S1—C8—C9—C10	−177.6 (2)	S1—C8—C9—C10	−179.3 (2)
C7—C8—C9—C10	−62.4 (3)	C7—C8—C9—C10	−63.2 (3)
C11—C8—C9—C10	62.9 (4)	C11—C8—C9—C10	62.8 (4)
S1—C8—C11—O1	−107.5 (3)	S1—C8—C11—O1	−104.8 (3)
S1—C8—C11—C12	70.2 (3)	S1—C8—C11—C12	72.9 (3)
C7—C8—C11—O1	137.6 (3)	C7—C8—C11—O1	140.7 (3)
C7—C8—C11—C12	−44.6 (4)	C7—C8—C11—C12	−41.6 (4)
C9—C8—C11—O1	15.3 (4)	C9—C8—C11—O1	17.3 (4)
C9—C8—C11—C12	−167.0 (3)	C9—C8—C11—C12	−165.0 (3)

Reflections were measured for whole space to determine the absolute configuration. The structure was refined for two configurations: R = 0.054 and wR = 0.072 for the R modification; R = 0.043 and wR = 0.056 for the S modification. The absolute configuration was assigned from the enantiomeric structure which refined with the lower R value.

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71094 (26 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AS1040]

References

Adachi, A., Masuya, K., Tanino, K. & Kuwajima, I. (1993). In preparation.

Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Molecular Structure Corporation (1985). *TEXSAN. TEXRAY Structure Analysis Package*. MSC, 3200A Research Forest Drive, The Woodlands, TX 77381, USA.

Sheldrick, G. M. (1986). *SHELXS86*. Program for the solution of crystal structures. Univ. of Göttingen, Germany.

Tanino, K., Shoda, H., Nakamura, T. & Kuwajima, I. (1992). *Tetrahedron Lett.* **33**, 1337-1340.

Acta Cryst. (1993). **C49**, 1511-1514

Structures of α-Phenyl-amino-stilbene Derivatives

Eriko Chiba

Research and Development Center, Ricoh Company Ltd, 16-1 Shin'ei-Cho, Kouhoku-ku, Yokohama, Kanagawa 223, Japan

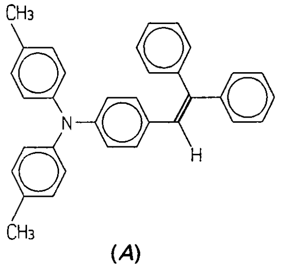
(*Received* 1 *December* 1992; *accepted* 22 *February* 1993)

Abstract

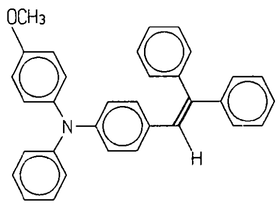
The crystal structures of two α-phenyl-amino-stilbene derivatives have been determined: (*A*) α-phenyl-4′-[bis(4-methylphenyl)amino]stilbene; (*B*) α-phenyl-4′-[(4-methoxyphenyl)phenylamino]stilbene. Compound (*A*) consists of two crystallographically independent molecules *A* and *A*′. The geometrical difference between molecules *A* and *A*′ lies mainly in the distortion between the two benzene rings of the *trans*-stilbene moiety. The *trans*-stilbene moiety in compound (*B*) is approximately planar, while those in the molecules *A* and *A*′ are not. Nevertheless, the planarity of the molecules *A* and *A*′, as a whole, is better than that of compound (*B*). The molecules in (*A*) are arranged on the *ac* plane in such a way that the directions of the *trans*-stilbene moiety are almost parallel and are stacked along the *b* axis. Planes of the *trans*-stilbene moiety in (*B*) are parallel; the anisole-group planes are nearly perpendicular to these planes.

Comment

The structures of the title compounds were determined as part of studies on charge-transport materials. The C(8)—C(31) and C(8)—C(41) bond lengths observed in these compounds are longer than the corresponding distances in *trans*-bis(4-dimethylaminonaphthalene-1-azo)-4,4′-stilbene [1.458 (3) Å (Foitzik, Paulus, Haase & Loub, 1991)]. The angle C(4)—C(7)—C(8) is larger and the angles C(7)—C(8)—C(31) and C(7)—C(8)—C(41) are smaller than the corresponding angles in *trans*-bis(4-dimethylaminonaphthalene-1-azo)-4,4′-stilbene [127.1 (2), 127.5 (2)° (Foitzik, Paulus, Haase & Loub, 1991)]. They are the result of the repulsion between the two phenyl groups bonded to the α-C atom.



