$wR = 0.062$
$S = 1.59$
974 reflections
289 parameters
$w = 1/[\sigma^2(F)+0.0010F^2]$
$(\Delta/\sigma)_{max} = 0.001$

Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Data collection: Enraf–Nonius CAD-4 software. Cell refinement: Enraf–Nonius CAD-4 software. Data reduction: *NRC-VAX DATRD2* (Gabe, Le Page, Charland, Lee & White, 1989). Program(s) used to solve structure: *NRCVAX SOLVER*. Program(s) used to refine structure: *NRCVAX LSTSQ*. Molecular graphics: *NRCVAX*. Software used to prepare material for publication: *NRCVAX TABLES*.

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* ($\mathring{A}^2$)

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

	x	y	z	U_{eq}
O1A	0.3516 (5)	0.3111 (5)	0.56704 (21)	0.048 (5)
O2A	0.1486 (8)	0.2170 (8)	0.6298 (3)	0.119 (8)
C1A	0.4474 (8)	0.3636 (8)	0.6008 (3)	0.040 (7)
C2A	0.5379 (8)	0.3388 (7)	0.6006 (3)	0.039 (7)
C3A	0.6334 (7)	0.4004 (8)	0.6334 (3)	0.042 (7)
C4A	0.6441 (8)	0.4898 (8)	0.6657 (3)	0.046 (7)
C5A	0.5520 (8)	0.5168 (8)	0.6642 (3)	0.047 (8)
C6A	0.4529 (7)	0.4546 (8)	0.6324 (3)	0.040 (7)
C7A	0.5462 (7)	0.2613 (7)	0.5580 (3)	0.042 (6)
C8A	0.7542 (7)	0.5658 (8)	0.6984 (3)	0.052 (7)
C9A	0.8194 (10)	0.6917 (9)	0.6761 (4)	0.086 (9)
C10A	0.8385 (11)	0.5171 (11)	0.6976 (5)	0.109 (11)
C11A	0.7241 (10)	0.5721 (12)	0.7541 (4)	0.107 (11)
C12A	0.2676 (10)	0.1877 (10)	0.5703 (5)	0.082 (10)
C13A	0.1585 (11)	0.1516 (11)	0.5970 (5)	0.080 (11)
C14A	0.0544 (10)	0.0353 (9)	0.5849 (5)	0.100 (10)
O1B	0.4159 (5)	0.2024 (5)	0.46228 (19)	0.043 (5)
O2B	0.2195 (7)	−0.0167 (6)	0.4742 (3)	0.090 (6)
C1B	0.5272 (8)	0.3052 (7)	0.4629 (3)	0.038 (7)
C2B	0.3787 (8)	0.5660 (8)	0.5798 (3)	0.038 (7)
C3B	0.4807 (8)	0.6793 (8)	0.5773 (3)	0.045 (7)
C4B	0.7493 (7)	0.5088 (7)	0.4667 (3)	0.040 (7)
C5B	0.7048 (8)	0.4342 (8)	0.5083 (3)	0.045 (7)
C6B	0.5947 (8)	0.3338 (8)	0.5082 (3)	0.040 (7)
C7B	0.3589 (7)	0.4908 (7)	0.6285 (3)	0.043 (6)
C8B	0.8736 (8)	0.6228 (8)	0.4687 (4)	0.056 (7)
C9B	0.9036 (11)	0.6988 (11)	0.4206 (5)	0.116 (11)
C10B	0.9678 (9)	0.5875 (10)	0.4745 (5)	0.110 (11)
C11B	0.8806 (12)	0.6974 (11)	0.5141 (6)	0.136 (12)
C12B	0.4135 (8)	0.1056 (9)	0.4386 (4)	0.062 (8)
C13B	0.2979 (11)	−0.0073 (10)	0.4441 (4)	0.073 (10)
C14B	0.2828 (11)	−0.1102 (9)	0.4132 (5)	0.111 (11)

Table 2. *Selected bond lengths* ($\mathring{A}$)

