StÃ©phane Humbel

List of Publications by Year
in descending order

66 papers	4,263 citations	279487 23 h-index	106150 65 g-index
74 all docs	74 docs citations	74 times ranked	3665 citing authors

#	Article	IF	Citations
1	ONIOM:Â A Multilayered Integrated MO + MM Method for Geometry Optimizations and Single Point Energy Predictions. A Test for Dielsâ^'Alder Reactions and Pt(P(t-Bu)3)2+ H2Oxidative Addition. The Journal of Physical Chemistry, 1996, 100, 19357-19363.	2.9	1,824
2	The IMOMO method: Integration of different levels of molecular orbital approximations for geometry optimization of large systems: Test for nâ€butane conformation and SN2 reaction: RCl+Clâ^. Journal of Chemical Physics, 1996, 105, 1959-1967.	1.2	659
3	Energetics using the single point IMOMO (integrated molecular orbital+molecular orbital) calculations: Choices of computational levels and model system. Journal of Chemical Physics, 1996, 105, 3654-3661.	1.2	282
4	Compact valence bond functions with breathing orbitals: Application to the bond dissociation energies of F2 and FH. Journal of Chemical Physics, 1994, 101, 5969-5976.	1.2	187
5	IMOMO(G2MS):â€‰ A New High-Level G2-Like Method for Large Molecules and Its Applications to Dielsâ^'Alder Reactions. Journal of Physical Chemistry A, 1997, 101, 227-233.	1.1	112
6	Nature of the Differential Electron Correlation in Three-Electron Bond Dissociations. Efficiency of a Simple Two-Configuration Valence Bond Method with Breathing Orbitals. The Journal of Physical Chemistry, 1994, 98, 11697-11704.	2.9	103
7	Diffusion coefficients of additives in polymers. I. Correlation with geometric parameters. Journal of Applied Polymer Science, 2001, 82, 2422-2433.	1.3	94
8	Diastereoselective Tandem Additionâ^'Cyclization Reactions of Unsaturated Tertiary Amines Initiated by Photochemical Electron Transfer (PET). Journal of Organic Chemistry, 2000, 65, 8690-8703.	1.7	88
9	What Is Physically Wrong with the Description of Odd-Electron Bonding by Hartree-Fock Theory? A Simple Nonempirical Remedy. Journal of the American Chemical Society, 1995, 117, 9003-9011.	6.6	58
10	Configurational Stability of Chlorophosphines. Inorganic Chemistry, 2003, 42, 420-427.	1.9	47
11	Tandem mass spectrometry of doubly charged poly(ethylene oxide) oligomers produced by electrospray ionization. International Journal of Mass Spectrometry, 2008, 272, 1-11.	0.7	45
12	Short Strong Hydrogen Bonds:â€‰ A Valence Bond Analysis. Journal of Physical Chemistry A, 2002, 106, 5517-5520.	1.1	42
13	From Prochiral N-Heterocyclic Carbenes to Optically Pure Metal Complexes: New Opportunities in Asymmetric Catalysis. Journal of the American Chemical Society, 2020, 142, 93-98.	6.6	39
14	HÃ¼ckel-Lewis Projection Method: A â€œWeights Watcherâ€•for Mesomeric Structures. Journal of Physical Chemistry A, 2008, 112, 13256-13262.	1.1	36
15	Role of the Adducted Cation in the Release of Nitroxide End Group of Controlled Polymer in Mass Spectrometry. Macromolecules, 2009, 42, 1849-1859.	2.2	36
16	Simultaneous Control of Central and Helical Chiralities: Expedient Helicoselective Synthesis of Dioxa[6]helicenes. Journal of the American Chemical Society, 2020, 142, 16199-16204.	6.6	36
17	Tandem Mass Spectrometry of Trimethylsilyl-Terminated Poly(Dimethylsiloxane) Ammonium Adducts Generated by Electrospray Ionization. Journal of the American Society for Mass Spectrometry, 2011, 22, 649-658.	1.2	34
18	Three-Electron Binding between Carbonyl-like Compounds and Ammonia Radical Cation. Comparison with the Hydrogen Bonded Complex. Journal of the American Chemical Society, 1999, 121, 5507-5512.	6.6	31

