

06-Crystallography of Organic Compounds

The observation of only one diastereoisomer of **6** is noteworthy and indicates highly stereospecific character of the oxidation step. This observation may be of great significance and we plan to utilize compound **6** as a chiral precursor in the synthesis of natural products.

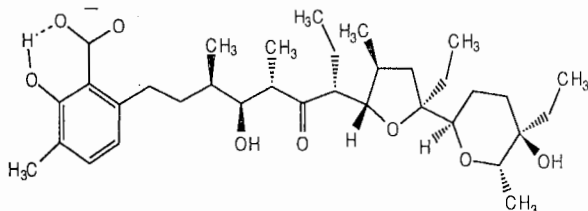
References.

- Bhat, K.L., Chen, S-Y. & Joullie, M. (1985) *Heterocycles*, **23**, 691-734; *Aldrichimica Acta*, **22** (2), 49,(1989).
 Czarnocki, Z. (1992) *J. Chem. Research (S)*, 334-335.
 Czarnocki, Z. (1992) *J. Chem. Research (M)*, 2801-2819.

PS-06.03.07 COMPLEXATION OF GUANIDINIUM AND AMIDIUM CATIONS WITH THE POLYETHER ANTIBIOTIC LASALOCID. Xiuqi Shui*, Drake S. Eggleston, Nelson Troupe and John W. Westley, SmithKline Beecham Pharmaceuticals, Box 1539, King of Prussia, PA 19406, USA

Studies directed toward the complexation of guanidinium and amidinium groups by organizable recognition sites are expected to be of value for a number of reasons. Among these is the potential for crystallization of otherwise recalcitrant natural products and peptides. As one approach to that goal, complex formation with the highly crystalline naturally occurring ionophore lasalocid A, which has previously been shown to be of value in the complexation and resolution of asymmetric amines (Westley, Evans & Blount, 1977, *J. Am. Chem. Soc.* **99**, 6057-6061), has been investigated for a variety of target molecules. Circular dichroism studies in various polar and nonpolar solvents have confirmed complex formation and several complexes of general formula I have been crystallized. Details of these studies where R = various molecules incorporating guanidinium and amidinium groups and comparisons of the recognition motifs will be presented.

R⁺



PS-06.03.08 CRYSTAL STRUCTURES OF CIS- α -NITROSTILBENE AND THE ADDUCT: TRANS-STILBENE. (CIS- α -NITROSTILBENE)₂

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Crystal structure of *cis*- α -nitrostilbene (I) and that of *trans*-stilbene. (*cis*- α -nitrostilbene)₂ (II) have been determined by X-ray diffraction at room temperature.

Crystal data:

I. formula: C₁₄H₁₁NO₂
 monoclinic, space group: P2₁/n
 a=5.839(2) b=16.034(4) c=24.851(5) Å
 β = 90.95(2)^o
 V=2326.3(9) Å³ Z = 8 D_x = 1.286 Mg/m³
 R = 0.034 wR = 0.043

II. formula: C₁₄H₁₂·(C₁₄H₁₁NO₂)₂
 monoclinic, space group: P2₁/n
 a=15.755(4) b=5.771(1) c=18.809(3) Å
 β = 101.84(2)^o
 V=1763.7(6) Å³ Z = 2 D_x = 1.251 Mg/m³
 R = 0.045 wR = 0.050

The unit cell of I contains two independent molecules. The two molecules have similar bond lengths, bond angles and geometry. The nitro group is close to coplanar with the central C=C bond with the two phenyl rings twisted at about 70^o and 30^o from this plane. The central C=C bond length is 1.329(4) Å.

The unit cell of II contains one molecule of *cis*- α -nitrostilbene and half a molecule of *trans*-stilbene per asymmetric unit. The geometry, bond lengths and angles of the *cis*- α -nitrostilbene are close to those found in I. The central C=C bond length is 1.323(4) Å. The nitro group is close to coplanar with the C=C bond with the two phenyl rings twisted at 70^o and 30^o. The *trans*-stilbene molecule is planar with a central C=C bond length of 1.330(4) Å. The crystal is packed with the *trans*-stilbene molecules wedged between layers of molecules of *cis*- α -nitrostilbene. The efficient packing accounts for the stability of II.

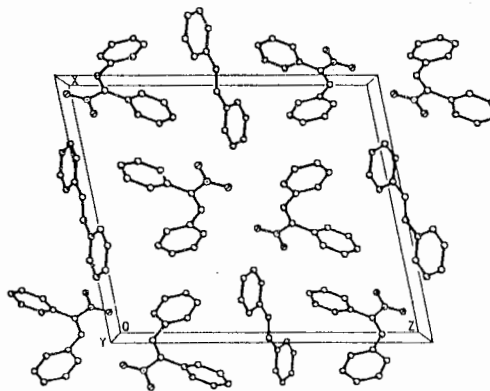


Fig. 1. Crystal packing of II.

PS-06.03.09

GUEST/HOST-COMPOUNDS WITH ³ NETWORKS OF HYDROGEN BONDED OLIGOMERIC BORATE ANIONS AND BORIC ACID MOLECULES

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The crystalline pentaborates NMe₄[B₅O₆(OH)₄]·0.25 H₂O, NEt₄[B₅O₆(OH)₄], NPhMe₃[B₅O₆(OH)₄] and pipH[B₅O₆(OH)₄] form a series of unique, closely related inclusion compounds with ³ host structures assembled by hydrogen-bonded pentaborate [B₅O₆(OH)₄]⁻ ions (Figure 1 a). The organic cations and water molecules occupy as guest species large straight channels of rectangular cross-section (Figure 1 b).