Bond	Range	Mean
C_{ar}—O_{ether}	1.384 (10)–1.392 (10)	1.388 (10)
Csp^3—O_{ether}	1.382 (12)–1.418 (13)	1.400 (13)
Csp^3—Csp^2	1.426 (18)–1.489 (15)	1.466 (16)
Csp^2=O	1.235 (16)–1.247 (17)	1.241 (17)
C_{ar}—C_{ar}	1.364 (13)–1.407 (13)	1.384 (13)
C_{ar}—Csp^3	1.512 (11)–1.550 (12)	1.528 (12)
Csp^3—C(^{t}Bu methyl)	1.492 (16)–1.528 (14)	1.508 (15)

H atoms, visible in difference maps, were allowed for as riding atoms with C—H 0.95 $\mathring{A}$. U_{ij} were refined for all non-H atoms.

The θ-scan width was $(0.6+0.35\tan\theta)°$ with a θ-scan rate of $2.75°$ min^{-1} and background counts for 15 s on each side of every scan.

The systematic absences (00l only present if $l = 3n$) and the observed $\bar{3}m$ Laue symmetry allow the space group to be one of the enantomorphous pairs $P3_112$ and $P3_212$ or $P3_121$ and $P3_221$.

0108-2701/93/030604-04$06.00

The structure was solved and refined in $P3_121$. No attempt was made to determine any absolute configuration in the light of the paucity of observed data and the low values of the anomalous-scattering components for C and O. Very few reflections were observed beyond $\theta = 15°$ and data collection was terminated at $\theta = 20°$.

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Structures of Furo[2,3-b]indolizine Derivatives

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Abstract

The indolizine and furan rings in the skeleton of 2-benzoyl-9-methylfuro[2,3-b]indolizine (2a) and 8-benzoyl-5,6-dihydro-4H-furo[2′,3′:4,5]pyrrolo[3,2,1-ij]quinoline (2b) are planar [mean deviations 0.023 (4) and 0.006 (4) $\mathring{A}$ (2a), 0.014 (3) and 0.005 (3) $\mathring{A}$ (2b), respectively] and inclined at $5.62°$ (2a) and $3.25°$ (2b) to one another. In (2b), The nearly planar cyclohexene ring (fused to the indolizine ring at the 1- and 8-positions) is also nearly coplanar with the indolizine ring [mean deviation 0.140 (3) $\mathring{A}$, dihedral angle $5.41°$]. The annelation of the cyclohexene ring in (2b)

causes a shortening of the N1—C8 bond (1.402 Å) and distortion of the bond angles around C8 in the indolizine ring. The delocalized ring system extends to the fused furan ring. The phenyl ring in the benzoyl group is inclined to the indolizine ring with a dihedral angle of 46.64° in (2a) and 44.20° in (2b).

Comment

A chloroform solution of ethyl 1-cyano-2-[1-methyl-2-(phenacyloxy)indolizin-3-yl]acrylate (1a) (1 mmol) and 1,8-diazabicyclo[5.4.0]undec-7-ene (500 mg) was heated under reflux for 30 min. After removal of the solvent under reduced pressure, the residual oil was separated by column chromatography on alumina using ether and then chloroform to afford 2-benzoyl-9-methylfuro[2,3-b]indolizine (2a) in a 92% yield (Kakehi, Ito, Furuta & Todoroki, 1985). Similar treatment of 1,8-annelated indolizines (1b) gave the corresponding product, 8-benzoyl-5,6-dihydro-4H-furo[2',3':4,5]pyrrolo[3,2,1-ij]quinoline (2b) in a 43% yield (Kakehi, Ito & Yotsuya, 1986).
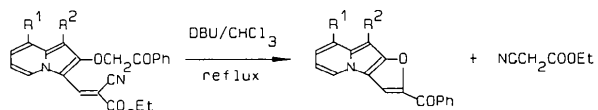
(1a) R¹ = H, R² = Me
(1b) R¹, R² = -(CH₂)₃-

