06-Crystallography of Organic Compounds

The observation of only one diastereoisomer of 6 is noteworthy and indicates highly stereosepecific 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.

pg-06.03.07 COMPLEXATION OF GUANIDINIUM AND AMIDINIUM CATIONS WITH THE POLYETHER ANTIBIOTIC LASALOCID: Xiaqi Shi, Drake S. Eggleton, 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 recognizable recognition sites are expected to be of value for a number of reasons. Among these is the potential for crystalization of otherwise recalcitrant natural products and peptides. As one approach to that goal, complex formation with the highly crystalline naturally occurring isoazole Lasalocid A, which has previously been shown to be of value in the complexation and resolution of asymmetric amines (Westley, Eggleton, Troupe & Schmitz, 1997, 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 1 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.

\[ \text{R}^+ \]

PS-06.02.08 CRYSTAL STRUCTURES OF CIS-α-NITROSTILBENE AND THE ANTAGONIST: TRANS-STILBENE. (CIS-α-NITROSTILBENE)²

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Crystal structure of cis-α-nitrostilbene (1) and that of trans-stilbene (cis-α-nitrostilbene)² (II) have been determined by X-ray diffraction at room temperature.

Crystal data:
1. formula: C₁₄H₁₁NO₂
   monoclinic, space group: P2₁/n
   a=5.839(2) Å, b=16.034(4) Å, c=24.851(5) Å
   \( \beta = 90.95(2)^\text{o} \)
   \( V=2326.3(19) \text{ Å}^3 \)
   \( Z = 8 \)
   \( D_x = 1.286 \text{ Mg/m}^3 \)
   \( R = 0.034 \quad wR = 0.043 \)

II. formula: C₁₄H₁₂O₂N₂
   monoclinic, space group: P2₁/c
   \( a=15.755(4) \text{ Å}, b=5.771(1) \text{ Å}, c=18.899(1) \text{ Å} \)
   \( \beta = 101.84(2)^\text{o} \)
   \( V=1763.7(6) \text{ Å}^3 \)
   \( Z = 2 \quad D_x = 1.251 \text{ Mg/m}^3 \)
   \( R = 0.045 \quad wR = 0.050 \)

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° and 30° 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° and 30°. 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.

![Crystal packing of II](image)

PS-06.03.09 GUEST-HOST COMPOUNDS WITH NETWORKS OF HYDROGEN BONDED OLIGOMERIC BORATE ANIONS AND BICRYSTAL MOLYBDENUM MOLECULES

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The crystalline assemblages NMe₄[BO₃(OH)₄] (0.75 H₂O), NMe₄[BO₃(OH)₂] (1.75 H₂O), NMe₄[BO₃(OH)₄] (1.75 H₂O), and piper[BO₃(OH)₂] form a series of unique, closely related inclusion compounds with the host structures assembled by hydrogen-bonded borate [BO₃(OH)₂]⁻ ions (Figure 1 a). The organic cations and water molecules occupy the guest species large straight channels of rectangular cross-section (Figure 1 b).