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# 9-Chloroacridine

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**Abstract.** $C_{13}H_8NCl$, orthorhombic, $P2_12_12_1$, $a$ = 6·850 (3), $b$ = 11·662 (5), $c$ = 12·705 (5) Å, $D_m$ = 1·40 (1), $D_c$ = 1·393 g cm$^{-3}$ for $Z = 4$. Equi-inclination Weissenberg intensities, scanned with an automatic densitometer. The structure, solved by direct methods, refined to $R$ 0·0577 and $R_w$ 0·0649 for 1653 reflexions. The crystal structure is characterized by partial stacking of the chromophores; these are slightly non-planar.

**Introduction.** As part of a study of the effects of various ring substitutions on the molecular geometry and solid-state packing of the acridines (Achari & Neidle, 1976) the crystal structure of the title compound was determined. Studies of several other acridines substituted only at the 9-position have been reported: 9-amino-acridine hydrochloride monohydrate (Talacki, Carrell & Glusker, 1974), 9-chloromethylacridine hydrochloride (Zacharias & Glusker, 1974), and 2-[3-(9-acridinylamino)propylamino]ethanol (Glusker, Gallen & Carrell, 1973).

Table 1. *Final positional parameters for the non-hydrogen* (×10$^4$) *and for the hydrogen atoms* (×10$^3$)

For H, the atom numbering denotes the atom to which each H is bonded. The *X*–H bond lengths, *r*, (Å) are given. Estimated standard deviations are in parentheses.

| | *x* | *y* | *z* | *r* |
|---|---|---|---|---|
| C(1) | 6119 (5) | 4889 (3) | 2379 (3) | |
| C(2) | 7303 (7) | 4785 (4) | 1505 (4) | |
| C(3) | 6833 (7) | 3998 (4) | 703 (4) | |
| C(4) | 5222 (6) | 3327 (4) | 760 (3) | |
| C(5) | −596 (7) | 2108 (4) | 2478 (4) | |
| C(6) | −1901 (7) | 2163 (4) | 3281 (4) | |
| C(7) | −1610 (7) | 2920 (5) | 4138 (4) | |
| C(8) | −3 (6) | 3605 (4) | 4180 (3) | |
| C(9) | 3101 (5) | 4249 (3) | 3328 (3) | |
| N(10) | 2340 (5) | 2733 (3) | 1643 (3) | |
| C(11) | 3923 (6) | 3405 (3) | 1645 (3) | |
| C(12) | 1414 (6) | 3576 (3) | 3355 (3) | |
| C(13) | 4408 (5) | 4207 (3) | 2476 (3) | |
| C(14) | 1105 (6) | 2824 (3) | 2478 (4) | |
| Cl | 3585 (2) | 5172 (1) | 4376 (1) | |
| H(1) | 618 (6) | 538 (4) | 301 (4) | 0·98 (4) |
| H(2) | 862 (11) | 518 (6) | 144 (7) | 1·02 (7) |
| H(3) | 749 (8) | 387 (4) | 0 (4) | 1·01 (5) |
| H(4) | 485 (8) | 281 (5) | 30 (4) | 0·88 (5) |
| H(5) | −71 (9) | 164 (5) | 192 (5) | 0·91 (5) |
| H(6) | −315 (9) | 169 (5) | 356 (5) | 1·08 (6) |
| H(7) | −250 (9) | 295 (5) | 477 (5) | 1·01 (6) |
| H(8) | 17 (9) | 402 (5) | 468 (6) | 0·81 (6) |

9-Chloroacridine was crystallized from fluorobenzene as light-yellow plates elongated along **a**. Photographs revealed the crystals to be orthorhombic, with systematic absences $h00$: $h = 2n + 1$, $0k0$: $k = 2n + 1$ and $00l$: $l = 2n + 1$, thus determining the space group

Table 2. *Non-hydrogen-atom bond lengths* (Å) *and valence angles* (°)

Estimated standard deviations are in parentheses.

| | | | |
|---|---|---|---|
| C(1)–C(2) | 1·381 (6) | C(8)–C(12) | 1·429 (5) |
| C(1)–C(13) | 1·421 (5) | C(9)–C(12) | 1·397 (5) |
| C(2)–C(3) | 1·409 (7) | C(9)–C(13) | 1·407 (5) |
| C(3)–C(4) | 1·355 (6) | C(9)–Cl | 1·744 (4) |
| C(4)–C(11) | 1·437 (5) | N(10)–C(11) | 1·338 (5) |
| C(5)–C(6) | 1·358 (6) | N(10)–C(14) | 1·362 (5) |
| C(5)–C(14) | 1·433 (5) | C(11)–C(13) | 1·449 (5) |
| C(6)–C(7) | 1·416 (7) | C(12)–C(14) | 1·434 (5) |
| C(7)–C(8) | 1·361 (6) | | |

| | | | |
|---|---|---|---|
| C(2)–C(1)–C(13) | 120·3 (4) | C(4)–C(11)–N(10) | 117·6 (3) |
| C(1)–C(2)–C(3) | 120·3 (4) | C(4)–C(11)–C(13) | 118·0 (3) |
| C(2)–C(3)–C(4) | 121·6 (4) | N(10)–C(11)–C(13) | 124·5 (3) |
| C(3)–C(4)–C(11) | 120·6 (4) | C(8)–C(12)–C(14) | 118·9 (3) |
| C(6)–C(5)–C(14) | 120·5 (3) | C(9)–C(12)–C(14) | 116·6 (3) |
| C(5)–C(6)–C(7) | 120·9 (4) | C(8)–C(12)–C(9) | 124·5 (3) |
| C(6)–C(7)–C(8) | 120·7 (4) | C(1)–C(13)–C(9) | 124·9 (3) |
| C(7)–C(8)–C(12) | 120·5 (4) | C(1)–C(13)–C(11) | 119·2 (3) |
| Cl–C(9)–C(12) | 119·0 (3) | C(9)–C(13)–C(11) | 116·0 (3) |
| Cl–C(9)–C(13) | 119·3 (3) | C(5)–C(14)–C(10) | 117·4 (3) |
| C(12)–C(9)–C(13) | 121·7 (3) | C(10)–C(14)–C(12) | 124·1 (3) |
| C(11)–N(10)–C(14) | 117·1 (3) | C(5)–C(14)–C(12) | 118·5 (3) |

