Brachtel, G. & Jansen, M. (1981). *Cryst. Struct. Commun.* **10**, 669–672.

Chananont, P., Hamor, T. A. & Martin, I. L. (1980). *Acta Cryst.* B**36**, 898–902.

Codding, P. W., Zeugner, H. & Finner, E. (1987). *Acta Cryst.* C**43**, 1394–1397.

Cromer, D. T. & Mann, J. B. (1968). *Acta Cryst.* A**24**, 321–324.

Gillespie, R. J. (1970). *J. Chem. Educ.* **47**, 18–23.

Gilli, G., Bertolasi, V., Sacerdoti, M. & Borea, P. A. (1978*a*). *Acta Cryst.* B**34**, 2826–2829.

Gilli, G., Bertolasi, V., Sacerdoti, M. & Borea, P. A. (1978*b*). *Acta Cryst.* B**34**, 3793–3795.

Harkema, S., van Hummel, G. J. & Gaymans, R. J. (1980). *Acta Cryst.* B**36**, 3182–3184.

Johnson, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.

Leiserowitz, L. & Tuval, M. (1978). *Acta Cryst.* B**34**, 1230–1247.

Main, P., Fiske, S. J., Hull, S. E., Lessinger, L., Germain, G., Declercq, J.-P. & Woolfson, M. M. (1980). *MULTAN*80. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univs. of York, England, and Louvain, Belgium.

Motherwell, W. D. S. & Clegg, W. (1978). *PLUTO*. Program for plotting molecular and crystal structures. Univ. of Cambridge, England.

Nardelli, M. (1983). *Comput. Chem.* **7**, 95–98.

North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.

Palmer, A. & Brisse, F. (1980). *Acta Cryst.* B**36**, 1447–1452.

Petcher, T. J., Widmer, A., Maetzel, U. & Zeugner, H. (1985). *Acta Cryst.* C**41**, 909–912.

Pineault, C. & Brisse, F. (1983*a*). *Acta Cryst.* C**39**, 1434–1437.

Pineault, C. & Brisse, F. (1983*b*). *Acta Cryst.* C**39**, 1437–1439.

Romer, D., Buscher, H. H., Hill, R. C., Maurer, R., Petcher, T. J., Zeugner, H., Benson, W., Finner, E., Milkowski, W. & Thies, P. W. (1982). *Nature* (*London*), **298**, 759–760.

Singh, J. & Thornton, J. M. (1985). *FEBS Lett.* **191**, 1–6.

Stewart, J. M., Machin, P. A., Dickinson, C. W., Ammon, H. L., Heck, H. & Flack, H. (1976). The *XRAY*76 system. Tech. Rep. TR-446. Computer Science Center, Univ. of Maryland, College Park, Maryland, USA.

Stewart, R. F., Davidson, E. R. & Simpson, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.

Stoe & Co. (1985). *REDU*4. *Data-Reduction Program*. Stoe & Co., Darmstadt, Germany.

Acta Cryst. (1992). C**48**, 512–515

Structures of New DNA Photocleaving Agents: 3,6-Bis(dimethylamino)-10-[6-(4-nitrobenzoyloxy)hexyl]acridinium Chloride (I) and 9-{[6-(4-Nitrobenzoyloxy)hexyl]amino}acridinium Chloride Monohydrate (II)

By R. Kuroda* and M. Shinomiya

Department of Chemistry, College of Arts and Sciences, The University of Tokyo, 3-8-1 *Komaba, Meguro, Tokyo* 153, *Japan*

