1973). There are indeed short intramolecular O(5′)···base contacts in all known structures of cyclic nucleosides with positive charge on the base, *i.e.* 2,2′-anhydro-1-β-D-arabinofuranosylcytosine-3′,5′-diphosphate (Yamagata, Suzuki, Fujii, Fujiwara & Tomita, 1979), 2,2′-anhydro-1-β-D-arabinofuranosyl-5-dimethylsulfonio-6-oxocytosine chloride (Yamagata, Koshibe, Tokuoka, Fujii, Fujiwara, Kanai & Tomita, 1979) and 2,2′-anhydro-1-β-D-arabinofuranosylcytosine hydrochloride (Brennan & Sundaralingam, 1973); and in just one structure with no formal charge: 2,2′-anhydro-1-(3′,5′-di-*O*-acetyl-β-D-arabinofuranosyl)-5-chloro-6-oxocytosine (Yamagata, Koshibe, Tokuoka, Fujii, Fujiwara, Kanai & Tomita, 1979).

The molecules in the crystal of the title compound are connected by a complicated system of hydrogen bonding employing all six H atoms bonded to oxygens, and O(4*A*) [bifurcated hydrogen bonding], O(4*B*), O(3′*B*), N(3*B*) and water as their acceptors. The donor···acceptor distances are between 2·67 and 2·86 Å while the *D*—H···*A* angles are between 162 and 178°. The absence of other than O(4) acceptors in molecule *A* may be related to the intramolecular O(5′*A*)···uracil(*A*) moiety interactions (Fig. 2).

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Structure of the 1/1 Complexes of [2.2.2]Paracyclophanetriene and [2.2]Paracyclophane with Tetracyanoethylene

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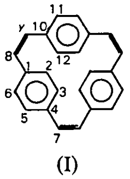
Abstract. $C_{24}H_{18}.C_6N_4$ (I), $M_r = 437·51$, monoclinic, $P2_1/m$, $a = 8·192\ (5)$, $b = 20·579\ (8)$, $c = 6·881\ (3)$ Å, $\beta = 94·70\ (4)°$, $V = 1156$ Å^3, $Z = 2$, $D_x = 1·26$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, $\mu = 0·604$ mm^{-1}, $F(000) = 452$, $T = 153$ K; $C_{16}H_{16}.C_6N_4$ (II), $M_r = 338·60$, triclinic, $P\bar{1}$, $a = 8·079\ (5)$, $b = 8·632\ (4)$, $c = 7·615\ (3)$ Å, $\alpha = 106·80\ (5)$, $\beta = 111·60\ (5)$, $\gamma = 101·00\ (5)°$, $V = 446$ Å^3, $Z = 1$, $D_x = 1·26$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0·066$ mm^{-1}, $F(000) = 176$, $T = 293$ K. The structures were refined to wR values of 0·053 (I) and 0·068 (II) for 869 and 726 observed intensities respectively. In (I), the paracyclophane molecule has a crystallographic mirror plane and a threefold pseudo-axis of symmetry, as was observed in [2.2.2]paracyclophane. In (II), the paracyclophane molecule has a centre of symmetry. In both compounds, the tetracyanoethylene (TCNE) molecules are disordered. The disorder corresponds to two perpendicular, almost coplanar orientations of TCNE with 58–42% in (I) and 93–7% in (II). Each

TCNE lies on a centre of symmetry in a sandwich arrangement between two cyclophane molecules. This leads to 1/1 complexes with the charge-transfer direction along the *b* axis in (I) and along the [111] direction in (II). The structure of (I) is closely related to that of [2.2.2]paracyclophane–TCNE. The structure of (II) is isomorphous to that of [3.3]paracyclophane–TCNE.

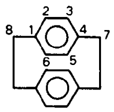
Introduction. This work is part of a series of structural studies on paracyclophanes and their complexes with metal ions or electron-acceptor molecules such as tetracyanoethylene, TCNE (Pierre, Baret, Chautemps & Armand, 1981; Pierre, Baret, Chautemps & Pierre, 1983; Cohen-Addad, Baret, Chautemps & Pierre, 1983).

