

were measured in the manner described for Cb:PMDA (Stezowski, Binder & Karl, 1982). No significant deviations were observed in the intensities of three periodically measured reference reflections. Data were corrected for Lorentz and polarization effects but not for absorption, $\mu = 1 \cdot 10 \text{ cm}^{-1}$.

The initial structural model was determined by direct methods and developed by difference Fourier and least-squares techniques. Refinement was carried out in

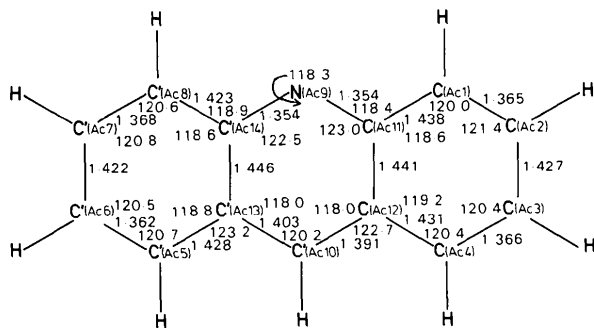


Fig. 1. Bond distances (Å) and bond angles (°) for acridine. E.s.d.'s in bond distances are $<0.003 \text{ Å}$ and in bond angles $<0.2^\circ$.

Table 1. Fractional atomic coordinates and isotropic temperature factors

	x	y	z	U_{eq} or $U(\text{Å}^2)$
C(P1)	-0.0281 (2)	0.3763 (2)	0.0579 (1)	0.01982
C(P2)	-0.1301 (2)	0.4372 (2)	-0.0001 (1)	0.01755
C(P3)	0.1034 (2)	0.4441 (2)	0.05544 (9)	0.01761
C(P4)	-0.2799 (2)	0.3949 (3)	-0.0165 (1)	0.02157
O(P4)	-0.3484 (1)	0.2959 (2)	0.01391 (8)	0.02900
O(P6)	-0.3394 (1)	0.4957 (2)	-0.08040 (7)	0.02256
C(P5)	0.2368 (2)	0.4058 (3)	0.1065 (1)	0.02123
O(P5)	0.2621 (1)	0.3113 (2)	0.16096 (8)	0.02760
N(Ac9)	0.0772 (1)	0.8889 (2)	0.11109 (7)	0.01648
C(Ac11)	-0.0556 (2)	0.8388 (2)	0.11019 (9)	0.01552
C(Ac12)	-0.0973 (2)	0.7324 (2)	0.16918 (9)	0.01623
C(Ac10)	0.0042 (2)	0.6807 (2)	0.22989 (9)	0.01801
C(Ac13)	0.1426 (2)	0.7310 (2)	0.23233 (9)	0.01653
C(Ac14)	0.1749 (2)	0.8369 (2)	0.17036 (9)	0.01529
C(Ac8)	0.3150 (2)	0.8878 (2)	0.1718 (1)	0.01898
C(Ac7)	0.4163 (2)	0.8404 (3)	0.2314 (1)	0.02080
C(Ac6)	0.3840 (2)	0.7395 (3)	0.2931 (1)	0.02161
C(Ac5)	0.2517 (2)	0.6852 (2)	0.2934 (1)	0.02054
C(Ac4)	-0.2396 (2)	0.6827 (3)	0.1628 (1)	0.02042
C(Ac3)	-0.3352 (2)	0.7370 (3)	0.1019 (1)	0.02206
C(Ac2)	-0.2945 (2)	0.8461 (2)	0.0445 (1)	0.01937
C(Ac1)	-0.1597 (2)	0.8951 (2)	0.04758 (9)	0.01819
H(P1)	-0.041 (2)	0.293 (3)	0.095 (1)	0.024 (6)
H(Ac10)	-0.019 (2)	0.604 (3)	0.275 (1)	0.020 (5)
H(Ac8)	0.330 (2)	0.956 (3)	0.127 (1)	0.028 (6)
H(Ac7)	0.525 (3)	0.884 (4)	0.234 (1)	0.046 (8)
H(Ac6)	0.458 (2)	0.710 (3)	0.336 (1)	0.037 (7)
H(Ac5)	0.234 (3)	0.619 (4)	0.338 (2)	0.063 (9)
H(Ac4)	-0.274 (2)	0.606 (3)	0.203 (1)	0.032 (6)
H(Ac3)	-0.424 (3)	0.697 (3)	0.099 (1)	0.044 (7)
H(Ac2)	-0.366 (2)	0.896 (3)	0.005 (1)	0.016 (5)
H(Ac1)	-0.134 (3)	0.999 (3)	0.008 (1)	0.048 (7)