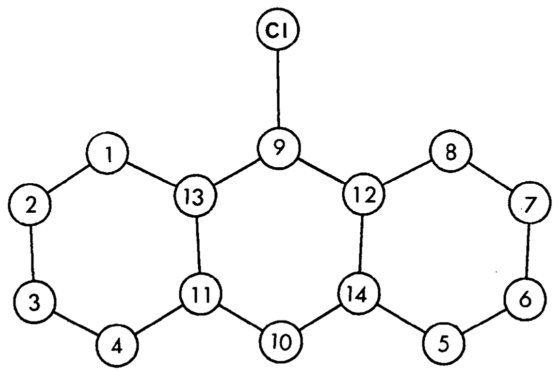

Fig. 1. The numbering scheme.

uniquely to be $P2_12_12_1$. Cell dimensions were obtained from least-squares refinement of $2\theta$ values measured from calibrated Weissenberg photographs. Intensities were collected by the equi-inclination Weissenberg method with multi-film packs. Layers *0kl*–*5kl* and *h0l*–*h10l* were photographed with Ni-filtered Cu *Kα* radiation. The films were scanned by the Science Research Council microdensitometer service with an Optronics P-1000 Photoscan. 1653 unique observed reflexions were obtained after interlayer scaling and merging of equivalent reflexions; the average agreement $R_s$ between multiple measurements of a reflexion was 0·102 ($R_s = \Sigma|\bar{I} - I_i|\,\Sigma I_i$, where $\bar{I}$ is the mean of multiple measurements $I_i$).

The structure was solved by direct methods, and refined by full-matrix least squares; the H atoms were located in a difference synthesis. The refinement converged with anisotropic temperature factors for the nonhydrogen atoms, and isotropic for H. *R* was 0·0577 and $R_w$ was 0·0649. Weights were of the form $w = 1/(\sigma^2|F| + 0{\cdot}001\,F^2)$. Table 1 lists the final positional parameters.*

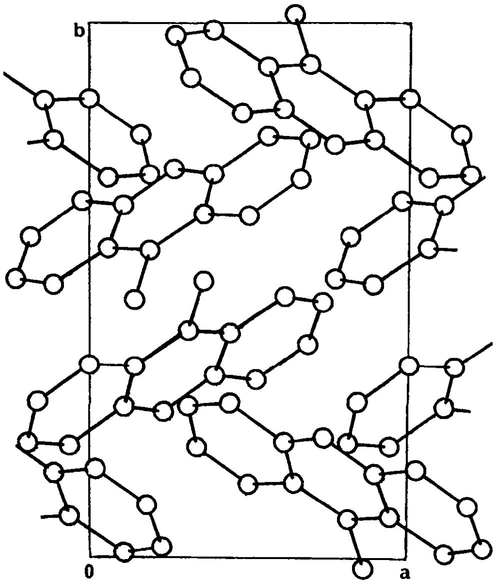

Fig. 2. The *c* axis projection of the crystal structure.

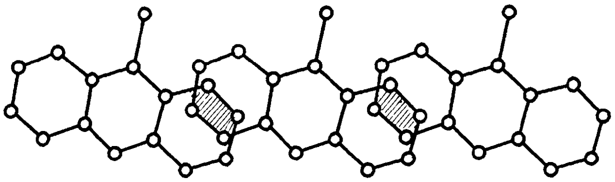

Fig. 3. The stacking of the chromophores in the crystal structure, viewed perpendicular to their planes.

**Discussion.** Fig. 1 shows the numbering scheme. Table 2 gives the bond lengths and angles. The crystal structure does not utilize any potential molecular symmetry [contrast 3,6-diaminoacridine, proflavine, which has crystallographically imposed mirror symmetry (Achari & Neidle, 1976)]. Within the limits of error, the molecule has mirror symmetry along the C(9)–N(10) plane; the differences between C(11)–C(13) and C(12)–C(14), and between N(10)–C(11) and N(10)–C(14) are not significant. A comparison of 9-chloroacridine with related structures shows that the electron-withdrawing Cl substituent has induced a significant shortening of C(9)–C(12) and C(9)–C(13), compared with their lengths in 9-aminoacridine (Talacki, Carrell & Glusker, 1974), and 2-[3-(9-acridinylamino)propylamino]ethanol (Glusker, Gallen & Carrell, 1973). Their average length here is 1·404 Å, as against 1·436 and 1·434 Å, respectively. As has been noted (Jones & Neidle, 1975), many acridines are significantly non-planar, the extent of the deviation increasing with the amount of side-chain substitution. In 9-chloroacridine, the two outer rings are mutually inclined at 1·8°.

The crystal structure is shown in Fig. 2. There is relatively little chromophore stacking: Fig. 3 shows the extent of this 3·51 Å interaction, which contrasts with the extensively stacked structures of many more complex acridines (Glusker, Carrell, Berman & Gallen, 1975).

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32799 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.