In the solid state, very few complexes have been investigated (Keehn & Rosenfeld, 1983). The complex [3.3]paracyclophane–TCNE (Bernstein & Trueblood, 1971) presents disordered TCNE molecules in a sandwich-type stacking. More recently, we determined the crystal structure of [2.2.2]paracyclophane and [2.2.2.2]paracyclophane complexes with TCNE (Cohen-Addad, Lebars, Renault & Baret, 1984). The charge transfer observed in these compounds involves only two of the aromatic rings of the paracyclophane molecules and is, therefore, one-dimensional. On the other hand, in [2.2.2]paracyclophanetriene (Trueblood, Mirsky, Maverick, Knobler & Grossenbacher, 1982), the three aromatic rings are linked together through —C=C— double bonds. This makes the molecule more conjugated than [2.2.2]paracyclophane and might strengthen the charge transfer in a complex with TCNE.

So, in order to carry on a study of the structural features related to the charge transfer in these complexes, we have undertaken the structure determination of the following two compounds: (I) [2.2.2]- or [2^3]paracyclophanetriene–TCNE and (II) [2.2]- or [2^2]paracyclophane–TCNE.



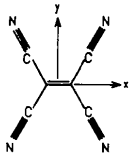
(I)



(II)

Experimental. Synthesis: [2^3]paracyclophanetriene prepared according to a method already described (Cram & Dewhirst, 1959); [2^2]paracyclophane is a commercial product (Aldrich).*

Compound (I): [2^3]paracyclophanetriene–TCNE (1/1), dark red, crystal $0{\cdot}2 \times 0{\cdot}15 \times 0{\cdot}2$mm. Compound (II): [$2^2$]paracyclophane–TCNE (1/1), purple, crystal $0{\cdot}25 \times 0{\cdot}3 \times 0{\cdot}15$ mm. Obtained by slow evaporation at 277 K from a solution of TCNE and paracyclophane in a mixture of dichloromethane and hexane. For compound (I), room-temperature (293 K) and low-temperature (153 K) data collections on an Enraf–Nonius CAD-4 diffractometer, graphite-monochromatized Cu $K\alpha$ radiation, θ–2θ-scan mode, no absorption correction. For compound (II), room-temperature (293 K) measurements with a Nicolet *P3F* diffractometer, graphite-monochromatized Mo $K\alpha$ radiation, ω-scan mode, no absorption correction. Lattice parameters (I and II) refined with 25 reflexions. Number of reflexions with $I \geq 3\sigma(I)$: (I) 869 independent (1980 measured reflexions), $\sin\theta/\lambda < 0{\cdot}56$ Å^{-1}, h $-8 \rightarrow 8$, k $0 \rightarrow 21$, l $0 \rightarrow 7$; (II) 726 independent (1521 measured reflexions), $\sin\theta/\lambda < 0{\cdot}57$ Å^{-1}, h $-9 \rightarrow 8$, k $-9 \rightarrow 8$, l $0 \rightarrow 7$. Standard reflexions: (I) 352, 352 (3% variation); (II) 021, 120, 132 (3% variation). Structures solved with multisolution direct methods (Germain, Main & Woolfson, 1971). For both compounds, from preliminary least-squares refinement minimizing $\sum w|F_o - F_c|^2$ (Busing & Levy, 1962), a Fourier difference map revealed disorder of TCNE. Final rigid-body refinement made with *ORION* (André, Fourme & Renaud, 1971). Following parameters refined: independent positional and anisotropic thermal parameters for paracyclophane atoms, orientation angles, occupancy factors and isotropic thermal parameters for the two TCNE. H positions calculated but not refined. For (II), a final refinement was performed with atoms of the cyclophane and TCNE1 (predominant molecule) treated independently with anisotropic thermal parameters while TCNE2 was kept fixed. For both compounds, TCNE: planar model calculated from TCNE crystal structure (Little, Pautler & Coppens, 1971). A coordinate system *S* is attached to the molecular group and is defined in the following way (see formula): origin, centre of symmetry; *x* axis, C=C double bond; *xy* plane, molecular plane of TCNE.



