
 Vol. C, Tables 4.2.6.8 and
 6.1.1.4)

Compound (III)

Crystal data

$C_{18}H_{11}ClF_3N_3$
$M_r = 361.75$
Triclinic
$P\bar{1}$
$a = 8.422$ (2) Å
$b = 9.042$ (1) Å
$c = 12.859$ (3) Å
$\alpha = 70.43$ (2)°
$\beta = 89.09$ (2)°
$\gamma = 62.25$ (1)°
$V = 804.9$ (3) Å^3
$Z = 2$
$D_x = 1.493$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 35
 reflections
$\theta = 9-25°$
$\mu = 0.275$ mm^{-1}
$T = 293$ (2) K
Needle
$0.60 \times 0.32 \times 0.24$ mm
Yellow

Data collection

Siemens *P*4 diffractometer
$\theta/2\theta$ scans
Absorption correction:
 none
3352 measured reflections
2742 independent reflections
2084 observed reflections
 $[I > 2\sigma(I)]$
$R_{int} = 0.0242$

$\theta_{max} = 25.00°$
$h = -1 \rightarrow 9$
$k = -9 \rightarrow 9$
$l = -15 \rightarrow 15$
3 standard reflections
 monitored every 97
 reflections
 intensity decay: $<4\%$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0416$
$wR(F^2) = 0.1191$
$S = 1.019$
2742 reflections
297 parameters
All H-atom parameters
 refined
$w = 1/[\sigma^2(F_o^2) + (0.0781P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}
Extinction correction: none
Atomic scattering factors
 from *International Tables*
 for Crystallography (1992,
 Vol. C, Tables 4.2.6.8 and
 6.1.1.4)

Compound (IV)

Crystal data

$C_{18}H_{11}BrF_3N_3$
$M_r = 406.21$
Triclinic
$P\bar{1}$
$a = 8.557$ (1) Å
$b = 8.954$ (1) Å
$c = 12.957$ (1) Å
$\alpha = 70.12$ (1)°
$\beta = 72.27$ (1)°
$\gamma = 63.19$ (1)°
$V = 819.62$ (15) Å^3
$Z = 2$
$D_x = 1.646$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 39
 reflections
$\theta = 8-25°$
$\mu = 2.544$ mm^{-1}
$T = 293$ (2) K
Needle
$0.62 \times 0.32 \times 0.16$ mm
Yellow

Data collection

Siemens P4 diffractometer
$\theta/2\theta$ scans
Absorption correction:
  empirical, ψ scans
  (XSCANS; Siemens, 1994)
  $T_{min} = 0.576$, $T_{max} = 0.949$
4432 measured reflections
3692 independent reflections
2183 observed reflections
  $[I > 2\sigma(I)]$

