



Original article

## Molecular structure simulation of (*E*)-2-(butan-2-ylidene)hydrazinecarbothioamide using the DFT approach, and antioxidant potential assessment of its complexes



Tahmeena Khan<sup>a,\*</sup>, Iqbal Azad<sup>a</sup>, Rumana Ahmad<sup>b</sup>, Alfred J. Lawrence<sup>c</sup>, Mohammad Azam<sup>d</sup>, Saikh Mohammad Wabaidur<sup>d</sup>, Saud I. Al-Resayes<sup>d</sup>, Saman Raza<sup>c</sup>, Abdul Rahman Khan<sup>a</sup>

<sup>a</sup> Department of Chemistry, Integral University, Dasauli, P.O. Bas-ha, Kursi Road, Lucknow 226026, UP, India

<sup>b</sup> Department of Biochemistry, Era's Lucknow Medical College and Hospital, Era's University, Lucknow 226003, U.P., India

<sup>c</sup> Department of Chemistry, Isabella Thoburn College, 7, Faizabad Road, Lucknow 226007, UP, India

<sup>d</sup> Department of Chemistry, College of Science, King Saud University, PO Box-2455, Riyadh 11451, Saudi Arabia

## ARTICLE INFO

## Article history:

Received 15 November 2020

Revised 10 December 2020

Accepted 17 December 2020

Available online 24 December 2020

## Keywords:

Gaussian

Optimization

Quantum

Mechanics

Thiosemicarbazone

Antioxidant

## ABSTRACT

The molecular structure of (*E*)-2-(butan-2-ylidene)hydrazinecarbothioamide (2-butanone thiosemicarbazone) was validated by density functional theory (DFT) calculations. The characterization of the ligand was done using various spectroscopic techniques. Four transition metal complexes were prepared with the ligand and their antioxidant activity was tested. Molecular docking studies of the complexes were also performed against nicotinamide adenine dinucleotide phosphate (NADPH) and myeloperoxidase (MPO). Structure validation of the ligand was done in Gaussian 09 software. The geometry optimization was done at B3LYP/6-31G++(d,p) level. The <sup>1</sup>H and <sup>13</sup>C NMR chemical shifts, FT-IR vibrations and UV–visible transitions were validated with the help of theoretical calculations. The frontier molecular orbital analysis, molecular electrostatic potential (MEP) and global reactivity descriptors were calculated to predict the stability of the molecule. Non-linear optical (NLO) properties were assessed and compared with urea. Natural bond orbital (NBO) analysis was done to predict the stability of the ligand resulting from hyper conjugative interactions and electron delocalization. Molecular docking studies of the complexes were performed with iGEMDOCK 2.1 and AutoDock 4.2.6. Antioxidant potential was assessed by 2,2-diphenyl-1-picrylhydrazyl (DPPH) Assay. <sup>1</sup>H and <sup>13</sup>C correlation coefficients (*R*<sup>2</sup>) were 0.9964 and 0.9974 respectively. In case of FT-IR, the correlation coefficient (*R*<sup>2</sup>) was 0.9984. [Fe(C<sub>5</sub>H<sub>11</sub>N<sub>3</sub>S)<sub>2</sub>(SO<sub>4</sub>)] possessed maximum antioxidant potential followed by [Cu(C<sub>5</sub>H<sub>11</sub>N<sub>3</sub>S)<sub>2</sub>(SO<sub>4</sub>)]. Molecular docking findings suggested that the Fe complex released the minimum binding energy. Computational structure validation is an important aspect in finding a lead moiety. The theoretical spectral findings correlated well with the experimental findings in the present study. The metal complexes showed appreciable antioxidant potential as predicted by the computational and experimental findings. The ligand possessed better NLO properties than urea.

© 2020 The Author(s). Published by Elsevier B.V. on behalf of King Saud University. This is an open access article under the CC BY-NC-ND license (<http://creativecommons.org/licenses/by-nc-nd/4.0/>).

## 1. Introduction

Through quantum mechanical simulations the structural characteristics of new materials can be easily and accurately predicted.

\* Corresponding author.

E-mail address: [tahminakhan30@yahoo.com](mailto:tahminakhan30@yahoo.com) (T. Khan).

Peer review under responsibility of King Saud University.



Production and hosting by Elsevier

<https://doi.org/10.1016/j.jksus.2020.101313>

1018–3647/© 2020 The Author(s). Published by Elsevier B.V. on behalf of King Saud University.

