The calculation of small molecular interactions by the differences of separate total energies. Some procedures with reduced errors

DOI: 10.1080/00268977000101561
Molecular Physics, 1970, 19, 553-566.

#	Paper	IF	Citations
2280	Two Geometrical Isomers of a 1D Coordination Polymer: Rationalization by Theoretical Calculations and Variation of Electrical Properties with the Change in Binding Mode of Dicarboxylate Linker.		
2279	Importance of Interactions Involving Chelate Rings in Addition to the Tetrel Bonds in Crystal Engineering: A Combined Experimental and Theoretical Study on a Series of Hemi- and Holodirected Nickel(II)/Lead(II) Complexes.		
2278	Understanding and Controlling PolymerOrganometallic Precursor Interactions in Sequential Infiltration Synthesis.		
2277	Descriptor-Based Rational Design of Two-Dimensional Self-Assembled Nanoarchitectures Stabilized by Hydrogen Bonds.		
2276	RhodiumOrganic Cuboctahedra as Porous Solids with Strong Binding Sites.		
2275	A Series of Lanthanide-Based MetalOrganic Frameworks Derived from Furan-2,5-dicarboxylate and Glutarate: Structure-Corroborated Density Functional Theory Study, Magnetocaloric Effect, Slow Relaxation of Magnetization, and Luminescent Properties.		
2274	Triple-Pnictogen Bonding as a Tool for Supramolecular Assembly.		
2273	Many-Body Interactions in Ice.		
2272	Comprehensive Thermochemical Benchmark Set of Realistic Closed-Shell Metal Organic Reactions.		
2271	Octapodal Corannulene Porphyrin-Based Assemblies: Allosteric Behavior in Fullerene Hosting.		
2270	Domino Reaction of Aromatic Aldehydes and 1,3-Indanediones for Construction of Bicyclo[2.2.2]octanes and Dibenzo[b,g]indeno[1,2:3,4]fluoreno[1,2d]oxonines.		
2269	Exploring the Reactivity of Hydrofluoropolyethers toward OH through a Cost-Effective Protocol for Calculating Multiconformer Transition State Theory Rate Constants.		
2268	Assignment of Infrared-Active Combination Bands in the Vibrational Spectra of Protonated Molecular Clusters Using Driven Classical Trajectories: Application to N4H+ and N4D+.		
2267	Structural Effects on the Norrish Type I Bond Cleavage of Tropospherically Important Carbonyls.		
2266	Collisional Energy Transfer from Vibrationally Excited Hydrogen Isocyanide.		
2265	Electronic Spectrum and Photodissociation Chemistry of the 1Butyn-3-yl Cation, H3CCHCCH+.		
2264	Chemisorption of Acetophenone on Si(111)7 7. Polar Aromatic Molecule on Electronically Complex Surface.		

2245 Systematic Modulation of Charge Transport in Molecular Devices through Facile Control of MoleculeElectrode Coupling Using a Double Self-Assembled Monolayer Nanowire Junction.

2244 Halogen Bonding Promotes Higher Dye-Sensitized Solar Cell Photovoltages.

2243 Three-in-One: Sensing, Self-Assembly, and Cascade Catalysis of Cyclodextrin Modified Gold Nanoparticles.

2242 Half-Sandwich Complexes of an Extremely Electron-Donating Redox-Active 6Diborabenzene Ligand.

2241 Nucleoside Analogue-Based Supramolecular Nanodrugs Driven by Molecular Recognition for Synergistic Cancer Therapy.

2240 Integrating Organic Lewis Acid and Redox Catalysis: The Phenalenyl Cation in Dual Role.

2239 Understanding and Exploitation of Neighboring Heteroatom Effect for the Mild NArylation of Heterocycles with Diaryliodonium Salts under Aqueous Conditions: A Theoretical and Experimental Mechanistic Study.

2238 Mechanistic Perspectives in the Regioselective Indole Addition to Unsymmetrical Silyloxyallyl Cations.

2237 Naphtho[2,1e]1,2-azaphosphorine 2Oxide Derivatives: Synthesis, Optoelectronic Properties and Self-Dimerization Phenomena.

2236 Ab Initio Characterization of the Electrostatic Complexes Formed by H2 Molecule and Cr+, Mn+, Cu+, and Zn+ Cations.

2235 Remarkable Structure and Elasticity Relaxation Dynamics of Poly(diallyldimethylammonium chloride)Poly(acrylic acid) Multilayer Films.

2234 Methane Adsorption in Zr-Based MOFs: Comparison and Critical Evaluation of Force Fields.

2233 Oxidation Enhances Aerosol Nucleation: Measurement of Kinetic Pickup Probability of Organic Molecules on Hydrated Acid Clusters.

2232 Influence of the Anomeric Conformation in the Intermolecular Interactions of Glucose.

2231 Rotational Characterization of an n * Interaction in a PyridineFormaldehyde Adduct.

2230 CF Bond Activation of a Perfluorinated Ligand Leading to Nucleophilic Fluorination of an Organic Electrophile.

2229 Structure and Dynamics of Iron Pentacarbonyl.

2228 Modeling Key Pathways Proposed for the Formation and Evolution of Cocktail-Type Systems in Pd-Catalyzed Reactions Involving ArX Reagents.

2227 High-Concentration Ether Electrolytes for Stable High-Voltage Lithium Metal Batteries.

2226 Gd-Dots with Strong LigandWater Interaction for Ultrasensitive Magnetic Resonance Renography.

2225 Functionalized Phosphorene Quantum Dots as Efficient Electrocatalyst for Oxygen Evolution Reaction.

2224 Pyridinium Containing Amide Based Polymeric Ionic Liquids for CO2/CH4 Separation.

2223 Dispersion and Halogen-Bonding Interactions: Binding of the Axial Conformers of Monohalo- and ()-trans-1,2-Dihalocyclohexanes in Enantiopure Alleno-Acetylenic Cages.

2222 .

2221 Anion Transport with Pnictogen Bonds in Direct Comparison with Chalcogen and Halogen Bonds.

2220 Chemiresistive Detection of Gaseous Hydrocarbons and Interrogation of Charge Transport in Cu[Ni(2,3-pyrazinedithiolate)2] by Gas Adsorption.

2219 Cocrystals of Fluconazole with Aromatic Carboxylic Acids: Competition between Anhydrous and Hydrated Solid Forms.

2218 Deciphering Solvent Effect on Crystal Growth of Energetic Materials for Accurate Morphology Prediction.

2217 Enhancement of CO2 Uptake and Selectivity in a MetalOrganic Framework by the Incorporation of Thiophene Functionality.

2216 On Transannulation in Azaphosphatranes: Synthesis and Theoretical Analysis.

2215 Intricacies of van der Waals Interactions in Systems with Elongated Bonds Revealed by Electron-Groups Embedding and High-Level Coupled-Cluster Approaches.

2214 Cation Interactions between Methylated Ammonium Groups and Tryptophan in the CHARMM36 Additive Force Field.

2213 PCILON. perturbative configuration interaction using localized orbitals and numerical integration. I. Numerical integration techniques for the calculation of Hamiltonian matrix elements between localized orbitals. **1972**, 6, 575-591 7

2212 Counterpoise orbital basis in SCF computations of conformational energies of molecules. **1974**, 29, 123-127 10

2211 Ab initio molecular orbital calculations on the water-carbon dioxide system: Molecular complexes. **1975**, 30, 58-59 76

2210 Weak intermolecular interaction. **1975**, 36, 215-220 60

2209	Semiempirical estimates of the correlation energy in small clusters of hydrogen atoms. **1975**, 40, 287-295		3
2208	Ghost orbitals and the basis set extension effects. **1976**, 39, 612-614		85
2207	Studies on the lithium bond. **1976**, 44, 465-467		20
2206	An application of counterpoise method to a hydrogen bonded system. **1976**, 34, 145-146		14
2205	Calculations of Intermolecular Interaction Energies. **1976**, 2, 1-66		1
2204	The computation of intermolecular forces with Gaussian basis functions. Illustration with He2. **1977**, 67, 4696-4700		15
2203	On basis set effects in SCF calculations of the interaction energy between closed-shell atoms. **1977**, 44, 399-404		43
2202	An ab initio investigation into the SN2 reaction: Frontside attack versus backside attack in the reaction of F with CH3F. **1977**, 44, 245-256		46
2201	Exchange polarization effects in the interaction of closed-shell systems. **1977**, 46, 277-290		79
2200	A simple theoretical model for the van der Waals potential at intermediate distances. II. Anisotropic potentials of He H2 and Ne H2. **1978**, 68, 5501-5517		135
2199	AB initio studies of chemical equilibria. Application of many-body rayleigh-schr dinger perturbation theory up to third order to the proton affinity of water. **1978**, 58, 83-86		5
2198	A Theoretical Study of Complex Formation between Formaldehyde and Lithium. **1978**, 61, 1193-1199		12
2197	The calculation of intermolecular forces. A critical examination of the Gordon-Kim model. **1978**, 27, 893-912		84
2196	A calculation of the helium pair polarizability including correlation effects. *Molecular Physics*, **1978**, 36, 541-551	1.7	74
2195	Ab initio molecular orbital calculations on hydrogen- and non-hydrogen-bonded complexes. H2CO H2O and H2CO H2S. *Molecular Physics*, **1979**, 38, 1051-1059	1.7	17
2194	Counterpoise-corrected SCF and Gordon Kim electron gas interaction potentials for NH3-He. **1979**, 71, 1418-1425		22
2193	Correction for basis superposition error in correlated wavefunctions. **1979**, 65, 127-131		29
2192	Ab initio studies of chemical equilibria. A refined approach to the reaction NH2 + H2 ? NH3 + H **1979**, 61, 85-87		3

2191	Possible improvements of the interaction energy calculated using minimal basis sets. **1979**, 51, 219-240		210
2190	Nonempirical calculations for molecules in restricted bases of Gaussian functions. **1979**, 19, 513-518		
2189	Minimal basis sets in calculations of intermolecular interaction energies. **1979**, 54, 187-203		58
2188	Modern state of intermolecular interaction theory. **1979**, 16, 445-465		6
2187	Symmetry-adapted double-perturbation analysis of intramolecular correlation effects in weak intermolecular interactions. *Molecular Physics*, **1979**, 38, 191-208	1.7	213
2186	Configuration interaction calculations of the helium pair potential including CI superposition corrections. *Molecular Physics*, **1979**, 37, 1529-1541	1.7	32
2185	Ab initio calculations of intermolecular potentials. *Molecular Physics*, **1980**, 40, 1273-1284	1.7	19
2184	Non-additivity in water-ion-water interactions. **1980**, 55, 257-266		115
2183	Many-orbital cluster expansion for the exchange-repulsion nonadditivity in the interaction of rare gas atoms. The neon trimer. **1980**, 56, 199-210		36
2182	Nonadditivity of interaction in water trimers. **1980**, 17, 377-398		161
2181	Interaction of methane molecules. **1980**, 17, 429-448		32
2180	Theoretical study of some Van der Waals molecules. **1980**, 17, 775-798		33
2179	Nonadditive effects in metal clusters and chemisorption. Pseudopotential study of palladium clusters. **1980**, 18, 595-600		11
2178	A systematic preparation of new contracted Gaussian-type orbital sets. III. Second-row atoms from Li through ne. **1980**, 1, 205-228		438
2177	Quantum chemical investigations of charge transfer interactions in relation to the electronic theory of cancer. IV. The interaction of formamide and the enol tautomers of several glyoxals. **1980**, 1, 400-406		4
2176	Ab initio study of β-lactam antibiotics. II. Potential energy surface for the amidic CN bond breaking in the 3-cephem + OH^- reaction and comparison with the β-lactam + OH^- reaction. **1980**, 45, 291-304		30
2175	Ab initio study of the hydration complexes of HCO_3^-. **1980**, 53, 95-103		7
2174	Ab initio calculations of the interaction of ions with neutral ligands. Pair potentials for Li^+/ether, Li^+/thioether and Li^+/amide systems. **1980**, 72, 3096-3102		25

2173	A systematic preparation of new contracted Gaussian-type orbital basis sets. II. Test basis set for Cu2 molecule with and without splitting of the outer orbitals. **1980**, 72, 399-405	96
2172	Correlation effects in the isomeric cyanides: HNC<-HCN, LiNC<-gLiCN, and BNC<-gBCN. **1980**, 72, 986-991	75
2171	The polarizability of H2 in the triplet state. **1980**, 72, 2832-2840	41
2170	Monte Carlo simulations of water clusters around Zn++ and a linear Zn++?CO2 complex. **1980**, 72, 260-263	54
2169	Ab initio studies of the interactions in Van der Waals molecules. **1980**, 1-51	182
2168	Refined ab initio calculation of the potential energy surface of the He–H2 interaction with special emphasis to the region of the van der Waals minimum. **1980**, 73, 1880-1897	202
2167	The CO2?HF complex: A theoretical study (4–31G, 6–31G* + dispersion energy) of the stationary points and thermodynamics of formation. **1981**, 85, 241-247	8
2166	Energy Decomposition Analysis of Molecular Interactions. **1981**, 215-242	107
2165	Monte Carlo simulations of liquid and solid nitrogen based on an ab initio MO–CAO–SCF–CI potential. **1981**, 74, 2896-2903	22
2164	Self-consistent, nonorthogonal group function approximation for polyatomic systems. II. Analysis of noncovalent interactions. **1981**, 74, 6298-6306	48
2163	EFFECTIVE POTENTIAL METHODS FOR USE IN ELECTRONIC STRUCTURE CALCULATIONS OF LARGE MOLECULES*. **1981**, 367, 17-34	9
2162	AB-INITIO MODPOT/VRDDO/MERGE CALCULATIONS ON LARGE BIOMEDICAL MOLECULES AND ELECTROSTATIC MOLECULAR POTENTIAL CONTOUR MAPS*. **1981**, 367, 452-477	7
2161	Molecular potential, cation binding, and hydration properties of the carboxylate anion. Ab initio studies with an extended polarized basis set. **1981**, 2, 87-95	25
2160	Methane in aqueous solution at 300 K. **1981**, 82, 147-152	26
2159	HF-ClF: minima on the 4-31G and 4-31G* energy hypersurfaces and thermodynamics of formation. **1981**, 82, 469-472	17
2158	Electron density redistribution in the stabilization of a molecular stacking complex: The nature and correction of basis set superposition errors. **1981**, 2, 73-82	11
2157	A systematic preparation of new contracted Gaussian-type orbital sets. IV. The effect of additional 3s functions introduced by the use of the six-membered 3dGTOs. **1981**, 2, 96-99	28
2156	A systematic preparation of new contracted Gaussian- type orbital sets. VII. MINI-3, MINI-4, MIDI-3, and MIDI-4 sets for transition metal atoms. **1981**, 2, 278-286	56

2155	SCF non-additivity of the interaction energy in the neon trimer. **1981**, 78, 361-365		33
2154	Anion-ligand interactions: ab initio study of the binding of H2O, CO2 and SO2 to the nitrite ion. **1981**, 81, 195-200		15
2153	Magnesium and calcium cation–ligand interactions within the pseudopotential approach. II. Cation–GABA interactions. **1981**, 19, 463-475		6
2152	Ghost orbitals in semiempirical methods. Estimation of basis set superposition error. **1981**, 19, 891-900		11
2151	Strategy for computer-generated theoretical and quantum chemical prediction of toxicity and toxicology (and pharmacology in general). **1981**, 20, 419-439		6
2150	Hydrogen bonding in oxirane–HF; an ab initio SCF-MO study. **1981**, 20, 71-76		5
2149	AB initio calculations of the OH?H2 potential energy surface. **1981**, 57, 217-225		45
2148	A theoretical study on the reactivity and spectra of H2CO and HCOH. A dimeric model for nonzero pressure formaldehyde photochemistry. **1981**, 74, 5744-5757		20
2147	Theoretical computation of the binding energy of BH3NH3, a difficult case. **1981**, 75, 4980-4982		25
2146	Intermolecular potentials for ammonia based on SCF–MO calculations. **1981**, 74, 1211-1216		70
2145	Intermolecular Forces. **1981**,		54
2144	Ab initio calculations as a source of intermolecular potential functions. Ethanol–water with a minimal basis set. **1981**, 74, 3980-3988		18
2143	Theoretical investigation of rotational rainbow structures in XNa2 collisions using CI potential surfaces. I. Rigid-rotor X = He scattering and comparison with state-to-state experiments. **1981**, 74, 3916-3928		50
2142	Pair polarizabilities of the heavy inert gases II. SCF calculations of the pair polarizabilities of krypton and xenon. *Molecular Physics*, **1982**, 47, 193-208	1.7	33
2141	Theoretical investigation of rotational rainbow structures in XNa2 collisions using CI potential surfaces. III. Rigid-rotor X = Ne scattering. **1982**, 76, 895-912		36
2140	Mo/ller–Plesset treatment of electron correlation effects in (HOHOH)–**1982**, 77, 4586-4593		58
2139	Improved procedure for analysis of electron density redistribution in molecular complexes. **1982**, 77, 4529-4541		26
2138	(Cl2)2: Planar or not planar? A charge transfer complex or a van der Waals molecule?. **1982**, 77, 2691-2692		1

2137	The (H2)2 potential surface and the interaction between hydrogen molecules at low temperatures. **1982**, 76, 6073-6087		56
2136	Ab initio calculations of exchange repulsion between two Ar atoms. *Molecular Physics*, **1982**, 45, 1271-1278	1.7	13
2135	Ab initio calculations of dilithiopropenes. **1982**, 79, 3922-6		18
2134	Basis set refinement in theoretical modelling of molecular electronic structures. *Molecular Physics*, **1982**, 47, 785-809	1.7	9
2133	An SCF calculation of the pair polarizability of argon. *Molecular Physics*, **1982**, 45, 1-15	1.7	53
2132	On the pair polarizability of helium. *Molecular Physics*, **1982**, 45, 17-32	1.7	63
2131	Intermolecular interaction energies from minimal-basis SCF calculations. Interactions pertinent to formaldehyde hydration. **1982**, 88, 23-35		16
2130	A molecular orbital study of the hydration of ions. The role of nonadditive effects in the hydration shells around Mg2+ and Ca2+. **1982**, 76, 5405-5413		54
2129	Ab-initio SCF potential energy surfaces for the nucleophilic attack of hydride on coordinated carbon monoxide. **1982**, 61, 587-595		17
2128	An investigation of basis sets and basis set superposition error in transition metals using frozen core and frozen orbital techniques. **1982**, 69, 185-192		85
2127	Methanol in water solution at 300 K. **1982**, 86, 299-306		54
2126	Ab initio study of the pair potentials and electric dipole moments of the ArHe and NeHe diatoms. **1982**, 22, 133-143		1
2125	Ab initio SCF-MO study of hydrogen bonding in benzene□HF. **1982**, 24, 245-249		
2124	Basis set superposition effects on properties of interacting systems. Dipole moments and polarizabilities. **1982**, 61, 1-9		105
2123	Computations of intermolecular interactions: Expansion of a charge-transfer energy contribution in the framework of an additive procedure. Applications to hydrogen-bonded systems. **1982**, 22, 199-215		37
2122	Theoretical investigation of the electrophilic attack. IX. Ab initio study of the C2H4 □HF molecular complex. **1982**, 22, 631-637		7
2121	Quantum chemical investigations on group IA and IIA metal ion?DNA base complexes. **1983**, 76, L209-L212		17
2120	Structure of aggregates of water and Li+, Na+, or K+ counterions with nucleic acid in solution. **1983**, 11, 33-42		25

2119	The interaction of gamma-aminobutiric acid with hydrated Ca2+ and Mg2+. A pseudopotential ab initio study. **1983**, 104, 571-90	7
2118	Van der Waals molecules: Quantum chemistry, physical properties, and reactivity. **1983**, 23, 325-338	16
2117	Improved SCF interaction energy decomposition scheme corrected for basis set superposition effect. **1983**, 23, 847-854	83
2116	Importance of exchange effects in the deformation of interacting ions. **1983**, 23, 1843-1853	21
2115	On the artificial structure of the water dimer in the CNDO/2 method. **1983**, 24, 131-133	7
2114	Ab initio calculation of the heptamer (NH3)7 as a reasonable starting point for a description of the ammonia crystal. **1983**, 24, 687-695	12
2113	Modifications of the program Gaussian-70 **1983**, 23, 648-648	
2112	A theoretical investigation on the role of solvent in solvolytic reactions. **1983**, 63, 245-253	4
2111	Guidelines for development of basis sets for the first-order intermolecular interaction energy calculations. **1983**, 4, 506-512	18
2110	Full CI calculations on BH, H2O, NH3, and HF. **1983**, 95, 386-391	193
2109	Intermolecular potential of the acetonitrile dimer obtained from ab initio calculations. **1983**, 103, 55-58	19
2108	Full CI calibration of model hamiltonian, large basis set studies of the H2-H2 van der Waals interaction.. **1983**, 100, 51-58	7
2107	van der Waals interaction potentials: Many-body basis set superposition effects. **1983**, 101, 429-434	136
2106	The water dimer: Theory versus experiment. **1983**, 94, 198-201	103
2105	Theoretical study on the structure and stability of hydrogen-ion clusters Hn+ and Hn (n = 3, 5, 7, 9, 11, 13). **1983**, 80, 237-243	45
2104	Conformational energetics in hydrogen-bonded dimers. The unobserved CO?HF complex. **1983**, 80, 273-278	28
2103	Theoretical methods of calculating solvation effects. **1983**, 27, 79-123	16
2102	The influence of small monovalent cations on the hydrogen bonds of base pairs of DNA. **1983**, 78, 81-86	18

2101	The influence of Mg2+ ion on the hydrogen bonds of the adenine?thymine base pair. **1983**, 78, 177-180		33
2100	Metal ion influence on hydrogen bonds in solvent and ligands. **1983**, 79, 58-59		1
2099	Model MG-FSGO calculations of short range interactions. **1983**, 94, 267-273		
2098	A self consistent field molecular orbital study of the lithium-formaldehyde system. **1983**, 94, 299-303		1
2097	Electronic structure of small copper clusters. II. Localized d hole in excited states and ionized states of Cu2 and Cu3. **1983**, 78, 815-826		65
2096	The intermolecular potential of HF. *Molecular Physics*, **1983**, 50, 885-899	1.7	41
2095	Perturbation calculations of the interaction energy between closed-shell Hartree-Fock atoms. *Molecular Physics*, **1983**, 49, 1353-1373	1.7	31
2094	The extramolecular contributions to the photoelectron and soft x-ray photon chemical shift in solid and liquid benzene. **1983**, 79, 587-592		17
2093	Model MG-FSGO calculations of short range interactions. **1983**, 94, 267-273		
2092	A self consistent field molecular orbital study of the lithium-formaldehyde system. **1983**, 94, 299-303		1
2091	M dependence in the analysis of NH3He microwave double resonance experiments. **1983**, 78, 2170-2174		13
2090	Contributions to interatomic and intermolecular forces. *Molecular Physics*, **1983**, 49, 871-879	1.7	16
2089	On the basis set superposition error in potential surface investigations. I. Hydrogen-bonded complexes with standard basis set functions. **1983**, 78, 4606-4611		59
2088	Networks of water molecules in a proflavine deoxydinucleoside phosphate complex. **1983**, 1, 263-85		19
2087	The in-crystal polarizability of the fluoride ion. *Molecular Physics*, **1983**, 49, 913-923	1.7	109
2086	The long range model of intermolecular forces. *Molecular Physics*, **1983**, 50, 1349-1361	1.7	75
2085	van der Waals interaction potentials. *Molecular Physics*, **1983**, 50, 1295-1309	1.7	60
2084	A theoretical study of the interaction of N2 with water molecules. (H2O)n:N2, n=1. **1984**, 80, 2022-2028		22

2083	The interaction potentials for He-He and He-Li+. *Molecular Physics*, **1984**, 53, 233-240	1.7	14
2082	The electronic structure of small zinc clusters. Resemblance of the clusters to bulk Zn. **1984**, 80, 344-352		20
2081	Changes in the electronic structure and vibrational potential of hydrogen fluoride upon dimerization: A well-correlated (HF)2 potential energy surface. **1984**, 81, 5998-6006		134
2080	Effects of basis set and electron correlation on the calculated properties of the ammonia dimer. **1984**, 81, 407-409		72
2079	Intermolecular potentials for CH4, CH3F, CHF3, CH3Cl, CH2Cl2, CH3CN, and CO2. **1984**, 81, 1389-1395		105
2078	Water□water interaction potential: An approximation of the electron correlation contribution by a functional of the SCF density matrix. **1984**, 81, 2646-2651		132
2077	Model potential study of the interactions in Ar2, Kr2 and Xe2 dimers. *Molecular Physics*, **1984**, 52, 1495-1513	1.7	56
2076	Valence body study of the potential energy surface for the system He □HF. *Molecular Physics*, **1984**, 53, 161-182	1.7	21
2075	Local Structure and Bonding in Zeolites by Means of Quantum Chemical Ab Initio Calculations: Metal Cations, Metal Atoms and Framework Modification. **1984**, 18, 313-320		7
2074	Ab-initio quantum mechanical calculations of NMR chemical shifts in nucleic acid constituents. I. The Watson-Crick base pairs. **1984**, 2, 233-48		18
2073	The molecular electronic structure of the twenty-six lowest lying states of Li2 at short and intermediate internuclear separations. **1984**, 84, 463-475		128
2072	Effects of group IVB substituents on the proton affinity of alcohols and amines: A theoretical study. **1984**, 264, 163-168		3
2071	An intermolecular perturbation theory for the region of moderate overlap. *Molecular Physics*, **1984**, 53, 83-105	1.7	232
2070	Three-body contributions to the dipole polarizability of He3 clusters. **1984**, 104, 583-586		15
2069	Improvement of polarized double-zeta basis sets for molecular interactions. Complexes of NH3, OH2, and FH with H+ and Li+. **1984**, 105, 435-439		47
2068	Complete Cl calculations on the ground state of HeH. **1984**, 110, 40-42		13
2067	Potential energy curves for ground and excited states of NaLi from ab initio calculations with effective core polarization potentials. **1984**, 112, 120-128		61
2066	An ab initio study of the binding of N2 to Na+ and K+. **1984**, 110, 346-350		12