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Abstract. (I) $C_{30}H_{35}N_4O_4^+.Cl^-$, $M_r = 551.07$, triclinic, $P\bar{1}$, $a = 10.512$ (2), $b = 11.203$ (2), $c = 14.469$ (2) Å, $\alpha = 111.49$ (1), $\beta = 105.74$ (1), $\gamma = 95.82$ (1)°, $V = 1487.4$ (4) Å^3, $Z = 2$, $D_m = 1.23$ (by flotation), $D_x = 1.231$ g cm^{-3}, λ(Cu $K\alpha$) = 1.5418 Å, $\mu = 14.68$ cm^{-1}, $F(000) = 584$, $T = 296$ K, $R = 0.109$ for 3100 unique reflections with $I > 3\sigma(I)$. (II) $C_{26}H_{26}N_3O_4^+.Cl^-.H_2O$, $M_r = 497.98$, triclinic, $P\bar{1}$, $a = 9.4810$ (8), $b = 14.495$ (2), $c = 9.255$ (1) Å, $\alpha = 95.48$ (1), $\beta = 98.17$ (1), $\gamma = 101.78$ (1)°, $V = 1222.3$ (5) Å^3, $Z = 2$, $D_m = 1.35$ (by flotation), $D_x = 1.353$ g cm^{-3}, λ(Cu $K\alpha$) = 1.5418 Å, $\mu = 17.34$ cm^{-1}, $F(000) = 524$, $T = 296$ K, $R = 0.052$ for 3589 unique reflections with $I > 3\sigma(I)$. The diffraction work confirmed the molecular structures of the newly synthesized DNA photocleaving compounds, in which the *p*-nitrophenyl group is nearly coplanar with the acridine moiety in (I), whereas the two planar groups form a dihedral angle of 98.7° in (II). The flexibility of the methylene chain and the substantial stacking ability of the aromatic groups observed may be essential for binding to DNA and reaction with the deoxyribose H atoms.

Introduction. Synthetic agents which interact with DNA, particularly those possessing base sequence selectivity have recently attracted much interest (Dervan, 1986). We have designed and synthesized a new series of DNA photocleaving compounds and studied their interaction with DNA. The compounds consist of a *p*-nitrobenzoyl group which cleaves DNA on UV irradiation, and of an acridine moiety [acridine orange in compound (I), and 9-aminoacridine in (II)] which is a potential intercalator and is essential for the compounds' photocleavage activity (R. Kuroda & M. Shinomiya, to be published). Molecular and crystal structures of (I) and (II) have been determined in order to understand the possible mechanism of the interaction of these compounds with DNA.

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* To whom correspondence should be addressed.

Experimental. Compound (I) was synthesized by reaction of 6-iodohexyl 4-nitrobenzoate with acridine orange, and (II) by reaction of 6-aminohexyl 4-nitrobenzoate hydrochloride with 9-phenoxyacridine. Deep-red column-shaped crystals of (I) were obtained by crystallization from a 1:1 acetone/ethanol solution, and yellow column-shaped crystals of (II) from a 1:1 chloroform/ethanol solution.

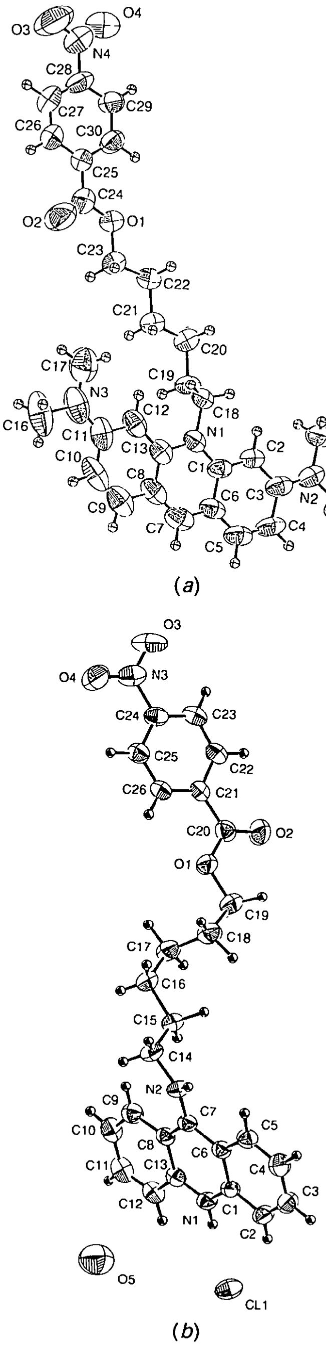

Fig. 1. *ORTEP*II drawing and the atomic numbering scheme of (*a*) compound (I) and (*b*) compound (II).

