MS34-P10 pH-Dependant crystalline forms of pyridoxal – a comparative crystallographic and theoretical study

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Vitamin B6 is unique among the B vitamins in that it is involved in the metabolism of all three primary macronutrients, namely proteins, lipids and carbohydrates and so it is aligned in high diversity of biochemical reactions.[1] In addition, it has been lately demonstrated that vitamin B6 has a second important function by being an effective antioxidant.[2]

The name 'vitamin B6' is a generic term for a group of six naturally occurring water-soluble vitamers, the 3-hydroxy-2-methylpyridine derivatives pyridoxine (PN), pyridoxal (PL) and pyridoxamine (PM) and their 5 -phosphorylated derivatives. Every form of vitamin has proven ability to form complexes with a broad spectrum of metal ions. Nevertheless, no PL complexes nor salts have been characterized in the solid state by X-ray diffraction so far.[1] The only described form is a hemiacteal PL zwitterion[3, 4] and a platinum hexachloride salt with protonated form of PL hemiacetal.[5]

The current contribution contains structural characterization of pyridoxal hemiacetal chloride and semichloride obtained by crystallization from controlled pH water solutions. The comparison of molecular packing of three PL forms will be presented. The identification of important, directional intermolecular interactions in crystal structures will be supported by the Hirshfeld surface analysis. Additionally, in the case of pyridoxal hemiacetal semichloride where the proton transfer between two PL hemiacetal is observed, the nature of this interaction will be investigated by quantum chemical methods.

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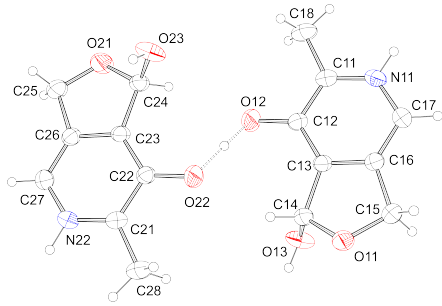

Figure 1.

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