$R_{int} = 0.0318$
$\theta_{max} = 27.50°$
$h = -1 \rightarrow 11$
$k = -10 \rightarrow 11$
$l = -16 \rightarrow 16$
3 standard reflections
  monitored every 97
  reflections
  intensity decay: <3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0523$
$wR(F^2) = 0.1444$
$S = 0.927$
3692 reflections
277 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0841P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.64$ e Å^{-3}
$\Delta\rho_{min} = -0.53$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from International Tables for Crystallography (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
(I)				
N1	0.2779 (2)	1.0662 (2)	0.9372 (2)	0.0543 (5)
N2	0.2702 (2)	0.9060 (2)	0.5837 (2)	0.0517 (4)
N3	0.2883 (2)	0.9770 (2)	0.7651 (2)	0.0463 (4)
C1	0.3670 (3)	0.9782 (2)	0.8579 (2)	0.0501 (5)
C2	0.5230 (3)	0.8911 (2)	0.8528 (2)	0.0595 (6)
C3	0.5944 (3)	0.8118 (2)	0.7586 (2)	0.0584 (5)
C4	0.5153 (2)	0.8123 (2)	0.6606 (2)	0.0498 (5)
C5	0.5853 (3)	0.7353 (2)	0.5564 (2)	0.0562 (5)
C6	0.4936 (3)	0.7453 (2)	0.4707 (2)	0.0610 (6)
C7	0.3403 (3)	0.8290 (2)	0.4887 (2)	0.0554 (5)
C8	0.3590 (2)	0.8962 (2)	0.6659 (2)	0.0471 (5)
C9	0.1426 (2)	1.0696 (2)	0.7910 (2)	0.0490 (5)
C10	0.1373 (2)	1.1246 (2)	0.8967 (2)	0.0484 (5)
C11	0.0100 (2)	1.2301 (2)	0.9631 (2)	0.0498 (5)
C12	-0.1263 (3)	1.3027 (3)	0.9151 (3)	0.0646 (6)
C13	-0.2425 (3)	1.4026 (3)	0.9780 (3)	0.0694 (6)
C14	-0.2314 (3)	1.4365 (2)	1.0919 (2)	0.0590 (6)
C15	-0.0972 (3)	1.3630 (3)	1.1404 (2)	0.0627 (6)
C16	0.0204 (3)	1.2621 (2)	1.0782 (2)	0.0576 (5)
C17	0.7519 (4)	0.6446 (4)	0.5398 (3)	0.0764 (7)
C18	0.2345 (3)	0.8319 (3)	0.4049 (3)	0.0710 (7)
C19	-0.3580 (4)	1.5474 (3)	1.1594 (3)	0.0803 (8)
F1	0.1459 (2)	0.9639 (2)	0.3628 (2)	0.0990 (6)
F2	0.3170 (2)	0.7939 (2)	0.2863 (2)	0.1213 (7)
F3	0.1331 (3)	0.7415 (2)	0.4791 (2)	0.1314 (8)
(II)				
N1	0.4158 (4)	0.2890 (4)	0.4375 (3)	0.0475 (8)
N2	0.0546 (4)	0.6224 (4)	0.6342 (2)	0.0476 (8)
N3	0.2386 (4)	0.4359 (4)	0.5432 (2)	0.0428 (8)