(2a) R¹ = H, R² = Me
(2b) R¹, R² = -(CH₂)₃-

The present study was undertaken to confirm the chemical structures of the title compounds and to compare their structural features with those of other indolizine and fused-indolizine derivatives. The bond distances and angles in the indolizine skeletons of (2a) and (2b) are similar to those in 1-acetoxy-2,3-diphenylindolizine (Wadsworth, Bender, Smith, Luss & Weidner, 1986), ethyl 1-trifluoromethylindolizine-3-carboxylate (Pritchard, 1988), ethyl 3,7-dimethyl-2-(p-methylbenzoyl)thieno[2,3-b]indolizine-9-carboxylate (Kakehi, Ito, Sakurai & Urushido, 1991), and 3-acetyl-6-methyl-2H-pyrano[2,3-b]indolizin-2-one (Kakehi, Kitajima, Ito & Takusagawa, 1992b). Those in (2b) are also similar to those in (2a) except for the shortened C8—N1 bond (1.402 Å) and enlarged N1—C8—C7 and N1—C8—C9 bond angles [119.6 (2) and 111.8 (2)°, respectively].

This distortion must be caused by the annelation at the 1- and 8-positions in the indolizine skeleton, as in ethyl 3,4-dihydrocyclopenta[hi]indolizine-1-carboxylate (Kakehi, Kitajima, Ito & Takusagawa, 1992a) in which there is a five-membered ring at the 1- and 8-positions of the indolizine ring. On the other hand, the furan ring attached to the 2- and 3-positions as well as the benzoyl group does not cause a large distortion of the indolizine skeleton. Furthermore, the distances and angles for the furan

rings in (2a) and (2b) differ considerably from those of the parent furan (Bak, Christensen, Dixon, Hansen-Nygaad, Andersen & Schottländer, 1962) and benzo[b]furan derivative (Fontaine, Dideberg & Dupont, 1975). The large difference between the two O—C bonds (O1—C2 and O1—C10) and the shortened C2—C3 bond are particular features of the furan ring in (2a) and (2b). We have recently reported similar relationships in the crystal structures of thieno[3,2-a]- and thieno[2,3-b]indolizine derivatives (Kakehi, Ito, Sakurai & Urushido, 1991). Ring planarity (as represented by χ^2) in the skeletons of the title compounds is summarized in Table 3.
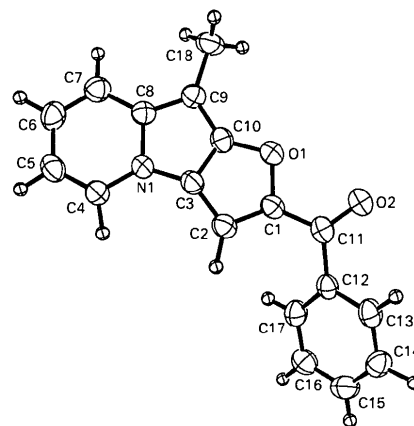

Fig. 1. ORTEP (Johnson, 1965) drawing of (2a) showing atomic numbering system.
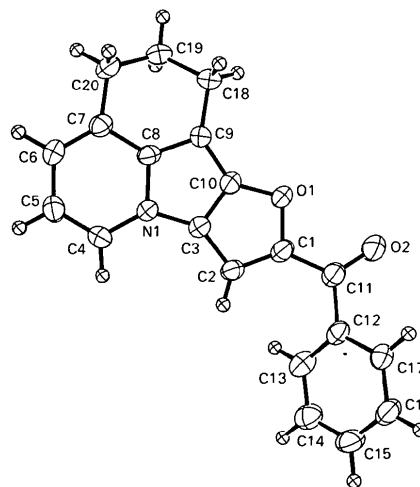

Fig. 2. ORTEP drawing of (2b) showing atomic numbering system.