The temperature factor has the form of $\exp(-T)$ where $T = 8\pi^2 U \cdot (\sin^2 \theta / \lambda^2)$ for isotropic atoms. The e.s.d. of the last significant digit is given in parentheses.

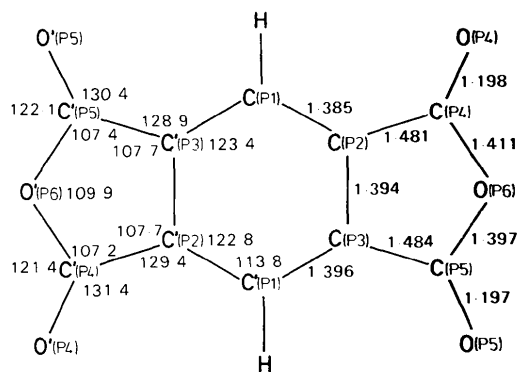


Fig. 2. Bond distances (Å) and bond angles (°) for PMDA. E.s.d.'s in bond distances are $<0.003 \text{ Å}$ and in bond angles $<0.2^\circ$.

a manner similar to that described for Cb:PMDA with the exception of the use of a slightly different weighting scheme: $w = \{\sigma^2(F_o) + 0.012|F_o| + 0.008|F_o|^2 + 0.00005|F_o|^3 + 2 \sin \theta\}^{-1}$. The conventional residuals* are presented in the *Abstract*. Atomic coordinates are contained in Table 1; bond distances and bond angles are displayed in Figs. 1 and 2.

Discussion. The bonding geometry of the PMDA molecule is representative of that found for the uncomplexed molecule (Aravamudhan, Haerberlen, Irngartinger & Krieger, 1979) and for the acceptor in the 1:1 donor-acceptor complexes with donors such as anthracene, A, (Robertson & Stezowski, 1978) and phenazine, Ph, (Karl, Ketterer & Stezowski, 1982). The maximum deviation of an atom from the least-squares mean plane fit to the PMDA molecule is 0.027 Å . The equation of the plane (in the coordinate system described for Cb:PMDA, Stezowski *et al.*, 1982) is: $-0.2874x + 0.7531y + 0.5918z = 2.855$ ($\sigma = 0.017 \text{ Å}$).

Common bonds in the Ac, A, and Ph molecules display very similar bonding geometry. The bond angle C(Ac12)-C(Ac10)-C(Ac13) is about 1° smaller than its analogue in A and the C(Ac11)-N(Ac9)-C(Ac14) angle is about 1° larger than its analogue in Ph. The respective C-C and C-N distances differ by no more than 0.01 Å . The equation for the least-squares plane fit to the Ac molecule is: $-0.2542x + 0.8299y + 0.496z = 6.460$ ($\sigma = 0.016 \text{ Å}$). The Ac molecule displays deviations from planarity (max. 0.025 Å) similar to those observed in the 1:1 PMDA complexes of A, Ph, and Ac (the Ac molecule is centrosymmetrically disordered in the 1:1 complex, Binder *et al.*, 1982).

