Ground states of molecules. 38. The MNDO method. Approximations and parameters

DOI: 10.1021/ja00457a004
Journal of the American Chemical Society, 1977, 99, 4899-4907

#	Paper	IF	Citations
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2292	Efficient Binding of Flexible and Redox-Active Coenzymes by Oxidoreductases.		
2291	ChemInform Abstract: GROUND STATES OF MOLECULES. 38. THE MNDO METHOD. APPROXIMATIONS AND PARAMETERS. **1977**, 8, no-no		
2290	Facile isomerization and oxidation by 3O2 of 1,2-dialkoxy-1-halogenoethenes. **1978**, 19, 4969-4970		4
2289	Theoretical study of complexes of cyclobutadiene with carbonmonoxide and carbondioxide. **1978**, 19, 1841-1844		5
2288	Some systematic errors in mindo/3 calculations. **1978**, 19, 1897-1900		8
2287	The ultraviolet photoelectron spectrum of O-benzoquinone methide. **1978**, 19, 2433-2436		13
2286	Analytical first derivatives of the energy in MNDO. **1978**, 2, 25-29		21
2285	Semiempirical calculations of molecular vibrational frequencies: The MNDO method. *Journal of Molecular Structure*, **1978**, 43, 135-138	3.4	96
2284	Iterative computer analysis of complex exchange-broadened NMR bandshapes. **1978**, 32, 145-152		25
2283	Photoelektronenspektren und MNDO-Rechnungen fˆ [n]Paracyclophane. **1978**, 111, 1958-1961		48
2282	MNDO calculations of molecular electric polarizabilities, hyperpolarizabilities, and nonlinear optical coefficients. **1978**, 59, 541-544		39
2281	Tris (methylidene)-cyclopropane ([3]Radialene)Part 1. Enthalpy of formation and strain energy. **1978**, 61, 741-753		26
2280	Chemical bonding. **1978**, 29, 1-31		52
2279	Ground states of molecules. 46. MNDO study of hydroboration of alkenes and alkynes. **1978**, 17, 1075-1082		31
2278	Ground states of molecules. 47. MNDO studies of boron hydrides and boron hydride anions. **1978**, 17, 1569-1581		36

2277	Theoretische Chemie 1977. **1978**, 26, 71-74		1
2276	THE SCF□CAO▽MO METHOD AND EXTENSIONS. **1978**, 309-346		
2275	SINGLET MOLECULAR OXYGEN CHEMISTRY AND IMPLICATIONS FOR FLAVIN-COFACTOR HYDROXYLATIONS. **1979**, 513-555		1
2274	NDDO MO calculations: isotropic hyperfine coupling constants and nuclear spin-spin coupling constants. **1979**, 68, 219-221		3
2273	The electronics structures of small strained rings. An investigation of the interaction between the oxygen and the □rbitals in 3-methyleneoxetane and 3-oxetanone. **1979**, 68, 237-241		9
2272	Coupling of stereochemistry and proton donor-acceptor properties of a schiff base, a model of a light-driven proton pump. **1979**, 64, 370-374		67
2271	On the degree of Koopmans' violations in alkylfulvenes. **1979**, 67, 479-482		1
2270	Planar Tetracoordinate Silicon. **1979**, 18, 553-554		53
2269	Existence of 1,2,3-Benzoxadiazole in the Gas Phase. **1979**, 18, 692-693		8
2268	Planar tetrakoordiniertes Silicium. **1979**, 91, 588-589		24
2267	Existenz von 1, 2, 3-Benzoxadiazol in der Gasphase. **1979**, 91, 737-738		17
2266	Structure of the tricyano ion. **1979**, 37, L469-L470		5
2265	A variable-temperature photoelectron spectral study of 2-oxa-bicyclo[2.2.0] hex-5-en-3-one and 2H-pyran-2-one (□pyrone). **1979**, 17, 67-70		9
2264	Structures and properties of fluorinated pyridines; assignment of the two homo's of pyridine. **1979**, 41, 21-33		31
2263	Mo studies of polymers. I. Use of MNDO to calculate geometries, vibrational frequencies and the electronic band structures of polymers; formalism and application to polyethylene. **1979**, 43, 145-156		43
2262	The combined use of SCF-MO calculations and frequency data in the evaluation of general harmonic force fields for molecules containing third row elements. *Journal of Molecular Spectroscopy*, **1979**, 78, 267-276	1.3	3
2261	The combined use of SCF-MO calculations and experimental data in the evaluation of quadratic force fields. *Journal of Molecular Spectroscopy*, **1979**, 78, 139-155	1.3	3
2260	MNDO study of transient species: the IR spectrum of benzyne. *Journal of Molecular Structure*, **1979**, 51, 275-279	3.4	16

2259	Detailed potential energy surfaces from MNDO semiempirical molecular orbital theory. *Journal of Molecular Structure*, **1979**, 51, 281-287	3.4	8
2258	Elucidation of thermal reactions by variable temperature photoelectron spectral detection of reactive intermediates. The UV photoelectron spectra of transient fulveneketene, fulvenethioketene, A ketoketene, and thiobenzpropiolactone. **1979**, 20, 59-62		25
2257	Diazothenes: evidence for their production by way of a Wittig reaction.. **1979**, 20, 4619-4622		15
2256	An intermediate neglect of differential overlap theory for transition metal complexes: Fe, Co and Cu chlorides. **1979**, 53, 21-54		750
2255	Geometry optimizations with explicit inclusion of electron correlation. **1979**, 52, 319-328		7
2254	Heptaphospha-Nortricyclene: Bindungsmodell fˆ P7H3 und Photoelektronen-Spektrum von P7[Si(CH3)3]3. **1979**, 458, 53-61		11
2253	Quantum chemical and physicochemical influences on structure activity relations and drug design. **1979**, 16, 221-241		21
2252	Diazo-, azo-, and azidoazoles. V. MNDO calculations on the 2-azidoimidazole/imidazo[1, 2-d]tetrazole equilibrium. **1979**, 16, 685-688		12
2251	A theoretical investigation on the systems C2H5O+ and C2H5S+. **1979**, 63, 326-331		8
2250	The use of SCF-MO calculations and experimental data in evaluating general quadratic force fields of light atom molecules. *Journal of Molecular Spectroscopy*, **1979**, 78, 125-138	1.3	6
2249	Quadratic potential functions for the boron trihalides. *Journal of Molecular Spectroscopy*, **1979**, 75, 363-367	1.3	6
2248	Semiempirical molecular orbital calculation of atom-pair interactions in a molecule. *Journal of the American Chemical Society*, **1979**, 101, 1087-1094	16.4	5
2247	Quantum chemical methods and their applications to chemical reactions. **1980**, 54, 263-300		33
2246	SINDO1. A semiempirical SCF MO method for molecular binding energy and geometry I. Approximations and parametrization. **1980**, 57, 95-106		228
2245	C2Li6 structural isomers. **1980**, 21, 2151-2154		13
2244	A MNDO study of the structures and stabilities of some substituted pentadienyl anions. **1980**, 185, 157-181		40
2243	Variation of calculated single bond lengths in saturated hydrocarbon and silicon hydride molecules. **1980**, 18, 1449-1463		2
2242	Multilayer X-ray spectrometry in the 2080 ˚ region: A molecular orbital analysis of CO and CO2 in the gas and solid states. **1980**, 9, 81-89		8

2241	Influence of the INDO parameterization on the indirect spin–spin coupling constants as calculated by the FPT INDO method. **1980**, 13, 137-142		14
2240	Dissoziative Ringˆ Öffnung halogensubstituierter Methylcyclopropan-Radikalkationen in der Gasphase. **1980**, 113, 1084-1094		20
2239	Reaktionen gekoppelter Dreiringe, X. Synthese und Bildungsweise eines donorstabilisierten Dicyclopropenylioallyl-Kations. **1980**, 113, 1746-1753		15
2238	Synthese bicyclischer, nicht-konjugierter Polyene. Stereochemie und transanulare Wechselwirkungen. **1980**, 113, 2589-2600		5
2237	Photoelektronenspektren von [8]Paracyclophan und [8]Paracyclophan-4-en. Eine Ermittlung des induktiven und hyperkonjugativen Effekts fˆ Ö[n]Paracyclophane. **1980**, 113, 3401-3403		14
2236	Mechanisms of unimolecular fragmentations of odd-electron cations in the gas phase: The importance of intramolecular hydrogen migration for [odd]+·→[even]+ transitions. **1980**, 15, 491-501		61
2235	Problems concerning the theoretical treatment of tautomeric equilibria of hetrocycles. **1980**, 69, 537-539		55
2234	The C4H4CO potential surface. Reactions involving bicyclo[2.1.0]pentenone. **1980**, 1, 129-133		11
2233	Evaluation of MINDO/3 calculated structures. II. Branching errors in alkanes and cycloalkanes. **1980**, 1, 233-239		8
2232	2-Vinylidene-2H-indene. **1980**, 19, 821-822		9
2231	Direkter Nachweis von Dicyanketen in der Gasphase. **1980**, 92, 751-752		15
2230	Direkter Nachweis von Dicyanthioketen in der Gasphase. **1980**, 92, 752-753		12
2229	2-Vinyliden-2H-inden. **1980**, 92, 846-847		9
2228	The use of the MNDO SCF MO method in UPS band-assignments for unsaturated hydrocarbons and fluorocarbons. **1980**, 21, 121-134		16
2227	Ground states of molecules. *Journal of Molecular Structure*, **1980**, 68, 105-118	3.4	15
2226	The 7,8-epoxy-2,3,5,6-tetrakis(methylene) bicyclo[2.2.2]octane; synthesis and diels-alder reactivity. **1980**, 36, 149-154		42
2225	Some remarkable oxidations of 2,3,5,6-tetrachloro--phenylenediamine, and products therefrom. **1980**, 21, 4119-4122		4
2224	Fluorinated chromenes. III. Synthesis of 3-fluoro-2,2-dimethyl-2H-chromenes. **1980**, 17, 1377-1379		14

2223	MNDO-Berechnungen der Nullpunktsenergien und der temperaturabh ̂ igigen Beitr ̂ ge zur Freien Reaktionsenthalpie von Protonen ̂ bertragungsreaktionen. **1980**, 20, 455-456	1
2222	Elucidation of thermal reactions by variable temperature photoelectron spectroscopy. A new synthesis of benzthiete and first direct evidence for transient benzothiete keten. **1980**, 21, 343-346	28
2221	OXYGEN AS A TWO-LEVEL TUNNELING SYSTEM IN SiO2. **1980**, 59-62	1
2220	MINDO/3-BERECHNUNGEN VON PHOSPHORORGANISCHEN VERBINDUNGEN. IV.1. **1980**, 8, 337-341	7
2219	Ab initio studies on polymers. IV. Polydiacetylenes. **1980**, 13, 5673-5689	64
2218	MNDO MOCIC evaluation of the uracil force field: Application to the interpretation of flavin vibrational spectra. **1980**, 73, 5482-5492	58
2217	MINDO/3-BERECHNUNGEN VON PHOSPHORORGANISCHEN VERBINDUNGEN. V.1. **1980**, 8, 343-350	8
2216	Ab Initio Calculation of One-Center Integrals of Semiempirical Theories of Valence. **1980**, 19, 99-108	19
2215	The application of gas phase and solid state X-ray photoelectron spectroscopy to the investigation of derivatives containing the repeating SN unit. **1980**, 1, 161-173	5
2214	Cyclononatetraenylidene. **1981**, 46, 2201-2202	15
2213	Struktur und eigenschaften der c ̂ siumamidolanthanatmonoammoniakate Cs3La(NH2)6 NH3 und Cs4La(NH2)7 NH3. **1981**, 81, 121-133	8
2212	Electronic structure and molecular topology of boron and aluminum suboxides. **1981**, 43, 2645-2647	16
2211	A study of the dimer bond on the reconstructed (100) surfaces of diamond and silicon. **1981**, 103, 404-415	68
2210	The adsorption of hydrogen on the (100) surfaces of silicon and diamond. **1981**, 108, 153-168	95
2209	Analyse conformationnelle th ̂ brique des mol ̂ cules de benzylid ̂ ne-aniline, stilb ̂ ne et azobenz ̂ ne. **1981**, 76, 299-311	28
2208	The molecular structures of SiX3OBX2 (X ? H, F, Cl). **1981**, 85, 373-380	4
2207	Jahn eller effects in the MNDO approximation: Structures of the molecular cations of silane and the fluoro and chlorosilanes. **1981**, 85, 87-98	5
2206	MNDO and INDO geometrical dependences of the hydrogen diamagnetic shielding tensor of some small molecules. **1981**, 86, 63-67	2

2205	An ab initio reinvestigation of the geometric and electronic structure of boron trioxide. **1981**, 76, 29-35	5
2204	MINDO/3 AND MNDO CALCULATIONS OF PHOSPHINES: CONFORMATIONAL ENERGIES, ROTATIONAL BARRIERS, BOND LENGTHS AND BOND ANGLES. **1981**, 11, 11-17	2
2203	Structure, spectra, and function of model cytochrome P450. **1981**, 367, 192-218	15
2202	SEMI-EMPIRICAL SCF-MO CALCULATIONS OF BACKBONE CONFORMATIONAL STATES IN SOME GLASSY POLYMERS. **1981**, 371, 299-300	
2201	MNDO study of some condensed (HnFn+1)□anions. **1981**, 85, 365-371	5
2200	Radical eliminations from gaseous cation radicals via multistep pathways □The concept of □hidden□hydrogen rearrangements. **1981**, 1-31	45
2199	Molecular Conformations of 4-Aminomethyl-1-cyclohexanecarboxylic Acids in Aqueous Solution. **1981**, 54, 2420-2426	
2198	A Photoelectron Spectroscopic Study of the 2-Azidopyridine ? Tetrazolo [1.5-□Pyridine Equilibrium between 391 and 533 K. **1981**, 14, 747-753	6
2197	Photoelektronen-Spektren und Molekˆ □eigenschaften: Echtzeit-Gasanalytik in strˆ □enden Systemen. **1981**, 93, 425-442	92
2196	Struktur- und Bindungsverhˆ □nisse in cyclischen Schwefel-Stickstoff-Verbindungen - Molekˆ □orbitalbetrachtungen. **1981**, 93, 442-450	31
2195	Cyclopentadienthion. **1981**, 93, 603-605	13
2194	Isobenzofulven. **1981**, 93, 1078-1079	9
2193	Transanulare Wechselwirkung des Azo-Chromophors in isodrinanalogen Systemen1). **1981**, 114, 423-432	26
2192	Die He(I)-Photoelektronenspektren von (CH3)2PSCH3, (CH3)2AsSCH3, (CH3)2AsSeCH3 und (CH3)2PSeCH31). **1981**, 114, 2300-2308	10
2191	Transannulare Wechselwirkungen zwischen Acetylenen □Photoelektronenspektroskopische Untersuchungen an 1,8-Diethinylnaphthalin und cyclischen Derivaten von 2,2?-Diethinylbiphenyl. **1981**, 114, 2309-2321	13
2190	Gasphasen-Reaktionen, 21. Thermische Erzeugung von Alkyl- und Halogenketenen. **1981**, 114, 2595-2608	49
2189	Gasphasen-Reaktionen, 22. Thermische Erzeugung von C4H4O: Vinylketen und Ethylidenketen. **1981**, 114, 2609-2621	16
2188	The electronic structures of some acyclic molecules containing phosphorus, nitrogen, and oxygen. **1981**, 79, 149-153	2

2187	Fragmentation mechanism for the loss of XCY (X and Y = O, OR, S) from 2-phenyl-1,3,4-oxadiazole-5-one and related sulfur-containing compounds. **1981**, 16, 29-33	7
2186	Etude par des techniques de partition d'ˆ hergie des facteurs qui conditionnent l'ˆ ¿uilibre conformationnel de propˆ Ïes disubstituˆ ¿-1,3 de configuration E. **1981**, 64, 1949-1958	1
2185	Bicyclo[1.1.0]butadiene (trialene): An experimentally viable molecule?. **1981**, 2, 207-211	9
2184	Three electron bonds. I. The H2SSH radical cation. **1981**, 2, 261-265	40
2183	MNDO calculations for compounds containing aluminum and boron. **1981**, 2, 433-445	86
2182	Limitations on mndo and mndo/ci computations of activation barriers. **1981**, 83, 151-155	7
2181	Quantum chemical studies on the conformational structure of bacterial peptidoglycan. I. MNDO calculations on the glycan moiety. **1981**, 88, 441-457	15
2180	Reaktivitˆ Ïder Pyrrolpigmente, 2. Mitt.: Deprotonierung von 3-Pyrrolin-2-onen. **1981**, 112, 359-368	11
2179	A MINDO/3 MO study of oxidized flavins. **1981**, 60, 127-141	10
2178	A CNDO/INDO molecular orbital formalism for the elements H to Br. theory. **1981**, 59, 127-151	177
2177	A CNDO/INDO molecular orbital formalism for the elements H to Br. applications. **1981**, 59, 153-179	61
2176	Semiempirical NDDO calculations with STO-3G and 4-31G basis sets. **1981**, 59, 191-208	10
2175	Strategy for computer-generated theoretical and quantum chemical prediction of toxicity and toxicology (and pharmacology in general). **1981**, 20, 419-439	6
2174	Alternative mechanisms for cyanide anion exchange with acetonitrile. **1981**, 22, 2957-2960	3
2173	2.4.5-Tris-(diethylamino)-4H-imidazol und davon abgeleitete fulvene und fulvalene. **1981**, 22, 2973-2976	10
2172	Rotational isomerism between the and forms of -substituted benzo--methyl hydroxamic acids in strong acid. **1981**, 22, 3007-3008	3
2171	Charge-transfer bands of bicyclic □unsaturated ketones. Circular dichroism of (+)-(1R)-5,6-dimethylidene-2-bicyclo[2.2.2]octanone and (+)-(1R)-2-bicyclo[2.2.2]oct-5-enone. **1981**, 22, 4721-4722	14
2170	The rearrangement of a tricyclic C8H11+ alkyl carbocation into a primary cyclopropylcarbinyl cation. **1981**, 22, 1191-1194	0

2169	The structure of silyl cyclopentadienes. **1981**, 221, 19-31		7
2168	Jahn-teller effects in the MNDO approximation: structures of the molecular cations of some simple organosilanes. **1981**, 217, 11-18		11
2167	Novel beryllium derivatives of (CH)n carbocycles: an MNDO study. **1981**, 219, 279-293		8
2166	Jahn-teller effects in the MNDO approximation: structures of the molecular cations of some simple organoberyllium compounds. **1981**, 217, 273-282		9
2165	Carbonyl sulfides as possible intermediates in the photolysis of oxathiiranes. **1981**, 37, 1257-1262		13
2164	On the planarity of tetracoordinate carbon enclosed by annulene perimeters. **1981**, 37, 921-927		41
2163	The gas-phase conformation of 3,7-dimethyl-3,7-diazabicyclo[3.3.1]nonane. **1981**, 37, 1853-1859		26
2162	The mechanism of [1,3] to acyl migrations. **1981**, 37, 3107-3110		2
2161	Gas phase and solid state X-ray photoelectron spectra of the substituted acetylenes (SF5)n C2 (CF3)2□ (n = 0, 1, 2): A comparison of the pentafluorosulfur and trifluoromethyl groups. **1981**, 22, 119-129		16
2160	A comparative theoretical study of photoionization cross sections and angular distributions. **1981**, 57, 227-243		35
2159	Difluoroborane, HBF2. A study by HeI photoelectron spectroscopy, and ab initio methods including perturbation corrections to Koopmans' theorem. **1981**, 59, 75-83		9
2158	Comparisons between crystallographic results and theoretical calculations on phenol molecules. *Journal of Molecular Structure*, **1981**, 70, 87-94	3.4	15
2157	Rotation and inversion in nitrosamines. *Journal of Molecular Structure*, **1981**, 73, 171-180	3.4	12
2156	The electronic structure of siloxyl sulfide, OSiS. **1981**, 53, L163-L164		4
2155	Application of the partitioning of energy in the mndo method to the study of the basicity of imidazole, pyrazole, oxazole, and isoxazole. **1981**, 18, 1189-1196		33
2154	Structural and electronic factors influencing the inhibition of aniline hydroxylation by alcohols and their binding to cytochrome P-450. **1981**, 34, 287-300		18
2153	Correlation between the observed infrared stretching frequency and the bond character of the Si□H bond. **1982**, 77, 4330-4332		24
2152	A Direct Photoelectron Spectroscopy Study of the 2-Azidopyridine Pyrolysis PES, 2-azidopyridine, thermic degradation, MNDO calculations. **1982**, 15, 435-438		3

2151	Reduzierte Zustandssummenverhˆ Ltnisse isotoper Molekˆ Le auf quantenchemischer Grundlage: I. Mitt. MNDO-Berechnungen von Siliziumverbindungen. **1982**, 18, 203-207	6
2150	Ligands of low electronegativity in the vsepr model: Isoelectronic molecules and ions (MX3)2 YE2n+. **1982**, 87, 273-282	7
2149	Ligands of low electronegativity in the VSEPR model: The structures of singlet carbenes. **1982**, 87, 71-79	4
2148	Molecular fragmentations. **1982**, 86, 377-385	5
2147	Isomerism and adduct formation in the Hector's base series: A MNDO study of model compounds. **1982**, 90, 227-239	0
2146	Ligands of low electronegativity in the VSEPR model: Molecular pseudohalides. **1982**, 89, 325-332	19
2145	Molecular fragmentations. **1982**, 89, 333-347	6
2144	The conformations of two enamines. **1982**, 89, 349-353	5
2143	Theoretical studies on the geometric and electronic structure of substituted SCN isomers. **1982**, 86, 239-253	8
2142	Non-empirical and MNDO study of the geometry and electronic structure of H2XO radicals. **1982**, 90, 59-64	8
2141	MNDO study of some cage molecules related to hexamethylenetetramine. **1982**, 90, 177-182	2
2140	Structure of bis(4-methylpyridine)hydrogen(I) tetraphenylborate. **1982**, 38, 667-669	11
2139	Structure of N,N'-bis[2-(5-tert-butyl-3H-1,2-dithiol-3-ylidene)ethylidene]hydrazine. **1982**, 38, 2281-2283	1
2138	Fast semiempirical calculations. **1982**, 3, 227-228	68
2137	Evaluation of MINDO/3 calculated structures. III. Saturated acyclic compounds with chlorine, nitrogen, oxygen, or sulfur. **1982**, 3, 229-233	3
2136	MNDO Calculations of silicon-containing molecules. **1982**, 3, 445-450	29
2135	Thermodynamical properties and structural data of radicals calculated by MNDOUHF. **1982**, 3, 486-494	66
2134	Interaction between Exocyclic s-cis-Butadiene and Homoconjugated Functions. Preparation and Diels-Alder Reactivity of Remotely Substituted 2,3-Dimethylidenebicyclo[2.2.2]octanes. **1982**, 65, 178-187	16

2133	Regioselectivity of the Diels-Alder Additions of 2-Substituted 5,6 Dimethylidenenorbornanes and-bicyclo[2.2.2]octanes. **1982**, 65, 188-203	28
2132	The Photoelectron Spectrum of [18]Annulene. **1982**, 65, 582-586	4
2131	Electronic and Molecular Structure of Simple 3,3?-Bicyclopropenyls. Photoelectron Spectroscopy and Model Calculations. **1982**, 65, 968-982	21
2130	The preferred structure of C2H2. **1982**, 85, 493-495	32
2129	Lettters to the editor. **1982**, 17, 151-153	6
2128	Letters to the editor. **1982**, 17, 448-460	7
2127	Gasphasen-Reaktionen, 24. Die thermische Erzeugung von Thiocarbonyl-Verbindungen. **1982**, 115, 492-503	48
2126	Azaborolinyl-Komplexe, VI. Synthese und Eigenschaften des 1,2-Azaborolinyl-Anions. **1982**, 115, 732-737	35
2125	Gasphasen-Reaktionen, 30. Thioacrolein: Das stabilste C3H4S-Isomere und sein PE-spektroskopischer Nachweis in der Gasphase. **1982**, 115, 1339-1348	47
2124	Aromatizitˆ als Funktion des Ionenpaarcharakters: Akzeptor-substituierte Cyclononatetraenyl-Anionen, Enolat-Anionen mit variablen Ladungsverteilungen und ungewˆ nlichen konformativen Eigenschaften. **1982**, 115, 3167-3190	19
2123	Siliciumverbindungen mit starken intramolekularen sterischen Wechselwirkungen, 13. Rotationshinderungen in Tri-tert-butylsilanen. **1982**, 115, 3444-3448	7
2122	Die thermische Umwandlung von 1,3-Cyclooctadien-5-in in Benzocyclobuten - eine neue Isomerisierung auf der C8H8-Hyperflˆ he. **1982**, 21, 85-90	1
2121	2,4,6-Cycloheptatrienylidenmalondialdehyd (8,8-Diformylheptafulven). **1982**, 21, 113-120	2
2120	Das Dianion 1,2-Diphenylbenzocyclobutadiendiid. **1982**, 21, 345-354	4
2119	Das Dianion 1,2,3,4-Tetraphenylcyclobutadiendiid. **1982**, 21, 355-360	5
2118	Ni(II) chromophores with the 2,6-bis(diphenylphosphinomethyl)pyridine ligand: XPS characterization of the electronic structure. **1982**, 63, 225-231	12
2117	Reaction profiles in sulfur?nitrogen chemistry I. The isomerization of cis thionylimide, HNSO, to cis thiazyl-S-hydroxide, HOSN. **1982**, 59, 165-169	3
2116	Factors influencing the stability of cations (amine) H-amine)+ and related ions. **1982**, 64, L73-L74	1

2115	MNDO-estimations of the standard heat of formation of some binary sulfur-nitrogen compounds and their derivatives. **1982**, 64, L161-L162		4
2114	On the electronic structure of the tetrathiazyl dication. **1982**, 65, L201-L202		2
2113	An MNDO SCF MO investigation of the electronic structures and conformational preferences of model polycarbonate systems. **1982**, 4, 83-94		9
2112	Theoretical description of conformational isomers in the azastilbenes: A study using modified neglect of differential overlap (MNDO) and intermediate neglect of differential overlap/spectroscopic (INDO/S). **1982**, 19, 329-335		10
2111	MNDO-rechnungen zum mechanismus der H2O-abspaltung aus protoniertem cyclohexanon in der gasphase. **1982**, 44, 81-90		8
2110	Gekreuzt-konjugierte polyene. *Journal of Molecular Structure*, **1982**, 81, 73-86	3.4	7
2109	The crystal structures of 2'-deoxy-2'-fluorocytidine and 2'-deoxy-2'-fluorouridine. *Journal of Molecular Structure*, **1982**, 82, 77-94	3.4	26
2108	Gekreuzt-konjugierte polyene. *Journal of Molecular Structure*, **1982**, 81, 207-221	3.4	11
2107	Molecular fragmentations Part XII. Mass spectral fragmentation of pyridine. *Journal of Molecular Structure*, **1982**, 91, 353-371	3.4	1
2106	Computation of nuclear quadrupole coupling constants by semiempirical quantum chemical techniques. *Journal of Molecular Structure*, **1982**, 91, 373-385	3.4	3
2105	Non-empirical and mndo study of the geometry and electronic structure of H2XO radicals. *Journal of Molecular Structure*, **1982**, 90, 59-64	3.4	7
2104	MNDO study of some cage molecules related to hexamethylenetetramine. *Journal of Molecular Structure*, **1982**, 90, 177-182	3.4	1
2103	Isomerism and adduct formation in the hector's base series: A MNDO study of model compounds. *Journal of Molecular Structure*, **1982**, 90, 227-239	3.4	2
2102	Quantum chemical studies of model cytochrome P450 hydrocarbon oxidation mechanisms II. Mechanisms and relative kinetics of oxene reactions with alkenes. **1982**, 17, 1-22		12
2101	Photoelectron spectra of thermally generated unstable organic compounds □2-Propene-1-imine. **1982**, 28, 33-43		21
2100	The UPS of some compounds containing the heteroatoms phosphorus, nitrogen, and oxygen. **1982**, 25, 135-147		3
2099	A non-empirical LCAO MO SCF investigation of the ground and core-hole states of the cyclopentyl cation. **1982**, 27, 57-62		
2098	He(I) Photoelectron spectroscopy of transient species: fluorothiocyanate (FSCN). **1982**, 26, 147-156		9

2097	The mechanism of NO3 formation from gaseous ethyl nitrate. **1982**, 67, 221-228	3
2096	Highly resolved optical spectra of o-durylene. **1982**, 72, 73-81	6
2095	Bond orders in 1,5-benzodiazepinium cations compared to those in biphenylenes. Another example of bonds of low bond order which isolated electron systems.. **1982**, 23, 4379-4380	4
2094	On the ground state and first excited state geometries of syn-sesquinorbornene. **1982**, 23, 927-930	21
2093	The cleavage of 2,5-dihydro-2-furanylcarbene. **1982**, 23, 2547-2550	0
2092	Y vs. cyclic delocalization in small ring dications and dianions: The dominance of charge repulsion over Huckel aromaticity. **1982**, 23, 3547-3550	38
2091	The crystal and molecular structure of 1,1,1,3,3,3-hexaphenyl-1,3-disilapropane. **1982**, 234, 15-25	16
2090	Regioselektive dimetallierung von aromaten. Bequemer zugang zu 2,2?-disubstituierten biphenylderivaten. **1982**, 228, 107-118	88
2089	Hexaorgano-substituted triatomics R3XYZR3: The configuration of (R3PNPR3)+ and the crystal and molecular structure of triphenyl(P,P,P-triphenylphosphine imidato-N)phosphorus(I) thiocyanate. **1982**, 226, 171-181	6
2088	MNDO study of reaction paths: Hydroboration of methyl cyanide. **1982**, 60, 451-454	0
2087	MNDO study of reaction paths: Diboration of acetylene. **1982**, 60, 573-578	6
2086	The interaction of nitrogen and carbon monoxide with certain ions and neutral species. **1982**, 60, 579-587	4
2085	Unrestricted Hartree-Fock instabilities in nuclear spin-spin coupling calculations. The MNDO method. **1982**, 61, 49-57	30
2084	Semiempirical and ab initio Calculations on the Tautomerism of Pyrazolin-5-ones in the Gas Phase and in Solution. **1982**, 324, 827-831	8
2083	Models for the Hydrogen-Related Defect Impurity Complexes and Si?H Infrared Bands in Crystalline Silicon. **1982**, 74, 329-341	83
2082	Critical examination of approximate LCAOMO methods. I. Reasons for the failure of the CNDO and INDO methods in theoretical conformational analysis of conjugated compounds. **1982**, 21, 833-843	25
2081	Proton transference in hydrogen bonded systems. I. Uracil tautomerism. **1982**, 22, 89-100	11
2080	Semi-empirical calculations concerning the geometry of the cycloheptatrienyl anion. **1982**, 101, 137-141	7

2079	Structure of N-[2-(5-tert-butyl-3H-1,2-dithiol-3-ylidene)ethylidene]-N',N'-dimethylhydrazine, C11H18N2S2. **1983**, 39, 106-108	1
2078	3,4,5,6-Tetrahydro-2H-1-benzothiocin 1,1-dioxide, C11H14O2S. **1983**, 39, 108-109	
2077	B-Z transition in methylated DNA. A quantum-chemical study. **1983**, 132, 55-62	23
2076	Metabolism and relative carcinogenic potency of chloroethylenes: a quantum chemical structure-activity study. **1983**, 43, 33-66	9
2075	Conformational analysis of cytokinins and analogs. **1983**, 43, 73-85	1
2074	Acid-catalyzed hydrolysis of 2-methoxypropenal. **1983**, 115, 85-94	1
2073	Theoretische Untersuchungen zum Zerfallsgleichgewicht des Harnstoffs in Gasphase und in w□ □iger L□ sung. **1983**, 325, 774-786	5
2072	Quantum study of the ground state of a series of unsaturated boron□itrogen compounds by the MNDO method. I. Geometries and stabilities. **1983**, 23, 891-904	15
2071	Mechanistic studies of oxene reactions with organic substrates: Reaction paths on MNDO enthalpy surfaces□odels for cytochrome P450 oxidations. **1983**, 23, 1257-1268	22
2070	Protonation of aminopyrone: A four centers problem, CNDO/2 versus MNDO study. **1983**, 24, 425-428	3
2069	A comparison of various MO methods for predicting regioselectivity in Diels-Alder reactions. **1983**, 62, 293-299	4
2068	Intrinsic reaction coordinate for the gas-phase pyrolysis of ethyl formate. **1983**, 62, 245-255	12
2067	Quantum chemical calculations on the structure of (Cl2F)+ and related molecules. **1983**, 22, 575-584	13
2066	Application de la spectroscopie moleculaire aux proprietes moleculaires. **1983**, 247, c17-c20	11
2065	Cyclisierung und fragmentierung aliphatischer azide an metall-metall-dreifachbindungen: Neuartige reaktionswege gegen□ □er ihrer thermischen zersetzung ln der gasphase [1,2]. **1983**, 254, 219-241	13
2064	Generation of dimethylgermathione and dimethylsilathione and their detection in the gas phase by photo-electron spectroscopy. **1983**, 249, c17-c20	23
2063	Correlation of 13C-1H spin-spin coupling constants and the sum of internuclear angle distortions in saturated hydrocarbons. **1983**, 39, 1783-1788	6
2062	Conformational analysis of 2,3-dialkoxy-1,4-dioxanes. **1983**, 39, 3959-3963	11

2061	Structure and reactivity of norbornene and syn-sesquinorbornene. **1983**, 39, 3345-3350	54
2060	Conformational dependent regio- and stereo-selectivity in transformations of germacrenes. **1983**, 39, 2981-2987	8
2059	[5]metacyclophanes a spectroscopic and theoretical investigation of structure and conformation. **1983**, 24, 1821-1824	16
2058	Halogenation of quinoxalino[2,3-ccinnolines by hydrogen halides. **1983**, 24, 3151-3154	2
2057	The stereochemistry of the dibenzylidene-ethylene dianion. **1983**, 24, 3985-3988	3
2056	Remarkably fast [2+2]cycloreversion in methoxy substituted Cookson's cage ketones assisted by the capto-dative substituent effect and by the through-bond interaction. **1983**, 24, 5645-5648	6
2055	Strong Distortion of the Tetrahedral Geometry in a Spirosilicate: Molecular Structure of Bis(tetramethylethylenedioxy)silane. **1983**, 22, 65-65	14
2054	Starke Verzerrung der Tetraedergeometrie bei einem Spirosilicat: Molekˆ [struktur von Bis(tetramethylethylendioxy)silan. **1983**, 95, 52-52	13
2053	Conjugative, Exciton and Charge-Resonance Interactions in D2d-9,9?-Spirobifluorene and D2d-Tetrabenzotricyclo [5.5.0.02,8]dodeca-3,5,9,11-tetraene. Photoelectron and Polarized Absorption Spectra. **1983**, 66, 1441-1455	12
2052	An ab initio study of the relative stabilities of the isomers of CH2N2 and SiH2N2. **1983**, 4, 1-8	44
2051	Ground states of molecules. 56. MNDO calculations for molecules containing sulfur. **1983**, 4, 84-103	85
2050	Ground states of molecules. 53.MNDO calculations for molecules containing chlorine. **1983**, 4, 158-169	66
2049	Reaction path calculations for the interaction of the ethylene radical cation with triplet oxygen. **1983**, 4, 488-493	13
2048	Ground states of molecules. 64.MNDO Calculations for compounds containing bromine. **1983**, 4, 542-551	47
2047	MNDO calculations of proton and methyl-and ethyl-cation affinities of neutral carbon, nitrogen, and oxygen bases. **1983**, 4, 594-604	21
2046	MINDO/3-Rechnungen und PE-Untersuchungen zur Reaktionsweise von Azabicyclen. **1983**, 116, 1097-1106	9
2045	Notizen: Das Tribenzylidenmethan-Dianion. **1983**, 116, 1669-1673	12
2044	1,2-Oxathiolane A Photoelectron Spectroscopic Study. **1983**, 116, 2374-2377	7

2043	Das Photoelektronenspektrum von 1,1-Diethoxy-3,3-bis(trifluormethyl)allen. Der Effekt von Trifluormethylgruppen auf kumulierte Systeme. **1983**, 116, 2888-2895	5
2042	The electronic structure of phosphorus cages with the nortricyclane skeleton. Model calculations and photoelectron spectroscopic investigations. **1983**, 116, 2972-2982	12
2041	cis,trans,cis- and trans,trans,trans-1,2,3,4-Tetravinylcyclobutane preparation and some spectroscopic properties. **1983**, 116, 2983-2993	5
2040	1-Acyl-4-alkyliden-1,4-dihydropyridine, 7. Aktivierung durch Bortrifluorid: Intermolekulare Acylgruppen Übertragung unter Bildung von 1-(4-Pyridyl)-2-alkanonen. **1983**, 116, 3192-3204	7
2039	Regioselektive Metallierung von Aromaten, II. Zweitmetallierung von 1-Lithionaphthalin und 9-Lithioanthracen. **1983**, 116, 3283-3292	50
2038	A Fourier Transform Ion Cyclotron Resonance Study of the Structure of some Phenyl-substituted 2-Azaallenium Ions. **1983**, 116, 3877-3883	13
2037	Crystal structure of merosinigrin, an (ap,ap)-monothioacetal; structural properties of the thioglycosidic linkage. **1983**, 123, 1-11	11
2036	On the formation of protonated acetic acid from ionized n-alkanoic acids in the gas phase. **1983**, 18, 147-149	15
2035	Stable C2H5X+ (X=Cl, Br) radical cations of structure [CH3CHXH+]. Their energetics and dissociation characteristics. **1983**, 18, 208-211	16
2034	Further examples of skeletal rearrangements of the Wagner-Meerwein type in chemical ionization mass spectrometry: The case of [C6H9]+ ions. **1983**, 18, 215-218	9
2033	The role of charge-site location in fragmenting ions. 1 [CH3 CHXCOOCH3]+ and [CH2XCH2 COOCH3]+ ions and the structures of daughter ions derived from the loss of X (X = I, Br, Cl and CH3). **1983**, 18, 335-339	19
2032	The structure of decomposing [C7H7O]+ ions: Benzyl versus tropylium ion structures. **1983**, 18, 474-485	28
2031	Transition state structure and isotope effects in unimolecular hydrogen elimination from carbocations. **1983**, 98, 463-466	5
2030	Shape resonances in the valence-shell photoionization of cyanogen. **1983**, 100, 351-357	13
2029	A semi-empirical MO study of a series of amide, imidic acid, and imidate isomers. **1983**, 94, 311-315	11
2028	The photoelectron spectrum of 1-azetine. **1983**, 102, 239-243	6
2027	Theory defects in silicon: Recent calculations using finite molecular clusters. **1983**, 116, 28-38	12
2026	Isomerisation des ions organiques en phase gazeuse. I. Thermochimie des migrations 1,2 de groupements XCOH (X = H, CH3, OH, OCH3, NH2). **1983**, 55, 47-53	24