Experimental

Compound (2a)

Crystal data

$C_{18}H_{13}NO_2$ Mo $K\alpha$ radiation
$M_r = 275.31$ $\lambda = 0.71069$ Å

Orthorhombic
$P2_12_12_1$
$a = 8.988 (2)$ Å
$b = 27.953 (3)$ Å
$c = 5.520 (2)$ Å
$V = 1386.8 (5)$ Å^3
$Z = 4$
$D_x = 1.318$ Mg m^{-3}

Cell parameters from 25
reflections
$\theta = 36.14–39.74°$
$\mu = 8.1$ mm^{-1}
$T = 297$ K
Prism
$0.48 \times 0.44 \times 0.32$ mm
Black

$wR = 0.047$
$S = 1.38$
1685 reflections
269 parameters
$w = 4F_o^2/[\sigma^2(F_o^2)]$
$(\Delta/\sigma)_{max} = 0.03$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}

Extinction coefficient:
0.61406×10^{-6}
Atomic scattering factors
from *International Tables*
for X-ray Crystallography
(1974, Vol. IV)

Data collection

Rigaku AFC-5S diffractometer
ω scans
1908 measured reflections
1908 independent reflections
1140 observed reflections
$[I > 3.0\sigma(I)]$
$\theta_{max} = 27.55°$

$h = 0 \rightarrow 11$
$k = 0 \rightarrow 36$
$l = 0 \rightarrow 7$
3 standard reflections
monitored every 150
reflections
intensity variation: average -0.4%

Refinement

Refinement on F
Final $R = 0.040$
$wR = 0.046$
$S = 1.47$
1140 reflections
243 parameters
$w = 4F_o^2/[\sigma^2(F_o)]$
$(\Delta/\sigma)_{max} = 0.10$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}

Extinction correction: analytical
Extinction coefficient:
0.29608×10^{-5}
Atomic scattering factors
from *International Tables*
for X-ray Crystallography
(1974, Vol. IV)

Compound (2b)

Crystal data

$C_{20}H_{15}NO_2$
$M_r = 301.34$
Monoclinic
$P2_1/c$
$a = 7.826 (2)$ Å
$b = 13.850 (2)$ Å
$c = 13.558 (2)$ Å
$\beta = 96.85 (1)°$
$V = 1459.1 (5)$ Å^3
$Z = 4$
$D_x = 1.372$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 25
reflections
$\theta = 19.11–19.83°$
$\mu = 8.3$ mm^{-1}
$T = 293$ K
Prism
$0.68 \times 0.36 \times 0.18$ mm
Brown

Data collection

Rigaku AFC-5S diffractometer
$\omega–2\theta$ scans
3748 measured reflections
3501 independent reflections
1685 observed reflections
$[I > 3.00\sigma(I)]$
$R_{int} = 0.025$
$\theta_{max} = 27.5°$

$h = 0 \rightarrow 10$
$k = 0 \rightarrow 17$
$l = -17 \rightarrow 17$
3 standard reflections
monitored every 150
reflections
intensity variation: average 0.6%