(*A*)



(*B*)

The dihedral angle between the two *trans*-stilbene benzene rings in (*B*) [25.0 (2)°] is much smaller than those in (*A*) [60.1 (2) and 77.0 (2)° in molecules *A* and *A*′, respectively]. Therefore, the *trans*-stilbene moiety in (*B*) is approximately planar, while those in (*A*) are not. The plane N(1)-C(1)-C(11)-C(21) and the plane C(7)-C(8)-C(31)-C(41) in molecules *A* and *A*′ of compound (*A*) are inclined in the same direction with respect to the plane formed by the C(1)-C(6) ring; but those in (*B*) are inclined in the opposite direction. The dihedral angles between the plane N(1)-C(1)-C(11)-C(21) and the plane C(7)-C(8)-C(31)-C(41) in molecules *A* and *A*′ are small [10.2 (3) and 2.9 (3)°, respectively], while that in (*B*) is as large

Acta Crystallographica Section C
ISSN 0108-2701 ©1993

as 75.6 (2)°. Therefore, the planarity of the molecules in (*A*), as a whole, is better than that in (*B*).

No intermolecular distances shorter than the sum of the van der Waals radii were observed.

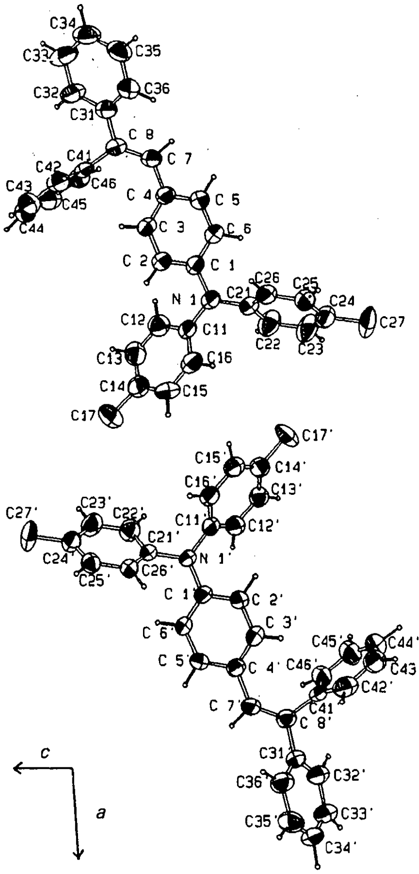


Fig. 1. *ORTEP*II (Johnson, 1976) view down the *b* axis of molecules *A* and *A'* in (*A*), showing the atom-numbering scheme. H atoms are represented by spheres of arbitary size (except the 12 H atoms bonded to the methyl C atoms which are omitted).

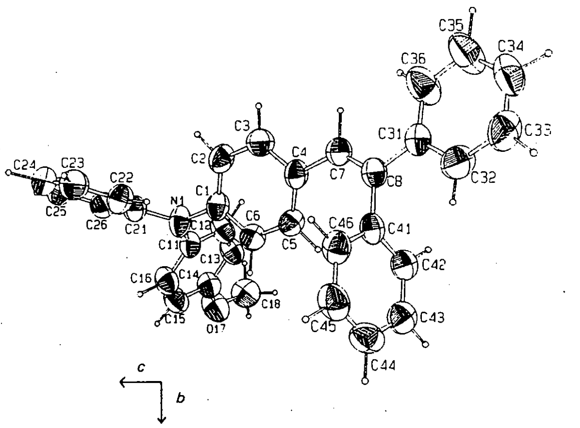


Fig. 2. *ORTEP*II (Johnson, 1976) view down the *a* axis of a molecule of (*B*), showing the atom-numbering scheme. H atoms are represented by spheres of arbitary size.

