

analogous disulfides with a *trans* S—S—P=S geometry (Buranda, Gallacher & Pinkerton, 1991; Gallacher, 1989; Lawton, 1970; Tkachev, Atovmyan & Shchepinov, 1976; Yadav, Bohra, Mehrotra, Rai & Srivastava, 1983). The S=P—C angle (116.8° average) is larger than the S—P—C angle (106.8° average) for steric reasons (S=P is shorter than S—P). The S=P distance (1.941 Å average) is comparable to that of alkyl-substituted disulfides but longer than that observed for the alkoxy analogs. The S—P distances (2.114 Å average) follow the same trend. The S—S distances (2.056 Å average) are as expected for normal single bonds (Meyer, 1976; Muller & Diemann, 1987) and the valence angles at sulfur are all close to tetrahedral values (106.6° average).

Analysis of the torsion angles of the S=P—S—S—P=S skeleton shows that each end of the molecule has a planar *trans* geometry (S=P—S—S = 179.6° average). Although this may be construed as a simple steric effect, from our studies of disulfide analogs we believe there is also an electronic driving force to obtain planarity of this unit (Buranda, Gallacher & Pinkerton, 1991; Gallacher, 1989). The geometry about the S—S bonds is more in keeping with simple sulfuranes with torsion angles close to 90° (Meyer, 1976; Muller & Diemann, 1987). The conformation of the P—S—S—P unit is similar to that of the *trans* S₅⁻ ion (Meyer, 1976; Muller & Diemann, 1987).

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Structures of Methyl 7-Phenyldibenz[*a,j*]anthracene-14-carboxylate and Methyl 7-Phenylbenzo[1,2-*h*:5,4-*h'*]diquinoline-14-carboxylate: Twisted Aromatic Spacers Containing Bay-Region Esters

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Abstract. C₃₀H₂₀O₂, (1), *M_r* = 412.49, triclinic, *P*1 (*C*₁), *a* = 11.301 (7), *b* = 12.069 (3), *c* =

9.777 (2) Å, α = 96.12 (2), β = 111.59 (4), γ = 114.68 (3)°, *V* = 1072 (2) Å³, *Z* = 2, *D_x* = 1.278 g cm⁻³, λ (Mo *K*α) = 0.71073 Å, μ = 0.73 cm⁻¹, *F*(000) = 432, *T* = 299 K, final *R* = 0.065 for 1231 observed reflections. C₂₈H₁₈N₂O₂, (2), *M_r* = 414.46, monoclinic, *I*2/*a* (*C*_{2h}⁶), *a* = 20.039 (10), *b* =

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11.762 (8), $c = 19.850$ (5) Å, $\beta = 117.61$ (3)°, $V = 4146$ (8) Å³, $Z = 8$, $D_x = 1.328$ g cm⁻³, $\lambda(\text{Mo } K\alpha) = 0.71073$ Å, $\mu = 0.79$ cm⁻¹, $F(000) = 1728$, $T = 298$ K, final $R = 0.048$ for 1924 observed reflections. Aromatic system (1) is highly twisted (43° from end to end) in a helical sense. Half of aromatic system (2) is nearly planar with the ester C atom, whereas the other half is twisted by *ca* 27° for planarity.

Introduction. Rigid spacer units have played an important role in the development of preorganized synthetic receptors as a result of their ability to hold groups in a well defined orientation and with a known separation. For example, we have used the dibenz[*c,h*]acridine chromophore as a spacer in the construction of novel non-macrocyclic receptors which we refer to as molecular tweezers (Zimmerman & VanZyl, 1987; Zimmerman, VanZyl & Hamilton, 1989). In the course of developing similar receptors containing active-site functional groups, one of us reported the synthesis and properties of two new aromatic spacers, (1) and (2), which contain bay-region ester groups (Zimmerman, 1988). Both compounds have been successfully incorporated into