Refinement

Refinement on F
Final $R = 0.043$

Extinction correction: analytical

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$$B_{eq} = (8\pi^2/3)\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
(2a)				
O1	0.7142 (3)	0.40012 (9)	0.5845 (5)	3.5 (1)
O2	0.9200 (3)	0.36606 (9)	0.8894 (6)	4.6 (1)
N1	0.3364 (3)	0.41063 (9)	0.4909 (6)	3.2 (1)
C1	0.6716 (4)	0.3684 (1)	0.7698 (7)	3.4 (2)
C2	0.5191 (4)	0.3647 (1)	0.7870 (8)	3.4 (2)
C3	0.4639 (4)	0.3953 (1)	0.6060 (8)	3.2 (2)
C4	0.1874 (4)	0.4034 (1)	0.5390 (8)	3.5 (2)
C5	0.0841 (5)	0.4211 (1)	0.3901 (9)	3.8 (2)
C6	0.1260 (5)	0.4481 (2)	0.1829 (9)	4.2 (2)
C7	0.2714 (5)	0.4576 (1)	0.1389 (9)	3.9 (2)
C8	0.3833 (4)	0.4400 (1)	0.2917 (7)	3.2 (2)
C9	0.5397 (4)	0.4431 (1)	0.2895 (7)	3.2 (2)
C10	0.5823 (4)	0.4152 (1)	0.4856 (7)	3.2 (2)
C11	0.7945 (4)	0.3489 (1)	0.9085 (8)	3.4 (2)
C12	0.7679 (4)	0.3068 (1)	1.0682 (7)	3.1 (2)
C13	0.8534 (5)	0.3027 (2)	1.2799 (8)	3.8 (2)
C14	0.8412 (5)	0.2631 (2)	1.4255 (9)	4.0 (2)
C15	0.7460 (5)	0.2265 (2)	1.3639 (9)	4.3 (2)
C16	0.6623 (5)	0.2295 (1)	1.1539 (9)	4.1 (2)
C17	0.6731 (5)	0.2695 (1)	1.0092 (8)	3.6 (2)
C18	0.6325 (6)	0.4715 (2)	0.1159 (10)	4.2 (2)
(2b)				
O1	0.4187 (2)	0.2041 (1)	0.1320 (1)	3.23 (8)
O2	0.5903 (3)	0.2738 (1)	0.3006 (1)	4.7 (1)
N1	0.2608 (3)	-0.0031 (1)	0.0128 (1)	2.62 (9)
C1	0.4831 (3)	0.1401 (2)	0.2076 (2)	3.0 (1)
C2	0.4411 (3)	0.0465 (2)	0.1827 (2)	2.9 (1)
C3	0.3489 (3)	0.0508 (2)	0.0879 (2)	2.7 (1)
C4	0.2342 (4)	-0.1008 (2)	0.0001 (2)	3.1 (1)
C5	0.1367 (4)	-0.1314 (2)	-0.0828 (2)	3.5 (1)
C6	0.0611 (3)	-0.0660 (2)	-0.1553 (2)	3.3 (1)
C7	0.0873 (3)	0.0305 (2)	-0.1442 (2)	2.8 (1)
C8	0.1925 (3)	0.0635 (2)	-0.0593 (2)	2.6 (1)
C9	0.2371 (3)	0.1577 (2)	-0.0323 (2)	2.8 (1)
C10	0.3354 (3)	0.1469 (2)	0.0598 (2)	2.8 (1)
C11	0.5738 (3)	0.1853 (2)	0.2948 (2)	3.2 (1)
C12	0.6388 (3)	0.1229 (2)	0.3813 (2)	3.0 (1)
C13	0.7193 (4)	0.0343 (2)	0.3722 (2)	3.7 (1)
C14	0.7742 (4)	-0.0199 (2)	0.4555 (2)	4.3 (1)
C15	0.7479 (4)	0.0133 (2)	0.5486 (2)	4.3 (2)
C16	0.6713 (4)	0.1014 (2)	0.5590 (2)	4.0 (1)
C17	0.6179 (4)	0.1560 (2)	0.4758 (2)	3.4 (1)
C18	0.1719 (5)	0.2385 (2)	-0.1009 (2)	3.9 (1)
C19	0.1310 (5)	0.1983 (2)	-0.2069 (2)	4.6 (2)
C20	0.0137 (4)	0.1099 (2)	-0.2130 (2)	3.7 (1)

Table 2. *Geometric parameters* (Å, °)

	(2a)	(2b)
O1—C1	1.407 (4)	1.403 (3)
O1—C10	1.372 (4)	1.364 (3)
O2—C11	1.231 (4)	1.234 (3)
N1—C3	1.379 (5)	1.379 (3)
N1—C4	1.381 (5)	1.377 (3)
N1—C8	1.436 (5)	1.402 (3)
C1—C2	1.378 (5)	1.370 (4)
C1—C11	1.450 (5)	1.447 (3)
C2—C3	1.404 (6)	1.398 (3)