C1	0.3347 (5)	0.2725 (5)	0.5285 (3)	0.0456 (9)
C2	0.3297 (6)	0.1207 (5)	0.6106 (3)	0.0547 (11)
C3	0.2385 (6)	0.1356 (5)	0.6994 (3)	0.0518 (10)
C4	0.1398 (5)	0.3057 (5)	0.7150 (3)	0.0440 (9)
C5	0.0437 (5)	0.3314 (5)	0.8061 (3)	0.0491 (10)
C6	-0.0467 (6)	0.5035 (6)	0.8081 (3)	0.0528 (10)
C7	-0.0384 (5)	0.6423 (5)	0.7206 (3)	0.0465 (9)
C8	0.1403 (5)	0.4583 (5)	0.6323 (3)	0.0406 (9)
C9	0.2649 (5)	0.5593 (5)	0.4529 (3)	0.0429 (9)
C10	0.3742 (5)	0.4666 (5)	0.3903 (3)	0.0421 (9)
C11	0.4401 (5)	0.5348 (5)	0.2847 (3)	0.0450 (9)
C12	0.4006 (6)	0.7134 (6)	0.2372 (3)	0.0550 (11)
C13	0.4588 (7)	0.7787 (7)	0.1375 (4)	0.0690 (13)
C14	0.5648 (7)	0.6616 (8)	0.0845 (3)	0.0648 (13)
C15	0.6059 (7)	0.4855 (7)	0.1308 (4)	0.0616 (12)
C16	0.5483 (6)	0.4192 (6)	0.2300 (3)	0.0550 (11)
C17	0.0383 (7)	0.1800 (6)	0.9001 (4)	0.0624 (12)
C18	-0.1319 (4)	0.8279 (5)	0.7226 (2)	0.0648 (13)
F1	-0.1809 (6)	0.9408 (4)	0.6259 (3)	0.1007 (15)
F2	-0.2866 (5)	0.8517 (5)	0.7681 (4)	0.0949 (14)
F3	-0.0321 (7)	0.8809 (6)	0.7744 (6)	0.143 (3)
F1'	-0.2914 (17)	0.927 (3)	0.675 (2)	0.1007 (15)
F2'	-0.154 (5)	0.844 (4)	0.8215 (8)	0.0949 (14)
F3'	-0.030 (4)	0.925 (4)	0.692 (3)	0.143 (3)
F4	0.6269 (5)	0.7200 (5)	-0.0131 (2)	0.0981 (12)
F5	0.7127 (5)	0.3779 (5)	0.0761 (3)	0.0998 (12)
(III)				
Cl	-0.34166 (8)	0.75144 (8)	-0.01306 (5)	0.0685 (2)
N1	0.3238 (2)	0.2834 (2)	0.44463 (13)	0.0487 (4)
N2	0.3258 (2)	0.6042 (2)	0.64892 (13)	0.0471 (4)
N3	0.3433 (2)	0.4250 (2)	0.55210 (12)	0.0400 (4)
C1	0.4172 (3)	0.2655 (2)	0.5328 (2)	0.0452 (4)
C2	0.5747 (3)	0.1132 (3)	0.6085 (2)	0.0556 (5)
C3	0.6459 (3)	0.1254 (3)	0.6955 (2)	0.0531 (5)
C4	0.5673 (3)	0.2906 (3)	0.7163 (2)	0.0443 (4)
C5	0.6329 (3)	0.3123 (3)	0.8071 (2)	0.0476 (5)
C6	0.5431 (3)	0.4795 (3)	0.8152 (2)	0.0544 (5)
C7	0.3934 (3)	0.6185 (3)	0.7355 (2)	0.0525 (5)
C8	0.4138 (2)	0.4424 (2)	0.64193 (15)	0.0400 (4)
C9	0.1944 (3)	0.5483 (3)	0.46980 (15)	0.0421 (4)
C10	0.1847 (3)	0.4595 (2)	0.40473 (15)	0.0418 (4)
