# Nadezhda M Vitkovskaya

List of Publications by Year
in descending order



| 89 | 556 | 840119 | 713013 |
|---|---|---|---|
| papers | citations | 11 h-index | 21 g-index |

| 90 | 90 | 90 | 465 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Theoretical study of the low-lying excited singlet states of furan. Journal of Chemical Physics, 2003, 119, 737-753. | 1.2 | 57 |
| 2 | Core-level electronic spectra in ADC(2) approximation for polarization propagator: Carbon monoxide and nitrogen molecules. Journal of Structural Chemistry, 2000, 41, 483-494. | 0.3 | 49 |
| 3 | Theoretical study of excitations in furan: Spectra and molecular dynamics. Journal of Chemical Physics, 2004, 121, 4585-4598. | 1.2 | 49 |
| 4 | Nucleophilic Addition of Ketones To Acetylenes and Allenes: AÂQuantum-Chemical Insight. Journal of Organic Chemistry, 2017, 82, 12467-12476. | 1.7 | 37 |
| 5 | Quantumâ€chemical models of KOH(KOBu<sup>t</sup>)/DMSO superbasic systems and mechanisms of baseâ€promoted acetylene reactions. International Journal of Quantum Chemistry, 2020, 120, e26158. | 1.0 | 27 |
| 6 | 3H-Pyrroles from ketoximes and acetylene: synthesis, stability and quantum-chemical insight. Tetrahedron, 2015, 71, 3273-3281. | 1.0 | 25 |
| 7 | Title is missing!. Russian Chemical Bulletin, 2002, 51, 774-782. | 0.4 | 23 |
| 8 | Exploring acetylene chemistry in superbasic media: A theoretical study of the effect of water on vinylation and ethynylation reactions with acetylene in KOH/DMSO and NaOH/DMSO systems. Journal of Physical Organic Chemistry, 2017, 30, e3669. | 0.9 | 22 |
| 9 | Theoretical investigation of photoelectron spectra of furan, pyrrole, thiophene, and selenole. Chemistry of Heterocyclic Compounds, 2008, 44, 1101-1112. | 0.6 | 20 |
| 10 | Methanol vinylation mechanism in the KOH/DMSO/CH<sub>3</sub>OH/C<sub>2</sub>H<sub>2</sub> system. International Journal of Quantum Chemistry, 2011, 111, 2519-2524. | 1.0 | 20 |
| 11 | A theoretical study of methanol vinylation reaction mechanism. International Journal of Quantum Chemistry, 2008, 108, 2630-2635. | 1.0 | 13 |
| 12 | Alkyland arylketone reactions with phenylacetylene promoted by KOHâ€”DMSO superbase: a quantum chemical study. Russian Chemical Bulletin, 2015, 64, 518-524. | 0.4 | 11 |
| 13 | Aluminium oxide-mediated cross-coupling of pyrroles with 1-bromo-2-(trifluoroacetyl)acetylene: a quantum-chemical insight. Mendeleev Communications, 2016, 26, 480-482. | 0.6 | 11 |
| 14 | A theoretical study of acetone reactions with acetylene and phenylacetylene in the KOH/DMSO superbasic system. Doklady Chemistry, 2014, 457, 126-128. | 0.2 | 9 |
| 15 | Self-Assembly of N-Phenyl-2,5-dimethylpyrrole from Acetylene and Aniline in KOH/DMSO and KOBu<sup>t</sup>/DMSO Superbase Systems: A Quantum-Chemical Insight. Journal of Organic Chemistry, 2020, 85, 10617-10627. | 1.7 | 9 |
| 16 | Cascade Assembly of 4,5,6,7-Tetrahydroindole from Cyclohexanone Oxime and Acetylene in the KOH/DMSO Superbase Medium: AÂQuantum Chemical Study. Journal of Organic Chemistry, 2020, 85, 6463-6470. | 1.7 | 9 |
| 17 | Nucleophilic addition of methanol and methanethiol to acetylene in the superbasic system KOH-DMSO: a quantum chemical model. Russian Chemical Bulletin, 2013, 62, 26-32. | 0.4 | 8 |