2065	Monte Carlo liquid water simulation with four-body interactions included. **1984**, 112, 426-430		117
2064	Ab initio study of the stepwise hydration of NO+. **1984**, 107, 107-111		18
2063	Compact contracted Gaussian-type basis sets for halogen atoms. Basis-set superposition effects on molecular properties. **1984**, 5, 146-161		81
2062	Quantum-mechanical and statistical mechanical studies of the torsional barrier of H2O2 in aqueous solution. **1984**, 25, 503-514		4
2061	Ab initio calculations of guanidinium□arboxylate interaction. **1984**, 26, 91-99		26
2060	Origin of high efficiency and specificity of biochemical reactions. **1984**, 26, 857-872		9
2059	Effective basis sets for calculations of exchange-repulsion energy. **1984**, 26, 971-982		68
2058	Monte Carlo liquid water simulations with four-body interactions included. **1984**, 26, 701-707		1
2057	Minimal basis set MINI-1 □powerful tool for calculating of molecular interactions. I. Neutral complexes. **1984**, 65, 279-290		70
2056	Interaction energy calculation scheme employing one-electron hamiltonian approximation for the evaluation of short-range interactions. **1984**, 66, 295-310		5
2055	In-crystal polarizabilities of alkali and halide ions. **1984**, 29, 1035-1042		181
2054	Studies of dispersion energy in hydrogen-bonded systems. H2O□HOH, H2O□HF, H3N□HF, HF□HF. **1984**, 80, 1535-1542		34
2053	Many-body energies in LiF. *Molecular Physics*, **1984**, 51, 1135-1139	1.7	12
2052	Ab initio quantum-chemical study on drug decomposition in solid state preparations. **1984**, 109, 177-193		2
2051	Intermolecular interactions : use of small basis sets in ab initio calculations. **1984**, 107, 49-57		6
2050	Quantum chemical investigations of charge transfer interactions in relation to the electronic theory of cancer. **1984**, 109, 73-86		
2049	Nonlocal polarizability densities and the effects of short-range interactions on molecular dipoles, quadrupoles, and polarizabilities. **1984**, 80, 393-407		53
2048	Ab initio calculations on the He□O2 potential energy surface. Hartree□ock instability of O2. **1984**, 81, 3168-3173		43

2047	Role of catalytic residues in the formation of a tetrahedral adduct in the acylation reaction of bovine beta-trypsin. A molecular orbital study. **1984**, 179, 103-23		19
2046	Ground-state properties of alkali dimers and their cations (including the elements Li, Na, and K) from ab initio calculations with effective core polarization potentials. **1984**, 80, 3311-3320		279
2045	Symmetry-adapted expansion and stable-conformation minima of the interaction potential of the H2O HF complex. *Molecular Physics*, **1984**, 51, 323-331	1.7	1
2044	An SCF-CI study of the water dimer potential surface and the effects of including the correlation energy, the basis set superposition error and the Davidson correction. *Molecular Physics*, **1985**, 55, 1097-1108	1.7	28
2043	van der Waals interaction potentials. *Molecular Physics*, **1985**, 54, 787-798	1.7	21
2042	Counterpoise corrections to the interaction energy components in bimolecular complexes. **1985**, 68, 271-283		91
2041	A pseudopotential study of the hydrogen bond in H2O H2S, H2S H2S and H2O H2Se systems. **1985**, 66, 375-393		9
2040	Ab initio studies of F (H2O)n and Cl (H2O)n clusters for n = 1, 2. **1985**, 27, 281-292		18
2039	Ab initio calculations on H transfer in the HF trimer. **1985**, 27, 781-786		12
2038	Steric and electronic structure of complexes of Li+, Na+, K+, Be2+, Mg2+, and Ca2+ Ions with N2 molecule. **1985**, 26, 350-354		3
2037	CEPA calculations of potential energy surfaces for open-shell systems.. **1985**, 92, 141-153		18
2036	Role of polarization functions in cation binding. H3N?Li+ and H2O?Li+. **1985**, 98, 59-70		13
2035	Interaction-optimized virtual orbitals. **1985**, 92, 255-262		7
2034	Determination of the basis set superposition error with DZP basis sets in SCF calculations: CO + H2, NH3 + H2, H2 + H2. **1985**, 92, 287-294		22
2033	Theoretical studies of lithium bonding in lithium chloride/aliphatic amine complexes. **1985**, 94, 55-63		18
2032	Model potential study of the interactions in ArHCl, ArHBr, KrHCl and XeHCl systems. **1985**, 100, 1-11		14
2031	The physical nature of catalytic activity due to the molecular environment in terms of intermolecular interaction theory: derivation of simplified models. **1985**, 30, 395-410		42
2030	Parallelism in computational chemistry: Applications in quantum and statistical mechanics. **1985**, 131, 74-102		9

2029	Energy decomposition analysis of borane monoammoniate: origin of the rotational barrier to nonrigid rotation. **1985**, 126, 381-384		4
2028	Non-empirical quantum chemical study of the siting and pairing of aluminium in the MFI framework. **1985**, 5, 165-172		143
2027	Ground- and excited-state properties of Li2 and Li2+ from ab initio calculations with effective core polarization potentials. **1985**, 92, 263-285		253
2026	The validity of electrostatic predictions of the shapes of van der Waals dimers. **1985**, 117, 400-408		84
2025	On the binding of water to the ammonium ion: The interplay of an improved basis set. Dispersion and zero-point energy. **1985**, 117, 419-423		28
2024	Second-quantization-based perturbation theory for intermolecular interactions without basis set superposition error. **1985**, 119, 538-542		39
2023	Ab initio calculations of intermolecular potentials. The ground state of the Ar?H2 van der Waals molecule. **1985**, 6, 39-45		13
2022	A systematic preparation of new contracted Gaussian-type orbitals. IX [54/5], [64/5], [64/6], [74/6], [74/7] and MAXI-1MAXI-5 from Li to Ne. **1985**, 6, 237-248		12
2021	Compact basis sets for LCAO-LSD calculations. Part II: Tests for Cr2 and Ni4. **1985**, 6, 533-537		21
2020	Dimer centred basis set in the calculations of the first-order interaction energy with CI wavefunction. *Molecular Physics*, **1985**, 54, 1173-1184	1.7	38
2019	The N2-N2 interaction. *Molecular Physics*, **1985**, 55, 1159-1169	1.7	75
2018	van der Waals interaction potentials. *Molecular Physics*, **1985**, 55, 199-210	1.7	45
2017	A variation-perturbation method for atomic and molecular interactions. I. Theory. **1985**, 83, 2316-2322		9
2016	Ab initio SCF and CI study of the NH+4?H2O complex. **1985**, 83, 2959-2964		14
2015	Model potential calculations for second-row transition metal molecules within the local-spin-density method. **1985**, 83, 4573-4580		165
2014	The excited states of Zn2 and Zn3. Inclusion of the correlation effects. **1985**, 82, 5608-5615		21
2013	Damped dispersion interaction energies for He-H2, Ne-H2, and Ar-H2. **1985**, 32, 1402-1411		11
2012	A minimal basis bond-orbital investigation of the linear water dimer. *Molecular Physics*, **1985**, 56, 1249-1269		23

2011	Systematic study of basis set superposition errors in the calculated interaction energy of two HF molecules. **1985**, 82, 2418-2426		539
2010	Rotationally inelastic scattering and potential calculations for He + CH4. *Molecular Physics*, **1985**, 55, 1255-1274	1.7	60
2009	Fluctuating dipoles and polarizabilities in ionic materials: Calculations on LiF. **1985**, 31, 5443-5455		80
2008	The electronic structure of the monomers, dimers, a trimer, the oxides and the borane complexes of the lithiated ammonias. **1985**, 122, 189-204		27
2007	A general approach to the potential energy functions of small polyatomic systems: Molecules and van der Waals molecules. **1985**, 120, 401-424		92
2006	Ab initio study of the alkali and alkaline-earth monohydroxides. **1986**, 84, 901-909		113
2005	Theoretical study of the diatomic alkali and alkaline-earth oxides. **1986**, 84, 4474-4480		97
2004	Extensive theoretical studies of the hydrogen-bonded complexes (H2O)2, (H2O)2H+, (HF)2, (HF)2H+, F2H□and (NH3)2. **1986**, 84, 2279-2289		621
2003	An ab initio investigation of possible intermediates in the reaction of the hydroxyl and hydroperoxyl radicals. **1986**, 84, 5013-5024		24
2002	Theoretical study of the X 1⊞ states of the alkali hydrides NaH□sH. **1986**, 85, 5158-5166		24
2001	The polarization-function counterpoise method. An application of the diagrammatic perturbation theory to the He⊞2 molecule in the region of the van der Waals minimum. **1986**, 85, 3448-3457		15
2000	Ab initio calculations on the positive ions of the alkaline-earth oxides, fluorides, and hydroxides. **1986**, 84, 4489-4496		41
1999	Intermolecular bonding and vibrations of the carbazole?B complexes (B=H2O, D2O, NH3). **1986**, 85, 1234-1246		49
1998	Intermolecular potentials for ammonia based on the test particle model and the coupled pair functional method. *Molecular Physics*, **1986**, 57, 1247-1264	1.7	109
1997	The role of electrostatics in molecular interactions: prediction of shapes and electronic properties of weakly bound complexes. **1986**, 5, 139-146		16
1996	The superposition error problem: The (HF)2 and (H2O)2 complexes at the SCF and MP2 levels. **1986**, 138, 377-385		42
1995	The introduction of polarization functions in the single-zeta bond-orbital method and an application to the ground state of the water molecule. **1986**, 135, 267-278		5
1994	On the acidic properties of compounds with C?C or N?N electrophilic double bonds. **1986**, 135, 299-328		11

1993	The hydrogen bonding influence on polarizability and hyperpolarizability. A derivative hartree-fock study of the electrical properties of hydrogen fluoride and the hydrogen fluoride dimer. **1986**, 135, 357-368		55
1992	The well-tempered GTF basis set and the ab initio molecular calculation. **1986**, 135, 403-408		14
1991	Ammonia dimer, linear or cyclic?. **1986**, 139, 233-240		13
1990	Charge distribution analysis on ArH2 system. **1986**, 136, 99-110		5
1989	The atom-surface interaction potential for He-NaCl: A model based on pairwise additivity. **1986**, 173, 337-350		43
1988	Simulations of complex chemical systems. **1986**, 127, 114-40		2
1987	Epstein-Nesbet calculation of interatomic interactions in the van der Waals region. *Molecular Physics*, **1986**, 59, 689-705	1.7	11
1986	van der Waals interaction potentials. *Molecular Physics*, **1986**, 57, 21-32	1.7	25
1985	Monte Carlo studies of aqueous solution of nitrogen using different potential energy surfaces. *Molecular Physics*, **1986**, 58, 65-83	1.7	7
1984	Perturbation calculations of molecular interaction energies: an example, HF....HF. **1986**, 128, 11-17		20
1983	Does the boys and bernardi function counterpoise method actually overcorrect the basis set superposition error?. **1986**, 129, 325-328		74
1982	Intermolecular interactions using small basis sets: Perturbation theory calculations avoiding basis set superposition error. **1986**, 128, 358-362		34
1981	Effect of secondary basis-set superposition error upon calculated vibrational intensities. **1986**, 131, 230-236		16
1980	The basis set superposition error in correlated electronic structure calculations. **1986**, 124, 370-375		196
1979	The full versus the virtual counterpoise correction for basis set superposition error in self-consistent field calculations. **1986**, 123, 56-61		58
1978	The interaction of O2 with water. **1986**, 125, 454-458		9
1977	A basis set superposition error from inadequate representation of the 1s core orbital in second-row elements. **1986**, 131, 367-369		1
1976	Ab initio determination of the proton affinities of small neutral and anionic molecules. **1986**, 7, 321-33		74

1975	The remarkably invariant interaction energies of lithium first-row compounds with water and with ammonia. **1986**, 7, 334-344		28
1974	Nonempirical Atom-Atom Potentials for Main Components of Intermolecular Interaction Energy. **1986**, 7, 693-700		32
1973	CEPA calculations of potential energy surfaces for open-shell systems. V. The O2-He Van der Waals potential. **1986**, 101, 243-257		12
1972	Counterpoise corrections to the evaluation of the bimolecular interaction energy components. **1986**, 69, 11-22		33
1971	Ab initio SCF calculations of the linear infinite chain of LiH according to the pseudo-lattice method. **1986**, 70, 227-236		1
1970	Intermolecular interactions: Elaboration on an additive procedure including an explicit charge-transfer contribution. **1986**, 29, 101-118		87
1969	Energetics of proton transfer between carbon atoms (H3CH ? CH3)⁺ **1986**, 29, 285-292		22
1968	Counterpoise corrections to the components of bimolecular energy interactions: An examination of three methods of decomposition. **1986**, 29, 373-378		24
1967	Weak intermolecular interactions: Statics and dynamics. **1986**, 29, 663-676		12
1966	Nitromethane dimer potential energy surface studies. **1986**, 30, 695-711		3
1965	A many-body perturbation theory and coupled cluster study of the water dimer. **1986**, 30, 437-443		24
1964	Investigation of the intermolecular interaction in the ethylene dimer by a modified CNDO method. **1986**, 21, 505-512		2
1963	Non-empirical study of the structure and stability of pentahalocarbonate anions CX_5^- (X ? F, Cl, Br). All-electron and valence-electron SCF calculations. **1986**, 101, 201-209		8
1962	MBPT studies of van der Waals molecules. III. The reliability of apparently accurate calculations for the magnesium dimer. **1986**, 103, 55-74		29
1961	Interaction of phospholipids (Lysophosphatidylethanolamines) with water and sodium cation. **1986**, 14, 49-56		4
1960	Intramolecular correlation correction to the first-order interaction energy between H2 molecules and its influence on the H2-H2 potential surface. *Molecular Physics*, **1986**, 57, 427-439	1.7	22
1959	Universal basis sets of elliptical functions. Applications to simple diatomic molecules. **1986**, 19, 17-32		16
1958	Stability and structure of cluster ions in the gas phase: Carbon dioxide with Cl⁻, H_3O^+, HCO_2^+, and HCO^+. **1986**, 84, 2091-2096		64

1957	Intermolecular potentials calculated by an extended geminal model: Theory. **1986**, 85, 262-273		28
1956	Pairwise-additive models for atom-surface interaction potentials: An ab initio study of He-LiF. **1986**, 33, 3724-3735		49
1955	Improved counterpoise corrections for the ab initio calculation of hydrogen bonding interactions. **1986**, 84, 2720-2725		71
1954	The importance of diffuse f functions for transition metals. **1986**, 84, 4485-4488		31
1953	STF HF wave functions from Sc to Zn and STF HF wave function for Cu2. **1986**, 85, 5895-5899		11
1952	Bound electronic states of HCl□**1986**, 85, 7232-7240		33
1951	Ab initio study of the hydrogen bonding interactions of formamide with water and methanol. **1986**, 84, 3271-3277		99
1950	About the overestimation of the basis set superposition error on interaction energy calculations for van der Waals systems. **1986**, 84, 5077-5080		28
1949	Vibrational relaxation of N2 by collision with He atoms. **1986**, 84, 3788-3797		52
1948	Correction of the basis set superposition error in SCF and MP2 interaction energies. The water dimer. **1986**, 84, 6328-6335		124
1947	Ab initio study of the ground state surface of Cu3. **1986**, 85, 7211-7215		34
1946	The potential energy surface of (NH3)2. **1986**, 84, 341-347		69
1945	MBPT studies of van der Waals molecules. *Molecular Physics*, **1986**, 59, 889-909	1.7	35
1944	Theoretical dissociation energies for the alkali and alkaline-earth monofluorides and monochlorides. **1986**, 84, 1687-1695		70
1943	Theoretical study of the 7□u state of N2. **1986**, 84, 6901-6906		23
1942	The electronic structure of small nickel clusters. **1986**, 85, 2875-2884		50
1941	Hartree-Fock ab initio approaches to the solution of some solid-state problems: state of the art and prospects. **1987**, 6, 367-384		3
1940	Proper correction for the basis set superposition error in SCF calculations of intermolecular interactions. *Molecular Physics*, **1987**, 61, 233-247	1.7	132

1939	Van der Waals interaction potentials. *Molecular Physics*, **1987**, 61, 1283-1293	1.7	18
1938	A test particle model potential for formamide and molecular dynamics simulations of the liquid. **1987**, 86, 5117-5126		81
1937	Ab initio ground state properties of neutral X2Y and ionic X2Y+ (X,Y=Li, Na, K) alkali trimers. **1987**, 87, 2854-2862		37
1936	An ab initio approach to the interaction of CF4 and CH4 with O2, CO2, N2, and CO. The nature of the interaction force in perfluorochemical artificial blood. **1987**, 87, 2158-2165		16
1935	Theoretical and experimental studies of the system Ca+(H2O)n for n=1 to 10. **1987**, 87, 1661-1665		34
1934	On the nonadditivity of the second-order exchange-dispersion energy in the interaction of three helium atoms. **1987**, 86, 937-946		40
1933	An ab initio quantum chemical study of the hydrogen- and □anti□hydrogen-bonded HF/ClF and HF/Cl2 dimers. **1987**, 87, 535-544		24
1932	The electronic and vibrational energies of two double-welled 3□u states of He2. **1987**, 87, 4000-4007		16
1931	Ab initio studies of the structures and energies of the H□(H2O) and H□(H2O)2 complexes. **1987**, 87, 2965-2975		37
1930	Neutral reactions in the presence of alkali ions. **1987**, 87, 6544-6552		11
1929	Mo/ller□Plesset perturbation theory for van der Waals complexes bound by electron correlation effects: Ground states of the Ar and Mg dimers. **1987**, 87, 3569-3579		68
1928	Primary and secondary basis set superposition error at the SCF and MP2 levels. H3N--Li+ and H2O--Li+. **1987**, 87, 1194-1204		77
1927	An ab initio study of hydrated chloride ion complexes: Evidence of polarization effects and nonadditivity. **1987**, 87, 5892-5894		35
1926	Structure, energetics, and vibrational spectrum of H2O□HCl. **1987**, 87, 5928-5936		62
1925	An ab initio study with counterpoise correction of ethylene dimer- and trimer-cations. **1987**, 151, 149-155		6
1924	Extended SCF calculations of repulsive interaction potential in Xe2. **1987**, 152, 185-188		1
1923	Potential energy surfaces for the X+?CO2 (X = Na, K) systems. **1987**, 149, 193-200		2
1922	Transition metal atom-water complexes: A quantum chemical study including electron correlation. **1987**, 149, 297-309		7

1921	Ab initio pseudopotential study of the first row transition metal monoxides and iron monohydride. **1987**, 86, 2123-2131	159
1920	Correlation correction to the Hartree-Fock total energy of solids. **1987**, 36, 891-897	71
1919	Interaction of atomic oxygen with copper clusters. **1987**, 86, 4030-4037	28
1918	Two-configuration potential energy surface for the Ca + HF -cCaF + H reaction. **1987**, 114, 241-249	6
1917	On the non-additivity of the basis set superposition error and how to prevent its appearance. **1987**, 72, 207-210	36
1916	Hydrogen-bonded complexes involving HF and HCl: the effects of electron correlation and anharmonicity. **1987**, 71, 41-57	48
1915	On the computational realization of planar tetracoordinate carbon. **1987**, 43, 1019-1026	6
1914	Hydrated carbonium ions as possible nitrosamine metabolites: An ab initio study. **1987**, 32, 123-131	2
1913	Direct calculation of the HartreeFock interaction energy via exchangePerturbation expansion. The He He interaction. **1987**, 32, 149-164	153
1912	The effect of ull and imited ounterpoise corrections with different basis sets on the energy and the equilibrium distance of hydrogen bonded dimers. **1987**, 32, 207-226	44
1911	Basis set extension effects on the He2 interaction energy components. **1987**, 32, 279-293	19
1910	Comparison of ab initio MODPOT interaction energy components against large basis set MBPT (4) calculations for nitromethane dimer. **1987**, 32, 645-660	7
1909	Equilbrium geometry and electrical polarizability of formic acid, formamide and their cyclic hydrogen-bonded paris. **1987**, 32, 85-103	13
1908	Frozen fragment reduced variational space analysis of hydrogen bonding interactions. Application to the water dimer. **1987**, 139, 15-22	363
1907	SCF theory of intermolecular interactions without basis set superposition error. **1987**, 136, 115-121	56
1906	Intermolecular SCF method without bsse: the closed-shell case. **1987**, 140, 558-564	56
1905	The electronic and vibrational energies of the 5g+ state of He2 which corresponds asymptotically to the interaction of two 1s2s 3S He atoms. **1987**, 139, 417-420	3
1904	Three-dimensional spatial characteristics of primary and secondary basis set superposition error. **1987**, 140, 338-344	14

1903	On the interaction hyperpolarisability of He2, He3 and Ne2. An AB initio study. **1987**, 135, 361-366	28
1902	Accurate ab initio calculations for the ground states of N2, O2 and F2. **1987**, 135, 543-548	56
1901	Theoretical structure of B2H6...HF. **1987**, 135, 549-552	6
1900	Non-additivity of SCF interaction energies in H3O+H2O)2. **1987**, 133, 143-149	23
1899	MP4 Interaction energies and basis set superposition errors for the (H2)2dimer. **1987**, 134, 418-422	22
1898	Applicability of the supermolecule MP2 approach to intermolecular interactions: He2 and Ne2. **1987**, 134, 553-559	25
1897	The electronic structure and stability of the H□ anion. **1987**, 139, 535-539	20
1896	Ab initio studies on van der Waals molecules. A comparative study with several basis sets of the C2v HeLi2 system. **1987**, 8, 51-56	1
1895	Polarization counterpoise corrections to correlated hydrogen bond interaction energies. **1987**, 8, 81-83	15
1894	Reliable Gaussian basis sets for closed-shell atoms. **1987**, 8, 117-131	11
1893	Basis sets for molecular interactions. 1. Construction and tests on (HF)2 and (H2O)2. **1987**, 8, 663-673	61
1892	Ab initio study of the He(1S)-Li2(X , 1□)interaction by the SCF and MP2 methods. **1987**, 8, 761-771	2
1891	Towards a valence-orbital/bond-orbital description of biochemical H-bonds from ab initio calculations. **1987**, 8, 816-825	7
1890	Cooperative effects in extended hydrogen bonded systems involving O?H groups. Ab initio studies of the cyclic S4 water tetramer. **1987**, 8, 1090-1098	64
1889	Investigations of Zn(II) complexes with DNA/RNA bases by means of quantum chemical calculations. **1987**, 137, 203-208	16
1888	Hartree-Fock calculations of crystalline packing of small linear n-alkanes. **1987**, 64, 827-829	5
1887	Study of the interaction between iron(0) and carbon dioxide, carbonyl sulphide and carbon disulphide: □b initio□calculations on the model compounds Fe(CO)2(PH3)2(□2-CO2), Fe(CO)2(PH3)2(□2-COS), Fe(CO)2(PH3)2(□2-CS2), and Fe(PH3)4(□2-CO2). **1987**, 332, 153-164	16
1886	Non-additive interactions between noble gas atoms by the model potential method. **1987**, 117, 105-111	7

1885	The impact of higher polarization functions of second-order dispersion energy. Partial wave expansion and damping phenomenon for He2. **1987**, 111, 271-283	90
1884	The H2O?Mg van der waals complex a theoretical study. **1987**, 113, 201-209	3
1883	Bond functions in molecular excited states: MRD CI calculations for the A3u, B3g and W3 states of N2. **1987**, 115, 23-32	13
1882	Molecular properties of FeCO as derived from AB initio molecular orbital calculations. **1987**, 36, 39-58	10
1881	The influence of intermolecular interactions on the electron-density distribution. A comparison of experimental and theoretical results for oxalic acid dihydrate. **1988**, 44, 609-616	22
1880	Ab initio investigation of interactions between models of local anesthetics and receptor: complexes involving amine, phosphate, amide, Na+, K+, Ca2+, and Cl-. **1988**, 77, 304-8	13
1879	On the structure, lattice energy and 14N nuclear quadrupole coupling constant of solid HCN. **1988**, 145, 399-406	11
1878	Configuration selection in the MC SCF method. The van der Waals X2 state of LiHe. **1988**, 147, 105-110	
1877	The C?H bond energy of formaldehyde. **1988**, 148, 202-204	11
1876	An efficient procedure for decomposition of the SCF interaction energy into components with reduced basis set dependence. **1988**, 153, 153-159	187
1875	An accurate ab initio calculation of the He2 potential curve. **1988**, 143, 435-438	40
1874	Acetylcholine in water: Ab-initio potential and Monte Carlo simulation. **1988**, 9, 1-10	14
1873	Determination of the water geometry in violuric acid monohydrate with a Monte Carlo simulation. **1988**, 9, 11-17	0
1872	Parallel computation of the MollerPlesset second-order contribution to the electronic correlation energy. **1988**, 9, 158-170	46
1871	Electron donor-acceptor complexes: Evaluation of MNDO as a computational tool to probe intermolecular interactions. **1988**, 9, 539-553	11
1870	MRD CI potential surfaces using balanced basis sets. V. Second-row diatomic hydrides. **1988**, 121, 381-391	18
1869	Van der Waals minima in excited states by Mller-Plesset perturbation theory: The a 3+ State of He2 And the 3state of MgHe. **1988**, 148, 289-295	17
1868	Intermolecular interaction energies between trimethylamine and benzene calculated using an ab initio SCF CI approximation. **1988**, 145, 537-540	3

1867	Theoretical study of the dependence of structural parameters of the H bond in the complex NH3H2CO2H+ on position of the proton. **1988**, 29, 463-466	
1866	Structure and molecular spectroscopy of gas-phase complexes. **1988**, 28, 735-764	3
1865	The structure and harmonic vibrational frequencies of the weakly bound complexes formed by HF with CO, CO2 and N2O. **1988**, 74, 415-428	37
1864	Counterpoise estimates of the BSSE in the evaluation of protonation energies. **1988**, 73, 307-316	11
1863	On the counterpoise correction for the basis set superposition error in large systems. **1988**, 74, 101-110	60
1862	Numerical Hartree-Fock and MCSCF calculations on diatomic copper: calibration of basis sets. **1988**, 74, 151-155	6
1861	Anab initio pair potential for the interaction between a water molecule and a formate ion. **1988**, 74, 1-10	6
1860	Ab initio pair potentials for the ionic lithium-formate system. **1988**, 74, 11-22	2
1859	A comparison of different many-body perturbation theory calculations of the ground state of SiS. **1988**, 33, 395-401	5
1858	Modified all-valence INDO/spd method for ground and excited state properties of isolated molecules and molecular complexes. **1988**, 34, 423-435	83
1857	An interaction potential between an alanine zwitterion and a water molecule based on ab initio calculations. **1988**, 34, 527-533	4
1856	3- and 5-Isoxazolol zwitterions: A model of interaction with the GABA-A receptor relating to agonism and antagonism. **1988**, 34, 149-165	5
1855	A possible explanation why doubly charged NeN2+, but no NeC2+ and NeO2+ were observed in charge-stripping mass spectrometry. **1988**, 82, 335-338	3
1854	Structure, energetics and vibrational spectra of H-bonded systems. Dimers and trimers of HF and HCl. **1988**, 122, 413-430	101
1853	A study of the reliability of different many-body methods: Potential energy curve for the ground state of Be2. **1988**, 125, 255-260	12
1852	The nature of the SCF basis set superposition error. Application of the indirect counterpoise method in polyatomic van der Waals molecules. **1988**, 127, 65-71	15
1851	A proposal for avoiding overestimation in the counterpoise basis set superposition error. Application to diatomic van der Waals systems. **1988**, 127, 343-350	13
1850	Decomposition of the interaction energy with counterpoise corrections to the basis set superposition error for dimers in solution. Method and application to the hydrogen fluoride dimer. **1988**, 122, 63-74	27