2025	An STO-3G investigation of barriers to rotation in model systems for aromatic polycarbonates. **1983**, 5, 23-28		6
2024	Charge distribution in alkylboranes and alkylamines and thier adducts with NH3 and BH3 respectively, as calculated by different methods. **1983**, 69, 61-69		10
2023	Application of quantum chemical calculations to chemical ionisation mass spectrometry. Protonation and adduct formation in stereoisomeric 7-norbornenyl compounds. **1983**, 46, 243-246		17
2022	Pyrolysis products in ion/molecule reactions. II. Amines, thiols, and esters. **1983**, 50, 235-243		5
2021	Development and status of MINDO/3 and MNDO. *Journal of Molecular Structure*, **1983**, 100, 41-50	3.4	96
2020	MNDO calculations applied to structural changes in 1,2,4-oxadiazole substituents. *Journal of Molecular Structure*, **1983**, 94, 203-207	3.4	2
2019	Semi-empirical molecular orbital conformational study of benzannelated cyclooctatetraenes and related compounds, and x-ray crystal structure of benzocyclooctatetraene. *Journal of Molecular Structure*, **1983**, 94, 285-291	3.4	4
2018	Molecular fragmentations. *Journal of Molecular Structure*, **1983**, 94, 305-318	3.4	10
2017	MNDO study of the proton affinity of fluorinated formaldehydes and acetones. *Journal of Molecular Structure*, **1983**, 94, 343-350	3.4	
2016	The structure and conformation of tetraoxaquaterene as an isolated molecule. *Journal of Molecular Structure*, **1983**, 94, 407-410	3.4	1
2015	MNDO study of the tautomers of nucleic bases. *Journal of Molecular Structure*, **1983**, 92, 255-265	3.4	18
2014	MNDO study of the tautomers of nucleic bases. *Journal of Molecular Structure*, **1983**, 92, 267-277	3.4	11
2013	AB initio and semiempirical molecular orbital studies on cytosine and N(4)-hydroxycytosine. *Journal of Molecular Structure*, **1983**, 92, 283-302	3.4	10
2012	Ligands of low electronegativity in the VSEPR model: Molecules and ions isoelectronic with primary, secondary and tertiary amines. *Journal of Molecular Structure*, **1983**, 92, 353-359	3.4	3
2011	Electrostatic solvent effect on the circular dichroism of The carbonyl transition. *Journal of Molecular Structure*, **1983**, 93, 277-281	3.4	2
2010	Ultraviolet photoelectron spectroscopic study of M?S □bonding energy and of spiroconjugation effects in group IVA thiospiranes. **1983**, 244, 343-354		3
2009	Semi-empirical Scf-Mo study of the mass spectral fragmentation of tetramethyldiphosphine. **1983**, 255, 49-60		6
2008	The positions of the hydrogen atoms in allyllithium and solvated allyllithium species. A MNDO study. **1983**, 259, 31-36		34

2007	Solitons and polarons in polyacetylene: Self-consistent-field calculations of the effect of neutral and charged defects on molecular geometry. **1983**, 28, 6927-6936	158
2006	The structure of pentacarbonyl(5,6-dihydro-4H-1,2-benzodithiole-7-carbothialdehyde-S7)tungsten(0), [W(C8H8S3)(CO)5]. **1983**, 39, 542-544	4
2005	Molecular fragmentations. **1983**, 104, 105-114	8
2004	The use of transformation matrices to follow the change in electronic structure of some simple organic molecules upon ionization. **1983**, 104, 233-239	6
2003	A new approach to the calculation of the molar Kerr constant in conjugated compounds: The conformation of 2-carbomethoxy-1,4-benzoquinone. **1983**, 105, 55-68	2
2002	On the structures of H+ (CO)5 and H+ (N2)5. **1983**, 105, 231-232	
2001	Molecular fragmentations. **1983**, 91, 353-371	8
2000	Computation of nuclear quadrupole coupling constants by semiempirical quantum chemical techniques. **1983**, 91, 373-385	3
1999	Electrostatic solvent effect on the circular dichroism of the carbonyl n-π* transition.. **1983**, 93, 277-281	9
1998	MNDO calculations applied to structural changes in 1,2,4-oxadiazole substituents. **1983**, 94, 203-207	1
1997	Semi-empirical molecular orbital conformational study of benzannelated cyclooctatetraenes and related compounds, and x-ray crystal structure of benzocyclooctatetraene. **1983**, 94, 285-291	2
1996	Molecular fragmentations. **1983**, 94, 305-318	5
1995	MNDO study of the proton affinity of fluorinated formaldehydes and acetones. **1983**, 94, 343-350	3
1994	The structure and conformation of tetraoxaquaterene as an isolated molecule. **1983**, 94, 407-410	5
1993	Isomerisation of gaseous C2H3O+ ions. **1983**, 104, 365-371	5
1992	Effect of conjugation beyond multiple bonds on geometry and acidity. **1983**, 105, 281-289	2
1991	MNDO study of the tautomers of nucleic bases. **1983**, 92, 255-265	35
1990	MNDO study of the tautomers of nucleic bases. **1983**, 92, 267-277	31

1989	AB initio and semiempirical molecular orbital studies on cytosine and N(4)-hydroxycytosine. **1983**, 92, 283-302	7
1988	Ligands of low electronegativity in the VSEPR model: Molecules and ions isoelectronic with primary, secondary and tertiary amines. **1983**, 92, 353-359	1
1987	A theoretical study of possible benzene dimerizations under high-pressure conditions. **1983**, 79, 4367-4375	35
1986	Neutral and charged soliton defects in polyacetylene. **1983**, 27, 1440-1442	21
1985	Helical versus planar cis-polyacetylene. **1983**, 28, 7387-7389	19
1984	Theoretical study of the reaction C(3P)+N2O(X 1⊞). I. Potential energy surfaces. **1983**, 78, 827-833	20
1983	Valence effective Hamiltonian technique for nitrogen containing polymers: Electronic structure of polypyrrole, pyrolized polyacrylonitrile, paracyanogen, polymethineimine, and derivatives. **1983**, 78, 6137-6148	125
1982	Isomerisation of Molecules in Organic Crystals, A Theoretical Study. **1983**, 96, 49-55	4
1981	Theory of strongly relaxed defects in crystalline and amorphous oxides. **1983**, 72, 27-38	16
1980	General trends in the molecular physics of azabiphenyls. **1983**, 49, 599-619	50
1979	Phase Transition and Vibrational Spectra of l-Leucine. **1983**, 87, 279-283	21
1978	CONFORMATIONAL ANALYSIS OF TRIMETHYLPHOSPHITE AND ITS METAL COMPLEXES. **1983**, 17, 205-220	9
1977	Pyrroles and their Benzo Derivatives: (i) Structure. **1984**, 155-200	11
1976	Molecular x-ray spectra: S-K□emission and K absorption spectra of SCO and CS2. **1984**, 81, 3375-3382	39
1975	A unified integral curve search technique for equilibrium- and transition- state geometries. **1984**, 80, 579-580	10
1974	Anisotropic rotational motion and internal rotation in liquid methylbenzenes. **1984**, 52, 1335-1354	20
1973	RADICAL IONS 64.1 IONIZATION AND OXIDATION OF 1,4,5,8-TETRATHIATETRALIN. **1984**, 21, 67-77	11
1972	Electronic structures of third-period interstitials in silicon. **1984**, 30, 771-774	5

1971	Theory of off-center impurities in silicon: Substitutional nitrogen and oxygen. **1984**, 29, 3193-3207		116
1970	Molecular aspect of the even□odd effect in cyanobiphenyls (nCB): Theoretical studies of the molecular geometrical conformation and optical anisotropy. I. n□. **1984**, 81, 344-348		6
1969	Electronic structure of hydrogen- and alkali-metal-vacancy complexes in silicon. **1984**, 29, 1819-1823		65
1968	Scale factor between fluorine-19 spin density and hyperfine coupling constant appropriate to the MNDO parameterization. **1984**, 83, L81-L82		4
1967	Semi-empirical MNDO SCF-MO of the lower phosphorus sulphides, and their molecular cation-radicals. **1984**, 81, 187-191		3
1966	Quantum-chemical description of the catalytic oxidation of benzene. **1984**, 26, 249-258		18
1965	X-Ray photoelectron spectrum of methylisocyanide gas. **1984**, 33, 153-162		2
1964	On the gas phase chemistry of ionized glycine and its enol. A combined experimental and ab initio molecular orbital study. **1984**, 62, 99-117		21
1963	Metastable radical cations of glycine methyl ester and its enol tautomer. **1984**, 62, 119-123		3
1962	Chemistry of gaseous ions. Part VIII. Bond strength and mass spectrometric fragmentation of 2-methoxycinnamic acid. **1984**, 56, 237-241		4
1961	On the formation of C2H5O2+ ions having the structure of hydroxy-protonated acetic acid. **1984**, 61, 87-95		11
1960	Mechanism of keto ˆ □enol tautomerism of ionized vinyl alcohol versus acetaldehyde and their dissociation to C2H3O+ and H□ An ab initio molecular orbital study. **1984**, 59, 21-37		56
1959	Gas-phase NMR. *Journal of Molecular Structure*, **1984**, 125, 97-107	3.4	7
1958	The structure of silylcycloheptatrienes. **1984**, 266, 25-32		3
1957	Gas phase reactions. **1984**, 271, 145-152		22
1956	Electronic properties of polyquinolines and poly(2,6-naphthylene). **1984**, 50, 1047-1050		10
1955	Surface relaxation and reconstruction in diamond-like crystals. **1984**, 49, 925-928		17
1954	ESR studies of acyclic delocalised radicals. **1984**, 5, 249-291		15

1953	MNDO studies on five-membered 1,3-heterocyclic systems. Part I. The acidity of the azolium cations. **1984**, 21, 1781-1784	3
1952	MNDO studies on five-membered 1,3-heterocyclic systems. Part II. Nucleophilicity and carbenic character of the conjugate bases of □lium□cations. **1984**, 21, 1785-1788	7
1951	Activated addition of sulfur chlorides and sulfenyl chlorides to hexafluorodimethylketene. **1984**, 33, 1261-1268	
1950	On the origin of the different activation energies for hydrogen additions at the C and O centres of R?CO+ ions (R = H, CH3): A theoretical interpretation. **1984**, 105, 490-494	8
1949	Theoretical and experimental investigation of the electron affinities of allene and propyne. **1984**, 104, 216-220	13
1948	Uv photoelectron spectrum of o-xylylene □detection of a low-energy non-koopmans (shake-up) ionization. **1984**, 108, 609-612	17
1947	LNDO/S PERTCI ionization spectra of trans-1,3,5-hexatriene and trans-1,3,5,7-octatetraene. **1984**, 106, 467-471	14
1946	A new procedure for calculating molecular polarizabilities; applications using MNDO. **1984**, 111, 416-420	69
1945	The heats of formation of some protonated olefinic carbonyl compounds: [C5H9O]+ and [C4H7O2]+ ions. **1984**, 19, 394-397	11
1944	Stereoisomeric fragment ions arising from decomposition of enol cation radicals of different internal energy content. **1984**, 19, 617-622	4
1943	MNDO study of catenated sulfur: The molecules and ions S3 to S8. **1984**, 5, 35-43	40
1942	Evaluation of MNDO calculated proton affinities. **1984**, 5, 230-236	56
1941	A computational study of the reaction of methane with methyl radical. **1984**, 5, 237-240	7
1940	Ground states of molecules. 67.MNDO Calculations for compounds containing iodine. **1984**, 5, 358-362	40
1939	Calculation of energies of excited states using MNDO. **1984**, 5, 480-485	37
1938	Molecular mechanics force-field parameterization procedures. **1984**, 5, 486-499	127
1937	MNDO Study of reaction pathways for SN2 reactions. Menschutkin reaction potential energy surfaces. **1984**, 5, 598-605	18
1936	Structure of a □-Conjugated□Dilithium Salt of an □-Keto Dianion: 1,3-Dilithiodibenzyl Ketone-(Me2NCH2CH2NMe2)2. **1984**, 23, 621-622	10

1935	Struktur eines ?-konjugierten?Dilithium-Salzes eines ?-Ketodianions: 1,3-Dilithiodibenzylketon-(Me2NCH2CH2NMe2)2. **1984**, 96, 623-625	9
1934	Radikalionen, 55. Die Einelektronen-Oxidation von Tetrahedran zum Cyclobutadien-Radikalkation. **1984**, 117, 172-186	25
1933	Darstellung, Reaktionen und Struktur von tert-Butyl(tert-butylimino)boran. **1984**, 117, 1089-1102	125
1932	Zur Struktur von N-Methylencarbons? ?reamiden: R? ?tgenstrukturergebnisse, spektroskopische Untersuchung und quantenmechanische Berechnungen. **1984**, 117, 1597-1605	34
1931	Photoelectron Spectra of Some Reduction Products of [2.2]Paracyclophane. **1984**, 117, 1987-1990	1
1930	The Structure of 2-Azaallenium Cations. **1984**, 117, 3365-3373	51
1929	Transformation matrices as tool to investigate the changes in the electronic structure of reacting molecules along the reaction coordinate. **1984**, 65, 65-76	1
1928	Le cation m? thyl? ?ecyclopropyle: Etude th? orique. Solvolyse des halog? hocycloprop? ?es et des halog? hom? thylenecyclopropanes. **1984**, 40, 315-325	1
1927	Colour and constitution of azo compounds derived from diaminoazines. **1984**, 40, 5081-5088	4
1926	MNDO calculations of the effects of substitution on antioxidant activity of phenols and Vitamin E. **1984**, 40, 3383-3385	10
1925	Orthogonene. **1984**, 40, 2799-2802	5
1924	Theoretical calculations of chemical interactions-111. **1984**, 40, 4227-4235	8
1923	Mndo study of bond orders in some conjugated BI- and tri-cyclic hydrocarbons. **1984**, 40, 4455-4472	70
1922	Photocycloaddition reactions of the first stable thioaldehyde: 2,4,6-tri(tert-butyl)thiobenzaldehyde with substituted allenes. **1984**, 25, 873-876	11
1921	A simple route to the 7-cyclopenta[a]pentalene system: preparation of the 1,2,3,4,5,6-hexachloro-derivative.. **1984**, 25, 2923-2924	1
1920	Pyryliumverbindungen, XXV. Quantenchemische Berechnungen zur Valenzisomerisierung von 2-Amino-2H-pyran und -thiopyran. **1984**, 326, 955-961	10
1919	Analysis of the inadequacies of some semi-empirical MO methods as theories of structure and reactivity. **1984**, 25, 367-390	20
1918	Localized molecular orbitals for multiple bonds in the ZDO approximation: The ?vs. banana bonds dilemma. **1984**, 26, 383-403	11

1917	Gas phase unimolecular 1,1-hydrogen elimination: Reaction mechanism and isotope effect. **1984**, 26, 621-636	4
1916	Modification of the MNDO method for calculations for systems with hydrogen bonds. **1984**, 25, 21-25	1
1915	MNDO calculations on hydrogen bonds. Modified function for core-core repulsion. **1984**, 64, 397-401	108
1914	A theoretical study of the relative stability of the isomeric forms of N2O3. **1984**, 64, 313-316	14
1913	The application of molecular orbital calculations to wood chemistry. **1984**, 18, 307-315	19
1912	Experimental and theoretical study of the effect of medium on chemical imidization. **1984**, 26, 2839-2848	15
1911	The molecular geometry of the elusive 1,4-dihydropyrazine. An MNDO study. **1984**, 109, 277-286	15
1910	MNDO study of the cyclopentathiazenium cation S5N5+. **1984**, 109, 367-371	1
1909	Theoretical study of internal rotation in perfluorobutadiene. **1984**, 109, 373-379	8
1908	An MNDO sudy OF H2□(0 1984, 109, 393-396	
1907	Theoretical determination of molecular structure and conformation. **1984**, 110, 277-291	25
1906	Internal rotations of vinylcyclopropane, cyclopropanecarboxaldehyde and cyclopropanecarboxylic acid studied by quantum chemical calculations. **1984**, 108, 49-58	5
1905	Partitioning of MNDO energy and description of bonding. **1984**, 108, 139-147	3
1904	Structures and stabilities of ion/dipole complexes. **1984**, 110, 49-59	9
1903	A GAUSSIAN 80(6-311G**) study of the species NHn and NHn+ (n = 1□). **1984**, 110, 155-166	10
1902	MNDO calculation of the molecular in-plane force field and vibrational intensities of nitrosyl cyanide. **1984**, 108, 241-245	1
1901	A HAM/3 study of photoelectron spectra of benzoic acid and its derivatives. **1984**, 108, 269-279	3
1900	Coupled calculation of vibrational frequencies and intensities by means of semiempirical quantum chemical methods. **1984**, 108, 299-306	6

1899	Volume 5 References. **1984**, 905-994		
1898	Model calculations of the interaction of two parallel antiaromatic 4n pi-electron systems. *Proceedings of the National Academy of Sciences of the United States of America*, **1984**, 81, 2589-91	11.5	10
1897	Volume 4 References. **1984**, 1085-1195		1
1896	PHOTOELECTRON SPECTRA OF DIARYLDIPHOSPHENES. **1984**, 13, 313-316		10
1895	Association between Polar Molecules. III.1H and13C NMR Studies on the Dipole Association of Acetonitrile Derivatives with Tetramethylurea and Dibutyl Sulfoxide in Nonpolar Solvents. **1984**, 57, 1299-1303		2
1894	Quantum Chemical Consideration of Substituent Effects on Tautomeric Properties of 2-Pyridones2-Pyridinols. **1984**, 57, 3454-3460		21
1893	SYNTHESIS AND PROPERTIES OF 1,4-DIHYDROPYRROLO[3,2-b]PYRROLE-2,5-DIONE DERIVATIVES. **1985**, 14, 1809-1812		5
1892	Alternative view of enzyme reactions. *Proceedings of the National Academy of Sciences of the United States of America*, **1985**, 82, 2225-9	11.5	173
1891	New Silicon (111) Surface (7ˆ 7) Reconstruction Benzene-Like Ring Model. **1985**, 63, 167		
1890	Rotational Isomerism in O-Methylphenol: Matrix-Isolation Infrared Study and MNDO Calculations. **1985**, 32, 207-213		
1889	Cluster Computations Related to Silicon Thermal Donors. **1985**, 59, 207		17
1888	An Examination of the Relationship Between Transition State Geometry in Hydron Transfer Reactions and the Temperature Dependence of the Primary Kinetic Isotope Effect. **1985**, 26, 378-386		2
1887	Description of interactions in molecular complexes by linear combination of educt orbitals. **1985**, 67, 477-483		
1886	An empirical scheme for evaluating in situ bond energy from MNDO data. **1985**, 66, 365-373		7
1885	A theoretical investigation of electron correlation and relaxation in organometallic polymers. **1985**, 27, 323-374		7
1884	A theoretical study of tautomerism: 2- and 4-oxopyrimidine and some of their derivatives. **1985**, 27, 567-583		11
1883	MNDO Calculation on Molecular Clusters Chosen to Model the Bonding of Oxygen in Silicon. **1985**, 130, 333-338		4
1882	On the stereochemistry of the aldol-addition. **1985**, 41, 5517-5524		42

1881	Studies on structurally simple butenolides. V. reactions of protoanemonin with piperidine and -nucleophiles. **1985**, 41, 5577-5587		18
1880	Flash vacuum thermolysis of spirocyclohexadienones. **1985**, 41, 3779-3784		1
1879	A mndo study of 3-, 5-, 7- and 9-membered carbocyclic, completely conjugated, planar carbenes and their nonplanar isomers. **1985**, 41, 1579-1586		52
1878	A study of electronic structures of some C9H9- carboanions. **1985**, 41, 5209-5212		
1877	Conformational behaviour of 3-phenyl- and 3-carbomethoxy-substituted cyclopropene derivatives. **1985**, 41, 5377-5382		13
1876	Protonation of cluster molecules: Bridging hydrogen sites in tetrahedral, octahedral and capped square pyramidal clusters: Be4H8, Be4H8. **1985**, 4, 687-695		16
1875	Potential-surface calculation for a model addition of a nucleophilic reagent to a carbonyl compound in the vapor state and in an aqueous medium. **1985**, 26, 332-336		
1874	Empirical correlation between the stretching force constant and the bond order for nitrogen-oxygen systems. **1985**, 116, 1305-1307		1
1873	Reactions of carbenes with bicyclobutanes and quadricyclane. **1985**, 41, 1453-1464		22
1872	Theoretical study of the reaction H + ClCH3 -fHCl + CH3. **1985**, 93, 265-275		7
1871	Base-pairing properties of O-methylated bases of nucleic acids. Energetic and steric considerations. **1985**, 22, 37-51		9
1870	Theoretical study of oxygen chemisorption on (111) and (100) silicon surfaces. **1985**, 113, 321-324		15
1869	Inversion of chalcogen defect levels in silicon: An MNDO study. **1985**, 112, 175-177		3
1868	Isomerisation des ions organiques en phase gazeuse. II. Etude des ions moleculaires metastables [CH3COCH(CH3)C2H5]+. **1985**, 64, 159-168		5
1867	Radical ions derived from hydrides and methyls of aluminum, silicon and phosphorus: A semi-empirical SCF?MO study. **1985**, 97, 173-178		4
1866	Semiempirical molecular orbital techniques applied to silicon dioxide: MINDO/3. **1985**, 46, 841-857		65
1865	Electronic structure and conformational properties of the amide linkage. *Journal of Molecular Structure*, **1985**, 131, 55-60	3.4	6
1864	Electronic structure and conformational properties of the amide linkage. *Journal of Molecular Structure*, **1985**, 131, 61-70	3.4	7

1863	The structures of dicyclopentadienylsilenes and related compounds. **1985**, 286, 289-295	13
1862	He(I) and He(II) photoelectron spectra of 1-aza-1,3-butadiene-tricarbonyliron complexes: [Fe(CO)3(R1N?CHCH?CHR2)]. **1985**, 288, 79-88	4
1861	The doubly bridged structure of 1,4-dilithio-cis-2-butene. A theoretical demonstration of the importance of counter-ion effects and of lithium multicenter bonding. **1985**, 280, C1-C5	15
1860	Double lithium bridging: The structure of 1,4-dilithio-1,4-diphenyl-cis-2-butene. **1985**, 280, C6-C10	32
1859	He(I) and He(II) photoelectron spectra of mononuclear transition metal carbonyl complexes containing a 1,4-diaza-1,3-butadiene ligand. **1985**, 281, 273-289	12
1858	Quantum-chemical analysis of silicon atom pentacoordination. **1985**, 292, 159-166	21
1857	The molecular and electronic structure of radical cations derived from tetramethyltin and hexamethylditin: An SCF-MO study. **1985**, 294, 173-178	10
1856	The infrared and Raman spectrum of trans-polyacetylene: A self-consistent-field study. **1985**, 53, 893-896	12
1855	The reactive excited state of naphthvalene and its photochemistry: a qualitative and quantitative theoretical investigation. **1985**, 28, 373-381	2
1854	Reaction of OH with phenylalanine in neutral aqueous solution. **1985**, 26, 103-108	19
1853	H attack on 2,2'-bipyridine in acid aqueous solution. **1985**, 26, 109-116	9
1852	Reaction of 3-aryl-2-benzoyloxiranes with alkyl thiocyanates. **1985**, 21, 1335-1338	
1851	Quantum-chemical study of the effect of hydration on the mechanism of the nucleophilic reactions of carbonyl compounds. **1985**, 34, 971-974	1
1850	Cyclooctadienine □hoch gespannte C8H8-Kohlenwasserstoffe. **1985**, 118, 176-181	6
1849	Untersuchungen zur Konformation und elektronischen Struktur von Cyclooctadieninen. **1985**, 118, 210-220	4
1848	C?C-Spaltungen bei ionisierten Carbons□ □ren als Umkehrung der [1,4]-Addition von Alkyl-Radikalen an protonierte □unges□ □tigte Carbons□ □ren. Zur Rolle von Enol-Radikalkationen als reaktive Zwischenstufen bei Isomerisierungs-/Dissoziationsprozessen in der Gasphase. **1985**, 118, 495-509	42
1847	Bicyclofulvene, XI. Zur Frage der Spirokonjugation bei Spiro[cycloheptatrien-7,7?-norbornadien]. **1985**, 118, 1000-1007	9
1846	Erzeugung von Cumulenen durch Lithium-Addition an 1,3-Diine. R□ □tgenstruktur von [3,6-Di(lithio-THF)-2,2,7,7-tetramethyl-3,4,5-octatrien]2, einem 1,4-Dilithiobutatrien-Dimeren. **1985**, 118, 1504-1516	18

1845	Synthese von 4-Oxo-4H-benzothiazolo[3,2-a]pyrimidin-1-ium-2-olaten und ihre Cycloadditionen an elektronenarme und elektronenreiche Alkine sowie an o-Chloranil. **1985**, 118, 2079-2094	20
1844	The molecular and electronic structure of dipiperidinosquaraine. **1985**, 118, 2118-2126	8
1843	PE- und 13C-NMR-spektroskopische Untersuchungen zur Homokonjugation in 7-Alkylidennorbornadienen. **1985**, 118, 2514-2543	14
1842	Brˆ Ekenkopf-olefinische Isomere des Triquinacens: Derivate des Tricyclo[5.2.1.04,10]deca-1,5,8- und -1,6,8-triens. **1985**, 118, 2757-2776	15
1841	Zur Positions- und Regioselektivitˆ Eneuer [3 + 2]-Cycloadditionen mesoionischer 1,3-Dithiol-4-one an elektronenarme und elektronenreiche Butatriene. **1985**, 118, 3438-3463	8
1840	Perhalogenierte 1,2,3,5-Dithiadiazolium-Salze und 1,2,3,5-Dithiadiazole. **1985**, 118, 3781-3804	68
1839	An analysis of the electronic structure of 6,7-dimethyl-3-oxabicyclo[3.2.0]hepta-1,4,6-triene. **1985**, 118, 3939-3943	1
1838	Chemospezifitˆ Eund Regioselektivitˆ Ebei der Cycloaddition von Diazoalkanen an 1H-1,2-Diazepine. **1985**, 118, 4682-4706	13
1837	Can 1,2,3-Oxadiazole be Stable?. **1985**, 24, 713-715	20
1836	Cl2C?Cl?Cl??, Cl2C?Cl?Br??, and Br2C?Br?Cl?? by Gas-Phase Decarbonylation of CX3COY??. **1985**, 24, 869-870	17
1835	Electron impact, chemical ionization and collisional activation mass spectrometry of methyl O-acetyl-ED-xylopyranosides. **1985**, 12, 49-58	15
1834	Structures and stabilities of [C3H3O]+ ions in the gas phase: A molecular orbital study. **1985**, 20, 560-564	23
1833	Fragmentation of trimethylsilyl derivatives of 2-alkoxyphenols: A further violation of the Even-electron rule**1985**, 20, 614-618	21
1832	Stable [C2H7O2]+ isomers: Experimental and theoretical evidence for the existence of protonated peroxides and proton-bound dimers in the gas phase. **1985**, 20, 665-673	18
1831	Vibronic coupling in the benzyl radical. **1985**, 115, 253-258	42
1830	Effect of ground and excited singlet-state geometry on the level ordering of 1,4-diphenylbutadiene: a theoretical study using MNDO. **1985**, 117, 583-588	18
1829	Spectral constants computed for C H22+ carbodications. **1985**, 118, 188-191	9
1828	Studies of a proposed mechanism for the reaction between 2H-pyran-2-ones and organomagnesium compounds. **1985**, 6, 9-12	1

1827	An MNDO treatment of sigma values. **1985**, 6, 437-440	20
1826	Bond Angles in Lactones and Lactams. **1985**, 68, 76-82	33
1825	The Molecular Ion of 5-Methylene-1,3-cyclohexadiene: Electronic Absorption Spectrum and Revised Enthalpy of Formation. **1985**, 68, 345-354	17
1824	The Synthesis of 4,7-Bis(dialkylamino)tricyclo[5.2.1.04,10]deca-1(10),2,5,8-tetraenes and their Reduction with Alkali Metal. **1985**, 68, 1658-1669	13
1823	Gas-Phase Basicities of Furan Compounds. The Role of Alkyl Substitution on Proton Affinity and on the Site of Protonation. **1985**, 68, 2037-2045	12
1822	1H-NMR Spectra of Cyclohexa-1,4-dienes and Cyclohexenes Annellated to Bicyclo[2.2.1]hept-2-enes. The Inter-Ring Homoallylic H,H Coupling Constants as Stereochemical Probes. **1985**, 68, 2182-2194	13
1821	Synthesen mit aliphatischen Dialdehyden, XLII. (2,4,6-Cycloheptatrien-1-yliden)malonaldehyd (8,8-Diformylheptafulven) Herstellung, Struktur und Reaktionen. **1985**, 1985, 1997-2011	9
1820	Kann 1,2,3-Oxadiazol best^ dig sein?. **1985**, 97, 704-705	8
1819	Cl2C?Cl??, Cl2C?Cl?Br?? and Br2C?Br?Cl?? durch Gasphasendecarbonylierung von CX3COY??. **1985**, 97, 855-857	4
1818	Computer-assisted mechanistic structure-activity studies: application to diverse classes of chemical carcinogens. **1985**, 61, 69-96	32
1817	The Application of Molecular Orbital Calculations to Wood Chemistry - III. The Chlorination of Lignin Model Compounds. **1985**, 39, 173-180	5
1816	Substitutional oxygen-oxygen pair in silicon. **1985**, 31, 3588-3592	35
1815	Investigation of off-center substitutional N in Si. **1985**, 31, 1208-1211	23
1814	Boron atom reactions with the halomethanes. **1985**, 83, 5595-5601	5
1813	Design and Synthesis of Diketones. The Cyclobutane-1,2-dione Chromophore: Synthesis, Dienophilic Reactivity and Electronic Properties of Cyclobutenedione and Polycyclic Cyclobutanediones [1]. **1985**, 25, 74-83	10
1812	RADIKALIONEN 661,2 THIOPARABANSAURE-DERIVATE: IONISATION ZUM RADIKALKATION UND REDUKTION ZUM RADIKALANION. **1985**, 22, 109-119	9
1811	New class of soliton-supporting polymers: Theoretical predictions. **1985**, 31, 652-655	37
1810	Hydrogen-acceptor pairs in silicon: Pairing effect on the hydrogen vibrational frequency. **1985**, 31, 6861-6864	160

1809	MENTHYLSUBSTITUIERTE PHOSPHORVERBINDUNGEN V1,2 R(P)-TERT.-BUTYL-1-MENTHYLTHIOPHOSPHORYLCHLORID KRISTALL- UND MOLEKˆ STRUKTUR, MNDO-RECHNUNGEN UND NMR-DATEN. **1985**, 25, 103-116	4
1808	An application of MNDO calculation to borate polyhedra. **1985**, 74, 25-36	14
1807	Geometric and electronic structures of isothianaphthene and thieno[3,4-C]thiophene: A theoretical investigation. **1985**, 11, 343-352	56
1806	Model Hamiltonians in the study of chemisorption and catalysis. **1985**, 152-153, 690-701	26
1805	Chemisorption of atomic and molecular oxygen on the (100) surface of silicon; a theoretical study. **1985**, 162, 230-238	31
1804	Structures and relative stabilities of [C2H6N]+ ions: A non-empirical and MNDO study. **1985**, 124, 319-324	11
1803	Electronic structure and conformational properties of the amide linkage. **1985**, 122, 35-45	32
1802	The MNDO potential energy surface and tunnelling dynamics of the cyclobutane radical cation. **1985**, 122, 59-65	5
1801	Theoretical study of organic solid state reactivity: Isomerisation of cyclohexadienones. **1985**, 121, 13-22	6
1800	A theoretical investigation by the MNDO method of the explosive complexes of hydroxide ion with 1,3,5-trinitrobenzene and 4,6-dinitrobenzofuroxan. **1985**, 121, 37-44	5
1799	An MNDO study of the CnNH carbenes. **1985**, 121, 109-114	9
1798	MNDO study of the tautomers of nucleic bases. **1985**, 121, 133-136	15
1797	MNDO and MNDO/H calculations on hydrogen bonds comparison with ab initio and CNDO/2 methods. **1985**, 122, 343-350	18
1796	Conformation and electronic structure of the di-sulfur nitride (S2N anion. **1985**, 123, 259-265	9
1795	A theoretical study of the bond dissociations of small molecules using MNDO/CI. **1985**, 123, 343-359	11
1794	Comparative study of some 5- and 6-membered rings of sulfur, nitrogen and carbon or phosphorus. A quantum chemical Hartree ock Slater analysis. **1985**, 133, 1-9	4
1793	SCPT-INDO calculation of coupling constants in five- and six-membered chalcogen heteroaromatics. **1985**, 133, 125-137	11
1792	Semiempirical and ab initio calculations on geometry and stability of intermediates. Stability of intermediates for nucleophilic reactions of carbonyl compounds in the gas phase and in solution. **1985**, 133, 263-268	9

1791	A non-Woodward and Hoffmann reaction path for photochemical sigmatropic rearrangements. **1985**, 119, 367-378	6
1790	A Theoretical study of 13C NMR chemical shifts in a series of rigid bicyclo[m.n.o.] alkanes. **1985**, 124, 25-40	5
1789	Beta-adrenergic activity and conformation of the antihypertensive specific alpha 2-agonist drug, guanabenz. **1985**, 34, 491-8	12
1788	Quantum chemical study of cyclization mechanism in polyamic acids. **1986**, 28, 919-927	1
1787	On the use of quantum chemical methods as an additional tool in studying corrosion inhibitor substances. **1986**, 26, 927-934	22
1786	Evidence for a 13,14-cis cycle in bacteriorhodopsin. **1986**, 50, 81-9	33
1785	MNDO studies of basicity in borate glasses. **1986**, 85, 290-308	14
1784	Heteroatom effects in heterocyclic ring chain polymers. **1986**, 16, 235-243	32
1783	Quantum-mechanical study of the chemisorption of atomic and molecular oxygen on graphite clusters. **1986**, 136, 313-322	10
1782	A theoretical study of the nitrogen□graphite system. **1986**, 139, 277-282	4
1781	Conformational transitions in N-linked oligosaccharides. **1986**, 25, 6342-50	111
1780	Characterization of high molecular weight polycyclic aromatic hydrocarbons by charge exchange chemical ionization mass spectrometry. **1986**, 58, 2114-2121	35
1779	Polyaniline: A theoretical study. **1986**, 15, 105-114	45
1778	A theoretical conformational study of s-tetrathiane, s-tetroxane and their methyl derivatives. **1986**, 135, 7-14	11
1777	Theoretical analysis of the isomerization of fluorocarbonyl thiocyanate. **1986**, 135, 15-19	1
1776	On the possibility of fluorescence from twisted intramolecular charge transfer states of 2-dimethylamino-6-acylnaphthalenes. A quantum-chemical study. **1986**, 139, 13-23	48
1775	Conformational analysis of several aliphatic alcohol molecules by means of PCILO and MNDO methods. **1986**, 137, 217-234	4
1774	Theoretical aspects of the inversion barriers in cyclotriphosphanes and related systems. **1986**, 137, 341-345	6

1773	Quantumchemical (MNDO SCF/CI) calculations of the chiroptical properties of twisted conjugated diene and dione chromophores. **1986**, 137, 347-364		6
1772	A MINDO/3 study of the ethylene dication. **1986**, 136, 209-214		9
1771	Photochromism of sydnones: Structural evidence for the blue colored species from 3-(3-pyridyl)sydnone. **1986**, 136, 261-273		14
1770	MINDO/3 computed proton affinities. **1986**, 136, 361-369		3
1769	An MNDOC study of 2,3-diazabicyclo[2.2.1]heptene and 2,3-diazabicyclo[2.2.2]octene. **1986**, 136, 381-385		
1768	Configuration interaction study of the lowest □ and □ states in the succinimidyl radical. **1986**, 138, 69-76		2
1767	Comparison of semiempirical and ab initio transition states for organic reactions. **1986**, 138, 141-150		5
1766	Calculation of bond dissociation energies of benzylic hydrogens: A comparative study. **1986**, 138, 157-161		5
1765	Geometric and electronic structure of vitamin C radicals. A semiempirical study. **1986**, 139, 179-195		11
1764	Electronic structure and conformational properties of the amide linkage. **1986**, 139, 315-325		13
1763	Molecular orbital description of the polythiazyl polymer. **1986**, 139, 327-332		8
1762	Hard basicity of borate anion clusters. **1986**, 88, 1-10		6
1761	Effects of substituent-induced strain on the electronic structure of polydiacetylenes. **1986**, 85, 4116-4119		76
1760	New synthetic technology for the construction of oxocenes. *Journal of the American Chemical Society*, **1986**, 108, 2468-9	16.4	59
1759	Theoretical Studies of Cytochrome P-450. **1986**, 36, 54-78		22
1758	Binding specificity of papain and cathepsin B. **1986**, 36, 141-9		8
1757	New ideas about enzyme reactions. **1986**, 36, 8-20		53
1756	A Novel Development for the Simulater of Intermolecular Potentials. **1986**, 59, 1317-1320		4

1755	The Origin of Regio- and Stereoselectivities in 1,3-Cycloadditions of Azomethine Ylides Generated fromN-(Benzylidene)trimethylsilylmethylamine and the Related Compounds. **1986**, 15, 1113-1116	7
1754	Studies of the influence of chloro-substituent sites and conformational energy in polychlorinated biphenyls on uroporphyrin formation in chick-embryo liver cell cultures. **1986**, 235, 291-6	32
1753	Biological activity of polychlorinated biphenyls related to conformational structure. **1986**, 240, 621-2	15
1752	Reference Energies in Semiempirical Parametrizations. **1986**, 7, 213-218	10
1751	Motional dynamics in liquid 1,2,3,4-tetrahydro-5,6-dimethyl-1,4-methanonaphthalene. **1986**, 59, 721-736	11
1750	Evaluation of the dioxane effect on the dipole moment of malonic acid. **1986**, 132, 305-310	3
1749	An analysis of predictions by the semi-empirical MNDO molecular orbital method for some aspects of molecular energetics. **1986**, 128, 31-37	14
1748	Theoretical calculation of vibrational polarizabilities. An application to the study of conformational and solvent effects. **1986**, 128, 177-181	31
1747	Uv photoelectron spectrum of cyclobutadiene. free cyclobutadiene stable up to high temperatures. **1986**, 124, 140-146	26
1746	Polarizabilites of organic ions. **1986**, 21, 449-450	1
1745	Isomerization and fragmentation of methylfuran ions and pyran ions in the gas phase. **1986**, 21, 459-466	25
1744	N-[1-(Acyloxy)alkyl]heteroaryliumsalze in der Synthese, 3. Intramolekulare ortho-Acylierung einiger N-heteroaromatischer Ringsysteme. **1986**, 119, 279-296	13
1743	Photoelectron and UV spectroscopic investigations of homoconjugative interactions between parallel C?C and N?N bonds. **1986**, 119, 543-553	20
1742	Photoelektronenspektroskopische Untersuchungen an Hexahydro-1,3,5-triazinen. **1986**, 119, 554-562	3
1741	Zur Positions- und Regioselektivitˆ Eneuer [3 + 2]-Cycloadditionen von Nitronen und einem Nitriloxid an Butatriene. **1986**, 119, 563-574	3
1740	Reaktionen von 1,2-Dimethyl-3,5-diphenylpyrazolium-4-olat und 3,5-Diphenyl-1,2-dithiolylium-4-olat mit Singulett-Sauerstoff. **1986**, 119, 762-765	2
1739	Photoelectron spectra of pteridine and its 4-methyl and 2,4,6,7-tetramethyl derivatives. **1986**, 119, 1275-1280	7
1738	Synthese von 2,6-Diazabicyclo[2.2.2]oct-7-en-3,5-dionen und 2(1H)-Pyridinonen. Ein Beitrag zum Mechanismus und zur Regiochemie 1,4-Dipolarer Cycloadditionen neuer und bekannter 3,6-Dihydro-6-oxo-1-pyrimidinium-4-olate an elektronenreiche und elektronenarme Alkine. **1986**, 119, 1315-1330	12

1737	Intramolecular interactions and hindered rotation in tropinone urethanes: A combined PE-, ET- and DNMR-spectroscopic study. **1986**, 119, 1613-1626	3
1736	Synthese und physikalische Eigenschaften stabiler 1,3-Oxathiolylium-4-olate. **1986**, 119, 2308-2316	5
1735	Zur Regio- und Stereoselektivitˆ Ëneuer thermischer [3 + 2]-Cycloadditionen mesoionischer 1,3-Oxathiol-4-one an Alkine und Alkene. **1986**, 119, 2317-2338	10
1734	Photoelectron spectra of N-substituted 1,4-dihydro-4,4-dimethylpyridines. **1986**, 119, 2381-2386	0
1733	Thieno[3,4-f]-2,1-benzisothiazol. ÜSynthese und physikalische Eigenschaften eines neuen kondensierten 14ËHeteroarens sowie dessen thermisches Cycloadditions-verhalten gegenˆ Über N,N-Doppelbindungssystemen. **1986**, 119, 3158-3164	3
1732	A Simple Route to the Intramolecular Quinhydrone of [2.2]Paracyclophanediene. **1986**, 25, 171-173	4
1731	The Structure of an Allenylsodium DerivativeÜCompetition between Carbanion Resonance Delocalization and Gegenion Charge Localization. **1986**, 25, 902-903	11
1730	2-Lithio-1-phenylpyrrole: X-Ray Structure Analysis and 6Li-1H 2D Heteronuclear Overhauser NMR Spectroscopy (2D HOESY). **1986**, 25, 1103-1104	51
1729	Divinylglyoxal and Methylvinylglyoxal. **1986**, 25, 1116-1117	4
1728	Einfacher Zugang zum intramolekularen Chinhydron von [2.2]Paracyclophandien. **1986**, 98, 162-163	5
1727	Die Struktur eines Propadienylnatrium-Derivats ÜKonkurrenz zwischen Ladungsdelokalisierung durch Resonanz und Ladungslokalisierung durch das Gegenion. **1986**, 98, 922-924	13
1726	2-Lithio-1-phenylpyrrol: Rˆ Ëntgen-Strukturanalyse und 6Li-1H-2D-heteronucleare Overhauser-NMR-Spektroskopie (2D-HOESY). **1986**, 98, 1130-1132	29
1725	Divinylglyoxal und Methylvinylglyoxal. **1986**, 98, 1134-1136	5
1724	The mass spectra of organic compounds. 8th Communication. 1-Buten-3-yn-2-ol. A new kinetically unstable C4H4O isomer. **1986**, 69, 683-691	6
1723	PE Spectra of Dewar Benzenes, Bridged by a Cyclohexadiene or a Butadiene Unit. **1986**, 69, 962-971	5
1722	Triaziridines. Part V. A semiempirical MNDO study of nitrogen inversion and amide rotation in Formyltriaziridines. **1986**, 69, 1461-1468	9
1721	An improved set of mndo parameters for sulfur. **1986**, 7, 140-143	240
1720	Matrix elements for anharmonic potentials: Application to I morse oscillator. **1986**, 7, 208-212	28

