Eluvathingal D Jemmis

List of Publications by Year in Descending Order

242 papers	7,293 citations	46 h-index	74 g-index
266 ext. papers	7,922 ext. citations	7.4 avg, IF	5.97 L-index

#	Paper	IF	Citations
242	Orbital Engineering in Chemistry. *Israel Journal of Chemistry*, **2022**, 62,	3.4	
241	Borophenes: Insights and Predictions From Computational Analyses **2021**, 27-49		0
240	Reversing Lewis acidity from bismuth to antimony. *Chemical Communications*, **2021**, 57, 8889-8892	5.8	6
239	Comparison of RNC Coupling and CO Coupling Mediated by Cr-Cr Quintuple Bond and B-B Multiple Bonds: Main Group Metallomimetics. *Journal of Physical Chemistry A*, **2021**, 125, 7207-7216	2.8	1
238	Metal-Stabilized [B H] Derivatives with Dodecahedral Structure in the Solid and Solution States: [(Cp MBH) B H] (Cp=□-C H ; M=Zr (1-Zr) and Hf (1-Hf)). *Chemistry - A European Journal*, **2021**, 27, 15634-15637	4.8	1
237	DFT Study of C□□ and C□N Coupling on a Quintuple-Bonded Cr2 Template: MECP (Minimum Energy Crossing Point) Barriers Control Product Distribution. *Organometallics*, **2020**, 39, 1700-1709	3.8	3
236	Electrophilic Organobismuth Dication Catalyzes Carbonyl Hydrosilylation. *Chemistry - A European Journal*, **2020**, 26, 12717-12721	4.8	14
235	Structures and bonding in [L]M(□CCR)M[L] and [L]M(□RCR)M[L]: requirements for C-C coupling. *Dalton Transactions*, **2020**, 49, 5157-5166	4.3	3
234	Continuum in H-bond and Other Weak Interactions (X□□□Y): Shift in X□ Stretch from Blue Through Zero to Red. *Journal of the Indian Institute of Science*, **2020**, 100, 127-133	2.4	1
233	A Neutral Three-Membered 2□Aromatic Disilaborirane and the Unique Conversion into a Four-Membered BSi2N-Ring. *Angewandte Chemie*, **2020**, 132, 23215-23219	3.6	1
232	A Neutral Three-Membered 2□Aromatic Disilaborirane and the Unique Conversion into a Four-Membered BSi N-Ring. *Angewandte Chemie - International Edition*, **2020**, 59, 23015-23019	16.4	6
231	trans-Influence in Heavy Main Group Compounds: A Case Study on Tris(pyrazolyl)borate Bismuth Complexes. *European Journal of Inorganic Chemistry*, **2020**, 2020, 2530-2536	2.3	7
230	Stabilization of Classical [B2H5]□Structure and Bonding of [(Cp*Ta)2(B2H5)(□H)L2] (Cp*=□5-C5Me5; L=SCH2S). *Angewandte Chemie*, **2019**, 131, 17848-17853	3.6	7
229	Stabilization of Classical [B H] : Structure and Bonding of [(Cp*Ta) (B H)(□H)L] (Cp*=□-C Me ; L=SCH S). *Angewandte Chemie - International Edition*, **2019**, 58, 17684-17689	16.4	12
228	A theoretical analysis of the structure and properties of BH isomers. Consequences to the laser and semiconductor doping capabilities of large borane clusters. *Physical Chemistry Chemical Physics*, **2019**, 21, 12916-12923	3.6	4
227	A Dicationic Bismuth(III) Lewis Acid: Catalytic Hydrosilylation of Olefins. *European Journal of Inorganic Chemistry*, **2019**, 2019, 3265-3269	2.3	22
226	Isolation of base stabilized fluoroborylene and its radical cation. *Dalton Transactions*, **2019**, 48, 8551-8555	4.3	7

225	A Dicationic Bismuth(III) Lewis Acid: Catalytic Hydrosilylation of Olefins. *European Journal of Inorganic Chemistry*, **2019**, 2019, 3257-3257	2.3	3
224	Overlap of Radial Dangling Orbitals Controls the Relative Stabilities of Polyhedral B H Isomers (n = 5-12, x = 0 to n - 1). *Inorganic Chemistry*, **2019**, 58, 3627-3634	5.1	6
223	Designing M-bond (X-M Y, M = transition metal): hole and radial density distribution. *Journal of Chemical Sciences*, **2019**, 131, 1	1.8	9
222	Organoaluminum cations for carbonyl activation. *Chemical Communications*, **2019**, 55, 14629-14632	5.8	13