| 18 | Two classes of heterocyclesâ€”6,8â€dioxabicyclo[3.2.1]octanes and cyclopentenols from the same reagents: A quantumâ€chemical comparison of mechanism. International Journal of Quantum Chemistry, 2018, 118, e25689. | 1.0 | 8 |

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|---|---|---|---|
| 19 | Multiple bond migration with participation of a protophilic agent. Russian Chemical Bulletin, 1999, 48, 35-41. | 0.4 | 7 |
| 20 | Synthesis of divinyl sulfide via addition of the hydrogen sulfide anion to acetylene in an alkaline metal hydroxide/DMSO superbasic system: A quantum-chemical insight. Tetrahedron Letters, 2017, 58, 92-96. | 0.7 | 7 |
| 21 | Transition-Metal-Free C-Vinylation of Ketones with Acetylenes: A Quantum-Chemical Rationalization of Similarities and Differences in Catalysis by Superbases MOH/DMSO and tBuOM/DMSO (M = Na, K). Journal of Organic Chemistry, 2018, 83, 3719-3726. | 1.7 | 7 |
| 22 | Quantum-chemical investigation of the silicon and carbon coordination bond in their isostructural compounds. International Journal of Quantum Chemistry, 1980, 17, 299-305. | 1.0 | 6 |
| 23 | Theoretical analysis of pyrrole anions addition to carbon disulfide and carbon dioxide. International Journal of Quantum Chemistry, 2002, 88, 542-548. | 1.0 | 6 |
| 24 | Theoretical study of the [1,3]-prototropic rearrangements of oximes and their ethers. Journal of Structural Chemistry, 2008, 49, 216-223. | 0.3 | 6 |
| 25 | A Theoretical study of vinylation of methanol, acetoxime, and methanethiol with acetylene in the KOH-DMSO system. Doklady Chemistry, 2011, 438, 167-169. | 0.2 | 6 |
| 26 | Aldol Condensation Versus Superbase-Catalyzed Addition of Ketones to Acetylenes: A Quantum-Chemical and Experimental Study. Journal of Organic Chemistry, 2021, 86, 7439-7449. | 1.7 | 6 |
| 27 | Theoretical Analysis and Experimental Study of the Spatial Structure and Isomerism of Acetone Azine and Its Cyclization to 3,5,5-Trimethyl-4,5-dihydro-1H-pyrazole. Journal of Structural Chemistry, 2004, 45, 748-755. | 0.3 | 5 |
| 28 | AB initio quantum chemical study of the reaction mechanism of ethynide ion formation in the C2H2/MOH/DMSO system (M = Li, Na, K). Journal of Structural Chemistry, 2009, 50, 27-33. | 0.3 | 5 |
| 29 | Interaction of methanol, methanthiol, and acetoxime with potassium and rubidium hydroxides in dimethyl sulfoxide. Journal of Structural Chemistry, 2011, 52, 659-663. | 0.3 | 5 |
| 30 | Hydrative trimerization of acetylene into 2-vinyloxy-1,3-butadiene in the KOH/DMSO system: a quantum chemical insight. Tetrahedron Letters, 2015, 56, 1063-1066. | 0.7 | 5 |
| 31 | Quantum chemical comparison of ethynylation and C-vinylation routes in superbase catalyzed reaction of acetylenes with imines. Mendeleev Communications, 2019, 29, 622-624. | 0.6 | 5 |
| 32 | Ambient access to a new family of pyrrole-fused pyrazine nitrones via 2-carbonyl-N-allenylpyrroles. Organic Chemistry Frontiers, 2020, 7, 4019-4025. | 2.3 | 5 |
| 33 | Ab initio quantum-chemical study of the reaction mechanisms of acetylene in superbasic media. Noncatalytic vinylation of methanol. Journal of Structural Chemistry, 2007, 48, S94-S99. | 0.3 | 4 |
| 34 | Methanol interaction with potassium and rubidium hydroxides in dimethyl sulfoxide. Journal of Structural Chemistry, 2011, 52, 652-658. | 0.3 | 4 |