1719	Substituent Effects on the Low-Lying Singlet and Triplet States of Methylene. **1986**, 7, 428-442		14
1718	13C NMR spectra of 7-, 8-, 9- and 10-fluorobenzo[a]pyrene. **1986**, 24, 287-291		4
1717	Reaktionen eines Thieno[3,4-c]isothiazols mit 1,2,4-Triazolin-3,5-dionen und Alkinen. **1986**, 1986, 1796-1803		4
1716	Evidence for keto-enol tautomerism in reduced acetylisoalloxazines. **1986**, 14, 211-221		1
1715	On the interaction of halogen atoms with (111) and (100) surfaces of silicon. **1986**, 59, 433-436		12
1714	Electronic structures and thermolyses of 2-tetrazenes. **1986**, 42, 2511-2518		13
1713	Hydrogen bonding studies of 2,4,6-trinitrotoluene. **1986**, 42, 461-466		16
1712	Vibrational spectra of 2,4,6-trinitrotoluene and its isotopically substituted analogues. **1986**, 42, 13-21		40
1711	The unimolecular decomposition of the fluoroethylene radical anions formed by electron attachment. **1986**, 41, 453-466		13
1710	Semi-empirical pertci ionization spectra of some cumulenes and cumulene-like systems. Low-energy non-koopmans' ionizations. **1986**, 103, 375-382		6
1709	An MNDO and CNDO / S(S + DES CI) study on the structural and electronic properties of a model squaraine dye and related cyanine. **1986**, 107, 159-174		113
1708	Molecular aspect of the even-odd effect in cyanobiphenyls (n-CB): Theoretical studies of the molecular geometrical conformation and optical anisotropy. II. n ? 6. **1986**, 101, 393-399		2
1707	Mechanism of resonant multiphoton ionization dissociation of p-xylene. **1986**, 108, 33-43		6
1706	Electron attachment by saturated nitriles, acrylonitrile (C2H3CN), and benzonitrile (C6H5CN). **1986**, 73, 127-144		61
1705	The isomers CF3NC and CF3CN. Formation and dissociation of the anions formed on electron attachment. **1986**, 71, 199-210		16
1704	Consideration of electrochemical dimerization reactions in terms of the perturbation molecular orbital theory. **1986**, 209, 43-56		8
1703	The dipole moment derivatives of nitrosyl cyanide theoretical calculations and analysis. *Journal of Molecular Structure*, **1986**, 140, 107-113	3.4	0
1702	Coupled calculation of vibrational frequencies and intensities. *Journal of Molecular Structure*, **1986**, 146, 51-60	3.4	6

1701	The atomic polar tensors, effective charges and vibrational intensities of the CHnN (n = 3, 5, 7 and 9) molecules. *Journal of Molecular Structure*, **1986**, 142, 209-212	3.4	3
1700	MNDO-UHF study of the molecular and electronic structures of cation radicals derived from tetramethylgermane, hexamethyldigermane, and other related organogermanes. **1986**, 303, 337-341		9
1699	2,6-Bis(lithiumtrimethylsilylmethyl)pyridine 2TMEDA: A monomeric dilithio compound exhibiting electrostatic charge communication. **1986**, 316, C4-C8		29
1698	Crystallographic and vibrational study of hexanitroethane. **1986**, 47, 1129-1137		8
1697	Operators that move the nuclei of a molecule along paths of constant orbital energy. **1986**, 127, 26-32		2
1696	He(I) and He(II) photoelectron spectra of Hyprrole-2-CH?N??t-Bu and the biscarbonyl Rh(I) and Ir(I) complexes of its anion. **1986**, 111, 83-87		5
1695	Bonding in nitrosylated molybdenum-sulphur clusters. **1986**, 120, 85-90		0
1694	Estimation using MNDO of skeletal bending frequencies in linear and quasi-linear silyl compounds. **1986**, 112, L5-L6		3
1693	Conformation, electronic structure and lectronic spectrum of the 1,2,3,4-thiatriazole-5-thiolate (CS2N3) anion and HCS2N3 acid. **1986**, 113, 71-74		14
1692	Theoretical studies on the acid hydrolysis of acetamide. **1986**, 42, 6627-6633		6
1691	Steric control of regiochemistry in the reactions of methyl substituted pentadienyl cations with isobutene. **1986**, 42, 6657-6662		2
1690	A simple algorithm for the calculation of the ionization energies of substituted benzenes. **1986**, 42, 4549-4555		10
1689	The conformational analysis of benzocycloalkanones using the lanthanide induced shift msthod. **1986**, 42, 3559-3568		4
1688	A CNDO/S study on the alkylbenzene-TCNE complexes. **1986**, 42, 735-738		4
1687	Lewis acid mediated aldol condensations using thioester silyl ketene acetals. **1986**, 42, 893-909		69
1686	A theoretical study of regioselectivity and synchronicity of 1,3 dipolar cycloaddition reactions. **1986** , 42, 5857-5862		7
1685	Small-ring cyclic cumulenes: Synthesis of a kinetically stable eight membered ring allene. **1986**, 27, 4679-4682		38
1684	An experimental and theoretical investigation of the influence of alkene homo energy level upon the hydroboration reaction. Additional evidence supporting an early transition state which has retention of alkene character.. **1986**, 27, 4693-4696		18

1683	Doubly-charged gas phase cations. **1986**, 69, 147-159	21
1682	A study of hydrogen bond strengths of neutral water clusters (H2O) n using modified MNDO. **1986**, 70, 3-10	26
1681	On the density matrix definition of valency. **1986**, 70, 67-71	20
1680	Etude MNDO des composes conjugues enneagonaux. **1986**, 29, 1599-1624	8
1679	An MNDO study of the reaction of methanol with fulminic acid and acetonitrile oxide. **1986**, 30, 213-224	3
1678	Tautomerism of uracil, cytosine, isocytosine, and some of their thio-derivatives. **1986**, 30, 225-237	22
1677	Calculation of polymer elastic moduli using semiempirical methods. **1986**, 30, 529-540	19
1676	Zuordnung von Schwingungsspektren organischer Molekˆ Łe durch MNDO-Berechnungen. **1986**, 328, 97-104	1
1675	Quantenchemische Berechnungen an Radikalen vom Allyltyp: Methylsubstituierte Allylradikale. **1986**, 328, 886-892	3
1674	Application of the MNDO/HB method for calculating systems with proton transfer in hydrogen bonds. **1986**, 27, 347-351	1
1673	Calculation of the potential surface for nucleophilic substitution reactions taking place by the SN 2 mechanism with allowance for solvation. **1986**, 27, 352-356	
1672	Quantum-chemical study of the influence of the electronegativity of substituents on the reactivity of Łchloroethylamine derivatives. **1986**, 27, 367-371	
1671	Mechanism and transition-state structure of hydride-transfer reactions mediated by nad(p)h-models. **1986**, 42, 975-992	56
1670	A mndo study of olefin epoxidation by peroxyacids.. **1986**, 42, 4017-4026	2
1669	Scope and limitations of the flash vacuum thermolysis approach to small [n]paracyclophanes. **1986**, 42, 1571-1574	19
1668	The mechanism of electrocleavage reactions and photorearrangements of some sulfonium salt derivatives. **1986**, 42, 6123-6129	30
1667	Structure of 4,7,12,15-tetrahydro[2.2]paracyclophane; a molecule with interdeck through-space interaction. **1986**, 42, 494-495	1
1666	Hydrolysis of cyclic nucleotides by a purified cGMP-stimulated phosphodiesterase: structural requirements for hydrolysis. **1986**, 871, 199-206	41

1665	19F NMR spectrum of perfluoropentadienyl cation, and calculation of its geometry by the LCAO MO method in the indo approximation. **1986**, 35, 1598-1600		
1664	Theoretical investigation of polyfluorinated allyl cations. **1986**, 35, 1357-1360		1
1663	Electronic and photoelectron spectra of amino-1-methylnitropyrazoles and their quantum-chemical interpretation. **1986**, 22, 1316-1321		1
1662	Spatial and electronic structure of the BEDT-TTF molecule. **1986**, 22, 337-340		
1661	Quantum chemical analysis of pentacoordination of the silicon atom. **1986**, 22, 62-67		
1660	Stability of water clusters: Implication for atmospheric hydrated clusters and aerosols. **1986**, 20, 2027-2032		1
1659	Ring inversion kinetics of radicals derived from Mu addition to cycloheptatriene. **1986**, 32, 747-752		4
1658	Electrophilic hydrogen-deuterium exchange of some deactivated pyrroles. **1986**, 23, 1475-1480		12
1657	A MNDO approach to the elementary reactions of atomic hydrogen with monosubstituted halomethanes (CH3X, X ? Cl, Br, I). **1986**, 104, 49-56		3
1656	The structure of the halogeno and nitro derivatives of N-vinylcarbazole. PMR spectral data and related MNDO calculations. **1986**, 42, 977-981		1
1655	An examination of the solution conformations of bicuculline using NMR and theoretical methods. *Journal of Molecular Structure*, **1986**, 140, 131-139	3.4	7
1654	Internal heavy atom effects for chloro- and bromoquinolines. *Journal of Molecular Structure*, **1986**, 141, 469-474	3.4	4
1653	The Use of Computer Graphics to Study Adsorption, Diffusion and Catalysis in Zeolites. **1986**, 475-479		6
1652	Theoretical studies on polyaniline. **1986**, 85, 4584-4590		146
1651	Nonempirical cluster-model study of the chemisorption of atomic hydrogen on the (111) surface of diamondlike crystals. **1986**, 34, 7203-7208		24
1650	Hydrogen-acceptor pairs in silicon. **1986**, 56, 402		49
1649	Kinetics of aggregation of carbon clusters. **1986**, 33, 7395-7398		72
1648	Molecular x-ray spectra: S-K□emission and K absorption spectra of thiophene. **1986**, 84, 4228-4234		15

1647	The Application of Molecular Orbital Calculations to Wood Chemistry. IV. The Formation of Methylol Derivatives. **1986**, 6, 505-521		5
1646	Semiempirical treatment of the benzophenone molecule as a function of twist angle. **1986**, 84, 1590-1597		35
1645	Absolute total cross sections for the scattering of low energy electrons by CCl4, CCl3F, CCl2F2, CClF3, and CF4. **1986**, 84, 813-819		110
1644	Kinetics of cluster formation in the laser vaporization source: Carbon clusters. **1986**, 85, 3258-3267		109
1643	A Theoretical Study of Silanol Polymerization. **1986**, 73, 529		3
1642	Calculation of bond strengths and optimized geometries of nitroaromatics by semi-empirical methods. **1987**, 5, 157-166		
1641	INFLUENCE OF ELECTRON-WITHDRAWING SUBSTITUENTS IN THE OXAPHOSPHOLE RING ON THE AXIAL CONFORMATIONAL TRANSMISSION IN Pv COMPOUNDS. **1987**, 31, 267-279		1
1640	Acylphosphonic Derivatives - New Precursors for Low Coordination Phosphorus Species. **1987**, 30, 113-116		4
1639	Some aspects of the chemistry of polylithiated aliphatic hydrocarbons. **1987**, 1-61		80
1638	Crystallographic and molecular mechanics calculations on the anti-tumor drugs N-[(2-dimethylamino)ethyl]-and N-[(2-dimethyl-amino)butyl]-9-aminoacridine-4-carboxamides and their dications: implications for models of DNA-binding. *Journal of Biomolecular Structure and Dynamics*, **1987**, 5, 145-58	3.6	12
1637	Ultra Violet and X-Ray Photoelectron Spectroscopy of Crystal Violet. **1987**, 35, 551-556		5
1636	Evaluation of semiempirical quantum-chemical methods in solid-state applications. I. Molecular-cluster calculations of defects in silicon. **1987**, 36, 9612-9618		36
1635	An effective Hamiltonian study of molecular clusters. **1987**, 87, 636-642		16
1634	Photoelectron spectra from local-density-functional calculations: Application to chain polymers. **1987**, 36, 3312-3318		13
1633	Hydrogen passivation of shallow acceptors in c-Si: An ab initio approach. **1987**, 36, 6228-6230		68
1632	Ab initio calculation of harmonic force fields and vibrational spectra for the methyl, silyl, germyl, and stannyl halides. **1987**, 86, 923-936		91
1631	Evaluation of semiempirical quantum-chemical methods in solid-state applications. II. Cyclic-cluster calculations of silicon. **1987**, 36, 9619-9627		55
1630	Hydrogen bonding and cation radical formation of methyl 4-(N,N-dimethylamino)phenyl carbamate, DMAPCMe. **1987**, 87, 4967-4971		12

1629	Prototropy of 1-Hydroxy-1,2,3-Triazole Studied by UV Photoelectron Spectroscopy. **1987**, 20, 105-110	6
1628	1,4-Dihydropyrrolo[3,2-b]pyrrole: The Electronic Structure Elucidated by Photoelectron Spectroscopy. **1987**, 60, 1981-1983	18
1627	The Chemistry of Isopyrene (Azuleno[2,1,8-ija]azulene). Oxidations. **1987**, 16, 33-36	4
1626	13C NMR Spectra of Substituted 2-Thiophenecarboxylic Acid Methyl Esters and MNDO Calculations. **1987**, 60, 953-961	17
1625	Fluorescence excitation spectra of hydrogen-bonded cresol-isomers in supersonic free jets. **1987**, 91, 140-152	21
1624	Structure and Molecular Orbital Calculations of a 29 Electron Species at the MgO Surface: The $CNO_2^{\square}$ Radical Ion*. **1987**, 152, 31-40	7
1623	Mo studies of solvation effects. **1987**, 153, 195-201	18
1622	Mo studies of solvation effects. **1987**, 153, 203-208	4
1621	Mo studies of solvation effects. **1987**, 153, 209-213	9
1620	Reliability of MNDO in determining the equilibrium structures of unionized amino acids. **1987**, 152, 293-303	19
1619	Charge iteration at CNDO/2 level of approximation. **1987**, 152, 341-346	
1618	Calculated properties of C60 isomers and fragments. **1987**, 153, 75-84	40
1617	Hyperpolarizability of conjugated organic systems. **1987**, 153, 185-190	5
1616	A semiempirical HAM/3 study of core-electron binding energies for uracil its related molecules. **1987**, 150, 309-317	3
1615	The meta photocycloaddition of benzene to ethylene semi-empirical calculations. **1987**, 151, 1-10	24
1614	Finite field calculations of molecular polarizability and hyperpolarizabilities for organic π-electron systems. **1987**, 151, 215-222	52
1613	Theoretical study of the coordination effect: The C?N bond stretch force constants of HCN?BF3 and HCN?BCl3. **1987**, 151, 223-226	2
1612	On the potential hypersurface of the dication of cyclotetraphospane. **1987**, 152, 145-154	1

1611	MNDO study of the tautomers of nucleic bases: Thiouracils. **1987**, 149, 185-192		10
1610	Picosecond solvation dynamics of coumarin 153: The importance of molecular aspects of solvation. **1987**, 86, 6221-6239		1061
1609	Dissolving-Metal Reduction of Polynuclear Aromatic Compounds in Liquid Ammonia. **1987**, 73-87		1
1608	MNDO analysis of the oxidised diamond (100) surface. **1987**, 183, 469-483		44
1607	The cluster approach in the study of atomic and molecular chemisorption on silicon. **1987**, 189-190, 106-113		23
1606	On the chemisorption of water on the (100) surface of silicon. **1987**, 180, 599-604		27
1605	Reaction of methylated urates with 1,1-diphenyl-2-picrylhydrazyl. **1987**, 3, 251-7		17
1604	Polaron lattice in highly conducting polyaniline: Theoretical and optical studies. **1987**, 59, 1464-1467		775
1603	Conformation and electronic structure of poly(3,4-diisopropylidenecyclobutene), a cross-conjugated conductive polymer. **1987**, 22, 171-178		1
1602	Electronic structure of the alkyl, benzyl and methoxy derivatives of polythiophene. **1987**, 21, 149-156		37
1601	Computer-aided molecular modeling of polymers. III. enthalpy of polymerization as a measure of stability. **1987**, 26, 495-508		
1600	Ion molecule reactions of carbon cluster ions with D2 and O2. **1987**, 86, 715-725		141
1599	The electronic spectrum of benz[a]anthracene. Linear and magnetic circular dichroism and fluorescence polarization studies. **1987**, 116, 411-420		18
1598	Electrostatic solvation energy in electrolyte solutions: A self-consistent inhomogeneous continuum model. **1987**, 112, 77-84		1
1597	On the problem of □electron delocalisation across sp3 carbon atoms introduced as defects in polyacetylene. **1987**, 64, 1183-1186		13
1596	Orbital interactions in 1,3-dithiane derivatives studied by UV photoelectron spectroscopy and MNDO method. *Journal of Molecular Structure*, **1987**, 160, 117-126	3.4	5
1595	Electronic structures and electronic spectra of the linkage isomers NSO□and SNO□*Journal of Molecular Structure*, **1987**, 162, 351-357	3.4	8
1594	WIZARD: AI in conformational analysis. **1987**, 1, 73-85		64

1593	Oxiranyl-β-aminovinylketones. 1. Preparation of oxiranyl-β-dialkylaminovinylketones from acetyloxiranes and acetals of amides. **1987**, 23, 821-823	
1592	Investigation of the electron structures of 2-substituted 1,3-dioxanes by the method of modified neglect of differential overlap (MNDO). **1987**, 23, 734-736	
1591	Calculation of coulomb integrals in molecules over an spd basis of STO. **1987**, 72, 47-55	11
1590	CNDO-S2α semiempirical SCF MO method for transition metal organometallics. **1987**, 72, 211-222	28
1589	MNDO calculations of systems containing hydrogen bonds. **1987**, 72, 223-228	46
1588	Theoretical study of the in-plane components of the 13C shielding tensors in condensed aromatic hydrocarbons. **1987**, 71, 277-288	22
1587	MNDO calculations of systems with hydrogen bonds S-H. **1987**, 71, 327-331	3
1586	On the regioselectivity of the fremy's salt oxidation of phenols. **1987**, 43, 3523-3532	19
1585	Mechanism of the biosynthesis of squalene from farnesyl pyrophosphate. **1987**, 43, 2661-2674	15
1584	Reaction of difluorocarbene with small bicyclic molecules. **1987**, 43, 653-662	5
1583	General approach to the synthesis of polyquinenes. IV. Studies directed toward the preparation of dicyclopenta[cd,gh]pentalene.. **1987**, 28, 4821-4824	5
1582	Photoelectron spectroscopy of monosubstituted benzenes and 4H-tetrafluorobenzenes : the effects of introduction of fluorine in the para-position and symmetry of highest occupied π levels. **1987**, 35, 627-641	1
1581	The structure and properties of flavins: Molecular orbital study based on totally optimized geometries. I. Molecular geometry investigations. **1987**, 31, 195-216	24
1580	Fixed closest distance of approach dipole potential mapping: An effective alternative to the monopole isopotential approach. **1987**, 32, 181-191	8
1579	The effect of additional fused rings on the stabilities and the band gaps of heteroconjugated polymers. **1987**, 32, 163-170	23
1578	A theoretical analysis of photoaddition reactions of hydroxylazoaromatic compounds and the related thione analogs with olefins. **1987**, 32, 283-295	1
1577	A possible solution to the rotational invariance and silicon parameter problem in the MNDO approximation. **1987**, 32, 547-554	3
1576	An MNDO molecular orbital study of the reactions of protonated oxirane with guanine. **1987**, 32, 57-64	3

1575	Crystal and molecular structure ofS-methyl(pentafluorosulfanyl)thiocarbamate. **1987**, 17, 187-196	2
1574	Treatment of anions in SINDO1. **1987**, 72, 373-378	13
1573	MNDO calculations on systems containing S-H hydrogen bonds. **1987**, 28, 5-8	1
1572	Revised semiempirical parameters for Br, I, Sn, Hg, and Pb in the MNDO method. **1987**, 28, 9-12	3
1571	Pseudocontinual model of point dipoles for taking into account solvation in quantum-chemical calculations. **1987**, 28, 169-174	
1570	A program for searching for semiempirical parameters by the MNDO method. **1987**, 28, 312-314	
1569	Quantum-chemical calculation of the geometry of 1-vinylazoles. **1987**, 27, 658-659	
1568	Synthesis and transformations of some pyrido[2,3-d]pyrimidines. **1987**, 118, 399-407	4
1567	Hydrogen in crystalline semiconductors. **1987**, 43, 153-195	865
1566	Identification of a glycine-like fragment on the strychnine molecule. **1987**, 17, 209-13	24
1565	NMR and theoretical (MNDO and Ab Initio) studies of lone-pair electron-□electron interactions: The conformation of 9-methoxyfluorene. **1987**, 25, 251-255	2
1564	ESR and theoretical study of tetrathiofulvalene and dibenzotetrathiofulvalene and their radical cations. **1987**, 25, 648-652	9
1563	NMR spectra of the porphyrins 32□conformational analysis of Pyrrolidine and 3-Hydroxypyrrolidine using CoIII meso-Tetraphenylporphyrin (CoTPP). **1987**, 25, 790-797	5
1562	15N and 17O NMR chemical shift calculations using the MNDO/GIAO method. **1987**, 25, 860-863	3
1561	Syntheses and Structures of 2-(O-Acylhydroxyimino)-1,3-indandiones. **1987**, 1987, 375-376	3
1560	Sulfonyl-Activated Cyclobutenes as Building Blocks for the Synthesis of Dihydrodiazepines. **1987**, 120, 171-175	10
1559	The Laticyclic [2 + 2 + 2] Conjugation: PE and UV Spectroscopical Investigation of the Interaction Between Three Parallel □Bonds. **1987**, 120, 195-201	19
1558	Bis(1,2-dimethyl-3-indolizinyl)methane: Structural Studies of a Two-Bladed Molecular Propeller. **1987**, 120, 231-237	4

1557	Diazepinones from Syndnones and Isopropylidenecyclobutenone. Extension of the Frontier Molecular Orbital Model for Sydnone Cycloadditions. **1987**, 120, 275-283	10
1556	Zur Regioselektivitˆ 1,4-Dipolarer Cycloadditionen von 3,6-Dihydro-6-oxo-1-pyrimidinium-4-olaten an elektronenreiche und elektronenarme Butatriene. **1987**, 120, 445-447	12
1555	Anomer kontrollierte Substitutionsreaktionen mit verschiedenen N-Alkylpyridiniumverbindungen. **1987**, 120, 735-745	25
1554	Beitrˆ ge zur Chemie des Bors, 186 Ein Allen-analoges Diborylamid-Ion. **1987**, 120, 907-909	6
1553	The Vinylogous Tricarbonyl Chromophore. Violerythrine End Groups and Related Six-Membered Ring Compounds. Their synthesis, Conformation, and Investigation by Photoelectron, UV, and NMR Spectroscopy and by Crystal Structure Analysis1). **1987**, 120, 1133-1149	16
1552	PMO Analysis of Cycloadditions, I Diels-Alder Reactions of 2,3-Bis(methylene)norbornane. **1987**, 120, 1323-1330	44
1551	Photoelektronenspektrum und elektronische Struktur von 4-Butadiinylmorpholin, einem Amino-substituierten 1,3-Diin. **1987**, 120, 1441-1443	1
1550	Die Rˆ tgenstruktur von N-Lithiocarbazol-Dimer: Experimentelle Bestˆ tigung der theoretischen Analyse von Strukturen des N-Lithiopyrrol-Typs. **1987**, 120, 1533-1538	46
1549	Gasphasen-Reaktionen, 601) Methanimine RR?C?NR?: Darstellung und Photoelektronen-Spektren2 . **1987**, 120, 1961-1970	32
1548	Gasphasen-Reaktionen, 611) Cycloalkanimine 2H-Azirin, 1-Azetin, 1-Pyrrolin, 1-Piperidein und 3,4,5,6-Tetrahydro-2H-azepin: Darstellung und Photoelektronen-Spektren2,3). **1987**, 120, 1971-1985	32
1547	Testing ab initio procedures; The 6 1G* model. **1987**, 138, 141-145	36
1546	Ab initio study of the chair cope rearrangement of 1,5-hexadiene. **1987**, 141, 521-524	55
1545	CN formation following electron attachment to cyanogen ((CN)2). **1987**, 135, 335-339	9
1544	Doubly charged ion mass spectra of alkyl-substituted furans and pyrroles. **1987**, 22, 389-399	5
1543	Charge reversal of the conjugate base of formamide. **1987**, 22, 534-540	14
1542	A comparison of three experimental techniques for ion structure studies via collision-induced reactions: The [C5H8]+ example. **1987**, 22, 779-789	13
1541	Angular Distortions at Tetracoordinate Carbon Planoid Configurations in Substituted Spiro[4.4]nonanes. **1987**, 70, 534-542	12
1540	Angular Distortions at Tetracoordinate Carbon Planoid Distortions in -Bridged Spiro[4.4]nonanes and [5.5.5.5]Fenestranes. **1987**, 70, 543-553	27

1539	Synthese und NMR-Spektren von Nonafulven sowie Vergleich mit 10-Phenylnonafulven. **1987**, 70, 862-880	13
1538	Oxidative Breaking of Long-Chain Acetylenic Enol Ethers of Glycerol of the Marine Sponges Raspailia pumila and of Model Compounds with Aerial Oxygen. **1987**, 70, 1400-1411	16
1537	Interactions between Oxygen Lone-Pair Orbitals and Double-Bond Orbitals in Unsaturated, Bicyclic Ketones; a PE-Spectroscopic Investigation. **1987**, 70, 1540-1550	12
1536	Face-to-Face Benzo-anellierte homologe Hypostrophene. Synthesen, Rˆ ntgenstrukturanalysen und PE-Spektren. **1987**, 70, 1816-1842	10
1535	On the importance of size-consistency corrections in semiempirical MNDOC calculations. **1987**, 8, 48-50	12
1534	Combination of MOMM and VEH methods to calculate electronic properties of polymers. **1987**, 8, 107-116	10
1533	Comparison of the use of the MNDO and MINDO/3 methods with ab initio methods to study tautomerism in histamine, 2- and 4-methylhistamine. **1987**, 8, 142-148	16
1532	Column design. 3. Theoretical studies of a chiral stationary phase used in column chromatography. **1987**, 8, 753-760	15
1531	Theoretical studies on the acid hydrolysis of methyl carbamate. **1987**, 8, 794-800	9
1530	Improvement of the hydrogen bonding correction to MNDO for calculations of biochemical interest. **1987**, 8, 835-849	47
1529	Application of SINDO1 to sulphur compounds. **1987**, 8, 1004-1015	29
1528	Systematic drug receptor mapping: A new approach to the analysis of conformational energy calculations of flexible molecules with application to dopaminergic and adrenergic agonists. **1987**, 8, 1075-1083	4
1527	Semi-empirical calculations of molecular trajectories: Method and applications to some simple molecular systems. **1987**, 8, 1117-1123	90
1526	MNDO Calculations on [n]metacyclophanes. **1987**, 8, 1154-1169	17
1525	An investigation of the relative stabilities of the isomers of CF2N2: Comparison of ab initio and MNDO calculations. **1987**, 8, 1170-1178	4
1524	Isolierung und Photoisomerisierung von einfach substituierten Nitriloxiden. **1987**, 99, 152-153	21
1523	P8iPr4 das erste Tricyclo[3.2.1.02,4]octaphosphan. **1987**, 99, 371-372	9
1522	Biphenylene mit stark trapezfˆ mig verzerrtem Vierring. **1987**, 99, 459-460	6

1521	Dihydrocyclobutafuran. **1987**, 99, 471-473	6
1520	Photooxidation von 2,5-Dimethyl-2,3,4-hexatrien Matrixisolation eines Trisdioxetans. **1987**, 99, 495-497	1
1519	Die Pyrolyse von Aziden in der Gasphase. **1987**, 99, 518-540	51
1518	Effects of isotopic substitution on the vibrational spectra of 2,4,6-trinitrotoluene. **1987**, 43, 1249-1255	17
1517	The amide bond stretch of cyclic cis-amides. **1987**, 43, 587-588	1
1516	Infrared intensity parameters of the diacetylene and acidity of acetylenic hydrogens. **1987**, 43, 345-348	2
1515	On the electroreduction mechanism of halobenzenes. **1987**, 219, 197-208	11
1514	Correlation of the anodic peak potentials with the quantum mechanical properties of various vinyl compounds. **1987**, 237, 187-190	1
1513	Competition between single and double electron transfer in collisions of doubly charged molecular pyrrole ions with neutral pyrrole molecules. **1987**, 79, 127-140	3
1512	Methylsulfonylamino phenethylamines and aryloxypropylamines as potential adrenergic agents. **1987**, 22, 165-167	1
1511	Electrostatic potentials of tumour promoters. **1987**, 5, 92-96	12
1510	A simple method to display molecular orbitals with computer graphics. **1987**, 5, 197-199	3
1509	A theoretical study of the decomposition of halogenated alkoxy radicals. I. Hydrogen and chlorine extrusions. **1987**, 116, 203-213	23
1508	Core ionization of nitrosobenzene-dimer compounds: phenazon-di-N-oxide. **1987**, 118, 101-112	4
1507	A theoretical study of the decomposition of halogenated alkoxy radicals. II. Fluorine extrusion. **1987**, 118, 265-272	8
1506	MNDO and MINDO/3 study of the reactivity of 3-pyrrolin-2-one tautomers and derivatives. **1987**, 24, 457-464	4
1505	Quantum chemical study of the interaction of acetylene with lithium hydroxide and hydrosulfide. **1987**, 36, 94-97	
1504	Quantum chemical investigation of allyl compounds with group iv elements. Communication I. Electron structure of molecules in the fundamental state. **1987**, 36, 2563-2567	1

1503	Quantum-chemical study of the electronic structure and geometry of 1-vinylimidazole derivatives. **1987**, 36, 1855-1857	
1502	Structure of pyridine and quinoline vinyl ethers according to data from1H and13C NMR spectra and quantum-chemical calculations. **1987**, 36, 279-284	
1501	Electronic structure of negative monothiocarbonate ions. **1987**, 36, 2036-2039	
1500	New parametrization for mindo/3 calculations of the structure of compounds with N-N Bonds. **1987** , 36, 2199-2201	
1499	Dependence of the reactivity of five-membered aromatic heterocycles on their structure. 2. Effect of aza substitution on the proton affinity of aminofurans. **1987**, 23, 143-146	
1498	Dependence of the reactivity of five-membered aromatic heterocycles on their structure. 1. Effect of the number, type, and position of nitrogen atoms on the proton affinity of aminoazoles. **1987**, 23, 44-48	1
1497	Investigation of the electronic structure and properties of cluster models of silica by the MNDQ method. **1987**, 22, 509-520	2
1496	Molecular electrostatic potential mapping using a dipole. *Journal of Chemical Sciences*, **1987**, 99, 113-118.8	3
1495	Model mndo calculations for rotamers of □acylnitroxides and of N-nitrosonitroxides. **1987**, 43, 405-408	10
1494	Facile construction of terpenoid frameworks by cycloadditions with methyl 2-chlorocyclopropylidenacetate. **1987**, 43, 3213-3223	28
1493	The effect of strain on the tropone ring. [3]- and [5](2,7)troponophanes. **1987**, 28, 977-980	5
1492	Rearrangements of bicyclo[n.1.1]alkylium cations. **1987**, 28, 3869-3872	2
1491	Structure and stereochemistry of 2-(N-methylaniline)-3-(N-methoxyaceto)-7-(p-chlorophenyl)-8-methoxy-4,5-benzo-3-aza-1-nonem. **1987**, 43, 269-272	
1490	Substituent effects of □acceptors to prismane. Structure of methyl 2,3,5,6-tetramethyl-4-phenylprismanecarboxylate and theoretical calculations on formylprismane. **1987**, 43, 266-269	8
1489	Die Umsetzung von Tropon mit einem Homopyrrol als Ergebnis einer computerunterstˆ □zten Suche nach prˆ □edenzlosen chemischen Reaktionen. **1988**, 100, 1618-1619	7
1488	Die Kristall- und Molekˆ □struktur von Gestoden. **1988**, 1988, 199-202	5
1487	Keto-enol tautomers and distonic ions: The chemistry of [CnH2nO] radical cations. Part I. **1988**, 7, 1-39	88
1486	Distonic radical cations in gaseous and condensed phase. **1988**, 7, 123-202	303

1485	The thermochemistry of polyoxides and polyoxy radicals. **1988**, 20, 455-466	34
1484	Conformational analysis and computer graphics in drug research. **1988**, 8, 1-25	16
1483	Deuterium-induced NMR isotope shifts for 13C resonance frequencies of norbornane. Quantitative data for the dihedral angle dependence of vicinal shifts. **1988**, 26, 408-411	16
1482	13C NMR chemical shift assignments for some 1-aminopyrrole derivatives. **1988**, 26, 714-719	4
1481	Bildung, Struktur und Reaktionen von Methyl(methylimino)boran. **1988**, 121, 61-66	9
1480	Pyrrolo[1,2-b]-1,3,4-thiadiazol-Derivate aus mesomeren Heteropentalenen und Azodicarbonestern. **1988**, 121, 95-104	4
1479	2,2?-Verbrˆ ckte Bis(thiophene) aus Bis(1,3-dithiolylium-4-olaten) und Alkinen. **1988**, 121, 313-322	13
1478	Photoelectron Spectrum and Electronic Structure of Triazadienyl Fluoride, N3F. **1988**, 121, 555-557	6
1477	2,3-Dihydro-2,3-dimethylenthiophen, Dihydrocyclobutathiophen und die gegenseitige Umwandlung beider Verbindungen. **1988**, 121, 791-793	21
1476	2H-1,3,4-Oxadiazin-2-one. Eine neue Klasse heterocyclischer Verbindungen. **1988**, 121, 887-894	9
1475	Darstellung von 1-Oxo-1H-pyrazolo[1,2-a][1,2,4]triazol-4-ium-3-olaten. Eine Ring-Ketten-Tautomerie in der Reihe bicyclischer dipolarer Heterocyclen. **1988**, 121, 895-907	11
1474	Neue 1,4-Dipolare Cycloadditionen von 6-Oxo-6H-1,3-oxazin-3-ium-4-olaten und eines 6-Oxo-6H-1,3-thiazin-3-ium-4-olats an Keten-Derivate und Enamine. **1988**, 121, 951-960	14
1473	Electronic Structure and Gas-Phase Thermolysis of Substituted Tetrazolines Studied by Photoelectron Spectroscopy. **1988**, 121, 1213-1217	14
1472	The Electronic Structure of 2-Azapentalenes. Photoelectron Spectroscopic Investigations. **1988**, 121, 1219-1223	1
1471	Herstellung von (Bicycloalkyl)essigsˆ ure-Derivaten durch zweifache nucleophile Substitution am Cyclopropan. **1988**, 121, 1487-1493	10
1470	Brˆ ckenkopf-gekoppelte Bicyclo[1.1.1]pentane: Synthese und Struktur. **1988**, 121, 1785-1790	41
1469	Bicyclo[6.1.0]nonine. **1988**, 121, 2013-2018	11
1468	Relationship of molecular radical anion abundance and calculated lowest unoccupied molecular orbital energies for polychlorinated dibenzofurans and dibenzodioxins in electron capture negative ion mass spectrometry: evidence for negative metastable ions. **1988**, 17, 63-7	14

1467	Charge neutralization of ions from benzene. **1988**, 23, 256-260	4
1466	Circular Dichroism of Planar, Exocyclic S-cis-Butadienes Remotely Perturbed. **1988**, 71, 419-428	1
1465	New Reactions of 3-Vinyl- and 3-(2-Propenyl)Indoles with N-Phenylmaleimide: [4 + 2] Cycloaddition, ene reaction, and dimerization. **1988**, 71, 467-471	33
1464	1H-and 13C-NMR study of the dilithium naphthalene and its TMEDA complex. **1988**, 71, 694-702	14
1463	First Synthesis of 2-Vinylindole and its diels-Alder Reactions with CC-Dienophiles. **1988**, 71, 1060-1064	24
1462	Application of SINDO1 to phosphorus compounds. **1988**, 9, 40-50	17
1461	Application of SINDO1 to silicon, aluminum, and magnesium compounds. **1988**, 9, 51-62	26
1460	Explorations on the multidimensional potential energy surface of a chiral stationary phase. **1988**, 9, 63-66	9
1459	AM1 calculations of rotation around essential single bonds and preferred conformations in conjugated molecules. **1988**, 9, 369-377	87
1458	Numerical sensitivity of trajectories across conformational energy hypersurfaces from geometry optimized molecular orbital calculations: AM1, MNDO, and MINDO/3. **1988**, 9, 387-398	64
1457	Electron donor-acceptor complexes: Evaluation of MNDO as a computational tool to probe intermolecular interactions. **1988**, 9, 539-553	11
1456	Comparison of semiempirical MO methods for open-shell systems. **1988**, 9, 702-707	13
1455	Theoretical calculations of proton affinities of azines. Prediction of the relative basicities and preferred protonation sites. **1988**, 9, 784-789	35
1454	A new tool for the rapid estimation of charge distribution. **1988**, 9, 893-904	20
1453	Theoretical investigation of the role of clay edges in prebiotic peptide bond formation. II. Structures and thermodynamics of the activated complex species. **1988**, 18, 107-19	26
1452	Computer simulation of the binding of quinocarcin to DNA. Prediction of mode of action and absolute configuration. **1988**, 2, 91-106	12
1451	Vibrational modes and frequencies of 2-pyrrolidinones and their deutero-isotopomers. **1988**, 44, 371-377	29
1450	Use of the semiempirical MNDO method for the prediction of equilibrium geometries and relative stability of exo- and endo-5-nitro-2-norbornenes. **1988**, 44, 1011-1014	1

1449 The first dissociation constant of uric acid. **1988**, 38, 118-124 17

1448 Intramolecular charge-transfer fluorescence of a new class of sterically hindered bichromophoric molecules. **1988**, 153, 357-364 10

1447 Resonant and near-resonant charge transfer reactions of gaseous organic ions. **1988**, 146, 113-120 5

1446 Negative-ion formation in fluoroacetonitrile and chloroacetonitrile following low-energy electron impact. **1988**, 153, 268-272 5

1445 New semiempirical SCF-MO method for calculating organometallic compounds. **1988**, 29, 349-356 2

1444 MNDO calculations of Mg compounds. **1988**, 28, 926-929 2

1443 Complexes with hydrogen bonds by the MNDO/M method. **1988**, 29, 192-197

1442 Structure and valence isomerizations of antiaromatic molecules. XIII. Relative stability of cyclobutadiene and its aza-substituted derivatives. **1988**, 28, 483-490 5

1441 Conformational behavior of methyldialkoxysilanes by the MNDO method and IR spectroscopy. **1988**, 28, 513-518

1440 Parameters of MNDO method for Zn atom. **1988**, 28, 649-652

1439 Program to implement MNDO/VS with analytic first-derivative computation and vibrational-spectrum calculation. **1988**, 28, 772-773

