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

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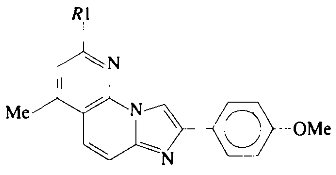
Abstract

The structures of 2-(4-methoxyphenyl)-6,8-dimethylimidazo[1,2-*a*][1,8]naphthyridine, (V), and 2-(4-methoxyphenyl)-6-methyl-8-phenylimidazo[1,2-*a*][1,8]naphthyridine, (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 derivatives (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 comparable with those observed in other imidazonaphthyridine derivatives (Fun *et al.*, 1996).



	R1
(V)	Me
(VI)	Ph

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 imidazonaphthyridines; 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 methoxyphenyl groups is 18.23 (6)° in (V*A*) and 14.56 (7)° in (V*B*). The angle between the planes of the imidazon-

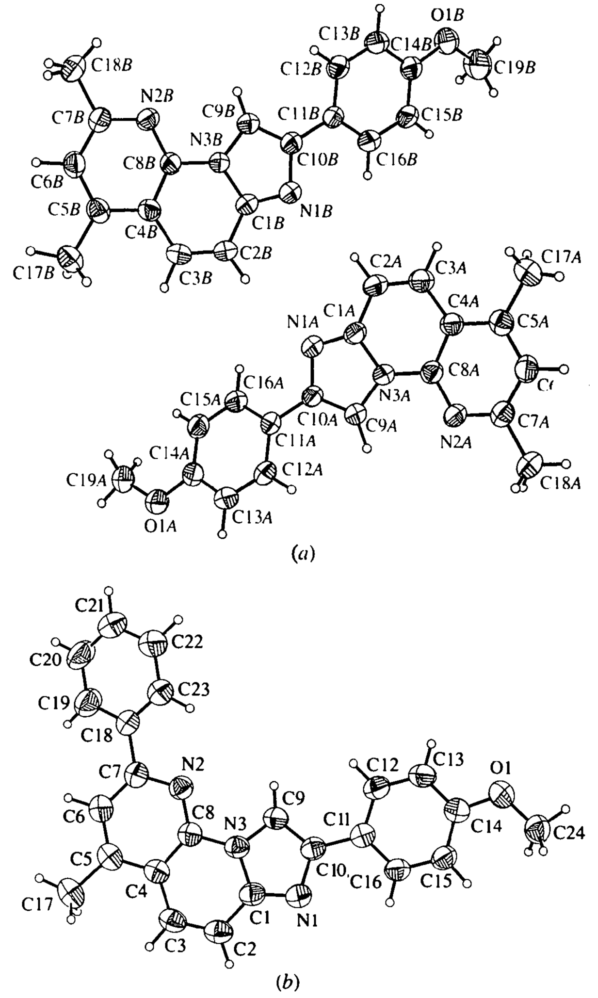


Fig. 1. Views of (*a*) the two molecules of (V) in the asymmetric unit, and (*b*) molecule (VI) showing numbering schemes; displacement ellipsoids are drawn at the 50% probability level.

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aphthyridine moieties in the dimeric pair is 40.19 (3)°. The methoxy atom O1*A* in (V*A*) is involved in an intermolecular hydrogen bond whereas O1*B* is not [C3*B*···O1*A*^{i} 3.476 (3) Å, C3*A*—H3*A*···O1*A*^{i} 177 (2)°; symmetry code: (i) $2-x$, $1-y$, $1-z$]. In the crystal the molecules of type *A* and *B* form alternate layers which are connected by the hydrogen bonds.

The imidazonaphthyridine moiety in (VI) is also planar, with a maximum deviation of 0.048 (2) Å for C7; the methoxyphenyl ring lies in the same plane, the dihedral angle is 2.29 (5)°. The plane of the phenyl ring at C7 makes an angle of 22.35 (5)° with the imidazonaphthyridine plane. In this case, the molecules also form dimeric pairs through C—H···N hydrogen bonds; C2···N1^{i} 3.496 (2) Å, C2—H2···N1^{i} 164 (2)°. In addition, an intermolecular C—H···O hydrogen bond between C21 and O1 is present; C21···O1^{ii} 3.525 (3) Å, C21—H21···O1^{ii} 143 (2)° [symmetry codes: (i) $-x$, $1-y$, $-z$; (ii) $1-x$, $y-\frac{3}{2}$, $\frac{1}{2}-z$].

