MS73.P21

**Crystal Structure of N-(4-heptylphenyl)acetamide**

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The crystal structure of the title compound, N-(4-heptylphenyl)acetamide ($C_{15}H_{23}NO$), is determined by X-ray diffraction method and crystallizes in the Triclinic space group *P-1* with cell parameters a = 9.5432(4)Å, b = 17.3533(7)Å, c = 18.8570(7)Å, V = 2892.6(2)Å^3, Z = 8, D_{calc} = 1.072mg/m^3, μ = 0.066mm^{-1}, F_{000}=1024, λ(Mok$_\alpha$) = 0.71073Å and the structure was refined to R = 0.0684.

The structure contains four independent molecules (A & C and B & D) linked by a strong N---H...O hydrogen bond. The aromatic rings and alkyl chains of each molecule are non coplanar; the dihedral angles between phenyl rings and alkyl chains of molecules A, B, C & D are 64.10(3)Å, 30.5(5)Å, 27.8(4)Å & 73.4(3)Å respectively. The molecular assembly in the structure is established by an intramolecular N---H...O & C---H...O, intermolecular N---H...O hydrogen bonds and as well as C---H....π-electron ring $C_g(3)$ [C10D-C15D] interactions. Intermolecular N---H...O hydrogen bonds involving different types of molecules generate an infinite ACAC...and BDBD ... chain running parallel to the [100] direction and packing of the molecules show the stacking when viewed along *a*.

Small biological molecules like amino acids, DNA bases or drug related molecules have been extensively studied for physisorption on electronically conducting surfaces. 4-acetaminophenol is a common antipyretic and analgesic drug used for the treatment of headaches and fever. In this molecule the 4-acetyl-amine group in *para* position to the phenol functionality owing to such remarkable biological activity.

The dihedral angles between the independent one pair of molecules with another pair molecules are 61.5(2) Å and 64.0(2) Å and heptylphenyl and acetamide groups of the molecules A, B, C and D are 16.32(15)Å, 15.78(15)Å, 15.30(15)Å and 6.14(16)Å respectively.
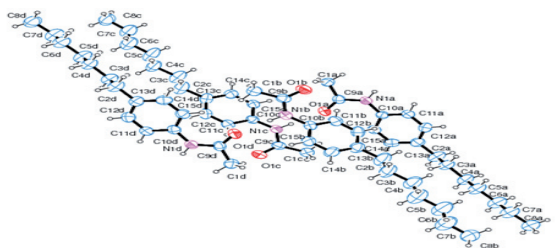
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Keywords: Crystal, Hydrogenbond, diffractometer

MS73.P22

**X-ray structure of poly substituted 1,2-dihydropyridine derivative**

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The crystal structure of the title derivative, methyl 6-(4-bromophenyl)-1-(2,4-dimethoxybenzyl)-4-hydroxy-2-oxo-1,2-dihydropyridine-3-carboxylate ($C_{22}H_{20}NO_6Br$) is determined by X-ray diffraction method and crystallizes in the Orthorhombic space group *Pca21* with cell parameters a = 16.1028(12) Å, b = 9.7450(7)Å, c = 27.0253(14)Å, V = 4240.9(5)Å^3, Z = 8, D_{calc} = 1.486mg/m^3, μ = 1.977mm^{-1}, F_{000}=1936, λ(Mok$_\alpha$) = 0.71073 Å and the structure was refined to R = 0.0622.

Polysubstituted pyridines represent molecular frameworks that serve as a platform for developing pharmaceutical agents for various applications. They show modulating activity on cardiovascular and neuronal processes and on corticosteroid regulatory circuits and prevent inflammatory and diabetic processes and some show antineoplastic , geroprotective, radioprotective and radiosensitizing effects.