1438 Induced circular dichroism spectra of 2-(2,4,6-cycloheptatrien-1-ylidene)-4-cyclopentene-1,3-dione included in□cyclodextrin. **1988**, 6, 249-252 1

1437 Intramolecular interactions and nature of the lowest electronically excited states in compounds modeling the structural unit of lignin. I. Molecular form. **1988**, 24, 227-235 1

1436 Intramolecular interactions and nature of the lowest electronically excited states in compounds modeling the structural unit of lignin. II. Phenolate anions. **1988**, 24, 235-241

1435 Spectral identification of Al3Cl10□in 1-methyl-3-ethylimidazolium chloroaluminate molten salt. **1988**, 7, 1139-1145 37

1434 Stabilization of polyheteroatomic aza and phospha analogs of cyclobutadiene and benzene. **1988**, 24, 210-215

1433 Minimal requirements for approximate wavefunctions of molecules. **1988**, 74, 275-288 8

1432 The lone-pair orbitals of triaziridine. **1988**, 1, 267-273 5

1431	The role of hydrophobicity in the Ames test. The correlation of the mutagenicity of nitropolycyclic hydrocarbons with partition coefficients and molecular orbital indices. **1988**, 34, 91-101		21
1430	Modified all-valence INDO/spd method for ground and excited state properties of isolated molecules and molecular complexes. **1988**, 34, 423-435		83
1429	The influence of geometrical fluctuations on electron tunneling barriers in proteins. **1988**, 34, 23-32		
1428	3- and 5-Isoxazolol zwitterions: A model of interaction with the GABA-A receptor relating to agonism and antagonism. **1988**, 34, 149-165		5
1427	Use of quantum mechanical models in studies of reaction mechanisms. **1988**, 34, 557-566		14
1426	Electrostatic potential maps of flavone acetic acids: A new class of antitumor drugs. **1988**, 34, 697-705		4
1425	Model Clusters and Electronic Characteristics of Deep-Level Impurities in Silicon. **1988**, 145, K125-K130		
1424	Electronic structures and thermolyses of cyclic 2-tetrazenes. *Journal of Molecular Structure*, **1988**, 175, 423-428	3.4	6
1423	Molecular orbital study on the metabolic pathway through the diol epoxide form of carcinogenic benzene in comparison with benzo[a]pyrene. **1988**, 135, 215-8		2
1422	An AMI study of the cope rearrangements of bullvalene, barbaralane, semibullvalene, and derivatives of semibullvalene. **1988**, 44, 1351-1358		41
1421	2,4-Dichloro-3-(dimethylaminomethylene)-1,4-cyclohexadiene-1,5- dicarboxaldehyde: X-ray structure, mndo calculations, and rotational barriers of a stable non-aromatic tautomer of a penta-substituted benzene. **1988**, 44, 3209-3214		6
1420	The tertiary amino effect in heterocyclic synthesis : mechanistic and computational study of the formation of six-membered rings. **1988**, 44, 4637-4644		37
1419	An experimental study on the mechanism and stereochemistry of a photochemical [1,3]-oh shift. A non-woodward and hoffmann reaction path for photochemic. **1988**, 44, 4821-4836		3
1418	Semiempirical mo studies on the proton transfer equilibria of amides1. **1988**, 44, 7345-7353		1
1417	Temperature dependent energies of formation for hydrogen-bonded water clusters using a modified mndo and a statistical mechanics approach. **1988**, 44, 7373-7378		4
1416	Electronic structure study of hydrogen-bonded water clusters and linear-chain ice crystal using a modified mndo. **1988**, 44, 7379-7384		3
1415	Semiempirical methods: current status and perspectives. **1988**, 44, 7393-7408		119
1414	Reexamination of the C2H4F+ potential surface. the status of the classical 2-fluoroethyl cation: a local minimum or transition structure?. **1988**, 44, 7489-7498		11

1413	An alternative parameterization of electron repulsion terms in mndo and aml. **1988**, 44, 7509-7515		5
1412	NMR spectra of organogermanium compounds. **1988**, 44, 7531-7539		4
1411	Theoretical studies on the hydride transfer between 1-methyl-1,4-dihydronicotinamide and its corresponding pyridinium salt. **1988**, 44, 7601-7610		11
1410	Regioselectivity in the diels-alder reactions of □pyrones with alkynes. **1988**, 44, 1915-1924		11
1409	Theoretical evaluation of stereoelectronic diastereofacial selectivity in the conjugate addition of cuprates to 5-substituted cyclopentenones. **1988**, 29, 443-446		10
1408	Spontaneous rearrangement in Corey's reaction. **1988**, 29, 851-852		14
1407	An mndo study of structures and stabilities of representative 1-chloro-1-alkenes and of their beryllium hydride derivatives. **1988**, 44, 6287-6294		4
1406	The siting, energetics and mobility of saturated hydrocarbons inside zeolitic cages: methane in zeolite Y. **1988**, 331, 601-604		107
1405	Negative ion formation in SF5NCO following low-energy electron attachment. **1988**, 85, 125-136		12
1404	Molecular orbitals of benzoxadiazole compounds with optical nonlinearities. **1988**, 127, 259-262		11
1403	Oxidation of o-xylene: a quantum chemical study. **1988**, 45, 183-191		13
1402	An improved SCF iteration scheme. **1988**, 12, 233-236		14
1401	Correlation of reduction potentials of cyanine dyes with their orbital energies. **1988**, 9, 217-220		2
1400	Nonempirical cluster model study of the on-top chemisorption of fluorine and chlorine on C(111) surface. **1988**, 65, 945-947		1
1399	Theoretical foundation of molecular structures useful in structure/property relationships. **1988**, 206, 239-251		9
1398	Modelling the morphology of molecular crystals; application to anthracene, biphenyl and □succinic acid. **1988**, 88, 159-168		86
1397	A dipole moment study on gradually hindered N-phenylpyrroles. *Journal of Molecular Structure*, **1988**, 178, 187-200	3.4	23
1396	Unexpected chirality in trans-1,4-dicyanocyclohexane. *Journal of Molecular Structure*, **1988**, 172, 355-367	3.4	11

1395	Solid-state structure and conformation of the cognition activator 3-phenoxypyridine sulphate: X-ray, two-dimensional 1H NMR and 13C NMR, and theoretical Mo-MNDO studies. *Journal of Molecular Structure*, **1988**, 172, 369-380	3.4	6
1394	The structures of hexaorgano-substituted triatomics R13M1XM2R23 and related species. **1988**, 356, 151-158		9
1393	Competition among multihapto bonding, solvation, and aggregation. The □1/□2 infinite-chain X-ray structure of indenylsodium □N,N,N?,N?-tetramethyl-1,2-diaminoethane. **1988**, 341, 19-38		13
1392	Electronic structure of hydantoin studied by He I photoelectron spectroscopy and MNDO quantum□hemical calculations. **1988**, 44, 289-292		2
1391	Absorption and vibrational spectra of the surface properties of molecular monolayers with large light-induced dipole alterations. **1988**, 44, 793-803		6
1390	Excited states and electronic spectra of monosubstituted benzenes. An AM1 study. **1988**, 44, 1427-1434		13
1389	Analysis of the long-range effect of the nitrogen unshared pair on the direct13C-1H coupling constants in the vinyl group of N-vinylazoles. **1988**, 37, 752-755		
1388	R^ ẏio et p^ ḥis^ lectivit^ 'de r^ ȧctions de diels-alder et des cycloadditions dipolaires-1,3 avec une triaz^ ƀine-1,2,4: Approche th^ ȯrique. **1988**, 25, 453-457		9
1387	The reaction of 2-substituted-4,5-dichloro-3(2H)-pyridazinones with alkoxides and alkylthiolates. **1988**, 25, 1757-1760		20
1386	Electronic structure of imidazole, its tautomerism and mechanism for H-D exchange in aqueous solution. **1988**, 37, 2504-2507		2
1385	Quantum-chemical study of the structure and electronic absorption spectrum of allyllithium. **1988**, 37, 2087-2091		1
1384	Quantum-chemical investigation of the electronic structure and geometry of 1-vinylpyrazole derivatives. **1988**, 37, 278-283		1
1383	Quantum-chemical investigation of the mechanisms of reactions involving nucleophilic addition to acetylene 1. Addition of a hydroxide ion. **1988**, 37, 1173-1176		1
1382	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. **1988**, 37, 1177-1180		
1381	Quantum-chemical investigation of the mechanisms of reactions involving nucleophilic addition to acetylene. 3. Mechanism of the formation of vinylthio anions. **1988**, 37, 1180-1182		
1380	Quantum-chemical study of the cleavage of the C-X bonds in the radical ions CH3X? (X=F, Cl, Br, I). **1988**, 37, 1837-1841		
1379	Quantum-chemical investigation of the mechanisms of reactions involving nucleophilic addition to acetylene. 4. Study of reactions in the acetylene-LIOH system. **1988**, 37, 1841-1846		
1378	Semiempirical models of the transannular bond in silatranes and phosphatranes. **1988**, 37, 1846-1851		

1377	Quantum chemical investigation of donor-acceptor reactions of silicon, phosphorus, and sulfur halides with the carbonyl group of formaldehyde. **1988**, 37, 500-502	
1376	Quantum-chemical study of donor-acceptor interactions between silicon, phosphorus, and sulfur halides and ammonia. **1988**, 37, 503-505	
1375	Parametrization in the AM 1 method. **1988**, 24, 682-686	1
1374	Vibrational spectrum and structure of nitrosothiocarbamylcyanomethanide ion. **1988**, 24, 303-309	2
1373	Electronic structure of polyphosphate ions. **1988**, 23, 621-627	2
1372	Distribution of electron density and internal rotation in phospha-alkenes according to data from quantum-chemical calculations by the MNDO method. **1988**, 23, 679-682	
1371	Quantum Chemical Studies of H2-Antagonist-Receptor Complexes. Cimetidine and Related Compounds. **1988**, 7, 7-12	5
1370	QSAR Studies on Mifentidine and Related Compounds. **1988**, 7, 60-71	2
1369	Molecular structure of dicumyl peroxide. **1988**, 37, 674-678	3
1368	Bonding Properties of Diphosphacyclobutadienes. **1988**, 121, 2071-2073	9
1367	Alkylation of barbituric acid under phase transfer catalysis conditions. **1988**, 37, 797-799	
1366	Mechanism of the chain extension step in the biosynthesis of fatty acids. **1988**, 27, 3302-8	32
1365	Structural factors of importance for 5-hydroxytryptaminergic activity. Conformational preferences and electrostatic potentials of 8-hydroxy-2-(di-n-propylamino)tetralin (8-OH-DPAT) and some related agents. **1988**, 31, 212-21	23
1364	Postulation of bis(thiazolin-2-ylidene)s as the catalytic species in the benzoin condensation catalyzed by a thiazolium salt plus base. **1988**, 53, 4433-4436	47
1363	The electronic structure of substituted all-trans-polyenes. **1988**, 25, 345-364	1
1362	The structure of a novel polymeric metal: Acceptor-doped polyaniline. **1988**, 25, 121-137	77
1361	Properties of trans-polyacetylene with sp3 defects. **1988**, 37, 8262-8268	28
1360	State and motion of hydrogen in crystalline silicon. **1988**, 37, 6887-6892	161

1359	Selective hydrogenation of neat isoquinoline. **1988**, 43, 71-84	3
1358	Structural modeling of the distamycin A-d(CGCGAATTCGCG)2 complex using 2D NMR and molecular mechanics. **1988**, 27, 8088-96	90
1357	Calculated physical properties of polychlorinated dibenzo-p-dioxins and dibenzofurans. **1988**, 17, 2355-2362	48
1356	The crystal structure of octachlorodibenzodioxin: Experimental and calculated. **1988**, 17, 2419-2422	8
1355	Quantitative structure-activity relationship studies of the fungitoxic properties of phenethyl 1,2,4-triazoles. **1988**, 30, 199-213	8
1354	Structural variations in small ring hydrocarbons bridged by allenic double bonds. **1988**, 164, 25-35	9
1353	Modified atoms in molecules. **1988**, 170, 39-57	20
1352	Theoretical study of the mechanism of halogenotropic rearrangement in dichlorovinylsulphones. **1988**, 170, 133-142	2
1351	Theoretical study of the addition of bromine atoms to monosubstituted and disubstituted derivatives of ethylene. **1988**, 170, 225-232	3
1350	An attempt to examine alternative MNDP reaction courses of the hydrogen transfer from NADH model to acetaldehyde. **1988**, 170, 239-244	5
1349	Extension of AM1 to the halogens. **1988**, 180, 1-21	214
1348	Molecular orbital description of the polythiazyl polymer: Part 2. MNDO calculations of a structure with chlorine as a model dopant. **1988**, 180, 325-328	0
1347	Theoretical modelling of pyrolysis reactions: Thermal retroaldol reactions of β-hydroxy compounds. **1988**, 180, 383-387	2
1346	Calculation of proton transfers in hydrogen bonding interactions with semi-empirical MNDO/H. **1988**, 179, 153-163	6
1345	Reliability of AM1 in determining the equilibrium structures of unionized amino acids. **1988**, 164, 299-311	21
1344	MNDO/M Calculations on hydrogen bonded systems. **1988**, 164, 343-349	42
1343	Hydrogen bonding and rotation barriers: A comparison between MNDO and AM1 results. **1988**, 164, 379-389	57
1342	Calculation of vibrational frequencies of (CF3)2CX2 (X ? H, D, F, Cl). **1988**, 167, 227-233	4

1341	Quantum chemical study of molecular components of the organic superconductor (BEDT-TTF)2I3. **1988**, 167, 269-273	1
1340	Substituent effect on the planarization energy and the relative stability of Winstein and Mˆ Bius structures of the homotropylium cation. **1988**, 167, 275-300	5
1339	Semiempirical MNDOCI calculations on photochemical reactions: Criteria for selecting configurations. **1988**, 167, 301-306	13
1338	Protonation and rehybridization: A combined ab initio and semiempirical study. **1988**, 169, 447-457	12
1337	Ab initio SCF calculations of the barrier to internal rotation in formamidine and its derivatives. **1988** , 168, 1-14	8
1336	Reliability of AM1 in conformational analysis of unionized amino acids. **1988**, 168, 227-234	10
1335	An MNDO-effective charge model study of the solvent effect: The internal rotation about partial double bonds and the nitrogen inversion in amine. **1988**, 168, 265-277	28
1334	A MNDO-study of solvent free and solvated dimeric lithium ion pairs of acetaldoxime. Models for dimeric aggregates of lithiated oxime ethers. **1988**, 163, 19-50	18
1333	An AM1 study of the preferential solvation of ammonium ion in ammonia water mixtures. **1988**, 163, 101-110	32
1332	AM1, MNDO and MM2 studies of concatenated cyclobutanes: Prismanes, ladderanes and asteranes. **1988**, 163, 133-141	36
1331	Calculation of vibrational frequencies using molecular trajectories. **1988**, 163, 143-149	22
1330	A MNDO study of the geometries and rotational barriers of conjugated cations and radical cations. **1988**, 163, 163-171	1
1329	Inverse sandwich compounds. **1988**, 163, 259-265	3
1328	Theoretical study of the reaction C(3P) + SH(X2) **1988**, 163, 267-283	10
1327	Reinvestigation of some thermally forbidden pericyclic reactions and biradical processes in the semiempirical TCSCF approach. **1988**, 163, 285-304	14
1326	Correlation between hydride transfer and one-electron oxidation of dihydropyridines and heterocycles. **1988**, 163, 315-330	8
1325	New formulas for integrals in semiemperical molecular orbital methods. **1988**, 163, 355-388	2
1324	Fast semiempirical geometry optimizations. **1988**, 163, 415-429	34

1323	CHIMISTE: A quantum chemistry computer program. **1988**, 166, 125-128	4
1322	Thermal rearrangements of the homotropylium cation: An MO investigation of some relevant stationary points on the potential energy surface. **1988**, 166, 431-438	1
1321	Quantum-chemical and experimental investigations of photochromic transformations in quinone compounds. **1988**, 181, 285-296	2
1320	Monte Carlo simulation of 1,2-dichloroethane in dilute benzene solution. **1988**, 181, 345-352	1
1319	2-R 2-Oxo 1,3,2-dioxaphosphorinans. **1988**, 181, 377-388	
1318	A theoretical study of the reaction nitrile oxides with methyl amine. **1988**, 181, 389-399	
1317	MNDO CI study of vertical excitation energies. **1988**, 165, 1-8	19
1316	Influence of substituents on bond lengths. **1988**, 165, 87-97	6
1315	MNDO study of □vs. □protonation of pyrrole and N-methyl pyrrole. **1988**, 165, 365-378	11
1314	SYNTHESIS OF THE 8-PHOSPHABICYCLO[3.2.1]OCTA-2,6-DIENE RING SYSTEM. **1988**, 35, 353-361	4
1313	Formation and dissociation of negative ion resonances in methanol and allylalcohol. **1988**, 88, 7453-7458	45
1312	ZUR DARSTELLUNG VON BENZODITHIET-DERIVATEN DURCH THERMOLYSE 1,2-DITHIO-SUBSTITUIERTER BENZOLE. **1988**, 35, 291-307	10
1311	Conformation and electronic structure of heterocyclic ring chain polymers. **1988**, 25, 109-119	15
1310	Photolysis of polycyclic aromatic hydrocarbons adsorbed on fly ash. **1988**, 22, 1311-1319	188
1309	The conformational structure of 1,2-dimethoxy-ethane in the gas phase. **1988**, 170, 69-74	13
1308	Chemisorption on the SiO2 and silicon surfaces and the influence of infrared laser excitation. **1988**, 203, 143-154	12
1307	Cluster modelling of the 2 ˆ □1 chain reconstruction of the diamond (111) surface. **1988**, 194, 535-547	9
1306	Associative and dissociative electron attachment by SF6 and SF5Cl. **1988**, 88, 149-155	97

1305	Theoretical studies on the acylation reactions of ammonia by ketenes: Determination of reactivity by molecular orbital theory (part 54). **1988**, 1, 83-90	4
1304	Displacement vectors of localized vibrational modes around a charged soliton in Trans-polyacetylene. **1988**, 24, 357-370	10
1303	MNDO calculations of stilbene potential energy properties relevant for the photoisomerization dynamics. **1988**, 88, 7030-7039	61
1302	Bond-centered interstitial hydrogen in silicon: Semiempirical electronic-structure calculations. **1988**, 38, 7520-7529	69
1301	Hyperfine interactions in cluster models of the Pb defect center. **1988**, 38, 9674-9685	57
1300	Hydrogen passivation of a substitutional sulfur defect in silicon. **1988**, 38, 9936-9940	30
1299	Ab initio study of charged polyenes as charge-carrier models in conducting polymers. **1988**, 37, 2520-2528	42
1298	Surface and size effects for impurities in Si clusters. **1988**, 37, 858-863	40
1297	ZUR EXISTENZ VON H3PS UND SEINES RADIKALKATIONS IN DER GASPHASE. **1988**, 40, 227-232	11
1296	Reactions of carbon cluster ions with small hydrocarbons. **1988**, 89, 2063-2075	73
1295	The effect of heteroatomic substitutions on the band gap of polyacetylene and polyparaphenylene derivatives. **1988**, 88, 2609-2617	148
1294	Wavelength regulation in bacteriorhodopsin and halorhodopsin: A Pariser Parr Pople multireference double excitation configuration interaction study of retinal dyes. **1988**, 88, 4884-4896	37
1293	Structure, vibrational spectra, and IR intensities of polyenes from ab initio SCF calculations. **1988**, 88, 1003-1009	66
1292	Thermochromism in poly(3-hexylthiophene) in the solid state: A spectroscopic study of temperature-dependent conformational defects. **1988**, 89, 4613-4619	229
1291	Band structure of silicon from the semiempirical modified neglect of diatomic differential overlap method. **1988**, 38, 13422-13425	2
1290	An experimental and theoretical study of the valence electron properties of crystal violet. **1988**, 37, 831-835	1
1289	X-ray fluorescence yields for light emitter atoms: carbon. **1988**, 21, 1173-1182	22
1288	Neutral and charged soliton defects in polyyne chains: self-consistent field calculations of the effect of kink solitons on molecular geometry. **1988**, 21, 1971-1982	7

1287	The Application of Molecular Orbital Calculations to Wood Chemistry. V. The Formation and Reactivity of Quinone Methide Intermediates. **1988**, 42, 233-240		18
1286	Stereodynamic Coupling of Light Energy and Ion Transport in the Retinal Proteins Bacteriorhodopsin and Halorhodopsin. **1988**, 92, 1040-1045		5
1285	Bacteriorhodopsin's L550 intermediate contains a C14-C15 s-trans-retinal chromophore. *Proceedings of the National Academy of Sciences of the United States of America*, **1988**, 85, 2156-60	11.5	77
1284	Estimation of thermodynamic and spatial properties of organic compounds for quantitative molecular design. **1988**, 60, 271-276		0
1283	The diffusion and electronic structure of hydrogen in silicon. **1988**, 163-174		2
1282	Computational Predictions of the Tensile and Compressive Properties of Rigid-Rod Polymers. **1988**, 134, 313		12
1281	Theoretical Predictions of Nonlinear Optical Properties of Molecules and Polymers. **1988**, 134, 609		3
1280	NMR Spectroscopic Study of the Conformational Preference of Methoxycarbonyl and Methyl Substituted Thiophenecarbaldehydes. Possibility of a Hydrogen-Bond-Like Interaction between Formyl C□H and the Ester Carbonyl Group. **1988**, 61, 2031-2037		53
1279	Development and Applications for the Simulater of Intermolecular Potentials. II. Hydration Effects on the Conformation of Tyramine. **1988**, 61, 329-332		
1278	A Remarkable Difference of the Positional Selectivity in Electrophilic Aromatic Substitution of Dibenzofuran between the Classical □Complex and Charge-Transfer Mechanisms. **1988**, 17, 1285-1288		8
1277	Reaction of 1,1,2,2-Tetrachloro-2,2a□4□8b□tetrahydrocydobuta[c]quinolin-3(1H)-one with Nucleophiles; Reaction, Product Structure, and Mechanism. **1988**, 61, 2387-2391		2
1276	Calculation of Localized Vibrational Modes and Infrared Spectra around a Soliton in Polyacetylene. **1988**, 57, 1327-1340		4
1275	Struktur und Eigenschaften isomerer C4H3-Radikale. **1989**, 270O, 1067-1072		2
1274	Static and Dynamic Stereochemistry of Alkyl and Analogous Groups. **1989**, 25, 1-97		5
1273	The molecular structures of 11-methyl and 1,12-dimethylbenz[a]anthracene: purely theoretical semi-empirical AM1 calculations are able to predict accurate structures of these polycyclic hydrocarbons. **1989**, 10, 317-20		12
1272	The conformations and electrostatic potential maps of phorbol esters, teleocidins and ingenols. **1989**, 10, 531-40		9
1271	Ab initio molecular orbital and resonance Raman studies of the structure of the lowest triplet state of N,N,N□N□tetramethyl-p-phenylenediamine. **1989**, 90, 2317-2319		8
1270	.		5

1269	Pressure dependence of the polarized reflectance spectrum of the solid charge-transfer complex, perylene□TCNQ: Estimation of microscopic parameters. **1989**, 91, 3450-3455	11
1268	Molecular Design for New Second-Order Nonlinear Optical Materials. **1989**, 170, 259-272	3
1267	Sulfur Phosphorus Heterocycles RP(S)Sn and [RP(S)Sm]2, Synthesis and Dynamic Properties. **1989**, 41, 57-62	6
1266	States of hydrogen in crystalline semiconductors. **1989**, 111-112, 323-344	5
1265	The Application of Molecular Orbital Calculations to Wood Chemistry. VI. The Reactions of Anthraquinone Under Pulping Conditions. **1989**, 9, 277-292	2
1264	UHF calculations of hyperfine coupling constants of anomalous muonium in C, Si, Ge. **1989**, 1, 8227-8234	8
1263	Site-and regioselective □4S + □2S cycloaddition of nitrileoxides to pyridazin-3-ones: Formation of novel 3a, 7a-dihydroisoxazolo[4, 5-d]pyridazin-4-ones. **1989**, 26, 553-555	5
1262	1,3-Dipolar cycloaddition reactions. Regioselective synthesis of heterocycles and theoretical studies. **1989**, 26, 1003-1008	2
1261	Studies of transnitrilation mechanism in the presence of trifluoroacetic acid. **1989**, 39, 449-455	3
1260	An NMR and computational study of diazepinediones. **1989**, 199, 175-181	4
1259	Ionization energies of azines from green's function method in semiempirical AM1 approximation. **1989**, 188, 159-166	7
1258	Studies on the relationship between the MO indices and anticholinesterase activity of suberogorgin. **1989**, 188, 167-174	3
1257	A critique of frontier orbital theory. **1989**, 200, 301-323	63
1256	Matrix isolation radiation chemistry and photochemistry: electronic absorption spectra of o-xylylene and benzocyclobutene radical cations; localization of koopmans and non-koopmans bands in the photoelectron spectra of o-xylylene, styrene, toluene, o-xylene and benzocyclobutene. **1989**, 200, 375-400	21
1255	MNDO/H and AM1 calculations on the formic acid-methylamine complexes. **1989**, 200, 533-541	5
1254	AM1 study of the tautomerism of 2- and 4-pyridones and their thio-analogs. **1989**, 184, 179-192	28
1253	AM1 study of hydrogen bonded complexes of water. **1989**, 187, 55-68	41
1252	AM1 outer valence green's function ionization energies of the azoles. **1989**, 187, 297-306	7

1251	Reaction paths of circumambulatory rearrangements of sulfur-substituted cyclopentadienes. **1989**, 186, 293-303	6
1250	SINDO1 study of sulphur isomers and sulphur fluorine compounds. **1989**, 186, 347-359	18
1249	Semiempirical calculations of anti/gauche enthalpy differences in acyclic cyano-derivatives. **1989**, 201, 113-116	1
1248	Cluster-model study on the adsorption of atoms and molecules on the basal plane of graphite. **1989**, 201, 149-159	5
1247	Equilibrium geometry, force field and stability of the 1,2-dihalogenocyclobutene-3,4-diones. **1989**, 201, 307-318	10
1246	Vibrational spectra and conformational equilibrium of 1,1-dichloro-1-nitrosoethane and its deuterium analog. **1989**, 38, 2326-2330	2
1245	Quantum chemical study of allyl halides. **1989**, 38, 2341-2345	1
1244	Spectroscopic and quantum-chemical investigation of alkyl- and alkenyltetrazoles. **1989**, 25, 30-36	2
1243	X-ray crystallographic and quantum-chemical investigation of tert-butyl hydroperoxide. **1989**, 25, 73-77	2
1242	Kinetics of the alkaline hydrolysis of alkoxyfluoroborate anions. **1989**, 25, 111-113	
1241	Conformational investigations of vinyl esters on the basis of spatial effects in multinuclear EPR spectroscopy (1H,13C,15N,17O) and quantum-chemical calculations. **1989**, 38, 776-784	
1240	Quantum-chemical study of the interactions of Ebrbitals of double bonds in divinyl compounds. **1989**, 38, 260-262	2
1239	Quantum-chemical study of the effect of solvation on the strength of the phosphamide bond in N-phosphorylammonium cations and zwitterions. **1989**, 38, 267-270	
1238	Molecular structure and electrostatic characteristics of 5-nitro- and 5-nitrosofuran. **1989**, 38, 1062-1064	
1237	Distribution of the electron density and proton chemical shifts in a series of nitromethane derivatives. **1989**, 38, 1619-1623	
1236	Quantum-chemical study of the mechanism of the hydrolysis of amides in the gas phase and in aqueous solution. **1989**, 38, 1635-1641	2
1235	Quantum-chemical investigation of the mechanisms of nucleophilic addition reactions to acetylene. **1989**, 38, 1641-1645	
1234	Quantum-chemical investigation of the mechanisms of nucleophilic addition reactions to acetylene. **1989**, 38, 1645-1648	1

1233	Syntheses based on the electrogeneration of carbenes. 6. Thermodynamics of the formation of carbenes from the anions of chloro- and bromomethanes. **1989**, 38, 1188-1192		
1232	Syntheses based on the electrogeneration of carbenes. 7. Kinetics of the formation of carbenes from the anions of bromomethanes. **1989**, 38, 1192-1196		
1231	Electrocarboxylation of aryl- and acylhydrazones in nonaqueous media. **1989**, 38, 1197-1201		
1230	Photoelectron and ultraviolet absorption spectra of allenyl vinyl ethers. **1989**, 38, 1848-1851		
1229	Vibrational spectra and conformational equilibrium of (CH3)2CClNO and (CD3)2CClNO. **1989**, 38, 1406-1412		
1228	Quantum chemical study of reactions of episulfonium ions. 1. Comparative MNDO study of opening of the episulfonium ion ring by neutral nucleophiles and SN2 substitution in protonated methylthiol. **1989**, 38, 1439-1445		
1227	Quantum chemical study of reactions of episulfonium ions. 2. Effect of substituents on the orientation of ring opening for episulfonium ions by neutral nucleophiles. **1989**, 38, 1445-1450		
1226	Cluster structures for water adsorbed on SiO2. **1989**, 24, 516-526		1
1225	Calculations for photoelectron spectra of azoles by the AM1 method using a green's function approximation for the outer valence molecular orbital. **1989**, 25, 659-661		
1224	Quantum-chemical investigation of the mechanism of nucleophilic addition in the HCNO molecule. **1989**, 25, 662-665		
1223	Estimate of the activation barriers of chemical reactions on a silica surface. **1989**, 25, 696-697		1
1222	Investigation of electronic structure of impurity and defect centers on the surface of silica by the MNDO method. **1989**, 24, 396-406		
1221	HeI photoelectron and theoretical study of the gas phase flash pyrolysis of tetrazole and analysis of CN2H2 energy hypersurface. **1989**, 138, 157-171		31
1220	A theoretical study of the Si-O bond in disiloxane and related molecules. **1989**, 2, 267-80		6
1219	Calculation of dye-dye and dye-AgX surface interaction energies. **1989**, 130, 568-577		1
1218	On the adsorption of oxy-anions on mercury electrodes from solutions of constant ionic strength. **1989**, 258, 391-401		5
1217	Geometry changes induced by negative hyperconjugative interactions involving carbonyl and thiocarbonyl groups. *Journal of Molecular Structure*, **1989**, 194, 135-147	3.4	15
1216	Structural studies of di-Schiff bases with a middle flexible group, relationship between the structure and liquid crystal properties. *Journal of Molecular Structure*, **1989**, 193, 147-159	3.4	4

1215	Locoselective [4 + 2] Cycloadditions of Vinylindoles with Inverse Electron Demand: A new access of indolyl-substituted and annellated pyridazines. **1989**, 72, 65-72	18
1214	The Photochemical Synthesis and Denitrogenation of 8,9-diazadibenzo[c, e]isobullvalene. **1989**, 72, 1722-1728	4
1213	Deorthogonalization of atomic originals in the CNDO approach. **1989**, 10, 17-34	20
1212	Combined bond polarization function basis sets for accurate ab initio calculation of the dissociation energies of AHn molecules (A=LI to F). **1989**, 10, 152-162	25
1211	Optimization of parameters for semiempirical methods I. Method. **1989**, 10, 209-220	6553
1210	Optimization of parameters for semiempirical methods II. Applications. **1989**, 10, 221-264	3335
1209	Probing the anomeric effect. The diaminomethylene group: Calculations of N?C?N-containing molecular systems1. **1989**, 10, 265-283	39
1208	Basis set dependence, precision, and accuracy of full ab initio gradient optimizations of molecular structures of nonstrained hydrocarbons. I. CC bond lengths. **1989**, 10, 329-343	19
1207	Ab initio study of the proton affinity of a number of ortho-substituted pyridines. **1989**, 10, 346-357	20
1206	An MNDO molecular orbital study of the reactions of protonated oxirane derivatives (XCHCH2OH+, X = CN, Cl, CH3, Ph) with simple nucleophiles. Implications for regioselectivity in the reactions of electrophiles with nucleic acid bases. **1989**, 10, 568-592	9
1205	Theoretical studies in molecular recognition: Rebek's cleft. **1989**, 10, 595-602	23
1204	3S- Versus 1s-type Gaussian primitives: Modifications of the 3-21G(*) basis set for the sulfur atom. **1989**, 10, 660-672	1
1203	The dynamics of gallamine: A potent neuromuscular blocker. A determination by quantum mechanics and molecular dynamics (i) in vacuo studies. **1989**, 10, 975-981	1
1202	A molecular mechanics analysis of molecular recognition by cyclodextrin mimics of □-chymotrypsin. **1989**, 10, 1038-1052	29
1201	On the GABAA receptor: a molecular modeling approach. **1989**, 23, 129-35	25
1200	Zur Regiochemie von [4 + 2]-Cycloadditionen mit Methylpyrano[3,4-b]indol-3-onen und unsymmetrischen Dienophilen. **1989**, 1989, 227-230	8
1199	Makrocyclen aus Alanin und Phenoxathiin, Synthese und Konformation in L^ □sung. **1989**, 1989, 459-468	17
1198	Konfigurative Stabilit^ □von S-Adenosylmethionin □Mutarotation ohne Pseudorotation. **1989**, 1989, 607-610	1

1197	NMR spectra of organogermanium compounds. 8Ø73Ge, 13C and 1H NMR spectra of methylvinylgermanes. **1989**, 27, 72-74	9
1196	13C NMR study of the substituent effects on the internal steric hindrances in amidines. **1989**, 27, 577-581	8
1195	Struktur, Deformationselektronendichte, Photoelektronenspektrum und Reaktivitˆ Ø von 3,4-Dihydro-1H-cyclobuta[a]cyclopropa[d]benzol. **1989**, 101, 209-211	7
1194	Erste PE-spektroskopische Untersuchungen von Lithium-, Natrium- und Kalium-tert-butoxid. **1989**, 101, 953-955	4
1193	Sehr kurze C-C-Einfachbindungen und ihre Ursache; die Lˆ Øge der zentralen Bindung in Bitetrahedryl. **1989**, 101, 1264-1266	4
1192	Erzeugung und Ionisationsmuster der iso(valenz)elektronischen Verbindungen ClP(?O)2 und ClP(?S)2. **1989**, 101, 1378-1381	16
1191	Grundlagen der Silicium-Chemie: Molekˆ Øzustˆ Øde Silicium enthaltender Verbindungen. **1989**, 101, 1659-1682	56
1190	On the use of mixed basis sets to compute accurate molecular electrostatic potentials. **1989**, 160, 305-310	17
1189	Isomerization and fragmentation of methyl benzofuran ions and chromene ions in the gas phase. **1989**, 24, 47-54	2
1188	Photodissociation and structures of [C6H4]+ Øons generated from cyanobenzene and other precursors. **1989**, 24, 59-62	8
1187	Collision-induced fragmentation reactions of doubly charged ions of polycyclic aromatic hydrocarbons. **1989**, 24, 327-337	15
1186	Fused-ring tropylium ion formation and fragmentation. **1989**, 24, 767-772	3
1185	Thermische Cycloadditionen von 1,2-Dihydropentalen. **1989**, 122, 101-104	7
1184	Øerngesteuerte Ønucleophile Eigenschaften der Anionen einiger 4-Alkylpyridine: AM 1- und MNDO-Berechnungen sowie experimentelle Untersuchungen. **1989**, 122, 105-111	8
1183	Beitrˆ Øge zur Chemie des Bors, 196. Darstellung und Reaktionen eines 3-Amino-1,2,3-azaphosphaboriridins. **1989**, 122, 423-426	10
1182	9-Oxabicyclo[6.1.0]nonine. **1989**, 122, 509-517	12
1181	The Electronic Structures of 4-Substituted 3,5-Dihydro-4H-pyrazoles and 5-Substituted 1,4-Dihydro-5H-tetrazoles. **1989**, 122, 985-991	11
1180	Cycloadditionen, 15. Einflu Øvon Substituenten in p-, m- und o-Position am Aromaten auf die intramolekulare Diels-Alder-Reaktion von Allencarbonsˆ Øre-aniliden und -phenylestern. **1989**, 122, 1161-1173	13

1179	Diels-Alder-Reaktionen mit Diakzeptor-substituierten Methylencyclopropanen Ein neuer Aspekt f^ die doppelte nucleophile Substitution an Cyclopropanen. **1989**, 122, 1277-1284	6
1178	Decamethylsilicocene The first stable silicon(II) compound: Synthesis, structure, and bonding. **1989**, 122, 1629-1639	105
1177	1,4-Dihydroisochinoline und 1H-Benzo[de]isochinoline aus 2-Azaallenium-Salzen. **1989**, 122, 1711-1718	7
1176	Experimental test of structural predictions of semiempirical methods: Bis (1,2-dioxa-4,6-diazacycloheptano)[4?,5?,6?: 1,6,5][4?,5?,6?: 2,3,4]-1,2,4,5-tetraazacyclohexane, A 7:6:7-Tricyclic system correctly calculated by AM1 as more stable than its 6:6:6-Tricyclic isomer. **1989**, 122, 1989-1993	4
1175	Niedermolekulare Phosphorsulfide in der Gasphase. **1989**, 122, 2265-2267	13
1174	-C6H5CH2Li THF TMEDA, Kristallstruktur eines Benzyllithium THF TMEDA-Komplexes mit einem pyramidalen Benzyl-C-Atom. **1989**, 122, 2303-2309	88
1173	Interactions of nucleic acids with distamycins. The drug monomeric chromophore. **1989**, 28, 2161-76	3
1172	Structure, Deformation Electron Densities, Photoelectron Spectra, and Reactivity of 3,4-Dihydro-1H-cyclobuta[a]cyclopropa[d]benzene. **1989**, 28, 206-208	24
1171	Generation and Ionization Pattern of the Iso(valence)electronic Compounds CIP(?O)2 and CIP(?S)2. **1989**, 28, 1373-1376	15
1170	Fundamentals of Silicon Chemistry: Molecular States of Silicon-Containing Compounds. **1989**, 28, 1627-1650	91
1169	Draw 2D, draw 3D: MOPAC 2- and 3-dimensional graphical output written using the PHIGS graphics standard. **1989**, 2, 223-232	
1168	Projection of molecular interaction possibilities onto a cylinder surface. **1989**, 2, 141-151	
1167	A Monte Carlo study of the benzene effect on the dipole moment of 1,2-dichloroethane. **1989**, 156, 525-532	2
1166	Quantum-chemical studies on the mechanism of conversion of alcohols on zeolites. **1989**, 54, 444-450	0
1165	CNDO-S2: a new semiempirical SCF MO method for transition metal organometallics. **1989**, 54, 462-477	20
1164	Liquid crystal birefringence and electric dipole moment relationship with temperature, weak magnetic field and molecular geometry.. *Journal of Molecular Liquids*, **1989**, 44, 63-71 6	6
1163	Gas phase negative ion chemistry. **1989**, 89, 1-72	139
1162	A study of C1s binding energies in some gaseous polycyclic aromatic hydrocarbons. **1989**, 48, 179-185	7