Position of the group in the cell is given by the crystallographic coordinates u_1, u_2, u_3 of the origin of *S* (not varied) and three orientation angles, θ_1, θ_2, θ_3, *S* being in coincidence with the conventional orthogonal system (*ABC*) related to the cell system (*abc*). Rotations of θ_1 around *A*, then θ_2 around *B*, and θ_3 around *C* bring *S* to its real orientation in the cell. At low temperature, the orientation disorder of TCNE may

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* *Chemical Abstracts* names: (I): tetracyclo[14.2.2.$2^{4,7}$.$2^{10,13}$]-tetracosa-2,4,6,8,10,12,14,16,18,19,21,23-dodecaene–ethenetetracarbonitrile (1/1); (II): tricyclo[8.2.2.$2^{4,7}$]hexadeca-4,6,10,-12,13,15-hexaene–ethenetetracarbonitrile (1/1).

Table 1. *Atomic coordinates* (× 10^4) *and isotropic thermal parameters of* [2^3]*paracyclophanetriene–TCNE* (I) *and* [2^2]*paracyclophane–TCNE* (II)

Standard deviations are within parentheses.

$$B_{eq} = (U_1U_2U_3)^{1/3}.$$

Compound (I)

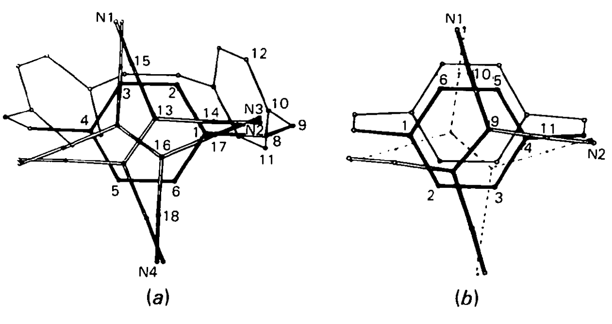
		x	y	z	B_{eq}(Å^2)
	C(1)	2969 (6)	1069 (2)	−1736 (7)	2·5
	C(2)	3175 (6)	1094 (2)	302 (7)	2·7
	C(3)	2080 (6)	1442 (2)	1338 (6)	2·7
	C(4)	750 (6)	1768 (2)	411 (6)	2·4
	C(5)	470 (6)	1695 (2)	−1603 (7)	3·1
	C(6)	1581 (6)	1357 (2)	−2651 (7)	2·8
	C(7)	−320 (6)	2176 (2)	1552 (7)	2·6
	C(8)	4220 (6)	761 (2)	−2926 (7)	3·0
	C(9)	5250 (6)	1097 (2)	−3920 (7)	2·6
	C(10)	5428 (5)	1815 (2)	−3899 (6)	2·3
	C(11)	5540 (5)	2162 (2)	−5624 (6)	2·5
	C(12)	5462 (5)	2163 (2)	−2164 (6)	2·4
TCNE1	C(13)	−670	147	−416	
	C(14)	−1761	510	705	
	C(15)	−1100	116	−2482	
	N(1)	−1485	103	−4121	
	N(2)	−2661	804	1546	
TCNE2	C(16)	147	−121	−872	
	C(17)	1611	−481	−1160	
	C(18)	−985	−37	−2563	
	N(3)	2762	−771	−1450	
	N(4)	−1855	20	−3945	

TCNE1: $\theta_1 = 81{\cdot}9$ (2), $\theta_2 = -25{\cdot}2$ (1), $\theta_3 = -29{\cdot}8$ (2)°
$u_1 = 0, u_2 = 0, u_3 = 0, m = 0{\cdot}58$ (1), $B = 2{\cdot}7$ (2) Å^2
TCNE2: $\theta_1 = 61{\cdot}0$ (2), $\theta_2 = 63{\cdot}2$ (1), $\theta_3 = -55{\cdot}9$ (3)°
$u_1 = 0, u_2 = 0, u_3 = 0, m = 0{\cdot}42, B = 2{\cdot}9$ (2) Å^2