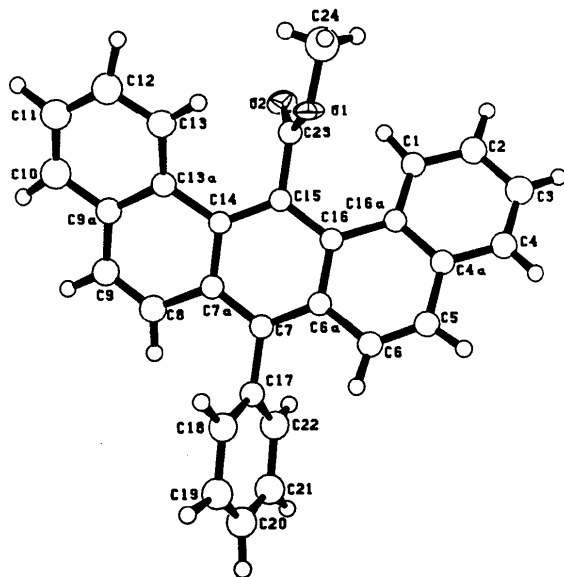


Fig. 1. View of spacer (1) showing atomic numbering.

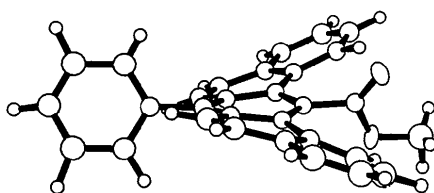


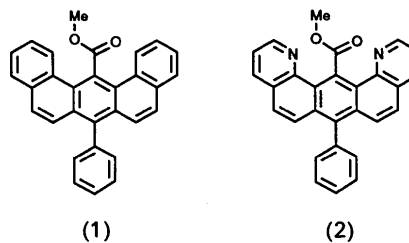
Fig. 2. Side view of spacer (1).

Table 1. *Positional and isotropic thermal parameters* (Å²) for (1)

The O atoms were refined with anisotropic thermal parameters; the equivalent isotropic thermal parameter, U_{eq} , is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U_{iso}(U_{eq})$
O(1)	0.4132 (5)	0.1478 (4)	0.3122 (5)	(0.053)
O(2)	0.3441 (5)	0.0154 (4)	0.4472 (5)	(0.053)
C(1)	0.6660 (9)	0.2646 (7)	0.6472 (8)	0.042 (2)
C(2)	0.8114 (9)	0.2960 (7)	0.7091 (9)	0.051 (2)
C(3)	0.9218 (9)	0.4223 (8)	0.7769 (9)	0.055 (2)
C(4)	0.8850 (9)	0.5161 (7)	0.7883 (8)	0.048 (2)
C(4a)	0.7397 (8)	0.4881 (7)	0.7320 (8)	0.042 (2)
C(5)	0.7042 (9)	0.5879 (7)	0.7578 (8)	0.045 (2)
C(6)	0.5710 (9)	0.5615 (7)	0.7310 (8)	0.043 (2)
C(6a)	0.4491 (8)	0.4315 (6)	0.6553 (8)	0.037 (2)
C(7)	0.3111 (8)	0.4041 (7)	0.6375 (8)	0.040 (2)
C(7a)	0.1899 (8)	0.2836 (6)	0.5459 (8)	0.039 (2)
C(8)	0.0484 (9)	0.2463 (8)	0.5407 (9)	0.053 (2)
C(9)	-0.0688 (9)	0.1322 (8)	0.4506 (9)	0.053 (2)
C(9a)	-0.0631 (9)	0.0497 (7)	0.3441 (8)	0.047 (2)
C(10)	-0.194 (1)	-0.0643 (8)	0.2358 (10)	0.067 (3)
C(11)	-0.193 (1)	-0.1408 (8)	0.1251 (10)	0.067 (3)
C(12)	-0.067 (1)	-0.1106 (8)	0.1108 (10)	0.066 (3)
C(13)	0.0639 (9)	0.0012 (8)	0.2161 (9)	0.057 (2)
C(13a)	0.0696 (8)	0.0788 (7)	0.3376 (8)	0.043 (2)
C(14)	0.2052 (8)	0.1925 (6)	0.4570 (7)	0.036 (2)
C(15)	0.3478 (8)	0.2160 (6)	0.4916 (7)	0.034 (2)
C(16)	0.4727 (8)	0.3333 (6)	0.5971 (7)	0.036 (2)
C(16a)	0.6239 (8)	0.3593 (6)	0.6534 (7)	0.038 (2)
C(17)	0.2930 (8)	0.5028 (6)	0.7194 (8)	0.041 (2)
C(18)	0.2304 (9)	0.5678 (7)	0.6396 (9)	0.055 (2)
C(19)	0.2220 (10)	0.6667 (8)	0.7205 (10)	0.065 (2)
C(20)	0.2770 (9)	0.6978 (8)	0.8782 (10)	0.061 (3)
C(21)	0.3386 (9)	0.6357 (8)	0.9580 (10)	0.063 (2)
C(22)	0.3462 (9)	0.5374 (7)	0.8775 (9)	0.057 (2)
C(23)	0.3673 (8)	0.1150 (7)	0.4183 (8)	0.040 (2)
C(24)	0.441 (1)	0.0578 (9)	0.237 (1)	0.075 (3)