221	Synthesis, Structure, Bonding, and Reactivity of Metal Complexes Comprising Diborane(4) and Diborene(2): [{Cp*Mo(CO)2}2{ 2: 2-B2H4}] and [{Cp*M(CO)2}2B2H2M(CO)4], M=Mo,W. *Angewandte Chemie*, **2018**, 130, 8211-8215	3.6	9
220	Synthesis, Structure, Bonding, and Reactivity of Metal Complexes Comprising Diborane(4) and Diborene(2): [{Cp*Mo(CO) } { : -B H }] and [{Cp*M(CO) } B H M(CO)], M=Mo,W. *Angewandte Chemie - International Edition*, **2018**, 57, 8079-8083	16.4	25
219	Origin of agostic interaction in d0 transition metal alkyl complexes: Influence of ligands. *Journal of Organometallic Chemistry*, **2018**, 865, 37-44	2.3	7
218	Metal Templates and Boron Sources Controlling Borophene Structures: An Ab Initio Study. *Journal of Physical Chemistry C*, **2018**, 122, 2268-2274	3.8	13
217	Nanoisozymes: Crystal-Facet-Dependent Enzyme-Mimetic Activity of V O Nanomaterials. *Angewandte Chemie - International Edition*, **2018**, 57, 4510-4515	16.4	124
216	Adamantane-Derived Carbon Nanothreads: High Structural Stability and Mechanical Strength. *Journal of Physical Chemistry C*, **2018**, 122, 7945-7950	3.8	5
215	Electronic Structure of Condensed Polyhedral Carboranes **2018**, 277-308		
214	B-B Coupling and B-B Catenation: Computational Study of the Structure and Reactions of Metal-Bis(borylene) Complexes. *Chemistry - A European Journal*, **2018**, 24, 17844-17851	4.8	1
213	Halogen bond shortens and strengthens the bridge bond of [1.1.1]propellane and the open form of [2.2.2]propellane. *Physical Chemistry Chemical Physics*, **2018**, 20, 25792-25798	3.6	6
212	Contrasting Behavior of the Z Bonds in X-Z Y Weak Interactions: Z = Main Group Elements Versus the Transition Metals. *Inorganic Chemistry*, **2017**, 56, 1132-1143	5.1	23
211	The Role of Holes in Borophenes: An Ab Initio Study of Their Structure and Stability with and without Metal Templates. *Angewandte Chemie - International Edition*, **2017**, 56, 10093-10097	16.4	36
210	The Role of Holes in Borophenes: An Ab Initio Study of Their Structure and Stability with and without Metal Templates. *Angewandte Chemie*, **2017**, 129, 10227-10231	3.6	6
209	A DFT Study on the Stabilization of the B?B Triple Bond in a Metallaborocycle: Contrasting Electronic Structures of Boron and Carbon Analogues. *Chemistry - A European Journal*, **2017**, 23, 9746-9751	4.8	18
208	The dynamic behavior of the exohedral transition metal complexes of (mathrm{B}_{40}: {upeta}^{6})- and ({upeta}^{7})-(mathrm{B}_{40}hbox {Cr(CO)}_{3}) and (hbox {Cr(CO)}_{3})-({upeta}^{7})-(hbox {B}_{40}) -({upeta}^{7})-(hbox {Cr(CO)}_{3}). *Journal of Chemical Sciences*, **2017**, 129, 1061-1067	1.8	2

207	Fragment approach to the electronic structure of □boron allotrope. *Physical Review B*, **2017**, 95,	3.3	5
206	Approaches to Sigma Complexes via Displacement of Agostic Interactions: An Experimental and Theoretical Investigation. *Organometallics*, **2017**, 36, 2736-2745	3.8	8
205	Consequence of Ligand Bite Angle on Bismuth Lewis Acidity. *Inorganic Chemistry*, **2017**, 56, 9391-9395	5.1	35
204	A halogen bond route to shorten the ultrashort sextuple bonds in Cr and Mo. *Chemical Communications*, **2017**, 53, 8168-8171	5.8	9
203	Computational design of Oligo-sulfuranes. *Journal of Chemical Sciences*, **2016**, 128, 1663-1669	1.8	
202	Exohedral Complexation of B , C and Arenes with Transition Metals: A Comparative DFT Study. *Chemistry - an Asian Journal*, **2016**, 11, 3350-3354	4.5	20