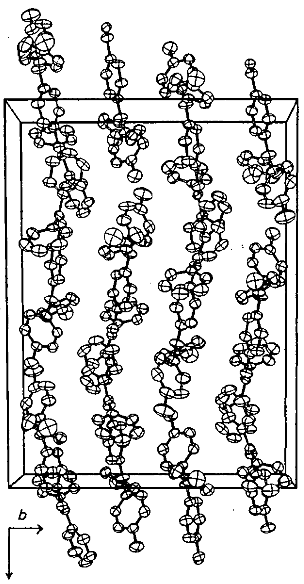


Fig. 3. The packing of molecules in (*A*) viewed down the *c* axis.

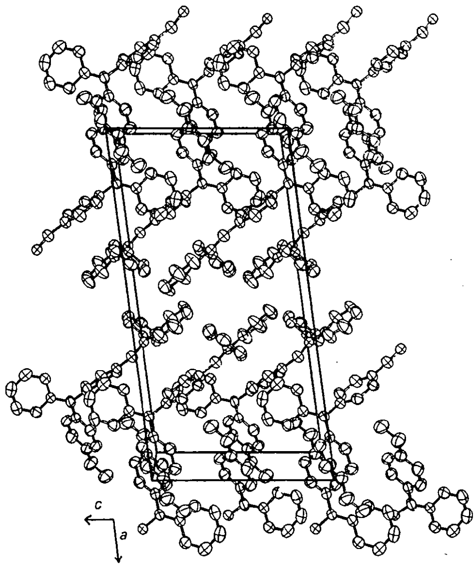


Fig. 4. The packing of molecules in (*B*) viewed down the *b* axis.

Experimental

Compound (*A*)

Crystal data

$C_{34}H_{29}N$
$M_r = 451.6$
Monoclinic
$P2_1/n$
$a = 25.126\ (4)$ Å
$b = 18.960\ (2)$ Å
$c = 11.014\ (2)$ Å
$\beta = 94.22\ (1)°$

Cu $K\alpha$ radiation
$\lambda = 1.5418$ Å
Cell parameters from 20 reflections
$\theta = 18.5\text{–}30.0°$
$\mu = 0.466\ \text{mm}^{-1}$
$T = 296$ K
Plate
$0.51 \times 0.35 \times 0.10$ mm

V = 5232.3 (14) Å^3
Z = 8
D_x = 1.146 Mg m^{-3}

Pale yellow
Crystal source: from methanol solution

Data collection

Mac Science MXC^3 four-circle diffractometer
ω-2θ scans of speed 4° min^{-1} and ω-scan width (1.31 + 0.5tanθ)°
Absorption correction: none
9830 measured reflections
9830 independent reflections

5469 observed reflections [$F_o > 3\sigma(F_o)$]
$\theta_{\max}$ = 65.0°
$h = -28 \rightarrow 28$
$k = 0 \rightarrow 21$
$l = 0 \rightarrow 12$
3 standard reflections monitored every 100 reflections intensity variation: ±3.1%

Refinement

Refinement on F
Final R = 0.079
wR = 0.076
S = 2.29
5469 reflections
815 parameters
46 H atoms refined
Unit weights applied

$(\Delta/\sigma)_{\max}$ = 0.31
$\Delta\rho_{\max}$ = 0.192 e Å^{-3}
$\Delta\rho_{\min}$ = −0.038 e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.3.1)