molecular tweezers (Zimmerman & Zeng, 1990; Zimmerman, Zeng, Wu & Reichert, 1990) and herein we report their novel structures.



Experimental. Both compounds (Zimmerman, 1988) were crystallized by slow evaporation from ethyl acetate. Lattice parameters for light-yellow columnar crystal, $0.1 \times 0.1 \times 0.3$ mm, (1), and colorless prismatic crystal, $0.4 \times 0.5 \times 0.6$ mm, (2), were derived by least-squares refinement of 25 automatically centered reflections, 2θ range 16 to 23° (1), 24 to 26° (2); Enraf-Nonius CAD-4 κ -axis diffractometer, graphite crystal monochromator; ω/θ scans, ω -scan angle $1.50[1.00 + 0.35\tan(\theta)]^\circ$ for (1), $1.5[1.20 + 0.35\tan(\theta)]^\circ$ for (2), variable scan speed from 2 to 8° min⁻¹ (1), 3 to 16° min⁻¹ (2); numerical absorption correction (Busing & Levy, 1957) for (2), transmission-factor range 0.972 to 0.952; maximum

Table 2. Selected distances (Å) and angles (°) for (1)

C(1)—C(2)	1.38 (1)	C(2)—C(3)	1.38 (1)
C(3)—C(4)	1.37 (1)	C(4)—C(4a)	1.39 (1)
C(4a)—C(5)	1.45 (1)	C(5)—C(6)	1.32 (1)
C(6)—C(6a)	1.451 (10)	C(6a)—C(7)	1.39 (1)
C(7)—C(7a)	1.397 (9)	C(7a)—C(8)	1.45 (1)
C(8)—C(9)	1.34 (1)	C(9)—C(9a)	1.40 (1)
C(9a)—C(10)	1.43 (1)	C(10)—C(11)	1.35 (1)
C(11)—C(12)	1.38 (1)	C(12)—C(13)	1.41 (1)
C(9a)—C(13a)	1.42 (1)	C(13)—C(13a)	1.40 (1)
C(7a)—C(14)	1.435 (9)	C(13a)—C(14)	1.477 (9)
C(14)—C(15)	1.41 (1)	C(6a)—C(16)	1.424 (10)
C(15)—C(16)	1.418 (9)	C(1)—C(16a)	1.41 (1)
C(4a)—C(16a)	1.423 (9)	C(16)—C(16a)	1.46 (1)
C(7)—C(17)	1.491 (10)	C(17)—C(18)	1.38 (1)
C(18)—C(19)	1.42 (1)	C(19)—C(20)	1.37 (1)
C(20)—C(21)	1.35 (1)	C(17)—C(22)	1.38 (1)
C(21)—C(22)	1.40 (1)	O(1)—C(23)	1.347 (9)
O(2)—C(23)	1.206 (9)	C(15)—C(23)	1.484 (10)
O(1)—C(24)	1.45 (1)		
C(23)—O(1)—C(24)	115.7 (6)	C(2)—C(1)—C(16a)	121.8 (7)
C(1)—C(2)—C(3)	121.0 (8)	C(2)—C(3)—C(4)	118.7 (8)
C(3)—C(4)—C(4a)	122.0 (7)	C(4)—C(4a)—C(5)	120.8 (7)
C(4)—C(4a)—C(16a)	120.2 (7)	C(5)—C(4a)—C(16a)	118.9 (7)
C(4a)—C(5)—C(6)	121.8 (7)	C(5)—C(6)—C(6a)	121.1 (7)
C(6)—C(6a)—C(7)	120.2 (7)	C(6)—C(6a)—C(16)	119.0 (7)
C(7)—C(6a)—C(16)	120.8 (6)	C(6a)—C(7)—C(7a)	120.2 (7)
C(6a)—C(7)—C(17)	119.9 (6)	C(7a)—C(7)—C(17)	119.9 (7)
C(7)—C(7a)—C(8)	121.6 (7)	C(7)—C(7a)—C(14)	119.8 (7)
C(8)—C(7a)—C(14)	118.6 (6)	C(7a)—C(8)—C(9)	121.8 (8)