Compound (II)

		x	y	z	B_{eq}(Å^2)
	C(1)	1130 (9)	2214 (7)	−31 (9)	3·2
	C(2)	2548 (8)	1479 (7)	266 (9)	3·7
	C(3)	2942 (8)	691 (7)	1630 (9)	3·4
	C(4)	1948 (8)	645 (7)	2789 (8)	3·2
	C(5)	859 (8)	1717 (7)	2812 (8)	2·9
	C(6)	455 (8)	2488 (7)	1417 (9)	3·2
	C(7)	1763 (9)	−722 (8)	3636 (9)	4·2
	C(8)	−86 (10)	−2385 (8)	2039 (9)	4·2
	C(9)	4652 (8)	4976 (8)	5671 (9)	3·3
TCNE1	C(10)	3330 (9)	5848 (8)	5869 (9)	3·4
	C(11)	5231 (9)	4088 (8)	7021 (10)	3·4
	N(1)	2294 (8)	6506 (8)	6082 (9)	4·5
	N(2)	5617 (9)	3408 (8)	8093 (9)	4·9
TCNE2	C(12)	5507	4515	5305	
	C(13)	5126	3586	6484	
	C(14)	7040	4343	4820	
	N(3)	4868	2827	7424	
	N(4)	8271	4173	4465	

TCNE1: $\theta_1 = -23{\cdot}8$ (1), $\theta_2 = 41{\cdot}3$ (2), $\theta_3 = 23{\cdot}3$ (1)°
$U_1 = 0{\cdot}5, U_2 = 0{\cdot}5, U_3 = 0{\cdot}5, M = 0{\cdot}93$ (1), $B = 4{\cdot}0$ (1) Å^2
TCNE2: $\theta_1 = 27$ (2), $\theta_2 = 17$ (1), $\theta_3 = 129$ (1)°
$u_1 = 0{\cdot}5, u_2 = 0{\cdot}5, u_3 = 0{\cdot}5, m = 0{\cdot}07, B = 4{\cdot}0$ (1) Å^2



(*a*) (*b*)

Fig. 1. Conformation of (*a*) [2^3]paracyclophanetriene–TCNE and (*b*) [2^2]paracyclophane–TCNE. [Projections on the plane C(1)–C(4)–C(6) (*a*) and C(1)–C(2)–C(4) (*b*).]

vary or even disappear; however, no change was observed for (I) at 153 K: at the two temperatures, the structures are identical with the same occupancy factors for TCNE (lower thermal parameters at 153 K). Only the low-temperature results are given. Final R values: compound (I) 869 reflexions, $R = 0{\cdot}046$, $wR = 0{\cdot}053$, $(\Delta/\sigma)_{max} = 0{\cdot}1$, final $\Delta\rho < 0{\cdot}25$ e Å^{-3}; compound (II) 726 reflexions, $R = 0{\cdot}066$, $wR = 0{\cdot}068$, $(\Delta/\sigma)_{max} = 0{\cdot}5$, final $\Delta\rho < 0{\cdot}3$ e Å^{-3}. No weighting scheme. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).*

Discussion. Final atomic parameters are given in Table 1, bond distances, valence angles and torsion angles in Table 2. Fig. 1 shows the conformations of the two complexes.

Table 2. *Interatomic distances* (Å), *valence and torsion angles* (°) *in compounds* (I) *and* (II)

Symmetry code: (i) $x, \frac{1}{2}-y, z$; (ii) $\bar{x}, \bar{y}, \bar{z}$; (iii) $1-x, 1-y, 1-z$.