The structure of methyl 6-(4-bromophenyl)-1-(2,4-dimethoxybenzyl)-4-hydroxy-2-oxo-1,2-dihydropyridine-3-carboxylate contains two independent molecules in the asymmetric unit. The aromatic rings and pyridine ring systems are non coplanar with one another. The Pyridine ring makes dihedral angles of 71.3(4)Å and 85.2(4)Å respectively with the two aromatic ring systems. The structure of the molecules is stabilized by intermolecular C--H...O and intramolecular C--H...O & O--H...O hydrogen bonds.
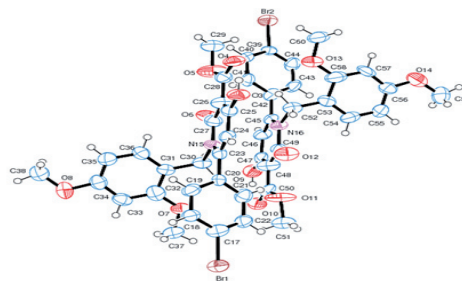
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Keywords: Crystal, Intermolecular, Diffractometer

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Conformational adaptations of a versatile podand

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Flexible anion receptors draw significant scientific attention in the last few decades [1]. Even though peak selectivity with flexible podands is not always accomplished, conformational adaptability of the host may be exploited for other purposes, such as sensor design or signal transduction [2]. Studies of spatial rearrangements of a host during interactions with a guest are important in crystal engineering for supramolecular template synthesis [3].

In our previous studies of binding properties and conformational adaptability of a known nitrate/sulfate receptor *N*,*N'*-3-azapentane-1,5-bis[3-(1-aminoethylidene)-6-methyl-3*H*-pyran-2,4-dione] (**L**) [4] toward various charge-dispersed monoanions (HSO_3^-, ClO_4^-, IO_4^-, PF_6^- and SbF_6^-) we have shown that **L** is able to discriminate anions on the basis of their charge density.

Herein we present two structures whit the same anion, SCN^-, achieves two different complexes with **L**, thus displaying versatile binding nature of this podand. Geometry and (hydrogen-bonding) acceptor properties of SCN^- allow two distinct binding modes. When anion uses a sulfur atom as an acceptor, all strong hydrogen bond donors of the podand become coordinatively saturated by interactions with the oxo-functionalities from neighboring podands, so the only weaker C−H groups are accessible for anion binding. On the other hand, when anion uses nitrogen atom as a hydrogen-bonding acceptor then podand uses its N−H groups to accomplish optimal binding.

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Keywords: anion receptors, podans, binding modes

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Recent Advances in Two-dimensional X-ray Diffraction

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The two most important developments in two-dimensional x-ray diffraction are area detectors and algorithms in analyzing 2D diffraction patterns [1]. Recent advances in area detectors, particularly the one based on the MikroGap technology, and the diffraction vector approach in 2D data analysis are discussed with experimental examples in phase identification, stress measurement, texture analysis and grain size determination.

The VÅNTEC-500 area detector, based on proprietary MikroGap technology, achieves high resolution and low detector noise with a very high dynamic range by combining the advantages of a gaseous detector with the new resistive anode micro-design. It is designed and optimized for the two-dimensional x-ray diffraction system for analytical applications in various materials research, such as nanotechnology, thin films, polymers, metals, biomaterials, forensics, and process control. The detector features a large active area and a tapered geometry which makes it possible to capture diffraction patterns in a large solid angle and to access high diffraction angles.