1161	Many-body effects in the ionization spectra of azides. **1989**, 48, 187-201		3
1160	An investigation of the minimal requirements for H2-receptor agonists: a computational study of N-(3-aminopropyl)formamidine tautomerism. **1989**, 24, 189-192		1
1159	X-ray crystal structure, dipole moment and theoretical molecular orbital study of the cognition activator dihydro-1H-pyrrolizine-3,5(2H, 6H)-dione (Ð□olziracetam)□ **1989**, 24, 81-85		5
1158	The active site of cytochrome P-450 nifedipine oxidase: a model-building study. **1989**, 7, 206-11		25
1157	Comparison of synchronous and asynchronous hydrogen transfer mechanisms in free-base porphyrins. **1989**, 136, 285-295		33
1156	Discrete-state approach to the time evolution of molecular states. **1989**, 139, 265-281		6
1155	An MNDO calculational study of selected oxazine, thiazine and oxazone dyes. **1989**, 138, 365-375		17
1154	Stability of the amylxanthate ion as a function of pH: Modelling and comparison with the ethylxanthate ion. **1989**, 25, 1-16		16
1153	Charge localisation in doped segmented polyacetylene. **1989**, 69, 281-284		2
1152	Determination of approximate force field parameters. **1989**, 13, 123-128		4
1151	A theoretical approach to zwitterionic derivatives of 4-vinylpyridine. **1989**, 30, 1747-1750		4
1150	Molecular orbital study of the initial processes in the electrochemical polymerizations of pyrrole, thiophene and furan. **1989**, 258, 303-311		15
1149	Correlation of anodic peak potentials with the semi-empirical orbital and HOMO energies of various vinyl compounds. **1989**, 261, 105-112		9
1148	Photoisomerization in bacteriorhodopsin studied by FTIR, linear dichroism and photoselection experiments combined with quantum chemical theoretical analysis. *Journal of Molecular Structure*, **1989**, 214, 257-288	3.4	88
1147	The electronic spectra of benzo[b]thiete and transient o-thiobenzoquinonemethide. Spectral assignments on the basis of the electronic spectra of aniline, thiophenol, thioanisole, all-trans-octatetraene and transient o-xylylene in conjunction with quantum-chemical calculations. *Journal of Molecular Structure*, **1989**, 198, 307-325	3.4	12
1146	Critical appraisal of some current semiempirical methods in calculating ESCA chemical shifts. *Journal of Molecular Structure*, **1989**, 198, 427-434	3.4	9
1145	Theoretical studies on the stabilities of 1,2- and 1,3-isomers of cyclic H4A2X2 (A?C, Si; X?O,S,CH2): the anomeric effect at silicon. *Journal of Molecular Structure*, **1989**, 194, 183-190	3.4	10
1144	Electronic structure and conformational properties of the amide linkage. *Journal of Molecular Structure*, **1989**, 196, 181-192	3.4	4

1143	Comparison of theoretical and experimental ionization potentials of nicotine and related molecules. *Journal of Molecular Structure*, **1989**, 212, 37-44	3.4	6
1142	Comparison between optimized and crystal structures of R5135, a potent steroidic GABA-A antagonist: ab initio molecular orbital charge population analysis. *Journal of Molecular Structure*, **1989**, 212, 315-322	3.4	6
1141	Electronic and geometric structures of oligothiophenes. *Journal of Molecular Structure*, **1989**, 197, 265-289	3.4	22
1140	Photoelectron spectra and electronic structure of some 1-substituted aziridines and of 1,1?-biaziridinyl. *Journal of Molecular Structure*, **1989**, 197, 291-305	3.4	7
1139	Molecular structures and reactivities of the antioxidant 8-hydroxy-2,2?,4-trimethyl-1,2,3,4-tetrahydroquinoline and the free-radical products of its oxidation. **1989**, 29, 688-691		
1138	MNDO parameters for the Ca atom. **1989**, 29, 793-795		
1137	Green's function method for photoelectron spectroscopy calculations based on MNDO and AM1 semiempirical approximations. **1989**, 30, 474-477		
1136	Fragment-by-fragment analysis of molecular orbitals in some substituted benzenes. **1989**, 30, 194-202		1
1135	Molecular structure of 1,1-dimethylhydrazine. **1989**, 30, 224-228		3
1134	Photoelectron spectrum and quantum-chemical structural analysis of N-methyl-N-methoxydiazene-N-oxide. **1989**, 30, 228-233		2
1133	New structural aspects of 3-vinyl-1H-indoles for predicting the outcome of Diels-Alder reactions. **1989**, 120, 27-34		16
1132	On the reaction of dithiocarbamates with nitrogen-containing derivates of oxalic acid. **1989**, 120, 561-569		11
1131	MNDO properties of heteroatom and phenyl substituted nitrenium ions. **1989**, 45, 1763-1776		45
1130	Molecular modeling of □lactam analogues of □lactam antibacterial agents: synthesis and biological evaluation of selected penem and carbapenem analoques. **1989**, 45, 1905-1928		44
1129	A conformational study of bis-, tris- and tetrakis-pyrazolylmethane. Crystallography, L.S.R., dipole moments and theoretical calculations. **1989**, 45, 7805-7816		17
1128	First reactions of vinylindoles with diethyl mesoxalate, nitrosobenzene, and chlorosulfonyl isocyanate: New functionalized and □annellated indoles. **1989**, 45, 6427-6438		21
1127	Diazabicycloalkanes with nitrogen atoms in bridgehead positions.. **1989**, 25, 305-310		
1126	Amine-imine tautomerism of 2-aminothiazolines. **1989**, 25, 824-829		

1125	Comparative evaluation of quantum-chemical methods for calculating aromatic and antiaromatic nitrogen heterocycles (review). **1989**, 25, 1321-1335	8
1124	Quantum-chemical study of the electrophilicities of ynamino and ynaziridino esters. **1989**, 25, 884-888	
1123	Direct 13C-13C spin-spin coupling constants in the vinyl group of N-vinylazoles. **1989**, 25, 157-160	2
1122	Dependence of the reactivity of five-membered heterocycles on their structure. 3. Proton affinity of azoles and oxazoles. **1989**, 25, 423-425	4
1121	Detection of nitrosofuran anion radicals in the electrochemical reduction of 5-nitrofuran. EPR investigations and quantum-chemical calculations. **1989**, 25, 983-988	
1120	The structures of HCOO□,CH3COO□,C2H5COO□and CH3O□in gas phase and in crystal structure by ab initio and resonance theory. **1989**, 75, 433-446	11
1119	Can normal mode analysis reveal the geometry of the L550 chromophore of bacteriorhodopsin?. **1989**, 16, 341	11
1118	A preliminary quantum-chemical study of the mechanisms for the reactions of perchlorofluoroethanes with nucleophiles initiated by chlorophilic attacks. **1989**, 2, 103-109	4
1117	Theoretical study of pyrazole elimination of N-alkyl pyrazoles. **1989**, 2, 225-231	7
1116	Theoretical studies on the hydrolysis of urea in acid solution. **1989**, 2, 281-299	5
1115	Quantum-Chemical-Calculations of Models for Surface Defects in Dehydroxylated Silica. **1989**, 156, 205-209	1
1114	Structure and electronic structure of polyacene. **1989**, 35, 305-313	47
1113	Correlation of mutagenicity of 1,1-dimethyl-3-(X-phenyl)-triazenes with molecular orbital energies and hydrophobicity. **1989**, 36, 19-33	9
1112	Theoretical studies on (□52CR) bridged cyclopentadienyl molybdenum dimers. **1989**, 162, 281-285	4
1111	Long-range interactions and molecular dynamics of polyenes: Polyacetylene. **1989**, 32, 151-169	16
1110	Theoretical design of small bandgap polypyrrole derivatives. **1989**, 28, 205-210	48
1109	The X-ray structure and MNDO calculations of □erthienyl: A model for polythiophenes. **1989**, 30, 381-389	181
1108	Electronic structure of small gap polymers. **1989**, 28, 545-552	35

1107	Localized vibrations around a soliton in polyacetylene. **1989**, 28, D381-D386	1
1106	MNDO calculations on tetrathiafulvalenes. **1989**, 32, 179-190	12
1105	Structure, electrical conductivity and dielectric relaxation of a 1,2-dimethoxybenzene-tetracyanoethene 1:1 complex. **1989**, 32, 79-89	11
1104	A theoretical study on the metabolic activation of paracetamol by cytochrome P-450: indications for a uniform oxidation mechanism. **1989**, 2, 60-6	45
1103	Theoretical study of the influence of thermochromic effects on the electronic structure of poly(3-hexylthiophene). **1989**, 28, 359-364	158
1102	Perchloro-organic Chemistry: Structure, Spectroscopy and Reaction Pathways. **1989**, 25, 267-445	17
1101	A SCF MO study on the reaction mechanism of quaternary ammonium cation with hydroxide ion. **1989**, 183, 311-318	
1100	Molecular structure and electronic properties of hexaethynylbenzene. **1989**, 183, 175-181	6
1099	Quantum-mechanically calculated properties for the development of quantitative structure-activity relationships (QSAR'S). pKA-values of phenols and aromatic and aliphatic carboxylic acids. **1989**, 19, 1595-1609	54
1098	Two helical conformations of polythiophene, polypyrrole, and their derivatives. **1989**, 40, 9661-9670	101
1097	Quantochemical analysis of the formation of crosslinked structures and volatile products on thermolysis of polyimides. **1989**, 31, 2538-2542	1
1096	Determination of Water Loss Mechanism in Amine Terminous Amino Acids Using Laser Mass Spectrometry. **1989**, 43, 1087-1092	4
1095	The different influences of ether and ester phospholipids on the conformation of gramicidin A. A molecular modelling study. **1989**, 979, 321-30	28
1094	Experimental and theoretical studies of anthelmintics: oxfendazole and its imidazo[1,2-a]pyridine-2-carbamate isomer. **1989**, 19, 363-8	2
1093	A study of the UV spectrum of the truncated icosahedral C60 molecule. **1989**, 183, 271-278	47
1092	Excited states of polyyne chains: Polarons and polarexcitons. **1989**, 31, 61-71	5
1091	Molecular orbital study of the initial reaction paths in the electrochemical polymerization of aniline. **1989**, 33, 19-26	6
1090	Electronic Interactions of Cyclopropyl Groups: Synthesis and Photoelectron Spectra of Model Compounds Derived from Triasterane, Nortricyclane and Norbornane. **1989**, 29, 153-164	8

1089	Localized vibrational modes and phonon dispersion curves of polyacetylene with a charged soliton. **1989**, 30, 227-244	4
1088	The structure of the poly(vinyl chloride) chain. I. Conformation of 2,4-dichloropentane. **1989**, 29, 321-328	2
1087	Effects of Hydrogen Atoms on Passivation and Growth of Microcrystalline Si. **1989**, 164, 205	9
1086	Helical Conformations of Conducting Polymers. **1989**, 173, 391	
1085	Interaction of Atomic Hydrogen with the (111) and (100) Surfaces of Diamond-Like Crystals. **1989**, 69-73	
1084	On the Reactivity of Diamond-Like Semiconductor Surfaces. **1989**, 809-816	2
1083	Nitric Oxide Adsorption on (111) and (001) Surfaces of Diamond-Like Crystals. A Theoretical Study on Model Finite Clusters. **1989**, 48, 893-902	
1082	Synthesis and biological activity of 7 alpha-hydroxyethyl-1-oxacephem derivatives. **1989**, 42, 1124-32	8
1081	Selectivities of Aromatic Methyl Metalation. Unexpectedly Strong Interactions of Carbanions with Aromatic Rings. **1989**, 62, 79-82	0
1080	Molecular and Electronic Structures of Thieno[3,4-b]thiophene-2-carboxylic Acid and Acetic Thieno[3,4-b]thiophene-2-carboxylic Anhydride. An AM1, MNDO, and CNDO/S Study. **1989**, 62, 1262-1268	13
1079	Kinetic Study on Hydrogenation of Isoquinoline over Supported Ruthenium Catalysts. **1989**, 62, 3622-3627	3
1078	The Reactivities of Polyaromatic Hydrocarbons in Catalytic Hydrogenation over Supported Noble Metals. **1989**, 62, 3994-4001	22
1077	Electron Densities in Molecules CHX1X2 and Correlation with the Intensity of the 00 Band of the Secondary Transition. **1990**, 23, 223-232	4
1076	Energy and Charge Transfer in Clusters of Organic Molecules Following Resonant Electron Capture. **1990**, 94, 1334-1338	1
1075	An Experimental and Theoretical Study of Acid-Base Properties of Di-Pyridyl Ketones. **1990**, 168, 55-63	3
1074	GaAs Total Energy Tight Binding Hamiltonians for Use in Molecular Dynamics. **1990**, 193, 219	1
1073	Hydrogenation Pathway of Quinolines over Raney Nickel and Ru/C. **1990**, 63, 3167-3174	13
1072	Synthesis and Lactamase Inhibitory Activity of 3-Cyano-3-cephem Derivatives. **1990**, 63, 412-416	6

1071	Substituent Effects on15N and17O NMR Chemical Shifts in 4?-Substitutedtrans-NNO-Azoxybenzenes. **1990**, 63, 702-707	9
1070	AnAb InitioMolecular Orbital Study on the Ene Reaction of Methyl Acrylate with Propene. **1990**, 63, 2246-2251	9
1069	Synthesis and Conformational Properties of 2-Carboxy-15-crown-5 and Its Cation Complexes. **1990**, 63, 383-388	2
1068	Synthesis and Tautomerism of 1,5-Bis(alkylamino)-4H-benzo[a]phenothiazin-4-ones. **1990**, 63, 1467-1477	7
1067	Extremely Long CC Single Bonds in Stereomers of 6,7,12a,12b-Tetrahydrodipyrido[1,2-a:2?,1?-c]pyrazine. **1990**, 19, 493-496	0
1066	ESR Spectra of Transient Radical Cations of NADH Analogues. **1990**, 19, 1275-1278	1
1065	Structural Determination of 4-Vinylcyclohexene Oxide Using 2D INADEQUATE NMR Spectroscopy and MNDO Calculation. **1990**, 22, 719-723	1
1064	15. Effect of Silane Compounds on Catalyst Isospecificity-A Plausible Model Based on MO Calculation. **1990**, 56, 177-183	8
1063	Anionic Polymerization of 2,3,4,5,6-Pentafluorostyrene. **1990**, 22, 171-174	16
1062	Nanometre-sized diamonds are more stable than graphite. **1990**, 343, 244-245	292
1061	Structure of 5-hydroxyindole-3-acetic acid. **1990**, 46, 2426-2428	0
1060	High-pressure X-ray diffraction study on the structure and phase transition of 1,3-cyclohexanedione crystals. **1990**, 46, 246-256	76
1059	QSAR analysis of the acute fish toxicity of organic phosphorothionates using theoretically derived molecular descriptors. **1990**, 9, 417-428	84
1058	Graph-set analysis of hydrogen-bond patterns in organic crystals. **1990**, 46 (Pt 2), 256-62	2078
1057	Quantum-chemical investigation of tautomerism of hydrophosphoryl compounds. **1990**, 25, 450-454	
1056	Energy of formation and structures of monoaquacomplexes of anions: Results of calculations by the MNDO/M method. **1990**, 26, 59-62	
1055	Structures of some polyfluorinated allyl cations calculated by the MO LCAO SCF method in the MNDO approximation. **1990**, 39, 1435-1440	
1054	MNDO estimates of the heats of isomerization of 2,5-oxazolines. **1990**, 39, 1515-1516	

1053	Conformation of S-vinyl-N,N-diethyldithiocarbamate and C-H...S intramolecular interaction between atoms of olefinic hydrogen and sulfur of thiocarbonyl group according to1H and13C NMR data. **1990**, 39, 1796-1800	1
1052	Substitution of the halogen atoms in □halogenonitro compounds of the aliphatic series. 5. Use of the MNDO method to explain the behavior of the chlorine atom in the substitution reactions of chloronitroacetic acid derivatives. **1990**, 39, 1826-1831	
1051	Electron structure and reactivity of organofluorine compounds. 3. Mndo and ami calculations of the ground state of perfluoroalkyl chlorides, bromides, and iodides. **1990**, 39, 947-950	3
1050	Electrochemical reduction and structural properties of borylphosphinoethene derivatives. **1990**, 39, 17-20	3
1049	Substituent effects on the nature of hydrogen bonding in organic hydroperoxides and the structure of triphenylmethyl hydroperoxide. **1990**, 39, 57-62	
1048	An attempt to structurally convert mu-selective morphine toward delta-receptor binding: dimerization based on enkephalin conformation. **1990**, 188, 359-68	0
1047	On the choice of the perturbed state for pmo prediction of selectivities in cycloaddition reactions. **1990**, 208, 235-251	3
1046	Ab initio study of internal rotation in 2-pyridincarboxaldehyde. **1990**, 210, 291-298	5
1045	Theoretical studies of hydrogen-bonded complexes using semiempirical methods. **1990**, 210, 405-426	35
1044	Comparison of semiempirical and bsse corrected mˆ ller-plesset ab initio calculations on the direct addition of water to formaldehyde. **1990**, 210, 427-440	19
1043	MNDO and AM1 estimation of the electrostatic, induction and dispersion contributions to the solvation energy by a continuum model. **1990**, 210, 441-446	5
1042	Molecular modelling of glutathione: a comparison with crystallographic data. **1990**, 210, 467-475	7
1041	The molecular structure of hydrazine and melamine: rotational barriers and hybridisation. **1990**, 209, 303-312	14
1040	Theoretical model of the electrophilic substitution in pentagonal unsaturated heterocycles. **1990**, 209, 361-372	6
1039	Theoretical studies of aza analogues of platonic hydrocarbons. **1990**, 206, 67-75	32
1038	Ab initio calculations of potential barbiers for ionic conductivity of the □PbF2 compound. **1990**, 206, 99-107	1
1037	An efficient procedure for calculating the molecular gradient, using SCF-CI semiempirical wavefunctions with a limited number of configurations. **1990**, 206, 123-133	44
1036	Study of the configurational isomerism of polar groups present in histamine H2-receptor antagonists. **1990**, 207, 269-283	5

1035	NPT ensemble Monte-Carlo simulation of ethanol in water. **1990**, 209, 69-75		1
1034	Rotational potential energy functions in ethylchlorosilane,(chloromethyl)methylsilane, and (chloromethyl) chlorosilane: MM2, MNDO, and ab initio calculations. **1990**, 204, 79-100		13
1033	Theoretical investigation of lipid peroxidation mechanism. **1990**, 204, 379-388		
1032	The influence of proton transfer on the metalsubstrate interaction in the active sites of zinc dependent enzymes. **1990**, 205, 113-118		1
1031	Molecular-orbital study of the relative stability of protonated nucleic acid base pairs. **1990**, 205, 119-128		7
1030	MNDO study of the radical addition of hydrogen halides to ethylene and propene. **1990**, 205, 213-221		
1029	Is the ethylenedione radical anion linear or bent?. **1990**, 205, 279-285		3
1028	Calculation of thermochemical parameters for CHnX3□□F CHnX2□+X□n = 0,1 and 2, X = Cl and Br. MO study of solvent and counter-ion effects. **1990**, 205, 287-293		3
1027	Electrostatic proximity effects in gas-phase acidities and basicities: a comparison of theoretical methods (INDO, MNDO, AM1 and ab initio). **1990**, 205, 367-372		16
1026	Tautomerism of hydroxypyridazines. A semiempirical (AM1, MNDO, MINDO/3, CNDO/S-CI) and ab initio molecular orbital study. **1990**, 206, 295-307		16
1025	Reactivity of biologically important reduced pyridines. **1990**, 206, 315-334		17
1024	Semiempirical MNDO/H calculations of opiates. **1990**, 207, 1-14		11
1023	MNDO effective charge model study of conformations of zwitterionic and neutral forms of glycine, alanine and serine in the gas phase and in solution. **1990**, 207, 103-114		27
1022	MNDO and IR spectroscopic studies of tautomerism of isocytosine. *Journal of Molecular Structure*, **1990**, 216, 77-90	3.4	24
1021	The molecular and electronic structures of ions and radicals derived from tetramethyllead, hexamethyldilead, dimethyllead, and tetramethyldilead: an SCF-MO study. **1990**, 398, 241-249		5
1020	New organic non-linear optical crystals of benzylidene-aniline derivative. **1990**, 166, 353-357		42
1019	Helical Peierls distortion: Formation of helices of polyketone and polyisocyanide. **1990**, 169, 445-449		7
1018	The structures of the [M-H] anions of the CH3NO 2 isomers nitromethane and methyl nitrite. **1990**, 1, 295-300		9

1017	Crystal lattice energy of ammonium and methanaminium chlorides. **1990**, 36, 2009-2013		2
1016	Note on the preference of aliphatic epoxides for the N-7 position of guanine in DNA. **1990**, 64, 504-5		4
1015	Germanium-carbon versus germanium-nitrogen double-bond formation in the reactions between germylenes and diazo compounds. *Structural Chemistry*, **1990**, 1, 317-323	1.8	4
1014	MINDO/3- und MMP2-Berechnungen zur Energetik isomerer Kohlenwasserstoffe der Formel C7H8. **1990**, 332, 519-524		4
1013	MNDOC-CI calculations for organic photoreactions. I. The □cleavage reaction of carbonyl compounds. **1990**, 3, 81-88		24
1012	Theoretical studies on the gas-phase pyrolysis of acetic anhydride and diacetyl sulphide. **1990**, 3, 279-284		7
1011	[4]Paracyclophane: MNDO and STO-3G molecular structure and strain energy. **1990**, 3, 295-300		13
1010	AM1 studies on the acid hydrolysis of acetamide. **1990**, 3, 397-403		1
1009	Interpretation of 1H NMR spectra of 2-benzopyrylium salts with the use of the CNDO/2 method. **1990**, 3, 575-580		3
1008	Theoretical study of the gas-phase thermal isomerization of isoxazoles. Part I. Isoxazole. **1990**, 3, 611-619		8
1007	Comparison between some semi-empirical and ab initio Hartree□ock models for the description of amides (formamide revisited). **1990**, 3, 711-722		4
1006	Absolute hardness and aromaticity: MNDO study of benzenoid hydrocarbons. **1990**, 3, 784-788		35
1005	Reaction field effects on the electronic structure of carbon radical and ionic centers. **1990**, 37, 1-13		51
1004	Electrostatic potential mapping of polycyclic aromatic hydrocarbon diol epoxides using a dipole. **1990**, 38, 11-23		7
1003	MNDO calculation of reaction heats determininig the mechanism of antioxidant action of the phenols in polyolefins. **1990**, 38, 221-224		2
1002	MNDO CI study of the photoisomerization about polar double bonds. **1990**, 38, 231-238		4
1001	Sur une tentative d'unification des th□ ories quantiques de la canc□ risation par les polyac□ nes: I. Th□ orie des r□ gions M, L, et B. **1990**, 38, 461-486		8
1000	A study of hydration effects on the conformational aspects of gaba mediators. **1990**, 38, 533-549		2

999	Semiempirical calculation of the hyperpolarizabilities of polyenes. **1990**, 38, 791-798		31
998	The cycloaddition reaction of □oxo sulfines and 2-trimethylsilyloxy-1,3-butadienes. **1990**, 109, 190-196		5
997	Theory of Germanium-Related Defects in Vitreous Silicon Dioxide. I. Germanium Atom in Silicon Site. **1990**, 162, 173-181		4
996	The OASIS concept for predicting the biological activity of chemical compounds. **1990**, 4, 207-215		30
995	Investigation of conformations and electronic structure of diphenylamine and the diphenylaminyl radical by means of MNDO and INDO methods. **1990**, 31, 24-28		6
994	Investigation of fragments of potential-energy surfaces of molecular systems of the CH2Cl□CH2CHX type by the MNDO method. **1990**, 31, 149-152		
993	Vibrational spectra of (CF3)2CFNCO and (CF3)2CC1NCO. **1990**, 52, 550-554		
992	Reproduction and the energy cost of defense in a Batesian mimicry complex. **1990**, 84, 69-73		8
991	Intermediates in the reactions of electron-rich germylenes with an acyl azide: An MNDO-SCF-MO investigation. *Structural Chemistry*, **1990**, 1, 511-516	1.8	0
990	The use of crystal data together with other experimental and computational results to discuss structure-reactivity and activity relationships. *Structural Chemistry*, **1990**, 1, 597-616	1.8	18
989	Germanium-oxygen interactions in acyl-substituted germyleneazines L2GeNNC(COX)(COY). *Structural Chemistry*, **1990**, 1, 151-157	1.8	7
988	The electronic spectrum of o-benzyne. *Structural Chemistry*, **1990**, 1, 89-100	1.8	18
987	A practical procedure for the determination of electrostatic charges of large molecules. **1990**, 4, 411-26		41
986	MOPAC: a semiempirical molecular orbital program. **1990**, 4, 1-105		2256
985	Gasf^ □miges □H3PS2□□Erzeugung und Charakterisierung. **1990**, 580, 181-187		10
984	Quantum-chemical investigation of the factors which determine stability of the 3,5-dimethyl-1H-pyrazole-4-diazonium ion. **1990**, 26, 298-300		
983	1,3-Dipolar cycloaddition reactions of ylides formed from pyridines and dichlorocarbene. **1990**, 26, 304-311		5
982	Mass spectrometric study of ring-substituted secondary and tertiary □aminopiperidines. **1990**, 26, 326-332		

981	Synthesis of allyl dichlorophosphines and arsines, precursors of transient 1-phosphadiene and 1-arsadiene.. **1990**, 31, 1147-1150	9
980	Synthesis and structure elucidation of new spirocephams. **1990**, 31, 7141-7144	1
979	Palladium(0) catalyzed substitution reactions of cyclopropyl group containing allylic esters. **1990**, 31, 4593-4596	24
978	Vibration-induced intramolecular charge transfer in the ring opening of 2,3-diaryl-1-methylenecyclopropane radical cation. **1990**, 31, 5175-5178	5
977	Ethoxyacetylene and ethyl vinyl ether, dipolarophiles of opposite regiochemistry in diazomethane cycloadditions. **1990**, 46, 783-792	20
976	Development of a molecular mechanics (MM2) force field for chlorosilanes. **1990**, 46, 8005-8018	9
975	Intramolecular diels-alder reactions of pyrazines with alkynylphenyl moieties as side-chain dienophiles. **1990**, 46, 3641-3650	17
974	Reactivity of biologically important reduced pyridines VI. Lack of through-resonance stabilization in the ferricyanide-mediated oxidation of substituted 1-Phenyl-1,4-Dihydronicotinamides. **1990**, 46, 319-324	9
973	Intermolecular potentials of EDA complexes by semi-empirical theory dispersion energy terms in the PM3 method. **1990**, 46, 423-432	5
972	5-Methylene-2(5H)-furanone in Diels-Alder reactions with cyclic dienes: endo/exo selectivity. **1990**, 46, 4371-4378	11
971	Generation of specifically substituted pyridines and pyridones from 2(1h) pyrazinones and acetylenes : A FMO description. **1990**, 46, 5715-5732	31
970	Theoretical studies of fluorocarbons. Part I. Small perfluoroalkane molecules. **1990**, 46, 317-337	12
969	Theoretical studies of fluorocarbons. Part II. Fluorine and chlorine substituted alkanes. **1990**, 47, 489-507	10
968	Effects of fluorination on conformation and bonding in diphenyl sulphides. **1990**, 48, 45-62	
967	MNDO MO theoretical study of electronic structure and homolytic dissociation of perfluoroalkanoyl peroxides. **1990**, 50, 393-410	12
966	Semiempirical studies on the structure and bonding of fluorosulfuranes and aminofluorosulfuranes. **1990**, 50, 427-432	
965	The Structure of Cyclic C6S6 and C6O6. **1990**, 29, 1410-1412	25
964	Die Struktur von cyclischem C6S6 und C6O6. **1990**, 102, 1516-1517	12

963	Interaction between Oxygen Lone-Pair Orbitals of Ether and π-Unsaturated Ketone Functions in 3,5,6-Trimethylidene-7-oxabicyclo[2.2.1]heptan-2-one and 3,6-Dimethylidene-7-oxabicyclo[2.2.1]heptane-2,5-dione: A PE-Spectroscopic Investigation. **1990**, 73, 1-12	7
962	Synthesis and Chemical Transformations of 4, 5-Homosnoutene Derivatives: An Attempted New Access onto the (CH)12 Energy Hypersurface. **1990**, 73, 1182-1196	3
961	The Solid-State and Solution Conformations of (+)-Chelidonine. **1990**, 73, 2171-2178	7
960	Hydrocarbon acidities calculated with MINDO/3, MNDO, and AM1. **1990**, 11, 94-104	13
959	Semiempirical AM1 electrostatic potentials and AM1 electrostatic potential derived charges: A comparison with ab initio values. **1990**, 11, 159-169	146
958	Theoretical study of the proton affinities of 2-, 3-, and 4-monosubstituted phenolate ions in the gas phase by means of MINDO/3, MNDO, and AM1. **1990**, 11, 269-290	16
957	Comparative study of the molecular electrostatic potential obtained from different wavefunctions. Reliability of the semiempirical MNDO wavefunction. **1990**, 11, 416-430	97
956	Atomic charges derived from semiempirical methods. **1990**, 11, 431-439	2668
955	Comments on a comparison of AM1 with the recently developed PM3 method. **1990**, 11, 541-542	57
954	A combined quantum mechanical and molecular mechanical potential for molecular dynamics simulations. **1990**, 11, 700-733	2017
953	Mechanistic aspects of biological redox reactions involving NADH 2: A combined semiempirical and ab initio study of hydride-ion transfer between the NADH analogue, 1-methyl-dihydronicotinamide, and folate and dihydrofolate analogue substrates of dihydrofolate reductase. **1990**, 11, 791-804	27
952	On the use of AM1 and MNDO wave functions to compute accurate electrostatic charges. **1990**, 11, 909-923	111
951	Partial charges by multipole constraint. Application to the amino acids. **1990**, 11, 978-993	16
950	Free energy perturbation calculations on models of active sites: Applications to adenosine deaminase inhibitors. **1990**, 11, 994-1002	8
949	Correlation of the acidity of substituted phenols, anilines, and benzoic acids calculated by MNDO, AM1, and PM3 with Hammett-type substituent constants. **1990**, 11, 1009-1016	29
948	The application of molecular similarity calculations. **1990**, 11, 1139-1146	121
947	Kinetics and mechanism of the reaction of Ozone with Aliphatic alcohols. **1990**, 22, 321-329	16
946	Cycloadditionen, 18. 5-Aminoisoxazole durch Cycloaddition von Nitriloxiden an Inamine. **1990**, 1990, 403-407	10

945	Quantum chemical study of the electronic and conformational characteristics of adenosine and 8-substituted derivatives: functional implications in the mechanism of reaction of adenosine deaminase. **1990**, 79, 133-7	8
944	29Si and 13C NMR spectra of 4-substituted 2-methoxytrimethylsiloxybenzenes. Factors determining the chemical shifts in models of lignin constituents. **1990**, 28, 973-978	1
943	Konformationsanalyse am Beispiel des N-Benzylpyridinium-bromids: Vergleich von kristallstrukturanalytischen Daten mit den Ergebnissen von semiempirischen Berechnungen (MINDO/3, MNDO, AM1 und PM3). **1990**, 123, 321-325	14
942	Die Borierung von Lactamen und Harnstoffen mit einem Amino-imino-boran. **1990**, 123, 455-458	6
941	Wasserstoffˆ Übertragungen, 15 Zum Ablauf der Dehydrierung von Dihydroarenen durch Chinone. **1990**, 123, 627-633	5
940	Starke P ,P-Wechselwirkungen in Tetraphosphacubanen, PE-spektroskopische Untersuchungen. **1990**, 123, 757-760	24
939	Gas-Phase Thermolysis of 4-Substituted 3,5-Dihydro-3,3,5,5-tetramethyl-4H- pyrazoles Studied by Photoelectron Spectroscopy and Flash Vacuum Pyrolysis. **1990**, 123, 1161-1168	18
938	N-[(2-Naphthyloxy)methyl] benzazoles: Synthesis and Investigation by X-ray Analysis and by Semiempirical MO Calculations. **1990**, 123, 1185-1191	5
937	1-Oxa-3-cyclooctin. **1990**, 123, 1411-1414	10
936	Chirale Homoenolat-Äquivalente, IV. Kristallstruktur einer chiralen 1-Aminoallyllithium-Verbindung: dimeres, intramolekular chelatisiertes (3S)-3-Lithio-1-[(S)-2-(methoxymethyl)pyrrolidino]-1,3-diphenylpropen. **1990**, 123, 1853-1858	29
935	Wittig-Synthese und Röntgen-Struktur eines 26-gliedrigen, zwei Bipyridin-Einheiten enthaltenden Makrocyclus. **1990**, 123, 2181-2185	16
934	Acetylierung von N-(Trimethylsilyl)keteniminen: N-Acylketenimine und β-Cyanketone. **1990**, 123, 2339-2347	21
933	Wasserstoffˆ Übertragungen, 16. Freie 1-Phenylallyl-Kationen bei der Aromatisierung von Dihydronaphthalinen mit Triphenylmethyl-tetrafluoroborat. **1990**, 123, 2373-2380	8
932	The characterization of the Hg|H3PO4 interface from studies of adsorption of dimethylsulfoxide. **1990**, 35, 1901-1906	2
931	A study of the structure-mesomorphism relationship in some polymers and low-molecular-weight model compounds. **1990**, 26, 1259-1265	2
930	Strong Mills-Nixon effect in biphenylene. **1990**, 171, 49-52	24
929	An estimation of energy parameters for the soliton movement in hydrogen-bonded chains. **1990**, 171, 217-221	18
928	The electronic structure of cis- and trans-decalin radical cations in halocarbon matrices: an ESR and MNDO study. **1990**, 174, 95-102	21

927	Atomic charges derived from semiempirical electrostatic potentials; an interaction energy method. **1990**, 174, 355-360		26
926	On the stability of doped conducting polymers: electrostatic contributions and sterical effects. **1990**, 175, 125-129		13
925	Reliability of the AM1 wavefunction to compute molecular electrostatic potentials. **1990**, 168, 269-275		43
924	The HeI PE spectrum and electronic structure of nitroethene. **1990**, 170, 113-116		7
923	Simulated annealing, classical molecule dynamics and the Hartree□Fock method: the NDDO approximation. **1990**, 172, 83-88		22
922	Model mechanisms for the thermal cis□trans isomerization of cyanines. **1990**, 172, 187-192		15
921	Electronic spectra of benzil in solution and thin film. **1990**, 51, 245-258		4
920	Classical dynamics of the O(3P)+CS(X1□)-□CO(X1□)+S(3P) reaction on the ground triplet potential energy surface. **1990**, 141, 401-415		18
919	The structure of trans- and cis-3-hexene radical cations stabilised in halocarbon matrices at low temperature: An ESR and MNDO/AM1 study. **1990**, 141, 417-430		24
918	Interpreting the visible absorption bands of 1,4-(dihydroxy)-9,10-anthraquinone and its metal chelates. **1990**, 36, 187-99		7
917	Electron capture induced processes in molecules and molecular aggregates. **1990**, 100, 753-784		13
916	Low-energy satellite lines in photoelectron spectra-how low is it possible?. **1990**, 51, 173-181		3
915	Aromaticity as a quantitative concept part V: A comparison of semi-empirical methods for the calculation of molecular geometries of heteroaromatic compounds and application of the AM1 and MNDO methods to the calculation of Bird's aromaticity indices. **1990**, 3, 247-269		10
914	An alternative method for the alignment of molecular structures: Maximizing electrostatic and steric overlap. **1990**, 3, 615-633		262
913	Absorption and emission properties of the six isomeric di-pyridyl-ketones. **1990**, 46, 425-427		7
912	Study of the conformations of stiff chain, rigid-rod and substituted rigid-rod polymers. **1990**, 31, 1637-1648		15
911	Two-dimensional n.m.r. characterization of cycloaliphatic epoxy resins. **1990**, 31, 2425-2430		10
910	Carbenes in matrices: reactions and rearrangements. *Journal of Molecular Structure*, **1990**, 222, 21-31	3.4	17

909	Internal Rotation and vibrational properties of polyfuran oligomers. *Journal of Molecular Structure*, **1990**, 219, 397-402	3.4	8
908	Electronic spectra of adenine: interaction with dissolved oxygen in solution, oscillation and intensification of n-π transition. *Journal of Molecular Structure*, **1990**, 220, 25-41	3.4	12
907	Surface intermediates in the transformation of allyl alcohol over zeolites. *Journal of Molecular Structure*, **1990**, 239, 185-192	3.4	3
906	Monte Carlo study of lactone formation kinetics. *Journal of Molecular Structure*, **1990**, 239, 193-203	3.4	2
905	Influence of the conjugation effect on the UV-spectra of 4-substituted pyridine N-oxides and their conjugated acids. *Journal of Molecular Structure*, **1990**, 218, 129-134	3.4	6
904	Investigation of a transition metal-assisted retro Diels-Alder reaction used in the synthesis of transition metal S2O complexes. **1990**, 384, 105-114		20
903	Theoretical study of the acidic strength of amino acid side chains. **1990**, 18, 361-372		2
902	Oligosaccharide conformations: Application of NMR and energy calculations. **1990**, 22, 55-81		90
901	Relation between effective conjugation, vibrational force constants and electronic properties in polyconjugated materials. **1990**, 74, 199-202		28
900	Thermal properties, crystal lattice energy, mechanism and energetics of the thermal decomposition of hydrochlorides of 2-amino acid esters. **1990**, 171, 253-277		3
899	The microcomputer OASIS system for predicting the biological activity of chemical compounds. **1990**, 14, 193-200		46
898	Characterization of TSSS paint coatings for solar collectors by FTIR spectroscopy. **1990**, 20, 435-454		14
897	Reactions in monolayers: The oxidation of thiols to disulfides. **1990**, 49, 281-287		8
896	TRANSITION-METAL COMPLEXES OF N2, CO2, AND SIMILAR SMALL MOLECULES. AB-initio MO STUDIES OF THEIR STEREOCHEMISTRY AND COORDINATE BONDING NATURE. **1990**, 95-177		4
895	Mutual Orientation of Oxygen and Hydrocarbon Molecules as Factor Determining The Reaction Pathway. **1990**, 55, 701-706		
894	A semi-empirical effective Hamiltonian study of electronic structures of molecular clusters and crystals based on geometry optimization. **1990**, 2, 9989-10001		
893	Antiproton storage materials: Response of neon, argon, and benzene to a negative particle. **1990**, 41, 2315-2321		1
892	Theoretical evaluation of Young's moduli of polymers. **1990**, 41, 11368-11378		8

891	Dependence of Young's modulus of trans-polyacetylene upon charge transfer. **1990**, 64, 3031-3034	13
890	Ab initio study of the infrared spectra of linear Cn clusters (n=6). **1990**, 93, 8850-8861	89
889	Spectroscopy and rotational dynamics of oxazine 725 in alcohols: A test of dielectric friction theories. **1990**, 92, 2891-2896	62
888	Using Theoretical Descriptors Tn St13ucture Activity Relationships: Acetylcholtnesterase Inhibition.	
887	Semiempirical electronic-structure calculations of the hydrogen-phosphorus pair in silicon. **1990**, 41, 7581-7586	33
886	Molecular modeling of reduction reactions of dicyandiamide on zinc: a theoretical study of epoxy adhesive/galvanized steel adhesion. **1990**, 4, 443-452	15
885	Chromium Interactions in CCA/CCB Wood Preservatives. Part I. Interactions with Wood Carbohydrates. **1990**, 44, 373-380	28
884	Theoretical Calculation of Nonlinear Optical Susceptibilities. **1990**, 182, 17-31	3
883	SYNTHESIS AND PROPERTIES OF COMPOUNDS RELATED TO 1-t-BUTYLACETYLENE-2-PHOSPHONIC ACID AND 1-t-BUTYLETHANE-1,2,2-TRIPHOSPHONIC ACID. STERICALLY OVERCROWDED PHOSPHORUS COMPOUNDS, PART I:. **1990**, 48, 131-140	12
882	Estimation of Δf of nitro derivatives of benzene and toluene using AM1 and DSC. **1990**, 8, 85-98	20
881	Conformational Studies on Mesogenic Monomers and Dimers. **1990**, 192, 155-160	
880	A quantitative molecular-orbital study of the structures and vibrational spectra of the hydrogen-bonded complexes H2O NH3, H2CO NH3 and (H2O)n, n= 2. **1990**, 943-951	37
879	A theoretical approach to the vibrational analysis of the nitroenamine system. **1990**, 1627-1636	5
878	Prediction of initial reduction potentials of compounds related to anthracyclines and implications for estimating cardiotoxicity. **1990**, 3, 244-7	17
877	Chain flexibility in polyheteroaromatic polymers part I. Electronic properties, structure and vibrational spectra of oligomers as models of polypyrrole and polythiophene. **1990**, 38, 299-312	49
876	Nitrated phenols in fog. **1990**, 24, 3067-3071	42
875	The structural basis for the mutagenicity of aristolochic acid. **1990**, 55, 7-11	20
874	Reactivity of diazoazoles with electron-rich double bonds. **1990**, 1943-1950	11