C(8)—C(9)—C(9a)	120.8 (8)	C(9)—C(9a)—C(10)	119.7 (8)
C(9)—C(9a)—C(13a)	121.4 (7)	C(10)—C(9a)—C(13a)	118.9 (7)
C(9a)—C(10)—C(11)	120.8 (9)	C(10)—C(11)—C(12)	121.4 (9)
C(11)—C(12)—C(13)	119.1 (8)	C(12)—C(13)—C(13a)	121.3 (8)
C(9a)—C(13a)—C(13)	118.3 (7)	C(9a)—C(13a)—C(14)	117.8 (6)
C(13)—C(13a)—C(14)	123.8 (7)	C(7a)—C(14)—C(13a)	117.4 (7)
C(7a)—C(14)—C(15)	118.1 (6)	C(13a)—C(14)—C(15)	124.5 (6)
C(14)—C(15)—C(16)	121.2 (6)	C(14)—C(15)—C(23)	119.3 (6)
C(16)—C(15)—C(23)	119.5 (7)	C(6a)—C(16)—C(15)	117.6 (7)
C(6a)—C(16)—C(16a)	117.8 (6)	C(15)—C(16)—C(16a)	124.5 (6)
C(1)—C(16a)—C(4a)	116.1 (7)	C(1)—C(16a)—C(16)	125.0 (6)
C(4a)—C(16a)—C(16)	118.8 (6)	C(7)—C(17)—C(18)	120.7 (6)
C(7)—C(17)—C(22)	121.0 (7)	C(18)—C(17)—C(22)	188.2 (7)
C(17)—C(18)—C(19)	120.0 (7)	C(18)—C(19)—C(20)	119.5 (8)
C(19)—C(20)—C(21)	121.2 (8)	C(10)—C(21)—C(22)	119.1 (8)
C(17)—C(22)—C(21)	121.9 (8)	O(1)—C(23)—O(2)	123.7 (7)
O(1)—C(23)—C(15)	111.1 (6)	O(2)—C(23)—C(15)	125.3 (7)

$\sin\theta/\lambda$ for (1) = 0.57 \AA^{-1} , for (2) = 0.59 \AA^{-1} ; index range h 0/12, k -13/13, l -11/11 for (1), h 0/23, k -13/0, l -23/23 for $h+k+l=2n$ for (2); three standard reflections monitored, no significant variation; for (1) 3647 reflections measured, 3345 unique, 1231 observed [$I > 2.58\sigma(I)$], $R_{\text{int}} = 0.013$, and for (2) 4228, 3647, 1924, 0.016, respectively.

Initial positions for non-H atoms were determined by direct methods (*SHELXS86*; Sheldrick, 1985); positions for non-H atoms were obtained from subsequent electron density syntheses; positions for H atoms obtained by calculation. Full-matrix least-squares refinement on F (*SHELX76*; Sheldrick, 1976) with $w = k/[(\sigma(F)^2 + (pF)^2)]$, k for (1) = 1.98, for (2) = 1.44, $p = 0.02$, included common isotropic H thermal parameters, isotropic (1) or anisotropic (2) thermal coefficients for C atoms, anisotropic coefficients for the remaining atoms and all positional parameters. Model for (1) converged with $R = 0.065$, $wR = 0.064$, $S = 1.65$, maximum $\Delta\sigma = 0.02$ and range $\Delta\rho = -0.31$ to 0.24 e \AA^{-3} . Model for (2) converged with $R = 0.048$, $wR = 0.056$, $S = 1.79$, maximum $\Delta\sigma = 0.08$ and range $\Delta\rho = -0.19$ to