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

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

	x	y	z	$U_{\rm eq}$
N(1)	0.6240 (2)	0.5867 (3)	0.6240 (4)	0.067 (3)
C(1)	0.5732 (2)	0.6026 (3)	0.6664 (5)	0.053 (3)
C(2)	0.5688 (2)	0.6370 (3)	0.7760 (5)	0.053 (3)
C(3)	0.5187 (2)	0.6516 (3)	0.8157 (5)	0.053 (3)
C(4)	0.4720 (2)	0.6342 (3)	0.7475 (5)	0.051 (3)
C(5)	0.4773 (2)	0.6011 (3)	0.6357 (5)	0.058 (3)
C(6)	0.5271 (2)	0.5848 (3)	0.5956 (5)	0.061 (4)
C(7)	0.4185 (2)	0.6523 (3)	0.7834 (5)	0.056 (3)
C(8)	0.4017 (2)	0.6593 (3)	0.8960 (5)	0.049 (3)
C(11)	0.6680 (2)	0.5740 (3)	0.7085 (5)	0.055 (3)
C(12)	0.6631 (3)	0.5278 (3)	0.8041 (6)	0.065 (4)
C(13)	0.7052 (3)	0.5171 (3)	0.8908 (6)	0.070 (4)
C(14)	0.7531 (3)	0.5516 (4)	0.8862 (6)	0.079 (5)
C(15)	0.7576 (3)	0.5970 (5)	0.7895 (7)	0.093 (6)
C(16)	0.7162 (3)	0.6082 (4)	0.7019 (6)	0.075 (4)
C(17)	0.7987 (3)	0.5414 (5)	0.9865 (7)	0.114 (6)
C(21)	0.6322 (2)	0.5975 (3)	0.4982 (5)	0.055 (3)
C(22)	0.6578 (3)	0.5471 (4)	0.4340 (6)	0.084 (5)
C(23)	0.6648 (3)	0.5588 (4)	0.3098 (6)	0.092 (5)
C(24)	0.6476 (3)	0.6200 (4)	0.2521 (6)	0.072 (4)
C(25)	0.6232 (2)	0.6707 (3)	0.3183 (5)	0.059 (4)
C(26)	0.6154 (2)	0.6596 (3)	0.4410 (5)	0.057 (3)
C(27)	0.6543 (3)	0.6330 (5)	0.1155 (6)	0.113 (6)
C(31)	0.3475 (2)	0.6857 (3)	0.9167 (5)	0.053 (3)
C(32)	0.3202 (2)	0.7314 (4)	0.8377 (6)	0.068 (4)
C(33)	0.2694 (3)	0.7543 (4)	0.8574 (7)	0.074 (4)
C(34)	0.2453 (3)	0.7336 (4)	0.9587 (8)	0.085 (5)
C(35)	0.2725 (3)	0.6911 (5)	1.0402 (8)	0.091 (5)
C(36)	0.3236 (2)	0.6672 (4)	1.0217 (6)	0.070 (4)
C(41)	0.4354 (2)	0.6377 (3)	1.0069 (4)	0.045 (3)
C(42)	0.4560 (2)	0.6877 (3)	1.0888 (6)	0.061 (4)
C(43)	0.4873 (3)	0.6673 (5)	1.1914 (6)	0.078 (5)
C(44)	0.4976 (3)	0.5977 (5)	1.2142 (6)	0.079 (5)
C(45)	0.4768 (2)	0.5464 (4)	1.1357 (6)	0.070 (4)
C(46)	0.4456 (2)	0.5666 (3)	1.0311 (5)	0.057 (3)
N(1)′	0.9985 (2)	0.6191 (3)	0.7596 (4)	0.058 (3)
C(1)′	1.0490 (2)	0.6304 (3)	0.7162 (4)	0.047 (3)
C(2)′	1.0538 (2)	0.6559 (3)	0.5994 (5)	0.052 (3)
C(3)′	1.1038 (2)	0.6665 (3)	0.5559 (5)	0.053 (3)
C(4)′	1.1508 (2)	0.6526 (3)	0.6253 (5)	0.050 (3)
C(5)′	1.1449 (2)	0.6281 (3)	0.7436 (5)	0.055 (3)
C(6)′	1.0957 (2)	0.6167 (3)	0.7879 (5)	0.055 (3)
C(7)′	1.2044 (2)	0.6637 (3)	0.5855 (5)	0.055 (3)
C(8)′	1.2213 (2)	0.6638 (3)	0.4738 (5)	0.048 (3)
C(11)′	0.9538 (2)	0.6040 (3)	0.6764 (4)	0.047 (3)
C(12)′	0.9563 (2)	0.5478 (3)	0.5960 (5)	0.056 (3)
C(13)′	0.9146 (2)	0.5354 (3)	0.5100 (5)	0.055 (3)
C(14)′	0.8694 (2)	0.5766 (3)	0.5017 (5)	0.053 (3)
C(15)′	0.8666 (2)	0.6316 (3)	0.5863 (5)	0.057 (3)
C(16)′	0.9080 (2)	0.6444 (3)	0.6735 (5)	0.051 (3)
C(17)′	0.8233 (2)	0.5632 (4)	0.4045 (6)	0.080 (4)
C(21)′	0.9904 (2)	0.6274 (3)	0.8868 (4)	0.046 (3)
C(22)′	0.9625 (2)	0.5766 (3)	0.9462 (5)	0.059 (3)
C(23)′	0.9549 (2)	0.5852 (3)	1.0698 (5)	0.064 (4)
C(24)′	0.9745 (2)	0.6437 (3)	1.1343 (5)	0.056 (3)
C(25)′	1.0012 (2)	0.6940 (3)	1.0721 (5)	0.053 (3)
C(26)′	1.0091 (2)	0.6865 (3)	0.9495 (4)	0.047 (3)
C(27)′	0.9668 (3)	0.6524 (4)	1.2709 (5)	0.090 (5)
C(31)′	1.2781 (2)	0.6794 (3)	0.4533 (5)	0.051 (3)
C(32)′	1.3033 (2)	0.7376 (3)	0.5042 (6)	0.067 (4)
C(33)′	1.3570 (3)	0.7500 (4)	0.4844 (7)	0.078 (5)
C(34)′	1.3850 (3)	0.7051 (4)	0.4177 (6)	0.074 (4)
C(35)′	1.3599 (2)	0.6470 (4)	0.3667 (6)	0.076 (4)
C(36)′	1.3064 (2)	0.6345 (4)	0.3817 (6)	0.065 (4)
C(41)′	1.1866 (2)	0.6452 (3)	0.3618 (5)	0.048 (3)
C(42)′	1.1713 (2)	0.6957 (4)	0.2763 (6)	0.069 (4)
C(43)′	1.1370 (3)	0.6752 (5)	0.1743 (7)	0.088 (5)
C(44)′	1.1206 (3)	0.6069 (5)	0.1610 (6)	0.081 (5)
C(45)′	1.1373 (3)	0.5573 (4)	0.2425 (6)	0.080 (5)
C(46)′	1.1700 (2)	0.5757 (3)	0.3435 (5)	0.063 (4)