201	Non-covalent C-Cl□interaction in acetylene-carbon tetrachloride adducts: Matrix isolation infrared and ab initio computational studies. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2016**, 157, 69-78	4.4	11
200	Continuum in the X-Z---Y weak bonds: Z= main group elements. *Journal of Computational Chemistry*, **2016**, 37, 270-9	3.5	21
199	Synthetic, Crystallographic, and Computational Studies of Extensively Hydrogen Bonded Bilayers in Thermally Stable Adamantane Hydroperoxides. *Asian Journal of Organic Chemistry*, **2016**, 5, 1398-1405	3	4
198	Experimental and theoretical study of intramolecular O?O interaction in structurally rigid □keto carboxylic esters. *RSC Advances*, **2016**, 6, 91689-91693	3.7	11
197	Implication of a □Methane Complex en Route to Elimination of Methane from a Ruthenium Complex: An Experimental and Theoretical Investigation. *Organometallics*, **2015**, 34, 1245-1254	3.8	8
196	Time and Space resolved Methods: general discussion. *Faraday Discussions*, **2015**, 177, 263-92	3.6	1
195	Structural variations in aromatic 2□electron three-membered rings of the main group elements. *Journal of Chemical Sciences*, **2015**, 127, 183-196	1.8	1
194	Ketocyanine dyes: impact of conjugation length on optical absorption and third-order polarizabilities. *Physical Chemistry Chemical Physics*, **2015**, 17, 12988-99	3.6	4
193	The Self-Association of Graphane Is Driven by London Dispersion and Enhanced Orbital Interactions. *Journal of Chemical Theory and Computation*, **2015**, 11, 1621-30	6.4	36
192	Relative stabilities of condensed face sharing mono- and di-carboranes: CB20H18 and C2B19H18+. *Journal of Organometallic Chemistry*, **2015**, 798, 91-98	2.3	4
191	Negative hyperconjugation and red-, blue- or zero-shift in X-Z□Y complexes. *Faraday Discussions*, **2015**, 177, 33-50	3.6	18
190	Designing stuffed hetero-fullerene nano-clusters: C26B46N12 and C14B58N12Li12. *RSC Advances*, **2014**, 4, 30013-30018	3.7	4

189	Metallacyclocumulenes: a theoretical perspective on the structure, bonding, and reactivity. *Accounts of Chemical Research*, **2014**, 47, 2917-30	24.3	57
188	Electron-Counting Rules in Cluster Bonding Polyhedral Boranes, Elemental Boron, and Boron-Rich Solids **2014**, 113-148		1
187	P3F9(2-): an all-pseudo- 2aromatic. *Journal of the American Chemical Society*, **2013**, 135, 16026-9	16.4	8
186	Stabilization of diborane(4) by transition metal fragments and a novel metal to Dewar-Chatt-Duncanson model of back donation. *Dalton Transactions*, **2013**, 42, 10633-9	4.3	14
185	Complexes of acetyleneluoroform: A matrix isolation and computational study. *Journal of Molecular Structure*, **2013**, 1049, 69-77	3.4	12
184	Experimental and Theoretical Studies of Unusual Four-Membered Metallacycles from Reactions of Group 4 Metallocene Bis(trimethylsilyl)acetylene Complexes with the Sulfurdiimide Me3SiN=S=NSiMe3. *European Journal of Inorganic Chemistry*, **2012**, 2012, 611-617	2.3	20
183	Reactions of titanocene bis(trimethylsilyl)acetylene complexes with carbodiimides: an experimental and theoretical study of complexation versus C-N bond activation. *Journal of the American Chemical Society*, **2012**, 134, 15979-91	16.4	37
182	(Dimethylamino)borylene and Related Complexes of Electron-Rich Metal Fragments: Generation of Nucleophile-Resistant Cations by Spontaneous Halide Ejection. *Organometallics*, **2012**, 31, 1092-1102	3.8	8
181	Polyhedral borane analogues of the benzynes and beyond: bonding in variously charged B12H10 isomers. *Journal of the American Chemical Society*, **2012**, 134, 5916-20	16.4	14