X-ray photographs for determining the crystal class. A rotating-anode Cu $K\alpha$ source with a graphite monochromator. Intensity data collection for (I) and (II) using a 2θ–ω scan mode on Rigaku AFC-5*R* and Enraf–Nonius CAD-4 diffractometers, respectively. 4990 unique reflections out of 5229 reflections measured with $2\theta < 130.8°$, $0 < h < 12$, $-13 < k < 13$, $-17 < l < 17$, $R_{\rm int} = 0.032$, crystal size $0.20 \times 0.25 \times 0.30$ mm for (I), and 4248 unique reflections out of 4549 reflections measured with $2\theta < 139.7°$, $0 < h < 11$, $-17 < k < 17$, $-10 < l < 10$, $R_{\rm int} = 0.054$, crystal size $0.25 \times 0.25 \times 0.45$ mm for (II). Accurate unit-cell parameters from setting of 25 reflections with $39 < \theta < 40°$ for (I) and $20 < \theta < 30°$ for (II). Lorentz and polarization corrections, but no absorption corrections. Three standard reflections measured after every 150 reflections and after every 2 h of X-ray exposure time for (I) and (II), respectively: no crystal and electronic instability for either compound. Structures solved by direct methods [*MITHRIL* (Gilmore, 1984) for (I), and *MITHRIL* and *DIRDIF* (Beurskens, 1984) for (II)] and refined by full-matrix least squares on *F*. All the H atoms of (I) were located assuming an ideal geometry and their positional and isotropic temperature factors not refined but included in the structure refinements. H atoms of (II), except those of the water molecule, were located from difference Fourier maps and refined with isotropic temperature factors. Atomic scattering factors and the values for $\Delta f'$ and $\Delta f''$ were those of Cromer & Waber (1974) and of Cromer (1974), respectively. $R = 0.0109$, $wR = 0.164$ for (I), and $R = 0.052$, $wR = 0.083$ for (II), $w =$

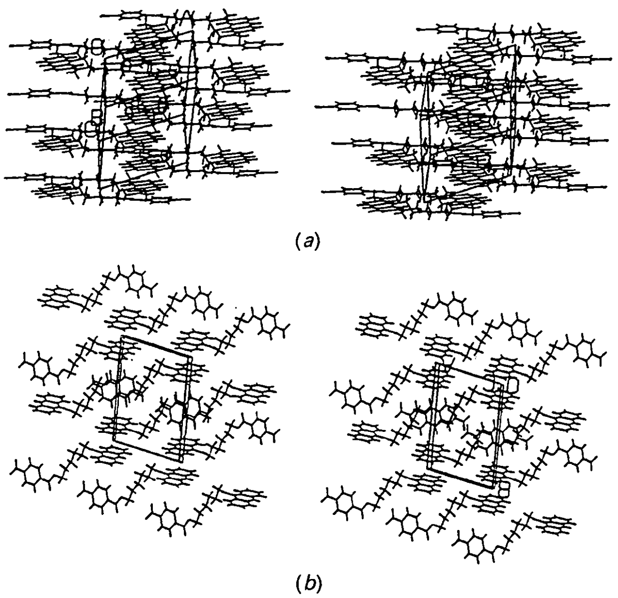

Fig. 2. Stereoview packing diagram for (*a*) compound (I) and (*b*) compound (II).

$4F_o^2/\sigma^2(F_o^2)$. Number of parameters = 370 (I) and 421 (II); goodness of fit = 4.45 (I) and 2.74 (II); $(\Delta/\sigma)_{\max} = 0.01$ (I) and 0.03 (II); $(\Delta\rho)_{\min} = -0.27$ (I) and -0.38 e Å^{-3} (II); $(\Delta\rho)_{\max} = 0.78$ (I) and 0.49 e Å^{-3} (II). The Cl atom in crystal (I) is disordered; the occupancy factors of three sites were fixed with similar $B_{\rm iso}$ values, and not refined. Because of this disorder, the crystal structure of (I) could not be determined accurately. All the computations were carried out using the *TEXSAN* (Molecular Structure Corporation, 1985) program system.