#	Article	IF	Citations
19	HOâˆ´OHâˆ': a model for stable three-electron bonded peroxide radical anions. Chemical Physics Letters, 1995, 247, 126-134.	1.2	29
20	In^{III}â€Catalysed Tandem Câ€"C and Câ€"O Bond Formation between Phenols and Allylic Acetates. European Journal of Organic Chemistry, 2010, 2010, 6239-6248.	1.2	28
21	The Nature of Resonance in Allyl Ions and Radical. Journal of Physical Chemistry A, 2008, 112, 13249-13255.	1.1	25
22	Bonding of Gold with Unsaturated Species. ChemPhysChem, 2012, 13, 2090-2096.	1.0	25
23	Gas-Phase Study of Phenylacetylene and Norbornadiene on a Palladium(II) Phosphinous Acid Complex: Importance of the Order of Introduction of the Organic Partners. Organometallics, 2009, 28, 2735-2743.	1.1	24
24	Lewis-Based Valence Bond Scheme:â€‰ Application to the Allyl Cation. Journal of Physical Chemistry A, 2006, 110, 2505-2509.	1.1	23
25	Theoretical Study of Intramolecular Aldol Condensation of 1,6-Diketones:Â Trimethylsilyl Substituent Effect. Journal of Organic Chemistry, 2000, 65, 5823-5830.	1.7	20
26	On the link atom distance in the ONIOM scheme. An harmonic approximation analysis. Computational and Theoretical Chemistry, 2003, 632, 61-69.	1.5	20
27	Theoretical study of the semihydrogenation of alkynes catalyzed by Pd(0) complexes: Is a zwitterionic pathway possible?. Theoretical Chemistry Accounts, 2004, 112, 305.	0.5	20
28	Valence Bond Approach of Metalâ"Ligand Bonding in the Dewarâ"Chattâ"Duncanson Model. Inorganic Chemistry, 2007, 46, 11390-11396.	1.9	18
29	HÃ¼ckel theory for Lewis structures: HÃ¼ckelâ€"Lewis Configuration Interaction (HL-CI). Computational and Theoretical Chemistry, 2007, 817, 99-109.	1.5	18
30	Modelling the Twoâ€Đimensional Polymerization of 1,4â€Benzene Diboronic Acid on a Ag Surface. ChemPhysChem, 2009, 10, 2480-2485.	1.0	16
31	Dissociation characteristics of Î±,Ï‰-dihydride poly(dimethylsiloxane) ammonium adducts generated by electrospray ionization. International Journal of Mass Spectrometry, 2011, 306, 70-76.	0.7	15
32	Substituent Effects on Two-Center Three-Electron Bonds and Hydrogen Bonds Involving Unsaturated Organic Functional Groups and an Ammonia Radical Cation-The Resonance Contribution. Chemistry - A European Journal, 2000, 6, 1592-1600.	1.7	13
33	Theoretical description of [2+2] photocycloadditions: enone and ethylene as a model of the reactivity of cycloenones. Computational and Theoretical Chemistry, 2001, 538, 165-177.	1.5	12
34	Specific solvent effect on R2ZrCl2 (R=butyl, ethyl) reactivity, a density functional study. Journal of Organometallic Chemistry, 2002, 664, 268-276.	0.8	12
35	Do Platinum(II) and Palladium(II) Phosphinito Phosphinous Acids Generate the Same Type of Reactive Intermediate in Alkyne Coordination? A Gas-Phase Study with Phenylethyne and Propargyl Acetate. Organometallics, 2011, 30, 4814-4821.	1.1	12
36	Chemodivergent Palladiumâ€Catalyzed Processes: Role of Versatile Ligands. ChemCatChem, 2015, 7, 3848-3854.	1.8	12