C11	0.0528 (2)	0.5299 (2)	0.30425 (15)	0.0414 (4)
C12	-0.0981 (3)	0.7025 (3)	0.2691 (2)	0.0484 (5)
C13	-0.2195 (3)	0.7707 (3)	0.1729 (2)	0.0522 (5)
C14	-0.1907 (3)	0.6656 (3)	0.1099 (2)	0.0481 (5)
C15	-0.0451 (3)	0.4939 (3)	0.1433 (2)	0.0552 (5)
C16	0.0759 (3)	0.4276 (3)	0.2392 (2)	0.0518 (5)
C17	0.7943 (4)	0.1594 (4)	0.8938 (2)	0.0650 (6)
C18	0.2926 (4)	0.8016 (4)	0.7428 (2)	0.0736 (7)
F1	0.1358 (11)	0.9039 (11)	0.6855 (11)	0.153 (4)
F2	0.2582 (17)	0.7788 (9)	0.8514 (5)	0.142 (3)
F3	0.3907 (13)	0.8735 (13)	0.7368 (11)	0.151 (5)
F1'	0.1482 (12)	0.8385 (9)	0.7786 (12)	0.133 (2)
F2'	0.3879 (12)	0.8421 (10)	0.7903 (9)	0.141 (5)
F3'	0.2468 (12)	0.9348 (5)	0.6369 (4)	0.105 (2)
(IV)				
Br	0.15267 (6)	0.23386 (6)	0.51849 (4)	0.0632 (2)
N1	0.8271 (5)	0.2285 (4)	0.0548 (3)	0.0477 (9)
N2	0.8231 (5)	0.7532 (4)	-0.1474 (3)	0.0464 (8)
N3	0.8444 (4)	0.4778 (4)	-0.0520 (2)	0.0395 (7)
C1	0.9193 (6)	0.3001 (5)	-0.0329 (3)	0.0462 (10)
C2	1.0780 (6)	0.2233 (6)	-0.1067 (4)	0.0543 (12)
C3	1.1479 (6)	0.3219 (5)	-0.1926 (4)	0.0501 (11)
C4	1.0688 (5)	0.5078 (5)	-0.2130 (3)	0.0439 (9)
C5	1.1330 (6)	0.6192 (5)	-0.3026 (3)	0.0461 (10)
C6	1.0389 (6)	0.7961 (6)	-0.3112 (4)	0.0544 (11)
C7	0.8903 (6)	0.8542 (5)	-0.2333 (4)	0.0536 (11)
C8	0.9129 (5)	0.5847 (5)	-0.1398 (3)	0.0393 (9)
C9	0.6931 (5)	0.5192 (5)	0.0283 (3)	0.0421 (9)
C10	0.6866 (5)	0.3642 (5)	0.0934 (3)	0.0424 (9)
C11	0.5549 (5)	0.3326 (5)	0.1924 (3)	0.0408 (9)
C12	0.4037 (6)	0.4674 (5)	0.2268 (3)	0.0484 (10)
C13	0.2847 (6)	0.4400 (6)	0.3218 (4)	0.0494 (11)
C14	0.3146 (5)	0.2751 (5)	0.3851 (3)	0.0476 (10)
C15	0.4621 (6)	0.1373 (6)	0.3531 (3)	0.0528 (11)
C16	0.5804 (7)	0.1686 (6)	0.2579 (4)	0.0517 (12)
C17	1.2938 (7)	0.5547 (8)	-0.3880 (4)	0.0639 (13)
C18	0.7891 (5)	1.0417 (6)	-0.2403 (3)	0.075 (2)
F1	0.7627 (16)	1.0698 (12)	-0.1381 (5)	0.0890 (12)
F1'	0.6171 (8)	1.1062 (11)	-0.2542 (11)	0.0890 (12)
F1''	0.8707 (13)	1.1547 (11)	-0.2936 (11)	0.0890 (12)