180	Theoretische Studien zu einem viergliedrigen Metallacycloallen, stabilisiert durch eine ungewnliche ergangsmetall-Kohlenstoff-Bindung. *Angewandte Chemie*, **2012**, 124, 5442-5446	3.6	10
179	Theoretical evidence of the stabilization of an unusual four-membered metallacycloallene by a transition-metal fragment. *Angewandte Chemie - International Edition*, **2012**, 51, 5347-50	16.4	31
178	Reactivity of bispropargyl sulfones under basic conditions: interplay between Garratt-Braverman and Schmittel/Myers-Saito cyclization pathway. *Chemistry - an Asian Journal*, **2012**, 7, 957-65	4.5	18
177	Structure-activity relationship of photocytotoxic iron(III) complexes of modified dipyridophenazine ligands. *Inorganic Chemistry*, **2011**, 50, 2975-87	5.1	52
176	Reactions of group 4 metallocene alkyne complexes with carbodiimides: experimental and theoretical studies of the structure and bonding of five-membered hetero-metallacycloallenes. *Journal of the American Chemical Society*, **2011**, 133, 5463-73	16.4	56
175	Synthesis, characterization, and electronic structure of new type of heterometallic boride clusters. *Inorganic Chemistry*, **2011**, 50, 9414-22	5.1	51
174	Cobalt(II) complexes of terpyridine bases as photochemotherapeutic agents showing cellular uptake and photocytotoxicity in visible light. *Dalton Transactions*, **2011**, 40, 1233-42	4.3	38
173	Mechanism of gallic acid biosynthesis in bacteria (Escherichia coli) and walnut (Juglans regia). *Plant Molecular Biology*, **2011**, 75, 555-65	4.6	70
172	Structure and bonding in stannadiphospholes and their dianions SnC2P2R2m (R=H, tBu m=0, -2): a comparative study with C5H5+ and C5H5- analogues. *Chemistry - A European Journal*, **2011**, 17, 9142-52	4.8	1

171	Selectivity in Garratt-Braverman cyclization: an experimental and computational study. *Organic Letters*, **2011**, 13, 888-91	6.2	27
170	Theoretical Studies on the Structure and Bonding of Metallacyclocumulenes, -cyclopentynes, and -cycloallenes. *Organometallics*, **2011**, 30, 2670-2679	3.8	36
169	Vertex-fused metallaborane clusters: synthesis, characterization and electronic structure of [(eta5-C5Me5Mo)3MoB9H18]. *Inorganic Chemistry*, **2010**, 49, 900-4	5.1	51
168	Generation of cationic two-coordinate group-13 ligand systems by spontaneous halide ejection: remarkably nucleophile-resistant (dimethylamino)borylene complexes. *Journal of the American Chemical Society*, **2010**, 132, 4586-8	16.4	20
167	Are Metallocene Acetylene (M = Ti, Zr, Hf) Complexes Aromatic Metallacyclopropenes?. *Organometallics*, **2010**, 29, 76-81	3.8	45
166	Stuffed fullerenelike boron carbide nanoclusters. *Applied Physics Letters*, **2010**, 96, 023108	3.4	9
165	Electronic structure and bonding in neutral and dianionic boradiphospholes: R'BC2P2R2 (R = H, tBu, R' = H, Ph). *Chemistry - A European Journal*, **2009**, 15, 8429-42	4.8	7
164	Relative stability of closo-closo, closo-nido, and nido-nido macropolyhedral boranes: the role of orbital compatibility. *Chemistry - an Asian Journal*, **2009**, 4, 1346-53	4.5	9
163	Chlorinated hypoelectronic dimetallaborane clusters: synthesis, characterization, and electronic structures of (eta(5)-C5Me5W)2B5H(n)Cl(m) (n = 7, m = 2 and n = 8, m = 1). *Inorganic Chemistry*, **2009**, 48, 6509-16	5.1	47
162	Closo versus hypercloso metallaboranes: A DFT study. *Inorganic Chemistry*, **2009**, 48, 7818-27	5.1	15
161	Reactivity of Cationic Terminal Borylene Complexes: Novel Mechanisms for Insertion and Metathesis Chemistry Involving Strongly Lewis Acidic Ligand Systems. *Organometallics*, **2009**, 28, 2961-2975	3.8	41