1849	Electronic structure of platinum(II) antitumor complexes and their interactions with nucleic acid bases. I. **1988**, 152, 151-157		14
1848	Calculation of NH...pi hydrogen bond energies in basic pancreatic trypsin inhibitor. **1988**, 954, 137-9		18
1847	A theoretical investigation of the electronic structure and some thermodynamic properties of PbF2. **1988**, 21, 5351-5359		31
1846	An analysis of the hydrogen bond in BASE-HF complexes using the theory of atoms in molecules. *Molecular Physics*, **1988**, 65, 695-722	1.7	296
1845	Theoretical studies of the potential surface for the F+H2-HF+H reaction. **1988**, 88, 1743-1751		66
1844	Ab initio investigation of hydrogen bonding by carbamates: Complexes including N-methyl methylcarbamate, N-phenyl methylcarbamate, dimethyl ether and methyl acetate. **1988**, 181, 19-24		3
1843	Intermolecular SCF theory without BSSE: The equations and some applications for small systems. **1988**, 170, 9-17		22
1842	Ab initio molecular orbital calculations of the infrared spectra of interacting water molecules: Part 1. Complexes of water with nitrogen, neon and argon. **1988**, 180, 241-265		14
1841	Models and modeling in theoretical chemistry. **1988**, 179, 273-292		49
1840	Ab initio molecular orbital calculations of the infrared spectra of hydrogen bonded complexes of water, ammonia and hydroxylamine. **1988**, 168, 247-264		21
1839	Construction of theoretical potentials in van der waals systems. An alternative to the polarization function counterpoise method.. **1988**, 166, 307-312		5
1838	Ab initio calculations on the hydration of dimethylpyrazole and indazole. Solvent effects on tautomeric energies.. **1988**, 165, 115-124		7
1837	Ab initio interaction potentials of guanidine-formic acid in the neutral and charged states. **1988**, 165, 319-327		15
1836	Theoretical study of the A 5 g and C 5 u states of N2: Implications for the N2 afterglow. **1988**, 88, 3174-3186		109
1835	Electron density distributions in hydrogen bonds: A local density-functional study of oxalic acid dihydrate and comparison with experiment. **1988**, 89, 4199-4208		34
1834	Theoretical study of the interaction of Fe, Fe+, and FeCO with Ar. **1988**, 89, 4867-4870		12
1833	Many-body effects in tetrahedral water clusters. **1988**, 89, 2149-2159		55
1832	Vibrational frequencies and intensities of H-bonded and Li-bonded complexes. H3N??HCl and H3N??LiCl. **1988**, 89, 3131-3138		39

1831	Adiabatic and diabatic potential energy surfaces for collisions of CN(X 2□, A 2□) with He. **1988**, 89, 3139-3151		194
1830	Ab initio molecular orbital calculations on linkage isomers of magnesium difluoride-carbon monoxide adducts. **1988**, 168, 317-322		
1829	Infrared spectrum of NeHF. **1988**, 61, 1576-1579		31
1828	Theoretical vibrational study of the FX???O(CH3)2 hydrogen-bonded complex. **1988**, 88, 4861-4866		18
1827	Stationary points on the potential energy surfaces of (C2H2)2, (C2H2)3, and (C2H4)2. **1988**, 88, 3811-3816		69
1826	The analytic gradient for the coupled pair functional method: Formula and application for HCl, H2CO, and the dimer H2CO???HCl. **1988**, 88, 7011-7023		33
1825	Ab initio investigation of the bound rovibrational states in the electronic ground state of HeN+2. **1988**, 89, 2178-2184		67
1824	Predictions of the rotational and vibrational spectra of SiF+, PO+, and NS+ by Mo/llerBlesset perturbation theory. **1988**, 89, 4929-4944		34
1823	Ab initio configuration interaction study of mixed BeLik clusters (k=1□). **1988**, 89, 5794-5802		46
1822	Ab initio calculation of argonBrgon potential. **1988**, 89, 6339-6347		45
1821	The HeNe interatomic potential from multiproperty fits and HartreeBock calculations. **1988**, 89, 2866-2880		27
1820	Correlation correction to the Hartree-Fock total energy of solids. II. **1988**, 38, 194-198		31
1819	A local density-functional study of the electron density distribution in the H2O dimer. **1988**, 89, 5787-5793		14
1818	A theoretical study of the water dimer interaction. **1988**, 89, 3662-3673		240
1817	Ab initio study of the interaction of polyoxymethylene with polyoxymethylene, ammonium perchlorate, and the aluminum (100) surface. **1988**, 37, 8915-8922		7
1816	Coupled-electron-pair approximation calculations on open-shell molecules: The two lowest states of HeNe+. **1988**, 38, 1289-1299		17
1815	On the connection between the supermolecular M□ller-Plesset treatment of the interaction energy and the perturbation theory of intermolecular forces. *Molecular Physics*, **1988**, 63, 205-224	1.7	291
1814	Interpretation of the Hartree-Fock interaction energy between closed-shell systems. *Molecular Physics*, **1988**, 64, 337-355	1.7	96

1813	van der Waals interaction potentials. *Molecular Physics*, **1988**, 65, 1363-1376	1.7	22
1812	Potential energy curves for the Rydberg states of LiHe and the spectrum of Li atoms interacting with He gas. **1988**, 21, 463-484		38
1811	Ab Initio Calculation for the Interaction Energy of HeH. **1988**, 61, 3141-3144		
1810	Ab Initio Calculation for Interaction Potential of HeHe. **1988**, 61, 1014-1016		5
1809	Quantum chemistry in the University of Cambridge. **1988**, 7, 351-370		2
1808	The water dimer potential surface. **1989**, 93-170		1
1807	Label-free operator in calculations of individual properties of atoms in a pair. **1989**, 40, 6702-6705		
1806	Ab initio configuration interaction study of the electronic and geometric structure of small, mixed neutral and cationic MgNak and MgLik (k=2) clusters. **1989**, 91, 4229-4241		42
1805	The role of bonding electrons in intermolecular forces; solid acetylene. *Molecular Physics*, **1989**, 67, 447-454	1.7	4
1804	A systematic study on the basis set superposition error in the calculation of interaction energies of systems of biological interest. **1989**, 90, 6361-6370		19
1803	Nonadditive effects in HF and HCl trimers. **1989**, 91, 7048-7056		113
1802	Weakly bound NeHF. **1989**, 91, 711-721		43
1801	Balance in interaction energy calculations. *Molecular Physics*, **1989**, 67, 1011-1020	1.7	8
1800	Mo/llerPlesset perturbation theory calculation of alkaline earthare gas complexes: Ground states of MgHe and MgAr. **1989**, 91, 1114-1120		19
1799	Analysis of the potential energy surface of ArNH3. **1989**, 91, 7809-7817		74
1798	Quantum scattering studies of electronically inelastic collisions of CN (X 2, A 2) with He. **1989**, 91, 5425-5439		104
1797	A comparison of defect energies in MgO using Mott-Littleton and quantum mechanical procedures. **1989**, 1, 7367-7384		55
1796	Structure and bonding of hydrogen halide complexes: An ab initio calculation of the 1:1 species. **1989**, 200, 483-496		31

1795	Ab initio molecular orbital calculations of the IR spectra of hydrogen bonded complexes of water, ammonia and hydroxylamine: Part 4. Two dimers of hydroxylamine. **1989**, 200, 507-532	22
1794	Interaction energy decomposition and basis set superposition error analysis in hydrogen abstraction from the nitroxyl molecule by atomic hydrogen. **1989**, 184, 373-380	2
1793	AB initio studies of the structure, energetics and vibrational spectra of hydrogen bonded systems. **1989**, 202, 177-192	14
1792	Intermolecular interactions, proton-transfer and charge-transfer transitions in biological hydrogen-bonded systems: thioguanine-cytosine, adenine-5-fluoro(bromo)-uracil, Mg2+-guanine-cytosine complexes and cis-Pt(NH3)22+-thioguanine (guanine). **1989**, 201, 87-98	17
1791	Ab initio study of hydrogen bonds and proton transfer in the systems (CH3)3NH+ □□COH and CH3NH3+□OCHOCH3 modelling a local-anaesthetic-receptor interaction. **1989**, 201, 287-294	8
1790	Metal ion interactions with water and ammonia. **1989**, 201, 339-350	20
1789	Bonding in zerovalent Ni compounds: NiN2 and Ni(N2)4 compared with NiCO and Ni(CO)4. **1989**, 129, 431-437	47
1788	Relativistic all electron configuration interaction calculation of ground and excited states of the gold hydride molecule. **1989**, 13, 363-375	42
1787	CEPA calculations of potential energy surfaces for open-shell systems. **1989**, 14, 143-148	18
1786	Theoretical study of linear LiCnLi (n=2□8) molecules. **1989**, 162, 479-485	3
1785	The structure of CH3NH3+ in aqueous solution: An ab initio study. **1989**, 162, 329-335	7
1784	A quantum chemical study of the HBr and HCN□HBr molecules: The effects of hydrogen bonding on molecular properties. **1989**, 157, 115-122	15
1783	Theoretical studies of sulfuric acid monohydrate: Neutral or ionic complex?. **1989**, 158, 111-115	28
1782	The dissociation energy of He2+. **1989**, 160, 183-188	35
1781	Ab-initio calculations on the protonation of simple amides by H3O+. Effects of discrete hydration and solvent cavity. **1989**, 194, 191-201	5
1780	Stationary points on the potential energy surface of O2□HF and O2□H2O. **1989**, 10, 55-62	10
1779	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
1778	Ab initio study of the proton affinity of a number of ortho-substituted pyridines. **1989**, 10, 346-357	20

1777	Degenerate lithium-hydrogen exchange reactions: Ab initio models for metallation mechanisms involving H2, CH4, NH3, H2O, and HF. **1989**, 10, 437-448	15
1776	Contraction of the well-tempered Gaussian basis sets: The first-row diatomic molecules. **1989**, 10, 753-769	35
1775	Combined bond-polarization basis sets for accurate determination of dissociation energies. II. Basis set superposition error as a function of the parent basis set. **1989**, 10, 875-886	26
1774	Effect of small cations on the hydrogen bond between an N-aromatic heterocycle and amine. **1989**, 160, 479-484	7
1773	The beryllium dimer potential. **1989**, 160, 494-501	48
1772	Stationary points on the potential energy surface of (C2H2)3. **1989**, 161, 166-174	20
1771	The HF-AlF3 gas-phase complex: An ab initio molecular orbital study. **1989**, 156, 125-128	12
1770	On the helium pair potential. **1989**, 155, 413-418	9
1769	Interaction in halide ion-rare gas systems: The Cl□e interaction potential. **1989**, 156, 269-274	15
1768	Interactions in the halide ion-rare gas systems: The F□e interaction potential. **1989**, 131, 215-225	21
1767	Mechanism of Hg(3P) relaxation in nitrogen matrices. I. Theoretical study of HgN2. **1989**, 133, 377-393	7
1766	Pseudopotential MRD CI calculations of nickel-containing molecules. II. The electronic 1□ ground state and 20 low-lying excited states of the NiSi molecule. **1989**, 138, 315-325	13
1765	On the reliability of SCF ab initio calculations of vibrational frequencies and intensities of hydrogen-bonded systems. **1989**, 194, 89-105	15
1764	On the many-body contributions to the interaction polarisability and hyperpolarisability of Hen. **1989**, 75, 53-65	4
1763	A quantum chemical study of the hydrogen bonding in the CO2?HF and N2O?HF complexes. **1989**, 76, 173-185	36
1762	Decomposition of the interaction energy between metal cations and water or ammonia with inclusion of counterpoise corrections to the interaction energy terms. **1989**, 76, 297-313	29
1761	Theoretical study of the calcium dication hydrates. **1989**, 75, 299-306	4
1760	Noncovalent interactions of medium strength. A revised interpretation and examples of its applications. **1989**, 35, 223-239	16

1759	Improved intermolecular SCF theory and the BSSE problem. **1989**, 36, 225-240		66
1758	Computational chemical studies of chiral stationary-phase models: The nature of the Pi interaction in complexes of methyl N-(2-naphthyl) alaninate with N-(3,5-dinitrobenzoyl)leucine n-propylamide. **1989**, 36, 313-317		7
1757	References. **1989**, 175-179		
1756	Ab initio MO calculations of hydrogen bonding between guanidine isosters and carboxylate. **1989**, 183, 371-379		2
1755	Silanol as a model for the free hydroxyl of amorphous silica: Ab initio calculations of the interaction with ammonia. **1989**, 224, 498-514		16
1754	The argon hydrogen□luoride differential scattering cross section. **1989**, 90, 2182-2191		33
1753	Theoretical study of the excited states of the heavier alkali dimers. II. The Rb2molecule. **1989**, 22, 2465-2483		69
1752	A theoretical study of the BeF molecule in the X 2□ state. *Molecular Physics*, **1989**, 67, 1129-1140	1.7	27
1751	The water flip barrier in the Li+HCOO□H2O crystal from ab initio and molecular mechanics calculations. **1989**, 91, 368-375		2
1750	Theoretical Calculations on Nonlinear Susceptibilities of Organic Crystals. **1989**, 173, 659		2
1749	Theoretical Investigation of the Interaction Potential of Helium Trimer. **1989**, 62, 1410-1414		1
1748	Ab Initio Calculation for the Interaction Energy of He□le+. **1989**, 62, 633-635		
1747	Theoretical Studies of Collision-induced Energy Transfer in Electronically Excited States. **1990**, 94, 1253-1262		15
1746	Theoretical Investigation of van der Waals Interaction Energy of Helium Trimer. Three-Body Effect. **1990**, 63, 958-960		1
1745	Modeling Localized Defects in Ionic Materials Using Mott-Littleton and Embedded Quantum Cluster Methodology. **1990**, 73, 3251-3256		15
1744	Perturbation theoretical vs supermolecule calculations on intermolecular interactions. **1990**, 67, 387-400		4
1743	Towards a third order perturbation theory of intermolecular interactions without BSSE. **1990**, 68, 241-251		3
1742	Non-covalent interactions in bimolecular up to mesoscopic systems. **1990**, 210, 311-322		1

1741	Comparison of semiempirical and bsse corrected mller-plesset ab initio calculations on the direct addition of water to formaldehyde. **1990**, 210, 427-440	19
1740	The structure of the CH2O-NH3 system. **1990**, 207, 259-268	5
1739	Investigations of the anaesthetic activity of nitrous oxide by quantum-chemical calculations. **1990**, 204, 1-14	19
1738	Pseudopotential MRD-CI calculations of nickel-containing molecules: Part I. The electronic ground state of NiH. **1990**, 205, 25-34	
1737	The decomposition of the SCF and Heitler-London interaction energies for small and medium size basis sets. **1990**, 206, 211-233	4
1736	Tautomerism, protonation, and interaction with formiate, of phenyliminoimidazoline and benzylimidazolidine: AM1 and ab initio 4-31G calculations. **1990**, 224, 285-296	6
1735	Ab initio molecular-orbital calculations on Pt, PtH and PtH2 with a quasirelativistic pseudopotential for Pt. **1990**, 166, 311-316	12
1734	New theoretical results on the CO-cyclobutadiene complex. **1990**, 173, 21-25	3
1733	Contrasting behaviour of hydrogen fluoride and hydrogen chloride in the formation of weak complexes with methane. **1990**, 175, 593-600	10
1732	Comparison of Morokuma and perturbation theory approaches to decomposition of interaction energy. (NH4)+-NH3. **1990**, 166, 57-64	66
1731	Semi-empirical calculation of the potential curves of NaNe, Na+Ne and Na-Ne. **1990**, 173, 573-578	5
1730	Quantum chemical study of the HCl molecule and its binary complexes with CO, C2H2, C2H4, PH3, H2S, HCN, H2O and NH3: Hydrogen bonding and its effect on the 35Cl nuclear quadrupole coupling constant. **1990**, 144, 53-69	40
1729	Induced infrared absoption bands of ethylene adsorbed on mordenites: Experimental and theoretical studies of electron-donor-acceptor interactions. **1990**, 147, 77-83	9
1728	Functional counterpoise corections for the NMR chemical shift in a model dimeric water system. **1990**, 147, 91-97	8
1727	The structure of C2H4 clusters from theoretical interaction potentials and vibrational predissociation data. **1990**, 15, 341-351	18
1726	CEPA calculations on open-shell molecules. **1990**, 16, 167-173	5
1725	Muscarine and water: Ab initio potentials. **1990**, 1, 385-390	
1724	Ab initio computations of one and two hydrogen or deuterium atoms in the palladium tetrahedral site. **1990**, 9, 383-389	1

1723	Localized orbitals for the description of molecular interaction. **1990**, 38, 665-673	26
1722	Enhanced Li+ binding energies of some azines: a molecular orbital study. **1990**, 77, 1-15	34
1721	Theoretical study of the6⊞,6⊡ and4⊞ van der Waals states of NO. **1990**, 77, 323-331	7
1720	The influence of Li+, Na+, Mg2+, Ca2+, and Zn2+ ions on the hydrogen bonds of the Watson-Crick base pairs. **1990**, 29, 757-69	78
1719	SCF, MP2, and CEPA-1 calculations on the OH .. O hydrogen bonded complexes (H2O)2 and (H2O-H2CO). **1990**, 11, 1-18	70
1718	Ab initio study of substituent effect on the addition of hydrogen fluoride to fluoroethylenes. **1990**, 11, 170-180	8
1717	Overestimation of the coupling component in the CP technique. Application of the indirect counterpoise correction to the H2O?HF hydrogen-bonded system. **1990**, 11, 576-588	16
1716	Combined application of pair potentials and the MM2 force field for the modeling of ionophores. **1990**, 11, 819-828	12
1715	The effect of diffuse functions on minimal basis set superposition errors for H-bonded dimers. **1990**, 11, 930-942	28
1714	Pseudopotential calculations for methyl compounds of zinc and magnesium. **1990**, 11, 1029-1037	20
1713	Comparative study of imidazole hydration: Ab initio and electrostatic calculations vs. Cambridge structural database analysis. **1990**, 11, 1038-1046	17
1712	The nature of the N ? H⊡O?C hydrogen bond: An intermolecular perturbation theory study of the formamide/formaldehyde complex. **1990**, 11, 1217-1233	96
1711	Effect of basis-set superposition on the atomic charges and valencies in hydrogen- and lithium-bonded complexes. **1990**, 172, 487-493	2
1710	The microwave spectrum and structure of the neon-phosphorus trifluoride complex. **1990**, 171, 542-546	3
1709	The beryllium atom⊡water molecule interaction A many-body perturbation theory study. **1990**, 174, 19-24	8
1708	Silanol as a model for the free hydroxyl of amorphous silica: Ab initio calculations of the interaction with formaldehyde. **1990**, 169, 501-508	21
1707	A matrix partitioning approach to the calculation of intermolecular potentials. General theory and some examples. **1990**, 140, 343-361	33
1706	Pseudopotential MRD CI calculations of nickel-containing molecules. III. NiSiH3 and NiAlH3 as minimum models of metal-support systems. **1990**, 142, 369-380	

1705	Infrared excitation and dissociation of methanol dimers and trimers. **1990**, 143, 423-435	53
1704	Monte Carlo method in the theory of solutions. **1990**, 12, 69-133	8
1703	The electron density distribution in the hydrogen bond. A quantum chemical and crystallographic study. **1990**, 237, 33-46	7
1702	Theoretical study of the acidic strength of amino acid side chains. **1990**, 18, 361-372	2
1701	CHAPTER 2. ATOMIC TREATMENT OF MINERAL-WATER SURFACE REACTIONS. **1990**, 17-86	21
1700	Ab initio calculation of the OH (X 2□ A 2⊞)+Ar potential energy surfaces and quantum scattering studies of rotational energy transfer in the OH (A 2⊞) state. **1990**, 93, 3351-3366	203
1699	Molecular dynamics studies on molten alkali hydroxides. I. Static properties of molten LiOH. **1990**, 92, 7505-7514	14
1698	Quantum scattering study of rotational energy transfer in OH(A 2⊞, v⊟0) in collisions with He(1S). **1990**, 93, 8757-8763	42
1697	Convergence to the configuration-set limit in multireference configuration-interaction calculations on the He dimer. **1990**, 93, 643-651	63
1696	Intermolecular potential of the methane dimer and trimer. **1990**, 93, 4243-4253	81
1695	On decomposition of second-order Mo/llerPlesset supermolecular interaction energy and basis set effects. **1990**, 92, 4357-4363	178
1694	Second-order exchange effects in intermolecular interactions. The water dimer. **1990**, 92, 6049-6060	34
1693	Ab initio potentials and pressure second virial coefficients for CH4⊟2O and CH4⊟2S. **1990**, 93, 7808-7812	25
1692	Calculations of nonadditive effects by means of supermolecular Mo/llerPlesset perturbation theory approach: Ar3 and Ar4. **1990**, 92, 2481-2487	97
1691	Theoretical study of the interaction of ionized transition metals (Cr,Mn,Fe,Co,Ni,Cu) with argon. **1990**, 41, 10447-10452	15
1690	Prediction of the spectrum for excitation of the van der Waals modes in ArHCN. **1990**, 93, 7666-7675	22
1689	An ab initio investigation of the spectroscopic properties of ClF, ArF+, SF□and ClO□n their ground electronic states. **1990**, 92, 7412-7417	27
1688	On the origin of metastable decay in Ar+2. **1990**, 93, 376-383	45

1687	Photodissociation of CO□: Product kinetic energy measurements as a probe of excited state potential surfaces and dissociation dynamics. **1990**, 92, 5935-5943		19
1686	About the first solvation shell of protonated hydrates: H3O+(H2O)6. **1990**, 93, 6648-6653		17
1685	Calculation of van der Waals spectra for H2HF, D2HF, and H2DF. **1990**, 93, 6334-6349		68
1684	Simulating Vacancy, Impurity And Electronic Defect States In Mgo, Lici And La2Cuo4 Using Quantum Cluster And Classical Lattice Simulation Techniques In A Consistent Manner.. **1990**, 209, 257		
1683	An analysis of hydrogen-bonded systems: (HF)2, (H2O)2 and H2O □HF. *Molecular Physics*, **1990**, 70, 353-37[illegible]7		25
1682	Molecular dynamics simulation of molten Li2CO3 and Na2CO3. *Molecular Physics*, **1990**, 69, 115-128	1.7	18
1681	On the Boys Bernardi□ethod to correct interaction energies calculated using M□ller-Plesset perturbation theory. **1990**, 185-186		14
1680	Ab initio calculation of relative ion concentrations of protonated water clusters at equilibrium. *Molecular Physics*, **1990**, 71, 207-215	1.7	15
1679	Floppy structure of the benzene dimer: Ab initio calculation on the structure and dipole moment. **1990**, 93, 5893-5897		139
1678	A User's Guide to Polarisabilities and Dispersion Coefficients for Ions in Crystals. **1990**, 4, 313-330		23
1677	An analysis of the hydrogen bond in ice. **1990**, 93, 8029-8035		149
1676	Gas phase acidities and molecular geometries of H3SiOH, H3COH, and H2O. **1990**, 93, 2575-2583		59
1675	On the dissociation energy of Mg2. **1990**, 92, 5377-5383		60
1674	Ab initio approach to molecular crystals: A periodic Hartree□ock study of crystalline urea. **1990**, 92, 7402-7411		187
1673	Many-body symmetry-adapted perturbation theory of intermolecular interactions. H2O and HF dimers. **1991**, 95, 6576-6601		288
1672	Accurate multireference configuration interaction calculations of the potential energy function and the dissociation energy of N2. **1991**, 94, 1264-1270		78
1671	A model calculation on the chemisorption of aluminum on graphite. **1991**, 255, L509-L515		8
1670	Characterization of oxide surfaces by infrared spectroscopy of adsorbed carbon monoxide: a theoretical investigation of the frequency shift of CO on MgO and NiO. **1991**, 255, 344-354		162

1669	Properties of urea□water solvation calculated from a new ab initio polarizable intermolecular potential. **1991**, 95, 8419-8429		65
1668	Exact perturbation treatment of the basis set superposition correction. **1991**, 95, 6705-6711		23
1667	A theoretical study of the low-lying states of Ti2 and Zr2. **1991**, 95, 1057-1063		42
1666	Effects of BSSE and d-orbital space in the calculation of the equilibrium geometry of CaF2. *Molecular Physics*, **1991**, 73, 941-951	1.7	11
1665	Interactions energies associated with short intermolecular contacts of C□H bonds. II. Ab initio computational study of the C□H???H□C interactions in methane dimer. **1991**, 94, 4835-4841		56
1664	Theoretical study of the low-lying bound states of O2. **1991**, 95, 8292-8300		75
1663	Potentials for the Classical Simulation of Molecular Systems: Current and Future Model Intermolecular Potentials. **1991**, 183-208		4
1662	Atomic Natural Orbital (ANO) Basis Sets for Quantum Chemical Calculations. **1991**, 301-373		98
1661	The electronic and molecular structure of ferrocene. **1991**, 95, 1829-1833		55
1660	New methods for electronic structure calculations on large molecules. **1991**, 42, 341-67		101
1659	An ab initio molecular orbital study of the anions O2 - □H2O and O2 - □CO2. *Molecular Physics*, **1991**, 74, 333-351	1.7	17
1658	A model calculation on the chemisorption of aluminum on graphite. **1991**, 255, L509-L515		
1657	Ab initio molecular orbital treatment of hydroxylamine-X+-water and hydroxylamine-X+-ammonia (X = H, Li) clusters. **1991**, 151, 21-36		11
1656	Adiabatic calculations and properties of the He2+ molecular ion. **1991**, 157, 75-87		42
1655	Interaction potentials in rare gas-halide ion systems. **1991**, 157, 123-133		16
1654	Ab initio study of the infrared photoconversion in the water-hydrogen iodide system. **1991**, 154, 23-32		11
1653	Theoretical investigation of the relative stabilities of singlet and triplet disulfides. **1991**, 185, 251-255		3
1652	Localized molecular orbitals of interacting molecular systems. **1991**, 70, 341-344		

1651	Theoretical investigation of the interaction energy in the Li++H2O ionic complex. **1991**, 70, 345-350	4
1650	A comparison ofa priori anda posteriori BSSE correction schemes for rare gas-proton potential curves. **1991**, 70, 403-413	1
1649	H-H bond activation in transition metal complexes: An MO-LCAO study of the ligands effect. **1991**, 2, 221-226	
1648	The use of MIDI basis set at the correlated level. **1991**, 236, 219-230	2
1647	Interaction energy of formaldehyde with ammonia. **1991**, 233, 139-145	13
1646	Ab initio molecular orbital calculations of the infrared spectra of hydrogen-bonded complexes of water, ammonia and hydroxylamine. **1991**, 235, 123-136	16
1645	The interaction between 5-hydroxytryptamine and tryptophan: a serotonin receptor model. **1991**, 235, 321-342	3
1644	Improved ab initio pair potentials for the interaction between nucleic acid bases and water. **1991**, 235, 355-389	18
1643	Ab initio studies of hydrogen-bonded complexes between uracil and HCl. **1991**, 235, 409-415	6
1642	Basis sets for molecular interactions. **1991**, 251, 245-260	16
1641	Substitution, addition and elimination reactions: a quantum chemical study of intermolecular complexes. **1991**, 230, 387-400	2
1640	Second quantization and exchange perturbation theory for intermolecular interactions. the basis set superposition error problem. **1991**, 232, 51-63	4
1639	An analytical investigation into the bsse problem. **1991**, 227, 43-65	39
1638	Geometry and electronic structure studies using computational quantum chemistry. **1991**, 234, 185-200	6
1637	An AB initio molecular orbital study of the structure, energetics and bond activation of Al+ complexes. **1991**, 234, 357-371	14
1636	Efficient techniques for the decomposition of intermolecular interaction energy at SCF level and beyond. **1991**, 234, 387-400	73
1635	Theoretical chemistry in solution. Some results and perspectives of the continuum methods and in particular of the polarizable continuum model. **1991**, 234, 401-424	169
1634	Theoretical calculations for low-lying adiabatic states of Be2+. **1991**, 187, 479-486	18

