

NBO Bibliography 2020

2531 publications – Revised and compiled by Ariel Andrea on Aug. 9, 2021

Aarabi, M.; Gholami, S.; Grabowski, S. J.

S-H ... O and O-H ... O Hydrogen Bonds-Comparison of Dimers of Thiocarboxylic and Carboxylic Acids
Chemphyschem, (21): 1653-1664 2020. 10.1002/cphc.202000131

Aarthi, K. V.; Rajagopal, H.; Muthu, S.; Jayanthi, V.; Girija, R.

Quantum chemical calculations, spectroscopic investigation and molecular docking analysis of 4-chloro-N-methylpyridine-2-carboxamide
Journal of Molecular Structure, (1210) 2020. 10.1016/j.molstruc.2020.128053

Abad, N.; Lgaz, H.; Atioglu, Z.; Akkurt, M.; Mague, J. T.; Ali, I. H.; Chung, I. M.; Salghi, R.; Essassi, E.; Ramli, Y.

Synthesis, crystal structure, hirshfeld surface analysis, DFT computations and molecular dynamics study of 2-(benzyloxy)-3-phenylquinoxaline

Journal of Molecular Structure, (1221) 2020. 10.1016/j.molstruc.2020.128727

Abbenseth, J.; Wtjen, F.; Finger, M.; Schneider, S.

The Metaphosphite (PO₂) Anion as a Ligand

Angewandte Chemie-International Edition, (59): 23574-23578 2020. 10.1002/anie.202011750

Abbenseth, J.; Goicoechea, J. M.

Recent developments in the chemistry of non-trigonal pnictogen pincer compounds: from bonding to catalysis

Chemical Science, (11): 9728-9740 2020. 10.1039/d0sc03819a

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A Terminal Chlorophosphinidene Complex

Zeitschrift Fur Anorganische Und Allgemeine Chemie, (646): 565-569 2020. 10.1002/zaac.202000010

Abbiche, K.; Acharjee, N.; Salah, M.; Hilali, M.; Leknifli, A.; Komiha, N.; Marakchi, K.

Unveiling the mechanism and selectivity of 3+2 cycloaddition reactions of benzonitrile oxide to ethyl trans-cinnamate, ethyl crotonate and trans-2-penten-1-ol through DFT analysis

Journal of Molecular Modeling, (26) 2020. 10.1007/s00894-020-04547-6

Abbiche, K.; Mohammad-Salim, H.; Salah, M.; Mazoir, N.; Zeroual, A.; El Abdallaoui, H. E.; El Hammadi, A.; Hilali, M.; Abdallah, H. H.; Hochlaf, M.

Insights into the mechanism and regiochemistry of the 1,3-dipolar cycloaddition reaction between benzaldehyde and diazomethane

Theoretical Chemistry Accounts, (139) 2020. 10.1007/s00214-020-02662-4

Abd El-Mageed, H. R.; Mustafa, F. M.; Abdel-Latif, M. K.

The ability of gold nanoclusters as a new nanocarrier for D-penicillamine anticancer drug: a computational chemistry study

Structural Chemistry, (31): 781-793 2020. 10.1007/s11224-019-01462-2

Abdel-Bary, A. S.; Tolan, D. A.; Nassar, M. Y.; Taketsugu, T.; El-Nahas, A. M.

Chitosan, magnetite, silicon dioxide, and graphene oxide nanocomposites: Synthesis, characterization, efficiency as cisplatin drug delivery, and DFT calculations
International Journal of Biological Macromolecules, (154): 621-633 2020.
10.1016/j.ijbiomac.2020.03.106

Abdel-Latif, M. K.; Abd El-Mageed, H. R.; Mohamed, H. S.; Mustafa, F. M.
Study the solvation effect on 6-phenyl-2-thioxo-1,2-dihydropyridine-3-carbonitrile derivatives by TD-DFT calculations and molecular dynamics simulations
Journal of Molecular Structure, (1200) 2020. 10.1016/j.molstruc.2019.127056

Abdel-Rahman, L. H.; Abu-Dief, A. M.; Moustafa, H.; Abdel-Mawgoud, A. A. H.
Design and nonlinear optical properties (NLO) using DFT approach of new Cr(III), VO(II), and Ni(II) chelates incorporating tri-dentate imine ligand for DNA interaction, antimicrobial, anticancer activities and molecular docking studies
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Theoretical investigation on the structure and stability of some neutral noble gas compounds containing Xe-Xe bond
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Abdi, N.; Seif, A.; Azizi, K.; Goodarzi, M.; Rashidi, A.
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Role of Asp190 in the Phosphorylation of the Antibiotic Kanamycin Catalyzed by the Aminoglycoside Phosphotransferase Enzyme: A Combined QM:QM and MD Study

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A molecular electron density theory study to understand the interplay of theory and experiment in nitrone-enone cycloaddition

Journal of Chemical Sciences, (132) 2020. 10.1007/s12039-020-01766-5

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Understanding the regio- and diastereoselective synthesis of a potent antinociceptive isoxazolidine from C-(pyridin-3-yl)-N-phenylnitrone in the light of molecular electron density theory

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Catalytic Effect of Electric Fields on the Kemp Elimination Reactions with Neutral Bases

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Deciphering the Curly Arrow Representation and Electron Flow for the 1,3-Dipolar Rearrangement between Acetonitrile Oxide and (1S,2R,4S)-2-Cyano-7-oxabicyclo 2.2.1 hept-5-en-2-yl Acetate Derivatives

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A DFT Investigation on Two Proposed Anticancer Platinum(IV) Drugs
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Blue Highly Fluorescent Boranil Derived From Anil Ligand: Synthesis, Characterization, Experimental and Theoretical Evaluation of Solvent Effect on Structures and Photophysical Properties
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Synthesis, crystal structure, DFT calculations, molecular docking study and Hirshfeld surface analysis of alkoxido-bridged dinuclear iron(III) complex

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