Table 2. *Geometric parameters* (Å, °) *for compound* (*A*)

N(1)—C(1)	1.421 (7)	N(1)′—C(1)′	1.405 (8)
N(1)—C(11)	1.414 (6)	N(1)′—C(11)′	1.426 (6)
N(1)—C(21)	1.430 (7)	N(1)′—C(21)′	1.438 (6)
C(4)—C(7)	1.469 (8)	C(4)′—C(7)′	1.462 (8)
C(7)—C(8)	1.345 (8)	C(7)′—C(8)′	1.331 (8)
C(8)—C(31)	1.485 (7)	C(8)′—C(31)′	1.491 (9)
C(8)—C(41)	1.491 (7)	C(8)′—C(41)′	1.500 (7)
C(1)—N(1)—C(11)	119.9 (4)	C(1)′—N(1)′—C(11)′	120.0 (4)
C(1)—N(1)—C(21)	119.0 (4)	C(1)′—N(1)′—C(21)′	120.7 (4)
C(11)—N(1)—C(21)	120.0 (4)	C(11)′—N(1)′—C(21)′	119.2 (4)
C(3)—C(4)—C(7)	123.6 (5)	C(3)′—C(4)′—C(7)′	125.1 (5)
C(4)—C(7)—C(8)	128.8 (5)	C(4)′—C(7)′—C(8)′	129.9 (5)
C(7)—C(8)—C(31)	122.0 (4)	C(7)′—C(8)′—C(31)′	121.0 (5)
C(7)—C(8)—C(41)	122.0 (4)	C(7)′—C(8)′—C(41)′	123.7 (5)

Compound (*B*)

Crystal data

$C_{33}H_{27}NO$
M_r = 453.6
Monoclinic
$P2_1/c$
a = 21.595 (5) Å
b = 10.311 (3) Å
c = 11.206 (1) Å
β = 97.44 (3)°
V = 2474.3 (7) Å^3
Z = 4
D_x = 1.217 Mg m^{-3}

