



Zn(II) complex derived from bidentate Schiff base ligand: Synthesis, characterization, DFT studies and evaluation of anti-inflammatory activity

Mohammad Azam^{a,*}, Saud I. Al-Resayes^a, Agata Trzesowska-Kruszynska^b, Rafal Kruszynski^b, Faiyaz Shakeel^c, Saied M. Soliman^{d,e}, Mahboob Alam^{f,**}, Mohammad Rizwan Khan^a, Saikh Mohammad Wabaidur^a

^a Department of Chemistry, College of Science, King Saud University, P. O. Box 2455, Riyadh, 11451, Saudi Arabia

^b Institute of General and Ecological Chemistry, Lodz University of Technology, Zeromskiego 116, 90-924, Lodz, Poland

^c Department of Pharmaceutics, College of Pharmacy, King Saud University, P. O. Box 2457, Riyadh, 11451, Saudi Arabia

^d Department of Chemistry, Rabigh College of Science and Art, King Abdulaziz University, P.O. Box 344, Rabigh, 21911, Saudi Arabia

^e Department of Chemistry, Faculty of Science, Alexandria University, P. O. Box 426, Ibrahimia, Alexandria, 21321, Egypt

^f Division of Chemistry and Biotechnology, Dongguk University, 123 Dongdae-ro, Gyeongju, Republic of Korea

ARTICLE INFO

Article history:

Received 17 March 2019
Received in revised form
9 September 2019
Accepted 1 October 2019
Available online 5 October 2019

Keywords:

Zn(II) complex
DFT studies
AIM study
Hirshfeld surfaces analyses
Anti-inflammatory activity

ABSTRACT

A novel zinc complex was prepared by the reaction of one equivalent of a bidentate Schiff base, N,N'-bis(2-chlorobenzylidene)-2,2-dimethylpropane-1,3-diamine, L with one equivalent of zinc chloride in methanol, and characterized by elemental analyses, NMR, IR and single crystal X-ray crystallography. The crystallographic studies revealed that the zinc ion in the complex is coordinated to two imine nitrogen atoms of L and two chloride ions of zinc chloride. Furthermore, to obtain insights into the structure and bonding, density functional theory (DFT) calculations were performed. The obtained results were found to be similar with the results obtained from the experimental findings. In addition, the anti-inflammatory activity of the studied zinc complex was also evaluated. The results obtained showed the studied complex could be a good candidate in treatment of inflammatory disorders.

© 2019 Published by Elsevier B.V.

1. Introduction

Over the years, zinc based complexes have shown diverse medicinal applications such as anti-inflammatory, anticonvulsant, antimicrobial, antidiabetic, antioxidant and anti-proliferative activities [1–10]. In addition, several zinc complexes are used as a major ingredient of the medicine used in the treatment of skin diseases [11], and find significant use as a catalyst in various catalytic reactions [1]. In last few decades, Schiff bases have emerged as strong chelating ligands in coordination chemistry [12] due to their ease in synthesis, structural variation [13] and several biological, catalytic and industrial applications [14–16]. The zinc complexes

derived from Schiff bases are extensively studied due to their wide applications in material and biological science [17,18]. In recent years, the pioneer work of Chai and co-workers have explored various transition metal complexes based on Schiff bases and their applications [19–25].

Non-steroidal anti-inflammatory drugs (NSAIDs) are the frequently used analgesic, anti-inflammatory and antipyretic medicines [26]. However, the use of these medicines is associated to several side effects [26–28]. Therefore, to overcome these problems, there are many reports showing that the therapeutic behavior of the drug is improved upon coordination to the metal ions as the metal complexes have higher lipophilicity enabling them to pass quickly from cell membrane to exert their effect [29]. Therefore, considering the medicinal and biological properties of Schiff base and zinc ion, we are reporting here a novel zinc complex derived from L and its characterization by elemental analyses, Infrared spectroscopy (IR), Nuclear Magnetic Resonance (NMR) spectroscopy and single crystal X-ray crystallography. Furthermore,

* Corresponding author.

** Corresponding author.

E-mail addresses: mhashim@ksu.edu.sa, azam_res@yahoo.com (M. Azam), mahboobchem@gmail.com (M. Alam).