From our studies on 2,6,8-substituted imidazo[1,2-*a*]1,8-naphthyridine derivatives, we observe that only (VI) is monoclinic, the other compound being triclinic (space group $P\bar{1}$). The 8-methyl and 8-trifluoromethyl compounds, (I)–(V) (Fun *et al.*, 1996) have the same mode of packing which differs from that of the 8-phenyl compound (VI).

Experimental

Single crystals of (V) and (VI) were obtained by slow evaporation of the ethanol solution of the compound.

Compound (V)

Crystal data

$C_{19}H_{17}N_3O$
$M_r = 303.36$
Triclinic
$P\bar{1}$
$a = 8.041$ (1) Å
$b = 13.567$ (1) Å
$c = 15.030$ (1) Å
$\alpha = 93.520$ (1)°
$\beta = 97.320$ (1)°
$\gamma = 105.93$ (1)°
$V = 1555.8$ (2) Å^3
$Z = 4$
$D_x = 1.295$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 35 reflections
$\theta = 9$–25°
$\mu = 0.082$ mm^{-1}
$T = 293$ (2) K
Prism
0.52 × 0.36 × 0.20 mm
Colourless

Data collection

Siemens *P*4 diffractometer
$\theta/2\theta$ scans
Absorption correction: none
8674 measured reflections
7152 independent reflections
3761 observed reflections [$I > 2\sigma(I)$]
$R_{int} = 0.0224$

$\theta_{max} = 27.50°$
$h = -1 \rightarrow 10$
$k = -17 \rightarrow 17$
$l = -19 \rightarrow 19$
3 standard reflections monitored every 97 reflections intensity decay: <5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0589$
$wR(F^2) = 0.1807$
$S = 0.894$
7151 reflections
551 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.1051P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ 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 (VI)

Crystal data

$C_{24}H_{19}N_3O$
$M_r = 365.42$
Monoclinic
$P2_1/c$
$a = 8.435$ (1) Å
$b = 7.146$ (1) Å
$c = 31.823$ (3) Å
$\beta = 92.00$ (1)°
$V = 1917.0$ (4) Å^3
$Z = 4$
$D_x = 1.266$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 40 reflections
$\theta = 9$–25°
$\mu = 0.079$ mm^{-1}
$T = 293$ (2) K
Rectangle
0.60 × 0.52 × 0.28 mm
Pale yellow

Data collection

Siemens *P*4 diffractometer
$\theta/2\theta$ scans
Absorption correction: none
6045 measured reflections
4362 independent reflections
2461 observed reflections [$I > 2\sigma(I)$]
$R_{int} = 0.0257$

$\theta_{max} = 27.50°$
$h = -1 \rightarrow 10$
$k = -1 \rightarrow 9$
$l = -41 \rightarrow 41$
3 standard reflections monitored every 97 reflections intensity decay: <2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0482$
$wR(F^2) = 0.1433$
$S = 0.899$
4361 reflections
329 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0767P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ 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 (Å^2)*

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

	x	y	z	U_{eq}
(V)				
O1*A*	1.2210 (2)	0.60958 (14)	0.43979 (14)	0.0636 (5)
N1*A*	0.4184 (3)	0.40470 (14)	0.24969 (13)	0.0465 (5)
N2*A*	0.1638 (3)	0.64000 (14)	0.13780 (13)	0.0449 (5)
N3*A*	0.2756 (2)	0.51109 (14)	0.19025 (12)	0.0405 (4)
C1*A*	0.2673 (3)	0.4101 (2)	0.2070 (2)	0.0425 (5)
C2*A*	0.1054 (4)	0.3326 (2)	0.1795 (2)	0.0497 (6)