Cu $K\alpha$ radiation
λ = 1.5418 Å
Cell parameters from 20 reflections
θ = 8.0-20.0°
μ = 0.526 mm^{-1}
T = 296 K
Needle
0.40 × 0.25 × 0.15 mm
Pale green
Crystal source: from methanol solution

Data collection

Mac Science MXC^3 four-circle diffractometer

2043 observed reflections [$F_o > 3\sigma(F_o)$]

ω-2θ scans of speed 4° min^{-1} and ω-scan width $(1.24 + 0.5\tan\theta)$°
Absorption correction: none
3133 measured reflections
3133 independent reflections
$\theta_{\max} = 50.0°$
$h = -21 \rightarrow 20$
$k = 0 \rightarrow 10$
$l = 0 \rightarrow 11$
3 standard reflections monitored every 100 reflections intensity variation: none

Refinement

Refinement on F
Final $R = 0.053$
$wR = 0.047$
$S = 1.19$
2043 reflections
424 parameters
All H-atom parameters refined
Unit weights applied
$(\Delta/\sigma)_{\max} = 0.316$
$\Delta\rho_{\max} = 0.089$ e Å^{-3}
$\Delta\rho_{\min} = -0.016$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.3.1)

Table 3. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2) *for compound* (*B*)

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

	x	y	z	$U_{\rm eq}$
N(1)	0.1540 (1)	0.0892 (4)	0.5108 (3)	0.061 (2)
C(1)	0.1915 (2)	0.0468 (4)	0.6176 (3)	0.054 (3)
C(2)	0.2102 (2)	−0.0822 (5)	0.6304 (4)	0.063 (3)
C(3)	0.2474 (2)	−0.1212 (5)	0.7340 (4)	0.062 (3)
C(4)	0.2682 (2)	−0.0359 (4)	0.8255 (3)	0.053 (3)
C(5)	0.2474 (2)	0.0924 (4)	0.8128 (4)	0.052 (3)
C(6)	0.2096 (2)	0.1320 (5)	0.7104 (4)	0.055 (3)
C(7)	0.3086 (2)	−0.0900 (4)	0.9297 (4)	0.057 (3)
C(8)	0.3512 (2)	−0.0335 (4)	1.0112 (3)	0.049 (2)
C(11)	0.0973 (2)	0.1566 (4)	0.5239 (3)	0.054 (3)
C(12)	0.0596 (2)	0.1137 (5)	0.6060 (4)	0.064 (3)
C(13)	0.0050 (2)	0.1791 (5)	0.6222 (4)	0.066 (3)
C(14)	−0.0121 (2)	0.2860 (4)	0.5533 (4)	0.063 (3)
C(15)	0.0248 (2)	0.3273 (5)	0.4684 (4)	0.071 (3)
C(16)	0.0794 (2)	0.2633 (5)	0.4559 (4)	0.065 (3)
O(17)	−0.0648 (1)	0.3588 (3)	0.5616 (3)	0.090 (2)
C(18)	−0.1034 (3)	0.3217 (7)	0.6477 (6)	0.090 (4)
C(21)	0.1685 (2)	0.0532 (4)	0.3976 (3)	0.051 (3)
C(22)	0.2305 (2)	0.0287 (4)	0.3810 (4)	0.062 (3)
C(23)	0.2455 (3)	−0.0087 (5)	0.2707 (5)	0.073 (3)
C(24)	0.2003 (3)	−0.0218 (5)	0.1743 (5)	0.077 (4)
C(25)	0.1395 (3)	0.0039 (5)	0.1881 (4)	0.072 (3)
C(26)	0.1237 (2)	0.0417 (4)	0.2982 (4)	0.060 (3)
C(31)	0.3870 (2)	−0.1102 (4)	1.1089 (3)	0.049 (2)
C(32)	0.4306 (2)	−0.0518 (5)	1.1924 (5)	0.082 (3)
C(33)	0.4624 (3)	−0.1206 (7)	1.2873 (5)	0.089 (4)
C(34)	0.4529 (2)	−0.2494 (6)	1.2996 (4)	0.081 (4)
C(35)	0.4117 (3)	−0.3092 (6)	1.2163 (5)	0.103 (4)
C(36)	0.3799 (3)	−0.2406 (6)	1.1226 (5)	0.090 (4)
C(41)	0.3665 (2)	0.1066 (4)	1.0059 (3)	0.048 (2)
C(42)	0.3446 (2)	0.1972 (5)	1.0820 (4)	0.056 (3)
C(43)	0.3596 (2)	0.3261 (5)	1.0758 (4)	0.064 (3)
C(44)	0.3970 (2)	0.3690 (5)	0.9932 (5)	0.069 (3)
C(45)	0.4194 (2)	0.2800 (6)	0.9190 (5)	0.075 (3)
C(46)	0.4046 (2)	0.1512 (5)	0.9248 (4)	0.063 (3)