Discussion. Fig. 1 shows *ORTEP*II drawings (Johnson, 1976) of the molecules and the atomic numbering schemes, and Fig. 2 stereoviews of the crystal structures. Table 1 gives the final atomic coordinates and equivalent isotropic thermal parameters for the non-H atoms.* Relevant bond lengths and torsion angles are listed in Table 2. Bond distances and angles are all normal. C(7)—N(2) bond of (II) is as short as 1.331 (3) Å, like the corresponding bond of many other 9-alkylaminoacridines (Glusker, Gallen & Carrell, 1973), consistent with an appreciable degree of double-bond character. In (I), the N(1)—C(18) bond is of single-bond character [1.504 (5) Å], while the N(2)—C(3) and N(3)—C(11) bonds are short. Many acridines are known to be significantly non-planar, and the extent of the deviation increases with the amount of side-chain substitution (Jones & Neidle, 1975). The acridines are nearly planar in both compounds and the two outer rings of an acridine are mutually inclined at only 1.23 (4) and 2.25 (3)° for (I) and (II), respectively.

Both of the structures show a dihedral angle of approximately 9.5° between the plane of the benzene ring and that of its substituent nitro group. This lack of coplanarity has been observed in many similar compounds (Colapietro & Domenicano, 1977). The plane of the ester group is almost coplanar with the benzene ring in (II), while the two average planes form a dihedral angle of 8.2° in (I). This may result from the strong intermolecular interaction between the carbonyl O atom and the adjacent *N*-methyl C atoms [O(2)···C(16) = 2.961 (8) Å] in (I).

The two compounds contain the same *p*-nitrobenzoyloxyhexyl side chain, and only the acridine moieties are different. However, the orientation of the nitrophenyl group with respect to the acridine moiety is very different for the two compounds. In (I), the acridine and the phenyl ring planes are

Table 1. *Fractional atomic coordinates and equivalent isotropic temperature factors* (Å^2) *of non*-H *atoms with e.s.d.'s in parentheses*

$B_{\rm eq} = (8\pi^2/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$. Site occupancy factors for Cl(1), Cl(2) and Cl(3) are 0.48, 0.37 and 0.15, respectively, for (I).