873	Lattice dynamics and vibrational spectra of pristine and doped polypyrrole: Effective conjugation coordinate. **1990**, 92, 3892-3898	221
872	Lattice dynamics and vibrational spectra of polypyrrole. **1990**, 92, 3886-3891	244
871	Calculation of properties of ionic water clusters by the MNDO method. **1990**, 24, 1397-1399	5
870	Reduction of nitrated phenols: A method to predict half-wave-potentials of nitrated phenols with molecular modeling. **1990**, 20, 717-728	2
869	Structure and Properties of N-Substituted Polyisoindoles. **1990**, 190, 9-18	2
868	Ground- and excited-state dipole moments of some nitroaromatics: Evidence for extensive charge transfer in twisted nitrobenzene systems. **1990**, 93, 7085-7093	38
867	Molecular orbital studies of molecular exciplexes. Part 1: AM1 and PM3 calculations of the ammonia□xygen complex and its solvation by water. **1990**, 877-883	19
866	MNDO study on infrared spectra of silicates. **1990**, 122, 276-284	14
865	Biochemical and behavioral responses of pilocarpine at muscarinic receptor subtypes in the CNS. Comparison with receptor binding and low-energy conformations. **1990**, 533, 232-8	23
864	Modulation of the affinity of aspartic proteases by the mutated residues in active site models. **1990**, 261, 241-4	12
863	Prominent stacking interaction with aromatic amino acid by N-quarternization of nucleic acid base: X-ray crystallographic characteristics and biological implications. **1990**, 278, 217-27	16
862	Prediction of nucleoside-carcinogen reactivity. Alkylation of adenine, cytosine, guanine, and thymine and their deoxynucleosides by alkanediazonium ions. **1990**, 3, 219-30	49
861	Weak bonds and atomic charge distribution in hydrogenated amorphous silicon. **1991**, 137-138, 295-298	4
860	Adatom-based (2 ˆ □2n) reconstruction on Ge(111). **1991**, 241, 135-145	6
859	The influence of inter-atomic transitions in Auger valence band spectroscopy: oxygen on Si(001)2 ˆ □ 1. **1991**, 258, 197-209	14
858	Quantum chemical study for genotoxic and antitumor activities of hydroxyanthraquinones. **1991**, 13, 185-94	8
857	Conformational and vibrational properties of poly (3-methylthiophene). **1991**, 43, 3501-3504	
856	Conformational preferences and energetics of N□ heterolyses in aryl nitrenium ion precursors: ab initio and semiempirical molecular orbital calculations. **1991**, 607-616	12

855	Interaction of indole derivatives with biologically important aromatic compounds. Part 22. Importance of simultaneous co-operation of hydrogen-bond pairing and stacking interactions for recognition of guanine base by a peptide: X-ray crystal analysis of 7-methylguanosine-5?-phosphate□ryptophanylglutamic acid complex. **1991**, 1847-1853	19
854	Coulombic energy in bromide salts of mononitrogen organic bases. **1991**, 87, 1333-1337	9
853	Conformational analysis. Part 17. An NMR and theoretical investigation of the conformation of bicyclo[5.2.1]decane-2,6-dione. **1991**, 1471-1475	2
852	Application of Bravais-Friedel-Donnay-Harker, attachment energy and Ising models to predicting and understanding the morphology of molecular crystals. **1991**, 24, 89-99	303
851	Electronic structure of conducting polymers with nonconjugated backbones: 1,4-polybutadiene and 1,4-polyisoprene. **1991**, 24, 3723-3724	8
850	Influence of ring-torsion dimerization on the band gap of aromatic conjugated polymers. **1991**, 44, 6002-6010	74
849	Response of the headgroup of phosphatidylglycerol to membrane surface charge as studied by deuterium and phosphorus-31 nuclear magnetic resonance. **1991**, 30, 10558-66	32
848	PAF-receptor. III. Conformational and electronic properties of PAF-like agonists and antagonists. **1991**, 1085, 91-105	10
847	Study of stress and birefringence relaxation of new amorphous polyarylates. **1991**, 131-133, 781-792	5
846	Predictive QSAR models estimating ecotoxic hazard of phenylureas: Mammalian toxicity. **1991**, 22, 613-623	7
845	Predictive QSAR models for estimating biodegradation of aromatic compounds. **1991**, 109-110, 253-9	14
844	Electronic properties of the base and protonated forms of polypyrrylenemethine, a small bandgap conjugated polymer. **1991**, 43, 3555-3558	10
843	Superconductivity in the fullerenes. **1991**, 254, 989-92	487
842	Effect of steric hindrance and □electrons on alcohol self-association. **1991**, 87, 1745-1750	24
841	New methods for electronic structure calculations on large molecules. **1991**, 42, 341-67	101
840	A class of narrow-band high-spin organic polymers I. Polymers with direct exchange interaction between orthogonal □orbitals. **1991**, 40, 127-135	24
839	A QUANTUM CHEMICAL REACTION DESIGN OF A PLASMA CHEMICAL REACTION OF VINYLSILANE. **1991**, 499-502	
838	Chapter 14 Computational Studies of Hydrogen-Containing Complexes in Semiconductors. **1991**, 511-546	7

837	Fluorescent Dyes as Probes of Voltage Transients in Neuron Membranes Progress Report. **1991**, 95, 1333-134557	
836	Demonstrating the Utility of Boron Based Precursor Molecules for Selective Area DepositIon in a Scanning Tunnelling Microscope. **1991**, 236, 153	
835	Theoretical Studies of Defects, Impurities, and Complexes in Semiconductors. **1991**, 240, 643	6
834	Hierarchy in Extended Chain Polymers 1. **1991**, 255, 119	0
833	Conformational Change of Benzoquinone Crown Ether Radical Anions Induced by Complexation with Alkali Metal Cation: An ESR Study. **1991**, 64, 3245-3250	9
832	1 : 1 Adduct Ion Formation of Permethylated Monosaccharides with Organic Cations in FAB Mass Spectrometry. **1991**, 64, 1243-1252	16
831	Solvent Effect on the ESR Parameters of Di-t-butyl Nitroxide and Galvinoxyl. Theoretical Application of the MNDO Effective Charge Model. **1991**, 64, 3511-3514	2
830	Structural Effects on Photochemical Intermolecular Cycloaddition of Phenanthrenecarboxylic Lactones. Dual Collapse Processes of an Exciplex Leading to Cycloadducts. **1991**, 20, 1683-1686	1
829	Unusual Bonding in the Isomers of 6,7,13a,13b-Tetrahydro-6H-dipyrido[l,2-a:2?,1?-c][1,4]diazepine. **1991**, 20, 705-708	1
828	Diels alder reactions of P-chloro (bistrimethylsilyl) methylene phosphine. **1991**, 47, 71-82	8
827	Ab initio and semiempirical molecular orbital studies of alpha and beta lithiated vinyl ethers. **1991**, 32, 6069-6072	3
826	The electrostatic energy in iodide salts of mono-nitrogen organic bases. **1991**, 176, 183-196	10
825	The secondary □deuterium isotope effect in dark adaptation of bacteriorhodopsin containing retinal-20,20,20-d3. **1991**, 19, 18-28	4
824	Computational studies on isomerization of imine from penicillin and electron transfer by carboxyiminium derived from □lactams. **1991**, 19, 314-326	10
823	Geometry optimization within a modified extended Hˆ □kel formalism: Modifications to the ASED program. **1991**, 15, 157-160	6
822	Growth of bulk single crystals of organic materials for nonlinear optical devices: An overview. **1991**, 22, 19-51	71
821	Semi-empirical studies of torsional potentials in halonitrosomethanes. **1991**, 47, 1661-1671	2
820	Electronic spectra of 2-aminopurine and 2,6-diaminopurine: phototautomerism and fluorescence reabsorption. **1991**, 47, 1685-1693	35

819	Role of hydrogen atoms in anodized porous silicon. **1991**, 170, 535-539		29
818	Photo-oxygenative polymerization of guanine: the formation of a new material. **1991**, 61, 281-284		7
817	Quantum chemical study of oxidation of unsaturated fragments of butene. **1991**, 66, 373-384		5
816	Oxidation of hydrocarbons on transition metal oxide catalysts quantum chemical studies. **1991**, 70, 277-333		41
815	Theoretical infrared spectra of large carbon clusters. **1991**, 151, 309-321		61
814	Resonant two-photon ionization of phenol in methylene chloride doped solid argon using 248 nm KrF laser and 254 nm Hg lamp radiation, a comparative study. The UV/VIS absorption spectrum of phenol radical cation. **1991**, 153, 511-517		24
813	Isomerization and unimolecular rearrangement channels of dithioformic acid. **1991**, 154, 221-225		5
812	On the disordered distribution of defects in transpolyacetylene. **1991**, 155, 1-5		9
811	A quantum chemical study on the alternative mechanisms of the thermal cis-trans isomerization of streptocyanines. **1991**, 153, 63-71		5
810	Electronic structure of nitroxyl radicals determined by means of photoelectron spectroscopy. **1991**, 56, 73-84		14
809	Birefringence and electric dipole moment relationship with temperature, weak magnetic field and molecular geometry of 6CB and 7CB.. *Journal of Molecular Liquids*, **1991**, 50, 107-114	6	3
808	Structure-activity studies of morphine fragments. II. Synthesis, opiate receptor binding, analgetic activity and conformational studies of 2-R-2(hydroxybenzyl)piperidines. **1991**, 26, 763-773		3
807	Structure-activity studies of morphine fragments. III. Synthesis, opiate receptor binding, analgetic activity and conformational studies of spiro-[tetralin-1,4?-piperidines]. **1991**, 26, 775-785		4
806	Pyranocoumarins as potential photochemotherapeutic agents: theoretical and physico-chemical studies on the mechanism of action. **1991**, 26, 875-887		7
805	DARC/PELCO and OASIS methods I. Methodological comparison. Modeling purine pKa and antitumor activity. **1991**, 26, 575-592		14
804	Conformational analysis of and lactam antibiotics. **1991**, 26, 43-50		22
803	Structure-resonance calculation of the ionization potential of saturated hydrocarbons. *Journal of Molecular Structure*, **1991**, 246, 289-300	3.4	1
802	On the correlation between ionization potentials and bond angles in heterocyclic compounds. *Journal of Molecular Structure*, **1991**, 249, 305-312	3.4	6

801	Conformational analysis of symmetric carbonic acid esters by quantum chemical calculations and dielectric measurements. *Journal of Molecular Structure*, **1991**, 249, 327-341	3.4	13
800	73Ge, 13C and 1H NMR spectra of methylethynylgermanes. **1991**, 410, 287-291		7
799	Polycarbonate-poly(methyl methacrylate) blends: the role of molecular interactions on miscibility and antiplasticization. **1991**, 32, 1155-1159		44
798	Co-ordination, isomerisation and disruption of the ligands Ph2PO2C(CH2)nCHCH2(n= 0 or 1). X-Ray crystal and molecular structure of chloro(tetraphenyldiphosphoxane-P,P?)(triphenylphosphine)rhodium(I)tetrahydrofuran (1/1). **1991**, 1765-1772		21
797	Ames assay mutagenicity and electronic structure calculations of bromomethylfluoranthenes, chloromethylfluoranthenes, and hydroxymethylfluoranthenes. **1991**, 77, 291-302		
796	Theoretical investigation of mechanism of antioxidant action of sterically hindered phenols. **1991**, 27, 152-156		3
795	Molecular models of aluminum hydroxide. **1991**, 27, 411-413		
794	Effect of essential oils, such as raspberry ketone and its derivatives, on antiandrogenic activity based on in vitro reporter gene assay. **2010**, 20, 2111-4		24
793	Evaluation of Density Functionals, SCC-DFTB, Neglect of Diatomic Differential Overlap (NDDO) Models and Molecular Mechanics Methods for Prolyl-Leucyl-Glycinamide (PLG) and Structural Derivatives. **2010**, 944, 76-82		1
792	Theoretical studies on the pKa values of perfluoroalkyl carboxylic acids. **2010**, 949, 60-69		69
791	New parameterization of the PM3 method for monosaccharides. **2010**, 500, 140-143		5
790	T-cell epitope prediction and immune complex simulation using molecular dynamics: state of the art and persisting challenges. **2010**, 6 Suppl 2, S4		22
789	MNDO- und MINDO/3-Berechnungen zum sekundär Isotopieeffekt. **2010**, 19, 235-236		3
788	MINDO/3- und MNDO-Berechnungen von Isotopenaustauschgleichgewichten. **2010**, 20, 426-426		1
787	Ab-initio-SCF- und FSGO-Potentialenergieberechnungen mit fixierter Geometrie. **2010**, 21, 339-340		
786	Theoretische Berechnung der Temperaturabhängigkeit primärer Zerfallsgleichgewichte des Harnstoffs in der Gasphase. **2010**, 24, 417-418		
785	MNDO-Studie zur Struktur und zum Schwingungsspektrum von SiO, Si2O2 und Si3O3. **2010**, 25, 257-259		1
784	Elektronische Eigenschaften und Struktur von Phenylisothiocyanaten und Benzoylisothiocyanaten; Applikation der MNDO-Methode. **2010**, 26, 401-402		

783	Harmonische Kraftkonstapten fˆ Si(OH)4- und Al(OH)4--Modelle primˆ er Bildungseinheiten in Zeolithgittern. **2010**, 30, 141-142	2
782	Stability of Non-isothermally Treated Double-Base Propellants Containing Different Stabilizers in Comparison with Molecular Orbital Calculations. **2010**, 35, 468-476	11
781	Dynamics of DNA. A quantumchemical study. **2010**, 102, 148-154	5
780	Molecular aspects of methylated adenine in DNA. A quantum-chemical study. **2010**, 103, 123-130	1
779	Linear versus bent transition-state structures in hydride-transfer processes mediated by NAD(P)H model systems; a theoretical investigation. **2010**, 103, 143-144	14
778	Synthesis and conformational analysis of halo[n.3.1]propellanes. **2010**, 104, 184-190	8
777	Spectroscopic characterization of 1-methylene-2-vinylcyclopropane and some of its derivatives. **2010**, 106, 48-53	3
776	An experimental and theoretical study of the dimetallation of vinylacetylene. **2010**, 107, 286-295	6
775	Conformational analysis of three simple organosilicon compounds. **2010**, 108, 230-234	5
774	The role of axial chirality in schiff bases of pyridoxal phosphate and amino acids in the mechanism of racemase enzymes. A quantum-chemical study. **2010**, 108, 413-417	1
773	Photochemical behaviour of cyclic s-cis oxo oxime ethers. Ab-initio investigation on ethanedial monooxime as model compound. **2010**, 109, 502-508	9
772	Photochemistry and spectroscopy of three oxo oxime ethers: 4-(methoxyimino)-2,2,3,3-tetramethylcyclobutanone, 3,3,5-trimethyl-4(5H)-isoxazolone and 6-(benzyloxyimino)-2,2,5,5-tetramethylcyclohexanone. **2010**, 110, 31-40	5
771	A convenient synthesis of aziridine-2-carboxylic esters. **2010**, 111, 1-15	57
770	Photochemistry of bis(methoxyimino)alkanes. **2010**, 111, 79-87	0
769	Conformational analysis of 1-arylpiperazines and 4-arylpiperidines. **2010**, 112, 151-160	15
768	Theoretical Studies of Substitutionally Doped Single-Walled Nanotubes. **2010**, 2010, 1-42	10
767	Quantum-Chemical Descriptors in QSAR/QSPR Modeling: Achievements, Perspectives and Trends. **2010**, 693-721	2
766	Thermodynamic Investigation of Enol<-Keto Tautomerism for Alcohol Sensors Based on Carbon Nanotubes as Chemical Sensors. **2010**, 18, 45-55	11

765	Thermodynamic and Electronic Investigation About Remove of MTBE from Environment by Single-Walled Carbon Nanotube (SWNT). **2010**, 114, 7-16		3
764	Compactness aromaticity of atoms in molecules. *International Journal of Molecular Sciences*, **2010**, 11, 1269-310	6.3	20
763	Molecular Modeling of Matter: Impact and Prospects in Engineering. **2010**, 49, 3026-3046		86
762	Implementing Quantum Mechanics into Molecular Mechanics□combined QM/MM Modeling Methods. **2010**, 1-15		9
761	N-Hydroxylamines for Peptide Synthesis. **2010**,		1
760	Accuracy of computational solvation free energies for neutral and ionic compounds: Dependence on level of theory and solvent model. **2010**,		10
759	On the Interfragment Exchange in the X-Pol Method. *Journal of Chemical Theory and Computation*, **2010**, 6, 2469-2476	6.4	24
758	Approximate Multiconfigurational Treatment of Spin-Coupled Metal Complexes. *Journal of Chemical Theory and Computation*, **2010**, 6, 1981-9	6.4	6
757	Handbook of Heterocyclic Chemistry - Pages 917-970. **2010**, 917-970		
756	Polarization propagators: A powerful theoretical tool for a deeper understanding of NMR spectroscopic parameters. **2010**, 29, 1-64		68
755	Stabilization and structure calculations for noncovalent interactions in extended molecular systems based on wave function and density functional theories. **2010**, 110, 5023-63		666
754	The role of structural chemistry in the inhibitive performance of some aminopyrimidines on the corrosion of steel. **2010**, 52, 2387-2396		137
753	A theoretical study of some hydroxamic acids as corrosion inhibitors for carbon steel. **2010**, 52, 3304-3308		42
752	A time-dependent semiempirical approach to determining excited states. **2010**, 132, 234106		18
751	Empirically corrected DFT and semi-empirical methods for non-bonding interactions. **2010**, 12, 307-22		71
750	Advances in quantum and molecular mechanical (QM/MM) simulations for organic and enzymatic reactions. **2010**, 43, 142-51		201
749	Benchmark of Electronically Excited States for Semiempirical Methods: MNDO, AM1, PM3, OM1, OM2, OM3, INDO/S, and INDO/S2. *Journal of Chemical Theory and Computation*, **2010**, 6, 1546-64	6.4	155
748	Theoretical study of phosphodiester hydrolysis in nucleotide pyrophosphatase/phosphodiesterase. Environmental effects on the reaction mechanism. *Journal of the American Chemical Society*, **2010**, 132, 6955-63	16.4	47

747	Electronic structure and the glass transition in pnictide and chalcogenide semiconductor alloys. I. The formation of the pp□hetwork. **2010**, 133, 234503		20
746	Investigations of enzyme-catalysed reactions with combined quantum mechanics/molecular mechanics (QM/MM) methods. **2010**, 29, 65-133		89
745	A DFT periodic study on the interaction between O2 and cation exchanged chabazite MCHA (M = H+, Na+ or Cu+): effects in the triplet-singlet energy gap. **2010**, 12, 442-52		16
744	Long Pitch Orthoconic Antiferroelectric Binary Mixture for Display Applications. **2010**, 525, 140-152		33
743	Accounting for non-optimal interactions in molecular recognition: a study of ion-□complexes using a QM/MM model with a dipole-polarisable MM region. **2011**, 13, 19401-8		5
742	A Dielectric Effect on Normal Mode Analysis and Symmetry of BNNT Nanotube. **2011**, 19, 182-196		4
741	Polarized Molecular Orbital Model Chemistry. II. The PMO Method. *Journal of Chemical Theory and Computation*, **2011**, 7, 857-867	6.4	24
740	Further evaluation of quantum chemical methods for the prediction of non-specific binding of positron emission tomography tracers. **2011**, 13, 21552-7		7
739	Chemical Preparation, Thermal Behavior, Kinetic, and IR Studies of MnK4(P3O9)2.2H2O, Crystallographic Data of a New Cyclotriphosphate MnK4(P3O9)2, and Quantum Chemical Calculations for the P3O3□9 Ion. **2011**, 186, 1501-1514		2
738	Performance assessment of semiempirical molecular orbital methods in describing halogen bonding: quantum mechanical and quantum mechanical/molecular mechanical-molecular dynamics study. **2011**, 51, 2549-59		31
737	The calculation of intermolecular interaction energies. **2011**, 107, 148		24
736	Time-Dependent Density Functional Tight Binding: New Formulation and Benchmark of Excited States. *Journal of Chemical Theory and Computation*, **2011**, 7, 3304-13	6.4	85
735	Theoretical prediction of drug-receptor interactions. **2011**, 26, 91-104		4
734	Importance of physicochemical properties for the design of new pesticides. **2011**, 59, 2909-17		35
733	A new parametrizable model of molecular electronic structure. **2011**, 135, 134120		40
732	Thermodynamic study of alcohol on SnO2 (100)-based gas nano-sensor. **2011**, 49, 626-638		4
731	INVESTIGATION OF POLYCHLORINATED BIPHENYLS (PCBs) REMOVAL BY SIGNAL WALLED CARBON NANOTUBES: STUDIES. **2011**, 10, 651-657		4
730	Controlling bandgap energy and multivibronic modes of a poly(2,5-thiophene-1,4-dialkoxyphenylene) derivative by gamma photons. **2011**, 115, 8288-94		5

729	References. 557-640		
728	Conformation-dependent QSPR models: logPOW. **2011**, 51, 2408-16		10
727	MSINDO-sCIS: A New Method for the Calculation of Excited States of Large Molecules. *Journal of Chemical Theory and Computation*, **2011**, 7, 3675-85	6.4	19
726	Fast calculation approach to semi-empirical molecular orbital method using real space division method. **2011**, 50, 3346-3349		1
725	Singlet□triplet (S0 -fT1) excitation energies of the [4 ˆ □n] rectangular graphene nanoribbon series (n = 2□): A comparative theoretical study. **2011**, 977, 163-167		11
724	The role of molecular modeling in confined systems: impact and prospects. **2011**, 13, 58-85		142
723	Polarized Molecular Orbital Model Chemistry. I. Ab Initio Foundations. *Journal of Chemical Theory and Computation*, **2011**, 7, 852-856	6.4	24
722	DFTB3: Extension of the self-consistent-charge density-functional tight-binding method (SCC-DFTB). *Journal of Chemical Theory and Computation*, **2012**, 7, 931-948	6.4	620
721	Semiempirical, Hartree-Fock, density functional, and second order Moller-Plesset perturbation theory methods do not accurately predict ionization energies and electron affinities of short- through long-chain [n]acenes. **2011**,		1
720	Membrane fusion induced by small molecules and ions. **2011**, 2011, 528784		48
719	A Chronicle About the Development of Electronic Structure Theories for Transition Metal Complexes. **2011**, 1-38		11
718	MNDO-Like Semiempirical Molecular Orbital Theory and Its Application to Large Systems. **2011**, 259-286		18
717	Ab initio and Semiempirical Methods. **2011**,		
716	Insight into the phosphodiesterase mechanism from combined QM/MM free energy simulations. **2011**, 278, 2579-95		19
715	Electron transfer with TD-Split, a linear response time-dependent method. **2011**, 391, 62-68		2
714	Semiempirical self-consistent polarization description of bulk water, the liquid-vapor interface, and cubic ice. **2011**, 115, 6046-53		21
713	A quantum-chemical perspective into low optical-gap polymers for highly-efficient organic solar cells. *Chemical Science*, **2011**, 2, 1200-1218	9.4	218
712	Theoretical study of the models of Ca2+ and Mg2+ ions binding by the methylidene rhodanine neutral and anionic forms. **2011**, 81, 576-585		3

711	Study of structure and spectral characteristics of the binuclear zinc complex with (E)-2-({2-[3-(pyridin-2-yl)-1H-1,2,4-triazol-5-yl]phenylimino}methyl)phenol. **2011**, 81, 2332-2344		11
710	Internal investigation of saturation carbon nanotubes molecular hydrogen. **2011**, 5, 530-536		
709	Quantum-chemical study of structure and spectral properties of triphenylamine-rhodanine dye 2-(5-(4-(diphenylamine)benzylidene)-4-oxo-2-thioxothiazolidine-3-yl) acetic acid. **2011**, 110, 216-223		11
708	MSCALE: A General Utility for Multiscale Modeling. *Journal of Chemical Theory and Computation*, **2011**, 7, 1208-1219	6.4	38
707	Semiempirical Calculations. **2011**, 391-444		0
706	Binding free energy calculation with QM/MM hybrid methods for Abl-Kinase inhibitor. **2011**, 37, 69-78		29
705	Using a quantum-chemical approach for the investigation of corrosion on surfaces of metals and alloys. **2011**, 47, 137-149		
704	AM1 parameters for palladium and silver. **2011**, 17, 2585-600		6
703	Using multipole point charge distributions to provide the electrostatic potential in the variational explicit polarization (X-Pol) potential. **2011**, 129, 3-13		10
702	Theoretical study of the electronic ground states and low-lying singlet excited states of thiophene-based spirofluorenes. **2011**, 54, 884-889		2
701	Intrinsic minimal atomic basis representation of molecular electronic wavefunctions. **2011**, 111, 2851-2867		21
700	Influence of electron doping on the hydrogenation of fullerene C60 : a theoretical investigation. **2011**, 12, 2581-9		3
699	A fast empirical GAFF compatible partial atomic charge assignment scheme for modeling interactions of small molecules with biomolecular targets. **2011**, 32, 893-907		40
698	Similarity analysis of the conformational potential energy surface of n-pentane. **2011**, 963, 378-383		9
697	The molecular basis of working mechanism of natural polyphenolic antioxidants. **2011**, 125, 288-306		717
696	Theoretical and experimental study of structures and properties of cement paste: The nanostructural aspects of C□H. **2011**, 72, 920-933		19
695	Theoretical studies of 2-nitrobenzaldehyde and furan-2-carbaldehyde Schiff base of 2-amino pyridine. **2011**, 15, 161-165		5
694	Thermochromism of perylenes: dynamics in aromatics. **2011**, 78, 1212-4		6

693	Lagrangian formulation with dissipation of Born-Oppenheimer molecular dynamics using the density-functional tight-binding method. **2011**, 135, 044122		58
692	QSAR studies on the depuration rates of polycyclic aromatic hydrocarbons, polybrominated diphenyl ethers and polychlorinated biphenyls in mussels (Elliptio complanata). **2011**, 22, 561-73		4
691	Theoretical predictions of red and near-infrared strongly emitting X-annulated rylenes. **2011**, 134, 074510		18
690	Comparison of different computational methods for water structure optimisation. **2012**, 59, 55-66		
689	http://www.omicsgroup.org/journals/insulin-as-therapeutic-agent-against-alzheimers-disease-2169-0138.1000e112.php? **2012**, 02,		1
688	Mechanism of Drug Action: Basic Concepts. **2012**, 9-38		
687	QM/MM investigations of organic chemistry oriented questions. **2014**, 351, 25-101		3
686	3D-RISM-Dock: A New Fragment-Based Drug Design Protocol. *Journal of Chemical Theory and Computation*, **2012**, 8, 3356-72	6.4	34
685	9.10 MNDO-PSDCI and the Analysis of the Photophysical Properties of Visual Chromophores and Retinal Proteins. **2012**, 162-189		0
684	Inelastic collisions of the uracil molecules with electrons. **2012**, 137, 184303		13
683	Improved chemical energy component analysis. **2012**, 14, 337-44		11
682	Radiationless S 1 -fS 0 phenyl deactivation pathway: an investigation of iodine-marked bi-phenyl on a silicon surface by means of time resolved core-level photoelectron spectroscopy. **2012**, 110, 207-216		
681	Modification of the secondary structure of angiotensin II by substitution of hydrogen with Cs cations: an experimental and theoretical study. **2012**, 14, 9301-5		
680	Theoretical justification for the fire-protection modification of textiles through the action of laser radiation. **2012**, 44, 90-94		1
679	Extended polarization in third-order SCC-DFTB from chemical-potential equalization. **2012**, 116, 9131-41		38
678	Molecular dynamics simulation of tri-n-butyl-phosphate liquid: a force field comparative study. **2012**, 116, 305-13		38
677	Molecular modeling assisted hapten design to produce broad selectivity antibodies for fluoroquinolone antibiotics. **2012**, 84, 4527-34		54
676	SCC-DFTB Parametrization for Boron and Boranes. *Journal of Chemical Theory and Computation*, **2012**, 8, 1153-63	6.4	23

675	Convergence of QM/MM free-energy perturbations based on molecular-mechanics or semiempirical simulations. **2012**, 14, 12592-604		62
674	Erratum: Polarized Molecular Orbital Chemistry. 2. The PMO Method. *Journal of Chemical Theory and Computation*, **2012**, 8, 2983	6.4	5
673	Isomerization energies of tetrahedranes to 1,3-cyclobutadienes: A challenge for theoretical methods. **2012**, 979, 1-9		8
672	Singlet□Triplet excitation energies of naphthyl cations: High level composite method calculations suggest a singlet ground state. **2012**, 983, 69-75		7
671	Schiff bases as corrosion inhibitor for aluminium in HCl solution. **2012**, 54, 251-259		182
670	Design, synthesis and pharmacophoric model building of novel substituted nicotinic acid hydrazones with potential antiproliferative activity. **2012**, 35, 1543-52		23
669	Theoretical Methods for Supramolecular Chemistry. **2012**, 743-793		
668	Synthesis of rubrolide analogues as new inhibitors of the photosynthetic electron transport chain. **2012**, 60, 10555-63		29
667	A Hierarchy of Methods for the Energetically Accurate Modeling of Isomerism in Monosaccharides. *Journal of Chemical Theory and Computation*, **2012**, 8, 2630-45	6.4	49
666	Pathways to Modern Chemical Physics. **2012**,		7
665	In silico strategies toward enzyme function and dynamics. **2012**, 87, 249-92		2
664	A computational methodology to screen activities of enzyme variants. **2012**, 7, e49849		15
663	. **2012**,		15
662	Elongation method for linear scaling. **2012**,		
661	Extensions of DFTB to investigate molecular complexes and clusters. **2012**, 249, 245-258		29
660	Computational strategy for graphene: Insight from odd electrons correlation. **2012**, 112, 3076-3090		14
659	Targeted prodrugs in oral drug delivery: the modern molecular biopharmaceutical approach. **2012**, 9, 1001-13		43
658	Semiempirical Quantum Chemical Calculations Accelerated on a Hybrid Multicore CPU-GPU Computing Platform. *Journal of Chemical Theory and Computation*, **2012**, 8, 2272-81	6.4	41

657	A Bifunctional Isocupreidine Derivative as Catalyst for the Enantioselective Morita–Baylis–Hillman Reaction and a Mechanistic Rationale for Enantioselectivity. **2012**, 2012, 4140-4152		10
656	The Mechanisms of Chemical Reactions. **2012**, 223-269		
655	Analytical Gradients for the MSINDO-sCIS and MSINDO-UCIS Method: Theory, Implementation, Benchmarks, and Examples. *Journal of Chemical Theory and Computation*, **2012**, 8, 986-96	6.4	10
654	Quantum kernel applications in medicinal chemistry. **2012**, 4, 1479-94		11
653	MMPBSA.py: An Efficient Program for End-State Free Energy Calculations. *Journal of Chemical Theory and Computation*, **2012**, 8, 3314-21	6.4	1807
652	The relationship between threshold voltage and dipolar character of self-assembled monolayers in organic thin-film transistors. *Journal of the American Chemical Society*, **2012**, 134, 12648-52	16.4	75
651	Theoretical study of the dimerization of rhodanine in various tautomeric forms. **2012**, 47, 1268-1279		10
650	Molecular dynamics investigations of chlorine peroxide dissociation on a neural network ab initio potential energy surface. **2012**, 131, 1		5
649	Gas-phase thermolysis reaction of formaldehyde diperoxide. Kinetic study and theoretical mechanisms. **2012**, 393, 37-45		5
648	A Benchmark Test Suite for Proton Transfer Energies and its Use to Test Electronic Structure Model Chemistries. **2012**, 400, 8-12		32
647	On the effect of a variation of the force field, spatial boundary condition and size of the QM region in QM/MM MD simulations. **2012**, 33, 363-78		33
646	Quantum chemical description of absorption properties and excited-state processes in photosynthetic systems. **2012**, 13, 386-425		97
645	Why sp2-like nanosilicons should not form: Insight from quantum chemistry. **2013**, 113, 612-618		19
644	Quantum chemical study of some triazoles as inhibitors of corrosion of copper in acid media. **2013**, 39, 1279-1289		7
643	Novel phenomena for aggregation induced emission enhancement: highly fluorescent hydrophobic TPE-BODIPY couples in both organic and aqueous media. **2013**, 3, 15866		41
642	The future of prodrugs - design by quantum mechanics methods. **2013**, 10, 713-29		14
641	CORROSION INHIBITION AND ADSORPTION BEHAVIOR OF SOME AZO DYE DERIVATIVES ON CARBON STEEL IN ACIDIC MEDIUM: SYNERGISTIC EFFECT OF HALIDE IONS. **2013**, 200, 1366-1393		31
640	The accuracy of quantum chemical methods for large noncovalent complexes. *Journal of Chemical Theory and Computation*, **2013**, 9, 3364-3374	6.4	223

639	Sparkle/RM1 parameters for the semiempirical quantum chemical calculation of lanthanide complexes. **2013**, 3, 16747		50
638	Parametrization scheme with accuracy and transferability for tight-binding electronic structure calculations with extended H□kel approximation and molecular dynamics simulations. **2013**, 19, 2363-73		4
637	Molecular structure and electronic properties of pyridylindolizine derivative containing phenyl and phenacyl groups: Comparison between semi-empirical calculations and experimental studies. *Journal of Molecular Structure*, **2013**, 1034, 162-172	3.4	9
636	Evaluation of optical activities by modern semi-empirical methods. **2013**, 113, 2447-2456		7
635	AM1 Specific Reaction Parameters for Reactions of Hydroxide Ion with Halomethanes in Complex Environments: Development and Testing. *Journal of Chemical Theory and Computation*, **2013**, 9, 4470-80	6.4	15
634	Carbon nanotubes, new material for purification of water-ethanol mixtures from isomers of propanol. **2013**, 83, 1601-1606		
633	Force Field Treatment of Proton and Hydrogen Transfer in Molecular Systems. **2013**, 253-276		1
632	Adsorption of atomic hydrogen on the surface of the boron-carbon nanotubes. **2013**, 83, 1580-1585		0
631	Sparkle/PM7 Lanthanide Parameters for the Modeling of Complexes and Materials. *Journal of Chemical Theory and Computation*, **2013**, 9, 3333-3341	6.4	86
630	Modern quantum chemical methods for calculating spin□spin coupling constants: theoretical basis and structural applications in chemistry. **2013**, 82, 99-130		94
629	Modeling of fluorescence quenching by lutein in the plant light-harvesting complex LHCII. **2013**, 117, 10974-86		59
628	In situ parameterisation of SCC-DFTB repulsive potentials by iterative Boltzmann inversion. **2013**, 111, 3595-3607		24
627	Polarized Molecular Orbital Model Chemistry 3. The PMO Method Extended to Organic Chemistry. *Journal of Chemical Theory and Computation*, **2013**, 9, 33-45	6.4	16
626	Ab initio, density functional theory, and semi-empirical calculations. **2013**, 924, 3-27		3
625	Optimization of parameters for semiempirical methods VI: more modifications to the NDDO approximations and re-optimization of parameters. **2013**, 19, 1-32		1126
624	Study of molecular behavior in oxidation of insulating oil using terahertz spectroscopy. **2013**, 183, 9-15		2
623	Quantum mechanical force field for water with explicit electronic polarization. **2013**, 139, 054503		31
622	Theoretical and experimental studies on the electronic, optical, and structural properties of poly-pyrrole-2-carboxylic acid films. **2013**, 425, 91-95		4

621	Benchmark Study for the Cysteine-Histidine Proton Transfer Reaction in a Protein Environment: Gas Phase, COSMO, QM/MM Approaches. *Journal of Chemical Theory and Computation*, **2013**, 9, 1765-77	6.4	33
620	Quantum Chemical Methods in the Design of Agrochemicals. **2013**, 43-71		1
619	Michael J. S. Dewar: A Model Iconoclast. **2013**, 139-153		1
618	Modeling of high-order terms in potential energy surface expansions using the reference-geometry Harris-Foulkes method. **2013**, 15, 10233-40		10
617	Assessing the Accuracy of Density Functional and Semiempirical Wave Function Methods for Water Nanoparticles: Comparing Binding and Relative Energies of (H2O)16 and (H2O)17 to CCSD(T) Results. *Journal of Chemical Theory and Computation*, **2013**, 9, 995-1006	6.4	43
616	Silica surface features and their role in the adsorption of biomolecules: computational modeling and experiments. **2013**, 113, 4216-313		414
615	Doped polycyclic aromatic hydrocarbons as building blocks for nanoelectronics: a theoretical study. **2013**, 78, 1894-902		28
614	Quantum-chemical investigation of the structure and electronic absorption spectra of electroluminescent zinc complexes. **2013**, 114, 30-40		11
613	Infrared and electron spin resonance spectral studies of some copper purine and pyrimidine complexes. **2013**, 102, 175-85		17
612	Specific Reaction Path Hamiltonian for Proton Transfer in Water: Reparameterized Semiempirical Models. *Journal of Chemical Theory and Computation*, **2013**, 9, 2672-86	6.4	36
611	Parametrization of the SCC-DFTB Method for Halogens. *Journal of Chemical Theory and Computation*, **2013**, 9, 2939-49	6.4	45
610	Electrochemical and Theoretical Studies of Adsorption and Corrosion Inhibition of N,N?-Bis(2-hydroxyethoxyacetophenone)-2,2-dimethyl-1,2-propanediimine on Low Carbon Steel (API 5L Grade B) in Acidic Solution. **2013**, 52, 6617-6632		76
609	Small optical gap molecules and polymers: using theory to design more efficient materials for organic photovoltaics. **2014**, 352, 1-38		13
608	Effect of hydroxyl group position on adsorption behavior and corrosion inhibition of hydroxybenzaldehyde Schiff bases: Electrochemical and quantum calculations. *Journal of Molecular Structure*, **2013**, 1035, 247-259	3.4	75
607	Acceleration of Semiempirical Quantum Mechanical Calculations by Extended Lagrangian Molecular Dynamics Approach. *Journal of Chemical Theory and Computation*, **2013**, 9, 3393-403	6.4	6
606	Quantum chemical studies of novel 2?-4? conformationally restricted antisense monomers. **2013**, 113, 2523-2533		4
605	Correlated ab Initio and Electroanalytical Study on Inhibition Behavior of 2-Mercaptobenzothiazole and Its Thiole□thione Tautomerism Effect for the Corrosion of Steel (API 5L X52) in Sulphuric Acid Solution. **2013**, 52, 14875-14889		72
604	Synthesis of Telechelic Poly(ether sulfone) Oligomers by Chain-Growth Condensation Polymerization. **2013**, 214, 2489-2499		1

603	Prodrugs design based on inter- and intramolecular chemical processes. **2013**, 82, 643-68	39
602	A QSPR Model for Prediction of the Impact Sensitivities of some Nitro Compounds. **2013**, 641-642, 109-112	3
601	Advances in Quantum Methods and Applications in Chemistry, Physics, and Biology. **2013**,	2
600	Modeling the bandstructures of B-DNA base stacks. **2013**, 113, 173703	5
599	Molecular Theory of Graphene. **2013**, 249-284	2
598	Interface of the polarizable continuum model of solvation with semi-empirical methods in the GAMESS program. **2013**, 8, e67725	12
597	Photoresponsive wettability in monolayer films from sinapinic acid. **2013**, 2013, 915237	2
596	. **2013**,	39
595	Some Recent Developments on the Synthesis, Chemical Reactivity, and Theoretical Studies of Tetroxanes. **2013**, 3, 48-73	1
594	Time-dependent Density Functional-based Tight-bind Method Efficiently Implemented with OpenMP Parallel and GPU Acceleration. **2013**, 26, 635-645	29
593	Theoretical study of interaction between Tacrine and finite-length Al-doped Carbon and Boron nitride Nanotubes: A Semiempirical drug delivery study in thermodynamic view. **2014**, 30, 1805-1813	
592	Synthesis, crystal structure, spectra and quantum chemical study on 1-phenyl-3-(4-nitrophenyl)-5-(2-thienyl)-2-pyrazoline. *Molecules*, **2014**, 19, 5313-24	4.8
591	Prodrugs for Masking the Bitter Taste of Drugs. **2014**,	3
590	Electronic and optical properties at organic/organic interfaces in organic solar cells. **2014**, 352, 103-50	5
589	Spin-orbit coupling and dissociation of CO2 molecules. **2014**, 117, 695-702	8
588	The CHARMM-TURBOMOLE interface for efficient and accurate QM/MM molecular dynamics, free energies, and excited state properties. **2014**, 35, 2076-86	40
587	Experimental and Theoretical Studies on Synthesized Compounds as Corrosion Inhibitor for Mild Steel in Hydrochloric Acid Solution. **2014**, 35, 1751-1763	7
586	Quantum mechanical force field for hydrogen fluoride with explicit electronic polarization. **2014**, 140, 204501	8