Table 4. *Geometric parameters* (Å, °) *for compound* (*B*)

N(1)—C(1)	1.425 (5)	C(8)—C(31)	1.484 (5)
N(1)—C(11)	1.430 (5)	C(8)—C(41)	1.484 (6)
N(1)—C(21)	1.396 (5)	C(14)—O(17)	1.376 (6)
C(4)—C(7)	1.473 (5)	O(17)—C(18)	1.409 (8)
C(7)—C(8)	1.343 (5)		
C(1)—N(1)—C(11)	117.6 (3)	C(7)—C(8)—C(31)	121.0 (4)
C(1)—N(1)—C(21)	120.7 (3)	C(7)—C(8)—C(41)	122.1 (4)
C(11)—N(1)—C(21)	121.3 (3)	C(13)—C(14)—O(17)	124.5 (4)
C(3)—C(4)—C(7)	116.7 (4)	C(14)—O(17)—C(18)	117.9 (5)
C(4)—C(7)—C(8)	131.1 (5)		

Locations of H atoms in both compounds were found from difference Fourier maps, but the 12 H atoms bonded to the methyl C atoms C(17), C(27), C(17)′ and C(27)′ in (*A*) could not be located owing to their free rotation. The high R value for compound (*A*) may result from the poor crystal quality and exclusion of the 12 H atoms from the structure-factor calculations.

Data collection: MXC^3 control. Data reduction: Mac Science software. Program(s) used to solve structure: *MULTAN78* (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978). Program(s) used to refine structure: *DS*SYSTEM* (Okada & Koyama, 1991).

The author is grateful to Professors Y. Saito and M. Tokonami (The University of Tokyo) for valuable discussions, as well as Dr K. Tani. Mr K. Okada (Ricoh Company Ltd) is thanked for the modification of his program.

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, complete geometry and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71127 (57 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AS1045]

References

Foitzik, J. K., Paulus, H., Haase, W. & Loub, J. (1991). *Acta Cryst.* C**47**, 1640-1642.

Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Main, P., Hull, S. E., Lessinger, L., Germain, G., Declercq, J.-P. & Woolfson, M. M. (1978). *MULTAN78. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univs. of York, England, and Louvain, Belgium.

Okada, K. & Koyama, H. (1991). *J. Appl. Cryst.* **24**, 1067-1070.

Acta Cryst. (1993). C**49**, 1514–1517

Two Novel Ten-Membered Ring Compounds: 1,2,5,8-Dithiadiazecine-6,7-diones

KENTARO YAMAGUCHI, TAKASHI ITOH, KAZUHIRO NAGATA, MAMIKO OKADA AND AKIO OHSAWA

School of Pharmaceutical Sciences, Showa University, 1-5-8 Hatanodai, Shinagawa-ku, Tokyo 142, Japan

(*Received* 8 *December* 1992; *accepted* 26 *January* 1993)

Abstract

The structures of two new ten-membered ring compounds, 3,4,5,8,9,10-hexamethyl-1,2,5,8-dithiadiazecine-6,7(5*H*,8*H*)-dione (I) and 11,14-dimethyldibenzo[*c*,*i*]-

Acta Crystallographica Section C
ISSN 0108-2701 © 1993