0.27 e \AA^{-3} . Atom-scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV). Molecular illustrations obtained using *ORTEPII* (Johnson, 1971).*

Discussion. The molecular structure of (1) is shown in Figs. 1 and 2, and atomic coordinates and non-H-atom bond angles and lengths are given in Tables 1 and 2. As a result of unfavorable non-bonded interactions between the ester group and H(1) and H(13), the aromatic system of (1) is highly deformed, exhibiting a marked helical twist in which C(2) and C(12) deviate from the mean plane of dibenzanthracene system by -0.68 and 0.75 \AA , respectively. The aromatic system is twisted *ca* 43° from end to end. However, this is a smaller deformation than that reported for a similarly twisted aromatic system

* Lists of structure factors, anisotropic thermal parameters, complete bond distances and angles, selected mean planes, and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54685 (32 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

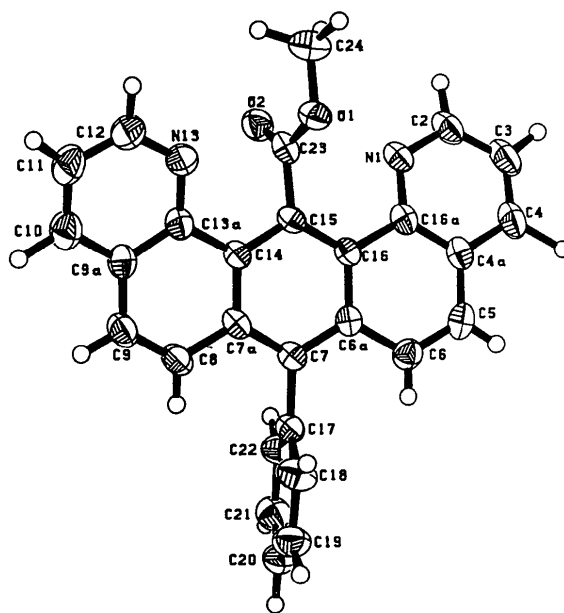


Fig. 3. View of spacer (2) showing atomic numbering.

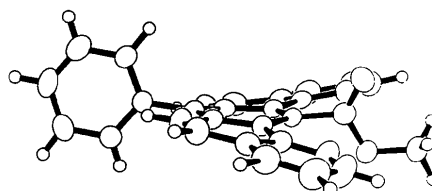


Fig. 4. Side view of spacer (2).