Compound (I)

C(1)–C(2)	1·400 (7)	C(7)–C(7^{i})	1·333 (9)
C(2)–C(3)	1·389 (7)	C(8)–C(9)	1·324 (7)
C(3)–C(4)	1·389 (6)	C(9)–C(10)	1·485 (7)
C(4)–C(5)	1·394 (6)	C(10)–C(11)	1·395 (6)
C(5)–C(6)	1·393 (7)	C(10)–C(12)	1·390 (6)
C(6)–C(1)	1·387 (7)	C(11)–C(11^{i})	1·391 (9)
C(4)–C(7)	1·484 (7)	C(12)–C(12^{i})	1·387 (9)
C(1)–C(8)	1·503 (7)		
C(1)–C(2)–C(3)	120·2 (4)	C(2)–C(1)–C(8)	122·0 (4)
C(2)–C(3)–C(4)	121·9 (4)	C(1)–C(8)–C(9)	123·6 (4)
C(3)–C(4)–C(5)	117·6 (4)	C(8)–C(9)–C(10)	125·5 (4)
C(3)–C(4)–C(7)	120·3 (4)	C(9)–C(10)–C(11)	121·0 (4)
C(5)–C(4)–C(7)	122·0 (4)	C(9)–C(10)–C(12)	121·1 (4)
C(4)–C(5)–C(6)	120·5 (4)	C(11)–C(10)–C(12)	118·0 (4)
C(5)–C(6)–C(1)	121·6 (4)	C(10)–C(11)–C(11^{i})	120·8 (3)
C(6)–C(1)–C(2)	117·8 (4)	C(10)–C(12)–C(12^{i})	121·0 (2)
C(6)–C(1)–C(8)	120·2 (4)		
C(1)–C(8)–C(9)–C(10)	5·1 (7)	C(11)–C(10)–C(9)–C(8)	−135·4 (5)
C(6)–C(1)–C(8)–C(9)	73·7 (6)	C(12)–C(10)–C(9)–C(8)	43·5 (7)
C(2)–C(1)–C(8)–C(9)	−104·4 (6)		

Compound (II)

C(1)–C(2)	1·392 (8)	C(4)–C(7)	1·507 (8)
C(2)–C(3)	1·375 (8)	C(7)–C(8^{i})	1·615 (8)
C(3)–C(4)	1·397 (8)	C(9)–C(9^{i})	1·342 (11)
C(4)–C(5)	1·394 (8)	C(9)–C(10)	1·445 (9)
C(5)–C(6)	1·384 (8)	C(9)–C(11)	1·450 (9)
C(1)–C(6)	1·381 (7)	C(10)–N(1)	1·129 (7)
C(1)–C(8)	1·518 (8)	C(11)–N(2)	1·126 (7)
C(1)–C(2)–C(3)	121·1 (5)	C(3)–C(4)–C(7)	121·5 (5)
C(2)–C(3)–C(4)	120·5 (5)	C(5)–C(4)–C(7)	120·8 (6)
C(3)–C(4)–C(5)	116·6 (5)	C(10)–C(9)–C(9^{iii})	121·3 (7)
C(4)–C(5)–C(6)	121·1 (6)	C(11)–C(9)–C(9^{iii})	121·5 (7)
C(5)–C(6)–C(1)	120·5 (5)	C(10)–C(9)–C(11)	117·2 (5)
C(6)–C(1)–C(2)	117·1 (5)	C(9)–C(10)–N(1)	177·2 (7)
C(8)–C(1)–C(2)	121·9 (6)	C(9)–C(11)–N(2)	176·9 (7)
C(8)–C(1)–C(6)	119·9 (6)		
C(4)–C(7)–C(8^{iii})	111·5 (5)		
C(1)–C(2)–C(3)–C(4)	−1·4 (9)	C(5)–C(6)–C(1)–C(2)	−14·2 (8)
C(2)–C(3)–C(4)–C(5)	−12·9 (8)	C(6)–C(1)–C(2)–C(3)	15·1 (8)
C(3)–C(4)–C(5)–C(6)	13·8 (8)	C(3)–C(4)–C(7)–C(8^{ii})	−89·9 (6)
C(4)–C(5)–C(6)–C(1)	−0·2 (8)	C(5)–C(4)–C(7)–C(8^{ii})	78·4 (7)
C(2)–C(1)–C(8)–C(7^{ii})	−78·0 (6)	C(6)–C(1)–C(8)–C(7^{ii})	89·7 (7)