C3—C10	1.373 (5)	1.384 (3)
C4—C5	1.335 (6)	1.350 (4)
C5—C6	1.421 (6)	1.414 (4)
C6—C7	1.356 (6)	1.357 (4)
C7—C8	1.402 (6)	1.410 (3)
C7—C20	—	1.511 (4)
C8—C9	1.408 (5)	1.389 (3)
C9—C10	1.388 (5)	1.394 (3)
C9—C18	1.498 (6)	1.504 (4)
C11—C12	1.490 (5)	1.496 (4)
C12—C13	1.404 (6)	1.391 (4)
C12—C17	1.383 (5)	1.389 (4)
C13—C14	1.373 (6)	1.382 (4)
C14—C15	1.377 (6)	1.383 (4)
C15—C16	1.384 (6)	1.374 (4)
C16—C17	1.380 (6)	1.380 (4)
C18—C19	—	1.539 (4)
C19—C20	—	1.527(4)
C1—O1—C10	104.3 (3)	104.8 (2)
C3—N1—C4	132.2 (4)	132.8 (2)
C3—N1—C8	106.7 (3)	105.9 (2)
C4—N1—C8	121.0 (3)	121.3 (2)
O1—C1—C2	111.6 (3)	111.3 (2)
O1—C1—C11	114.4 (3)	115.0 (2)
C2—C1—C11	133.9 (4)	133.7(2)
C1—C2—C3	104.9 (4)	105.6(2)
N1—C3—C2	144.2 (4)	144.4 (2)
N1—C3—C10	107.1 (3)	107.6 (2)
C2—C3—C10	108.5 (3)	108.0 (2)
N1—C4—C5	120.1 (4)	118.3 (2)
C4—C5—C6	120.6 (4)	121.7 (3)
C5—C6—C7	120.3 (4)	120.6 (2)
C6—C7—C28	121.0 (4)	118.3 (2)
C6—C7—C20	—	127.4 (2)
C8—C7—C20	—	114.2 (2)
N1—C8—C7	116.8 (3)	119.6 (2)
N1—C8—C9	109.5 (4)	111.8 (2)
C7—C8—C9	133.6 (4)	128.6 (2)
C8—C9—C10	103.6 (4)	103.2 (2)
C8—C9—C18	126.4 (4)	118.7 (2)
C10—C9—C18	130.0 (4)	138.1 (2)
O1—C10—C3	110.7 (3)	110.3 (2)
O1—C10—C9	136.2 (4)	138.2 (2)
C3—C10—C9	113.0 (3)	111.5 (2)
O2—C11—C1	120.4 (4)	121.3 (2)
O2—C11—C12	120.4 (4)	120.0 (2)
C1—C11—C12	119.2 (3)	118.6 (2)
C11—C12—C13	117.9 (3)	123.7 (2)
C11—C12—C17	123.6 (4)	117.8 (3)
C13—C12—C17	118.2 (4)	118.5 (3)
C12—C13—C14	120.5 (4)	120.5 (3)
C13—C14—C15	120.4 (4)	119.9 (3)
C14—C15—C16	119.9 (4)	120.2 (3)
C15—C16—C17	119.7 (4)	119.8 (3)
C12—C17—C16	121.2 (4)	121.0 (3)
C9—C18—C19	—	109.1 (2)
C18—C19—C20	—	113.3 (3)
C7—C20—C19	—	111.6 (2)

Table 3. *Comparison of ring planarity in (2a) and (2b) as represented by χ^2 values*

	Pyridine	Pyrrole	Furan	Indolizine	Phenyl
(2a)	159.4	9.9	21.0	425.5	7.3
(2b)	114.1	15.1	20.0	385.4	40.6

Azimuthal scans of several reflections indicated that there was no need to correct for absorption for either compound. In both cases, the H atoms were located from a difference Fourier map and refined isotropically. The structures were solved by direct methods (*MITHRIL*; Gilmore, 1984), utilizing the *TEXSAN* system (Molecular Structure Corporation, 1985).

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Quinine Model Study: Stereospecific Aldol Condensation/Reduction

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Abstract

The racemate *rel*-(1*R*,2*R*,α*S*)-3-acetoxy-2-(α-acetoxy-4-quinolinemethyl)-1-azabicyclo[2.2.2]octane is obtained as the exclusive product in the condensation/reduction reaction sequence. The 1-azabicyclo[2.2.2.]octane moiety is twisted away from the ideal eclipsed geometry.