1633	Iodine-polyphenylacetylene charge-transfer complex: an ab initio quantum-chemical assessment. **1991**, 181, 582-587	2
1632	Interaction energies associated with short intermolecular contacts of C–H bonds. Structure and energetics of the interaction between CH4 and CN– **1991**, 177, 483-490	8
1631	A parallel vectorized implementation of triple excitations in CCSD(T): application to the binding energies of the AlH3, AlH2F, AlHF2 and AlF3 dimers. **1991**, 178, 462-470	74
1630	Ab initio molecular orbital calculations of the infrared spectrum of the hydroxylamine–ammonia complex. **1991**, 178, 266-272	18
1629	Second-order BSSE-free perturbation theory: intermolecular interactions within supermolecular approach. **1991**, 180, 114-120	23
1628	Basis-set superposition errors in tightly bound systems. **1991**, 176, 1-6	17
1627	Two very different B–N bond distances: electronic structure calculations on BF3–NCCN and BF3–NCCH3. **1991**, 176, 263-265	33
1626	The vapour-phase complex AlF3(HF)2: an ab initio molecular orbital study. **1991**, 182, 556-560	8
1625	The ammonia dimer potential energy surface: resolution of the apparent discrepancy between theory and experiment?. **1991**, 183, 449-456	46
1624	Computation of spectroscopic properties of van der Waals systems from post-SCF ab initio potentials including the EICP alternative counterpoise technique. **1991**, 12, 611-619	5
1623	MRD-CI potential surfaces using balanced basis sets. VI. Correlation of bond order with bond function composition for first-row diatomic molecules. **1991**, 12, 690-696	12
1622	Bond functions, covalent potential curves, and the basis set superposition error. **1991**, 12, 697-704	18
1621	Parametrization of calcium binding site in proteins and molecular dynamics simulation on phospholipase A2. **1991**, 12, 717-730	13
1620	Self-consistent, nonorthogonal group function approximation. III. Approaches for modeling intermolecular interactions. **1991**, 12, 811-828	23
1619	Counterpoise corrected calculations at the correlated level: A simplified method using LMOs. **1991**, 12, 953-958	15
1618	Ab initio investigation of interactions between models of membrane-active compounds and polar groups of membranes: complexes involving amine, ether, amide, phosphate, and carboxylate. **1991**, 80, 328-32	13
1617	Ab initio calculation of the second virial coefficient of neon and the potential energy curve of Ne2. **1991**, 156, 395-401	30
1616	Test-particle model potentials for hydrogen-bonded complexes: Complexes formed from HCN, HF, H2O, NH3, HCONH2, HCONHCH3, guanine and cytosine. **1991**, 156, 439-456	23

1615	Basis set superposition errors in intermolecular structures and force constants. **1991**, 183, 223-226	25
1614	Nonclassical hydrogen complexes of the alkaline earths. **1991**, 185, 529-534	15
1613	Interaction energies between H2O and HXCH=Y/X=CHYH for X, Y=CH2, NH or O the chemical Hamiltonian approach. **1991**, 183, 25-30	2
1612	Dual basis sets in calculations of electron correlation. **1991**, 178, 451-454	61
1611	Pseudopotential calculations for the potential energy curves and transition dipole moments of the NaHg system. **1991**, 178, 246-252	11
1610	Interaction energies associated with short intermolecular contacts of C?H bonds. 4. Ab initio computational study of C?Hanion interactions in CH4X(X=F, Cl, Br, I). **1991**, 180, 241-248	17
1609	A microwave spectral and ab initio investigation of O3?H2O. **1991**, 146, 493-512	51
1608	AM1 and ab initio calculations on nitric acid mono- and trihydrates. **1991**, 247, 225-236	14
1607	Proton transfer in ammonia cluster cations: molecular dynamics in a self consistent field. **1991**, 18, 413-426	37
1606	On the existence of free doubly negative molecular ions. **1991**, 18, 299-305	64
1605	SCF theory of molecular interactions. **1991**, 40, 97-126	2
1604	A BSSE-free SCF algorithm for intermolecular interactions. **1991**, 40, 139-148	42
1603	Perturbation theory calculations of intermolecular interaction energies. **1991**, 40, 23-36	10
1602	An examination of the effects of basis set and charge transfer in hydrogen-bonded dimers with a constrained HartreeFock method. **1991**, 40, 193-207	30
1601	Ab initio studies of internal rotation barriers and vibrational frequencies of (C2H2)2, (CO2)2, and C2H2-CO2. **1991**, 78, 133-163	68
1600	Application of open-shell coupled cluster theory to the ground state of GaAs. **1991**, 80, 215-219	8
1599	Anab initio study of the molecules P2O and P2O+. **1991**, 79, 105-114	7
1598	Structure of the O2(H2O)5 cluster ion. **1991**, 31, 649-650	1

1597	Nonlinear schr□dinger equations and intermolecular interactions. **1991**, 8, 151-160	4
1596	Excitation of the C(2p2.3Pj) fine structure states in collisions with He(1s21S0). **1991**, 24, 2343-2351	30
1595	Chapter 9 Introduction to Zeolite Theory and Modelling. **1991**, 58, 317-358	8
1594	Excitation of the fine-structure transitions of C in collisions with ortho- and para-H2. **1991**, 24, 2487-2502	77
1593	Ab initio calculations on the structure, stabilization, and dipole moment of benzene???Ar complex. **1991**, 95, 391-394	74
1592	Ab initio study of intermolecular potential for ArHCl. **1991**, 94, 6677-6685	57
1591	Rotationally inelastic collisions of Li2(A 1□u) with Ne: Fully ab initio cross sections and comparison with experiment. **1991**, 95, 6524-6535	22
1590	Bonding geometry and bonding character of thiocyanate adsorbed on a Ag(100) surface. **1991**, 95, 4678-4684	33
1589	Ab initio study of the structure, infrared spectra, and heat of formation of C4. **1991**, 94, 3753-3761	63
1588	Ab initio study of the nonadditive effects in the trimer of ammonia. **1991**, 95, 5169-5178	35
1587	Ab initio study of the intermolecular potential of Ar□2O. **1991**, 94, 2807-2816	78
1586	Quantum Monte Carlo perturbation calculations of interaction energies. **1991**, 43, 2139-2151	14
1585	The role of symmetry in collisions of N2 with N+2. **1991**, 94, 6500-6507	15
1584	Obtaining accurate pressure second virial coefficients for methane from an ab initio pair potential. **1991**, 95, 9106-9114	17
1583	A coupled cluster study of the classical barrier height of the F+H2-□H+H reaction. **1991**, 95, 7426-7436	32
1582	Interaction energies associated with short intermolecular contacts of C□ bonds. Ab initio computational study of the C□???O contact interaction in CH4???OH2. **1991**, 95, 5179-5186	76
1581	Ab initio theoretical study of small GaAs clusters. **1991**, 95, 6602-6606	52
1580	Accurate ab initio potential energy computations for the H4 system: Tests of some analytic potential energy surfaces. **1991**, 95, 4331-4342	39

1579	Potential energy surface of H???H2O. **1991**, 95, 1080-1085		22
1578	Calculations of H2O microwave line broadening in collisions with He atoms: sensitivity to potential energy surfaces. **1991**, 94, 1346-59		32
1577	Structure and decomposition path of the HIF radical. **1991**, 95, 433-440		2
1576	Calculation of the dispersion interaction energy by using localized molecular orbitals. **1991**, 94, 5565-5573		29
1575	Ab initio study of intermolecular potential of H2O trimer. **1991**, 94, 2873-2883		138
1574	Structures of Organonitrogen□lithium Compounds: Recent Patterns and Perspectives in Organolithium Chemistry. **1991**, 37, 47-142		336
1573	Structure and vibrational properties of water hydrogen halide complexes. **1991**, 94, 2915-2922		31
1572	An Ab Initio molecular orbital study of protonated water clusters, H(H2O) n + n = 1 to 5, at the SCF and MP2 levels. *Molecular Physics*, **1991**, 73, 375-405	1.7	54
1571	The structure of molten CsAu: ab initio and Monte Carlo study. **1991**, 3, 5615-5620		4
1570	AB Initio Molecular Orbital Calculations of Bond Index and Valency. **1992**, 301-351		64
1569	On the metastability of the1Sigma+gground state of He2+2and Ne2+2: a case study of binding metamorphosis. **1992**, 25, 4069-4098		44
1568	The interatomic potential for the X1Sigma state of NeLi+. **1992**, 25, 1795-1809		25
1567	Excitation of the fine-structure transitions of O(3PJ) in collisions with ortho- and para-H2. **1992**, 25, 285-297		71
1566	Electronic structure, bonding, geometry, and some spectroscopic properties of the scandium-nickel molecule. **1992**, 96, 8277-8282		7
1565	Basic Theory of Intermolecular Forces. **1992**, 121-145		4
1564	Structures and adsorption energetics for chemisorbed fluorine atoms on Si(100)-2 x 1. **1992**, 45, 9065-9081		78
1563	Ab initio potential-energy surfaces for Cd(1P)+H2=CdH(X 2□)+H, HCdH(X 1□g), Cd(3P)+H2, and Cd(1S)+H+H. **1992**, 96, 6555-6564		17
1562	Ab initio second- and fourth-order Mo/llerPlesset study on structure, stabilization energy, and stretching vibration of benzene???X (X=He,Ne,Ar,Kr,Xe) van der Waals molecules. **1992**, 97, 335-340		101

1561	A comparison of approximate techniques for the determination of potential energy surfaces of ion□molecule charge transfer systems. **1992**, 97, 6579-6587	6
1560	A quasiclassical trajectory study of OH rotational excitation in OH+CO collisions using ab initio potential surfaces. **1992**, 96, 7465-7473	52
1559	Infrared spectroscopy of CO2□D(H)Br: Molecular structure and its reliability. **1992**, 97, 5392-5402	26
1558	Ab initio theoretical study of arsine and trimethylgallium: The formation of GaAs by a stable adduct. **1992**, 96, 3723-3731	20
1557	Ab initio study of the structure, cooperativity, and vibrational properties of the H2O: (HF)2 hydrogen bonded complex. **1992**, 97, 1911-1918	22
1556	Convergence to the basis-set limit in ab initio calculations at the correlated level on the water dimer. **1992**, 97, 5019-5030	148
1555	Convergence properties of coupled Hartree□ock theory of intermolecular interactions. **1992**, 97, 7545-7554	36
1554	Intermolecular potential of H2O???H2 in the van der Waals region. An ab initio study. **1992**, 96, 6039-6047	36
1553	Proton□onor properties of water and ammonia in van der Waals complexes with rare-gas atoms. Kr□H2O and Kr□NH3. **1992**, 97, 8181-8187	28
1552	Multireference configuration-interaction potential surfaces for the collinear F+H2 reaction. **1992**, 97, 8296-8311	9
1551	Ab initio calculations of the intermolecular chemical shift in nuclear magnetic resonance in the gas phase and for adsorbed species. **1992**, 97, 417-434	90
1550	Molecular adsorption of NH3 on MgO(001) and hydrogen abstraction from NH3 on gaseous LiO and Li-doped MgO(001). A computational study. **1992**, 96, 6281-6290	18
1549	The role of nonbond and charge flux in hydrogen bond interactions. The effect on structural changes and spectral shifts in water dimer. **1992**, 97, 9161-9172	22
1548	Inversion of experimental data and ab initio studies of a pseudo-atom□iatom model for the vibrational dynamics of HCN□HF. **1992**, 97, 2209-2223	20
1547	Stationary points on the potential energy surfaces of (SO2)2 and (SO2)3. **1992**, 96, 8390-8410	27
1546	Ab initio calculations for the adsorption of small molecules on metal oxide surfaces. I. Cluster calculations for carbon monoxide CO on nickel oxide NiO(100). **1992**, 97, 2583-2592	75
1545	Anisotropic repulsive potential energy surfaces from Hartree□ock calculations for HeCO2 and HeOCS. **1992**, 96, 6621-6628	24
1544	Basis set superposition error effects on electronic and □X, □???N stretching modes of hydrogen bonded systems FX???NCX (X=H,D). **1992**, 96, 6033-6038	23

1543	Evaluation of the multipole-induced-multipole model: incremental dipole polarizabilities in the CH4He system. *Molecular Physics*, **1992**, 75, 221-231	1.7	9
1542	The polarizabilities of species present in ionic solutions. *Molecular Physics*, **1992**, 76, 353-372	1.7	87
1541	Development and Applications of an Extended-Hückel-Based Reactivity Index for Organometallic Complexes. **1992**, 14, 27-62		14
1540	Lateral Interaction between Adsorbates at Ionic Surfaces: Theoretical Investigation of the CO Vibrational Frequency Shift at MgO(001). **1992**, 96, 1711-1715		29
1539	On the stability of the singly and doubly charged beryllium trimers Be+ 3 and Be++ 3. *Molecular Physics*, **1992**, 76, 1489-1499	1.7	6
1538	Accurate proton affinities: Ab initio proton binding energies for N2, CO, CO2, and CH4. **1992**, 97, 1087-1094		33
1537	The van der Waals potential-energy surfaces and the structures of ArClF and ArCl2. **1992**, 97, 440-451		75
1536	Ab initio calculation of the deuterium quadrupole coupling in liquid water. **1992**, 97, 5898-5904		75
1535	On the performance of large Gaussian basis sets for the computation of total atomization energies. **1992**, 97, 5012-5018		93
1534	Existence of doubly-negative charged ions and relation to solids. **1992**, 25, 2257-2265		65
1533	Calculated rovibrational energy levels and infrared spectrum of He-C2H2. *Molecular Physics*, **1992**, 77, 111-134	1.7	20
1532	The contribution of metal sp electrons to the chemisorption of CO: theoretical studies of CO on Li, Na, and Cu. **1992**, 278, 427-436		71
1531	Chemisorption of CO on defect sites of MgO. **1992**, 275, 450-458		103
1530	Ab initio study of the bare and hydrated (001) surface of tetragonal zirconia. **1992**, 275, 482-492		38
1529	Application of systematic sequences of wave functions to the water dimer. **1992**, 96, 6104-6114		1007
1528	Using monomer properties to obtain integrated intensities for vibrational transitions of van der Waals complexes. *Molecular Physics*, **1992**, 77, 823-835	1.7	12
1527	Ab initio potential-energy curves for the molecular ions NeH+ and ArH+. *Molecular Physics*, **1992**, 77, 279-290	1.7	15
1526	Hydrogen bonded complexes of HCl with CO, C2H2, C2H4, PH3, H2S, HCN, H2O and NH3. *Molecular Physics*, **1992**, 77, 61-73	1.7	46

1525	Ab initio pseudopotential study of Yb and YbO. **1992**, 97, 1162-1173	59
1524	Ab initio methods in mineral surface reactions. **1992**, 30, 269	33
1523	Ab initio Hartree-Fock study of tetragonal and cubic phases of zirconium dioxide. **1992**, 45, 592-601	83
1522	An ab initio investigation of clusters NanCln. **1992**, 97, 3487-3497	59
1521	Analysis of the intermolecular potential of Ar□CH4: An ab initio study. **1992**, 96, 463-469	37
1520	Theoretical calculations on nonlinear susceptibilities of organic materials. **1992**, 49-62	
1519	Self-Consistent-Field potential-energy surfaces for hydrogen atom pairs within small palladium clusters. **1992**, 41, 793-810	2
1518	Near-Hartree□ock wave functions for solids: The case of crystalline silicon. **1992**, 42, 5-33	43
1517	An essay on the theory and calculations of intermolecular interactions. **1992**, 42, 581-590	28
1516	Evolution of polarizabilities and hyperpolarizabilities with molecular aggregation: A model study of acetylene clusters. **1992**, 43, 135-146	18
1515	A BSSE-free SCF algorithm for intermolecular interactions. II. Sample calculations on hydrogen-bonded complexes. **1992**, 43, 801-811	32
1514	Constrained self-consistent-field wave functions with improved long-range behavior. **1992**, 44, 985-995	3
1513	Hydrogen bonding: Methodology and applications to complexes of HF and HCl with HCN and CH3CN. **1992**, 44, 527-541	43
1512	Quantum chemical modeling of chiral catalysis. Part 6. On the relative stability of dimers of chiral oxazaborolidines used in the catalytic enantioselective reduction of ketones. **1992**, 3, 933-945	30
1511	The combined use of ab initio molecular orbital theory and matrix isolation infrared spectroscopy in the study of molecular interactions. **1992**, 3, 75-93	33
1510	Basis set validation for polyatomic cation-water interactions. **1992**, 2, 137-152	5
1509	Ab initio calculations of silicon-halogen-silicon double bridges. **1992**, 123, 17-24	1
1508	A new approach to theab initio energy of the homodesmic reaction for the resonance energy of benzene. **1992**, 83, 377-388	13

1507	Water dimer in liquid water. **1992**, 84, 181-194	37
1506	Molecular structure of mono- and dicarbonyls of rhodium and palladium. **1992**, 84, 217-235	36
1505	Analysis of the interaction energy in the Cu+-H2O and Cl⁻-H2O systems, with CP corrections to the BSSE of the separate terms, and MC simulations of the aqueous systems with and without CP corrections. **1992**, 82, 165-187	8
1504	Ab initio molecular orbital calculations of the infrared spectra of hydrogen-bonded complexes of water, ammonia and hydroxylamine. **1992**, 81, 255-268	25
1503	Influence of the counterpoise correction on the optimized relative degrees of freedom in the H-bonded complex water-formamide. **1992**, 81, 281-290	9
1502	Ab initio studies of ground and excited electronic states of MgAr, CdAr, and BeAr. **1992**, 83, 209-225	7
1501	Nonempirical calculation of the potential energy surface for the O ⁻ H2O system. **1992**, 33, 138-141	
1500	Ab initio molecular orbital calculations of the infrared spectra of interacting water molecules part 2. complexes of water with carbon monoxide and nitrogen. **1992**, 275, 33-54	30
1499	Many-body symmetry-adapted perturbation theory study of the He?F⁻ interaction. **1992**, 166, 329-339	23
1498	An analysis of electron donor-acceptor complexes: BH3CO and BH3NH3. **1992**, 162, 271-284	25
1497	The torsional dependence of an interaction potential: the CH3OH?He system. **1992**, 162, 285-292	10
1496	Ab initio CI calculations of electronic and vibrational spectra of ZnCH3. **1992**, 164, 191-196	7
1495	CO bonding and vibrational modes on a perfect MgO(001) surface: LCGTO-LDF model cluster investigation. **1992**, 168, 267-280	69
1494	An ab initio investigation of the potential energy surface of the benzene-neon van der Waals complex. **1992**, 195, 482-486	20
1493	Ab initio BSSE-EICP calculations of thermodynamic properties on linear hydrogen fluoride dimerization. **1992**, 254, 219-228	2
1492	Ab initio calculation of protonation and lithiation energy of acetamidoxime. **1992**, 254, 473-480	1
1491	Degenerate Li-H exchange in first-row hydrides: a charge density analysis. **1992**, 255, 309-325	5
1490	Ab initio MO calculations of high temperature gaseous fluorine complexes MAlF4 (M = H, Li or Na): a comparative study using different basis sets. **1992**, 258, 251-260	16

1489	M□ller-Plesset fourth order perturbations and group theoretical formalism for C2v and D3h isomers of ozone. **1992**, 262, 131-146	9
1488	Ab initio MO study of the potential energy surface of the HF?.Cl2 binary complex. **1992**, 259, 211-227	3
1487	Theoretical study of carbamic acid [1H-imidazol-2-yl-]methyl ester. **1992**, 259, 265-272	1
1486	Ab initio calculations of nonadditive effects. **1992**, 261, 37-54	38
1485	Effects of hydration on scale factors for ab initio force constants III: supermolecules. **1992**, 253, 57-72	9
1484	A quantum chemical study of the hydrogen bonding in a weakly bound SCO-HF complex. **1992**, 253, 187-197	3
1483	Structure, energetics, and vibrational spectrum of H2O-X□(X = F, Cl) complexes. **1992**, 253, 225-241	13
1482	Methods for determining the reliability of semiempirical electrostatic potentials and potential derived charges. **1992**, 256, 249-269	27
1481	Ab initio vibrational spectra of hydrogen-bonded N-methylacetamide. **1992**, 257, 57-73	13
1480	Intermolecular potential function for methanol dimer interactions from ab initio calculations. **1992**, 166, 341-360	25
1479	A theoretical study of the (H2)2 dimer. II. The potential energy surface. **1992**, 167, 263-275	27
1478	Ab initio study of the infrared absorption bands and their intensities for ethylene-halogen and amine-halogen complexes. **1992**, 163, 297-305	16
1477	Electronic structure and spectra of [Fe(CN)6SO3]4□**1992**, 48, 1773-1777	1
1476	Basis set superposition error effects on □X, □XN stretching modes of hydrogen-bonded systems FX□NCH (X=H, D). **1992**, 198, 491-497	9
1475	Symmetry-adapted perturbation theory calculations of uracil□water interaction energy. **1992**, 199, 567-573	16
1474	Ab initio interaction potentials between an Ar atom and the NH radical in the states X 3□a 1□and b 1□. **1992**, 192, 21-28	19
1473	An accurate ab initio calculation of the Ne2 potential. **1992**, 194, 162-166	56
1472	Electron-density distribution in fluorobenzene derivatives. **1992**, 48, 849-854	19

1471	Calculation of the potential energies and transition dipole moments of the KHg pair. **1992**, 199, 47-54	9
1470	The peculiar potential surface of the carbon dioxide dimer. **1992**, 199, 525-529	13
1469	Monomer geometry relaxation and the basis set superposition error. **1992**, 191, 497-499	107
1468	Ab initio calculations of tetrahedral hydrogenated buckminsterfullerene. **1992**, 191, 527-532	38
1467	Relative propensity of methanol and silanol towards hydrogen bond formation. **1992**, 191, 537-547	30
1466	Relativistic pseudo-potential analysis of the weak Au(I)Au(I) attraction. **1992**, 197, 586-590	107
1465	Perturbation analysis of the supermolecule interaction energy and the basis set superposition error. **1992**, 197, 591-598	38
1464	Prediction of non-transition-metal hydrogen complexes. **1992**, 196, 213-219	12
1463	Comparison between limited CI and valence bond calculations for van der Waals systems: application to the H2?H2 potentials. **1992**, 196, 377-383	4
1462	Basis set superposition error in proton transfer potentials. **1992**, 196, 384-389	25
1461	Calculation of the potential energies and transition dipole moments of the CdHg pair. **1992**, 197, 187-194	15
1460	Properties and reactions of protonated molecules in the gas phase. Experiment and theory. **1992**, 11, 389-430	56
1459	The counterpoise method and bond functions in molecular dissociation energy calculations. **1993**, 206, 560-564	7
1458	Relativistic corrections to the properties of the alkali fluorides. **1993**, 206, 565-567	5
1457	An efficient procedure for calculations of interaction energy in large molecular systems. **1993**, 201, 33-36	
1456	The energetical and structural properties of FeO+. An application of multireference perturbation theory. **1993**, 211, 242-248	48
1455	Finite-difference versus finite-element methods. **1993**, 202, 7-12	70
1454	Theoretical study of the (H2O)6 cluster. **1993**, 213, 181-188	198

1453	Ab initio study of the gas-phase equilibrium between (H2O)4 and (H2O)8. **1993**, 212, 644-648	26
1452	An investigation of the structure of weakly bound (OCS)2. **1993**, 206, 260-270	30
1451	Analysis of the intermolecular interactions in the FCN dimer. **1993**, 206, 312-317	6
1450	Accurate modeling of intermolecular forces: a systematic Møller-Plesset study of the argon dimer using correlation consistent basis sets. **1993**, 204, 29-35	92
1449	Ab initio theoretical study of the electronic structure, stability and bonding of dialkali halide cations. **1993**, 204, 73-79	21
1448	Bond strengths of the gas-phase cluster ions X−(CS2)n (X = F, Cl, Br and I). **1993**, 208, 491-496	8
1447	Reactions between H+3 and rare gas atoms. **1993**, 208, 497-502	17
1446	Calculation of the interaction energies for the ZnHg and ZnCd system. **1993**, 212, 534-542	11
1445	The vibrational contribution to the polarisability of endohedral [C60M]n+ complexes (where M = metal atom). **1993**, 207, 332-338	32
1444	Ab initio investigation of the ground state potential surfaces of He?NO+ and Ar?NO+. **1993**, 210, 170-174	30
1443	Ab initio study of the long-range interaction between He+ and H2. **1993**, 213, 531-536	8
1442	Non-additivity in cation–peptide interactions. A molecular dynamics and ab initio study of Na+ in the gramicidin channel. **1993**, 212, 231-240	44
1441	Stability and the CO stretching vibrational frequency of molecular AgCo. **1993**, 215, 582-586	12
1440	Structures and energetics of Zn(NH3)2+n (n=4–8). Coordination number of Zn2+ by ammine. **1993**, 216, 309-312	17
1439	Die Stärke von C-H···O-Wasserstoffbrücken und die ekliptische Anordnung einer Csp3-CH3-Bindung in einem tricyclischen Orthoamid-Trihydrat. **1993**, 105, 640-641	4
1438	Comparison of a posteriori and a priori BSSE correction schemes for SCF intermolecular energies. **1993**, 14, 401-409	38
1437	Molecular interaction potential: A new tool for the theoretical study of molecular reactivity. **1993**, 14, 587-602	45
1436	Ab initio copper–water interaction potential for the simulation of aqueous solutions. **1993**, 14, 629-638	30