F2	0.6701 (15)	1.0878 (12)	−0.1478 (6)	0.0890 (12)
F2'	0.7076 (15)	1.1257 (12)	−0.3310 (7)	0.0890 (12)
F2''	0.9181 (12)	1.1026 (14)	−0.2598 (11)	0.0890 (12)
F3	0.6148 (8)	1.0854 (12)	−0.1902 (11)	0.0890 (12)
F3'	0.7859 (15)	1.1275 (12)	−0.3496 (5)	0.0890 (12)
F3''	0.8763 (14)	1.1216 (14)	−0.2205 (11)	0.0890 (12)

Table 2. *Selected geometric parameters (Å, °) for (I)–(IV)*

	(I)	(II)	(III)	(IV)
N1—C1	1.311 (3)	1.306 (5)	1.311 (2)	1.319 (5)
N1—C10	1.382 (3)	1.378 (5)	1.381 (2)	1.379 (5)
N2—C7	1.331 (3)	1.324 (5)	1.329 (2)	1.335 (5)
N2—C8	1.333 (2)	1.328 (5)	1.332 (2)	1.332 (5)
N3—C1	1.397 (2)	1.393 (5)	1.388 (2)	1.383 (5)
N3—C8	1.392 (2)	1.377 (5)	1.394 (2)	1.383 (5)
N3—C9	1.366 (3)	1.386 (5)	1.373 (2)	1.381 (5)
C1—C2	1.416 (3)	1.424 (6)	1.430 (3)	1.430 (6)
C2—C3	1.341 (3)	1.337 (6)	1.338 (3)	1.334 (6)
C3—C4	1.440 (3)	1.450 (5)	1.443 (3)	1.446 (6)
C4—C5	1.407 (3)	1.397 (5)	1.408 (3)	1.401 (5)
C4—C8	1.408 (3)	1.422 (5)	1.406 (3)	1.413 (5)
C5—C6	1.383 (3)	1.393 (6)	1.381 (3)	1.398 (6)
C5—C17	1.498 (3)	1.502 (6)	1.506 (3)	1.497 (6)
C6—C7	1.378 (3)	1.395 (6)	1.387 (3)	1.373 (6)
C7—C18	1.499 (3)	1.497 (6)	1.505 (3)	1.487 (6)
C9—C10	1.374 (3)	1.358 (5)	1.365 (3)	1.373 (5)
C10—C11	1.461 (3)	1.466 (5)	1.464 (3)	1.468 (5)
C14—R1	1.500 (4)	1.350 (5)	1.744 (2)	1.901 (4)
C15—R2	–	1.350 (5)	–	–
C1—N1—C10	106.2 (2)	106.1 (3)	105.5 (2)	105.3 (3)
C7—N2—C8	115.0 (2)	116.2 (3)	115.0 (2)	115.0 (3)
C1—N3—C8	122.4 (2)	123.8 (3)	123.2 (2)	123.4 (3)
C1—N3—C9	106.8 (2)	106.1 (3)	106.7 (2)	106.8 (3)
C8—N3—C9	130.8 (2)	130.2 (3)	130.1 (2)	129.7 (3)
N1—C1—N3	110.8 (2)	111.1 (3)	111.2 (2)	111.5 (3)
N1—C1—C2	130.6 (2)	131.2 (4)	130.8 (2)	130.4 (4)
N3—C1—C2	118.6 (2)	117.7 (4)	117.9 (2)	118.1 (3)
C1—C2—C3	120.5 (2)	120.8 (4)	120.4 (2)	120.3 (4)
C2—C3—C4	121.3 (2)	121.5 (4)	121.6 (2)	121.6 (4)
C3—C4—C5	124.1 (2)	124.7 (4)	124.7 (2)	124.6 (4)
C3—C4—C8	119.0 (2)	118.2 (3)	118.8 (2)	118.4 (3)
C5—C4—C8	116.9 (2)	117.1 (3)	116.6 (2)	116.9 (4)
C4—C5—C6	117.4 (2)	117.7 (4)	117.8 (2)	117.4 (4)
C4—C5—C17	121.3 (2)	121.8 (4)	121.8 (2)	122.3 (4)
C6—C5—C17	121.3 (2)	120.5 (4)	120.4 (2)	120.3 (4)
C5—C6—C7	120.1 (2)	119.6 (4)	119.8 (2)	119.9 (4)
N2—C7—C6	124.7 (2)	124.1 (4)	124.6 (2)	124.8 (4)
N2—C7—C18	114.3 (2)	115.6 (3)	114.5 (2)	114.3 (4)
C6—C7—C18	120.9 (2)	120.2 (3)	120.8 (2)	120.8 (4)
N2—C8—N3	115.9 (2)	116.7 (3)	115.6 (2)	115.9 (3)
N2—C8—C4	125.9 (2)	125.2 (3)	126.3 (2)	125.9 (3)
N3—C8—C4	118.2 (2)	118.0 (3)	118.1 (2)	118.1 (3)
N3—C9—C10	106.2 (2)	105.9 (3)	105.8 (2)	105.3 (3)
N1—C10—C9	110.0 (2)	110.7 (3)	110.7 (2)	111.1 (3)
N1—C10—C11	120.9 (2)	121.3 (3)	121.0 (2)	120.6 (3)
C9—C10—C11	129.1 (2)	127.9 (3)	128.2 (2)	128.4 (4)
C13—C14—R1	121.9 (3)	120.6 (5)	119.5 (2)	120.1 (3)
C15—C14—R1	121.4 (2)	119.6 (5)	119.6 (2)	119.2 (3)
C14—C15—R2	–	117.0 (4)	–	–
C16—C15—R2	–	120.9 (5)	–	–