	x	*y*	*z*	$B_{\rm eq}$
(I)				
Cl(1)	1.0106 (3)	0.4560 (4)	−0.9167 (4)	11.9 (1)
Cl(2)	1.0300 (4)	0.1566 (5)	−0.9094 (3)	11.7 (2)
Cl(3)	1.152 (1)	0.341 (1)	−0.8114 (9)	13.0 (4)
O(1)	1.4028 (3)	0.7873 (3)	0.4055 (2)	6.7 (1)
O(2)	1.3976 (4)	0.6653 (5)	0.4945 (4)	13.8 (2)
O(3)	2.0891 (5)	0.7834 (5)	0.6520 (4)	13.8 (2)
O(4)	2.0946 (4)	0.9055 (5)	0.5699 (4)	11.3 (2)
N(1)	0.6285 (3)	0.7114 (3)	0.0619 (3)	5.2 (1)
N(2)	0.5366 (4)	0.9320 (4)	−0.1703 (3)	6.6 (1)
N(3)	0.7236 (5)	0.5058 (4)	0.3040 (3)	8.4 (2)
N(4)	2.0336 (5)	0.8343 (5)	0.5967 (4)	8.6 (2)
C(1)	0.5413 (4)	0.7567 (4)	−0.0006 (3)	5.2 (1)
C(2)	0.5846 (4)	0.8243 (4)	−0.0533 (3)	5.4 (1)
C(3)	0.4935 (4)	0.8673 (4)	−0.1187 (3)	5.7 (1)
C(4)	0.3529 (4)	0.8400 (5)	−0.1282 (4)	6.8 (1)
C(5)	0.3110 (4)	0.7750 (5)	−0.0751 (4)	6.7 (2)
C(6)	0.3999 (4)	0.7322 (4)	−0.0108 (3)	5.9 (1)
C(7)	0.3578 (4)	0.6656 (5)	0.0424 (4)	6.8 (2)
C(8)	0.4467 (5)	0.6257 (4)	0.1087 (4)	6.5 (1)
C(9)	0.4060 (5)	0.5585 (5)	0.1649 (4)	7.4 (2)
C(10)	0.4924 (6)	0.5173 (5)	0.2269 (4)	7.7 (2)
C(11)	0.6349 (6)	0.5456 (4)	0.2409 (4)	7.0 (2)
C(12)	0.6781 (5)	0.6130 (4)	0.1873 (3)	6.3 (1)
C(13)	0.5888 (4)	0.6504 (4)	0.1209 (3)	5.6 (1)
C(14)	0.6786 (5)	0.9598 (5)	−0.1608 (4)	7.7 (2)
C(15)	0.4441 (5)	0.9733 (5)	−0.2414 (4)	8.0 (2)
C(16)	0.6865 (8)	0.4375 (6)	0.3644 (5)	10.5 (3)
C(17)	0.8677 (8)	0.5262 (6)	0.3154 (5)	10.2 (3)
C(18)	0.7755 (4)	0.7325 (4)	0.0701 (3)	5.2 (1)
C(19)	0.8560 (4)	0.8640 (4)	0.1556 (3)	5.8 (1)
C(20)	1.0088 (4)	0.8722 (4)	0.1860 (3)	6.0 (1)
C(21)	1.0591 (4)	0.8070 (5)	0.2579 (4)	6.4 (1)
C(22)	1.2117 (4)	0.8244 (5)	0.2956 (3)	6.3 (1)
C(23)	1.2550 (4)	0.7582 (5)	0.3674 (4)	7.4 (2)
C(24)	1.4594 (5)	0.7324 (5)	0.4680 (4)	7.2 (2)
C(25)	1.6094 (4)	0.7650 (4)	0.5029 (3)	6.1 (1)
C(26)	1.6814 (5)	0.7254 (5)	0.5773 (4)	7.5 (2)
C(27)	1.8201 (5)	0.7485 (5)	0.6078 (4)	7.8 (2)
C(28)	1.8852 (5)	0.8107 (5)	0.5648 (4)	6.5 (1)
C(29)	1.8202 (5)	0.8528 (5)	0.4914 (4)	7.1 (2)
C(30)	1.6785 (5)	0.8278 (5)	0.4597 (4)	6.7 (2)
(II)				
Cl(1)	−0.45703 (6)	0.11898 (6)	−0.71877 (8)	5.76 (3)
O(1)	0.8405 (2)	0.4928 (1)	0.1366 (2)	5.83 (7)
O(2)	0.8776 (3)	0.6479 (1)	0.2072 (3)	7.0 (1)
O(3)	1.4890 (3)	0.6101 (2)	0.6819 (3)	9.0 (1)
O(4)	1.4235 (3)	0.4588 (2)	0.6353 (3)	8.1 (1)
O(5)	−0.6659 (4)	0.0189 (3)	−0.0321 (4)	11.4 (2)
N(1)	−0.1221 (2)	0.1386 (1)	−0.6108 (2)	4.15 (7)
N(2)	0.3191 (2)	0.1529 (2)	−0.4965 (2)	4.32 (7)
N(3)	1.4063 (3)	0.5377 (2)	0.6192 (3)	6.1 (1)
C(1)	−0.0295 (2)	0.1727 (1)	−0.7016 (2)	3.72 (7)
C(2)	−0.0866 (3)	0.1991 (2)	−0.8369 (3)	4.7 (1)
C(3)	0.0044 (3)	0.2339 (2)	−0.9292 (3)	5.1 (1)
C(4)	0.1558 (3)	0.2434 (2)	−0.8911 (3)	5.2 (1)
C(5)	0.2124 (3)	0.2176 (2)	−0.7605 (3)	4.50 (9)
C(6)	0.1220 (2)	0.1811 (1)	−0.6609 (2)	3.59 (7)
C(7)	0.1772 (2)	0.1525 (1)	−0.5215 (2)	3.54 (7)
C(8)	0.0750 (2)	0.1235 (1)	−0.4244 (2)	3.65 (7)
C(9)	0.1113 (2)	0.0970 (2)	−0.2821 (3)	4.7 (1)
C(10)	0.0065 (4)	0.0641 (2)	−0.2016 (3)	5.5 (1)
C(11)	−0.1407 (4)	0.0566 (2)	−0.2558 (3)	5.5 (1)
C(12)	−0.1816 (3)	0.0811 (2)	−0.3902 (3)	4.9 (1)
C(13)	−0.0751 (2)	0.1152 (1)	−0.4764 (3)	3.86 (8)
C(14)	0.4196 (3)	0.1452 (2)	−0.3653 (3)	4.8 (1)
C(15)	0.4566 (3)	0.2357 (2)	−0.2578 (3)	5.0 (1)
C(16)	0.5698 (4)	0.2327 (2)	−0.1244 (4)	6.0 (1)
C(17)	0.6054 (4)	0.3250 (2)	−0.0152 (3)	5.9 (1)
C(18)	0.6822 (4)	0.4085 (3)	−0.0800 (3)	6.3 (1)
C(19)	0.7213 (5)	0.5000 (2)	0.0223 (4)	6.7 (1)
C(20)	0.9118 (3)	0.5733 (2)	0.2174 (3)	4.62 (9)
C(21)	1.0395 (3)	0.5608 (2)	0.3213 (2)	4.06 (8)
C(22)	1.1243 (3)	0.6403 (2)	0.4125 (3)	5.0 (1)
C(23)	1.2451 (3)	0.6343 (2)	0.5090 (3)	5.1 (1)
C(24)	1.2787 (3)	0.5465 (2)	0.5144 (3)	4.70 (9)
C(25)	1.1975 (3)	0.4660 (2)	0.4259 (3)	4.8 (1)
C(26)	1.0770 (3)	0.4737 (2)	0.3292 (3)	4.41 (8)

