

## 06-Crystallography of Organic Compounds

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accompanied by the dimerization are smaller than those estimated from the structure of ACD4. The water molecules move maintaining their relative distance almost constant to keep the hydrogen bonding between them. The modes of hydrogen bonding at the intermediate stage and the features of the atomic movements are discussed.

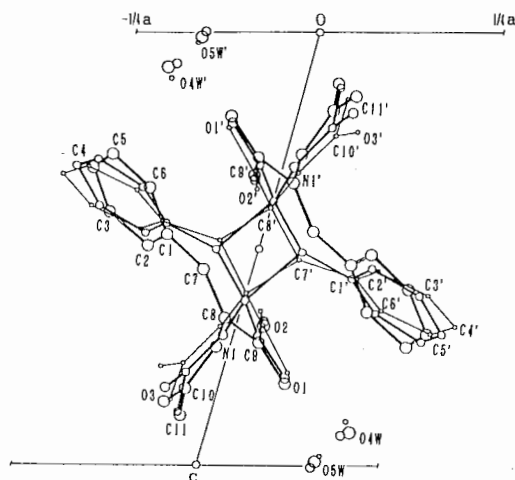


Fig. 1. The composite diagram around a center of symmetry of the photodimer components, and the molecules in AC2 and ACD4. Open bonds and large circles for AC2, bold bonds and medium circles for the photodimer component, and thin bonds and small circles for ACD4.

## PS-06.02.06 MOLECULAR STRUCTURES OF DIANTHRACENES

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The molecular structures of bridgehead substituted dianthracenes **1a-e**, prepared photochemically from 9-methoxy-, 9-methoxy-10-methyl-, and 9-(2-hydroxy-2-propyl)anthracene, have been established by X-ray diffraction.

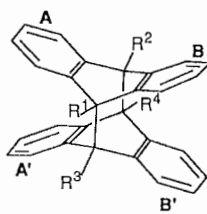


Fig. 1. Schematic presentation of stereoisomeric dianthracenes **1d** and **1e**.

	Bond Length (Å)	Dihedral Angles (deg)			
		A/A'	B/B'	A/B	A'/B'
<b>1a</b>	1.630(6)	41.2;	41.2;	138.8;	138.8
<b>1b</b>	1.639(2)	41.9;	41.9;	138.1;	138.1
<b>1c</b>	1.657(4)	43.2;	43.4;	130.7;	143.0
	1.637(4)				

In *i*- and  $C_2$ -symmetrical dianthracenes **1d** and **1e**, the difference in spatial demand due to the rotationally blocked 2-hydroxy-2-propyl groups is borne out by distinctly different dihedral angles between aromatic rings (see Fig. 1).

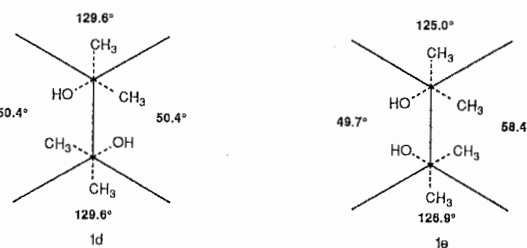
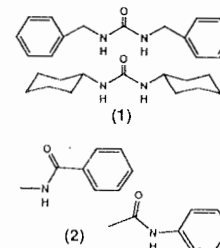


Fig. 1. Schematic presentation of stereoisomeric dianthracenes **1d** and **1e**.

PS-06.02.07 CRYSTAL STRUCTURES OF SOME ORGANIC CO-CRYSTALS. By Hidehiro UEKUSA\*, Yuji OHASHI, Tokyo Institute of Technology, Japan, and Fumio TODA, Ehime University, Japan.

Recently, many types of solid-solid organic reactions, such as a coupling of phenols, Wittig-Horner reaction and aldol condensation, have been found. Only mixing a powdery crystals of some organic compounds, these reactions can easily occur. In the solid-solid reaction, regio and stereo selective reactions are expected. In a course of the study of developing a new reaction field for the solid-solid reaction, the crystal structures of two co-crystals, (1) *N,N'*-dibenzyl-urea and *N,N'*-dicyclohexane-urea 1:1 complex crystal and (2) PhCONHMe and PhNHCOMe 1:1 mixed crystal, have been determined. Especially using a mixed crystal as a reactant or host compound, a new sophisticated reaction field may be obtained.

Crystal	(1)	(2)
a(Å)	26.013(2)	19.363(3)
b	9.164(1)	8.084(1)
c	11.324(1)	9.486(1)
$\beta$ (°)	90.843(9)	
V(Å <sup>3</sup> )	2699.1(4)	1484.9(3)
Z	4	4
Space group	C2/c	Pbca



**1a**:  $R^1=R^4=OMe$ ;  $R^2=R^3=Me$ .

**1b**:  $R^1=R^4=OMe$ ;  $R^2=Me$ ;  $R^3=H$

**1c**:  $R^1=R^3=OMe$ ;  $R^2=Me$ ;  $R^4=H$ .

**1d/1e**:  $R^1=R^4=2\text{-hydroxy-2-propyl}$ ;  $R^2=R^3=H$

For dianthracenes **1a-c**, topological features in terms of lengths of photochemically formed bonds, and dihedral angles between planes of aromatic rings are summarized in Table 1.