

# Dual Descriptor also reveals the Janus-Faced Behaviour of Diiodine

Jorge Martinez<sup>1</sup>

<sup>1</sup>Universidad Andres Bello

May 5, 2020

## Abstract

The diiodine molecule as Janus-faced ligand was evidenced by Rogachev and Hoffmann [A.Y. Rogachev *et al.*, *JACS*, 2013, **135**, 3262] through an exhaustive investigation based on the Molecular Orbital Theory (MOT), Natural Bond Orbital (NBO), and Energy Decomposition Analysis (EDA). In the present article the same conclusions were attained when applying the dual descriptor (DD or second-order Fukui function) on the same molecule. An advantage of DD lies on the fact of being an orbital-free descriptor, meaning that it is based only upon total electron density when written in its most accurate operational formula. In addition, the present work is an application of the generalized operational formula of the dual descriptor published in 2016 so allowing to predict the same coordination modes as experimentally known: bent “end-on” and linear “end-on”

## Hosted file

IJQC\_definite\_LaTeX\_version\_JMartinez.pdf available at <https://authorea.com/users/291665/articles/419091-dual-descriptor-also-reveals-the-janus-faced-behaviour-of-diiodine>

## Hosted file

Figure01.eps available at <https://authorea.com/users/291665/articles/419091-dual-descriptor-also-reveals-the-janus-faced-behaviour-of-diiodine>

## Hosted file

Figure02.eps available at <https://authorea.com/users/291665/articles/419091-dual-descriptor-also-reveals-the-janus-faced-behaviour-of-diiodine>

## Hosted file

Figure03.eps available at <https://authorea.com/users/291665/articles/419091-dual-descriptor-also-reveals-the-janus-faced-behaviour-of-diiodine>

## Hosted file

Figure04.eps available at <https://authorea.com/users/291665/articles/419091-dual-descriptor-also-reveals-the-janus-faced-behaviour-of-diiodine>