This is an open access article under the CC BY-NC-ND license (<http://creativecommons.org/licenses/by-nc-nd/4.0/>).

The computational predictions can also validate the experimental findings. Owing to the fast and accurate predictions by automated softwares, computational chemistry has received considerable attention (Matulkova et al., 2008; Boo et al., 2008). Due to the remarkable growth in the field of computational resources, many theoretical algorithms have been proposed to calculate various properties of a compound using semi-empirical and DFT methods. The theoretical data can be easily compared with the experimental one (Brewerton, 2008; Ravna and Sager, 2008). DFT has become a major tool for structure prediction and understanding the mechanistic approach (Lipkowitz et al., 2009; Lorenc et al., 2008). Quantum studies enable to envisage the structure of a chemical entity with the help of computer aided softwares. With the added



## MINI-REVIEW ARTICLE

## Psychological and Mental Health Issues During the SARS-CoV-2 Global Pandemic: A Critical Analysis



Tahmeena Khan<sup>1,\*</sup>, Iqbal Azad<sup>1</sup> and Alfred J. Lawrence<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Integral University, Lucknow, India; <sup>2</sup>Department of Chemistry, Faculty of Science, Isabella Thoburn College, Lucknow, India

**Abstract: Introduction:** With the outbreak of the SARS-CoV-2 in Wuhan, China in December, 2019, presently over 200 countries have been facing gruesome health effects of the deadly virus, with cases and casualties on the rise. So far, no concrete medicinal drug or vaccine has been developed to check the lethal viral infection, henceforth authorities have emphasized on practicing social distancing and imposed strict lockdowns forcing people to confine in their homes.

**Material and Methods:** This review was aimed to analyze the effects on mental health and well being during the pandemic. The studies cited in the review were sourced from journals, books and digital media reports. The research papers indexed in databases such as PUBMED, SCOPUS, INDEX COPERNICUS, CHEMICAL AND BIOLOGICAL ABSTRACTS, MEDLINE, EMBASE, EBSCO, DOAJ and THOMSON REUTERS were reviewed and have been included in the review.

**Results:** The coronavirus mayhem has not only posed a threat to human health, but also jolted different aspects of society, including mental and psychological health. Loss of freedom, boredom, fear and angst are some of the mild psychological effects, whereas a rise in domestic violence and suicidal tendencies is the more serious consequence reported from different parts of the world during the lockdown period.

**Conclusion:** This article is a comprehensive analysis of the effects on mental and psychological well being during this critical time. Strategic measures to be adopted by individuals and administration to cope up with the situation are also suggested as it should be an immediate priority to address the overall distress caused by the pandemic in public.

## ARTICLE HISTORY

Received: May 11, 2020  
Revised: August 19, 2020  
Accepted: September 17, 2020

DOI:  
10.2174/2666796701999201117103132



**Keywords:** Coronavirus, psychological, distress, mental, lockdown, suicide, violence, economic.

### 1. INTRODUCTION

The Severe Acute Respiratory Syndrome (SARS) coronavirus (SARS-CoV-2) has emerged as the greatest epidemic in recent times. The World Health Organization (WHO) and the International Committee on Taxonomy of Viruses have designated the virus as SARS-CoV-2. The virus originated in Wuhan, China, in 2019, has spread from animals to humans and later on from inter-personal transmission across hundreds of nations [1]. The coronaviruses belonging to the family *Coronaviridae* are known to cause respiratory and intestinal infections in living beings. The *Coronaviridae* sub-family is divided into four main genera viz.  $\alpha$ ,  $\beta$ ,  $\gamma$  and  $\delta$  according to the International Committee for Taxonomy of Viruses. The term corona is Latin in origin, meaning "crown", which has been designated owing to the crown-like morphology of the virus under electron microscopy [2].

They are zoonotic because of their mode of transmission from animals to humans. Two major outbreaks caused by coronaviruses viz. SARS in 2003 resulted in approximately 1,000 and Middle East Respiratory Syndrome (MERS) in 2012 caused 862 fatalities. MERS-CoV was first detected in Saudi Arabia. It was responsible for 2,494 confirmed cases [3]. The SARS was first reported in 2003, which resulted in about 8096 cases and 774 deaths taking place in 30 countries [4].

