

Sucrose is one of the most abundant pure organic chemicals in the world and the one most widely known to nonchemists. In recent years, sucrose is reported as a functional material for developing alternative biofuel cells which use biocatalysts to convert energy from sugar into electrical power. However, melting points among sucrose crystals with high purity are occasionally different with each other and the melting points quoted references range from 160°C to 192 °C . Although many researchers have studied on the melting point by using differential scanning calorimetry (DSC) or optical microscope, there are few reports on the microscopic observation of the crystalline - noncrystalline phase transition of sucrose. In the present work, using high-temperature X-ray diffraction (HTXRD) and simultaneous instruments for X-ray diffractometry and differential scanning calorimetry (XRD-DSC), we have investigated some possible factors involved in the noncrystallization from the crystalline state under isothermal and non-isothermal conditions. The sucrose from commercial source and its recrystallized one were used. XRD-DSC results showed the occurrence of two peaks around 150 °C and 175°C for recrystallized sucrose at heating rate of 10°C/min, while no significant change in the XRD patterns at the first peak was observed during the heating process. The noncrystallization point moved to high temperature as the rate of heating was increased. The Rietveld analysis of HTXRD data is a key point for understanding the mechanism and kinetics of crystalline – noncrystalline phase transition of sucrose under isothermal condition.

Keywords: sucrose, noncrystallization, kinetics

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Structure of sodium L-malate monohydrate

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An X-ray investigation of the title compound was carried out in order to elucidate unequivocally its molecular conformation in the solid state. The structure of sodium L-malate monohydrate Na₂(C₄H₄O₅).H₂O has been determined at room temperature using single-crystal MoKa diffraction techniques with 2011 measured independent reflections at diffraction angles lower than 30°, and 1096 were considered as observed (2s(I)), giving R= 0.05 in the structure refinements. The structure crystallizes in the monoclinic *P*2₁2₁, Z=4, with unit cell parameters *a*= 6.312(1), *b*= 9.766(1) and *c*= 11.221 Å. The crystal packing is governed by hydrogen bonds. L-malic acid, used as a means for creating two-dimensional anionic networks held together by O-H...O hydrogen bonds, has also been demonstrated to be a suitable anionic building block. We have synthesised a new crystal with an interesting hydrogen bonding network, the L-malate ions are linked together with H-bonds involving carboxylate and OH groups forming infinite helical molecular chains parallel to the *a* direction. These chains, in turn, are interconnected in the *bc* plane via H-bond links to intermediate water molecules.

Keywords: crystal engineering, single-crystal X-ray diffraction, hydrogen bonding

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X-ray structure and hydrogen bonding study of taurine and N-(glucitol-1-yl)taurine

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As a part of our continuing interest in this field we report here the crystal structure by X-ray diffraction of these active molecules, taurine (2-aminoethanesulfonic acid) and their derivative N-(glucitol-1-yl)taurine at low temperature in order to establish their conformational and configurational characteristic unequivocally and also to describe their hydrogen-bonding patterns, as they are important constituents of living organism found in nature. Taurine is one of the lesser-known amino acids, nevertheless it plays a role in the body and is essential to newborns of most mammal species, and it also protects our bodies against damage from radiation, is present in relatively high concentration in the central nervous system and brain, acts as neurotransmitter in retine, and shows cardio protective activity. The stability of these compounds that shown zwitterions structure, with electrostatic and hydrogen bonding interaction between the protonated aminogroups and the sulfonate groups results from a network of hydrogen bonds, which maintain the cohesion in the crystal and have been scarcely studied in solid state.

Keywords: zwitterions, hydrogen bonds, X-ray diffraction

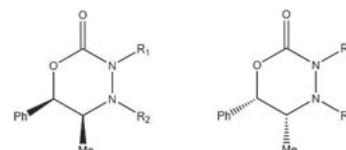
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Binary mixtures of a series of oxa-3,4-diazinan-2-ones

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Structural characterization of a series of 5-methyl-6-phenyl-oxa-3,4-diazinan-2-ones has been carried out. The molecules of interest have been isolated as enantiomerically pure samples. All have two chiral centers, both on the heterocycle in the five and six positions. In addition to structurally characterizing several of the enantiomerically pure samples, various binary mixtures of racemates and pseudoracemates have been prepared, crystallized, and structurally characterized. The likely form of the crystallized products could be mixtures of optically pure crystals, racemic twins, centrosymmetric racemates, pseudo-centrosymmetric racemates, or mixtures of two compounds roughly occupying the same crystallographic positions, where the varying R group appears at half occupancy. For example, (5*R*, 6*S*) 4-isopropyl-5-methyl-6-phenyl-2*H*-1,3,4-oxadiazinan-2-one and (5*S*, 6*R*) 4-isopropyl-5-methyl-6-phenyl-2*H*-1,3,4-oxadiazinan-2-one crystallize individually as isostructural non-centrosymmetric structures in *P*2₁2₁2₁; however, a binary mixture of these two enantiomers crystallize as the racemate in *C*2/*c*.



Keywords: oxadiazinanones, racemates, pseudoracemates