1435	Theoretical study of protonated pyruvate. A methylhydroxycarbene. carbon dioxide complex. Implications for the decarboxylation of pyruvic acid. **1993**, 14, 699-714	9
1434	Ab initio study of hydrogen bonding in the phenol. water system. **1993**, 14, 1027-1035	92
1433	Calculation of the interaction energy in a localized representation for a trimer (Ne3) system. **1993**, 14, 1136-1141	6
1432	Ab initio models for multiple-hydrogen exchange: Comparison of cyclic four- and six-center systems. **1993**, 14, 1149-1163	37
1431	Electrostatic and chemical bonding contributions to the cation core level binding energy shifts in MgO, CaO, SrO, BaO. A cluster model study. **1993**, 63, 189-205	23
1430	Promotion by alkali metals: a theoretical analysis of the vibrational shift of CO coadsorbed with K on Cu(100). **1993**, 177, 373-385	15
1429	Bonding and vibrations of CO molecules adsorbed at transition metal impurity sites on the MgO (001) surface. A density functional model cluster study. **1993**, 177, 561-570	44
1428	Are there geometric isomers of the van der Waals dimers Ar?OCS and Ar?SO2?. **1993**, 178, 255-277	8
1427	Super-cell versus embedded cluster simulation of a lithium vacancy in a lithium fluoride monolayer. **1993**, 169, 297-303	7
1426	Calculations on clusters of Li and F ions at LiF crystal geometries. **1993**, 171, 145-151	3
1425	Ab initio calculations on the geometry and OH vibrational frequency shift of cyclic water trimer. **1993**, 175, 271-281	80
1424	Computed gas-phase thermodynamics of N2 association. **1993**, 223, 1-6	3
1423	Gas-phase association of O2: a computational thermodynamic study. **1993**, 228, 9-14	6
1422	Computed gas-phase thermodynamics of the N2?O2 complexes. **1993**, 225, 1-7	6
1421	Ab initio molecular orbital studies of the vibrational spectra of nitrosyl fluoride and chloride monomers and dimers. **1993**, 297, 265-275	7
1420	Charge populations of, and water binding at, the oxygen atoms of some simple esters. **1993**, 300, 233-238	4
1419	The vibrational spectra of the boron halides and their molecular complexes Part 2. Ab initio predictions of the structure and vibrational spectra of the boron trifluoride dimer. **1993**, 300, 325-338	16
1418	Comparative study of all-electron and core pseudo-potentials basis sets for periodic AB INITIO hartree-fock calculation: The case of MgSiO3-ilmenite. **1993**, 54, 281-287	3

1417	Theoretical study on crown compounds as building blocks of functional molecules I. The relation between the hole size and the number of atoms in the ring of cyclic ethers and amines. **1993**, 49, 3959-3970	9
1416	MÖllerPlesset expansion of the dispersion energy in the ring approximation. **1993**, 45, 409-431	57
1415	A study of the weak interaction in SCO/He and SCO/N2 systems. **1993**, 46, 623-634	17
1414	Decomposition and interpretation of the SCF interaction and deformation energies by the modified Pauli Blockade method. **1993**, 47, 145-153	1
1413	Ab initio potential energy function for the dynamics of the fluoronium ion. **1993**, 47, 335-373	2
1412	Some comments on the counterpoise correction for the basis set superposition error at the correlated level. **1993**, 48, 375-384	70
1411	Active site dynamics of acyl-chymotrypsin. **1993**, 16, 172-94	34
1410	Structure, energetics, and vibrational frequencies of the pyrazole-water complex. **1993**, 124, 259-266	2
1409	Energy analysis on small to medium sized H-bonded complexes. **1993**, 85, 409-421	35
1408	Ab initio study on the methanol-water cation radical potential energy surface. **1993**, 87, 97-105	9
1407	Theoretical studies on the topographical features and energetics of diacetylene-hydrogen fluoride complexes. **1993**, 280, 191-197	2
1406	Ab initio MO study of the potential energy surface of the N2□1F binary complex. **1993**, 280, 239-252	1
1405	Basis set effects on the intermolecular interaction of the H2-H2 system obtained using ab initio molecular orbital calculations with the Möller-Plesset perturbation correction. **1993**, 280, 273-281	8
1404	Potential energy surface of the 1:1 acetone-iodine molecular complex at the SCF and MP2 levels. **1993**, 281, 67-74	4
1403	Computational studies of atmospheric chemistry species. **1993**, 282, 271-275	14
1402	Computational studies of atmospheric chemistry species. **1993**, 285, 77-87	3
1401	Computational studies of atmospheric chemistry species. **1993**, 285, 273-276	9
1400	A decomposition of intermolecular interaction energy in MNDO and AM1 semiempirical MO theories. **1993**, 280, 59-65	2

1399	Ab initio and AM1 calculations on model systems of Acctylcholine binding: complexes of tetramethylammonium with aromatics, neutral and ionic formic acid. **1993**, 283, 305-312	25
1398	On the stability of XH3YH3 charge-transfer complexes (X = B, Al, Ga, In and Y = N, or P for X = B, Al): an ab initio study. **1993**, 283, 317-320	25
1397	Ab initio quantum chemical analysis of Schiff base-water interactions in bacteriorhodopsin. **1993**, 286, 231-245	27
1396	Ab initio molecular orbital calculations on ion-molecule and ion pair-molecule complexes of the water-lithium cyanide system. **1993**, 284, 147-156	5
1395	A generalized valence bond + configuration interaction description of the P2O molecule. **1993**, 287, 67-75	4
1394	MBPT study of the CO-H2 van der Waals interaction. **1993**, 287, 139-147	4
1393	Ab initio and semiempirical calculations on the interaction of tetramethylammonium with a water molecule. **1993**, 279, 311-319	6
1392	Computational studies of atmospheric chemistry species. Part XI. A computational study of two Ar?N2 complexes. **1993**, 288, 17-20	9
1391	Association of metal cations with alkanes: Na(CH4)+ versus Cu(CH4)+ as molecular models. **1993**, 85, 121-126	6
1390	Ab initio and experimental study of the interaction of nitrous oxide with the isolated hydroxyl of silica. **1993**, 49, 1221-1234	7
1389	Ab initio molecular orbital study on R3SiCO+/R3SiOC+ (R = H or CH3). **1993**, 127, 183-190	12
1388	An MP2 study of the C2H2⊡O complex and its isotopomers. **1993**, 169, 185-193	7
1387	Ab initio potential energy surface for the collisional system H⊞H2 and properties of its van der Waals complex. **1993**, 176, 83-95	57
1386	Ab initio and semiempirical investigations of the complexation of methyl pyruvate by ammonia and the ammonium cation. **1993**, 297, 285-293	32
1385	Helium atom as a probe of molecular shape and properties: He?H2O complex. **1993**, 297, 313-325	17
1384	Molecular recognition in aqueous media. New binding studies provide further insights into the cation-.pi. interaction and related phenomena. **1993**, 115, 9907-9919	247
1383	Bonding and vibration of CO molecules adsorbed on low-coordinated surface sites of MgO: a LCGTO-LDF cluster investigation. **1993**, 297, 223-234	59
1382	N2O adsorption and decomposition at a CaO(100) surface, studied by means of theory. **1993**, 292, 317-324	29

1381	Physisorbed and chemisorbed CO2 at surface and step sites of the MgO(100) surface. **1993**, 281, 207-219		130
1380	Theoretical reaction pathways for the formation of [Si(OH)5]1− and the deprotonation of orthosilicic acid in basic solution. **1993**, 57, 3847-3853		47
1379	Ab initio intermolecular potentials of methane, nitrogen and methane + nitrogen and their use in Monte Carlo simulations of fluids and fluid mixtures. *Molecular Physics*, **1993**, 80, 1413-1429	1.7	29
1378	Symmetry-adapted perturbation theory calculation of the Ar–H2 intermolecular potential energy surface. **1993**, 98, 1279-1292		135
1377	On the use of bond functions in molecular calculations. **1993**, 98, 2481-2483		35
1376	Ab initio study of the potential energy surface of CH4-H2O. **1993**, 98, 3078-3089		95
1375	Stability of MX2− ions in the gas phase and when do ionic molecules have large ionization potentials. **1993**, 99, 441-455		86
1374	The History and Evolution of Gaussian Basis Sets. **1993**, 33, 357-367		47
1373	Free doubly negative tetrahalides. **1993**, 99, 8877-8891		62
1372	Adsorption of hydrocarbons on a diamond (111) surface: An ab initio quantum-mechanical study. **1993**, 48, 2666-2674		45
1371	Accuracy of the Boys and Bernardi function counterpoise method. **1993**, 98, 4728-4737		195
1370	Intermolecular potentials calculated by an extended group function model: Theory. **1993**, 99, 277-285		17
1369	Ab initio studies of open-shell complexes of CO+ with rare gases. **1993**, 99, 436-440		19
1368	Ab initio theoretical predictions of C28, C28H4, C28F4, (Ti@C28)H4, and M@C28 (M=Mg, Al, Si, S, Ca, Sc, Ti, Ge, Zr, and Sn). **1993**, 99, 352-359		149
1367	Quantum-chemical study of the CH4?HCl complex. **1993**, 89, 2363-2367		6
1366	Structures and binding energies of benzene–methane and benzene–benzene complexes. An ab initio SCF/MP2 study. **1993**, 89, 659-664		84
1365	An ab initio investigation of the molecular structure and vibrational spectrum of the silanol–hydrogen molecular complex. **1993**, 89, 983-989		4
1364	Effects of external ions on the energetics of proton transfer in hydrogen-bonded systems modelling a membrane-active drug–receptor interaction. **1993**, 89, 1321-1326		8

1363	Scattering of NH3 by ortho- and para-H2: Expansion of the potential and collisional propensity rules. **1993**, 98, 4662-4671		31
1362	Theoretical study of the ground states of the rare-gas hydrides, HeH, NeH, and ArH. **1993**, 99, 9776-9782		21
1361	Properties of fluorobenzene???Ar and p-difluorobenzene???Ar complexes: Ab initio study. **1993**, 99, 2809-2811		29
1360	Ionization potential and electron affinity of the Au atom and the AuH molecule by all-electron relativistic configuration interaction and propagator techniques. **1993**, 98, 3945-3951		64
1359	The use of midbond functions for ab initio calculations of the asymmetric potentials of He□Ne and He□Ar. **1993**, 98, 3049-3059		82
1358	The Ar□2H2 intermolecular potential from high resolution spectroscopy and ab initio theory: A case for multicenter interactions. **1993**, 99, 8585-8598		87
1357	Large Amplitude Motion in Oxalyl Chloride. **1993**, 409-421		
1356	Investigation of the CS structure of CO- 4 using ab initio calculations. *Molecular Physics*, **1993**, 79, 875-885.	1.7	4
1355	Quadrupole polarizabilities of anions in crystals. *Molecular Physics*, **1993**, 80, 135-143	1.7	16
1354	Towards the one-particle basis set limit of second-order correlation energies: MP2-R12 calculations on small Ben and Mgn clusters (n=1□). **1993**, 99, 5167-5177		76
1353	Ab initio group model potentials: Application to the study of intermolecular interactions. **1993**, 99, 1255-1261		12
1352	Ab initio study of intermolecular potential for dimers XO□E (X=N,C). **1993**, 99, 2855-2864		10
1351	Ab initio study of the H2CO□Ar complex. **1993**, 99, 5211-5218		10
1350	Measures of ionicity of alkaline-earth oxides from the analysis of ab initio cluster wave functions. **1993**, 48, 11573-11582		101
1349	Calculation of the interaction energy in a localized representation for several diatomic systems. *Molecular Physics*, **1993**, 80, 1059-1065	1.7	2
1348	Ab initio search for the equilibrium structure of the ammonia dimer. **1993**, 99, 5976-5982		91
1347	Differential and integral cross sections for the inelastic scattering of NO (X 2□) by Ar based on a new ab initio potential energy surface. **1993**, 99, 7725-7738		92
1346	Energetics, structure, and compressibility of NaF determined by the periodic Hartree□ock method. **1993**, 99, 336-344		9

1345	Ground state potential surface for van der Waals complexes: Ab initio second-order Mo/llerPlesset study on benzene...N2 van der Waals molecule. **1993**, 98, 6223-6226	35
1344	A Gaussian-2 ab initio study of van der Waals dimers R1R2 and their cations R1R+2 (R1, R2=He, Ne, Ar, and Kr). **1993**, 99, 3617-3621	34
1343	Experimental and theoretical characterization of the BAr van der Waals complex: The X 2, A 2, and B 2 electronic states. **1993**, 98, 8484-8495	53
1342	Intermolecular bonding and vibrations of phenol?H2O (D2O). **1993**, 98, 3763-3776	173
1341	Theoretical study of the gallium chloride molecule and its interaction with arsenic dangling bonds. **1993**, 47, 13420-13431	9
1340	The nonadditive interactions in the Ar2HF and Ar2HCl clusters: An ab initio study. **1993**, 99, 6732-6741	46
1339	Spin orbit branching in the photofragmentation of HCl. **1993**, 99, 1752-1764	107
1338	Structure and energetics of Cr(CO)6 and Cr(CO)5. **1993**, 98, 3978-3989	50
1337	On the nature of the interaction energy in the ArClF complex. **1993**, 99, 3700-3706	22
1336	Efficient elimination of basis set superposition errors by the local correlation method: Accurate ab initio studies of the water dimer. **1993**, 98, 2170-2175	204
1335	Relativistic effects on the bonding and properties of the hydrides of platinum. **1993**, 98, 9678-9686	49
1334	An exact quantum Monte Carlo calculation of the helium helium intermolecular potential. **1993**, 99, 345-351	107
1333	Accurate coupled cluster reaction enthalpies and activation energies for X+H2-XH+H (X=F, OH, NH2, and CH3). **1993**, 99, 5306-5315	72
1332	A global potential energy surface for ArH2. **1993**, 98, 4738-4744	20
1331	Adiabatic and approximate diabatic potential energy surfaces for the B...H2 van der Waals molecule. **1993**, 99, 6014-6026	68
1330	Fluxionality and low-lying transition structures of the water trimer. **1993**, 99, 5228-5238	116
1329	Proton-donor properties of water and ammonia in van der Waals complexes. BeH2O and BeNH3. **1993**, 98, 7020-7028	4
1328	Ca and Be substitution in bulk MgO: 'ab initio' Hartree-Fock and ionic model supercell calculations. **1993**, 5, 4793-4804	22

1327	Theoretical Studies on Hydrogen Bonding Interactions between Peptide Units. **1993**, 66, 3423-3429		13
1326	Theoretical study of acetylene- and ethylene-palladium complexes. *Molecular Physics*, **1993**, 78, 1449-1460	1.7	1
1325	Proton transfer in zeolites: a comparison between cluster and crystal calculations. **1994**, 2, 921-932		37
1324	Spin coupled valence bond theory of van der Waals systems: application to LiH He. *Molecular Physics*, **1994**, 83, 89-100	1.7	15
1323	Rotationally inelastic and bound state dynamics of H2-OH(X2). *Molecular Physics*, **1994**, 83, 405-428	1.7	40
1322	The molecular structure of the (NCCN)2 and (PCCP)2 van der Waals dimers. *Molecular Physics*, **1994**, 81, 1397-1410	1.7	8
1321	Interactions between amino groups in DNA. An Ab initio study and a comparison with empirical potentials. **1994**, 11, 1357-76		25
1320	A quantum-mechanical ab initio simulation of neutral and charged point defects in alpha-quartz. **1994**, 2, 965-974		10
1319	Ab initio potential energy surface and dynamics of HeCO. **1994**, 101, 8680-8686		50
1318	Structure, vibrational frequencies, and thermodynamic properties of hydrogen peroxide dimers: An ab initio molecular orbital study. **1994**, 100, 2871-2877		33
1317	Mechanical and molecular properties of ice VIII from crystal-orbital ab initio calculations. **1994**, 100, 2128-2138		56
1316	Accurate spectroscopic constants for the Cd(1S,3P,1P)H2 van der Waals complexes: A theoretical study. **1994**, 100, 8251-8256		6
1315	Ab initio study of He(1S)+Cl2(X 1g,3u) potential energy surfaces. **1994**, 101, 6800-6809		33
1314	Variation of interatomic distances in ice VIII to 10 GPa. **1994**, 49, 12540-12550		105
1313	Symmetry-adapted perturbation theory potential for the HeK+ molecular ion and transport coefficients of potassium ions in helium. **1994**, 101, 4697-4707		20
1312	Quantum scattering studies of electronically inelastic collisions of N+2(X 2g, A 2u) with He. **1994**, 100, 1953-1967		46
1311	Differential cross sections for fine structure transitions in O(3P2)+Ar collisions. **1994**, 100, 8026-8039		32
1310	Ab initio computations close to the one-particle basis set limit on the weakly bound van der Waals complexes benzeneneon and benzeneargon. **1994**, 101, 9747-9754		82

1309	The fraternal twins of quartet O+4. **1994**, 100, 224-237	39
1308	Ab initio study of the intermolecular potential of the water–carbon monoxide complex. **1994**, 100, 4272-4283	58
1307	Study of the LiHg excimer: Blue–green bands. **1994**, 101, 929-936	17
1306	Potential energy curves of M(np 2P)?RG(2) excited states and M+?RG ground states (M=Li, Na; RG=He, Ne). **1994**, 100, 8212-8218	34
1305	Supermolecular approach to many-body dispersion interactions in weak van der Waals complexes: He, Ne, and Ar trimers. **1994**, 101, 8860-8869	54
1304	Accurate ab initio potential energy surfaces of Ar–HF, Ar–H2O, and Ar–NH3. **1994**, 101, 1129-1145	123
1303	Investigation of the ground vibrational state structure of H35Cl trimer based on the resolved K, J substructure of the vibrational band. **1994**, 100, 7101-7108	20
1302	An ab initio molecular orbital study of the structures and energetics of the neutral and cationic CuO2 and CuNO molecules in the gas phase. **1994**, 101, 3898-3905	69
1301	About the nature of intermolecular three-body forces in ionic systems: The case of protonated hydrates. **1994**, 100, 1589-1598	12
1300	The dissociation energy of CN and C2. **1994**, 101, 3857-3861	73
1299	Potential energy surfaces for the interaction of BH(X 1,A 1) with Ar and a theoretical investigation of the stretch-bend levels of the ArBH(A) van der Waals molecule. **1994**, 101, 2887-2902	64
1298	Benchmark calculations with correlated molecular wave functions. V. The determination of accurate ab initio intermolecular potentials for He2, Ne2, and Ar2. **1994**, 100, 2838-2850	168
1297	A water–water potential derived using a quantum Monte Carlo vibrational analysis. **1994**, 100, 2865-2870	40
1296	Nonadditivity effects in the molecular interactions of H2O and HF trimers by the symmetry-adapted perturbation theory. **1994**, 101, 3062-3072	19
1295	Ab initio study of the phenol-water cation radical. **1994**, 101, 990-997	63
1294	How large is the effect of 1s correlation on the De, , and re of N2?. **1994**, 100, 4329-4335	64
1293	A computational thermodynamic evaluation of the altitude profiles of (N2)2, N2-O2 and (O2)2 in the Earth's atmosphere. **1994**, 231, 55-60	8
1292	Thermodynamics of Ar-N2 complexes and their abundance in Titan's atmosphere. **1994**, 232, 111-116	2

1291	Ab initio molecular orbital calculations of the energetic, structural, vibrational and electronic properties of some hydrogen bonded complexes of water, ammonia and hydroxylamine. **1994**, 50, 5-18	15
1290	Vibrational analysis of phenol/(methanol)1. **1994**, 29, 223-229	30
1289	Theoretical study of hydrogen-bonded formaldehyde complexes. **1994**, 32, 241-247	9
1288	Theoretical studies on specific interactions between biological molecules: interaction of cationic arginine with anionic glutamic acid. **1994**, 311, 45-53	2
1287	Directional hydrogen bonding in the MM3 force field. I. **1994**, 7, 591-609	79
1286	A comparative basis-set study of NeH+ using coupled-cluster techniques. **1994**, 49, 495-509	10
1285	Structure of the ammonia dimer studied by density functional theory. **1994**, 49, 613-623	21
1284	Theoretical study of the structure and vibrational spectra of the (H2O)2HF and H2O(HF)2 molecular complexes. **1994**, 52, 177-189	9
1283	Theoretical investigation of the enantioselective hydrogenation of ketoesters over pt/alumina modified with cinchonidine. **1994**, 52, 191-197	24
1282	Cooperativity and electron correlation effects on hydrogen bonding in infinite systems. **1994**, 52, 395-412	26
1281	Density functional studies on hydrogen-bonded complexes. **1994**, 52, 465-478	38
1280	Bonding of acetylene to copper atom, dimer, and trimer. **1994**, 52, 973-985	22
1279	Density functional treatment of water carbon dioxide van der waals complex. **1994**, 52, 1011-1015	19
1278	Effect of the ionic field on vibration spectroscopy of molecules in solvate complexes. **1994**, 34, 638-640	
1277	A theoretical determination of the dissociation energy of the nitric oxide dimer. **1994**, 88, 425-435	35
1276	The polarisability of Hg and the ground-state interaction potential of Hg2. **1994**, 87, 313-320	56
1275	A possible definition of basis set superposition error. **1994**, 217, 48-54	98
1274	Predicted ligand dependence of the Au(I)Au(I) attraction in (XAuPH3)2. **1994**, 218, 133-138	235

1273	Adiabatic potential curves for the KZn and KCd excimers. **1994**, 218, 454-461	5
1272	Structure, vibrational frequencies and thermodynamic properties of hydrogen peroxide□water dimers. An ab initio molecular orbital study. **1994**, 219, 45-52	20
1271	A theoretical study of NO□complexes with neutral water solvent molecules. **1994**, 221, 255-258	8
1270	Ab initio calculations on the stabilization energy and vibrational frequencies of the C6H6□F6 dimer. **1994**, 221, 241-248	1
1269	Theoretical study of the H2O?2CO hydrogen-bonded ternary complexes. **1994**, 222, 33-39	10
1268	The neglect of basis set superposition error in the accurate theoretical determination of heats of formation. **1994**, 223, 7-11	4
1267	Prediction and characterization of magnesium fluoride dimers and their non-classical hydrogen complexes. **1994**, 223, 233-239	10
1266	Coupled-pair functional calculations on the Ar?-CO and Ar2 van der Waals complexes. **1994**, 223, 377-382	29
1265	Potential energy surface for the ligand substitution reaction of the square-planar platinum(II) complex. Essential role of the repulsive three-body effect. **1994**, 224, 139-144	5
1264	A full-CI investigation into the BSSE problem. **1994**, 224, 166-174	36
1263	Adiabatic potential curves for the Cd2 dimer. **1994**, 225, 233-239	33
1262	The reliability of the point charge model representing intermolecular effects in ab initio calculations. **1994**, 225, 258-264	19
1261	A numerical evaluation of the counterpoise method on hydrogen bond complexes using near complete basis sets. **1994**, 225, 240-246	55
1260	Structures and bond energies of the noble gas complexes NgBeO (Ng?Ar, Kr, Xe). **1994**, 226, 11-16	74
1259	Correlation energies in the interaction energy of molecules. The water dimer. **1994**, 226, 484-490	17
1258	Kinetics and thermochemistry of the reversible gas phase reaction HONO+NH3?H3H-HONO studied by infrared diode laser spectroscopy. **1994**, 227, 6-12	13
1257	A new configuration selection method for configuration interaction calculations. **1994**, 227, 327-336	7
1256	An accurate determination of three-body intermolecular forces in the helium trimer. **1994**, 227, 401-404	8

1255	Theoretical studies on VPI-5. Origin of the hydrophilicity. **1994**, 227, 545-550	8
1254	Electron correlation effects in the cohesive properties of ice. **1994**, 228, 471-477	
1253	Extended basis set calculations of the interaction energy and properties of the ammonia dimer. **1994**, 228, 451-457	24
1252	Can (semi)local density functional theory account for the London dispersion forces?. **1994**, 229, 175-180	888
1251	Reduction of the basis set superposition error at the correlation level. **1994**, 230, 35-40	4
1250	Calculation of the fundamental vibrational frequencies and intensities of H2, D2, and N2 in the presence of Li+ or Na+. **1994**, 230, 177-181	22
1249	Theoretical modelling of metal oxides. Influence of field strength on atomic oxygen adsorption and a simple model reaction: Oads+CO -œCO2. **1994**, 230, 456-462	34
1248	H2S•HOH or H2O•HSH, which is more stable in the water-hydrogen sulfide complex?. **1994**, 230, 480-484	13
1247	The chemical Hamiltonian approach in density functional theory. **1994**, 230, 485-490	21
1246	Reaction of the copper dimer with ethylene. A theoretical study. **1994**, 231, 18-24	7
1245	Ab initio investigation of the stationary points on the potential energy surface for the ethylene-sulfur dioxide complex. **1994**, 231, 283-288	2
1244	An evaluation of the performance of density functional theory, MP2, MP4, F4, G2(MP2) and G2 procedures in predicting gas-phase proton affinities. **1994**, 231, 345-351	124
1243	Theoretical probation of FClCO?Cl2 molecular complex. **1994**, 231, 359-365	3
1242	Quantum chemical study of the trimethylamine•hydrogen chloride complex. **1994**, 221, 167-174	5
1241	Entropy-driven structures of the water octamer. **1994**, 219, 243-246	72
1240	Stability of Charge-Transfer Complexes of CS2 with PH3 and its derivatives: Ab initio MRSDCI/CASSCF Study. **1994**, 77, 1810-1816	2
1239	The structures of LiNC, NaNC, and KNC: Potential energy surface for the orbiting motion of the metal cation around the CN group. **1994**, 15, 322-332	36
1238	Triazene proton affinities: A comparison between density functional, Hartree•ock, and post-Hartree•ock methods. **1994**, 15, 875-892	29

1237	Decomposition analyses of the intermolecular interaction energies in two π-stacking complexes: Quinhydrone and N,N,N?, N?-tetramethyl-P-diaminobenzene-chloranil complex. **1994**, 15, 1013-1018	9
1236	Energetics of proton transfer in liquid water. I. Ab initio study for origin of many-body interaction and potential energy surfaces. **1994**, 180, 239-269	65
1235	Quantum chemical investigation of the Ar?CHI interaction potential. Steepness and asymmetry with implications for energy transfer. **1994**, 184, 67-83	2
1234	Theoretical study of the mono- and di-hydrated divalent ions of the first-row transition metals. **1994**, 184, 85-95	14
1233	Accurate computation of the normal and reverse complexes between water and hydrogen fluoride. **1994**, 186, 175-183	11
1232	Matrix isolation FTIR and ab initio study of complexes between formic acid and nitrogen. **1994**, 189, 245-260	47
1231	Neon in condensed phase: quantitative calculations of structural, thermodynamic and transport properties from pure theory. **1994**, 187, 317-327	20
1230	The insertion of acetylene into the palladium carbon bond of square planar Pd(II) complexes: a theoretical investigation. **1994**, 478, 121-129	47
1229	A New Potential Model for Carbon Dioxide from AB Initio Calculations. **1994**, 12, 343-353	18
1228	An ab initio study of anticonvulsants. **1994**, 315, 245-251	4
1227	Coordination of (CH3)2X (X ? O, S, and Se) to borane: an ab initio molecular orbital study. **1994**, 315, 109-115	1
1226	Cooperative effects in the cyclic trimer of methanol. An ab initio molecular orbital study. **1994**, 314, 73-81	128
1225	Bonded hydrogen and hydrogen bonding in reciprocal space. Simulation of diffraction by a water molecule and dimer. **1994**, 314, 155-167	
1224	Traps in modelling intermolecular three-body forces: example of the water system and protonated hydrates. **1994**, 314, 191-210	12
1223	A theoretical study of hydrogen-bonded complexes in solution: BSSE and decomposition of interaction energy. **1994**, 314, 229-239	15
1222	Structures and relative stabilities of bisulfite ion isomers. **1994**, 304, 1-11	9
1221	An ab initio study of the molecular structure of chlorine nitrate. **1994**, 309, 31-35	13
1220	Accurate calculation of the binding energy of the water dimer. **1994**, 309, 235-239	29