Table 3. *Hydrogen-bonding geometry (Å, °) for (I)–(IV)*

D—H···A	D—H	H···A	D···A	D—H···A
(I)				
C2—H2···N1[i]	1.00 (3)	2.50 (3)	3.486 (4)	175 (2)
C9—H9···F1[ii]	0.97 (3)	2.73 (3)	3.662 (4)	163 (2)
C15—H15···F3[iii]	1.00 (3)	2.80 (3)	3.642 (3)	143 (2)
C17—H17C···F3[iv]	0.95 (5)	2.78 (4)	3.649 (5)	154 (3)
(II)				
C2—H2···N1[v]	1.02 (6)	2.56 (6)	3.575 (6)	169 (5)
C12—H12···F1'[ii]	0.93 (1)	2.69 (3)	3.36 (3)	130 (1)
C12—H12···F2'[ii]	0.93 (1)	2.76 (3)	3.458 (3)	133 (1)
C12—H12···F3[ii]	0.93 (1)	2.77 (1)	3.637 (6)	155 (1)
C3—H3···F3[vi]	1.09 (5)	2.78 (6)	3.458 (8)	120 (3)
C17—H17B···F3[vi]	1.16 (9)	2.59 (9)	3.56 (1)	140 (5)
C17—H17A···F5[vii]	0.97 (6)	2.70 (5)	3.642 (6)	165 (4)
C17—H17C···F4[viii]	1.15 (6)	2.63 (8)	3.519 (8)	133 (4)
(III)				
C2—H2···N1[v]	0.90 (3)	2.72 (4)	3.582 (3)	160 (3)
C12—H12···F3'[ii]	0.95 (3)	2.64 (3)	3.545 (6)	160 (2)
C13—H13···F2'[ii]	0.92 (2)	2.63 (3)	3.311 (10)	131 (2)
(IV)				
C2—H2···N1[ix]	0.90 (5)	2.73 (6)	3.605 (6)	164 (5)
C3—H3···F1'[x]	0.96 (4)	2.75 (4)	3.548 (7)	141 (4)
C12—H12···F1[xi]	0.95 (6)	2.71 (6)	3.600 (9)	156 (5)
C13—H13···F1''[xi]	0.82 (4)	2.56 (5)	3.180 (10)	134 (4)
C12—H12···F2[xi]	0.95 (6)	2.66 (6)	3.558 (12)	159 (5)
C12—H12···F3''[xi]	0.95 (6)	2.69 (5)	3.354 (11)	128 (4)

Symmetry codes: (i) $1 - x, 2 - y, 2 - z$; (ii) $-x, 2 - y, 1 - z$; (iii) $-x, 2 - y, 2 - z$; (iv) $1 + x, y, z$; (v) $1 - x, -y, 1 - z$; (vi) $x, y - 1, z$; (vii) $x - 1, y, 1 + z$; (viii) $1 - x, 1 - y, 1 - z$; (ix) $2 - x, -y, -z$; (x) $1 + x, y - 1, z$; (xi) $1 - x, 2 - y, -z$.

The trifluoromethyl group was found to have rotational disorder in (II), (III) and (IV); each F atom is distributed over two sites (Fn and Fn') in (II) and (III) with final occupancies of 87.6 (5) and 12.4 (5)% in (II) and 50% each in (III) while in (IV), three sites with equal occupancy were assigned to each F atom. Some disordered F atoms have high U values. H atoms were located from difference maps and refined isotropically. The poor quality of the crystal resulting in poor data leads to the high R value for (II).

For all compounds, data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL/PC* (Sheldrick, 1990) (direct methods); program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993); molecular graphics: *SHELXTL/PC*; software used to prepare material for publication: *SHELXL93, PARST* (Nardelli, 1983).