160	Half-Sandwich Group 8 Borylene Complexes: Synthetic and Structural Studies and Oxygen Atom Abstraction Chemistry. *Organometallics*, **2009**, 28, 2947-2960	3.8	52
159	Which one is preferred: Myers-Saito cyclization of ene-yne-allene or Garratt-Braverman cyclization of conjugated bisallenic sulfone? A theoretical and experimental study. *Journal of the American Chemical Society*, **2009**, 131, 15695-704	16.4	48
158	A Theoretical Investigation of the Ni(II)-Catalyzed Hydrovinylation of Styrene. *Organometallics*, **2009**, 28, 3552-3566	3.8	43
157	Bond Prevents Short Bonds: A Detailed Theoretical Study on the Compounds of Main Group and Transition Metal Complexes **2009**, 165-181		
156	Theoretical Studies in Organolithium Chemistry **2009**,		1
155	Differing Reactivities of Zirconium and Titanium Alkoxides with Phenyl Isocyanate: An Experimental and Computational Study. *Organometallics*, **2008**, 27, 955-960	3.8	9
154	pH Dependence of a 310-Helix versus a Turn in the M-Loop Region of PDE4: Observations on PDB Entries and an Electronic Structure Study. *Journal of Chemical Theory and Computation*, **2008**, 4, 974-84	6.4	2

153	Theoretical study of the reaction of B20H16 with MeCN: closo/closo to closo/nido conversion. *Inorganic Chemistry*, **2008**, 47, 4375-82	5.1	14
152	Design, synthesis, and DNA binding properties of photoisomerizable azobenzene-distamycin conjugates: an experimental and computational study. *Bioconjugate Chemistry*, **2008**, 19, 2332-45	6.3	28
151	Structure and bonding in cyclic isomers of B2AlH(n)(m) (n = 3-6, m = -2 to +1): a comparative study with B3H(n)(m), BAl2H(n)(m) and Al3H(n)(m). *Journal of Physical Chemistry A*, **2008**, 112, 13080-7	2.8	12
150	Stuffing improves the stability of fullerenelike boron clusters. *Physical Review Letters*, **2008**, 100, 165504	7.4	135
149	Subtype selectivity in phosphodiesterase 4 (PDE4): a bottleneck in rational drug design. *Current Pharmaceutical Design*, **2008**, 14, 3854-72	3.3	49
148	Orbital compatibility in the condensation of polyhedral boranes. *Angewandte Chemie - International Edition*, **2008**, 47, 5561-4	16.4	8
147	Photophysical and duplex-DNA-binding properties of distamycin dimers based on 4,4'- and 2,2'-dialkoxyazobenzenes as the core. *Chemistry - an Asian Journal*, **2008**, 3, 1949-61	4.5	13
146	A theoretical study on the mechanism of boron metathesis. *Inorganic Chemistry*, **2007**, 46, 6091-8	5.1	8
145	New insights into the visible-light-induced DNA cleavage activity of dipyridoquinoxaline complexes of bivalent 3d-metal ions. *Inorganic Chemistry*, **2007**, 46, 11122-32	5.1	62
144	Bimetallic Complexes of Metallacyclopentynes: cis versus trans and Planarity versus Nonplanarity. *Organometallics*, **2007**, 26, 2149-2156	3.8	11
143	Structure and bonding in cyclic isomers of BAl2Hnm (n=3-6, m=-2 to +1): preference for planar tetracoordination, pyramidal tricoordination, and divalency. *Chemistry - A European Journal*, **2007**, 13, 2622-31	4.8	13
142	Tandem Si-C and C-H activation for decamethylhafnocene and bis(trimethylsilyl)acetylene. *Angewandte Chemie - International Edition*, **2007**, 46, 6907-10	16.4	23
141	Electronic structure and bonding studies on triple-decker sandwich complexes with a P6 middle ring. *Journal of Computational Chemistry*, **2007**, 28, 310-9	3.5	6
140	Red-, blue-, or no-shift in hydrogen bonds: a unified explanation. *Journal of the American Chemical Society*, **2007**, 129, 4620-32	16.4	625