#### 1.1. Mode of Spread and Symptomology

Upon the onset of the infection, initially, symptoms of Acute Respiratory Distress Syndrome (ARDS) are developed. Viral pneumonia is another common symptom leading to respiratory damage in severe cases. Fever, chills, myalgia and cough are the more prominent and common symptoms, along with sore throat and rhinorrhea [5]. Watery diarrhea is caused after one week of the onset of the disease [6].

The interpersonal transmission has been recognized as the major mode of spread of the viral infection. The most important route of contamination is through the contact of the

\*Address correspondence to this author at the Department of Chemistry, Faculty of Science, Integral University, P.O. Box: 226026, Lucknow, India; Tel/Fax: 09793232443; E-mails: tahminakhan30@yahoo.com, tahmeenak@iul.ac.in

## Occurrence Of Indoor Air Pollution And Health Symptoms In Households Of Nanpara (Bahraich)-A Survey Based Study

Alfred J. Lawrence<sup>1</sup>, Tahmeena Khan<sup>2\*</sup>, Iqbal Azad<sup>2</sup>, Saman Raza<sup>1</sup> and Abdul Rahman Khan<sup>2</sup>

1. *Isabella Thoburn College, Department of Chemistry, Lucknow - 226 007*

2. *Integral University, Department of Chemistry, Lucknow - 226 026*

\*Corresponding author, Email : [tahmeenak@iul.ac.in](mailto:tahmeenak@iul.ac.in); [alfred\\_lawrence@yahoo.com](mailto:alfred_lawrence@yahoo.com)

The study was conducted in seventy households in Nanpara town of Bahraich district from February-March 2019 to study the house characteristics, energy choices and health symptoms faced by the dwellers. The aim of the study was to identify probable occurrences of indoor air pollution (IAP) and health status of the occupants along with their socio-demographic profile. 50% of the sampled population was employed. 40.15% of the houses had a closed cooking space. In 77.74% of households, the kitchen had improper ventilation conditions whereas only 22% of households had adequate ventilation in the kitchen. The overall sanitary condition of the houses was very poor. Usage of LPG was frequent, still, 50% of households had traditional cooking stoves used for cooking and other heating purposes. Although the households had an electricity connection, showing their progression, yet they relied on crude fuel (44%) for cooking their meals due to easy availability and affordability. Educational status has a direct influence on the choices we make in day to day life. Majority of the inhabitants had secondary educational status (54.71%) and a meagre percentage of people went for higher education (11%). The correlation was further made with the willingness of the people to change their energy source. Eye irritation (81.13%), chest tightness (56.60%), shortness of breath (41.5%), headache (92.4%), heartburn (50.9%), dizziness (39%) and fatigue (79.24%) and phlegm (86.79%) were some of the common symptoms reported by the dwellers which were more frequent in the winter season. These symptoms are usually linked to the increased inhalation of particulates and CO<sub>2</sub> originating from smoke and due to inadequate ventilation.

### KEYWORDS

Questionnaire, Indoor, Health, Pollutants, Eye irritation

### 1. INTRODUCTION

Air pollution is responsible for around a million deaths globally, according to the World Health Organization (WHO) findings [1]. In the past, air pollution was linked to vehicular exhaust and smoke and confined within urban boundaries. Today air pollution has spread like an epidemic and become a global issue of grave concern. The actual exposure to air pollutants includes all micro-environments a person spends time in [2]. Indoor air pollution (IAP) is a direct consequence of outdoor pollution. IAP is one of the leading causes of health risks to the exposed population. Literature survey has shown that in developing countries, health impacts of indoor air pollution far outweigh those of outdoor air pollution [3]. There are many sources, like heating, cooking, cleaning, smoking and building materials which affect the indoor ambience considerably. Around half of the world's population and upto 90% of the rural population relies on biomass fuels in the form of wood, crop

residue and animal dung [4]. People belonging to low and middle income countries in southeast Asia and western Pacific regions are highly susceptible to the problem. Women and children are more vulnerable as they spend a substantial amount of their time indoors.