| 35 | Quantum-chemical study of regioselectivity and stereoselectivity of methanol vinylation with substituted acetylenes in a KOH/DMSO superbasic medium. Doklady Chemistry, 2013, 452, 227-229. | 0.2 | 4 |
| 36 | Quantum-chemical study of the stereoselectivity of methanethiol nucleophilic addition to substituted acetylenes in KOH/DMSO superbasic medium. Doklady Chemistry, 2014, 456, 91-93. | 0.2 | 4 |

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|---|---|---|---|
| 37 | Baseâ€Promoted Formation of an Annelated Pyrroloâ€1,4â€oxazine Ensemble from 1Hâ€pyrroloâ€2â€ylmethanol and Propargyl Chloride: A Theoretical and Experimental Study. ChemPlusChem, 2020, 85, 88-100. | 1.3 | 4 |
| 38 | Pyrrole anion addition to carbon disulfide: An ab initio study. International Journal of Quantum Chemistry, 2004, 100, 360-366. | 1.0 | 3 |
| 39 | An ab initio quantum chemical study of reaction mechanisms in the C2H2/CH3OH/KOH/DMSO system. Journal of Structural Chemistry, 2010, 51, 428-436. | 0.3 | 3 |
| 40 | Headâ€toâ€Tail Dimerization of 4â€Fluoroacetophenone in the KOH/DMSO Superbase Suspension and Related S<sub>N</sub>Ar Reaction. European Journal of Organic Chemistry, 2020, 2020, 3480-3485. | 1.2 | 3 |
| 41 | Nonempirical calculation of various derivatives of methane, silane, and the monofluorides of the elements of the third period. Journal of Structural Chemistry, 1977, 17, 678-681. | 0.3 | 2 |
| 42 | Ab initio investigation of the electron structure in bis-Cu+ acetylene and vinylidene complexes. Reaction Kinetics and Catalysis Letters, 1986, 31, 167-172. | 0.6 | 2 |
| 43 | Multiple bond migration with participation of a protophilic agent. Russian Chemical Bulletin, 1999, 48, 653-658. | 0.4 | 2 |
| 44 | Multiple bond migration with participation of a protophilic agent. Russian Chemical Bulletin, 2000, 49, 415-420. | 0.4 | 2 |
| 45 | Sulfur Versus Oxygen in Interaction with the Double Bond: AB Initio Study of Electronic Structure and Prototropic Rearrangement of 1-Methoxy-2-propene and 1-Methylthio-2-propene. Phosphorus, Sulfur and Silicon and the Related Elements, 2002, 177, 2931-2940. | 0.8 | 2 |
| 46 | Ab initio quantum-chemical study of vinylation of pyrrole and 2-phenylazopyrrole with acetylene in a KOH/DMSO system. Journal of Structural Chemistry, 2007, 48, S100-S110. | 0.3 | 2 |
| 47 | Theoretical evaluation of some interactions in the system of acetylene-alkali metal hydroxide-DMSO. Journal of Structural Chemistry, 2009, 50, 18-26. | 0.3 | 2 |
| 48 | Quantum chemical modeling of superbase-catalyzed reactions of acetophenone and methyl mesityl ketone with acetylene. Russian Chemical Bulletin, 2017, 66, 2227-2233. | 0.4 | 2 |
| 49 | Competitive Deprotonation in Vicinal O=SCH2CH2P=O Moieties. Letters in Organic Chemistry, 2006, 3, 720-722. | 0.2 | 2 |
| 50 | Structures of 2-hydroxypyridine and its vinyl derivatives. Chemistry of Heterocyclic Compounds, 1972, 8, 89-94. | 0.6 | 1 |
| 51 | Nonempirical quantum-chemical studies on Cu+ carbonyl and isocarbonyl complexes. Reaction Kinetics and Catalysis Letters, 1986, 30, 361-367. | 0.6 | 1 |
| 52 | Quantum chemical study of the interaction of acetylene with lithium hydroxide and hydrosulfide. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1987, 36, 94-97. | 0.0 | 1 |