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* Lists of structure factors, anisotropic thermal parameters, calculated H-atom parameters and mean-plane equations have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43066 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Conformation of the paracyclophane molecules

In complex (I) (Fig. 2), the paracyclophane has a mirror-plane symmetry. The aromatic rings are not distorted [maximum deviation to the ring plane, 0·03 (3) Å]. The threefold pseudo-axis of symmetry observed in [2^3]paracyclophane and in its complex with TCNE (Cohen-Addad, Baret, Chautemps & Pierre, 1983; Cohen-Addad, Lebars, Renault & Baret, 1984) is much less pronounced in the present compound as shown in Table 3. In particular, the phenyl rings are not perpendicular to the reference plane defined by their centres of gravity. This was already observed in [2^3]paracyclophanetriene (Trueblood *et al.*, 1982). In complex (II) (Fig. 3), the paracyclophane is located around a centre of symmetry. The aromatic rings are distorted in the same way as in [2^2]paracyclophane (Hope, Bernstein & Trueblood, 1972). The C(1) and C(4) atoms are 0·16 Å out of the C(2) C(3) C(5) C(6) plane in a boat conformation.

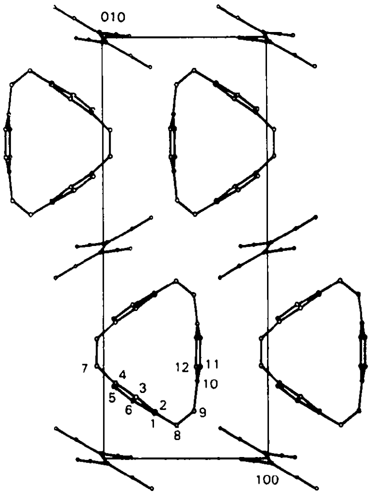

Fig. 2. Intermolecular arrangement in [2^3]paracyclophanetriene. Projection on the (110) plane. Only one TCNE is drawn.

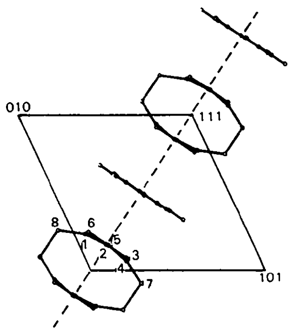

Fig. 3. Intermolecular arrangement in [2^2]paracyclophane–TCNE. Projection on the (101) plane.

Table 3. *Angles between mean planes* (°) *in compounds* (I) *and* (II)

Standard deviations: 0·5–0·7°.

*P*1: C(1) C(2) C(3) C(4) C(5) C(6)
*P*2: C(10) C(11) C(12) C(10^i) C(11^i) C(12^i)
P: (I), centres of gravity of the three rings
(II), C(1) C(4) origin
TCNE1, TCNE2: see Table 1
Origin: (0,0,0), (i): $x, \frac{1}{2}-y, z$

Dihedral angle	Compound (I)	Compound (II)
(*P*1, *P*2)	57·7	
(*P*1, *P*1^i)	67·4	
(*P*1, *P*)	76·1	86
(*P*2, *P*)	48·7	
(*P*1, TCNE1)	2·2	0
(*P*1, TCNE2)	8·2	

In both compounds, the complexation leads to a stabilization of the paracyclophane molecules, which are not disordered. In contrast, they were found to be disordered in the crystal structures of [2^3]paracyclophanetriene and [2^2]paracyclophane (Trueblood *et al.*, 1982; Hope *et al.*, 1972).