C3*A*	−0.0338 (4)	0.3577 (2)	0.1390 (2)	0.0484 (6)
C4*A*	−0.0252 (3)	0.4627 (2)	0.12347 (15)	0.0419 (5)
C5*A*	−0.1671 (3)	0.4956 (2)	0.0845 (2)	0.0463 (6)
C6*A*	−0.1372 (4)	0.5993 (2)	0.0736 (2)	0.0508 (6)
C7*A*	0.0275 (3)	0.6692 (2)	0.0997 (2)	0.0466 (6)
C8*A*	0.1338 (3)	0.5401 (2)	0.14900 (14)	0.0404 (5)
C9*A*	0.4430 (3)	0.5704 (2)	0.2239 (2)	0.0444 (6)
C10*A*	0.5280 (3)	0.5046 (2)	0.26042 (15)	0.0428 (6)
C11*A*	0.7085 (3)	0.5298 (2)	0.30686 (15)	0.0429 (5)
C12*A*	0.8012 (4)	0.6314 (2)	0.3416 (2)	0.0564 (7)
C13*A*	0.9691 (4)	0.6553 (2)	0.3857 (2)	0.0601 (7)
C14*A*	1.0529 (3)	0.5780 (2)	0.3956 (2)	0.0475 (6)
C15*A*	0.9628 (3)	0.4778 (2)	0.3629 (2)	0.0477 (6)
C16*A*	0.7930 (3)	0.4545 (2)	0.3193 (2)	0.0479 (6)
C17*A*	−0.3458 (4)	0.4211 (3)	0.0550 (3)	0.0622 (8)
C18*A*	0.0631 (5)	0.7814 (2)	0.0857 (3)	0.0675 (9)
C19*A*	1.3088 (4)	0.5340 (3)	0.4560 (2)	0.0613 (8)
O1*B*	−0.5193 (3)	−0.16133 (15)	−0.05096 (12)	0.0694 (6)
N1*B*	0.1100 (3)	0.09550 (15)	0.26198 (13)	0.0481 (5)
N2*B*	0.1647 (3)	−0.08080 (14)	0.50614 (12)	0.0426 (5)
N3*B*	0.1504 (2)	0.01965 (13)	0.38748 (12)	0.0393 (4)
C1*B*	0.2053 (3)	0.1065 (2)	0.3424 (2)	0.0441 (6)
C2*B*	0.3436 (3)	0.1904 (2)	0.3875 (2)	0.0504 (6)
C3*B*	0.4201 (3)	0.1839 (2)	0.4712 (2)	0.0496 (6)
C4*B*	0.3652 (3)	0.0929 (2)	0.5170 (2)	0.0419 (5)
C5*B*	0.4446 (3)	0.0791 (2)	0.6033 (2)	0.0447 (6)
C6*B*	0.3794 (3)	−0.0141 (2)	0.6365 (2)	0.0476 (6)
C7*B*	0.2416 (3)	−0.0920 (2)	0.5874 (2)	0.0436 (6)
C8*B*	0.2278 (3)	0.0097 (2)	0.47378 (15)	0.0382 (5)
C9*B*	0.0137 (3)	−0.0481 (2)	0.3316 (2)	0.0428 (6)
C10*B*	−0.0104 (3)	0.0000 (2)	0.25509 (15)	0.0411 (5)
C11*B*	−0.1427 (3)	−0.0392 (2)	0.17497 (15)	0.0419 (5)
C12*B*	−0.2842 (4)	−0.1256 (2)	0.1751 (2)	0.0506 (6)
