Discussion. The atomic coordinates are listed in Table 1,* bond distances and bond angles are displayed in Figs. 1 and 2 for PMDA and Tcn. The bonding geometry of the PMDA molecule agrees well with that found for the acceptor in quite a number of 1:1 D:A complexes with donors such as anthracene (Robertson & Stezowski, 1978), phenazine (Bulgarovskaya, Vozzhennikov, Krasavin & Kotov, 1982), carbazole (Stezowski, Binder & Karl, 1982). Tcn bond distances and bond angles may be compared with the average values found in the free Tcn (Robertson, Sinclaire & Trotter, 1961). Each of the component molecules is planar. The maximum deviations from the mean planes of the PMDA and Tcn molecules (neglecting H atoms) are 0-021 and 0-012 Å respectively.

The structure of the complex consists of columns of alternately stacked molecules of Tcn and PMDA. The a axis of the crystal is the stack axis. The molecular planes are parallel to each other and perpendicular to a (the angle between the plane normals is 1-7°, those between the normals to the Tcn and PMDA planes and the a axis are 0-7 and 1-5°, respectively), the interplanar separation being 3.36 Å. Because the stacks are not shifted with respect to one another along the a axis, the structure can also be described in terms of alternating sheets of Tcn and PMDA molecules. Adjacent Tcn and PMDA molecules are orientated in such a manner that the bonds of the Tcn molecule common to two rings lie over (or under) the centres of the rings of the neighbouring PMDA molecule, Fig. 3.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43514 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References


Structure of the 1:1 π-Molecular Complex of Chrysene with 1,2:4,5-Pyromellitic Dianhydride*

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Abstract. C_{18}H_{12}\cdot C_{10}H_{20}O_4. M_r = 446.4, monoclinic, P2_1/n, a = 8.093 (3), b = 16.479 (5), c = 7.746 (2) Å, \( \gamma = 97.62 (3) ^\circ \), \( V = 1023.9 (6) \) Å³, \( Z = 2 \), \( D_x = 1.45 \) g cm\(^{-3} \), \( \lambda(\text{Mo } K\alpha) = 0.71069 \) Å, \( \mu(\text{Mo}) = 0.96 \) cm\(^{-1} \), \( F(000) = 460 \), \( T = 295 \) K, \( R = 0.041 \) for 845 observed reflections \( I > 3\sigma(I) \). Alternate planar centrosymmetric molecules form stacks along c. The mean separation of the molecular planes is 3.32 Å, the interplanar angle is 2.0°.

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Introduction. The title compound is a charge-transfer (CT) complex formed by pyromellitic dianhydride (PMDA) as an acceptor with chrysene (Crs). The crystals of the compound studied exhibit moderately high photoconductivity in the regions corresponding to the CT-absorption band and to the singlet transitions of the component molecules. We report here the results of the X-ray analysis undertaken as part of our investigations with the object of establishing the role of the crystal structure in photoconductivity.

Experimental. Prismatic red crystals 0.35 x 0.25 x 0.15 mm grown by high-vacuum plate sublimation method. Syntex P1 diffractometer, graphite-monochromated Mo Ka radiation, lattice parameters from 12 reflections, $\theta/2\theta$ scan mode, $2\theta < 48^\circ$, three standard reflections with variation within counter statistics. 991 unique reflections collected, 845 non-zero $|I| > 3\sigma(I)$, range of $hkl$: $h +9$, $k 0-18$, $l 0-8$; Lp correction, absorption ignored. Direct methods, refinement by full-matrix least squares on $F$. H positions calculated using geometric considerations: final $R = 0.041$, $wR = 0.047$, $w = 1/|\sigma^2(F) + 0.0005F^2|$. Atomic scattering factors from International Tables for X-ray Crystallography (1974), for H from Stewart, Davidson & Simpson (1965). $(\Delta/\sigma)_{max} = 0.06$, $(\Delta\rho)_{max} = 0.10$ e Å$^{-3}$. Calculations carried out with SHELXTL (Sheldrick, 1978) on the Nova 3 computer incorporated in the Nicolet R3 crystallographic system.

Discussion. The atomic coordinates are listed in Table 1, interatomic distances and bond angles are presented in Figs. 1 and 2. The dimensions of the PMDA molecule agree well with those in the complexes with anthracene (Robertson & Stezowski, 1978),

Table 1. Fractional atomic coordinates (and e.s.d.'s) of non-hydrogen atoms (x 10$^4$) and hydrogen atoms (x 10$^3$), and equivalent isotropic thermal parameters (Å$^2$ x 10$^3$)

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* $U_{iso}$.
phenanthrene (Evans & Robinson, 1977), phenazine (Bulgarovskaya, Vozzhennikov, Krasavin & Kotov, 1982). The dimensions of the Crs molecule compare well with those of the free Crs (Burns & Iball, 1960) and of Crs in the complexes with 7,7,8,8-tetracyanoquinodimethane (Munnoch & Wright, 1974) and fluoranil (Munnoch & Wright, 1975). The PMDA molecule is planar, the maximum deviation from the least-squares best plane through the molecule being 0.008 Å. The Crs molecule is approximately planar. The individual rings are each planar; the maximum deviation from the best planes is 0.019 Å.

In the crystal the component molecules are arranged in mixed stacks extending along the c axis. The molecular planes are parallel to each other (the dihedral angle between the planes of the PMDA and Crs molecules is 2.0°) and make angles of 31.2 and 30.4° respectively with the c axis. The mean separation between the PMDA and Crs planes is 3.32 Å. The overlap diagram is shown in Fig. 3. A particular PMDA molecule is located above one portion of the neighbouring Crs molecule; the next PMDA molecule in the stack takes up an analogous position and orientation with respect to the other centrosymmetric portion of the Crs molecule sandwiched between them, and so on along the stack.

**References**


