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A novel Schiff base complex of brain fuel (sugar) coordinated with intelligence mineral (Zn): Synthesis, conjoint DFT-experimental evaluation and super oxide dismutation

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Abstract

Sugar–metal ion interaction is involved in many biological phenomena. In the evident interests towards Zn(II) compounds and motivated to extrapolate the search for more persuasive zinc compounds to emerge the ability of sugars towards metallotherapy, a systematic hyphenated DFT-experimental study of a novel sugar Schiff base Zn(II) complex of N-dehydroacetic acid-glucosamine (dha-glsH$_2$) is presented. In addition to its formulation based on various spectroscopic and spectrometric techniques, superoxide dismutation of the title complex is also the active goal of the work. A suitable distorted square planar geometry was revealed and the study stems a well promising biological efficiency of target compounds.

Keywords: Sugar Schiff base; Zn(II); Synthesis; SOD; DFT

1. Introduction

Bivalent zinc ranks as the second most abundant metal ion in humans [1]. The deficiency of this metal results in Crohn's disease and possesses a well-defined relation with the symptoms such as growth failure and immunological disorders [2–4]. Myocardial infarction and congestive heart failure are among other faults that have been liked with decreased levels of zinc in the blood [5,6]. Disruption of glucose homeostasis and diabetes may also intervene under the zinc inefficiency [7,8]. In addition to biological relevance [9], this metal is involved in the pathogenesis of Alzheimer's disease [10].

The coordination chemistry of sugar Schiff base derivates is a fascinating area [11,12] and appends metals to design desirable scaffolds [13]. The property of having anchoring functional groups to form stable chelate complexes is an interesting asset of its form [14–17]. These tunable ligands have found excellent use in medicinal inorganic chemistry [18] and alteration in constituent functionalities establishes well tuned metal binding capabilities [19–22].

On one hand, zinc is called as intelligence mineral because it is involved in so many brain functions [23] through the co-enzyme roles of periodate lysine paraformaldehyde (PLP) and flavine adenine dinucleotide

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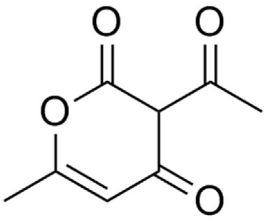
(FAD) in folate and homocysteine metabolism [24]. On the other hand, glucose is called as brain fuel [18] and is the direct source of energy for neurons, which cannot store glucose. In addition, both of the selected ligand and metal systems are contemporary quests to treat Alzheimer's disease. In such purview of the application as has been described, sugar Schiff base appended Zn(II) complex of DHA and Glucosamine was aimed. The superoxide dismutase activity was meticulously done and IC_{50} value was determined. Herein, the goal is to define the probability to extend the pharmacological profile of sugar based Schiff base ligands and the detailed comparative analysis of structural and coordination properties of zinc(II) complexes by a combined density functional theory (DFT) and experimental verification. Compounds that were used in synthesis of Schiff bases are given in Scheme 1.

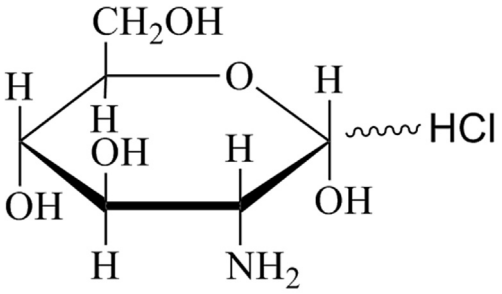
2. Experimental

2.1. Materials and methods

Zinc(II) sulphate heptahydrate was purchased from E. Merck India Chemicals, Bombay, Dehydroacetic acid and Glucosamine hydrochloride were the products



dehydroacetic acid



D-glucosamine hydrochloride

Scheme 1. 2-D structure of compounds used for the synthesis of Schiff bases.

of Sigma Aldrich, USA. All chemicals were of analytical reagent (A.R.) and were used without any further purification.

Elemental composition was performed on an Elemental Vario ELIII Carlo Erba 1108 analyzer from SAIF, CDRI, Lucknow. The percentage of zinc present in the complex was determined following the methodology applied elsewhere [25]. Sherwood Scientific magnetic susceptibility balance (UK) was used to carry out the magnetic susceptibility measurement applying mercury(II) tetrathiocyanatocobaltate(II) as calibrant. The solid state (KBr pellet based) IR spectra were recorded on a Bruker α-T FTIR Series spectrophotometer. Electronic spectral data was recorded by the help of Varian UV–Vis/NIR spectrophotometer in quartz cells using U.V. Visible-NIR Spectrophotometer (Cary-5000), Agilent Technology Germany. A Bio Analytical System Inc. (BASI), USA, Epsilon electrochemical analyzer was used for cyclic voltammetric experiments in DMSO solution of the complex, containing tetrabutylammonium perchlorate (TBAP) as the supporting electrolyte. Thermogravimetric analysis was done by heating the sample at a rate of 10 °C min^{-1} in a temperature range of 30–1000 °C on thermal analyzer at Sophisticated Analytical Instrument Facility, IIT, Mumbai. ^{1}HNMR and ^{13}CNMR spectrum in DMSO-d_6 were recorded at SAIF, C. D.R.I., Lucknow. The electron spray ionization (ESI) mass spectra were recorded on a THERMO Finnigan LCQ advantage max ion trap mass spectrometer.

The optimization of molecular structures of Schiff base dha-glsH_2 and its complex, [Zn(dha-gls)(H_2O)] were carried out by Gaussian 09 program package [26] at the Becke3–Lee–Yang–Parr (B3LYP) hybrid exchange-correlation functional [27,28] with the standard 6-311G/LANL2DZ basic set. After obtaining the energy minimal state of the structure the remaining vibrational frequency calculations, molecular topographies and TD-DFT computations were done to validate our experimental results.

2.2. Preparation of the ligand

The synthesis of Schiff base was carried out as follows. 10 mL aqueous solution of sodium bicarbonate (0.01 M) was poured in a 0.01 M solution of glucosamine hydrochloride prepared in 20 mL methanol-water (v/v 1:1). After lyophilization the solution was filtered followed by the addition of (0.01 M) dehydroacetic acid solution (20 mL methanol) to the filtrate. The solution was then allowed to reflux for 4 h at 30–40 °C under constant stirring using magnetic

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