C13*B*	−0.4075 (4)	−0.1639 (2)	0.0996 (2)	0.0548 (7)
C14*B*	−0.3918 (3)	−0.1170 (2)	0.0208 (2)	0.0497 (6)
C15*B*	−0.2538 (4)	−0.0307 (2)	0.0193 (2)	0.0545 (7)
C16*B*	−0.1318 (4)	0.0083 (2)	0.0959 (2)	0.0509 (6)
C17*B*	0.5937 (4)	0.1616 (3)	0.6566 (2)	0.0586 (7)
C18*B*	0.1715 (5)	−0.1942 (2)	0.6232 (2)	0.0620 (8)
C19*B*	−0.4971 (7)	−0.1238 (4)	−0.1361 (2)	0.0873 (12)
(VI)				
O1	0.5973 (2)	1.3243 (2)	0.08702 (4)	0.0656 (4)
N1	0.1728 (2)	0.5778 (2)	0.05260 (4)	0.0510 (4)
N2	0.1606 (2)	0.2014 (2)	0.16694 (4)	0.0471 (4)
N3	0.1498 (2)	0.3812 (2)	0.10666 (4)	0.0458 (3)
C1	0.1097 (2)	0.4172 (3)	0.06496 (5)	0.0488 (4)
C2	0.0118 (2)	0.2866 (3)	0.04266 (6)	0.0580 (5)
C3	−0.0384 (2)	0.1317 (3)	0.06240 (6)	0.0563 (5)
C4	0.0061 (2)	0.0922 (3)	0.10542 (5)	0.0487 (4)
C5	−0.0375 (2)	−0.0687 (3)	0.12803 (6)	0.0522 (4)
C6	0.0204 (2)	−0.0880 (3)	0.16880 (6)	0.0543 (5)
C7	0.1207 (2)	0.0459 (2)	0.18742 (5)	0.0491 (4)
C8	0.1041 (2)	0.2199 (2)	0.12764 (5)	0.0453 (4)
C9	0.2425 (2)	0.5278 (2)	0.12091 (6)	0.0474 (4)
C10	0.2555 (2)	0.6461 (2)	0.08760 (5)	0.0461 (4)
C11	0.3423 (2)	0.8239 (2)	0.08657 (5)	0.0459 (4)
C12	0.4246 (2)	0.8924 (3)	0.12211 (6)	0.0547 (5)
C13	0.5063 (2)	1.0579 (3)	0.12123 (6)	0.0579 (5)
C14	0.5110 (2)	1.1624 (3)	0.08461 (5)	0.0503 (4)
C15	0.4288 (2)	1.0990 (3)	0.04909 (6)	0.0553 (5)
C16	0.3458 (2)	0.9320 (3)	0.05044 (6)	0.0534 (4)
C17	−0.1391 (3)	−0.2175 (3)	0.10770 (8)	0.0662 (6)
C18	0.1968 (2)	0.0231 (3)	0.22997 (5)	0.0522 (4)
C19	0.1395 (3)	−0.0948 (4)	0.26016 (7)	0.0757 (6)
C20	0.2164 (3)	−0.1139 (4)	0.29877 (7)	0.0823 (7)
C21	0.3503 (3)	−0.0175 (3)	0.30849 (7)	0.0721 (6)
C22	0.4126 (3)	0.0988 (4)	0.27883 (7)	0.0886 (8)
C23	0.3353 (3)	0.1204 (3)	0.24012 (7)	0.0781 (7)
C24	0.6003 (3)	1.4376 (3)	0.05026 (7)	0.0660 (6)