Two-dimensional diffraction pattern contains information in a large solid angle. The 2D image can be described by the diffraction intensity distribution in both 2θ and γ directions. Unit diffraction vector is used in the data analysis of the 2D diffraction pattern. The unit diffraction vector for all the pixels in the 2D pattern can be calculated in the laboratory coordinates. The data analysis requires the unit diffraction vector to be expressed in the sample coordinates, which can be obtained by vector transformation. The the unit vector in the sample coordinates for Eulerian geometry are given by its three components $\{h_1, h_2, h_3\}$:

$$h_1 = \sin\theta\,(\sin\phi\,\sin\psi\,\sin\omega + \cos\phi\,\cos\omega) + \cos\theta\,\cos\gamma\,\sin\phi\,\cos\psi$$
$$- \cos\theta\,\sin\gamma\,(\sin\phi\,\sin\psi\,\cos\omega - \cos\phi\,\sin\omega)$$

$$h_2 = -\sin\theta\,(\cos\phi\,\sin\psi\,\sin\omega - \sin\phi\,\cos\omega) - \cos\theta\,\cos\gamma\,\cos\phi\,\cos\psi$$
$$+ \cos\theta\,\sin\gamma\,(\cos\phi\,\sin\psi\,\cos\omega + \sin\phi\,\sin\omega)$$

$$h_3 = \sin\theta\,\cos\psi\,\sin\omega - \cos\theta\,\sin\gamma\,\cos\psi\,\cos\omega - \cos\theta\,\cos\gamma\,\sin\psi$$

The three components can then be used to derive fundametal eauation for many applications or data corrections. The fundamental equation for stress analysis, for instance, is given by the scalar product of the strain tensor ε_{ij} with the unit vector components $\{h_1, h_2, h_3\}$:

$$\varepsilon_{(\gamma,\omega,\psi,\phi)}^{\{hkl\}} = \varepsilon_j \cdot h_i \cdot h_j$$

where $\varepsilon_{(\gamma,\omega,\psi,\phi)}^{\{hkl\}}$ is the measured strain at the Eulerian angles ω, ψ and ϕ, and on the portion of the diffraction ring given by γ.

For texture analysis, the pole figure angles (α,β) are given by pole mapping equations:

The diffraction unit vector is also used in polarization correction, absorption correction and effective volume calculation for crystal size evaluation by γ-profile analysis.

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Keywords: area detector, stress, texture

MS74.P02

Nullification of extinction effects in XRD analysis

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Based on the different behaviour of the empirical extinction coefficient k [1] and the secondary extinction (SE) coefficient g [2] with respect to the levels of interaction of the diffraction process, the present study outlines a pioneer approach to *analytical* nullification of the SE effects. Both the incident-beam intensity I_0 and the pole density P that represent the relative volume fraction of crystallites contributing to reflection define the variation of the levels of interaction of the diffraction process. Accounting for crystal and textural anisotropy, we have shown that the above coefficients are interconnected by $k=2g\mu/PI_0S$ or $g=PI_0S/2k\mu$ and depend on all the parameters describing the diffraction process of a reflection, excluding only the reflectivity Q. Here, S is the cross-section of the beam, and μ is the linear absorption coefficient. Whereas g is proportional to the product PI_0, the coefficient k is proportional to the g/PI_0 ratio. Therefore, by virtue of the *interdependence* between g and PI_0, any change of P or I_0 or both does not change the ratio g/PI_0 and, hence, k is constant that is independent of the level of interaction. For a pair of levels of interaction defined by variation of incident beam intensities from $I_{0,i}$ to $I_{0,i*}$, one can show that $k_i=k_{i*}$, where i and $i*$ denote a generator current values causing the respective I_0 intensity values that are related by $I_{0,i}/I_{0,i*}=i/i*=R_{i,i*}$. Here, $R_{i,i*}$ is the ratio between the generator current values. The equality $k_i=k_{i*}$ allows analytical nullifying the SE effects by using two expressions of k defined by the intensities of a reflection measured at a series of levels of interaction. The procedure for applying this approach starts with kinematic definition of the parameter (R or P) under study, and finishes with derivation of an operative formula for determining its extinction-free value. For the purposes of comparison, the extinction-affected pole density P_m is expressed using intensities measured at the same reflection of textured sample and powder standard. The object of this study was a nickel sample representing a moderate texture with <100> preferred orientation. The results show that whereas the extinction-free values