139	Heterolytic activation of H-X (X = H, Si, B, and C) bonds: an experimental and theoretical investigation. *Journal of the American Chemical Society*, **2007**, 129, 5587-96	16.4	45
138	Geometries of Three-Membered Rings in Triangulanes and Spirocyclopropanated Bicyclopropylidenes: Experimental Studies and a General Bond Increment Scheme. *Liebigs Annalen*, **2006**, 1996, 913-919		5
137	Bond length and bond multiplicity: sigma-bond prevents short pi-bonds. *Chemical Communications*, **2006**, 2164-6	5.8	32
136	Electrostatic repulsion as an additional selectivity factor in asymmetric proline catalysis. *Organic and Biomolecular Chemistry*, **2006**, 4, 2685-9	3.9	20

135	Hypercarbons in polyhedral structures. *Chemical Society Reviews*, **2006**, 35, 157-68	58.5	50
134	Reversal of stability on metalation of pentagonal-bipyramidal (1-MB6H7(2-) 1-M-2-CB5H7(1-) and 1-M-2,4-C2B4H7) and Icosahedral (1-MB11H12(2-) 1-M-2-CB10H12(1-) and 1-M-2,4-C2B9H12) boranes (M = Al, Ga, In, and Tl): energetics of condensation and relationship to binuclear metallocenes. *Journal of the American Chemical Society*, **2006**, 128, 10915-22	16.4	23
133	Icosahedral B12, macropolyhedral boranes, rhombohedral boron and boron-rich solids. *Journal of Solid State Chemistry*, **2006**, 179, 2768-2774	3.3	38
132	Boron and MgB2 analogs of fullerenes and carbon nanotubes: A density functional theory study. *Computational and Theoretical Chemistry*, **2006**, 771, 111-115		14
131	Binuclear organometallic compounds containing planar tetra co-ordinated carbon atoms: theoretical study on geometrical and bonding patterns. *Molecular Physics*, **2005**, 103, 897-903	1.7	12
130	Condensed two- and three-dimensional aromatic systems: a theoretical study on the relative stabilities of isomers of CB19H16+, B20H15Cl, and B20H14Cl2 and comparison to B12H10Cl22-, C6H4Cl2, C10H7Cl, and C10H6Cl2. *Inorganic Chemistry*, **2005**, 44, 7184-8	5.1	6
129	Characteristics of novel sandwiched beryllium, magnesium, and calcium dimers: C5H5BeBeC5H5, C5H5MgMgC5H5, and C5H5CaCaC5H5. *Chemical Physics Letters*, **2005**, 402, 414-421	2.5	110
128	Electronic structure and bonding of rhombohedral boron using cluster fragment approach. *Physical Review B*, **2005**, 72,	3.3	53
127	Reduction of 1,4-dichlorobut-2-yne by titanocene to a 1,2,3-butatriene. Formation of a 1-titanacyclopent-3-yne and a 2,5-dititanabicyclo[2.2.0]hex-1(4)-ene. *Chemical Communications*, **2004**, 2074-5	5.8	49
126	Does a sterically bulky group occupy the equatorial site in trigonal bipyramidal phosphorus?. *Organic Letters*, **2004**, 6, 145-8	6.2	28
125	Structure, reactivity and aromaticity of acenes and their BN analogues: a density functional and electrostatic investigation. *Inorganic Chemistry*, **2004**, 43, 5824-32	5.1	57
124	Stabilization of Tricoordinate Pyramidal Boron: Theoretical Studies on CBSiH5, BSi2H5, CBGeH5, and CBSnH5. *Angewandte Chemie*, **2003**, 115, 557-560	3.6	8
123	Stabilization of tricoordinate pyramidal boron: theoretical studies on CBSiH5, BSi2H5, CBGeH5, and CBSnH5. *Angewandte Chemie - International Edition*, **2003**, 42, 539-42	16.4	25
122	Condensed polyhedral boranes and analogous organometallic clusters: a molecular orbital and density functional theory study on the cap□ap interactions. *Applied Organometallic Chemistry*, **2003**, 17, 480-492	3.1	9
121	Face-selectivity in [4+2]-cycloadditions to novel polycyclic benzoquinones. Remarkable stereodirecting effects of a remote cyclopropane ring and an olefinic bond. *Tetrahedron Letters*, **2003**, 44, 3109-3113	2	6