Table 2. *Selected geometric parameters (Å, °) for (V) and (VI)*

	(V*A*)	(V*B*)	(VI)
N1—C1	1.323 (3)	1.323 (3)	1.330 (2)
N1—C10	1.385 (3)	1.377 (3)	1.382 (2)
N2—C7	1.339 (3)	1.333 (3)	1.337 (2)
N2—C8	1.334 (3)	1.339 (3)	1.329 (2)
N3—C1	1.394 (3)	1.390 (3)	1.382 (2)
N3—C8	1.391 (3)	1.396 (3)	1.393 (2)
N3—C9	1.377 (3)	1.369 (3)	1.375 (2)
C1—C2	1.424 (3)	1.418 (3)	1.420 (3)
C2—C3	1.342 (4)	1.347 (4)	1.348 (3)
C3—C4	1.442 (3)	1.441 (3)	1.435 (2)
C4—C5	1.409 (3)	1.418 (3)	1.412 (3)
C4—C8	1.405 (3)	1.400 (3)	1.406 (2)
C5—C6	1.384 (3)	1.380 (3)	1.377 (3)
C5—C17	1.507 (4)	1.497 (4)	1.499 (3)
C6—C7	1.392 (4)	1.394 (3)	1.395 (3)
C7—C18	1.503 (4)	1.507 (4)	1.487 (2)
C9—C10	1.367 (3)	1.376 (3)	1.363 (2)
C10—C11	1.466 (3)	1.466 (3)	1.467 (2)
C11—C12	1.406 (3)	1.392 (3)	1.395 (2)
C11—C16	1.382 (3)	1.388 (3)	1.386 (2)
C12—C13	1.368 (4)	1.378 (3)	1.369 (3)
C13—C14	1.399 (4)	1.383 (3)	1.386 (3)
C14—C15	1.379 (3)	1.378 (4)	1.382 (2)
C15—C16	1.379 (4)	1.386 (4)	1.385 (3)
O1—C14	1.368 (3)	1.369 (3)	1.368 (2)
O1—C19	1.412 (3)	1.420 (4)	1.423 (2)
C1—N1—C10	105.6 (2)	105.7 (2)	105.2 (1)
C7—N2—C8	116.4 (2)	116.3 (2)	116.9 (2)
C1—N3—C8	123.5 (2)	123.4 (2)	123.5 (1)
C1—N3—C9	106.8 (2)	107.1 (2)	107.0 (1)
C8—N3—C9	129.8 (2)	129.5 (2)	129.5 (1)
N1—C1—N3	110.9 (2)	110.8 (2)	111.0 (2)
N1—C1—C2	131.0 (2)	130.9 (2)	130.6 (2)
N3—C1—C2	118.1 (2)	118.3 (2)	118.4 (2)
C1—C2—C3	120.1 (2)	120.0 (2)	119.6 (2)
C2—C3—C4	121.5 (2)	121.6 (2)	122.0 (2)
C3—C4—C5	124.8 (2)	124.6 (2)	125.6 (2)
C3—C4—C8	119.3 (2)	119.2 (2)	118.8 (2)
C5—C4—C8	115.9 (2)	116.2 (2)	115.6 (2)
C4—C5—C6	117.8 (2)	117.3 (2)	118.1 (2)
C4—C5—C17	121.6 (2)	121.8 (2)	120.9 (2)
C6—C5—C17	120.6 (3)	120.9 (2)	120.9 (2)
C5—C6—C7	121.4 (2)	121.6 (2)	121.4 (2)
N2—C7—C6	121.9 (2)	122.2 (2)	121.5 (2)
N2—C7—C18	116.1 (2)	116.2 (2)	115.2 (2)
C6—C7—C18	122.0 (3)	121.6 (2)	123.2 (2)
N2—C8—N3	115.9 (2)	116.0 (2)	115.9 (2)
N2—C8—C4	126.5 (2)	126.4 (2)	126.4 (2)
N3—C8—C4	117.5 (2)	117.6 (2)	117.6 (2)
N3—C9—C10	106.0 (2)	105.8 (2)	106.0 (2)
N1—C10—C9	110.7 (2)	110.6 (2)	110.8 (2)
N1—C10—C11	121.6 (2)	121.7 (2)	121.7 (1)
C9—C10—C11	127.7 (2)	127.7 (2)	127.5 (2)
C10—C11—C12	121.1 (2)	121.4 (2)	121.4 (2)
C10—C11—C16	121.4 (2)	121.3 (2)	121.7 (2)
C12—C11—C16	117.5 (2)	117.3 (2)	116.9 (2)
C11—C12—C13	121.4 (2)	121.8 (2)	121.5 (2)
C12—C13—C14	119.9 (3)	120.0 (2)	120.8 (2)
C13—C14—C15	119.3 (2)	119.3 (2)	118.9 (2)
C14—C15—C16	120.3 (2)	120.3 (2)	119.8 (2)
C11—C16—C15	121.6 (2)	121.3 (2)	122.1 (2)
C13—C14—O1	115.6 (2)	115.8 (2)	116.1 (2)
C15—C14—O1	125.1 (2)	124.9 (2)	125.1 (2)
C14—O1—C19	118.1 (2)	117.8 (2)	117.4 (2)