Table 3. *Positional and equivalent isotropic thermal parameters (Å²) for (2)*

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
O(1)	0.2731 (1)	-0.0480 (2)	0.1923 (1)	0.062
O(2)	0.1677 (1)	-0.1414 (2)	0.1728 (1)	0.066
N(1)	0.2642 (1)	-0.0395 (3)	0.3291 (2)	0.058
C(2)	0.3125 (2)	-0.0815 (4)	0.3961 (2)	0.070
C(3)	0.3403 (2)	-0.0184 (5)	0.4625 (2)	0.081
C(4)	0.3157 (2)	0.0903 (4)	0.4610 (2)	0.071
C(4a)	0.2623 (2)	0.1354 (3)	0.3914 (2)	0.056
C(5)	0.2300 (2)	0.2449 (4)	0.3859 (2)	0.066
C(6)	1.1727 (2)	0.2814 (3)	0.3201 (2)	0.060
C(6a)	0.1493 (2)	0.2179 (3)	0.2504 (2)	0.048
C(7)	0.0902 (2)	0.2574 (3)	0.1825 (2)	0.051
C(7a)	0.0749 (2)	0.2036 (3)	0.1142 (2)	0.050
C(8)	0.0138 (2)	0.2426 (4)	0.0434 (2)	0.064
C(9)	-0.0020 (2)	0.1942 (3)	-0.0228 (2)	0.066
C(9a)	0.0451 (2)	0.1077 (3)	-0.0275 (2)	0.059
C(10)	0.0341 (2)	0.0644 (4)	-0.0971 (2)	0.077
C(11)	0.0826 (3)	-0.0147 (4)	-0.0985 (3)	0.091
C(12)	0.1413 (3)	-0.0506 (4)	-0.0302 (3)	0.090
N(13)	0.1532 (2)	-0.0136 (3)	0.0375 (2)	0.073
C(13a)	0.1055 (2)	0.0652 (3)	0.0394 (2)	0.054
C(14)	0.1181 (2)	0.1090 (3)	0.1134 (2)	0.048
C(15)	0.1704 (2)	0.0606 (3)	0.1828 (2)	0.048
C(16)	0.1867 (2)	0.1144 (3)	0.2517 (2)	0.046
C(16a)	0.2397 (2)	0.0687 (3)	0.3257 (2)	0.052
C(17)	0.0418 (2)	0.3552 (3)	0.1823 (2)	0.052
C(18)	0.0528 (2)	0.4641 (4)	0.1652 (2)	0.076
C(19)	0.0048 (2)	0.5511 (4)	0.1622 (2)	0.078
C(20)	-0.0546 (2)	0.5277 (4)	0.1759 (2)	0.072
C(21)	-0.0648 (2)	0.4212 (4)	0.1945 (2)	0.080
C(22)	-0.0174 (2)	0.3342 (3)	0.1976 (2)	0.069
C(23)	0.2028 (2)	-0.0549 (3)	0.1818 (2)	0.055
C(24)	0.3059 (3)	-0.1581 (4)	0.1919 (3)	0.085

