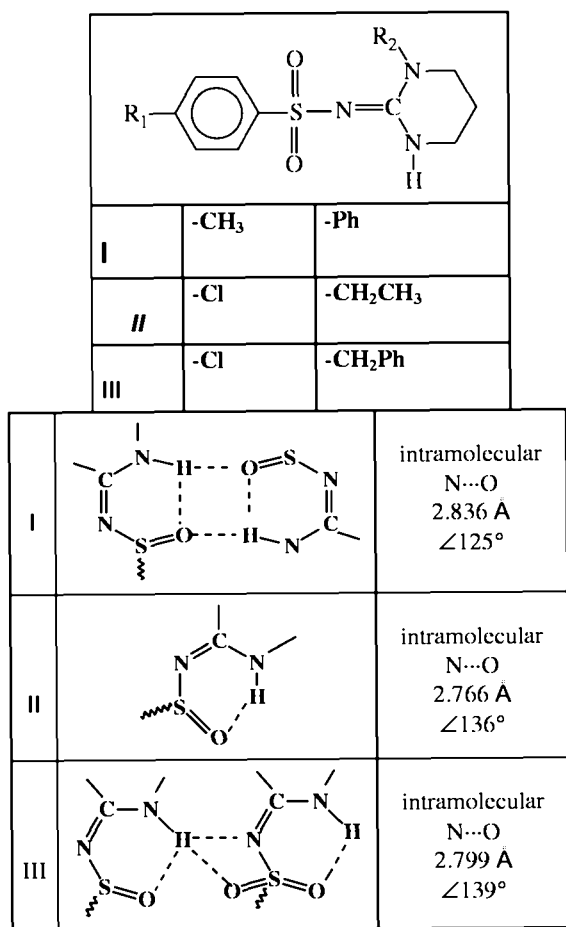


**[s9.m1.p7]** The role of intra- and intermolecular hydrogen bonding in the crystal structure of arylsulfonyl-guanidine derivatives. I. Dybala<sup>1</sup>, A.É. Koziol<sup>1</sup>, E. Szacoń<sup>2</sup>, D. Matosiuk<sup>2</sup>. <sup>1</sup>Dept. of Chemistry, Maria Curie-Skłodowska Univ., Lublin, Poland, <sup>2</sup> Dept. of Medicines Technology, Faculty of Pharmacy, Medical Univ., Lublin, Poland.

Keywords: arylsulfonylguanidine, hydrogen bond, guanidine derivative.

Three structures of arylsulfonylguanidine derivatives (I *N*-aryl-; II and III *N*-alkyl-) have been determined by X-ray crystal structure analysis. The intramolecular N-H...O hydrogen bonding is observed in all molecules, while various substituents present in analysed compounds determine different types of intermolecular hydrogen bonds.



**I:** Molecules linked by the intermolecular N-H...O hydrogen bonds form dimers (N...O distance 2.942 Å).

**II:** The intramolecular N-H...O hydrogen bond closes a six-membered ring.

**III:** Molecules form chains by weak bifurcated N-H...O and N-H...N intermolecular hydrogen bonds (N...O and N...N distances are 3.282 and 3.408 Å, respectively).

Intermolecular interactions influence a conformation of the O2-S-N2-C2-N3 fragment and orientation of substituents at the N and S atoms.

**[s9.m1.p8]** Inclusion crystals of finasteride. I. Wawrzycka<sup>a</sup>, A.É. Koziol<sup>a</sup>, E. Cendrowska<sup>b</sup>, <sup>a</sup>Department of Chemistry, M. Curie-Skłodowska Univ. Lublin, Poland, <sup>b</sup>Department of Chemistry, A. Mickiewicz Univ. Poznan, Poland.

Keywords: finasteride, steroids, inclusion crystals.

Finasteride [17β-(*N*-*tert*-butylcarbamoyl)-4-aza-5α-androst-1-en-3-one] is a modified steroid derivative. The ring A contains lactam group and the C17 atom is substituted with the *tert*-butylamide residue.

Finasteride crystallizes from ethanol<sup>[1]</sup> and DMSO solutions as the homomolecular crystal. It seems that the size of a solvent molecule has influence on form of inclusion crystals. The crystallization from other organic solvents gives isostructural clathrates (in the orthorhombic space group *P*2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>) with the bis-finasteride monohydrate unit as a host.

Solvent	Unit cell dimensions [Å]
1 ethyl acetate <sup>[1]</sup>	<i>a</i> = 8.173(3) <i>b</i> = 18.364(6) <i>c</i> = 35.65(2)
2 toluene	<i>a</i> = 8.138(2) <i>b</i> = 18.526(4) <i>c</i> = 34.770(7)
3 2-butanol	<i>a</i> = 8.113(2) <i>b</i> = 17.979(4) <i>c</i> = 35.802(7)
4 2-propanol	<i>a</i> = 8.162(5) <i>b</i> = 18.29(2) <i>c</i> = 35.92(3)
5 butyl acetate	<i>a</i> = 8.185(7) <i>b</i> = 18.33(3) <i>c</i> = 35.82(3)
6 chloroform	<i>a</i> = 8.167(2) <i>b</i> = 17.897(6) <i>c</i> = 36.24(1)

Structures of 2 and 3 have been determined by X-ray crystallography using data collected on a KM4CCD diffractometer at 130K. Unit cell dimensions for crystals of 3, 4 and 5 were determined on a KM4 diffractometer.

In the crystal lattice, two symmetrically independent finasteride molecules are linked by N-H...O hydrogen bonds between the lactam groups of the ring A. The water molecule is a double H-bond donor to the lactam O-atoms and an acceptor from the amide N-atom, which gives three-dimensional net with channels. The size of these channels is suitable for enclathration of solvent molecules, both polar and nonpolar.

[1] Wawrzycka I. *et al.* "Structural characterization of polymorphs and molecular complexes of finasteride." *J. Mol. Struct.* (1999) 474: 157 - 166.