For both compounds, data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structures: *SHELXTL/PC* (Sheldrick, 1990) (direct methods); program(s) used to refine structures: *SHELXL*93 (Sheldrick, 1993); molecular graphics: *SHELXTL/PC*; software used to prepare material for publication: *SHELXL*93, *PARST* (Nardelli, 1983).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry, along with packing diagrams of the molecules, have been deposited with the IUCr (Reference: MU1239). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Substituted Imidazonaphthyridine Derivatives. III. $C_{24}H_{28}N_4$, $C_{24}H_{28}N_4O$ and $C_{23}H_{25}BrN_4$

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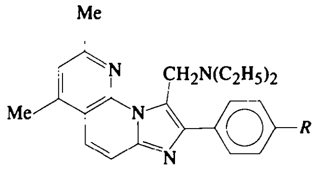
Abstract

The structures of three 1,2,6,8-tetrasubstituted imidazonaphthyridine derivatives, 1-diethylaminomethyl-6,8-dimethyl-2-(4-methylphenyl)imidazo[1,2-*a*][1,8]naphthyridine, (VII), 1-diethylaminomethyl-2-(4-methoxyphenyl)-6,8-dimethylimidazo[1,2-*a*][1,8]naphthyridine, (VIII), and 2-(4-bromophenyl)-1-diethylaminomethyl-6,8-dimethylimidazo[1,2-*a*][1,8]naphthyridine, (IX), are reported. Two molecules related by a pseudo inversion centre are present in the asymmetric unit of (IX). Intramolecular C—H···N hydrogen bonds are observed in (VII) and (IX) whereas an intermolecular C—H···O hydrogen bond is present in (VIII).

Comment

We continue our reports of the crystal structures of imidazonaphthyridine compounds (Fun *et al.*, 1996; Sivakumar *et al.*, 1996) with those of three 1,2,6,8-tetrasubstituted imidazonaphthyridine compounds, (VII), (VIII) and (IX). All three compounds were prepared by the Mannich reaction (Chua & Jackson, 1995). The bond lengths and angles observed in these structures (Table 2) are normal and comparable with those observed in other imidazonaphthyridine derivatives. However, the orientations of the phenyl rings and of the diethylaminomethyl groups show some differences in the three compounds.



	*R*1
(I)	Me
(II)	OMe
(III)	Br

In (IX) two molecules are present in the asymmetric unit and are related by a pseudo inversion centre at (0.22, 0.50, 0.25). The diethylaminomethyl groups in the two molecules (IX*A*) and (IX*B*) lie on opposite sides of the imidazonaphthyridine plane (see the relevent torsion angles in Table 2). The dihedral angles between the planes of the imidazonaphthyridine moiety and the phenyl ring are 15.66 (4), 29.07 (3), 20.6 (1) and 17.1 (1)° in (VII), (VIII), (IX*A*) and (IX*B*), respectively. In (VII), (IX*A*) and (IX*B*), the orientation of the diethylaminomethyl group is favourable for intramolecular C12—H12···N4 hydrogen bonding whereas in (VIII) the orientation of this group is entirely different and an intermolecular C—H···O hydrogen bond involving the O1 methoxy atom is observed instead. Hydrogen-bond details: in (VII) C12···N4 3.258 (2) Å, C12—H12···N4 151 (2)°; in (VIII) C18···O1^{i} 3.473 (3) Å, C18—H18*A*···O1^{i} 154 (3)°; in (IX) C12*A*···N4 3.258 (8) Å, C12*A*—H12*A*···N4 154 (4)°, C12*B*···N4*B* 3.270 (8) Å, C12*B*—H12*B*···N4*B*, 152 (4)° [symmetry code: (i) $1-x$, $1-y$, $1-z$]. The planar imidazonaphthyridine moieties stack parallel to the $(2\bar{2}2)$ planes (spacing 3.412 Å) in (VII), to $(20\bar{2})$ (spacing 3.351 Å) in (VIII), and to (004) (spacing 3.443 Å) in (IX). In all three structures, the packing involves intermolecular π–π interactions.

In 2,6,8-trisubstituted imidazonaphthyridine derivatives, the molecules readily form dimers through C2—H2···N1 bonds (Fun *et al.*, 1996; Sivakumar *et al.*,

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