| 53 | Quantum-chemical investigation of the mechanisms of reactions involving nucleophilic addition to acetylene 1. Addition of a hydroxide ion. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1988, 37, 1173-1176. | 0.0 | 1 |
| 54 | Quantum-chemical investigation of the mechanisms of nucleophilic addition reactions to acetylene. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1989, 38, 1645-1648. | 0.0 | 1 |

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|---|---|---|---|
| 55 | Question of the reverse polarization of triple bonds. Journal of Structural Chemistry, 1991, 32, 59-64. | 0.3 | 1 |
| 56 | Multiple bond migration with participation of a protophilic agent. Russian Chemical Bulletin, 1997, 46, 1677-1682. | 0.4 | 1 |
| 57 | Multiple bond migration with participation of a protophilic agent. Russian Chemical Bulletin, 2000, 49, 408-414. | 0.4 | 1 |
| 58 | Ab initio Study of the Reaction of Pyrrole Anions with Carbon Disulfide. Journal of Structural Chemistry, 2001, 42, 536-543. | 0.3 | 1 |
| 59 | Ab Initio Study of the Acetyleneâ€“Allene Rearrangement in 2-Propargylpyrrole, 2-Propargylfuran, and 2-Propargylthiophene. Journal of Structural Chemistry, 2004, 45, 5-11. | 0.3 | 1 |
| 60 | Theoretical study of the double bond migration mechanism with participation of hydroxide ion. International Journal of Quantum Chemistry, 2004, 100, 367-374. | 1.0 | 1 |
| 61 | A theoretical study of ethynylation of formaldehyde with acetylene in the KOH-DMSO system. Doklady Chemistry, 2011, 439, 181-182. | 0.2 | 1 |
| 62 | Quantum chemical study of the formation of acetylenic alcohols and 7-methylidene-6,8-dioxabicyclo[3.2.1]octanes from acetylene and carbonyl compounds. Russian Chemical Bulletin, 2013, 62, 2306-2310. | 0.4 | 1 |
| 63 | Quantum chemical study of the stereoselectivity of nucleophilic addition of 2-methylcyclohexanone to phenylacetylene. Doklady Chemistry, 2015, 461, 100-103. | 0.2 | 1 |
| 64 | Formation mechanism and conformational structure of 2,3,4-trimethyl-1,5-di(thiophen-2-yl)pentane-1,5-dione: quantum chemical study. Russian Chemical Bulletin, 2016, 65, 394-400. | 0.4 | 1 |
| 65 | Baseâ€Promoted Formation of an Annelated Pyrroloâ€1,4â€oxazine Ensemble from 1 H â€pyrrolâ€2â€ylmethanol and Propargyl Chloride: A Theoretical and Experimental Study. ChemPlusChem, 2020, 85, 4-4. | 1.3 | 1 |
| 66 | A program for nonempirical molecular SCF lcao mo calculations. Journal of Structural Chemistry, 1972, 13, 332-333. | 0.3 | 0 |
| 67 | AB initio calculation of acetylide anion. Journal of Structural Chemistry, 1975, 16, 309-310. | 0.3 | 0 |
| 68 | Analysis of electronic absorption spectra and structure of group IV-B heteroorganic compounds by means of semiempirical SCF MO LCAO method. Journal of Structural Chemistry, 1975, 15, 539-543. | 0.3 | 0 |
| 69 | Ab initio calculation of acetylene and its monoderivatives. Journal of Structural Chemistry, 1975, 15, 584-587. | 0.3 | 0 |
| 70 | Nonempirical calculation of surface area of potential energy of ammonium ion. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1976, 25, 2210-2212. | 0.0 | 0 |
| 71 | Electronic structure of anionic nitro compounds. Journal of Structural Chemistry, 1977, 17, 519-526. | 0.3 | 0 |
| 72 | Nonempirical calculation of the potential surface for the formation of the hydrazinium ion. Journal of Structural Chemistry, 1979, 19, 615-617. | 0.3 | 0 |