1219	A quantum chemical study of the F- and H-bonded isomers of HF/ClF. **1994**, 307, 9-22	5
1218	Molecular modelling of the antiarrhythmic-receptor interaction. **1994**, 307, 35-46	7
1217	The role of valence interaction in some cation-molecule complexes. **1994**, 307, 99-105	16
1216	Basis set effects on the intermolecular interaction of hydrocarbon molecules obtained by an ab initio molecular orbital method: evaluation of dispersion energy. **1994**, 307, 107-118	86
1215	Quantum mechanical studies of weakly bound molecular clusters. **1994**, 307, 119-133	9
1214	Symmetry-adapted perturbation theory of potential-energy surfaces for weakly bound molecular complexes. **1994**, 307, 135-151	33
1213	Ab initio calculations of the structural, energetic and vibrational properties of some hydrogen bonded and van der Waals dimers. **1994**, 307, 153-169	27
1212	On the nature of the interaction energy in the Ar-Cl2 complex. **1994**, 307, 187-199	24
1211	Filling of solvent shells about ions. **1994**, 307, 217-238	6
1210	Ab initio Hartree- Fock calculations of the interaction energy of bimolecular complexes. **1994**, 307, 239-259	8
1209	Reliability of the ab initio potentials for simple van der Waals systems based on second virial and thermal diffusion coefficients. **1994**, 305, 69-78	1
1208	Ab initio study of a Br□sted acid site model and complex with CO, with and without symmetry constraints. **1994**, 303, 65-70	4
1207	Calculations of the second virial coefficient and of the transport properties using BSSE-corrupted ab initio potentials. **1994**, 303, 119-129	2
1206	Ab initio study of methanol sorption and proton transfer on a zeolite acid site model. **1994**, 306, 57-65	41
1205	An extended basis set ab initio study of Li+(H2O)n, n=1□. **1994**, 100, 4981-4997	151
1204	Structural, vibrational and electronic properties of a crystalline hydrate from ab initio periodic Hartree□ock calculations. **1994**, 50, 268-279	41
1203	Ab initio molecular orbital calculations of the infrared spectra of interacting water molecules. Part 4. Interaction energies and band intensities of the complexes of water with carbon dioxide and nitrous oxide. **1994**, 312, 101-108	25
1202	A preliminary study of monomer geometry effects in theoretical calculations of the interaction energy for weak molecular complexes. **1994**, 312, 109-114	2

1201	Theoretical studies on specific interactions between biological molecules: interaction of cationic arginine with anionic glutamic acid. **1994**, 311, 45-53		2
1200	Ab initio calculations on ArNO+: Structure and vibrational frequencies. **1994**, 100, 5403-5410		27
1199	Ab initio studies of hydrogen bonds: the water dimer paradigm. **1994**, 45, 23-56		163
1198	Ab initio potential energy curves and binding energies of Ar2 and Mg2. *Molecular Physics*, **1994**, 81, 507-518	1.7	85
1197	A new ab initio potential for the neon dimer and its application in molecular dynamics simulations of the condensed phase. *Molecular Physics*, **1994**, 82, 689-699	1.7	42
1196	Many-body theory of intermolecular induction interactions. **1994**, 100, 4998-5010		103
1195	The structure and stability of BH5. Does correlation make it a stable molecule? Qualitative changes at high levels of theory. **1994**, 101, 7625-7632		72
1194	An accurate ab initio potential energy surface of the HeH2 interaction. **1994**, 100, 4947-4954		34
1193	Structure and energetics of van der Waals complexes of carbon monoxide with rare gases. HeCO and ArCO. **1994**, 101, 4964-4974		82
1192	A new approach to the efficient basis set for accurate molecular calculations: Applications to diatomic molecules. **1994**, 100, 3645-3650		53
1191	The NMR Chemical Shift: Insight into Structure and Environment. **1994**, 29, 1-69		41
1190	Charge separation and covalent bonding in metal oxide surfaces: A local density functional study on the MgO(001) surface. **1994**, 100, 6826-6836		79
1189	Symmetry-adapted perturbation theory calculation of the HeHF intermolecular potential energy surface. **1994**, 101, 2811-2824		69
1188	The interatomic potential for the X1Sigma state of ArLi+. **1994**, 27, 5603-5620		22
1187	A theoretical study of the adsorption and reaction of SO2 at surface and step sites of the MgO(100) surface. **1994**, 315, 337-350		93
1186	Crystal field effects on the topological properties of the electron density in molecular crystals: The case of urea. **1994**, 101, 10686-10696		577
1185	Cyclization of acetylene over Pd(111): a theoretical study of reaction mechanisms and surface intermediates. **1994**, 304, 208-222		77
1184	Modeling of supported metal clusters: a density functional study of CO chemisorption on Ni clusters deposited on alumina. **1994**, 306, 169-178		47

1183	Atomic oxygen chemisorption on Cu(110) and Ag(110): an ab initio study. **1994**, 301, 89-96		34
1182	Anisotropic rigid rotor potential energy function for H2O□H2. **1994**, 101, 5824-5830		65
1181	Natural energy decomposition analysis: An energy partitioning procedure for molecular interactions with application to weak hydrogen bonding, strong ionic, and moderate donor□cceptor interactions. **1994**, 100, 2900-2909		354
1180	The complex of N2 with H2O, D2O, and HDO: A combined ab initio and diffusion Monte Carlo study. **1994**, 101, 1378-1391		60
1179	Potential energy surfaces for the interaction of CH(X 2□,B 2□)with Ar and an assignment of the stretch-bend levels of the ArCH(B) van der Waals molecule. **1994**, 101, 4547-4560		53
1178	Bonding between CO and the MgO(001) surface: A modified picture. **1994**, 100, 2010-2018		168
1177	Ab initio study of nonadditive interactions in the Ar2HF and Ar2HCl clusters. II. Analysis of exchange and induction effects. **1994**, 101, 10708-10716		30
1176	Symmetry-adapted perturbation theory of the intramonomer correlation effects in intermolecular forces. **1994**, 100, 1995-2009		9
1175	Hydroxylamine□water: intermolecular potential function and simulation of hydrated NH2OH. **1994**, 90, 2337-2344		9
1174	Derivation and application of ab initio Nb5+-O2- short-range effective pair potentials in shell-model simulations of KNbO3 and KTaO3. **1994**, 49, 3746-3754		28
1173	Ab initio studies of cyclic water clusters (H2O)n, n=1□6. II. Analysis of many-body interactions. **1994**, 100, 7523-7534		600
1172	CO adsorption on the (001) surface of MgO: a comparison of Hartree-Fock and local density functional results. **1994**, 69, 13-21		39
1171	Adsorption of small molecules on metal oxides. **1994**, 69, 43-53		12
1170	Ab initio calculations for the adsorption of small molecules on metal oxide surfaces. Part 3. Adsorption of H and CH3 radicals on NiO(100). **1994**, 69, 99-109		10
1169	An ab initio investigation of structure and energetics of clusters KnCln and LinFn. **1994**, 98, 34-47		42
1168	Decomposition of the interaction correlation energy in terms of localized orbital contributions. *Molecular Physics*, **1994**, 82, 343-349	1.7	4
1167	Totallyab InitioPrediction of the Structures of CO2Molecular Crystal. **1995**, 24, 1073-1074		5
1166	Proton-transfer reactions within ionized methanol clusters: Mass spectrometric and molecular orbital studies. **1995**, 30, 969-976		37

1165	Hydration of cis and trans N-methylformamide as revealed by the use of 17O-NMR, molecular mechanics, and ab initio calculations. **1995**, 36, 415-428	13
1164	Relative stability of alternative chair forms and hydroxymethyl conformations of β-d-glucopyranose. **1995**, 276, 219-251	174
1163	Weak intermolecular interactions between nitrogen and oxygen atoms. **1995**, 232, 479-485	35
1162	Validation of self-consistent hybrid approaches for the study of transition metal complexes. NiCO and CuCO as case studies. **1995**, 233, 129-133	55
1161	Ab initio calculations for small iodo clusters. Good performance of relativistic effective core potentials. **1995**, 233, 249-256	31
1160	Loss of hydrogen fluoride from C2H2F3O+. A theoretical study of a reaction mechanism. **1995**, 233, 340-346	7
1159	Adsorption energies of NH3 and NH4+ in zeolites. An embedded cluster model including electron correlation. **1995**, 234, 367-372	31
1158	A theoretical study of isomeric C6H4Br□ ions. **1995**, 235, 436-443	18
1157	Quantum simulation of weakly bound complexes using direct ab initio energy points. **1995**, 237, 39-44	16
1156	Structure and EPR parameters of CuC2H2 from a density functional approach. **1995**, 237, 189-194	18
1155	The vibrational frequency of the donor OH group in the H-bonded dimers of water, methanol and silanol. Ab initio calculations including anharmonicities. **1995**, 238, 243-252	58
1154	MP2 studies of relativistic effects on the linear stationary points of the H + Cl2 -dHCl + Cl and Cl + HCl -dClH + Cl reactions. **1995**, 239, 181-185	11
1153	Anisotropic repulsion in complexes B.Cl2 and B.HCl: The shape of the chlorine atom-in-a-molecule. **1995**, 240, 130-134	29
1152	An ab initio study on the equilibrium structure and torsional potential energy function of dinitrogen tetroxide. **1995**, 240, 553-559	17
1151	Acidic properties of [Al], [Ga] and [Fe] isomorphously substituted zeolites. Density functional model cluster study of the complexes with a probe CO molecule. **1995**, 240, 547-552	46
1150	Comment on □A possible definition of basis set superposition error□**1995**, 241, 140-145	23
1149	Large basis set study of the stability of (H2S)2: the importance of 3d functions in weak interaction of second row molecules. **1995**, 243, 158-164	27
1148	Calculated spectroscopic properties for NH3□C4H. **1995**, 243, 378-386	10

1147	Methyl addition to acetylene and ethylene from a density functional approach. **1995**, 246, 45-52	24
1146	The dissociation energies of AlH2 and AlAr. **1995**, 246, 33-39	21
1145	Accurate hydrogen-bonding energies between 1-naphthol and water, methanol and ammonia. **1995** , 246, 291-299	102
1144	Transition metal monocarbonyls in the first excited electronic state. A hybrid density functional study. **1995**, 246, 463-468	15
1143	Adsorption of CO molecules on a MgO(001) surface. Model cluster density functional study employing a gradient-corrected potential. **1995**, 246, 546-554	75
1142	Calculated properties of XeH2. **1995**, 246, 239-244	35
1141	Can contemporary density functional theory yield accurate thermodynamics for hydrogen bonding?. **1995**, 247, 112-119	47
1140	Potential energy function for cation peptide interactions: An ab initio study. **1995**, 16, 690-704	52
1139	The electronic structure of weakly bound systems. I. Rare-gas bimolecular cations. **1995**, 16, 758-767	7
1138	Density functional theory and molecular clusters. **1995**, 16, 1315-1325	473
1137	Ab initio computation of the potential energy surfaces of the water hydrocarbon complexes H2O C2H2, H2O C2H4 and H2O CH4: minimum energy structures, vibrational frequencies and hydrogen bond energies. **1995**, 200, 319-335	58
1136	SCF calculations of the interactions of alkali and halide ions with the mercury surface. **1995**, 200, 347-355	32
1135	Ab initio investigation on stability and properties of XYCO... HZ complexes. II: Post hartree-fock studies on H2CO... HF. **1995**, 6, 255-259	7
1134	Laser ionization spectroscopy of Ag(NH3) n clusters. **1995**, 33, 119-124	10
1133	Modelling the interactions of protein side-chains. **1995**, 5, 89-105	1
1132	Large basis sets and geometry optimizations in embedded cluster calculations. **1995**, 54, 73-81	3
1131	Ab initio conformational study of the CO H2 van der Waals dimer. **1995**, 55, 251-260	12
1130	Ab initio molecular orbital calculations on the associated complexes of lithium cyanide with ammonia. **1995**, 55, 477-484	7

1129	Theoretical studies of organonickel compounds. I. A density functional and ab initio HF study. **1995**, 56, 575-587	7
1128	Determining and extending the domain of exchange and correlation functionals. **1995**, 56, 61-78	75
1127	A procedure to generate ab initio intermolecular potential function. **1995**, 104, 57-69	5
1126	Vibrational relaxation in NO+?He: accurate quantum mechanical study. **1995**, 149-150, 207-215	11
1125	An ab initio study of the chemical bond and the 129Xe NMR chemical shifts in M+ Xe compounds, M = Li, Na, K, Cu, Ag. **1995**, 192, 267-280	38
1124	Na+ in liquid hydroxylamine: pair potential function from ab initio calculations and Monte Carlo computer simulation of a 0.36 M NaCl solution (2 NaCl/200 NH2OH). **1995**, 199, 129-144	2
1123	Does the electronegativity scale apply to ionic crystals as to molecules? A theoretical study of the bonding character in molecular and crystalline alkaline-earth oxides based on dipole moments. **1995**, 199, 155-162	24
1122	The interatomic potential for the X1 state of ArNa+, NeNa+ and HeNa+. **1995**, 199, 33-52	39
1121	Molecular structure and internal motion in the (CO2)3 ? HCN tetramer. **1995**, 51, 653-660	5
1120	An ab initio study of hydrogen complexes of the X-H type between acetylene and HF or HCl. **1995**, 51, 821-830	65
1119	Ab initio calculations of the structural, energetic and vibrational properties of some hydrogen bonded and van der Waals dimers. Part 2. Sulphur dioxide. **1995**, 51, 1847-1860	12
1118	Vibrational frequencies, relative stability and angular geometry of some vinyl halide/HCl Van der Waals complexes observed in liquefied argon. **1995**, 348, 481-484	3
1117	A FTIR study of the Van der Waals complexes between boron trifluoride and carbon monoxide in liquefied argon. **1995**, 349, 461-464	7
1116	Preliminary density functional calculations on the formic acid dimer. **1995**, 19, 181-187	12
1115	Basis set superposition errors for Slater vs. gaussian basis functions in H-bond interactions. **1995**, 330, 77-83	11
1114	The application of localized representation in the calculation of interaction energy. **1995**, 332, 141-149	7
1113	Structure and energetics of SO2?X (X = F, Cl, Br, and I) complexes. **1995**, 333, 291-296	1
1112	Macroscopic properties of the argon system using molecular dynamics simulation with different ab initio energies and analytic functions. **1995**, 332, 241-249	

1111	Open-shell van der Waals complexes of the coinage metals: CuH2O, AgH2O, CuH2S, and AgH2S. **1995**, 332, 197-207		19
1110	On the angular geometry of the CH3Cl HCl van der Waals complex in the gas phase and in liquefied noble gas solutions. **1995**, 332, 231-240		8
1109	Ab initio study of acetonitrile coordinated with metal cations. **1995**, 334, 215-222		9
1108	Cation binding effect on hydrogen bonding and the energetics of proton transfer in the system (CH3)3NH+ DCOH. **1995**, 336, 7-15		3
1107	Bond functions in the description of the water dimer. **1995**, 337, 1-7		8
1106	Ab initio calculations on the water-carbon dioxide system. **1995**, 337, 129-138		29
1105	Hydrogen bonding between aromatics and cationic amino groups. **1995**, 338, 303-315		41
1104	Ab initio calculations on the C-H D hydrogen-bonded systems CH4-H2O, CH3NH2-H2O and CH3NH3+-H2O. **1995**, 341, 63-73		36
1103	On the energetics of the dimerization of boron trifluoride. **1995**, 357, 59-65		9
1102	Site-site function and successive reaction counterpoise calculation of basis set superposition error for proton transfer. **1995**, 342, 153-159		6
1101	Interaction of local anaesthetics with an anionic receptor site. An ab initio SCF study on procaine, lidocaine, tocainide and mexiletine and their HCO2 complexes. **1995**, 343, 141-147		5
1100	N2 and CO molecules as probes of zeolite acidity: an infrared spectroscopy and density functional investigation. **1995**, 31, 273-285		95
1099	Ab initio study of the structure of guanine-cytosine base pair conformers in gas phase and polar solvents. *Molecular Physics*, **1995**, 84, 469-480	1.7	29
1098	An accurate computational model for the study of intermolecular interactions. **1995**, 102, 7088-7094		7
1097	Experimental and theoretical determination of the temperature dependence of deuteron and oxygen quadrupole coupling constants of liquid water. **1995**, 103, 6941-6950		114
1096	The rotational relaxation of NH(c 1) in collisions with Ar: A combined theoretical and experimental investigation. **1995**, 102, 4069-4083		28
1095	Novel model for calculating the intermolecular part of the infrared spectrum for molecular complexes. **1995**, 102, 3534-3554		89
1094	Vibrational spectra of water complexes with H2, N2, and CO. **1995**, 102, 4804-4818		89

1093	Partitioning of interaction energy in van der Waals complexes involving excited state species: The He(1S)+Cl2(B 3Πu) interaction. **1995**, 103, 10116-10127	46
1092	Theoretical study of the interaction of AlH(X 1Σ+,A 1Π) with Ar: Potential energy surfaces and bend–stretch levels of the ArAlH(X,A) van der Waals complex. **1995**, 102, 2413-2425	21
1091	The HeCl2 potential: Atom–atom and ab initio compared to experiment. **1995**, 102, 8846-8854	52
1090	The potential energy function for a ligand substitution reaction of square-planar platinum (II) complex in water: The important role of three-body effect. **1995**, 103, 9274-9291	10
1089	Ab initio prediction of the structure, harmonic vibrational frequencies, and dissociation energy of the H2⋯eH+3H2 cluster ion. **1995**, 102, 3667-3673	11
1088	Ab initio potential energy surface for the HCl dimer. **1995**, 103, 950-956	42
1087	Ab initio calculations of van der Waals interactions in one- and two-dimensional infinite periodic systems. **1995**, 103, 2603-2614	24
1086	Mechanisms for molecular oxygen desorption from the CaO(100) surface. **1995**, 103, 7626-7630	22
1085	Nearest-neighbor influence on hydrocarbon adsorption on diamond (111) studied by ab initio calculations. **1995**, 51, 10003-10012	18
1084	Ab initio studies of the complexes of benzene with carbon monoxide and formaldehyde. **1995**, 102, 6812-6821	13
1083	Intermolecular potentials and rovibrational energy levels of the Ar complexes with HCN and HCCH. **1995**, 102, 7289-7297	38
1082	Compact model potentials for ab initio embedded cluster calculations. Part I. Basic formulation. **1995**, 102, 327-336	35
1081	Structure and bonding in the formamide crystal: A complete fourth-order many-body perturbation theoretical study. **1995**, 103, 7030-7039	40
1080	Intermolecular vibrations of phenol?(H2O)3 and d1-phenol?(D2O)3 in the S0 and S1 states. **1995**, 103, 6350-6361	57
1079	Ab initio study of the dication carbon trimer C32+. **1995**, 102, 3281-3291	24
1078	On the adequacy of pairwise additive potentials for rare gas–halogen systems: The effect of anisotropy of interactions between atoms. **1995**, 103, 3392-3399	52
1077	A hybrid density functional study of the first-row transition-metal monocarbonyls. **1995**, 103, 10605-10613	96
1076	Electronic spectrum of S2-, the electron affinity of S2, and the binding energies of neutral and anionic S3 clusters. **1995**, 52, 1024-1038	18

1075	Quantum scattering studies of the doublet resolved rotational energy transfer of OH(X 2) in collisions with He and Ar. **1995**, 103, 2067-2082		57
1074	Fully ab initio investigation of bound and predissociating states of the NeOH(X) complex. **1995**, 103, 3400-3417		26
1073	Towards an analytical three-body potential of Ar2Cl **1995**, 103, 299-308		22
1072	Relativistic and correlation effects in CuH, AgH, and AuH: Comparison of various relativistic methods. **1995**, 102, 2024-2031		81
1071	Towards a new correction method for the basis set superposition error: Application to the ammonia dimer. **1995**, 102, 3648-3654		31
1070	Ab initio studies of the nuclear magnetic resonance chemical shifts of a rare gas atom in a zeolite. **1995**, 103, 3885-3894		18
1069	Ab initio investigation of internal rotation in the ethylene sulfur dioxide dimer. **1995**, 102, 4184-4188		8
1068	Temperature dependence of hydrogen bonding in neat, liquid formamide. **1995**, 103, 3636-3642		47
1067	Structure and vibrations of phenol(H2O)2. **1995**, 103, 7392-7400		92
1066	Ab initio potential energy surfaces and quantum scattering studies of NO(X 2) with He: doublet resolved rotational and electronic fine-structure transitions. **1995**, 103, 6973-6983		48
1065	Benchmark full configuration interaction calculations on the helium dimer. **1995**, 102, 7479-7483		88
1064	An accurate calculation of the three-body potential for the ground state of the helium trimer. **1995**, 102, 7095-7105		25
1063	A perturbational study of some hydrogen-bonded dimers. **1995**, 103, 8043-8057		31
1062	Theoretical study of the Cu(H2O) and Cu(NH3) complexes and their photolysis products. **1995**, 103, 1860-1870		33
1061	Experimental and theoretical studies of hydrogen bonding in neat, liquid formamide. **1995**, 102, 5118-5125		80
1060	Quantum chemical predictions of the electron affinities of carbon-hydrogen clusters C2n H the CH binding energies and the gas phase acidities of polyacetylenes C2n H2 for n = 1. *Molecular Physics* , **1995**, 84, 691-706	1.7	18
1059	Microwave electronic spectrum of the He+2 ion. **1995**, 102, 5979-5988		55
1058	MP2/6-311++G(d,p) study of ten ionic hydrogen-bonded binary systems: Structures, normal modes, thermodynamics, and counterpoise energies. **1995**, 102, 8029-8039		58

1057	Structure and vibrations of the phenol-ammonia cluster. **1995**, 102, 9197-9204		49
1056	An extended basis set ab initio study of alkali metal cation□water clusters. **1995**, 103, 3526-3542		214
1055	Atomic-hydrogen interaction with metallic lithium: An ab initio embedded-cluster study. **1995**, 51, 7805-7816		19
1054	Ab initio methane dimer intermolecular potentials. *Molecular Physics*, **1995**, 85, 1179-1192	1.7	27
1053	An ab initio investigation of the charge-transfer complexes of alkali atoms with oligo (□) thiophenes and oligoparaphenylenes: A model calculation on polaronic and bipolaronic defect structures. **1995**, 103, 1508-1522		44
1052	Ab initio potential energy surface and near-infrared spectrum of the He□2H2 complex. **1995**, 102, 8385-8397		65
1051	On the importance of core polarization in heavy post-d elements: a pseudopotential calibration study for X2H6 (X = Si, Ge, Sn, Pb). *Molecular Physics*, **1995**, 86, 317-326	1.7	19
1050	Polarizabilities of anions in anisotropic environments The fluoride ion in the perovskite lattices NaMgF3, KMgF3 and KCaF3. *Molecular Physics*, **1995**, 84, 787-797	1.7	7
1049	Benchmark calculations with correlated molecular wave functions. VII. Binding energy and structure of the HF dimer. **1995**, 102, 2032-2041		254
1048	On the effectiveness of monomer-, dimer-, and bond-centered basis functions in calculations of intermolecular interaction energies. **1995**, 103, 7374-7391		202
1047	Adsorption of NH3 on MgO(100): a comparative study of ab initio and semi-classical calculations. **1995**, 325, 139-150		46
1046	The photoelectron spectrum of ethylene oxide adsorbed at metal surfaces: a density functional model cluster study of. **1995**, 326, 53-58		5
1045	Geometry and binding of acetylene on Cu(111): ab initio cluster studies. **1995**, 337, 205-214		39
1044	Theoretical study of the adsorption of carbon monoxide on a NaCl (100) surface. **1995**, 322, 342-360		19
1043	An explicitly correlated coupled cluster calculation of the helium□helium interatomic potential. **1995**, 103, 6127-6132		98
1042	On the role of bond functions in interaction energy calculations: Ar???HCl, Ar???H2O, (HF)2. **1995**, 103, 1498-1507		78
1041	Characterization of C-H-O Hydrogen Bonds on the Basis of the Charge Density. **1995**, 99, 9747-9754		2443
1040	An ab initio derived torsional potential energy surface for (H2O)3. II. Benchmark studies and interaction energies. **1995**, 103, 1085-1098		121

1039	Structure and spectroscopy of (HCN)n clusters: Cooperative and electronic delocalization effects in C H???N hydrogen bonding. **1995**, 103, 333-347		210
1038	Quantum chemical studies of the pyrrole-water and pyridine-water complexes. *Molecular Physics*, **1995**, 85, 573-585	1.7	32
1037	Experimental and theoretical study of the B Ne nonbonding interaction: The free-bound B 2 X 2 electronic transition. **1995**, 103, 2779-2786		33
1036	Harmonic vibrational frequencies of the water monomer and dimer: Comparison of various levels of ab initio theory. **1995**, 102, 310-317		74
1035	Theoretical study of the protonation of square-planar palladium(II) complexes. Assessment of basis set and correlation effects. **1995**, 92, 361-367		11
1034	Density functional calculations of the structures and bond energies of Cr(CO)6 and (6-C6H6) Cr(CO)2(CX) (X=O, S) complexes. **1995**, 91, 157-167		1
1033	Hydrogen-bonded and van der Waals complexes studied by a Gaussian density functional method. The case of (HF)2, ArHCl and Ar2HCl systems. **1995**, 91, 169-177		4
1032	Ab initio potential energy surface, infrared spectrum, and second virial coefficient of the He O complex. **1995**, 103, 321-332		75
1031	Towards phase transferable potential functions: Methodology and application to nitrogen. **1995**, 103, 2272-2285		29
1030	Low-lying stationary points and torsional interconversions of cyclic (H2O)4: An ab initio study. **1995**, 103, 6114-6126		88
1029	Dispersion energy in the coupled pair approximation with noniterative inclusion of single and triple excitations. **1995**, 103, 4586-4599		61
1028	Intermolecular potential and rovibrational levels of Ar HF from symmetry-adapted perturbation theory. **1995**, 103, 6076-6092		64
1027	Theoretical investigation of weakly-bound complexes of B with H2. **1995**, 103, 7956-7965		39
1026	Basis Set Effects in Density Functional Calculations on the Metal igand and Metal Metal Bonds of Cr(CO)5 O and (CO)5Mn Mn(CO)5. **1996**, 100, 5690-5696		115
1025	Aromatic van der Waals Clusters: Structure and Nonrigidity. **1996**, 100, 13348-13366		122
1024	Local treatment of electron correlation in coupled cluster theory. **1996**, 104, 6286-6297		650
1023	A relativistic Kohn Sham density functional procedure by means of direct perturbation theory. II. Application to the molecular structure and bond dissociation energies of transition metal carbonyls and related complexes. **1996**, 105, 5485-5493		37
1022	UNDERSTANDING NMR CHEMICAL SHIFTS. **1996**, 47, 135-169		88