Table 4. *Selected distances (Å) and angles (°) for (2)*

N(1)—C(2)	1.326 (5)	C(2)—C(3)	1.384 (6)
C(3)—C(4)	1.366 (7)	C(4)—C(4a)	1.403 (5)
C(4a)—C(5)	1.423 (6)	C(5)—C(6)	1.349 (5)
C(6)—C(6a)	1.446 (5)	C(6a)—C(7)	1.399 (4)
C(7)—C(7a)	1.396 (5)	C(7a)—C(8)	1.445 (5)
C(8)—C(9)	1.330 (5)	C(9)—C(9a)	1.419 (5)
C(9a)—C(10)	1.391 (5)	C(10)—C(11)	1.354 (7)
C(11)—C(12)	1.387 (6)	C(12)—N(13)	1.325 (5)
C(9a)—C(13a)	1.411 (5)	N(13)—C(13a)	1.344 (5)
C(7a)—C(14)	1.415 (4)	C(13a)—C(14)	1.463 (5)
C(14)—C(15)	1.408 (4)	C(6a)—C(16)	1.424 (4)
C(15)—C(16)	1.401 (4)	N(1)—C(16a)	1.355 (5)
C(4a)—C(16a)	1.405 (5)	C(16)—C(16a)	1.457 (4)
C(7)—C(17)	1.503 (5)	C(17)—C(18)	1.369 (5)
C(18)—C(19)	1.388 (6)	C(19)—C(20)	1.365 (6)
C(20)—C(21)	1.348 (7)	C(17)—C(22)	1.376 (5)
C(21)—C(22)	1.377 (6)	O(1)—C(23)	1.327 (4)
O(2)—C(23)	1.202 (5)	C(15)—C(23)	1.510 (5)
O(1)—C(24)	1.454 (5)		
C(23)—O(1)—C(24)	113.2 (3)	C(2)—N(1)—C(16a)	118.7 (3)
N(1)—C(2)—C(3)	122.7 (4)	C(2)—C(3)—C(4)	120.0 (4)
C(3)—C(4)—C(4a)	118.5 (4)	C(4)—C(4a)—C(5)	122.0 (3)
C(4)—C(4a)—C(16a)	118.3 (4)	C(5)—C(4a)—C(16a)	119.6 (3)
C(4a)—C(5)—C(6)	121.0 (3)	C(5)—C(6)—C(6a)	120.9 (3)
C(6)—C(6a)—C(7)	120.3 (3)	C(6)—C(6a)—C(16)	119.4 (3)
C(7)—C(6a)—C(16)	120.3 (3)	C(6a)—C(7)—C(7a)	119.5 (3)
C(6a)—C(7)—C(17)	120.9 (3)	C(7a)—C(7)—C(17)	119.6 (3)
C(7)—C(7a)—C(8)	120.4 (3)	C(7)—C(7a)—C(14)	120.5 (3)
C(8)—C(7a)—C(14)	119.1 (3)	C(7a)—C(8)—C(9)	122.1 (4)
C(8)—C(9)—C(9a)	120.7 (3)	C(9)—C(9a)—C(10)	121.5 (3)
C(9)—C(9a)—C(13a)	120.0 (3)	C(9)—C(9a)—C(13a)	118.5 (3)
C(9a)—C(10)—C(11)	119.1 (4)	C(10)—C(11)—C(12)	118.8 (4)
C(11)—C(12)—N(13)	124.3 (4)	C(12)—N(13)—C(13a)	117.3 (3)
C(9a)—C(13a)—N(13)	122.0 (3)	C(9a)—C(13a)—C(14)	119.6 (3)
N(13)—C(13a)—C(14)	118.5 (3)	C(7a)—C(14)—C(13a)	117.8 (3)
C(7a)—C(14)—C(15)	119.2 (3)	C(13a)—C(14)—C(15)	122.9 (3)
C(14)—C(15)—C(16)	120.3 (3)	C(14)—C(15)—C(23)	118.7 (3)
C(16)—C(15)—C(23)	120.8 (3)	C(6a)—C(16)—C(15)	119.0 (3)
C(6a)—C(16)—C(16a)	117.7 (3)	C(15)—C(16)—C(16a)	123.3 (3)
N(1)—C(16a)—C(4a)	121.6 (3)	N(1)—C(16a)—C(16)	118.3 (3)
C(4a)—C(16a)—C(16)	120.0 (3)	C(7)—C(17)—C(18)	122.6 (3)
C(7)—C(17)—C(22)	118.9 (3)	C(18)—C(17)—C(22)	118.5 (3)
C(17)—C(18)—C(19)	120.8 (4)	C(18)—C(19)—C(20)	119.6 (4)
C(19)—C(20)—C(21)	119.9 (4)	C(20)—C(21)—C(22)	120.9 (4)
C(17)—C(22)—C(21)	120.2 (4)	O(1)—C(23)—O(2)	125.4 (3)
O(1)—C(23)—C(15)	112.1 (3)	O(2)—C(23)—C(15)	122.5 (3)

where a phenyl substituent is attached to two central bay-region C atoms (Pascal, McMillan & van Engen, 1986). The C(2)⋯C(12) distance, which is 7.24 Å in dibenz[*c,h*]acridine (Mason, 1960), has expanded to 8.20 Å in (1) as a result of (a) the twist, (b) increased C(13a)—C(14) and C(16)—C(16a) bond lengths (*ca* 1.47 Å), and (c) decreased C(5)—C(6) and C(8)—C(9) bond lengths (*ca* 1.33 Å). As a result of the *peri* interactions, both the ester and phenyl substituents are twisted from planarity with the aromatic spacer unit by 68 and 111°, respectively.

The molecular structure of (2) is shown in Figs. 3 and 4, and atomic coordinates and non-H-atom bond angles and lengths are given in Tables 3 and 4. The deformations are smaller than in (1). The C(2)⋯C(12) distance is 7.52 Å and the twist is 27° from end to end. As in ester (1), C(2) and C(12) deviate from the mean plane of the aromatic system, in this case by -0.42 and 0.46 Å, respectively. However, it is clear from Fig. 4 that one half of (2) is nearly planar with the ester C atom so that the twist resides almost exclusively in the other half. As in (1) both the ester and phenyl substituents are twisted from planarity with the aromatic spacer unit. The ester and phenyl substituents are twisted by 76 and 99°, respectively. Although both N(1) and N(13) have close contacts with the C(23) of the ester (*ca* 2.60 Å), the ester group appears undistorted and has normal spectroscopic properties (Zimmerman, 1988).

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