120	Effect of metal complexation on ring opening of bowl-shaped hydrocarbons: Theoretical study. *International Journal of Quantum Chemistry*, **2003**, 95, 810-815	2.1	7
119	Analogies between boron and carbon. *Accounts of Chemical Research*, **2003**, 36, 816-24	24.3	90
118	Nonplanarity at tri-coordinated aluminum and gallium: cyclic structures for X3Hn(m) (X = B, Al, Ga). *Journal of the American Chemical Society*, **2003**, 125, 16397-407	16.4	22

117	Magic electron counts and bonding in tubular boranes. *Inorganic Chemistry*, **2003**, 42, 4650-9	5.1	27
116	The rearrangement of dicarboranyl methyl cation: a possible synthetic strategy toward cationic closo-tricarbaboranes. *Inorganic Chemistry*, **2003**, 42, 7725-7	5.1	9
115	Structure and Neutral Homoaromaticity of Metallacyclopentene, -pentadiene, -pentyne, and -pentatriene:A Density Functional Study. *Organometallics*, **2003**, 22, 4958-4965	3.8	66
114	The Relation Between Polyhedral Borane Sandwiches and Endohedral Complexes; the Electronic Structure and Stability of X@YmBnHn+mq (X = He, Ne, Li, Be; Y = B, C, Si; m = 0-3; n = 12-9; q = -2 to +2), (C2B4H6)2Xq (X = Li, Al, Si; q = -3, -1, 0) and X2@B17H17q (X = He, Li; q = -2, 0). *Collection of Czechoslovak Chemical Communications*, **2002**, 67, 965-990		10
113	Dependence of the Structure and Stability of Cyclocumulenes and Cyclopropenes on the Replacement of the CH2 Group by Titanocene and Zirconocene: A Density Functional Theory Study. *Organometallics*, **2002**, 21, 2254-2261	3.8	51
112	Electronic requirements for macropolyhedral boranes. *Chemical Reviews*, **2002**, 102, 93-144	68.1	181
111	Control of stability through overlap matching: closo-carborynes and closo-silaborynes. *Journal of the American Chemical Society*, **2002**, 124, 4402-7	16.4	40
110	Structures, Stabilities, and Ionization Potentials of Dodecahedrane Endohedral Complexes. *Journal of Physical Chemistry A*, **2002**, 106, 5144-5154	2.8	61
109	Structure and bonding of metallacyclocumulenes, radialenes, butadiyne complexes and their possible interconversion: a theoretical study. *Journal of Organometallic Chemistry*, **2001**, 635, 204-211	2.3	21
108	A theoretical study of transition metal complexes of C60 and C70 and their ring-opened alternatives. *Journal of Molecular Graphics and Modelling*, **2001**, 19, 256-65	2.8	6
107	Cationic Closo CarboranesPromising Weakly Coordinating Ions. *Journal of Computational Chemistry*, **2001**, 22, 1542-1551	3.5	12
106	Polyhedral boranes and elemental boron: direct structural relations and diverse electronic requirements. *Journal of the American Chemical Society*, **2001**, 123, 4324-30	16.4	62
105	A unifying electron-counting rule for macropolyhedral boranes, metallaboranes, and metallocenes. *Journal of the American Chemical Society*, **2001**, 123, 4313-23	16.4	158
104	Is borazine aromatic? Unusual parallel behavior between hydrocarbons and corresponding B-N analogues. *Inorganic Chemistry*, **2001**, 40, 3615-8	5.1	117
103	Missing hydrogens in B(19)H(20)(-)? Application of electron counting rule for edge-sharing macropolyhedral boranes. *Inorganic Chemistry*, **2001**, 40, 1730-1	5.1	14
102	CH?Interactions involving acetylene: an ab initio MO study. *Journal of Molecular Structure*, **2000**, 556, 315-320	3.4	23
101	Aza-bowls: synthesis and molecular structure of triaza-[3]-peristylane. *Tetrahedron Letters*, **2000**, 41, 2999-3002	2	15
100	Will an B-Si3H3Ligand Form Sandwich Compounds with Main Group Elements?. *Journal of the American Chemical Society*, **2000**, 122, 1725-1728	16.4	26

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