1021	Comparing ab initio computed energetics with thermal experiments in surface science: CO/MgO(001). **1996**, 105, 9339-9348	66
1020	Isomerization of the Molecular Ion of Allyl Bromide. **1996**, 100, 18048-18056	11
1019	Density Functional Studies on N-Methylacetamide−Water Complexes. **1996**, 100, 3942-3949	96
1018	Structures and Energies of Hydrogen-Bonded DNA Base Pairs. A Nonempirical Study with Inclusion of Electron Correlation. **1996**, 100, 1965-1974	378
1017	Molecular Dynamics Potential of Mean Force Calculations: A Study of the Toluene−Ammonium +Cation Interactions. **1996**, 118, 2998-3005	85
1016	Perturbative calculation of intermolecular interactions in orthogonalized or biorthogonal basis sets. **1996**, 94, 333-344	4
1015	29Si NMR Chemical Shifts of Silicate Species: Ab Initio Study of Environment and Structure Effects. **1996**, 118, 13015-13020	77
1014	Spontaneous DNA Mutations Induced by Proton Transfer in the Guanine−Cytosine Base Pairs: An Energetic Perspective. **1996**, 118, 3010-3017	252
1013	Natural Energy Decomposition Analysis:The Linear Response Electrical Self Energy. **1996**, 100, 17152-17156	116
1012	Natural Energy Decomposition Analysis: Explicit Evaluation of Electrostatic and Polarization Effects with Application to Aqueous Clusters of Alkali Metal Cations and Neutrals. **1996**, 118, 2473-2482	168
1011	An Ab Initio Investigation of the Structure and Alkaline Earth Divalent Cation Selectivity of 18-Crown-6. **1996**, 118, 6052-6059	91
1010	Contracted Gaussian-type basis functions revisited. **1996**, 104, 8493-8499	38
1009	Density-Functional-Derived Structures, Spin Properties, and Vibrations for Phenol Radical Cation. **1996**, 100, 10554-10563	47
1008	Valence selectivity of the gramicidin channel: a molecular dynamics free energy perturbation study. **1996**, 71, 3177-85	96
1007	Theoretical study of adsorption of Cu, Ag, and Au on the NaCl(100) surface. **1996**, 53, 10281-10288	19
1006	Tautomerism and Protonation of Guanine and Cytosine. Implications in the Formation of Hydrogen-Bonded Complexes. **1996**, 118, 6811-6821	292
1005	Density Functional Theory of Molecular Solids: Local versus Periodic Effects in the Two-Dimensional Infinite Hydrogen-Bonded Sheet of Formamide. **1996**, 100, 3950-3958	36
1004	BSSE-Free SCF Algorithm for Treating Several Weakly Interacting Systems. **1996**, 100, 6332-6335	21

1003	Conformers, Energetics, and Basicity of 2,2□Bipyridine. **1996**, 118, 10269-10274		104
1002	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 9. Intermolecular versus Intramolecular Carbon□Hydrogen Bond Activation in Zirconium, Rhodium, and Iridium Complexes. **1996**, 15, 1889-1897		37
1001	Ab initio calculations for propyne and the hydrogen bonded complex NH H C C CH 3 3. *Molecular Physics*, **1996**, 89, 1553-1565	1.7	11
1000	Properties of Closed-Shell, Octahedral, Multiply-Charged Hexafluorometallates MF63-, M = Sc, Y, La, ZrF62-, and TaF6-. **1996**, 118, 1173-1180		55
999	An Experimental and Theoretical Study of the Long-Lived Radical Cation of CH3OCH2CH2OH. **1996**, 118, 3914-3921		3
998	Cluster Models of Cu Binding and CO and NO Adsorption in Cu-Exchanged Zeolites. **1996**, 100, 6032-6046		83
997	Ab Initio Study of Endo/Exo and Diastereofacial Selectivities in Diels-Alder Reactions between Chiral Butenolides and Cyclopentadiene. **1996**, 61, 621-626		19
996	Ab Initio Modeling of the Endohedral Reactivity of Polyoxometallates:□1. Host□Guest Interactions in [RCN?(V12O32)4-] (R = H, CH3, C6H5). **1996**, 118, 13007-13014		58
995	Transition State Imbalances in Gas Phase Proton Transfers. Ab Initio Study of the Carbon-to-Carbon Proton Transfer from the Protonated Acetaldehyde Cation to Acetaldehyde Enol. **1996**, 118, 10494-10504		30
994	Theoretical Investigations on the Retro-Ene Rearrangement of Propargyl Ethers. **1996**, 61, 5831-5836		13
993	An Analysis of Electron Donor□Acceptor Complexes:□H2O□F2, H2O□Cl2, and H2O□ClF. **1996**, 118, 4152-4158		15
992	Direct Dynamics Calculation for the Double Proton Transfer in Formic Acid Dimer. **1996**, 118, 1522-1528		135
991	Anab InitioMolecular Orbital Study on Hyperpolarizabilities of an Interacting 2-Methyl-4-nitroaniline Molecular Pair:□A Molecular Study on the Oriented-Gas Approximation. **1996**, 100, 8777-8781		32
990	The Vibrational Spectra of the Boron Halides and Their Molecular Complexes. 3.Ab InitioPredictions of the Structures, Energetics, and Mulliken Atomic Charges of the Complexes of Boron Trifluoride with Some Linear Nitrogen Donors. **1996**, 36, 377-384		29
989	Ab Initio Study of the Hydrogen Exchange Reaction at Group 3 and 4 Metals in Comparison to That at Alkali Metals. **1996**, 15, 3688-3695		11
988	First-sphere and second-sphere electrostatic effects in the active site of a class mu gluthathione transferase. **1996**, 35, 4753-65		66
987	Response Function Basis Sets: Application to Density Functional Calculations. **1996**, 100, 6231-6235		27
986	Symmetry-adapted perturbation theory for the calculation of Hartree-Fock interaction energies. *Molecular Physics*, **1996**, 88, 741-758	1.7	90

985	Potential Energy Surface for the Benzene Dimer. Results of ab Initio CCSD(T) Calculations Show Two Nearly Isoenergetic Structures: T-Shaped and Parallel-Displaced. **1996**, 100, 18790-18794		546
984	On the Hylleraas functional for a non-Hermitian unperturbed Hamiltonian. *Molecular Physics*, **1996**, 89, 515-519	1.7	14
983	Combining ab initio computations, neural networks, and diffusion Monte Carlo: An efficient method to treat weakly bound molecules. **1996**, 105, 7597-7604		122
982	Acetylene on Cu and Pd(111) surfaces: a comparative theoretical study of bonding mechanism, adsorption sites, and vibrational spectra. **1996**, 346, 91-107		51
981	Cluster and band structure ab initio calculations on the adsorption of CO on acid sites of the TiO2(110) surface. **1996**, 350, 159-175		115
980	Analysis of the bonding mechanism of benzene on Cu(110), Cu(111), Pd(111) and the effect of coadsorbed C1 atoms. **1996**, 365, 297-309		29
979	An ab initio analytical potential energy surface for the O(3P)+CS(X 1Σ)-ЄO(X 1Σ)+S(3P) reaction useful for kinetic and dynamical studies. **1996**, 105, 10999-11006		18
978	Symmetry-adapted perturbation theory applied to interaction-induced properties of collisional complexes. *Molecular Physics*, **1996**, 89, 81-110	1.7	61
977	Nature of Nucleic AcidBase Stacking: Nonempirical ab Initio and Empirical Potential Characterization of 10 Stacked Base Dimers. Comparison of Stacked and H-Bonded Base Pairs. **1996** , 100, 5590-5596		376
976	Metal Deposition on Oxide Surfaces: A Quantum-Chemical Study of the Interaction of Rb, Pd, and Ag Atoms with the Surface Vacancies of MgO. **1996**, 100, 9032-9037		161
975	On the importance of the fragment relaxation energy terms in the estimation of the basis set superposition error correction to the intermolecular interaction energy. **1996**, 104, 8821-8824		607
974	Potential energy surface for interactions between N2 and He: Ab initio calculations, analytic fits, and second virial coefficients. **1996**, 104, 2541-2547		27
973	Interaction of CO Molecules with Electron-Deficient Pt Atoms in Zeolites: A Density Functional Model Cluster Study. **1996**, 100, 3482-3487		21
972	Directionality of Hydrogen Bonds to Sulfur and Oxygen. **1996**, 118, 2726-2733		192
971	Quantum chemical evidence for CH ? C hydrogen bonding. **1996**, 63-64		39
970	Ab initio study of the individual interaction energy components in the ground state of the mercury dimer. *Molecular Physics*, **1996**, 89, 139-156	1.7	60
969	Effects of monomer geometry and basis set saturation on computed depth of water dimer potential. **1996**, 104, 7606-7614		142
968	Structure of Water Clusters. The Contribution of Many-Body Forces, Monomer Relaxation, and Vibrational Zero-Point Energy. **1996**, 100, 18014-18022		233

967	Theoretical Characterization of the Structures and Vibrational Spectra of Benzene(H2O)n (n = 1−3) Clusters. **1996**, 100, 7810-7821	175
966	Ab Initio Study of the Interaction of Guanine and Adenine with Various Mono- and Bivalent Metal Cations (Li+, Na+, K+, Rb+, Cs+; Cu+, Ag+, Au+; Mg2+, Ca2+, Sr2+, Ba2+; Zn2+, Cd2+, and Hg2+). **1996**, 100, 7250-7255	196
965	An accurate multireference configuration interaction calculation of the potential energy surface for the F+H2→HF+H reaction. **1996**, 104, 6515-6530	353
964	Ab initio potential energy surface and rovibrational energies of Ar? ? ?CO. **1996**, 104, 183-190	36
963	Linear and Cyclic Clusters of Hydrogen Cyanide and Cyanoacetylene: A Comparative ab Initio and Density Functional Study on Cooperative Hydrogen Bonding. **1996**, 100, 13474-13486	47
962	Electron donor−acceptor complex of ICl with diethyl ether. He I photoelectron spectroscopy and ab initio molecular orbital study. **1996**, 92, 1677-1679	4
961	Simulation of the charge transfer absorption of the H2O/O2 van der Waals complex using high level ab initio calculations. **1996**, 104, 3198-3204	21
960	Samuel Francis Boys. **1996**, 100, 6007-6016	11
959	Multipole-based calculation of the polarization energy. **1996**, 94, 287-295	2
958	Fully relativistic pseudopotentials for alkaline atoms: Dirac-Hartree-Fock and configuration interaction calculations of alkaline monohydrides. **1996**, 93, 141-156	8
957	A quantum chemistry study of benzene dimer. **1996**, 105, 2780-2788	258
956	Refinement of Nonbonding Interaction Parameters for Carbon Dioxide on the Basis of the Pair Potentials Obtained by MP2/6-311+G(2df)-Level ab Initio Molecular Orbital Calculations. **1996**, 100, 4400-4407	36
955	Hydrogen Bond Energy of the Water Dimer. **1996**, 100, 2993-2997	433
954	Single and Multiple Lewis Sites of MgO: A Combined IR and ab Initio Study with CD3CN as a Molecular Probe. **1996**, 100, 5011-5016	35
953	Novel intermolecular C−H ?π interactions: an ab initio and density functional theory study. **1996**, 563-568	33
952	Study of electron densities of methyl acetate, N-methylacetamide and N,N?-dimethylurea by quantum mechanical investigations. Part 2. Solvent models. **1996**, 1403-1408	9
951	Variable hydrogen bond lengths in hydrated complexes of formate and methylammonium ions. **1996**, 2213-2219	15
950	Density functional study on the mechanism of the Simmons−Smith reaction. **1996**, 877-881	16

949	Proximity effects on nuclear spin□spin coupling constants. Part 2.□The electric field effect on 1J(CH) couplings. **1996**, 92, 3029-3033		44
948	An eclipsed Csp3-CH3 bond? An ab initio investigation of an atypical rotation barrier. *Molecular Physics*, **1996**, 89, 315-329	1.7	3
947	Analysis of the Thermochemistry of NOx Decomposition over CuZSM-5 Based on Quantum Chemical and Statistical Mechanical Calculations. **1996**, 100, 17582-17592		113
946	Crystal Structures and Properties of Nylon Polymers from Theory. **1996**, 118, 12291-12301		180
945	Calculated Structure and Optical Properties of Tl(2)Pt(CN)(4). **1996**, 35, 7450-7451		41
944	Effective O-17 quadrupole moments for the calibrated computation of quadrupole coupling parameters at different levels of theory. **1996**, 105, 8223-8230		29
943	The interaction polarizability and interaction second-hyperpolarizability for He□He. *Molecular Physics*, **1996**, 88, 887-898	1.7	16
942	The structure and binding energy of K+□ether complexes: A comparison of MP2, RI-MP2, and density functional methods. **1996**, 105, 1940-1950		55
941	Binding energy of the ring form of (H2O)6: Comparison of the predictions of conventional and localized-orbital MP2 calculations. **1996**, 105, 11091-11099		101
940	An investigation of the reaction of O- with CH2F2 with ab initio molecular orbital calculations. *Molecular Physics*, **1996**, 88, 143-160	1.7	1
939	On the dissociation energy of Ti(OH2)+. An MCSCF, CCSD(T), and DFT study. **1996**, 74, 1824-1829		17
938	Dihydrogen bonds (A□H?H□). **1996**, 1633-1634		84
937	Nature of the non-bonded (C□H)?O interaction of ethers CH3O□(CH2)n□OCH3(n= 4□). **1996**, 92, 4885-4888		19
936	Structural Trends in the Monocyanides of the Second-Row Metal Ions Na+, Mgm+ (m = 1, 2), and Aln+ (n = 1□). **1996**, 100, 11581-11588		29
935	Theoretical Studies on VPI-5. 2. Energy Decomposition Analysis of the Hydrophilicity. **1996**, 100, 12424-12430		9
934	Dipole moment derivatives and integrated intensities for the vibrational transitions of N2 □HF. **1996**, 17, 1339-43		
933	Adsorption complexes on oxides: Density functional model cluster studies. **1996**, 569-619		23
932	Geometry of Acetylene and Ethylene Adsorbed on Cu(111): Theoretical Cluster Studies. **1996**, 197, 219-235		11

931	Ab initio study on the stability and properties of XYCO? ? ?HZ complexes. III. A comparative study of basis set and electron correlation effects for H2CO? ? ?HCl. **1996**, 104, 1441-1451	15
930	Small Clusters of Water Molecules Using Density Functional Theory. **1996**, 100, 8701-8711	176
929	A Density Functional Study of Acidic Hydroxyl Groups in Zeolites and Their Interaction with Carbon Monoxide. **1996**, 100, 1814-1819	28
928	Ab initio molecular orbital calculations on ion-molecule and ion-pair-molecule complexes of formamide with LiF and LiCl. **1996**, 361, 229-242	5
927	Weakly bonded clusters of H2S. **1996**, 362, 275-282	20
926	Ab initio calculations of the properties of simple alkali and alkaline earth organometallics. **1996**, 364, 107-119	18
925	Examination of some new configurations of methanol-water hetero dimer system by molecular orbital and density functional calculations. **1996**, 366, 123-129	6
924	An ab initio study of the molecular properties of the acetylene-HX hydrogen complexes. **1996**, 366, 233-240	48
923	Selective oxidation of methane by dinitrogen monoxide on FeZSM-5 zeolites. Ab initio quantum chemical analysis. **1996**, 40, 17-23	24
922	A density functional study of CO adsorption on three- and five-coordinate Al in oxide systems. **1996**, 40, 183-188	26
921	High-quality theoretical potential energy surface for Be2 by using the multireference averaged quadratic coupled-cluster (MR-AQCC) method and large basis sets. **1996**, 258, 400-408	45
920	Helium dimer potential from symmetry-adapted perturbation theory. **1996**, 262, 431-436	54
919	A complete active-space self-consistent-field study on cubic N8. **1996**, 18, 1395-1405	8
918	Cooperative effects in water trimers. The performance of density functional approaches. **1996**, 371, 1-10	117
917	Notes on the use of bond functions for ab initio intermolecular energy calculations. **1996**, 367, 55-57	8
916	MP2 and CCSD(T) calculations on H?bonded and stacked formamide□formamide and formamidine□formamidine dimers. **1996**, 388, 115-120	3
915	An extended geminal calculation of the three-body potential for the ground state of the helium trimer. **1996**, 388, 331-337	4
914	Gaussian basis sets for use in correlated molecular calculations. VI. Sextuple zeta correlation consistent basis sets for boron through neon. **1996**, 388, 339-349	806

913	An ab initio study of terminal ?SiOH and bridging ?Si(OH)Al? groups in zeolites and their interaction with carbon monoxide. **1996**, 368, 93-110	39
912	MCSCF vibrational spectra of the symmetric and asymmetric dihydronium cations. **1996**, 368, 173-196	29
911	Theoretical investigations on 1,2-ethanediol: The problem of intramolecular hydrogen bonds. **1996**, 17, 133-147	50
910	The 1:1 glycine zwitterion-water complex: An ab initio electronic structure study. **1996**, 17, 338-349	87
909	Merck molecular force field. II. MMFF94 van der Waals and electrostatic parameters for intermolecular interactions. **1996**, 17, 520-552	799
908	Base stacking in cytosine dimer. A comparison of correlated ab initio calculations with three empirical potential models and density functional theory calculations. **1996**, 17, 841-850	134
907	Applications of spectral-Representation model as a potential method for Cu clusters. **1996**, 17, 1056-1067	8
906	Theoretical study of the reaction of P+ with methane. **1996**, 9, 419-426	4
905	Chemisorption of hydrogen and oxygen atoms on a cobalt surface: A quantum chemical cluster model study. **1996**, 57, 105-111	9
904	Calculation of bond dissociation energies of diatomic molecules using bond function basis sets with counterpoise corrections. **1996**, 57, 207-212	11
903	An ab initio study on HXC(double bond)O □HY molecular complexes (X, Y = F, Cl). **1996**, 57, 757-766	5
902	Application of the localized representation for studying interaction energies. **1996**, 57, 775-780	7
901	A BSSE-free SCF algorithm for intermolecular interactions. III. Generalization for three-body systems and for using bond functions. **1996**, 57, 1049-1055	12
900	Comparative study of DFT methods applied to small titanium/oxygen compounds. **1996**, 59, 427-443	50
899	Modification of the Roothaan equations to exclude BSSE from molecular interaction calculations. **1996**, 60, 157-166	179
898	Optimized spin-coupled virtual orbitals. **1996**, 60, 225-233	18
897	Interatomic potential for the X1□g state of Be2. **1996**, 60, 453-466	57
896	A comparison of Hartree□ock, MP2, and DFT results for the HCN dimer and crystal. **1996**, 60, 767-778	22

895	Basis sets for ab initio periodic Hartree–Fock studies of zeolite/adsorbate interactions: He, Ne, and Ar in silica sodalite. **1996**, 60, 809-820	54
894	Energetic and conformational study of four benzylimidazole compounds with α2 agonist profile: The mivazerol and three methylated derivatives. **1996**, 60, 911-930	5
893	Post-Hartree-Fock and DFT level studies on the Cl2CO···Cl2 complex: Accurate molecular parameters, harmonic vibrational frequencies, and interaction energies. **1996**, 60, 1007-1013	1
892	Direct reaction field force field: A consistent way to connect and combine quantum-chemical and classical descriptions of molecules. **1996**, 60, 1111-1132	56
891	Kohn-Sham equations with constrained electron density: an iterative evaluation of the ground-state electron density of interacting molecules. **1996**, 248, 71-76	214
890	Electron donor-acceptor complexes of I2 with diethyl ether and diethyl sulphide. An ab initio MO study. **1996**, 248, 153-157	19
889	Searching for the ylide structure. An ab initio study of the H2O···Cl2 complex. **1996**, 249, 136-140	11
888	Comparison of convetional and hybrid density functional approaches. Cationic hydrides of first-row transition metals as a case study. **1996**, 249, 290-296	40
887	Ab initio calculations on the structure, vibrational frequencies, and valence excitation energies of the benzene–Ar and benzene–Ar2 cluster. **1996**, 250, 402-408	30
886	Ab initio study of AgNH3 and its cation. **1996**, 250, 415-420	21
885	On the usefulness of the counterpoise method on hydrogen-bonded complexes: a numerical test using near complete basis sets on H2O···HF, (H2O)2, (HF) 2 and CH4···H2O. **1996**, 251, 33-46	79
884	Basis set effects on the calculated bonding energies of neutral benzene dimers: importance of diffuse polarization functions. **1996**, 252, 206-210	84
883	A computational study of the structures of Van der Waals and hydrogen-bonded complexes of ethene and ethyne. **1996**, 254, 135-140	21
882	Proton-ordered ice structures at zero pressure. A quantum-mechanical investigation. **1996**, 253, 201-208	59
881	On the nature of the cobalt-nitrogen bond in the CON+2 complex. A theoretical study. **1996**, 254, 314-320	
880	Cluster models of O2 adsorption on regular and defect sites and Fs centers of the MgO (100) surface. **1996**, 255, 58-64	75
879	An accurate ab initio potential energy surface of He?H2O. **1996**, 255, 179-186	29
878	The ground state potential of the beryllium dimer. **1996**, 258, 421-426	57

877	Ab initio SCF and DFT models of met-car adducts: Ti8C12(L)n (L = Cl, NH3, CO, C6H6; n = 4, 8). **1996**, 260, 577-581	22
876	Zero kinetic energy photoelectron study of the naphthalene-Ar van der Waals complex. **1996**, 261, 481-485	25
875	The magnitude of intramolecular basis set superposition error. **1996**, 261, 633-636	68
874	Halogen ions adsorption at silver and platinum surfaces: A quantum chemical study. **1996**, 41, 2285-2291	30
873	Cation-aromatic bonding in Group 14 organometallics. **1996**, 242, 191-200	14
872	How many conformers of the 1, 2, 3-propanetriol triacetate are present in gas phase and in aqueous solution?. **1996**, 52, 677-686	9
871	How good is fluorine as a hydrogen bond acceptor?. **1996**, 52, 12613-12622	597
870	The structure of the boron trifluoride-ammonia complex: a Fourier transform matrix isolation infrared spectroscopic and ab initio molecular orbital study. **1996**, 12, 221-235	32
869	Nonempirical ab initio calculations on DNA base pairs. **1996**, 204, 365-372	28
868	Theoretical study for the basicities of methylamines in aqueous solution: A RISM-SCF calculation of solvation thermodynamics. **1996**, 203, 53-67	41
867	Theoretical study of the low-lying electronic spectrum of C22+. **1996**, 202, 63-80	16
866	A theoretical study of tunneling in the (HCCH)2 complex. **1996**, 206, 1-8	15
865	Density functional based structure optimization for molecules containing heavy elements: analytical energy gradients for the Douglas-Kroll-Hess scalar relativistic approach to the LCGTO-DF method. **1996**, 210, 413-425	121
864	Ab initio calculation of three-body interaction in the (H2)3 trimer. **1996**, 211, 179-189	14
863	Ab initio studies on the interactions of water with tetramethylurea and tetramethylthiourea. **1996**, 381, 181-187	12
862	Comment on A computational study of the structures of van der Waals and hydrogen-bonded complexes of ethene and ethyne**1996**, 263, 345-347	9
861	Isomerization versus hydrogen exchange reaction in the HNC ? HCN conversion. **1996**, 263, 385-392	25
860	Deprotonation of distonic ions. Proton affinities of the radicals. **1996**, 157-158, 275-282	10

859	The ArClF Van der Waals complex as an example of how atoms inside a molecule interact with those outside. **1996**, 213, 33-43		9
858	The agonistic binding site at the histamine H2 receptor. I. Theoretical investigations of histamine binding to an oligopeptide mimicking a part of the fifth transmembrane alpha-helix. **1996**, 10, 461-78		12
857	Quantitative Description of Hydrogen Bonding in Chloride□Water Clusters. **1996**, 100, 9703-9713		206
856	Infrared Matrix Isolation Study of Acetone and Methanol in Solid Argon. **1996**, 100, 17124-17132		63
855	Dimers of rare gas atoms: CCSD(T), CCSDT and FCI calculations on the (He)2 dimer, CCSD(T) and CCSDT calculations on the (Ne)2 dimer, and CCSD(T) all-electron and pseudopotential calculations on the dimers from (Ne)2 through (Xe)2. *Molecular Physics*, **1996**, 89, 425-432	1.7	37
854	An ab Initio Study on Reactivity of Fluoroethane with Hydroxyl Radical: Application of G2 Theory□ **1996**, 100, 6212-6224		36
853	Theoretical study of the water pentamer. **1996**, 105, 6957-6971		114
852	Fluorescence-dip infrared spectroscopy of the tropolone-H2O complex. **1996**, 105, 2605-2617		44
851	Ab initio collision-induced polarizability, polarized and depolarized Raman spectra, and second dielectric virial coefficient of the helium diatom. **1996**, 104, 6997-7007		61
850	Convergence of symmetry-adapted perturbation theory expansions for pairwise nonadditive interatomic interactions. **1996**, 105, 8178-8186		27
849	Ab initio study of van der Waals interaction of formamide with a nonpolar partner. Ar???H2NCOH complex. **1996**, 105, 8213-8222		5
848	Ab initio pair potential parameter set for the interaction of a rigid and a flexible water model and the complete series of the halides and alkali cations. **1996**, 105, 5518-5524		48
847	Periodic Hartree□Fock calculations on crystalline HCN. **1996**, 105, 4668-4674		32
846	Second-order Epstein□Nesbet correction to □ynamic□onfiguration interaction energies. **1996**, 105, 10487-10492		12
845	Theoretical study of properties of H□and NH2□complexes with neutral ammonia solvent molecules. **1996**, 105, 7569-7572		13
844	Basis set superposition problem in interaction energy calculations with explicitly correlated bases: Saturated second- and third-order energies for He2. **1996**, 104, 3306-3319		70
843	Ab initio investigation of the N2□HF complex: Accurate structure and energetics. **1996**, 104, 5883-5891		39
842	Ground State Properties of Hg2. 1. A Pseudopotential Configuration Interaction Study. **1996**, 100, 6147-6151		70

841	Ground-state potentials for Co+/rare-gas interactions. *Molecular Physics*, **1996**, 89, 473-488	1.7	10
840	Ab initio potential-energy surfaces and electron-spin-exchange cross sections for H-O2 interactions. **1996**, 53, 766-771		15
839	Adsorption of water and methanol on zeolite Bro/nsted acid sites: An ab initio, embedded cluster study including electron correlation. **1996**, 105, 3770-3776		67
838	Laser-induced desorption of NO from NiO(100): Ab initio calculations of potential surfaces for intermediate excited states. **1996**, 104, 10030-10040		68
837	Ab initio study of the He(1S)+CH(X 2) interaction. **1996**, 105, 9525-9535		23
836	Relativistic and correlation effects on molecular properties. II. The hydrogen halides HF, HCl, HBr, HI, and HAt. **1996**, 105, 1987-1994		114
835	Ab initio study of van der Waals interaction of CO2 with Ar. **1996**, 104, 6569-6576		67
834	The rovibrational spectrum of the ArCO complex calculated from a semiempirically extrapolated coupled pair functional potential energy surface. **1996**, 105, 89-103		21
833	Ab initio study of the adducts of carbon monoxide with alkaline cations. **1996**, 105, 4129-4139		102
832	Post-Hartree–Fock study on Ar–HCO+ and He–HCO+ complexes: A critical examination of experimental data. **1996**, 105, 6388-6394		22
831	Solvent effects on the potential energy surface of the 1:1 complex of water and formamide: Application of the polarizable continuum model to the study of nonadditive effects. **1996**, 104, 5539-5546		33
830	Ab initio and scaled potential energy surfaces for Ar–2H2: Comparison with scattering and spectroscopic experiments. **1996**, 105, 10462-10471		30
829	Theoretical studies of geometric structures of phenol-water clusters and their infrared absorption spectra in the O–H stretching region. **1996**, 105, 420-431		98
828	Ab initio study of the O2(X 3g)+He(1S) van der Waals cluster. **1996**, 104, 7997-8002		34
827	Hydrogen bond spectroscopy in the near infrared: Out-of-plane torsion and antigeared bend combination bands in (HF)2. **1996**, 105, 4488-4503		57
826	The argon–diacetylene complex: An example of distributed interactions and transferable potentials. **1996**, 105, 10171-10177		7
825	Energy Decomposition Analyses for Many-Body Interaction and Applications to Water Complexes. **1996**, 100, 14316-14328		240
824	Supported nickel and copper clusters on MgO(100): A first-principles calculation on the metal/oxide interface. **1996**, 104, 7329-7337		151

