



## Research article

## Comparative study of the antioxidant capability of EDTA and Irganox

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## ARTICLE INFO

## Keywords:

DFT

HAT

IP

PA

Ethylenediaminetetraacetic acid

## ABSTRACT

Oxidative stress makes it difficult to preserve food and negatively affect the applicability of polymeric packaging. It is typically caused by an excess of free radicals, and it is dangerous to human health, resulting in the onset and development of diseases. The antioxidant ability and activity of ethylenediaminetetraacetic acid (EDTA) and Irganox (Irg) as synthetic antioxidant additives were studied. Three different antioxidant mechanisms were considered and compared by calculating bond dissociation enthalpy (BDE), ionization potential (IP), proton dissociation enthalpy (PDE), proton affinity (PA), and electron transfer enthalpy (ETE) values. Two density functional theory (DFT) methods were used, M05-2X and M06-2X with the 6-311++G(2d,2p) basis set in gas phase. Both additives can be used to protect pre-processed food products and polymeric packaging from oxidative stress related material deterioration. By comparing the two studied compounds, it was found that EDTA has a higher antioxidant potential than Irganox. To the best of our knowledge several studies have been carried out to understand the antioxidant potential of various natural and synthetic species, but EDTA and Irganox were not compared and investigated before. These additives can be used to protect pre-processed food products and polymeric packaging and prevent material deterioration caused by oxidative stress.

## 1. Introduction

Free radicals can damage biologically important species in the body such as carbohydrates, proteins, lipids, DNA strains, cells, and tissues through the oxidative stress [1, 2]. Oxidative stress is dangerous to human health, resulting in the development of numerous diseases [3]. There are reactive oxygen (ROS), reactive nitrogen (RNS), and reactive sulfur species (RSS). These are responsible for many diseases such as cancer, cardiovascular diseases like atherosclerosis and stroke, neurological disorders, renal disorders, liver disorders, hypertension, rheumatoid arthritis and others [4, 5, 6]. The growing understanding of the dual nature of radicals has sparked a rise of interest in the compounds that might reduce excessive quantities of reactive oxygen, nitrogen, and sulfur species, hence limiting their damaging action. These substances, referred to as antioxidants, are a diverse set of molecules with the capacity to lessen oxidative stress [6, 7]. Antioxidants are compounds that may give free radicals an electron, which detoxifies them [8].

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<https://doi.org/10.1016/j.heliyon.2023.e16064>

Received 3 March 2023; Received in revised form 27 April 2023; Accepted 4 May 2023

Available online 13 May 2023

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