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| 73 | Nonempirical study of the structure of complexes of acetylene with H+, Li+, and Na+ cations. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1982, 31, 785-788. | 0.0 | 0 |
| 74 | AB initio investigation of complexes of acetylene with alkali metal cations. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1982, 31, 1314-1317. | 0.0 | 0 |
| 75 | AB initio investigation of complexes of acetylene with alkali metal cations. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1982, 31, 1317-1319. | 0.0 | 0 |
| 76 | A program for nonempirical calculations for systems with open shells. Journal of Structural Chemistry, 1982, 22, 930-931. | 0.3 | 0 |
| 77 | Nonempirical investigation of acetylene complexes with cations of alkali metals 4. Vinylidene structures and barriers to their isomerization. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1983, 32, 1783-1787. | 0.0 | 0 |
| 78 | Modifications of the program ?Gaussian-70?. Journal of Structural Chemistry, 1983, 23, 648-648. | 0.3 | 0 |
| 79 | Nonempirical calculations of the affinity of the acetylene molecule for the lithium cation. Journal of Structural Chemistry, 1983, 24, 474-475. | 0.3 | 0 |
| 80 | Theoretical study of the structure of molecules of alkali metal acetylenides and carbides. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1987, 36, 2575-2579. | 0.0 | 0 |
| 81 | Nonempirical study of the interaction of CO and Co, Co+, and Co2+. Journal of Structural Chemistry, 1988, 28, 766-767. | 0.3 | 0 |
| 82 | Quantum-chemical investigation of the mechanisms of reactions involving nucleophilic addition to acetylene. 2. Interconversions of products of the reaction of acetylene with the hydroxide ion. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1988, 37, 1177-1180. | 0.0 | 0 |
| 83 | Quantum-chemical investigation of the mechanisms of reactions involving nucleophilic addition to acetylene. 3. Mechanism of the formation of vinylthio anions. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1988, 37, 1180-1182. | 0.0 | 0 |
| 84 | Quantum-chemical investigation of the mechanisms of reactions involving nucleophilic addition to acetylene. 4. Study of reactions in the acetylene-LIOH system. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1988, 37, 1841-1846. | 0.0 | 0 |
| 85 | Quantum-chemical investigation of the mechanisms of nucleophilic addition reactions to acetylene. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1989, 38, 1641-1645. | 0.0 | 0 |
| 86 | Quantum-chemical investigation of mechanisms of reactions of nucleophilic addition to acetylene. 7. Evaluation of possible interactions in C2H2/MOH/DMSO system. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1990, 39, 1624-1627. | 0.0 | 0 |
| 87 | Quantum-chemical investigation of the protonated forms of 2-(2-furyl)pyrrole. Chemistry of Heterocyclic Compounds, 1991, 27, 583-590. | 0.6 | 0 |
| 88 | Quantum-Chemical Study of the Profiles of Reactions that Form Pyrrole Anion N-Adducts with CS2 and CO2. Journal of Structural Chemistry, 2004, 45, 940-944. | 0.3 | 0 |
| 89 | Propagator quantum chemical study of S-cis-(Z)-2-(2-formylethenyl)pyrrole: electronic structure and aspects of intramolecular hydrogen bond manifestation in ionization spectra. Russian Chemical Bulletin, 2017, 66, 2241-2247. | 0.4 | 0 |