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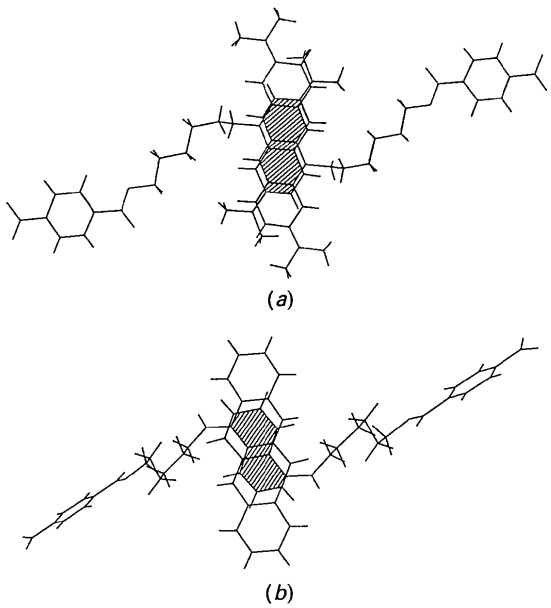
* Lists of structure factors, bond lengths and angles, anisotropic thermal parameters, and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54615 (36 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AS0520]

Table 2. *Selected bond lengths* (Å) *and torsion angles* (°) *with e.s.d.'s in parentheses*

(I)			
N(1)—C(1)	1.378 (5)	N(3)—C(16)	1.454 (8)
N(2)—C(3)	1.343 (6)	O(1)—C(23)	1.458 (5)
N(3)—C(11)	1.351 (7)	N(4)—C(28)	1.467 (6)
C(18)—C(19)	1.504 (5)	N(1)—C(18)	1.504 (5)
O(2)—C(24)	1.177 (6)	N(2)—C(15)	1.454 (6)
N(4)—O(4)	1.206 (7)	N(3)—C(17)	1.464 (9)
N(1)—C(13)	1.389 (6)	O(1)—C(24)	1.318 (6)
N(2)—C(14)	1.452 (6)	N(4)—O(3)	1.206 (7)
C(1)—N(1)—C(18)—C(19)	87.1 (4)	C(13)—N(1)—C(18)—C(19)	−91.0 (4)
N(1)—C(18)—C(19)—C(20)	164.0 (4)	C(18)—C(19)—C(20)—C(21)	−79.5 (5)
C(19)—C(20)—C(21)—C(22)	−175.2 (4)	C(20)—C(21)—C(22)—C(23)	179.5 (4)
O(1)—C(23)—C(22)—C(21)	−176.1 (4)	C(22)—C(23)—O(1)—C(24)	−177.8 (4)
C(23)—O(1)—C(24)—C(25)	179.5 (4)	O(1)—C(24)—C(25)—C(26)	173.2 (4)
O(1)—C(24)—C(25)—C(30)	−10.1 (7)	O(3)—N(4)—C(28)—C(27)	8.0 (7)
O(4)—N(4)—C(28)—C(29)	10.6 (7)		
(II)			
N(1)—C(1)	1.354 (3)	O(1)—C(20)	1.321 (3)
C(7)—C(8)	1.441 (3)	N(3)—O(3)	1.213 (4)
C(19)—O(1)	1.462 (3)	C(6)—C(7)	1.452 (3)
C(24)—N(3)	1.474 (4)	N(2)—C(14)	1.461 (3)
N(1)—C(13)	1.358 (3)	O(2)—C(20)	1.199 (3)
N(2)—C(7)	1.331 (3)	N(3)—O(4)	1.208 (4)
C(6)—C(7)—N(2)—C(14)	167.9 (2)	C(7)—N(2)—C(14)—C(15)	−73.6 (4)
N(2)—C(14)—C(15)—C(16)	−175.9 (3)	C(14)—C(15)—C(16)—C(17)	−179.5 (3)
C(15)—C(16)—C(17)—C(18)	−66.8 (4)	C(16)—C(17)—C(18)—C(19)	−179.2 (3)
O(1)—C(19)—C(18)—C(17)	75.5 (4)	C(18)—C(19)—O(1)—C(20)	165.3 (3)
C(19)—O(1)—C(20)—C(21)	−174.7 (3)	O(1)—C(20)—C(21)—C(22)	179.8 (5)
O(1)—C(20)—C(21)—C(26)	0 (1)	O(3)—N(3)—C(24)—C(23)	−10.3 (4)
O(4)—N(3)—C(24)—C(25)	−8.7 (4)		


