# Rifaat Hilal

List of Publications by Year
in descending order

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|---|---|---|---|
| 23 papers | 149 citations | 1306789 7 h-index | 1199166 12 g-index |
| 23 all docs | 23 docs citations | 23 times ranked | 159 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Time dependent â€“ density functional theory characterization of organic dyes for dye-sensitized solar cells. Molecular Simulation, 2017, 43, 1523-1531. | 0.9 | 22 |
| 2 | Molecular orbital treatment of phenylfurans and bifurans. International Journal of Quantum Chemistry, 1981, 19, 383-399. | 1.0 | 17 |
| 3 | Electronic structure of the peptide linkage. I. Equilibrium geometry and electronic properties of formhydroxamic acid. International Journal of Quantum Chemistry, 1984, 26, 183-196. | 1.0 | 17 |
| 4 | Equilibrium geometry and gas-phase proton affinity of 2-thiouracil derivatives. International Journal of Quantum Chemistry, 2002, 87, 378-388. | 1.0 | 12 |
| 5 | Theoretical investigation of the proton affinities of benzazoles in the gas phase and in solution. International Journal of Quantum Chemistry, 2005, 103, 332-343. | 1.0 | 12 |
| 6 | Electronic structure of orotic acid III geometric feature and thermal properties of some transition metal orotic acid complexes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 63, 740-748. | 2.0 | 11 |
| 7 | Molecular charge distribution and chemical binding in five-membered heterocycles. I. Journal of Computational Chemistry, 1980, 1, 348-357. | 1.5 | 10 |
| 8 | Thermal dissociation of 1,2-dioxethane. I. Charge density distribution along the reaction path and in differentHF solutions. International Journal of Quantum Chemistry, 1981, 19, 805-819. | 1.0 | 7 |
| 9 | On the electronic structure of transition metal complexes. I. An <scp>INDOâ€MO</scp> investigation of some octahedral complex ions. International Journal of Quantum Chemistry, 1985, 28, 877-887. | 1.0 | 5 |
| 10 | A QSAR study for 2-(4-aminophenyl)benzothiazoles: using DFT optimisation of geometry of molecules. Molecular Simulation, 2011, 37, 62-71. | 0.9 | 5 |
| 11 | Unconventional CHÎ´+â‹¯N hydrogen bonding interactions in the stepwise solvation of the naphthalene radical cation by hydrogen cyanide and acetonitrile molecules. Physical Chemistry Chemical Physics, 2016, 18, 2580-2590. | 1.3 | 5 |
| 12 | Thermal dissociation of 1,2-dioxethane. II. Quantum topology of the charge distributions. International Journal of Quantum Chemistry, 1981, 19, 821-831. | 1.0 | 4 |
| 13 | DFT investigation of sites of protonation of antitumor of 2-(4-aminophenyl)benzazoles in the gas phase and in solution. International Journal of Quantum Chemistry, 2005, 103, 449-459. | 1.0 | 4 |
| 14 | Electronic Absorption Spectra of Some Triazolopyrimidine Derivatives. International Journal of Spectroscopy, 2011, 2011, 1-8. | 1.4 | 4 |
| 15 | Localized molecular orbitals and chemical binding in five-membered heterocycles. II. Journal of Computational Chemistry, 1980, 1, 358-367. | 1.5 | 3 |
| 16 | Thermal dissociation of 1,2-dioxethane. III. Localized molecular-orbital study. International Journal of Quantum Chemistry, 1981, 19, 833-845. | 1.0 | 3 |
| 17 | Solvent-assisted excited state proton transfer and photoacidity of 2-hydroxypyridine. A nonadiabatic dynamics study. Molecular Simulation, 2019, 45, 165-177. | 0.9 | 3 |
| 18 | Electronic structure of the peptide linkage. II. A molecular orbital treatment of the electronic spectra of benzohydroxamic acids. International Journal of Quantum Chemistry, 1985, 27, 115-133. | 1.0 | 2 |

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|---|---|---|---|
| 19 | On the electronic structure of transition-metal complexes II. Bonding characteristics in titanium chloride systems. International Journal of Quantum Chemistry, 1985, 28, 715-721. | 1.0 | 2 |
| 20 | Photodissociation of 1,2-dioxetane: An excited state nonadiabatic dynamics study. Journal of the Indian Chemical Society, 2022, 99, 100440. | 1.3 | 1 |
| 21 | Closed-shellSCF-CIMO treatment of all-reactive electrons in complex heteroorganic molecules. International Journal of Quantum Chemistry, 1979, 15, 37-47. | 1.0 | 0 |
| 22 | Electronic Structure and Spectra of Some Carbamates INDO/Sâ€CI Treatment. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1991, 95, 192-197. | 0.9 | 0 |
| 23 | Electronic structure of some adenosine receptor antagonists: I. Equilibrium geometries, charge density distributions, and substituent effects. International Journal of Quantum Chemistry, 2002, 87, 389-399. | 1.0 | 0 |