A strong association has been established between smoke exposure and chronic bronchitis in women as they are the primary cooks [5]. Studies in India have reported increased child deaths in solid-fuel consuming households aged between 1-4 years. Girls were found to be more affected than boys in the same study [6]. Tuberculosis in the occupants has been attributed to cooking smoke in the age group of 20 years and above [7]. High odd ratio, namely 2.65 was obtained for women in rural areas in the same study. Results from a study among elderly men and women (age  $\geq$  60 years) showed a higher prevalence of asthma in biomass fuel users (odd ratio (OR) = 1.59; 95% confidence interval (CI) : 1.30-1.94) as compared to men (OR = 1.83; 95% CI: 1.32-2.53) [8]. Prevalence of asthma was greater in women as they are directly exposed to cooking smoke. The present study was

## Air Quality in Six Northern Indian Cities During Diwali 2020: The Real Tragedy in Disguise

A.J. LAWRENCE<sup>1</sup>, A. ABRAHAM<sup>1</sup>, F. ALI<sup>1</sup>, S. ARIF<sup>1</sup>, S. FATIMA<sup>2</sup>, U. FATIMA<sup>1</sup> and T. KHAN<sup>3,\*</sup>

<sup>1</sup>Department of Chemistry, Isabella Thoburn College, Lucknow-226007, India

<sup>2</sup>Department of Education, Unity Degree College, Lucknow-227107, India

<sup>3</sup>Department of Chemistry, Integral University, Lucknow-226026, India

\*Corresponding author: Fax: +98 21 2222512; E-mail: tahminakhan30@yahoo.com

Received: 19 December 2020;

Accepted: 17 February 2021;

Published online: 20 March 2021;

AJC-20303

North Indian cities have been highly polluted, especially in winters, which coincide with the Diwali festival. This year, the government imposed ban on the burning of firecrackers. This study was undertaken from 4<sup>th</sup>-21<sup>st</sup> November, 2020 to monitor the air quality variation with respect to PM<sub>10</sub> and PM<sub>2.5</sub> for Delhi, Lucknow, Ghaziabad, Muzaffarnagar, Greater Noida and Bulandshahar cities during and post Diwali period, to know whether there was any impact of the warnings. The hourly variations in the AQI were very poor between 8:00 p.m.-10:00 p.m. on Diwali day. Significant short term variation in the AQI was observed during the night. A weak positive correlation was obtained between the temperature and AQI, whereas a negative relationship was established with humidity. As compared to last year's AQI, higher values were obtained this year. The short-term variation in air quality may prove crucial in future in the wake of COVID-19 pandemic.

**Keywords:** COVID-19, Firecrackers, Correlation, Pollution.

### INTRODUCTION

The winter season in Northern India onsets from October and extends till February. It has been observed that air pollution is usually worse in winter season due to greater suspension time of pollutants in the air, owing to lower temperature, wind speed and high moisture content [1]. Proper mixing and dispersion do not take place at low wind speed, leading to frequent smog and longer retention time of pollutants at a particular place. The winter months coincide with Diwali (festival of lights), one of the largest festivals in India, celebrated with great fervour especially in northern India. The traditional firecrackers burning during the festival leads to a huge variation in air quality as the perilous aftermath. A distinct association between air pollution and firecracker burning has been established in the previous studies [1]. The research has been mainly concentrated on measuring pollutants' concentration before, during and after the festival [2]. The havoc caused during the festival led to a ban on the selling of firecrackers by the Supreme Court of India in 2017. The air quality variation during Diwali, which is of short-term in nature is gaining considerable interest

as the short-term variation causes long term adverse health effects [3]. In 2019, after Diwali, metropolitan cities like Delhi, Patna and Lucknow were worst hit in terms of air quality.

According to the Central Pollution Control Board's (CPCB) network of monitoring centres, the Air Quality Index (AQI) of these cities reached around 400 which was far more worse than the previous year's data. The deterioration in Delhi's air was also due to the stubble burning in neighbouring states, which was exacerbated by the burning of firecrackers [4]. Elaborating on the last year's variation in the air quality of the national capital during the Diwali episode, about a week before the festival the AQI crossed 300, which was categorized as very poor. On Diwali day, the AQI reached to 340 and the morning after, it went further higher reaching upto 368. What makes firecrackers so hazardous is the pollutants which are released in the environment, including sulphur dioxide and nitrogen oxides, particulate matter (PM<sub>10</sub> and PM<sub>2.5</sub>), water soluble ions and heavy metals [5]. Out of these pollutants, PM<sub>2.5</sub> is extremely harmful, owing to its small size and deeper penetration in the respiratory tract and to lungs. Firecracker burning led to a high hourly average of the PM<sub>2.5</sub> concentration during