(*a*)

(*b*)

Fig. 3. Stacking of acridine rings for (*a*) compound (I) and (*b*) compound (II).

almost coplanar with a dihedral angle of 5.9°, while they are nearly perpendicular to each other in (II) with an angle of 98.7°. These different conformations are achieved by the rotation around the methylene chains: the single bonds along the methylene chain adopt either *gauche* or *trans* conformations (Table 2). The crystal packing is governed mainly by the stacking nature of the aromatic rings. In (II), mutually parallel acridine rings, as a result of the space-group symmetry, stack on top of each other with overlap of two out of three constituent six-membered rings (Figs. 2*b*, 3*b*). The closest distance between the midpoint of the stacked six-membered rings is 3.497 Å. The mutually parallel phenyl rings of the nitrobenzoyl groups in (II) also stack on top of each other with a midpoint distance of 3.721 Å. The chloride ion may form very weak hydrogen bonds with water of crystallization [Cl(1)···O(5) = 3.291 (4), 3.391 (4) Å]. In (I), all the acridine and phenyl rings are almost parallel to each other (Fig. 2*a*). There is substantial stacking of acridine rings similar to (II), with overlap of two six-membered rings (Fig. 3*a*). There are no phenyl–phenyl contacts in (I) and the phenyl rings are surrounded by parallel acridine rings.

On interaction of the compounds with DNA, it is most likely that the acridine moiety intercalates between the base pairs of DNA which are aromatic in nature, and the side chain containing the reactive nitro group may be located in the grooves of DNA. The flexibility of the side chain may allow the nitro group to reach sugar H atoms rather easily, which is required for the subsequent scission of phosphodiester bonds. The stacking nature of the acridine rings as well as the side-chain flexibility observed in the crystal structures may suggest mechanisms for DNA photocleavage by these compounds.

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References

Beurskens, P. T. (1984). *DIRDIF*. Tech. Rep. 1984/1. Crystallography Laboratory, Toernooiveld, 6525 ED Nijmegen, The Netherlands.

Colapietro, M. & Domenicano, A. (1977). *Acta Cryst.* **B33**, 2240–2243.

Cromer, D. T. (1974). *International Tables for X-ray Crystallography*, Vol. IV, p. 148. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Cromer, D. T. & Waber, J. T. (1974). *International Tables for X-ray Crystallography*, Vol. IV, p. 71. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Dervan, P. E. (1986). *Science*, **232**, 464–471.

Gilmore, C. J. (1984). *J. Appl. Cryst.* **17**, 42–46.

Glusker, J. P., Gallen, B. & Carrell, H.-L. (1973). *Acta Cryst.* **B29**, 2000–2006.

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

Jones, A. & Neidle, S. (1975). *Acta Cryst.* **B31**, 1324–1333.

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