585	Impact of low molecular weight excipient octaacetylmaltose on the liquid crystalline ordering and molecular dynamics in the supercooled liquid and glassy state of itraconazole. **2014**, 88, 1094-104		14
584	Universal tight binding model for chemical reactions in solution and at surfaces. I. Organic molecules. **2014**, 141, 044503		6
583	Synthesis and prospects of application of branched polyarylenes in electroluminescent devices. **2014**, 83, 1062-1089		1
582	Nanostructured chalcogenide materials for memory switching devices. **2014**,		1
581	A New Approach to Dynamical Determination of the Active Zone in the Framework of the Hybrid Model (Quantum Mechanics/ Molecular Mechanics). **2014**, 6, 256-264		6
580	Semiempirical quantum chemical methods. **2014**, 4, 145-157		175
579	Molecular dynamics simulation and quantum chemical calculations for the adsorption of some Azo-azomethine derivatives on mild steel. *Journal of Molecular Structure*, **2014**, 1060, 80-87	3.4	51
578	An extensible interface for QM/MM molecular dynamics simulations with AMBER. **2014**, 35, 95-108		99
577	Explicit proton transfer in classical molecular dynamics simulations. **2014**, 35, 657-71		34
576	Computational catalysis--past, present, and future. **2014**, 53, 8605-13		68
575	Quantum and Molecular Mechanical (QM/MM) Monte Carlo Techniques for Modeling Condensed-Phase Reactions. **2014**, 4, 422-435		31
574	Study of thioureas derivatives synthesized from a green route as corrosion inhibitors for mild steel in HCl solution. **2014**, 79, 108-118		134
573	On the inter-ring torsion potential of regioregular P3HT: a first principles reexamination with explicit side chains. **2014**, 16, 3983-94		23
572	Charge transport across insulating self-assembled monolayers: non-equilibrium approaches and modeling to relate current and molecular structure. **2014**, 8, 12428-36		25
571	Katalyseforschung auf dem Computer. **2014**, 126, 8748-8757		7
570	An assessment to evaluate the validity of different methods for the description of some corrosion inhibitors. **2014**, 20, 2422		7
569	Studying chemical reactivity in a virtual environment. **2014**, 169, 89-118		26
568	Differentiation of alkane isomers through binding energy spectra and total momentum cross sections. *New Journal of Chemistry*, **2014**, 38, 1031	3.6	9

567	Electronic Effects in Organic Chemistry. **2014**,		1
566	One-way rotation of a molecule-rotor driven by a shot noise. **2014**, 6, 2793-9		21
565	Water interactions with hydrophobic groups: assessment and recalibration of semiempirical molecular orbital methods. **2014**, 141, 034106		15
564	One hundred years of the Max-Planck-Institut f ˆ Kohlenforschung. **2014**, 53, 8562-86		5
563	100 Jahre Max-Planck-Institut f ˆ Kohlenforschung. **2014**, 126, 8702-8727		1
562	Isotropic Periodic Sum Treatment of Long-Range Electrostatic Interactions in Combined Quantum Mechanical and Molecular Mechanical Calculations. *Journal of Chemical Theory and Computation*, **2014**, 10, 134-45	6.4	22
561	Excitation energy transfer in the peridinin-chlorophyll a-protein complex modeled using configuration interaction. **2014**, 118, 9141-54		18
560	AM1/d-CB1: A Semiempirical Model for QM/MM Simulations of Chemical Glycobiology Systems. *Journal of Chemical Theory and Computation*, **2014**, 10, 4694-4707	6.4	30
559	EMPIRE: a highly parallel semiempirical molecular orbital program: 1: self-consistent field calculations. **2014**, 20, 2331		42
558	Parameterization to NDDO-based polarizable force field. **2014**, 6,		78
557	Optimized Synthesis and Antimalarial Activity of 1,2-Dioxane-4-carboxamides. **2014**, 2014, 1607-1614		13
556	Experimental and theoretical study of sulfathiazole as environmentally friendly inhibitor on aluminum corrosion in NaCl. **2014**, 50, 244-253		13
555	Toward QM/MM Simulation of Enzymatic Reactions with the Drude Oscillator Polarizable Force Field. *Journal of Chemical Theory and Computation*, **2014**, 10, 1795-809	6.4	34
554	Molecular dynamics simulations of tri-n-butyl-phosphate/n-dodecane mixture: thermophysical properties and molecular structure. **2014**, 118, 10750-60		21
553	Reaction Path Force Matching: A New Strategy of Fitting Specific Reaction Parameters for Semiempirical Methods in Combined QM/MM Simulations. *Journal of Chemical Theory and Computation*, **2014**, 10, 3038-54	6.4	36
552	Accuracy of dispersion interactions in semiempirical and molecular mechanics models: the benzene dimer case. **2014**, 118, 9561-7		22
551	Vibrational energy relaxation of the amide I mode of N-methylacetamide in D D studied through Born-Oppenheimer molecular dynamics. **2014**, 118, 6186-97		25
550	Electrochemical and quantum chemical investigation of inhibitory of 1,4-Ph(OX)2(Ts)2 on corrosion of 1005 aluminum alloy in acidic medium. **2014**, 20, 4363-4370		44

549	Nitrogen and Sulfur Compounds in Atmospheric Aerosols: A New Parametrization of Polarized Molecular Orbital Model Chemistry and Its Validation against Converged CCSD(T) Calculations for Large Clusters. *Journal of Chemical Theory and Computation*, **2014**, 10, 3129-39	6.4	8
548	Cyclopent-4-ene-1,3-diones: a new class of herbicides acting as potent photosynthesis inhibitors. **2014**, 62, 5772-80		11
547	Structures and stabilities of (MgO)n nanoclusters. **2014**, 118, 3136-46		64
546	Thermodegradability of soluble polydiphenylsilane copolymers. **2014**, 107, 82-90		1
545	Improving intermolecular interactions in DFTB3 using extended polarization from chemical-potential equalization. **2015**, 143, 084123		38
544	A multi-agent quantum Monte Carlo model for charge transport: Application to organic field-effect transistors. **2015**, 143, 044114		10
543	Simulating charge transport in flexible systems. **2015**, 6, 58-65		3
542	. **2015**,		13
541	Current Challenges in Development of a Database of Three-Dimensional Chemical Structures. **2015**, 3, 66		3
540	References. **2015**, 199-213		
539	Mixed quantum-classical dynamics for charge transport in organics. **2015**, 17, 12395-406		69
538	EMPIRE: a highly parallel semiempirical molecular orbital program: 2: periodic boundary conditions. **2015**, 21, 144		23
537	An 'all pigment' model of excitation quenching in LHCII. **2015**, 17, 15857-67		52
536	Energy Alignment of Frontier Orbitals and Suppression of Charge Recombinations in P3HT/SWNT. **2015**, 119, 26258-26265		7
535	Benchmarking Ground-State Geometries and Vertical Excitation Energies of a Selection of P-Type Semiconducting Molecules with Different Polarity. **2015**, 119, 12876-91		22
534	The adaptive buffered force QM/MM method in the CP2K and AMBER software packages. **2015**, 36, 633-48		38
533	Analysis of self-consistent extended Hˆ kel theory (SC-EHT): a new look at the old method. **2015**, 53, 528-550		9
532	Quantum chemical and experimental investigations on inhibitory behavior of aminoimino tautomeric equilibrium of 2-aminobenzothiazole on steel corrosion in H2SO4 solution. **2015**, 26, 81-94		34

531	Adsorption and corrosion inhibition effect of Schiff base molecules on the mild steel surface in 1 M HCl medium: a combined experimental and theoretical approach. **2015**, 17, 5679-90		260
530	Relationship between structure and inhibition behaviour of quinolinium salts for mild steel corrosion: Experimental and theoretical approach. **2015**, 95, 71-87		112
529	Pyrrolyl-Silicon Compounds as Precursors for Donor-Acceptor Systems Stabilized by Noncovalent Interactions. **2015**, 119, 7038-51		5
528	Automated computational screening of the thiol reactivity of substituted alkenes. **2015**, 29, 725-35		17
527	Semiempirical Molecular Dynamics (SEMD) I: Midpoint-Based Parallel Sparse Matrix-Matrix Multiplication Algorithm for Matrices with Decay. *Journal of Chemical Theory and Computation*, **2015**, 11, 3145-52	6.4	16
526	Structures and energetics of (MgCO3)n clusters (n □16). **2015**, 119, 3419-28		13
525	Efficient pathways of excitation energy transfer from delocalized S2 excitons in the peridinin-chlorophyll a-protein complex. **2015**, 119, 5755-64		19
524	Mixed Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulations of Biological Systems in Ground and Electronically Excited States. **2015**, 115, 6217-63		277
523	Technical advances in molecular simulation since the 1980s. **2015**, 582, 3-9		11
522	Domain Based Pair Natural Orbital Coupled Cluster Studies on Linear and Folded Alkane Chains. *Journal of Chemical Theory and Computation*, **2015**, 11, 2137-43	6.4	45
521	Alcamines as corrosion inhibitors for reinforced steel and their effect on cement based materials and mortar performance. **2015**, 5, 36957-36968		43
520	Electrochemical and theoretical study of the inhibition effect of two synthesized thiosemicarbazide derivatives on carbon steel corrosion in hydrochloric acid solution. **2015**, 5, 20838-20847		30
519	Computational Chemistry. **2015**, 151-189		9
518	Large-Scale Computations in Chemistry: A Bird's Eye View of a Vibrant Field. **2015**, 115, 5797-890		152
517	Synthesis, DNA interaction and anticancer activity of 2-anthryl substituted benzimidazole derivatives. *New Journal of Chemistry*, **2015**, 39, 4882-4890	3.6	27
516	Corrosion inhibition effect of spiropyrimidinethiones on mild steel in 15% HCl solution: insight from electrochemical and quantum studies. **2015**, 5, 70832-70848		71
515	Quantum chemical and experimental investigations on equipotent effects of (+)R and (□S enantiomers of racemic amisulpride as eco-friendly corrosion inhibitors for mild steel in acidic solution. *Journal of Molecular Liquids*, **2015**, 212, 168-186	6	54
514	First-Principles Prediction of Enthalpies of Formation for Polycyclic Aromatic Hydrocarbons and Derivatives. **2015**, 119, 11329-65		28

513	Vibrational relaxation as the driving force for wavelength conversion in the peridinin-chlorophyll a-protein. **2015**, 1847, 1509-17	5
512	Conformational studies of dammarane-type triterpenoids using computational and NMR spectroscopic methods. **2015**, 53, 1035-42	2
511	Structural modifications of graphyne layers consisting of carbon atoms in the sp- and sp 2-hybridized states. **2015**, 120, 820-830	22
510	Synthesis, spectral, DFT, and semi-empirical study of trimetallic complexes with pyrazole-3,5-dicarboxylic acid containing Sn(IV) and Hg(II). **2015**, 85, 1725-1733	1
509	Quasi-three-coordinate iron and cobalt terphenoxide complexes {Ar(iPr8)OM(□O)}2 (Ar(iPr8) = C6H-2,6-(C6H2-2,4,6-(i)Pr3)2-3,5-(i)Pr2; M = Fe or Co) with M(III)2(□O)2 core structures and the peroxide dimer of 2-oxepinoxy relevant to benzene oxidation. **2015**, 54, 8914-22	7
508	Stretching and Breaking of Chemical Bonds, Correlation of Electrons, and Radical Properties of Covalent Species. **2015**, 70, 111-161	10
507	GTP is an allosteric modulator of the interaction between the guanylate-binding protein 1 and the prosurvival kinase PIM1. **2015**, 91, 132-44	8
506	Density functional theory and molecular dynamics simulation study on corrosion inhibition performance of mild steel by mercapto-quinoline Schiff base corrosion inhibitor. **2015**, 66, 332-341	276
505	On the origins of regioselectivity in the orthoester Claisen rearrangement of bisallylic alcohols. **2015**, 56, 1297-1301	1
504	Correct electrostatic treatment of noncovalent interactions: the importance of polarization. **2015**, 5, 169-177	87
503	Prediction of absorption wavelengths using a combination of semi-empirical quantum mechanics simulations and quantitative structure□property relationship modeling approaches. **2015**, 299, 183-188	2
502	Computational insights into function and inhibition of fatty acid amide hydrolase. **2015**, 91, 15-26	30
501	Zinc(II) Complexes of Acetophenone and 5-Chloro-2-hydroxy-benzophenone Thiosemicarbazones. Synthesis, Characterization, and Nonlinear Optical Properties from Quantum Chemical Calculations. **2015**, 190, 53-65	4
500	Comparative analysis of various electrostatic potentials on docking precision against cyclin-dependent kinase 2 protein: a multiple docking approach. **2015**, 85, 107-18	8
499	Schiff base compound as a corrosion inhibitor for mild steel in 1 M HCl. **2015**, 41, 4943-4960	5
498	Parametrization of DFTB3/3OB for magnesium and zinc for chemical and biological applications. **2015**, 119, 1062-82	90
497	Molecular-Level Modeling and Simulation in Process Safety. **2016**, 111-210	0
496	Approximate Molecular Orbital Theories. **2016**, 127-153	0

495	Computational Tools for the Study of Biomolecules. **2016**, 583-648		5
494	Shift-and-invert parallel spectral transformation eigensolver: Massively parallel performance for density-functional based tight-binding. **2016**, 37, 448-59		14
493	Cost-Effective Implementation of Multiconformer Transition State Theory for Peroxy Radical Hydrogen Shift Reactions. **2016**, 120, 10072-10087		55
492	Carbon nanotubes: Sensor properties. A review. **2016**, 2, 95-105		246
491	Enhanced MPSM3 for Applications to Quantum Biological Simulations. **2016**,		1
490	Structure, ferroelectric ordering, and semiempirical quantum calculations of lanthanide based metal-organic framework: [Nd(C4H5O6)(C4H4O6)][3H2O]. **2016**, 119, 144104		5
489	Ambient-Potential Composite Ewald Method for ab Initio Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation. *Journal of Chemical Theory and Computation*, **2016**, 12, 2611-32	6.4	26
488	Molecular Modeling on the Role of Local Concentration in the Crystallization ofl-Methionine from Aqueous Solution. **2016**, 16, 3454-3464		12
487	Brain-Targeting Chemical Delivery Systems and Their Cyclodextrin-Based Formulations in Light of the Contributions of Marcus E. Brewster. **2016**, 105, 2589-2600		13
486	Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. **2016**, 116, 5301-37		210
485	Design, synthesis, chemical stability, packing, cyclic voltammetry, ionisation potential, and charge transport of [1]benzothieno[3,2-b][1]benzothiophene derivatives. **2016**, 4, 4863-4879		26
484	Molecular Recognition in Biomimetic Receptors. **2016**, 146-164		
483	Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Benchmarks of Electronically Excited States. *Journal of Chemical Theory and Computation*, **2016**, 12, 4400-22	6.4	42
482	Structural and Electronic Property Study of (ZnO)n, n ≤ 68: Transition from Zinc Oxide Molecular Clusters to Ultrasmall Nanoparticles. **2016**, 120, 20400-20418		38
481	Application of classical simulations for the computation of vibrational properties of free molecules. **2016**, 18, 28325-28338		8
480	Calculating distribution coefficients based on multi-scale free energy simulations: an evaluation of MM and QM/MM explicit solvent simulations of water-cyclohexane transfer in the SAMPL5 challenge. **2016**, 30, 989-1006		20
479	Inhibitive properties, adsorption and theoretical study of 3,7-dimethyl-1-(prop-2-yn-1-yl)quinoxalin-2(1H)-one as efficient corrosion inhibitor for carbon steel in hydrochloric acid solution. *Journal of Molecular Liquids*, **2016**, 222, 239-252	6	87
478	Enhanced Basicity of Push-Pull Nitrogen Bases in the Gas Phase. **2016**, 116, 13454-13511		64

477	Reparameterization of PM6 Applied to Organic Diradical Molecules. **2016**, 120, 8750-8760		14
476	The simulation of carbon material structure based on polyacrylonitrile obtained under IR heating. **2016**, 2, 13-17		3
475	FASP: a framework for automation of SlaterKoster file parameterization. **2016**, 135, 1		11
474	Amide and Peptide Bond Formation: Interplay between Strained Ring Defects and Silanol Groups at Amorphous Silica Surfaces. **2016**, 120, 24817-24826		24
473	Unimolecular decomposition pathways of negatively charged nitriles by ab initio molecular dynamics. **2016**, 18, 31017-31026		9
472	Encyclopedia of Geochemistry. **2016**, 1-6		
471	Overview of Electronic Structure Methods. **2016**, 39-66		2
470	Quantitative Evaluation of Dissociation Mechanisms in Phenolphthalein and the Related Compounds. **2016**, 15, 13-21		2
469	Semiempirical Quantum Chemistry. **2016**, 239-258		5
468	Empirical correction for PM7 band gaps of transition-metal oxides. **2016**, 22, 24		
467	Comparative Molecular Dynamics Study on Tri-n-butyl Phosphate in Organic and Aqueous Environments and Its Relevance to Nuclear Extraction Processes. **2016**, 120, 5183-93		27
466	Evaluation of L-tyrosine mixed with sodium dodecyl sulphate or cetyl pyridinium chloride as a corrosion inhibitor for mild steel in 1 M HCl: experimental and theoretical studies. **2016**, 6, 61235-61248		23
465	PdAg/CNT catalyzed alcohol oxidation reaction for high-performance anion exchange membrane direct alcohol fuel cell (alcohol = methanol, ethanol, ethylene glycol and glycerol). **2016**, 199, 494-503		114
464	The effect of various atomic partial charge schemes to elucidate consensus activity-correlating molecular regions: a test case of diverse QSAR models. *Journal of Biomolecular Structure and Dynamics*, **2016**, 34, 540-59	3.6	13
463	A comparative density functional theory and molecular dynamics simulation studies of the corrosion inhibitory action of two novel N-heterocyclic organic compounds along with a few others over steel surface. *Journal of Molecular Liquids*, **2016**, 215, 486-495	6	67
462	Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Theory, Implementation, and Parameters. *Journal of Chemical Theory and Computation*, **2016**, 12, 1082-96	6.4	90
461	Quantum chemical studies and atomistic simulations of some inhibitors for the corrosion of al surface. **2016**, 52, 156-168		6
460	Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Benchmarks for Ground-State Properties. *Journal of Chemical Theory and Computation*, **2016**, 12, 1097-120	6.4	63

459	L-Phenylalanine methyl ester hydrochloride as a green corrosion inhibitor for mild steel in hydrochloric acid solution and the effect of surfactant additive. **2016**, 6, 5890-5902		55
458	Experimental, quantum chemical and Monte Carlo simulation studies of 3,5-disubstituted-4-amino-1,2,4-triazoles as corrosion inhibitors on mild steel in acidic medium. *Journal of Molecular Liquids*, **2016**, 218, 281-293	6	124
457	The effect of structure parameters on the corrosion inhibition effect of some heterocyclic nitrogen organic compounds. *Journal of Molecular Liquids*, **2016**, 219, 128-141	6	56
456	Automatized Parameterization of the Density-functional Tight-binding Method. II. Two-center Integrals. **2016**, 63, 57-68		11
455	Understanding the anion-□interactions with tetraoxacalix[2]arene[2]triazine. **2016**, 18, 6913-24		32
454	Synthesis of Main-Chain Poly(fullerene)s from a Sterically Controlled Azomethine Ylide Cycloaddition Polymerization. **2016**, 49, 1681-1691		16
453	Anti-corrosive properties of 4-amino-3,5-bis(disubstituted)-1,2,4-triazole derivatives on mild steel corrosion in 2 M H3PO4 solution: Experimental and theoretical studies. *Journal of Molecular Liquids*, **2016**, 216, 874-886	6	47
452	Diverse Optimal Molecular Libraries for Organic Light-Emitting Diodes. *Journal of Chemical Theory and Computation*, **2016**, 12, 1942-52	6.4	14
451	Empirical and quantum chemical studies on the corrosion inhibition performance of some novel synthesized cationic gemini surfactants on carbon steel pipelines in acid pickling processes. **2016**, 108, 94-110		130
450	Real-Time TD-DFT with Classical Ion Dynamics: Methodology and Applications. *Journal of Chemical Theory and Computation*, **2016**, 12, 466-76	6.4	41
449	Multicomponent reactions of phosphines, enynedioates and benzylidene malononitriles generated highly substituted cyclopentenes through an unexpected phosphine □addition-□evolvement of an anion pathway. **2016**, 14, 2306-17		5
448	Schiff's base derived from 2-acetyl thiophene as corrosion inhibitor of steel in acidic mediumPeer review under responsibility of Taibah University.View all notes. **2016**, 10, 774-785		21
447	Benchmarking semiempirical, Hartree□Fock, DFT, and MP2 methods against the ionization energies and electron affinities of short- through long-chain [n]acenes and [n]phenacenes. **2016**, 94, 251-258		6
446	Development, applications and challenges of ReaxFF reactive force field in molecular simulations. **2016**, 10, 16-38		60
445	Consistent Embedding Frameworks for Predictive Multi-theory Multiscale Simulations. *Springer Series in Materials Science*, **2016**, 249-297	0.9	
444	Cationic porphyrins are tunable gatekeepers of the 20S proteasome. *Chemical Science*, **2016**, 7, 1286-1297	9.4	27
443	Computational Tools To Model Halogen Bonds in Medicinal Chemistry. **2016**, 59, 1655-70		99
442	Nonorthogonal tight-binding model with H□□□ parameterisation. **2016**, 42, 305-311		46

441	Experimental and theoretical studies on the removal of polycarboxy-benzoic acids by adsorption onto polyaniline from aqueous solution. **2016**, 57, 15176-15189		15
440	Inhibition effect of E and Z conformations of 2-pyridinealdazine on mild steel corrosion in phosphoric acid. **2017**, 64, 23-35		10
439	Guide to Programs for Nonrelativistic Quantum Chemistry Calculations. **2017**, 861-883		0
438	Fundamental Structural, Electronic, and Chemical Properties of Carbon Nanostructures: Graphene, Fullerenes, Carbon Nanotubes, and Their Derivatives. **2017**, 1175-1258		2
437	Bloch equations for intense x-rays. **2017**, 22, 51-54		
436	Quantum chemical and thermodynamic calculations of fulvic and humic copper complexes in reactions of malachite and azurite formation. **2017**, 79, 9-16		3
435	Novel synthesized Schiff Base-based cationic gemini surfactants: Electrochemical investigation, theoretical modeling and applicability as biodegradable inhibitors for mild steel against acidic corrosion. *Journal of Molecular Liquids*, **2017**, 232, 478-498	6	70
434	Assessment of semi-empirical molecular orbital calculations for describing magnetic interactions. **2017**, 136, 52-57		6
433	Quantum Chemical Estimation of Acetone Physisorption on Graphene Using Combined Basis Set and Size Extrapolation Schemes. **2017**, 121, 8999-9010		2
432	Catalytic synthesis and stereostructure of 1,2,3-trisubstituted decahydroisoquinolines. **2017**, 53, 222-225		
431	The chemical bond as an emergent phenomenon. **2017**, 146, 174502		6
430	Anticorrosion Effect of 4-Amino-5-(4-pyridyl)-4H-1,2,4-triazole-3-thiol for Mild Steel in HCl Solution. **2017**, 2, 3676-3682		9
429	A Comparison of Quantum and Molecular Mechanical Methods to Estimate Strain Energy in Druglike Fragments. **2017**, 57, 1265-1275		34
428	Benchmarking of computational approaches for fast screening of lithium ion battery electrolyte solvents. **2017**, 681, 64-68		6
427	Reinvestigation of the crystal structure of barium cesium cyclotriphosphate dihydrate and vibrational study. **2017**, 192, 1286-1293		3
426	Automatic generation of reaction energy databases from highly accurate atomization energy benchmark sets. **2017**, 19, 9798-9805		23
425	The power of exact conditions in electronic structure theory. **2017**, 669, 54-70		27
424	Metal Ion Modeling Using Classical Mechanics. **2017**, 117, 1564-1686		189

423	Theory and Simulation of the Ultrafast Double-Bond Isomerization of Biological Chromophores. **2017**, 117, 13502-13565		160
422	Electrochemical Study of Self-Assembled Aminothiol Substituted Phthalonitrile Layers for Corrosion Protection of Copper. **2017**, 2, 8256-8261		6
421	Structure and Stability of Hydrolysis Reaction Products of MgO Nanoparticles Leading to the Formation of Brucite. **2017**, 121, 21750-21762		13
420	Mediating Reductive Charge Shift Reactions in Electron Transport Chains. *Journal of the American Chemical Society*, **2017**, 139, 17474-17483	16.4	28
419	Efficient Geometry Minimization and Transition Structure Optimization Using Interpolated Potential Energy Surfaces and Iteratively Updated Hessians. *Journal of Chemical Theory and Computation*, **2017**, 13, 6424-6432	6.4	28
418	Quantum mechanical force fields for condensed phase molecular simulations. **2017**, 29, 383002		18
417	Semiempirical Molecular Orbital Methods. **2017**, 159-202		2
416	Energy band structure and electronic transport properties of chlorine-doped polyaniline from ab initio calculations. **2017**, 231, 89-94		8
415	Experimental and Theoretical Investigation of Inhibition Efficiency of 2-(2-Hydroxyphenyl)-benzothiazole Using Impedance Spectroscopy, Experimental Design, and Quantum Chemical Calculations. **2017**, 56, 9035-9044		10
414	The hpCADD NDDO Hamiltonian: Parametrization. **2017**, 57, 1907-1922		11
413	Study on the interactions of Ag nanoparticles with low molecular weight organic matter using first principles calculations. **2017**, 200, 270-279		7
412	Density matrix approach to orbital relaxation dynamics in ionization. **2017**, 117, e25442		1
411	Amorphous chalcogenides as random octahedrally bonded solids: I. Implications for the first sharp diffraction peak, photodarkening, and Boson peak. **2017**, 147, 114505		7
410	Ionic conductivity in BC3 type boron carbon nanolayers. **2017**, 3, 91-94		1
409	Acceleration of Semiempirical QM/MM Methods through Message Passage Interface (MPI), Hybrid MPI/Open Multiprocessing, and Self-Consistent Field Accelerator Implementations. *Journal of Chemical Theory and Computation*, **2017**, 13, 3525-3536	6.4	11
408	Theoretical description of protein field effects on electronic excitations of biological chromophores. **2017**, 29, 013002		10
407	Corrosion inhibition and adsorption behaviour of some bis-pyrimidine derivatives on mild steel in acidic medium. *Journal of Molecular Liquids*, **2017**, 225, 406-417	6	68
406	Determination of consistent semiempirical one-centre integrals based on coupled-cluster theory. **2017**, 115, 538-544		5

405	De novo lead optimization of triazine derivatives identifies potent antimalarials. **2017**, 71, 96-103		7
404	Sensor activity with respect to alkali metals of a carbon nanotube edge-modified with amino group. **2017**, 62, 1458-1463		6
403	Looking Back, Looking Forward at Halogen Bonding in Drug Discovery. *Molecules*, **2017**, 22,	4.8	86
402	Semiempirical Theoretical Studies of 1,3-Benzodioxole Derivatives as Corrosion Inhibitors. **2017**, 2017, 1-10		5
401	Modeling the Sensing Activity of Carbon Nanotubes Functionalized with the Carboxyl, Amino, or Nitro Group Toward Alkali Metals. **2017**, 46, 580-584		2
400	Molecular Dynamics Study of Combustion Reactions in Supercritical Environment. Part 3: Boxed MD Study of CH + HO -fCHO + OH Reaction Kinetics. **2018**, 122, 3337-3345		3
399	Testing Semiempirical Quantum Mechanical Methods on a Data Set of Interaction Energies Mapping Repulsive Contacts in Organic Molecules. **2018**, 122, 2801-2808		13
398	Random versus Systematic Errors in Reaction Enthalpies Computed Using Semiempirical and Minimal Basis Set Methods. **2018**, 3, 4372-4377		9
397	Pyrazoline derivatives as possible corrosion inhibitors for mild steel in acidic media: A combined experimental and theoretical approach. **2018**, 5, 1441585		12
396	An efficient implementation of semiempirical quantum-chemical orthogonalization-corrected methods for excited-state dynamics. **2018**, 148, 154103		16
395	How Does Silica Catalyze the Amide Bond Formation under Dry Conditions? Role of Specific Surface Silanol Pairs. **2018**, 8, 4558-4568		36
394	Semiempirical configuration interaction calculations for ru-centered dyes. **2018**, 39, 1259-1266		1
393	In-silico prediction of sweetness using structure-activity relationship models. **2018**, 253, 127-131		17
392	Impact of long-range electrostatic and dispersive interactions on theoretical predictions of adsorption and catalysis in zeolites. **2018**, 312, 51-65		22
391	Molecular Dynamics Study of Combustion Reactions in a Supercritical Environment. Part 2: Boxed MD Study of CO + OH -fCO + H Reaction Kinetics. **2018**, 122, 897-908		7
390	Switching the Proton Conduction in Nanoporous, Crystalline Materials by Light. **2018**, 30, 1706551		78
389	Gas Phase Synthesis of Protonated Glycine by Chemical Dynamics Simulations. **2018**, 122, 869-877		15
388	The inhibition action of analgin on the corrosion of mild steel in acidic medium: A combined theoretical and experimental approach. *Journal of Molecular Liquids*, **2018**, 263, 454-462	6	80

387	Overview of Computational Methods for Organic Chemists. **2018**, 31-67		3
386	Voltammetric determination of meclizine HCL and its application in pharmaceuticals and biological fluid using CNTS/ZnO nano-carbon modified electrode. **2018**, 15, 1881-1888		1
385	The influence of isolated and penta-hydrated Zn on some of the intramolecular proton-transfer processes of thymine: a quantum chemical study.. **2018**, 8, 11021-11026		1
384	Investigation of the electronic, optoelectronics, and linear and nonlinear optical properties of the molecules heptacene ([7]acene) (C30H18) and [7]acene doped with potassium atom (C30H9K9). **2018**, 75, 637-652		6
383	Schiff-base derivatives as corrosion inhibitors for carbon steel materials in acid media: quantum chemical calculations. **2018**, 53, 36-43		10
382	Conjoint experimental□heoretical evaluation of pyrone-salicylic acid hydrazide copper(II) Schiff base complexes: their synthesis, SOD and electrochemical fronts. **2018**, 6, 55-80		12
381	Rigorous and Empirical Approaches to Correlated Single-Particle Theories. **2018**, 1-20		1
380	Charge calculation studies done on a single walled carbon nanotube using MOPAC. **2018**, 92, 479-485		4
379	Theoretical Investigations of the Interaction of Gaseous Pollutants Molecules with the Polyacrylonitrile Surface. **2018**, 6, 39		0
378	Constricted Variational Density Functional Theory Approach to the Description of Excited States. **2018**,		
377	Bibliography. **2018**, 209-228		
376	Experimental and theoretical tools for corrosion inhibition study of mild steel in aqueous hydrochloric acid solution by new indanones derivatives. **2018**, 12, 30-42		29
375	A Feynman dispersion correction: a proof of principle for MNDO. **2018**, 24, 338		7
374	Big data analysis of ab Initio molecular integrals in the neglect of diatomic differential overlap approximation. **2019**, 40, 638-649		6
373	Synthesis, characterization and corrosion inhibition studies of novel 8-hydroxyquinoline derivatives on the acidic corrosion of mild steel: Experimental and computational studies. **2018**, 12, 43-54		38
372	Chemical preparation, crystal structure and vibrational study of a new dihydrogenotriphosphate trihydrate of 4-aminobenzoic acid fertilizer type NP. **2018**, 71, 3510-3520		4
371	Experimental and theoretical evaluation of some synthesized imidazolidine derivatives as novel corrosion inhibitors for X60 steel in 1 M HCl solution. **2018**, 32, 2569-2589		5
370	Enforcing Extended Porphyrin J-Aggregate Stacking in Covalent Organic Frameworks. *Journal of the American Chemical Society*, **2018**, 140, 16544-16552	16.4	72

369	Semiempirical molecular orbital models based on the neglect of diatomic differential overlap approximation. **2018**, 118, e25799		29
368	Charge transfer dynamics at the boron subphthalocyanine chloride/C interface: non-adiabatic dynamics study with Libra-X. **2018**, 20, 25275-25294		15
367	Accelerated Computation of Free Energy Profile at ab Initio Quantum Mechanical/Molecular Mechanics Accuracy via a Semi-Empirical Reference Potential. I. Weighted Thermodynamics Perturbation. *Journal of Chemical Theory and Computation*, **2018**, 14, 5583-5596	6.4	30
366	4-(2-(2-(2-(2-(Pyridine-4-yl)ethylthio)ethoxy)ethylthio)ethyl)pyridine as New Corrosion Inhibitor for Mild Steel in 1.0 M HCl Solution: Experimental and Theoretical Studies. *Journal of Bio- and Tribo-Corrosion*, **2018**, 4, 1	2.9	13
365	Comprehensive Analysis of the Neglect of Diatomic Differential Overlap Approximation. *Journal of Chemical Theory and Computation*, **2018**, 14, 5169-5179	6.4	12
364	COBRAMM 2.0 - A software interface for tailoring molecular electronic structure calculations and running nanoscale (QM/MM) simulations. **2018**, 24, 271		29
363	Application of Semiempirical Methods to Transition Metal Complexes: Fast Results but Hard-to-Predict Accuracy. *Journal of Chemical Theory and Computation*, **2018**, 14, 3428-3439	6.4	29
362	Transition State Search Using rPM6: Iron- and Manganese-Catalyzed Oxidation Reactions as a Test Case. **2018**, 91, 1377-1389		3
361	Assessing the Performance of MM/PBSA, MM/GBSA, and QM-MM/GBSA Approaches on Protein/Carbohydrate Complexes: Effect of Implicit Solvent Models, QM Methods, and Entropic Contributions. **2018**, 122, 8113-8121		35
360	Multireference Approaches for Excited States of Molecules. **2018**, 118, 7293-7361		181
359	Encyclopedia of Geochemistry. **2018**, 1-6		
358	The Design, Synthesis, and Characterizations of Spore Germination Inhibitors Effective against an Epidemic Strain of Clostridium difficile. **2018**, 61, 6759-6778		10
357	Towards a Deeper Understanding of the Anticorrosive Properties of Hydrazine Derivatives in Acid Medium: Experimental, DFT and MD Simulation Assessment. **2018**, 49, 5180-5191		15
356	Benchmarking Semiempirical Methods To Compute Electrochemical Formal Potentials. **2018**, 122, 6809-6818		9
355	A new schiff base derivative as an effective corrosion inhibitor for mild steel in acidic media: Experimental and computer simulations studies. *Journal of Molecular Structure*, **2018**, 1168, 39-48	3.4	60
354	Study of some properties of quinone derivatives from quantum chemical calculations. **2018**, 50, 1		10
353	Corrosion inhibition performance of imidazolidine derivatives for J55 pipeline steel in acidic oilfield formation water: Electrochemical, surface and theoretical studies. **2019**, 95, 341-356		37
352	An Exploration about the Interaction of Mild Steel with Hydrochloric Acid in the Presence of N-(Benzo[d]thiazole-2-yl)-1-phenylethan-1-imines. **2019**, 123, 22897-22917		51

351	Electron enrichment of zigzag edges in armchair-oriented graphene nanoribbons increases their stability and induces pinning of the Fermi level. **2019**, 154, 211-218		4
350	Study of the Properties of Oxide Melts in a Model Experiment. **2019**, 2019, 176-181		1
349	Insights into corrosion inhibition behavior of a triazole derivative For mild steel in hydrochloric acid solution. **2019**, 13, 1008-1022		6
348	Examination of the performance of semiempirical methods in QM/MM studies of the SN2-like reaction of an adenylyl group transfer catalysed by ANT4?. **2019**, 138, 1		1
347	Size-Dependent Local Ordering in Melanin Aggregates and Its Implication on Optical Properties. **2019**, 123, 9403-9412		2
346	Graphynes: Advanced Carbon Materials with Layered Structure. **2019**, 113-150		7
345	Molecular dynamics of combustion reactions in supercritical carbon dioxide. Part 4: boxed MD study of formyl radical dissociation and recombination. **2019**, 25, 35		4
344	On the mechanism of pore formation in pyrolized polyacrylonitrile. **2019**, 1281, 012031		2
343	Assessment of localized and randomized algorithms for electronic structure. **2019**, 1, 033001		5
342	Molecular Models of Suprastructural Units for Alkaline Borates. **2019**, 2019, 142-145		
341	Towards Understanding the Anticorrosive Mechanism of Novel Surfactant Based on Mentha pulegium Oil as Eco-friendly Bio-source of Mild Steel in Acid Medium: a Combined DFT and Molecular Dynamics Investigation. **2019**, 35, 85-100		16
340	Background, Tasks, Modeling Methods, and Challenges for Computational Toxicology. **2019**, 15-36		1
339	Mechanism of triboactivity of Schiff bases: Experimental and molecular dynamics simulations studies. *Journal of Molecular Liquids*, **2019**, 289, 111171	6	10
338	Molecular modeling and computational study of the chiral-dependent structures and properties of self-assembling diphenylalanine peptide nanotubes. **2019**, 25, 199		20
337	QM/MM Benchmarking of Cyanobacteriochrome Slr1393g3 Absorption Spectra. *Molecules*, **2019**, 24,	4.8	15
336	The Feynman dispersion correction for MNDO extended to F, Cl, Br and I. **2019**, 25, 156		2
335	Relative stability of diamond and graphite as seen through bonds and hybridizations. **2019**, 21, 10961-10969		8
334	Vase-Kite Equilibrium of Resorcin[4]arene Cavitands Investigated Using Molecular Dynamics Simulations with Ball-and-Stick Local Elevation Umbrella Sampling. **2019**, 102, e1900060		3

333	End functionalization of a double walled carbon nanotube for biomedical application. **2019**,		
332	ZnxMg60□O60 Nanoclusters with Tunable Near-Ultraviolet Energy Gaps. **2019**,		
331	Diabatization by Localization in the Framework of Configuration Interaction Based on Floating Occupation Molecular Orbitals (FOMOCI). **2019**, 3, 933-944		8
330	Advanced quantum chemical and electrochemical analysis of ravage drugs for corrosion inhibition of mild steel. **2019**, 33, 1066-1089		19
329	Eco-friendly disposal of expired anti-tuberculosis drug isoniazid and its role in the protection of metal. **2019**, 7, 102971		21
328	Solvent-free microwave assisted synthesis and corrosion inhibition study of a series of hydrazones derived from thiophene derivatives: Experimental, surface and theoretical study. *Journal of Molecular Liquids*, **2019**, 283, 788-803	6	32
327	Description of halogen bonding in semiempirical quantum-mechanical and self-consistent charge density-functional tight-binding methods. **2019**, 40, 1633-1642		5
326	Semiempirical Quantum-Chemical Methods with Orthogonalization and Dispersion Corrections. *Journal of Chemical Theory and Computation*, **2019**, 15, 1743-1760	6.4	25
325	Investigation of BC5 nanotube interaction with alkaline metal atoms. **2019**,		1
324	BAR-based multi-dimensional nonequilibrium pulling for indirect construction of QM/MM free energy landscapes: from semi-empirical to ab initio. **2019**, 21, 21942-21959		9
323	Vibrational Study and Crystal Structure of Barium Cesium Cyclotriphosphate Dihydrate. **2019**,		
322	An examination of the nature of localized molecular orbitals and their value in understanding various phenomena that occur in organic chemistry. **2018**, 25, 7		8
321	Lone pairs vs. covalent bonds: conformational effects in bicyclo[3.3.1]nonane derivatives. *Structural Chemistry*, **2019**, 30, 509-522	1.8	5
320	An Apparent Binary Choice in Biochemistry: Mutual Reactivity Implies Life Chooses Thiols or Nitrogen-Sulfur Bonds, but Not Both. **2019**, 19, 579-613		6
319	Experimental and theoretical investigation of aqueous and methanolic extracts of Prunus dulcis peels as green corrosion inhibitors of mild steel in aggressive chloride media. *Journal of Molecular Liquids*, **2019**, 276, 347-361	6	49
318	Exploring the applicability of density functional tight binding to transition metal ions. Parameterization for nickel with the spin-polarized DFTB3 model. **2019**, 40, 400-413		11
317	Machine Learning–Based Charge Transport Computation for Pentacene. **2019**, 2, 1800136		18
316	Theoretical developments and applications of polarization propagators. **2019**, 119, e25722		7