* Lists of structure factors and anisotropic temperature factors have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36929 (41 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

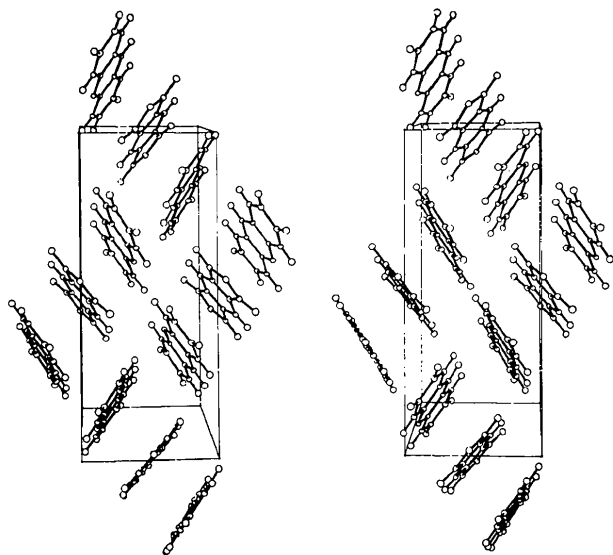


Fig. 3. A stereoscopic projection on the *bc* plane displaying one layer of crystal packing. The tilt of the acridine molecules with respect to the PMDA molecules can be seen clearly.

The 2:1 donor-acceptor complex can be appropriately characterized as a sandwich of one acceptor between two donor molecules, Fig. 3. A schematic drawing of the packing and of the dipole orientations is displayed in Fig. 4. The angle between the plane normals of the donor and acceptor molecules is 7.3° . The average distance of an Ac atom (excluding H atoms) from the plane of the acceptor is 3.434 \AA , which is approximately 0.1 \AA greater than that in the 1:1 complex. The angle between the intrasandwich stack axis (as determined from the coordinates of the molecular centroids neglecting H atoms) and the plane of the acceptor molecule is *ca* 25° .

Space-group symmetry (e.g. the glide reflection operator) generates a second unit of the complex as

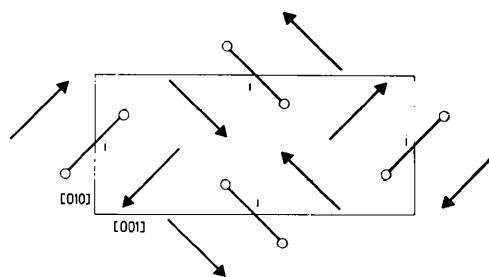


Fig. 4. A schematic drawing of the packing and of the dipole orientations of the donors.

illustrated in Fig. 3. The angle between plane normals of symmetry-related donor molecules is 82.3° , that between symmetry-related acceptor molecules is 67.8° . The angle between the intrasandwich stack axis and the *b* axis (the stack axis in the crystal) is 41° . Remarkably, the $\cdots DADADA \cdots$ sequence, typical for 1:1 complexes with weak charge-transfer interactions in the (electronic) ground state, is reduced to discrete *DAD* units which display little overlap of π -orbitals with neighbouring units.

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2,2,8,9-Tetramethyl-1,2-dihydropurine-6-carboxamide

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Abstract. $C_{10}H_{15}N_5O$, $M_r = 221.26$, monoclinic, $C2/c$, $a = 13.900$ (4), $b = 8.992$ (1), $c = 18.091$ (7) \AA , $\beta = 98.98$ (2) $^\circ$, $V = 2233.5 \text{ \AA}^3$, $Z = 8$, $D_x = 1.32 \text{ Mg m}^{-3}$, $F(000) = 944$, Mo $K\alpha$ radiation, $\lambda = 0.71069 \text{ \AA}$, $\mu =$

0.99 mm^{-1} , $R = 0.037$ for 1243 data with $I > 3\sigma$. The 1,2-dihydropurine ring system approaches planarity except for C(2) where the full ring conjugation found in purines is broken. The carbamoyl group is nearly