#	Article	IF	Citations
37	Substituent Effects on Two-Center Three-Electron Bonds and Hydrogen Bonds Involving Unsaturated Organic Functional Groups and an Ammonia Radical Cation-The Resonance Contribution. Chemistry - A European Journal, 2000, 6, 1592-1600.	1.7	12
38	Getting the Weights of Lewis Structures out of HÃ¼ckel Theory: HÃ¼ckelâ€“Lewis Configuration Interaction (HL-CI). Journal of Chemical Education, 2007, 84, 1056.	1.1	11
39	Quantifying resonance through a Lewis Valence Bond approach: application to haloallyl and carbonylcations. Faraday Discussions, 2007, 135, 273-283.	1.6	11
40	Successful MALDIâ€MS Analysis of Synthetic Polymers with Labile Endâ€Groups: The Case of Nitroxideâ€Mediated Polymerization Using the MAMAâ€SG1 Alkoxyamine. Chemistry - A European Journal, 2012, 18, 7916-7924.	1.7	11
41	Hyperconjugation in Carbocations, a BLW Study with DFT approximation. Frontiers in Chemistry, 2014, 1, 37.	1.8	11
42	trans-Bis-[(â¯)ephedrinate]-palladiumII complex: synthesis, molecular modeling and use as catalyst. Journal of Organometallic Chemistry, 2003, 687, 377-383.	0.8	10
43	On the Catalysis of the Cycloisomerization of 1,6â€Dienes with Tin(IV) Salts: The Important Role of a Water Molecule. ChemCatChem, 2014, 6, 500-507.	1.8	10
44	Large Hyperconjugation in Strained Systems. Chemistry - A European Journal, 2014, 20, 12601-12606.	1.7	8
45	Labile ligands on some Lewis super acids: a computational study. Physical Chemistry Chemical Physics, 2009, 11, 7130.	1.3	7
46	The Valence Bond Workshop in Paris: The Phoenix Rises from the Ashes or, Has a Love Story with MO-Based Theories Begun?. ChemPhysChem, 2012, 13, 4029-4030.	1.0	7
47	Computational insights about the dynamic behavior for the inclusion process of deprotonated and neutral aspirin in Î²-cyclodextrin. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2018, 92, 115-127.	0.9	7
48	On the suggestion of a heteronuclear CâµO through-space three-electron bond in tetrahydropyran radical. Computational and Theoretical Chemistry, 1998, 424, 57-65.	1.5	6
49	Integrated molecular orbital+molecular orbital (IMOMO) treatment of single electron transfer (SET) via a two-center three-electron (2câ€“3e) bonded complex: substituted carbonylâ€“ammonia example. Computational and Theoretical Chemistry, 1999, 461-462, 153-166.	1.5	6
50	Transition metal complexes bearing atropisomeric saturated NHC ligands. Chirality, 2022, 34, 13-26.	1.3	6
51	Differentiation of heterocyclic regioisomers: a combined tandem mass spectrometry and computational study of Nâ€acridinâ€4â€ylbenzylamide and Nâ€acridinâ€2â€ylâ€benzylamide. Rapid Communications in Mass Spectrometry, 2008, 22, 687-693.	0.7	5
52	Recasting wave functions into valence bond structures: A simple projection method to describe excited states. Journal of Computational Chemistry, 2016, 37, 771-779.	1.5	5
53	C₁â€Symmetric Atropisomeric NHC Palladium(II) Complexes: Synthesis, Resolution and Characterization. Advanced Synthesis and Catalysis, 2021, 363, 4229-4238.	2.1	5
54	Metal-catalyzed rearrangement of allenylsulfides to furan: A theoretical mechanistic approach. Molecular Catalysis, 2017, 443, 148-154.	1.0	4

#	Article	IF	Citations
55	Computational studies of Ni(II) photosensitizers complexes containing 1,1â€²-bis(diphenylphosphino)ferrocene and dithio ligands. Canadian Journal of Chemistry, 2020, 98, 194-203.	0.6	4
56	A theoretical and NMR experimental study of N1,N3-di(3-aminoacridin-6-yl)-isophthalamide and N2,N6-di(3-aminoacridin-6-yl)-2,6-dicarboxamide. Journal of Molecular Structure, 2009, 928, 132-137.	1.8	3
57	Methylenecyclopropene: local vision of the first 1B2 excited state. Journal of Molecular Modeling, 2017, 23, 22.	0.8	3
58	Predicted Gasâ€Phase and Liquidâ€Phase Acidities of Carborane Carboxylic and Dicarboxylic Acids. ChemistrySelect, 2018, 3, 4344-4353.	0.7	3
59	HuLiS, a program to teach mesomerism and more. Journal of Physics: Conference Series, 2016, 738, 012015.	0.3	2
60	Localized Structures at the HÃ¼ckel Level, a HÃ¼ckel-Derived Valence Bond Method. Challenges and Advances in Computational Chemistry and Physics, 2016, , 337-360.	0.6	2
61	A generalized Brillouin theorem (GBT)-like implementation to optimize Valence Bond wave function for excited states. Computational and Theoretical Chemistry, 2017, 1116, 184-189.	1.1	2
62	Determination of dissolved nickel in natural waters using a rapid microplate fluorescence assay method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 275, 121170.	2.0	2
63	Palladium-catalysed oxidation of alcohols to carbonyl compounds with 1,2-dichloroethane as the primary oxidant: a theoretical studyElectronic supplementary information (ESI) available: Tables of absolute energies and structural parameters for all of the computed species. See http://www.rsc.org/suppdata/p2/b1/b102256n/. Perkin Transactions II RSC, 2001, , 1998-2004.	1.1	1
64	Hydrometalation or Condensation in the Reaction of Cl2ZrEt2with H2CO. A Theoretical Account. Organometallics, 2004, 23, 2892-2899.	1.1	1
65	Reactivity of dialkylzirconium species and solvent polarity. International Journal of Quantum Chemistry, 2006, 106, 704-711.	1.0	1
66	Electronic densities and valence bond wave functions. Journal of Chemical Physics, 2022, 156, 204310.	1.2	1