315	Theoretical study of optoelectronic properties of the molecule 2-cyano-3-[4-(diphenylamino)phenyl] acrylic acid. **2020**, 17, 533-543		12
314	Synthesis, cytotoxic activity and quantum chemical calculations of new 7-thioxopyrazolo[1,5-f]pyrimidin-2-one derivatives. *Journal of Molecular Structure*, **2020**, 1202, 127261	3.4	8
313	Theoretical Investigation of the Key Roles in Fullerene-Formation Mechanisms: Enantiomer and Enthalpy. **2020**, 3, 547-554		6
312	Synthesis and corrosion inhibition evaluation of a new schiff base hydrazone for mild steel corrosion in HCl medium: electrochemical, DFT, and molecular dynamics simulations studies. **2020**, 34, 1283-1314		28
311	Corrections of Molecular Morphology and Hydrogen Bond for Improved Crystal Density Prediction. *Molecules*, **2019**, 25,	4.8	4
310	Electrochemical and theoretical study of newly quinoline derivatives as a corrosion inhibitors adsorption onmild steel in phosphoric acid media. **2020**, 121, 108222		13
309	Investigating the pernicious effects of heparan sulfate in serum amyloid A1 protein aggregation: a structural bioinformatics approach. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-15	3.6	3
308	Synthesis, experimental and theoretical studies of triazine derivatives with surface activity as effective corrosion inhibitors for medium carbon steel in acid medium. *Journal of Molecular Liquids*, **2020**, 315, 113711	6	6
307	Lemon seeds as green coating material for mitigation of mild steel corrosion in acid media: Molecular dynamics simulations, quantum chemical calculations and electrochemical studies. *Journal of Molecular Liquids*, **2020**, 316, 113797	6	16
306	Bis(silanetellurone) with C-H□□Te Interaction. **2020**, 59, 17811-17821		3
305	Conformational Control of the Photodynamics of a Bilirubin Dipyrrinone Subunit: Femtosecond Spectroscopy Combined with Nonadiabatic Simulations. **2020**, 124, 10457-10471		1
304	Simulation of pyrolysed polyacrylonitrile based composite with amorphising boron additives. **2020**, 1479, 012131		
303	Calculation of Quantum Chemical Values of Corrosion Inhibitors Molecules by Heterocyclic Compounds. **2020**, 459, 022064		
302	Deductive molecular mechanics of carbon allotropes (Review article). **2020**, 46, 655-670		2
301	Theoretical and experimental studies of pyranopyrazoles and their tribological compatibility with a borate ester. **2020**, 606, 125497		3
300	Real-Time Time-Dependent Electronic Structure Theory. **2020**, 120, 9951-9993		60
299	Computer simulation of collision induced dissociation and isolobal analogy: The case of biotin and its analogs. **2020**, 457, 116417		
298	Comparison of computational chemistry methods for the discovery of quinone-based electroactive compounds for energy storage. **2020**, 10, 22149		9

297	Predicting in silico electron ionization mass spectra using quantum chemistry. **2020**, 12, 63		12
296	Study of Synergistic Effect of Some Pyrazole Derivatives as Corrosion Inhibitors for Mild Steel in 1 M H2SO4. *Surface Engineering and Applied Electrochemistry*, **2020**, 56, 601-609	0.8	3
295	The ORCA quantum chemistry program package. **2020**, 152, 224108		479
294	Chemical Bonding: The Journey from Miniature Hooks to Density Functional Theory. *Molecules*, **2020**, 25,	4.8	5
293	Luminescence of Cytosine Vapor in an Electric Discharge. **2020**, 87, 256-259		1
292	Comparative Investigation of Corrosion-Mitigating Behavior of Thiadiazole-Derived Bis-Schiff Bases for Mild Steel in Acid Medium: Experimental, Theoretical, and Surface Study. **2020**, 5, 13503-13520		33
291	Pyrolyzed Polyacrylonitrile Based Composite with Amorphizing Silicon Additives. **2020**,		1
290	EMPIRE: a highly parallel semiempirical molecular orbital program: 3: Born-Oppenheimer molecular dynamics. **2020**, 26, 43		5
289	Accuracy of the PM6 and PM7 Methods on Bare and Thiolate-Protected Gold Nanoclusters. **2020**, 124, 2601-2615		6
288	Non-Covalent Interactions Atlas Benchmark Data Sets: Hydrogen Bonding. *Journal of Chemical Theory and Computation*, **2020**, 16, 2355-2368	6.4	21
287	Graphics Processing Unit-Accelerated Semiempirical Born Oppenheimer Molecular Dynamics Using PyTorch. *Journal of Chemical Theory and Computation*, **2020**, 16, 4951-4962	6.4	12
286	NEXMD Software Package for Nonadiabatic Excited State Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2020**, 16, 5771-5783	6.4	27
285	Inhibitory effect of 2-Nitroacridone on corrosion of low carbon steel in 1 M HCl solution: An experimental and theoretical approach. **2020**, 9, 4061-4075		16
284	Density matrix formalism for femtosecond x-ray absorption and its excitonic enhancement. **2020**, 53, 095602		0
283	SAMPL6 host-guest binding affinities and binding poses from spherical-coordinates-biased simulations. **2020**, 34, 589-600		16
282	Density-functional tight-binding: basic concepts and applications to molecules and clusters. **2020**, 5, 1710252		19
281	Impact of refractive index increment on the determination of molecular weight of hyaluronic acid by muti-angle laser light-scattering technique. **2020**, 10, 1858		6
280	Exploring the charge configuration of an armchair single walled carbon nanotube for drug delivery. **2020**, 28, 185-187		2

279	Thiazolo thiadiazole derivatives as anti-corrosion additives for acid corrosion. **2020**, 26, 100358		11
278	Synthesis of Macromolecular Aromatic Epoxy Resins as Anticorrosive Materials: Computational Modeling Reinforced Experimental Studies. **2020**, 5, 3151-3164		8
277	Crystal structure, hydrogen bonding, Hirshfeld surface analysis and inhibition efficiency of a Schiff base 2-methoxy-6-(naphthalene-2-yliminomethyl)-phenol. **2020**, 25, 100337		7
276	Quantum Mechanics in Drug Discovery. **2020**,		10
275	New spirocyclopropane derivatives: synthesis and evaluation of their performances toward corrosion inhibition of mild steel in acidic media. **2020**, 46, 2881-2918		7
274	Green approach of synthesis of thiazolyl imines and their impeding behavior against corrosion of mild steel in acid medium. **2020**, 599, 124824		17
273	A new release of MOPAC incorporating the INDO/S semiempirical model with CI excited states. **2021**, 42, 365-378		4
272	Understanding Corrosion Inhibition of C38 Steel in HCl Media by Omeprazole: Insights for Experimental and Computational Studies. **2021**, 21, 213-227		7
271	Review: Simulation Models for Materials and Biomolecules. **2021**, 27-82		1
270	Theoretical and Computational Investigations of Carbon Nanostructures. **2021**, 139-164		
269	Bond order predictions using deep neural networks. **2021**, 129, 064701		1
268	One-Dimensional Organic-Inorganic Material (CHN)BiCl: From Synthesis to Structural, Spectroscopic, and Electronic Characterizations. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	0
267	Mathematical modeling of the process of interaction of sulfur dioxide with pyrolyzed polyacrylonitrile. **2021**, 1745, 012092		
266	A quantitative evaluation of computational methods to accelerate the study of alloxazine-derived electroactive compounds for energy storage. **2021**, 11, 4089		3
265	Machine Learning Force Fields. **2021**, 121, 10142-10186		147
264	A map of mass spectrometry-based in silico fragmentation prediction and compound identification in metabolomics. **2021**, 22,		8
263	Anticorrosive Effects of Derivatives of 4-{[4-(Dimethylamino) Benzylidene]amino}-1,2,4-Triazole on 316 Stainless Steel in HCl Medium: Experimental and Computational Study. **2021**, 21, 1057		
262	Learning to Model G-Quadruplexes: Current Methods and Perspectives. **2021**, 50, 209-243		8

261	Quantum Chemistry Calculations for Metabolomics. **2021**, 121, 5633-5670		18
260	Alkane/Water Partition Coefficient Calculation Based on the Modified AM1 Method and Internal Hydrogen Bonding Sampling Using COSMO-RS. **2021**, 61, 3453-3462		1
259	Experimental, DFT and MD Assessments of Bark Extract of as Corrosion Inhibitor for Carbon Steel Used in Desalination Plants. *Molecules*, **2021**, 26,	4.8	2
258	Machine learned Hˆ Ekel theory: Interfacing physics and deep neural networks. **2021**, 154, 244108		12
257	Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems. **2021**, 121, 9816-9872		53
256	Lack of Environmental Sensitivity of a Naturally Occurring Fluorescent Analog of Cholesterol. **2021**, 31, 1401-1407		2
255	MECHANISMS OF TRANSMISSION OF THE SPIN-SPIN INTERACTION OF CARBON-CARBON IN A SERIES OF BICYCLOBUTANE DERIVATIVES. **2021**, 2021, 77-87		
254	CONSTANTS OF SPIN-SPIN INTERACTION BETWEEN CARBON NUCLEI IN STERICALLY STRESSED SYSTEMS ON THE EXAMPLE OF BICYCLOPENTANES AND BICYCLOHEXANES. **2021**, 2021, 97-95		
253	Synthesis, Characterization of New Polytriazole Derivatives from Polyacryloyl chloride and Theoretical with Corrosion Inhibitor Study for Stainless steel in acidic medium. **2021**, 3721-3726		
252	Influence of the maturity of Musa paradisica peels on mild steel corrosion in sulfuric acid. 1-21		0
251	Connecting Gas-Phase Computational Chemistry to Condensed Phase Kinetic Modeling: The State-of-the-Art. **2021**, 13,		4
250	Finite-temperature effect in the O-acylation of (R,S)-propranolol catalyzed by Candida antarctica lipase B. **2021**, 107, 107951		
249	Probing Contact Electrification: A Cohesively Sticky Problem. **2021**, 13, 44935-44947		4
248	Application of molecular docking in elaborating molecular mechanisms and interactions of supramolecular cyclodextrin. **2022**, 276, 118644		6
247	Do It YourselfDock It Yourself: General Concepts and Practical Considerations for Beginners to Start Molecular LigandTarget Docking Simulations. **2021**, 205-227		
246	Corrosion Inhibition of Mild Steel with Tolyltriazole. **2021**, 24,		2
245	Combined Quantum Mechanical and Molecular Mechanical Potentials.		1
244	MSINDO.		4

243	Successes of Computer-Assisted Molecular Design. 355-371	25
242	Aspects of Molecular Modeling. 321-354	17
241	Some Theoretical Studies of Electronic Substituent Effects in Organic Chemistry. 125-191	24
240	3D QSAR of Flexible Molecules Using Tensor Representation. **1998**, 167-182	4
239	Mapping of molecular electric potentials and fields. **1995**, 27-43	19
238	Encyclopedia of Complexity and Systems Science. **2009**, 7931-7953	1
237	QM Calculations in ADMET Prediction. **2020**, 2114, 285-305	4
236	High-Pressure Hydrogenated Carbon Nanostructures. **2010**, 225-250	1
235	Unraveling the Mechanisms of Ribozyme Catalysis with Multiscale Simulations. **2009**, 377-408	1
234	Towards an Accurate Semi-Empirical Molecular Orbital Treatment of Covalent and Non-Covalent Biological Interactions. **2009**, 105-136	1
233	Modeling The Effect of Solvation on Structure, Reactivity, and Partitioning of Organic Solutes: Utility in Drug Design. **1999**, 51-72	10
232	Thermally Irreversible Photochromic Materials for Erasable Optical Data Storage Media. **1989**, 105-116	1
231	Potential Energy Surfaces for Ion-Molecule Reactions: Summary of the Panel Discussion. **1979**, 1-29	4
230	MNDO and AM1 Molecular Orbital and Molecular Mechanics Analyses of (+)-Catechin, (-)-Epicatechin, and their 3-O-Acetyl Derivatives. **1992**, 459-478	2
229	Correlation of Crystal Data and Charge Density with the Reactivity and Activity of Molecules: Towards a Description of Elementary Steps in Enzyme Reactions. **1991**, 287-318	4
228	MNDO Molecular Orbital Analyses of Models for Proanthocyanidin-Methylolphenol Reactions. **1989**, 205-226	4
227	Partitioning of Free Energies of Solvation into Fragment Contributions: Applications in Drug Design. **2001**, 143-168	8
226	Mechanisms of Regulation of Crystal Growth in Selected Biological Systems. **1995**, 183-206	1

225	Hydrogen on Semiconductor Surfaces. **1986**, 61-79		10
224	Simulation of Zn/Cd binding in mammalian metallothionein domains. **1999**, 45-49		1
223	Semiempirical Calculations. **2016**, 421-482		1
222	The Modelling of Molecules as Collections of Modified Atoms. **1990**, 283-324		3
221	Theoretical Calculations of the Structures of Some Prostaglandins and Inhibitors of Lipoxygenase. **1988**, 125-134		1
220	Molecular Orbital and Force-Field Calculations for Structure and Energy Predictions. **1988**, 95-102		1
219	Durch die Berechnung von Molekˆ Eigenschaften zum gezielten Entwurf von neuen Wirkstoffen. **1989**, 147-160		1
218	Synthetic Studies on Molecular Recognition. **1991**, 115-174		20
217	Electronic Properties of Polyaniline. **1987**, 238-243		4
216	Effective Coordinate and the Interpretation of IR and Raman Spectra of Polypyrrole, Pristine and Doped. **1989**, 113-118		2
215	Hydrogen Incorporation in Crystalline Semiconductors. *Springer Series in Materials Science*, **1992**, 4-27	0.9	4
214	Quantum Parabolic Effects of Electronegativity and Chemical Hardness on Carbon Systems. **2011**, 1-32		5
213	Theoretical Studies of the Energetics of Radicals. **1996**, 110-149		1
212	Applications of Quantum Chemistry in Mass Spectrometry. **1996**, 89-102		1
211	Theoretical Studies on the Reactions of Free Radicals. **1989**, 221-231		0
210	Electronic Devices from Molecules: Overview, Prospects and Theoretical Chemistry. **1988**, 185-198		3
209	Binary SN Ring Systems and Related Heterocyclothiazenes. **1986**, 269-298		1
208	Structure and Spectra of Stable and Transient States and Mechanisms of Oxidation of Model Cytochrome P-450. **1982**, 295-312		2

207	Modelling the Habit Modification of Molecular Crystals by the Action of Tailor-Made Additives. **1995**, 179-192		4
206	Building A Bridge Between AB Initio and Semiempirical Theories of Molecular Electronic Structure. **1995**, 25-67		3
205	An Introduction to Quantumchemical Organometallic Chemistry. **1995**, 3-13		0
204	Practical Tools for Molecular Modeling of Complex Carbohydrates and Their Interactions with Proteins. **1995**, 425-454		14
203	Structure of Molecules: Experiments and Theory. **1992**, 135-147		0
202	Some Applications of the Quantum-Mechanical Semiempirical Methods to the Gas-Phase Chemistry of Bio-Organic Ions. **1992**, 311-322		3
201	Molecular Modelling. Semi-Empirical and Empirical Methods of Theoretical Chemistry. **1991**, 229-259		1
200	Kinetics of Photochromic Processes in Dihydropyridine Derivatives. **2000**, 249-260		3
199	Using the Reaction Path Concept to Obtain Rate Constants From ab initio Calculations. **1995**, 191-228		2
198	Electronic spectra of adenine and guanine: Assignments and effects of solution environment. *Journal of Chemical Sciences*, **1992**, 104, 649-660	1.8	9
197	Investigations on C70H30 obtained by the Birch reduction of C70. *Journal of Chemical Sciences*, **1993**, 105, 303-309	1.8	3
196	The Feynman dispersion correction for MNDO extended to F, Cl, Br and I. **2019**, 25, 1		1
195	Electronic and Nonlinear Optical Properties of Conjugated Molecules and Polymers: A Quantum Chemistry Approach. **1993**, 127-153		2
194	Computational studies of the morphology of molecular crystals through solid-state intermolecular force calculations using the atom–atom method. **1994**, 95-135		5
193	Theoretical study of the product specificity in the hydroxylation of camphor, norcamphor, 5,5-difluorocamphor, and pericyclocamphanone by cytochrome P-450cam.. **1988**, 263, 3164-3170		38
192	Ion-molecule chemistry. **1996**, 193-217		3
191	Methods of incorporating quantum mechanical calculations into molecular dynamics simulations. **1999**, 7, 1-29		2
190	Relative stabilities of isomeric fullerenes. **1999**, 185-235		22

189	SEMI-EMPIRICAL SCF-MO CALCULATIONS OF BACKBONE CONFORMATIONAL STATES IN SOME GLASSY POLYMERS. **1981**, 371, 299-300		10
188	Quantum Chemical Descriptors in Structure-Activity Relationships Calculation, Interpretation, and Comparison of Methods. **2004**,		1
187	Semi-Empirical Evaluation of the Probability of Structural Rearrangements in Nitrone Spin Traps. **2013**, 1, 17-21		1
186	Kinetics and Mechanism of the Ozone Reaction with Alcohols, Ketones, Ethers and Hydroxybenzenes. **2016**, 10, 531-551		6
185	DFT and ab initio calculations of ionization potentials, proton affinities and bond dissociation enthalpies of aromatic compounds. **2019**, 12, 225-240		2
184	Computational Surface Modelling of Ices and Minerals of Interstellar Interest Insights and Perspectives. **2021**, 11, 26		2
183	Application of GC/EIMS in Combination with Semi-Empirical Calculations for Identification and Investigation of Some Volatile Components in Basil Essential Oil. **2016**, 04, 14-25		9
182	Photocatalytic Degradation of Surfactants. XX. Photooxidation of Sodium Butylnaphthalenesulfonates. **2003**, 52, 245-253		2
181	Quantum-chemical modelling radiation damage of DNA components during inelastic interaction with slow electrons. Desoxyribose irradiation. **2005**, 21, 351-357		1
180	Local perturbations of periodic systems. Chemisorption and point defects by GoGreenGo. **2021**, 42, 2352-2368		
179	Diaryl Sulfide Derivatives as Potential Iron Corrosion Inhibitors: A Computational Study. *Molecules*, **2021**, 26,	4.8	0
178	Electrochemical Behaviour of Some Substituted Thiadiazoles. **2001**, 69, 652-658		
177	Deposition Chemistry. **2002**,		
176	Free Energy Perturbation Calculations within Quantum Mechanical Methodologies. **2002**, 103-123		
175	Semiempirical Vibrational Frequencies (Including Scaling).		
174	Semiempirical Methods: Integrals and Scaling.		
173	MNDO/d.		
172	Hydrogen Bonds: Semiempirical Methods.		

171 Green's Function Ionization Potentials in Semiempirical MO Theory.

170 Quantitative Structure-Property Relationships (QSPR).

169 Divide and Conquer for Semiempirical MO Methods.

168 PM3.

167 MNDO.

166 Population Analyses for Semiempirical Methods.

165 Configuration Interaction: Semiempirical Calculations.

164 Quantum Mechanical/Molecular Mechanical (QM/MM) Coupled Potentials.

163 Parameterization of Semiempirical MO Methods.

162 Rotational Barriers and Molecular Mechanics Corrections.

161 AM1.

160 Accuracy and Applicability of Quantum Chemical Methods in Computational Medicinal Chemistry. **2003**,

159 The SCF-LCAO-MO Method and Extensions. **2006**, 348-390

158 Models of Molecular Structure: Hybrid Perspective. **2008**, 95-204

157 EQUILIBRIUM CONFIGURATION AND ELECTRONIC STRUCTURE OF THE C32H8 MOLECULE ISOMERS. **2008**, 375-378

156 INFLUENCE OF IMPURITIES AND DEFECTS ON ELECTRONIC STRUCTURE OF CARBON NANOTUBES. **2008**, 365-368

155 Deductive Molecular Mechanics: Bridging Quantum and Classical Models of Molecular Structure. **2008**, 205-274

154 Telluropyrylium Compounds. 219-291

153 Rational Design of Inhibitors of HIV-1 Reverse Transcriptase. 121-127

152 Quantum Mechanics. 947-976

151 Some recent developments in quantum organic chemistry. **1978**, 107-29 1

150 Electronic Properties and Reactivities of Perfect, Defected, and Doped Single-Walled Carbon Nanotubes. **2010**, 421-471

149 Investigation Mechanism of MTBE on Wall of Carbon Nanotube (CNT) to Other Products from Air-groundwater (in Environment): MNDO. **2010**, 269-274

148 QM/MM Energy Functions, Configuration Optimizations, and Free Energy Simulations of Enzyme Catalysis. **2010**, 331-353

147 Study on Molecular Behavior in Oxidation of Insulating Oil using Terahertz Spectroscopy. **2011**, 131, 943-948 2

146 Grounds of computational science of fullerenes. **2011**, 17-30

145 THE SCF□CAO□MO METHOD AND EXTENSIONS. **1978**, 309-346

144 Reliable Ab Initio Quantum Chemical Calculations for Energetic Species. **1981**, 569-609 1

143 A THEORETICAL CALCULATION OF THE O K ISOTHERM FOR SHOCKED NITROMETHANE**Supported in part by the NSWC Independent Research Program.. **1984**, 621-624

142 Electronic Localization and Delocalization in Organic Metals and Semiconductors. **1984**, 325-335

141 Praktische Anwendung von MO-Verfahren. **1984**, 154-172

140 Molecules. **1985**, 76-86

139 Density functional theory. **1985**, 17-35

138 Total energy. **1985**, 272-276

137 Fluorine and Oxygen. **1986**, 1-161

136 Computer-Based Approaches to Drug Design. **1987**, 73-96 1

135	Electronic Properties of Water Clusters by an Effective Hamiltonian Treatment. **1987**, 407-412	
134	Uber die Parameterisierung empirischer Rechenprogramme zur Simulation von Molekˆ Bstrukturen. **1988**, 81-94	
133	On the Reconstruction of the Diamond (111) Surface. **1988**, 316-319	2
132	Theoretical Calculations of the Electrostatic Potential of Some Tumor Promoters. **1988**, 301-311	
131	Molecular Dynamics Simulation of the Primary Processes in the Photosynthetic Reaction Center of Rhodopseudomonas Viridis. **1988**, 513-525	
130	Investigation of the Electronic Structure of Polymeric Vinylene Derivatives of Pyrene. **1989**, 65-68	
129	Practical Applications of New Theoretical Concepts in Organic Chemistry. **1989**, 373-385	
128	Electronic Structure and Nonlinear Optical Properties of Polythiophene, Polythieno[3,4-C]thiophene and Polyisothianaphthene Oligomers and Their Vinylene Derivatives. **1989**, 209-213	
127	Quantum Chemical Methods for Calculating Potential Energy Surfaces. **1990**, 61-87	
126	Vinylene-Linked Low-Band-Gap Conducting Polymers: Electronic Structure And Defects. **1990**, 305-320	1
125	Role of hydrogen atoms in anodized porous silicon. **1991**, 535-539	
124	Inhibition of cysteine proteinases by a series of peptidyl-diazomethanes structurally related to the binding center of cystatins. **1991**, 799-800	
123	Calculation of Molecular Structures on Distributed Computer Systems by Use of Quantum Chemical and Vibrational Spectroscopic Methods. **1991**, 169-182	
122	The Orbital Concept as a Foundation for Photoelectron Spectroscopy. **1991**, 63-97	2
121	A Theoretical Treatment of the Structural Aspects of the Topochemical Polymerization of Diacetylenes. **1992**, 161-170	
120	Grand Challenges und Supercomputer Beispiele groˆ Br Herausforderungen fˆ BGesellschaft, Technik und Wissenschaft. **1992**, 1-20	
119	Electronic Properties of Nonconjugated Polymers: 1,4-Polybutadiene and 1,4-Polyisoprene. **1992**, 63-67	
118	SYNCHROTRON BASED DIFFRACTION STUDIES OF SORPTION IN ZEOLITE Y AT ROOM TEMPERATURE. **1993**, 619-626	1

117 THE SCF-LCAO-MO METHOD AND EXTENSIONS. **1993**, 350-391

116 Quantitative description of nucleic acid sequences based on chemical characterization of the monomers. **1993**, 483-484

115 Computational Studies of Organolithium Compounds. **1994**, 228-232

114 Molecular design of photochromic diarylethenes for photonics. **1994**, 319-322

113 Molecular Mechanics: Problems and Potential. **1994**, 53-88

112 Determination of Conformationally Dependent Point Charges for Potential of Mean Force Simulations. **1994**, 199-204

111 Molecular Modelling Methods. **1994**, 1-52

110 3D QSAR The Integration of QSAR with Molecular Modeling. **1994**, 9-88

109 Proton Affinities and Intrinsic Basicities of Alanine and Glycine Studied by Means of AM1 and PM3 Methods. **1996**, 103-108

108 Volume 2 References. **1996**, 969-1102

107 Second Order Static Hyperpolarizabilities of Insaturated Polymers. **1996**, 297-311

106 METAL-COATED FULLERENES. **1996**, 169-180

105 Computational materials design and processing: perspectives for atomistic approaches. **1996**, 72-82

104 Komponenten des Molecular Modelling. **1997**, 19-83

103 Systematic procedure for the development of accurate QM/MM model Hamiltonians. **1997**, 177-195

102 Computer Modeling of Poly(Acrylic Acid) and its Salts. **1997**, 165-170

101 Geometries and Stabilities of G□GC, T□AT, A□AT an C□GC Nucleic Acid Base Triplets. **1997**, 285-297

100 To the question of tautomerism of nucleic acid bases. **1997**, 13, 185-190 1

99	Developing a Semiempirical Method. **1999**, 83-97		
98	Guide to Programs for Nonrelativistic Quantum Chemistry Calculations. **2015**, 1-23		
97	Material modeling for large scale and complex nanostructures: A semi-empirical Hamiltonian method. **2015**, 64, 187302		
96	Liquid Interfaces: Dielectric Constants and Electrical Properties of Monolayers. 3858-3867		
95	Fundamental Structural, Electronic, and Chemical Properties of Carbon Nanostructures: Graphene, Fullerenes, Carbon Nanotubes, and Their Derivatives. **2016**, 1-84		
94	Quantum Mechanics for Quantum Chemistry. **2016**, 357-549		
93	Modeling Molecular Aromaticity. **2016**, 441-522		
92	Open-Shell Systems and Local Spins. **2016**, 115-136		
91	Study of vacancy migration as a function of boron substitution in carbon nanolayers. *Izvestiya Vysshikh Uchebnykh Zavedenii Materialy Elektronnoi Tekhniki = Materials of Electronics Engineering*, **2016**, 19, 249-253	0.2	
90	Experimental and Quantum Chemical Studies of the Inhibition of Copper with Sodium Dodecyl Sulphate (SDS) in Acidic Medium. *Engineering*, **2018**, 10, 851-862	0.4	0
89	Quantum Mechanics. 320-344		
88	ESTUDO DE PRIMEIROS PRINC^ PIOS DE DERIVADOS DA 2-METIL IMIDAZOLINA: MODELO DE INIBIDOR DE CORROS^ O.		
87	Vacancy Transport Properties in Boron-Carbon BC3 Nanotubes. *NBI Technologies*, **2019**, 38-44	0	
86	Inhibition Performance of Some Sulfonylurea on Copper Corrosion in Nitric Acid Solution Evaluated Theoretically by DFT Calculations. *Open Journal of Physical Chemistry*, **2020**, 10, 139-157	0.5	1
85	Inhomogeneities of charge distribution in porous graphitic carbon nitride g-CxNy nanosheets. *European Physical Journal D*, **2020**, 74, 1	1.3	
84	Investigation of mechanisms of interaction of components of medicinal coating of medical stents based on PVP with introduced carbon nanotubes. **2020**,		
83	Molecular Modelling. *Springer Series in Materials Science*, **2020**, 3-48	0.9	
82	The research of the possibility of using carbon nanotubulenes in dentistry. **2020**,		

81	The nanowire modeling on the two-dimensional hexagonal boron nitride surface. **2020**,		
80	Hybrid Potentials for Molecular Systems in the Condensed Phase. **2002**, 125-151		
79	Photoelectron Spectroscopy of Low-Dimensional Organic Systems. **2002**, 283-315		
78	Semiempirical Thermochemistry: A Brief Survey. **2001**, 235-245		
77	Theoretical Studies of Growth Reactions on Diamond Surfaces. **2004**, 266-307		1
76	Towards Fast and Reliable Quantum Chemical Modelling of Macromolecules. **2006**, 315-341		0
75	Potential chemical relationships of polycyclic aromatic hydrocarbons and c-C3H2. **1988**, 178-179		
74	An Introduction to Molecular Modeling. 1-25		
73	About the Creation of Sensor of New Firefighting, Devices Based on Nanostructures for Determination of Carbon Monoxide and Carbon Dioxide Components. *Lecture Notes in Networks and Systems*, **2021**, 277-287	0.5	
72	Nanofilters Based on Carbon Nanomaterials for Cleaning Liquids. *Lecture Notes in Networks and Systems*, **2021**, 297-306	0.5	
71	Theoretical and experimental studies for different compounds to calculate: electronic transfer, energy gap and NLO properties. *IOP Conference Series: Materials Science and Engineering*, **2020**, 928, 072010	0.4	
70	Structural and Electronic Factors Governing the Action of Anticonvulsants. *Journal of Drug Delivery and Therapeutics*, **2020**, 10, 67-73	1.3	
69	Two sides of thermal stability of energetic liquid: Vaporization and decomposition of 3-methylfuroxan. *Journal of Molecular Liquids*, **2021**, 348, 118059	6	1
68	A review of quantum chemical methods for treating energetic molecules. *Energetic Materials Frontiers*, **2021**, 2, 292-292	3.3	3
67	Construction of poly-N-heterocyclic scaffolds via the controlled reactivity of Cu-allenylidene intermediates. *Communications Chemistry*, **2021**, 4,	6.3	3
66	Electrochemical and Computational Examination of Camellia Sinensis Assamica Biomolecules Ability to Retard Mild Steel Corrosion in Sodium Chloride Solutions. *Journal of Bio- and Tribo-Corrosion*, **2022**, 8, 1	2.9	2
65	Estimation of electron absorption spectra and lifetime of the two lowest singlet excited states of pyrimidine nucleobases and their derivatives. *Journal of Molecular Structure*, **2021**, 1250, 131863	3.4	2
64	Is tetramethyleneethane a ground state triplet?. *Journal of Chemical Sciences*, **1993**, 105, 53-62	1.8	3

63	Molecular electric field mapping of some anions and cations of 2- aminopurine and 6- thioguanine. *Journal of Chemical Sciences*, **1994**, 106, 277-282	1.8	1
62	Intermediate hardness decoupling schemes for chemical reactivity. *Journal of Chemical Sciences*, **1994**, 106, 353-378	1.8	3
61	Experimental and computational (AM1, MNDO, PM3) studies on the hydrolysis rates of ethylene ketals in 1,3-cyclohexanediones. *Journal of Chemical Sciences*, **1996**, 108, 51-56	1.8	
60	Effect of optimised hybridization displacement charge on the description of molecular electrostatic potentials of some substituted acetaldehydes. *Journal of Chemical Sciences*, **1996**, 108, 469	1.8	1
59	A semiempirical MO study of tautomerism and the electronic structure of barbituric acid. *Journal of Chemical Sciences*, **1998**, 110, 535	1.8	8
58	MNDO-EHP method for the calculation of vertical excitation energies. *Journal of Chemical Sciences*, **1990**, 102, 751	1.8	1
57	Density functional theory and molecular dynamics simulation studies of bio-based fatty hydrazide-corrosion inhibitors on Fe (1 1 0) in acidic media. *Journal of Molecular Liquids*, **2022**, 347, 118321	6	2
56	Synthesis, characterizations of aryl-substituted dithiodibenzothioate derivatives, and investigating their anti-Alzheimer's properties.. *Journal of Biomolecular Structure and Dynamics*, **2022**, 1-18	3.6	
55	Evaluating the Accuracy of the QCEIMS Approach for Computational Prediction of Electron Ionization Mass Spectra of Purines and Pyrimidines.. *Metabolites*, **2022**, 12,	5.6	0
54	Theoretical Studies of Conducting Polymers: A Mini Review. *New Journal of Chemistry*,	3.6	1
53	Quantum-chemical studies of the antioxidant effectiveness of para -phenylene diamines. *Journal of Vinyl and Additive Technology*,	2	1
52	X-ray diffraction and vibrational data for a series of triphosphates type MIINa3P3O10.12H2O (MII = Cu, Ni and Mg) and their anhydrous forms MIINa3P3O10. *Journal of the Indian Chemical Society*, **2022**, 100449		
51	Synthesis, characterizations, crystal structure, inhibition effects and theoretical study of novel Schiff base on the corrosion of carbon steel in 1 M HCl. *Journal of Molecular Structure*, **2022**, 1261, 132852	3.4	0
50	Chemical preparation, crystal structure and vibrational study of MnNa3P3O10.12H2O and X-ray characterization of the new anhydrous triphosphate MnNa3P3O10. *Phase Transitions*, **2022**, 95, 50-63	1.3	1
49	Electronic Ionization of Cytosine Molecules. *Surface Engineering and Applied Electrochemistry*, **2022**, 58, 82-86	0.8	
48	Review on the QM/MM Methodologies and Their Application to Metalloproteins.. *Molecules*, **2022**, 27,	4.8	1
47	Toward Chemical Accuracy in Predicting Enthalpies of Formation with General-Purpose Data-Driven Methods.. *Journal of Physical Chemistry Letters*, **2022**, 3479-3491	6.4	5
46	Tracing the Primordial Chemical Life of Glycine: A Review from Quantum Chemical Simulations.. *International Journal of Molecular Sciences*, **2022**, 23,	6.3	0

45	Bio-Inspired Macromolecular Ordering of Elastomers for Enhanced Contact Electrification and Triboelectric Energy Harvesting. *Advanced Materials Technologies*, 2200162	6.8	2
44	Quantum Chemical Approaches to the Calculation of NMR Parameters: From Fundamentals to Recent Advances. *Magnetochemistry*, **2022**, 8, 50	3.1	3
43	Computational Modelling of Supramolecular Polymers. **2022**, 341-384		
42	Nano-metallic Semiconductor towards the Vibrational Analysis and Harmonic Linear Combination. *Russian Journal of Physical Chemistry A*, **2022**, 96, 1051-1061	0.7	
41	Modulation of the 20S Proteasome Activity by Porphyrin Derivatives Is Steered through Their Charge Distribution. *Biomolecules*, **2022**, 12, 741	5.9	
40	MolE8: Finding DFT Potential Energy Surface Minima Values from Force-Field Optimised Organic Molecules with New Machine Learning Representations. *Chemical Science*,	9.4	
39	A theoretical study of the valence tautomerism of 1H-pyrazolium-4-olates (X = O) and related compounds (X = S, Se, NH): relative stabilities, protonation effects, and tautomerization barriers. *Structural Chemistry*,	1.8	
38	Electrostatic potential mapping of nucleic acid constituents: I. Guanine, cytosine and the G-C base pair. **1989**, 101,		1
37	Detection of impurities in water by using nanostructures. *AIP Conference Proceedings*, **2022**,	0	
36	Identification of the impurities in the alcohol-containing substances with the use of nanostructures. *AIP Conference Proceedings*, **2022**,	0	
35	The Conformational Landscape Of Aminoglycine. *Journal of Molecular Spectroscopy*, **2022**, 111667	1.3	
34	Nonadiabatic Molecular Dynamics with Extended Density Functional Tight-Binding: Application to Nanocrystals and Periodic Solids. *Journal of Chemical Theory and Computation*,	6.4	1
33	Deep learning of dynamically responsive chemical Hamiltonians with semiempirical quantum mechanics. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119,	11.5	2
32	A quantum-chemical study of the mechanism of ionic conductivity in alkali borate glasses. *Glass Physics and Chemistry*, **2000**, 26, 418-424	0.7	4
31	Investigation of Two Corrosion Inhibitors in Acidic Medium Using Weight Loss, Electrochemical Study, Surface Analysis, and Computational Calculation. *Journal of Bio- and Tribo-Corrosion*, **2022**, 8,	2.9	0
30	ULYSSES: An Efficient and Easy to Use Semiempirical Library for C++. **2022**, 62, 3685-3694		2
29	Different timescales during ultrafast stilbene isomerization in the gas and liquid phases revealed using time-resolved photoelectron spectroscopy.		5
28	Carbon Nanodots from an In Silico Perspective. **2022**, 122, 13709-13799		2

27	Semiempirical quantum mechanical methods. **2023**, 67-92	0
26	Partition of the electronic energy of the PM7 method via the interacting quantum atoms approach. **2022**, 24, 19521-19530	1
25	A B3LYP/DFT Study on the Structure Activity Relationship for Benzimidazole Derivatives in Water Solution. **2022**, 16, 579-589	0
24	Beyond the Ground State: Predicting Electron Ionization Mass Spectra Using Excited-State Molecular Dynamics. **2022**, 62, 4403-4410	0
23	Cost-Effective Implementation of Multiconformer Transition State Theory for Alkoxy Radical Unimolecular Reactions. **2022**, 126, 6483-6494	1
22	Comparative study of electronic, optoelectronic, optical, and thermodynamic properties of two ovalene molecules and their derivatives functionalized with potassium and chlorine atoms.	0
21	The Accuracy of Semi-Empirical Quantum Chemistry Methods on Soot Formation Simulation. **2022**, 23, 13371	1
20	Smooth polymers charge negatively: Controlling contact electrification polarity in polymers. **2022**, 104, 107914	1
19	Photochemistry of Biological Systems: Excited-State Electronic Structure Calculations and Nonadiabatic Dynamics Simulations with QM/MM Methods. **2022**,	0
18	The vertical excitation energies and a lifetime of the two lowest singlet excited states of the conjugated polyenes from C2 to C22 : Ab initio, DFT, and semiclassical MNDO-MD simulations.	1
17	Accuracy of Computational Chemistry Methods to Calculate Organic Contaminant Molecular Properties. **2022**, 7,	0
16	An Improved Parameterization Procedure for NDDO-Descendant Semiempirical Methods.	0
15	Interactions of heparin derivatives with recombinant human keratinocyte growth factor: Structural stability and bioactivity effect study.	0
14	Investigation on Hydrazonobenzenesulfonamides as Human Carbonic Anhydrase I, II, IX and XII Inhibitors. **2023**, 28, 91	0
13	Ultra-Fast Semi-Empirical Quantum Chemistry for High-Throughput Computational Campaigns with Sparrow.	0
12	Long-range Corrected Fragment Molecular Orbital Density-Functional Tight-binding Method for Excited States in Large Molecular Systems.	1
11	Theoretical Investigation of the Nonlinear Optical and Charge Transport Properties of N-(4-Methoxybenzylidene) Isonicotinohydrazone and Some of Its Derivatives: A DFT and TD-DFT Study. **2023**, 2023, 1-14	0
10	A specific MNDO parameterization for water. **2023**, 158, 034106	0

9	Anti-corrosive non-aqueous DBSA/MEA lamellar liquid crystal lubrication system. **2023**, 639, 454-463	0
8	Discovery of a spirocyclic 3-bromo-4,5-dihydroisoxazole covalent inhibitor of hGAPDH with antiproliferative activity against pancreatic cancer cells. **2023**, 254, 115286	0
7	Study of Some Azo Derivatives as Corrosion Inhibitors for Mild Steel in 1 M H2SO4. **2022**, 58, 708-719	0
6	Model selection in atomistic simulation. **2023**, 158, 134103	0
5	Corrosion inhibition efficiency and quantum chemical studies of some organic compounds: theoretical evaluation. **2023**,	0
4	Vertical Excitation Energies and Lifetimes of the Two Lowest Singlet Excited States of Cytosine, 5-Aza-cytosine, and the Triazine Family: Quantum Mechanics/Molecular Mechanics Studies. **2023**, 19, 1976-1985	0
3	An improved parameterization procedure for NDDO-descendant semi-empirical methods. **2023**, 29,	0
2	Density functional theory (DFT)-based molecular modeling. **2023**, 115-133	0
1	Mechanistic Study of Lithium-Ion Battery Cathode Recycling Using Deep Eutectic Solvents. **2023**, 11, 6914-6922	0