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	R1
(V)	Me
(VI)	Ph

Substituted Imidazonaphthyridine Derivatives. II. $C_{19}H_{17}N_3O$ and $C_{24}H_{19}N_3O$

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Abstract

The structures of 2-(4-methoxyphenyl)-6,8-dimethyl-
imidazo[1,2-*a*][1,8]naphthyridine, (V), and 2-(4-methoxy-
phenyl)-6-methyl-8-phenylimidazo[1,2-*a*][1,8]naphthyrid-
ine, (VI), are reported. Two molecules of (V) are
present in the asymmetric unit and they exist as dimers
connected by C—H···N hydrogen bonds. In (VI) the
imidazonaphthyridine moiety and the methoxyphenyl
group lie in one plane with which the 8-phenyl makes
an angle of 22.35 (5)°. Molecules of (VI) also form
dimeric pairs connected by C—H···N bonds around the
inversion centres.

Comment

Continuing our studies of imidazonaphthyridine deriva-
tives (Fun *et al.*, 1996), we report the structures
of 2-(4-methoxyphenyl)-6,8-dimethylimidazo[1,2-*a*]-
[1,8]naphthyridine, (V), and 2-(4-methoxyphenyl)-6-
methyl-8-phenylimidazo[1,2-*a*][1,8]naphthyridine, (VI),
(see Fig. 1 and Table 2). The bond lengths and angles
observed in these structures are normal and compara-
ble with those observed in other imidazonaphthyridine
derivatives (Fun *et al.*, 1996).

Compound (V) crystallizes with two molecules
(*A* and *B*) in the asymmetric unit and they exist
as dimers connected by C—H···N hydrogen bonds,
which commonly stabilize the packing of imi-
dazonaphthyridines; C2*A*···N1*B* 3.525 (3) Å, C2*A*—
H2*A*···N1*B* 165 (2)° and C2*B*···N1*A* 3.633 (3) Å,
C2*B*—H2*B*···N1*A* 167 (2)°. The dihedral angle between
the planes of the imidazonaphthyridine and methoxy-
phenyl groups is 18.23 (6)° in (V*A*) and 14.56 (7)° in
(V*B*). The angle between the planes of the imidazon-
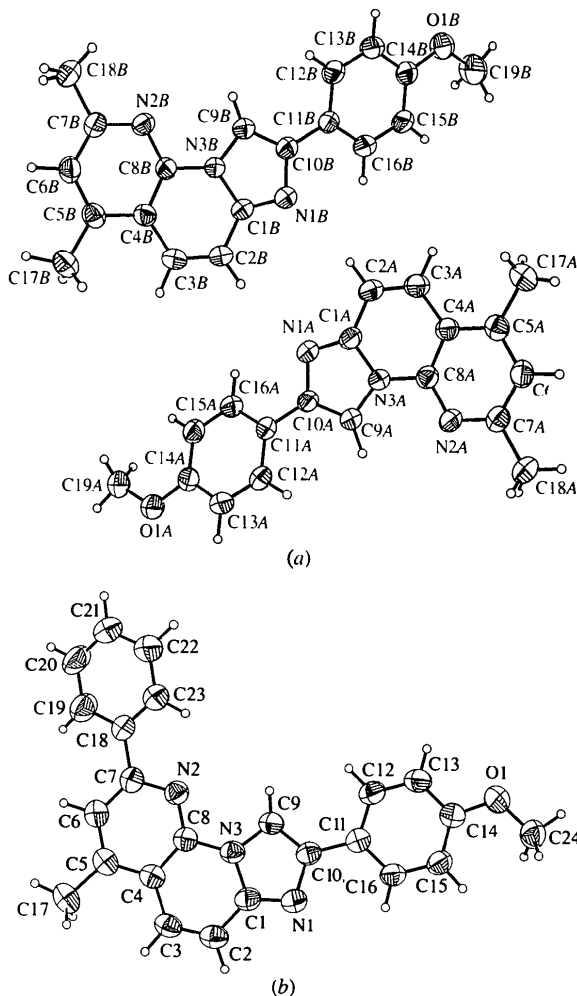
(*a*)

(*b*)

Fig. 1. Views of (*a*) the two molecules of (V) in the asymmetric unit,
and (*b*) molecule (VI) showing numbering schemes; displacement
ellipsoids are drawn at the 50% probability level.