

STRUCTURE OF ALANINE:GLYOXYLATE AMINOTRANSFERASE

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The human hereditary disease primary hyperoxaluria type 1 is caused by a deficiency of the liver-specific peroxisomal enzyme alanine:glyoxylate aminotransferase (AGT). This leads to the cumulative deposition of calcium oxalate stones in the kidney and urinary tract and eventually kidney failure. In this study, the X-ray crystallographic structures of normal human AGT and two polymorphic variants are reported. At least two crystal forms were obtained using similar conditions for AGT, AGT[P11L] and AGT[P11L, I340M]. Complete SAD and MAD data were collected on beamline ID14-4 and ID29 of ESRF (Grenoble, France), and native data at station 14.1 of SRS (Daresbury, UK). The crystals of AGT and AGT[P11L] diffracted to a resolution of 2.2 Å with spacegroup $P4_12_1$ and unit-cell parameters $a = b = 90.81$, $c = 142.62$ Å. The structures were solved with the phasing information from 7 Se atoms found in AGT sequence. The structures obtained provide insights into the mechanism of dimerization and mistargeting of AGT from peroxisomes to mitochondria.

Keywords: ALANINE GLYOXYLATE AMINOTRANSFERASE
PRIMARY HYPEROXALURIA TYPE 1 KIDNEY STONE

MESOMORPHIC PHENANTHROLINE: A NOVEL ARCHITECTURE BASED ON HYDROGEN WELDING AND MULTIPLE π - π STACKING

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The tailoring and design of new materials with multifunctional properties is a subject giving access to nanostructures with well-defined channels. Along these lines, intermolecular hydrogen bonding is a way to access to these materials. We present a mesomorphic structure derivatized-phenanthroline core presenting interesting π - π stabilizing interactions in multiple directions associated to an additional infinite hydrogen bond network. This compound possesses two dimethoxy benzamide and one phenanthroline rings connected to an aryl template and forms a unique coordination system. This results in a trimerization in the crystalline state, strongly stabilized through intricate π - π bondings. Crystals are only obtained as micro plates with a maximum of 50 microns in length. They were recorded at 100 K at the LURE synchrotron facility in Orsay, France.

Keywords: π - π STACKING PHENANTHROLINE MESOMORPHIC

HIGH-RESOLUTION X-RAY STRUCTURE OF A Mg^{2+} COMPLEX OF 5'-GTP

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The first high-resolution structure (0.97Å) of 5'-guanosine triphosphate or a derivative of 5'-GTP is described. Crystals of a mixed Mg^{2+}/Na^+ salt of 5'-GTP were grown by hanging drop vapor diffusion against a precipitant containing PEG 400, sodium citrate and Tris buffer. The title compound, $(Mg^{2+})(Na^+)_4(5'-GTP^{3-})_2 \cdot 32H_2O$, crystallizes in space group $P2_12_12_1$, with unit cell parameters $a = 13.012$, $b = 20.771$, $c = 51.022$ Å. Synchrotron data were collected at SSRL at $-177^\circ C$ up to a resolution of 0.97 Å [8667 independent reflections; overall $R(\text{merge}) = 5.3\%$]. The structure was solved with the program SnB and refined with SHELXL to a current agreement factor of 9.2% for 8365 non-zero reflections [$I > 2\sigma(I)$]. The main core of the molecule consists of a Mg^{2+} ion surrounded by six oxygens from two triphosphate units which forms a tight octahedral array of oxygen atoms in a facial (cis) fashion. Each of the four 5'-GTP molecules in the asymmetric unit contains a ribose sugar in a C_2 -endo conformation, and the guanine bases from neighboring molecules are π -stacked against each other. At the current stage of the structural analysis, one last remaining detail that needs to be worked out concerns the nature of small but persistent peaks that are situated near the 2'-OH and 3'-OH oxygens of two adjacent ribose sugars. It is hoped that the identity of these peaks will be resolved by the time this work is presented at the IUCr Congress.

Keywords: GTP MAGNESIUM NUCLEOTIDE

THE FIRST EVIDENCE OF CH/ π COMPLEX OF DE-TERT-BUTYL CALIX[4]ARENE

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No covalent interactions, such as hydrogen bond, π - π interaction, cation- π interaction, CH/ π interaction etc., play a crucial role in many forefront areas of modern chemistry. p-tert-Butylcalix[4]arene derivatives as the three-dimensional molecules exhibited good receptor properties in the field of supramolecular chemistry. The tert-butyls on the upper-rim of the calix scaffold are reckoned as fairly important in the formation of the host-guest complexes for they act as part of the hydrophobic cavity. However, the de-tert-butylcalix[4]arene derivatives are thought to be too shallow to include guest for a long time. We reported herein two crystal structures of calix[4]arene derivatives, 26,28-dipropoxycalix[4]arene-25,27-diol (1) and 27,28-dipropoxycalix[4]arene-25,26-diol (2), which exhibit host-guest properties in their solid state. (1) forms a dimer structure via self-inclusion of the two cavities, namely one of the four phenyl groups of one cavity embedded into another cavity. The attraction leading to the supramolecular structure is π - π stacking, which is formed by the partial overlapping of the two aromatic groups, and with an interplanar angle of 0° , as well as a distance of 3.46 Å between the two arenes. More interestingly, (1) forms infinite channel architecture via intermolecular CH/ π and π - π interactions. (2) adopts a commonly found in calix[4]arenes in the cone conformation, with one molecule of dichloromethane imbedded within the cavity of four aromatic groups as a guest via a CH/ π interaction. Dichloromethane C(35) to the centroids of the four aromatic rings are 3.606, 4.357, 3.426 and 3.960 Å, respectively.

Keywords: CALIX[4]ARENES SUPRAMOLECULAR CHEMISTRY
CH/ π INTERACTION