TCNE molecules, stacking and charge transfer

In both (I) and (II), as was observed in other structures (Bernstein & Trueblood, 1971; Cohen-Addad *et al.*, 1984), TCNE lies on a centre of symmetry between two paracyclophane molecules. The overlap between TCNE and the benzene rings is shown in Fig. 1. Both structures present a disorder of the TCNE molecule on two positions, related by a 90° rotation. In (I), the occupancies (*m*) of the two positions are 58 (1)–42%. In (II), the disorder is very small with occupancies of 93 (2)–7%. The TCNE molecules are almost parallel to the associated phenyl rings (Table 3). The plane-to-plane averaged distances are 3·3 Å, similar to those found in the other paracyclophane–TCNE complexes (Bernstein & Trueblood, 1971; Keehn & Rosenfeld, 1983; Cohen-Addad *et al.*, 1984). The shortest interatomic distances are (I) C(3)—C(18) 3·162 (6), C(2)—C(14), 3·291 (6) Å; (II) C(5)—C(9) 3·211 (8) Å.

The relative orientations of donor and acceptor can be characterized by the angle between the C(1)–C(4) axis of the phenyl ring and the C=C double bond of TCNE. This angle has the values of 34·1 (7) and 123·1 (7)° in (I) and 51·2 (5) and 142 (1)° in (II).

In (I), as was found in [2^3]paracyclophane–TCNE (Cohen-Addad *et al.*, 1984), only two of the benzene rings of each cyclophane molecule are involved in the association with TCNE (Fig. 2). This leads to a one-dimensional and not a two-dimensional stacking of the TCNE molecules along the *b* axis. The shortest TCNE–TCNE distance is 10·289 (5) Å (10·23 Å in [2^3]paracyclophane–TCNE). The two structures are closely related: the *b* axis in the present compound corresponds to the [111] direction in the previous one. Nevertheless, the two structures are not isomorphous.

The structure of compound (II) is isomorphous to that of [3^2]paracyclophane–TCNE (Bernstein & Trueblood, 1971). The charge-transfer direction is along the [111] direction in a sandwich arrangement. The shortest TCNE–TCNE distance is 9·374 (5) Å (9·63 Å in [3^2]paracyclophane–TCNE). The relative arrangement of TCNE and the benzene rings is the same in both compounds: the value of 52° defined above is equal to 45° in [3^2]paracyclophane–TCNE. However, the TCNE disorder is less important in the present compound than in the [3^2] complex where a 75–25% orientation disorder was found.

Both compounds show normal intermolecular distances involving van der Waals interactions.

Energy calculations are in progress on these complexes.

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Structure of 2,5-Dihydroxy-3,8-dimethyl-1,4-naphthalenedione (Aristolindiquinone)*

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Abstract. $C_{12}H_{10}O_4$, $M_r = 218{\cdot}21$, monoclinic, $P2_1/n$, $a = 4{\cdot}894\ (2)$, $b = 11{\cdot}595\ (6)$, $c = 18{\cdot}039\ (6)$ Å, $\beta = 106{\cdot}27\ (3)°$, $V = 982{\cdot}6$ Å^3, $Z = 4$, $D_x = 1{\cdot}47$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $\mu = 0{\cdot}068$ mm^{-1}, $F(000) = 456$, $T = 293$ K, $R = 0{\cdot}072$ for 866 reflexions. The aristolindiquinone molecule is essentially planar and exhibits intramolecular hydrogen bonding involving the 5-hydroxy group and the 4-keto O atom, O···O 2·568 (7) Å, angle O—H···O 140 (8)°. Short O···O contacts, C(2)—OH···O=C(1), intramolecularly of 2·643 (7) Å and intermolecularly of 2·731 (8) Å also occur.

Introduction. Aristolindiquinone (1) was extracted from the roots of the Indian medicinal plant *Aristolochia indica* L. (Aristolochiaceae). A complete description of phytochemical and biological studies of the compound

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* Studies on *Aristolochia*. IV. Part III: Che *et al.* (1984).
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