823	Interaction of Water with Brønsted Acidic Sites of Zeolite Catalysts. Ab Initio Study of 1:1 and 2:1 Surface Complexes. **1996**, 100, 6199-6211		152
822	Ground- and excited-state properties of neutral and anionic selenium dimers and trimers. **1996**, 54, 1979-1993		24
821	Adsorption of CO on TiO2 (110) studied by means of a cluster model surrounded by multipoles obtained from slab calculations. **1996**, 54, 14812-14821		33
820	Structure and vibrations of catechol and catechol?H2O(D2O) in the S0 and S1 state. **1996**, 104, 9362-9375		75
819	The long-range interaction between He and H+2: an ab initio and dynamical study. *Molecular Physics* , **1996**, 88, 647-662	1.7	11
818	The solvation of sodium ions in water clusters: intermolecular potentials for Na+-H2O and H2O-H2O. *Molecular Physics*, **1996**, 87, 1083-1116	1.7	24
817	Cation–Ether Complexes in the Gas Phase: Bond Dissociation Energies and Equilibrium Structures of Li+(1,2-dimethoxyethane)x, x = 1 and 2, and Li+(12-crown-4). **1996**, 100, 16116-16125		140
816	Cation–Ether Complexes in the Gas Phase: Bond Dissociation Energies and Equilibrium Structures of Li+[O(CH3)2]x, x = 1–4. **1996**, 100, 1605-1614		138
815	Toward an Understanding of the Drug–DNA Recognition Mechanism. Hydrogen-Bond Strength in Netropsin–DNA Complexes. **1996**, 100, 11480-11487		17
814	Dication–Water Interactions: M2+(H2O)n Clusters for Alkaline Earth Metals M = Mg, Ca, Sr, Ba, and Ra. **1996**, 100, 4790-4797		140
813	Base stacking and hydrogen bonding in protonated cytosine dimer: the role of molecular ion-dipole and induction interactions. **1996**, 13, 695-706		107
812	Significance of higher-order many-body interaction energy terms in water clusters and bulk water. **1996**, 73, 107-115		46
811	Hydrogen bonding and stacking of DNA bases: a review of quantum-chemical ab initio studies. **1996** , 14, 117-35		202
810	Decomposition of the total energy at the HF-SCF level and at several levels of correlation. *Molecular Physics*, **1996**, 87, 569-579	1.7	
809	Molecular Modeling of Small Molecules. **1996**, 55-92		3
808	Structure and Vibrational Features of Complexes between Unsaturated Hydrocarbons and Acidic Sites in Silica and Zeolites: An ab Initio Study. **1996**, 100, 3632-3645		38
807	Ab Initio Study of Proton Affinities of Three Crown Ethers. **1996**, 100, 7367-7371		28
806	Hydrogen Bond Energies of Hydrogen Chloride–Carbonyl Complexes. **1996**, 100, 2083-2088		15

805	Spectroscopic and Theoretical Studies of the Complexes between Nitrous Acid and Ammonia. **1996**, 100, 539-545	72
804	Ab Initio Calculations on the Use of Helium and Neon as Probes of the van der Waals Surfaces of Molecules. **1996**, 100, 2588-2596	46
803	Validation of Hybrid Density Functional/Hartree Fock Approaches for the Study of Homogeneous Catalysis. **1996**, 100, 2094-2099	32
802	Intermolecular Potential for the 1,2-Dimethoxyethane Water Complex. **1996**, 100, 6950-6957	48
801	Energetics and Mechanism of Decomposition of CF3OH. **1996**, 100, 6097-6103	42
800	Ab Initio Study of Nonadditive Effects in the (H2O)2 H2 Cluster. **1996**, 100, 10875-10881	4
799	Basis Set and Correlation Effects on Computed Lithium Ion Affinities **1996**, 100, 6284-6287	31
798	Critical Study of Fluoride Water Interactions. **1996**, 100, 3989-3995	96
797	Speciation in Aqueous Zinc Chloride. An ab Initio Hybrid Microsolvation/Continuum Approach. **1996** , 100, 9689-9693	28
796	Ab Initio Study of the Endohedral Complexes of C60, Si60, and Ge60 with Monoatomic Ions: Influence of Electrostatic Effects and Hardness. **1996**, 100, 7440-7448	35
795	A Direct Comparison between Structure Correlations and Reaction Paths. **1996**, 100, 6904-6909	22
794	Intermolecular Forces in van der Waals Complexes between Argon and Aromatic Molecules: Rotational Spectrum and ab Initio Investigation of Isoxazole Argon. **1996**, 100, 14298-14309	40
793	Vibrational Analysis of the van der Waals Complexes between Vinyl Fluoride and Hydrogen Chloride in Liquefied Argon. **1996**, 100, 15695-15703	5
792	High-Resolution Rovibrational Absorption Spectrum of CO2 N2O. **1996**, 100, 17772-17779	29
791	Carbenes and Silylenes as Hydrogen Bond Acceptors. **1996**, 100, 19367-19370	74
790	Matrix Infrared Spectra and ab Initio Calculations of the Nitrous Acid Complexes with N2 and CO. **1996**, 100, 11610-11615	48
789	Generalization of the Molecular Electrostatic Potential for the Study of Noncovalent interactions. **1996**, 3, 181-218	37
788	MEP: a tool for interpretation and prediction. From molecular structure to solvation effects. **1996**, 1-103	13

787	Charge-Transfer Complexes: Stringent Tests for Widely Used Density Functionals. **1996**, 100, 12265-12276	176
786	Optical transitions in excited alkali + rare-gas collision molecules and related interatomic potentials:. **1996**, 29, 3891-3910	39
785	Chemical storage of data. **1997**, 8, 1-5	12
784	A nontypical atom-diatom van der Waals interaction: Ar□2. **1997**, 107, 1185-1194	14
783	Pair potential for water from symmetry-adapted perturbation theory. **1997**, 107, 4207-4218	122
782	Application of the generalized-gradient approximation to rare-gas dimers. **1997**, 56, R2495-R2498	102
781	Novel Structures for the Excess Electron State of the Water Hexamer and the Interaction Forces Governing the Structures. **1997**, 79, 2038-2041	93
780	Anisotropic interface characteristics of bilayer GeSe based field effect transistors. **2022**, 115317	
779	The effect of platinum decoration on the sensing characterisation of AlP nanosheets towards mercaptopurine drug. **2022**, 96,	0
778	Correlated rotational excitations in NO-CO inelastic collisions.	
777	A DFT study on the adsorption behavior of antiviral Favipiravir drug on B N (n = 12, 16, 20, and 24) nanocages: the size effect. **2022**, 119388	1
776	Influence of magnetite incorporation into chitosan on the adsorption of the methotrexate and in vitro cytotoxicity.. **2022**,	1
775	Dispersion Interactions in Exciton-Localized States. Theory and Applications to □□ and n-□□ Excited States.. **2022**,	
774	The p Hydrogen-Bond Basicity Scale: From Molecules to Anions.. **2022**,	0
773	Eighth-Order Virial Equation of State for Methane from Accurate Two-Body and Nonadditive Three-Body Intermolecular Potentials.. **2022**,	0
772	Base pairs with 4-amino-3-nitrobenzonitrile: comparison with the natural WC pairs. Dimer and tetramer forms, Infrared and Raman spectra, and several proposed antiviral modified nucleosides.. **2022**, 1-23	0
771	Resonance-assisted intramolecular triel bonds.	0
770	New 2-cyanobenzyl-nitrile-dithiolate to di-n-butyltin(IV)-bis-(1-alkoxy-isoquinoline-4-nitrile thiolate): Crystallographic and Computational Studies.	3

769	Benzene and Triazine-Based Porous Organic Polymers with Azo, Azoxy and Azodioxy Linkages: A Computational Study.	0
768	Doxorubicin-peptide-gold nanoparticle conjugate as a functionalized drug delivery system: exploring the limits.	0
767	Theoretical study on potential energy surface and bound states of the Kr-CNCN complex: Compared with the Kr-NCCN system. **2022**, 386, 111645	
766	DFT study of the therapeutic potential of borospherene and metalloborospherenes as a new drug-delivery system for the 5-fluorouracil anticancer drug. **2022**, 119457	0
765	Unique O?N...O Pnicogen Interactions in Nitromethane Dimers: Evidence Using Matrix Isolation Infrared Spectroscopy and Computational Methodology.	1
764	Exploration of supramolecular and theoretical aspects of two new Cu(II) complexes: On the importance of lone pair(chelate ring) and (chelate ring) interactions. **2022**, 133358	0
763	Mechanical Bond Enhanced Lithium Halide Ion-Pair Binding by Halogen Bonding Heteroditopic Rotaxanes.	0
762	A computational inspection of the dissociation energy of mid-sized organic dimers. **2022**, 156, 204303	0
761	Mg12O12 and Be12O12 Nanocages as Sorbents and Sensors for H2S and SO2 Gases: A Theoretical Approach. **2022**, 12, 1757	0
760	Beryllium ion coordination in Ammonia, methanol and water solvents. **2022**, 360, 119414	0
759	Importance of R-CH3?O tetrel bonding and vinyl?aryl stacking interactions in stabilizing the crystal packing of 2,4-dihydroxy-3-methoxychalcone: Exploration of antileishmanial activity and molecular docking studies. **2022**, 1265, 133357	0
758	Solvation stabilizes intercarbonyl n-π interactions and polyproline II helix.	1
757	Quantum Effects in Biological Systems. **2022**, 201-247	
756	2,2,3,3,3-pentafluoro-1-propanol and its dimer: structural diversity, conformational conversion, and tunnelling motion.	1
755	Characterizing the n-π interaction of pyridine with small ketones: a rotational study of pyridine⋯acetone and pyridine⋯2-butanone.	2
754	A Minimum Quantum Chemistry CCSD(T)/CBS Data Set of Dimeric Interaction Energies for Small Organic Functional Groups: Heterodimers.	0
753	Inhibition of the Peroxygenase Lytic Polysaccharide Monooxygenase by Carboxylic Acids and Amino Acids. **2022**, 11, 1096	1
752	A DFT Study of the Hydrogen Bonded Structures of Pyruvic Acid⋯Water Complexes. 10,	0

751	Understanding the role of non-Watson-Crick base pairs in DNA–protein recognition: Structural and energetic aspects using crystallographic database analysis and quantum chemical calculation.	
750	Adsorption of Industrial Gases (CH4, CO2, and CO) on Olympicene: A DFT and CCSD(T) Investigation.	1
749	Role of Functional Groups in an Ionic Liquid Decorated Au(111) Surface for CO2 Capture and Activation: A First Principle Approach. **2022**, 169, 056524	1
748	Experimental and Theoretical Evidence of a Pb???Pb Ditetrel Bond Without a σ-Hole.	0
747	Modeling the Adsorption of Polycyclic Aromatic Hydrocarbons on Graphynes: An Improved Lennard-Jones Formulation.	0
746	Interaction of Cysteine with Li+ and LiF in the Presence of (H2O)n (n = 0–3) Clusters.	
745	Polymorphic transition due to grinding: the case of 3-[1-(tert-butoxycarbonyl)azetidin-3-yl]-1,2-oxazole-4-carboxylic acid. **2022**, 78, 510-519	0
744	Influence of side-chain length on antifungal efficacy of N-alkyl nicotinamide-based compounds.	1
743	Propylthiouracil drug adsorption on pristine, Cu, Ag, and Au decorated AlP nanosheets. **2022**, 128236	1
742	Dichlorosilane adsorption on the Al, Ga, and Zn-doped fullerenes.	4
741	Rydberg states of ZnAr complex. *Molecular Physics*,	1.7
740	Ab initio study for superior sensitivity of graphyne nanoflake towards nitrogen halides over ammonia. **2022**, 28,	0
739	Composition-selective full inclusion host–guest interaction of azobenzene-containing photoresponsive nanoring with fullerene C 60 .	1
738	New hydrate cocrystal of l-proline with 4-acetylphenylboronic acid obtained via mechanochemistry and solvent evaporation: An experimental and theoretical study. **2022**, 123282	1
737	Surface Modification Strategy for Enhanced NO2 Capture in Metal–Organic Frameworks. **2022**, 27, 3448	2
736	Fast and Accurate Determination of the Singlet–Triplet Gap in Donor–Acceptor and Multiresonance TADF Molecules by Using Hole–Hole Tamm–Dancoff Approximated Density Functional Theory. 2200056	1
735	Study to molecular insight into the role of Aluminum nitride nanotubes on to deliver of 5-Fluorouracil (5FU) drug in smart drug delivery. **2022**, 109617	1
734	DFT investigation of graphene quantum dot-Ixora floral natural dye (GQD-NDIX) nanocomposites as visible light harvesters in dye-sensitized solar cells. **2022**, 119531	0

733	Theoretical assessment of the solvent effect on the functionalization of Au32 and C60 nanocages with fluorouracil drug. **2022**, 126, 109142	4
732	Intermolecular Dynamics of Positively and Negatively Charged Aromatics and Their Isoelectronic Neutral Analogs in Aqueous Solutions.	0
731	Characterization of Competing Halogen- and Hydrogen-Bonding Motifs in Simple Mixed Dimers of HCN and HX (X = F, Cl, Br, and I).	0
730	Dissociation of Bipyridine and Coordination with Nitrosyl: Cyclometalated Ruthenium Nitrosyl Complex.	1
729	Breaking Covalent Bonds in the Context of the Many-Body Expansion (MBE): I. The purported "first row anomaly" in XHn (X = C, Si, Ge, Sn; n = 1-4).	2
728	Atenolol-imprinted polymer: a DFT study. **2022**, 28,	
727	Crystal structure of N-(1,3-benzothiazol-2-yl)-4-iodobenzene-1-sulfonohydrazide: the unexpected importance of l N-H???□and I???□nteractions on the supramolecular arrangement.	
726	Diffusion behavior of gas molecules in the one-dimensional channel of AlPO4-5 molecular sieves. **2022**, 340, 112024	1
725	Molecular design for all-in-one self-assembled donor□cceptor organic solar cells. **2022**, 244, 111798	0
724	Phenol-cyclohexanol eutectic mixtures: Phase diagram and microscopic structure by experimental and computational studies. **2022**, 360, 119492	0
723	A DFT study of the adsorption and surface enhanced Raman spectroscopy of pyridine on Au20, Ag20, and bimetallic Ag8Au12 clusters. **2022**, 115, 108234	1
722	Vacancy defects in monolayer boron carbon nitride for enhanced adsorption of paraben compounds from aqueous stream: A quantum chemical study. **2022**, 723, 122131	0
721	Intermolecular interactions in binary mixtures of formamide and acetone. **2022**, 560, 113517	
720	Simulating the Hydration Structure of Low- and High-Spin [Fe(bpy)3]2+: Long-Range Dispersion and Many-Body Effects.	1
719	Effect of Hydrogen Bonds and □.□nteractions on the Crystallization of Phenyl-perfluorophenyl Amides: Understanding the Self-organization of a Cocrystal.	
718	Non-Covalent Interactions Atlas benchmark data sets 5: London dispersion in an extended chemical space. **2022**, 24, 14780-14793	1
717	N/O?B dative bond supplemented by N-HN/HC Hydrogen Bonds make BN-cages an attractive candidate for DNA-nucleobase adsorption □An MP2 prediction.	0
716	Combined Computational/Experimental Investigation of new cocrystals of the drug bosentan.	2

715	Halogen bond-directed self-assembly in bicomponent blends at the solid/liquid interface: Effect of the alkyl chain substitution position.	2
714	Mitigating Cerium Migration for Perfluorosulfonic Acid Membranes Using Organic Ligands.	
713	Non-covalent interactions atlas benchmark data sets 4: hole interactions. **2022**, 24, 14794-14804	3
712	An accurate vibrational signature in halogen bonded molecular crystals. **2022**, 24, 15103-15109	
711	INVESTIGATION OF DIHYDROGEN BOND INTERACTION BETWEEN CYCLOALKENES AND ALKALI METAL HYDRIDES: A DFT APPROACH. **2022**, 63, 501-509	
710	The microwave spectra and molecular structures of the chiral and achiral rotamers of 2,3,3-trifluoropropene and their gas-phase heterodimers with the argon atom. **2022**, 387, 111656	0
709	Hydrophobic stacking interactions and hydrogen bonds drive self-aggregation of luteolin in water. **2022**, 108243	0
708	How Does Electronic Activity Drive Chemical Reactions? Insights from the Reaction Electronic Flux for the Conversion of Dopamine into Norepinephrine.	0
707	Enhancing of CO Uptake in Metal-Organic Frameworks by Linker Functionalization: A Multi-Scale Theoretical Study. **2022**, 4, 603-614	1
706	Alkaline Earth Metals Doped C2N With Enhanced Non-Linear Optical Properties. **2022**, 169514	0
705	Regioselective Synthesis of 2-Aryl-5-cyano-1-(2-hydroxyaryl)-1H-imidazole-4-carboxamides Self-Assisted by a 2-Hydroxyaryl Group.	0
704	Monolayered Carbides of Main Group Elements (Si, Ge, Sn and Pb) for NO2 Gas Sensing: Insights from First-Principle Studies.	0
703	Combination of FTIR and DFT to study the regulation law of [EMIM][OAc] on the microstructure of the acetone–methanol azeotrope system. **2022**, 119601	0
702	Potential application of some metal decorated AlP nano-sheet for detection of boron trichloride. **2022**, 113792	0
701	Investigation on the feasibility of recycled polyvinylidene difluoride polymer from used membranes for removal of methylene blue: experimental and DFT studies.	1
700	Determining Repulsion in Cyclophane Cages. **2022**, 27, 3969	0
699	Assessment of density functional approximations for N 2 and CO 2 physisorption on benzene and graphene. **2022**, 43, 1403-1419	
698	Revision of the Crystal Structure of the Orthorhombic Polymorph of Oxyma: On the Importance of Hole Interactions and Their Interplay with HBonds. **2022**, 12, 823	0

697	Enhanced adsorption of fluoroquinolone antibiotic on the surface of the Mg-, Ca-, Fe- and Zn-doped C60 fullerenes: DFT and TD-DFT approach. **2022**, 31, 103798	1
696	RNABPDB: Molecular Modeling of RNA Structure From Base Pair Analysis in Crystals to Structure Prediction.	0
695	The proton and the lithium cation linked with electron and electron systems: are such interactions beyond or within the definition of hydrogen/lithium bond?.	
694	Dissociation mechanism of a C60-Li+ complex by microscopic hydration: density functional theory study.	
693	DFT Study of Adsorption of Methyl Red on the Surface of Pure, Pyrrolidine-Functionalized, Silicon- and Germanium-Doped Zigzag (6, 0) Carbon Nanotubes. **2022**, 96, 1280-1290	0
692	Tetramethylammonium Cation: Directionality and Covalency in Its Interactions with Halide Ions. **2022**, 61, 9082-9095	1
691	A Classical Model for 3-body Interactions in Aqueous Ionic Systems.	2
690	Through-Bond-Driven Through-Space Interactions in a Fullerene C60 Noncovalent Dyad: An Unusual Strong Binding between Spherical and Planar Electron Clouds and Culmination of Dyadic Fractals. **2022**, 126, 3629-3641	2
689	Efficient and Accurate Description of Diels-Alder Reactions using Density Functional Theory.	0
688	Various Sorts of Chalcogen Bonds Formed by an Aromatic System.	1
687	High CT-Fluorophore Featuring a Basic Moiety into DA Chain as a pKa Probe. **2022**, 87, 7618-7634	0
686	Investigation of NH???HM Dihydrogen Bonded Interactions in Adenine, Cytosine, Guanine, and Thymine with HM (M = Li and Na) Complexes: A DFT Study. **2022**, 96, 1258-1267	
685	Bifurcated Chalcogen Bonds Based on One-Hole.	
684	Explicitly Correlated Electronic Structure Calculations with Transcorrelated Matrix Product Operators.	2
683	Synergistic Enhancement of Hydrogen-Bonding and Charge-Transfer Interactions in a Crystal of an AnthranolAcridine Dyad Comprised of a Hydrogen-Bonded Chain Aggregate.	
682	Structure, Spectra and Photochemistry of 2-Amino-4-Methylthiazole: FTIR Matrix Isolation and Theoretical Studies. **2022**, 27, 3897	
681	Extensive Analyses on Expanding the Scope of AcidAminopyrimidine Synthons for the Design of Molecular Solids.	1
680	Potential application of AlP nanosheet semiconductor in the detection of toxic phosgene, ?thiophosgene, and formaldehyde gases.	0

679	[2+3] Amide Cages by Oxidation of [2+3] Imine Cages - Revisiting Molecular Hosts for Highly Efficient Nitrate Binding.	1
678	Quantum chemical and theoretical kinetics studies on the reactions of hydroperoxy radical with methanethiol and ethanethiol. **2022**, 1214, 113787	
677	Carbonyl fluoride gas adsorption and detection by the pristine and Ni-doped inorganic boron nitride nanoclusters. **2022**, 142, 109652	0
676	Interactions between benzene and graphene by means of large-scale DFT-D4 calculations. **2022**, 561, 111606	1
675	Unravelling the interaction between boron nitride nanosheets and organic pesticides through density functional theory studies. **2022**, 649, 129550	0
674	Hydrogen and halogen bonding in H2O-HF and H2O-F2 complexes. **2022**, 561, 111605	
673	Herringbone Reconstruction-Mediated assembly of 2-(Hydroxymethyl)benzimidazole molecules on Au(1 1 1) studied by scanning tunneling microscope. **2022**, 803, 139799	
672	Structure and hydrogen-bond properties of N-alkyl-N-methyl-pyrrolidinium bis(trifluoromethylsulfonyl)imide and ethanol: A combination of FTIR and theoretical studies. **2022**, 1265, 133488	
671	Effective separation of toluene from n-heptane with imidazolium-based deep eutectic solvents. **2022**, 326, 124992	1
670	On the energetics of binding and hydride exchange in the RuH2(H2)2[P(C5H9)3)]2 complex as revealed by inelastic neutron scattering and DFT studies.	
669	Adsorption of Glyphosate on Graphene and Functionalized Graphenes: A Dft Study.	
668	On the Influence of Pnictogen Bonding on Aciditydeclaration of Interests.	
667	Evolution of microstructures and hydrogen bond interactions within choline amino acid ionic liquid and water mixtures.	0
666	Molecular modeling and nonlinear optical properties of new isostructural halogenated dihydroquinolinones.	
665	Unravelling a New Conformer of Psilocin Through Computational Methods.	
664	Centroid?centroid and hydrogen bond interactions as robust supramolecular units for crystal engineering: X-ray crystallographic, computational and urease inhibitory investigations of 1,2,4-triazolo[3,4-a]phthalazines.	0
663	Cooperative pentavalent pnicogen bonding versus dominant hydrogen bonding in POCl3-diethylether dimer characterized using matrix isolation infrared spectroscopy and ab initio computations. **2022**, 387, 111672	0
662	Quantum study of the bending relaxation of H2O by collision with H. **2022**, 514, 4426-4432	0

661	In silico Study of Solvent Effects on the Intramolecular Hydrogen Bond of Hydroxy Proline. **2022**, 38, 676-680	
660	Single-molecule DNA sequencing using two-dimensional Ti2C(OH)2 MXene nanopores: A first-principles investigation.	1
659	Hydrogen-Atom-Assisted Uphill Isomerization of N-Methylformamide in Darkness. **2022**, 144, 12339-12346	1
658	Exploring the effect of complexant on remarkably high static and dynamic second hyperpolarizability of aziridine-based diffuse electron systems: a theoretical study.	2
657	The role of weak C–H···O hydrogen bond in alcohol–water mixtures.	1
656	Highly Efficient and Accurate Computation of Multiple Orbital Spaces Spanning Fock Matrix Elements on Central and Graphics Processing Units for Application in F12 Theory. **2022**, 18, 4218-4228	
655	Rotational Spectroscopy of the 2,2,3,3,3-Pentafluoropropanol–Water Complex: Conformations and Large Amplitude Motions.	
654	Methoxyl-Substituted Phosphine Ligand Properties and a Case Study of Formation Adducts to Indium(III) Bromide by DFT Calculations. **2022**, 116043	
653	Antiparallel π and C–H···C Contacts in a Novel Zn(II) Coordination Solid involving π-hole Tetrel Bonding Interactions: A Combined Experimental and Theoretical Study, Hirshfeld Surface Analysis, Molecular Docking and Potential Drug Property.. **2022**, 133686	1
652	Preparation, Characterization and Anticancer Activity of Inclusion Complexes between Genistein and Amino-Appended β-Cyclodextrins. **2022**, 7,	
651	Post-synthetic halogen incorporation in Zr-based MOF for enhancement of the catalytic oxidation reactions. **2022**, 136, 104438	
650	Noncovalent Interactions between Aromatic Heterocycles and Carboxylic Acids: Rotational Spectroscopy of the Furan–Formic Acid and Thiophene–Formic Acid Complexes.	
649	Influence of Alkali Metal Doping and BN Substitution on the Second-Order Nonlinear Optical Properties of Graphyne: A Theoretical Perspective. **2022**, 61, 10756-10767	1
648	Theoretical investigation for the reactions of triplet oxygen atom with dimethyl sulphide, ethyl methyl sulphide: mechanism and kinetics properties. *Molecular Physics*,	1.7
647	Gas-Phase Internal Ribose Residue Loss from Mg-ATP and Mg-ADP Complexes: Experimental and Theoretical Evidence for Phosphate-Mg-Adenine Interaction.	
646	Ab initio studies on complexes of ozone with diatomic molecules.	0
645	Bifurcated Halogen Bond-Driven Supramolecular Double Helices from 1,2-Dihalotetrafluorobenzene and 2,2?-Bi(1,8-naphthyridine). **2022**, 12, 937	1
644	Intermolecular interactions between cyclo[18]carbon and XCN (X = H, F, Cl, Br, I): a theoretical study. **2022**, 28,	1

643 Effects of Ag-decoration on the adsorption and detection of toxic OF2 gas on a GaN nanotube. 1-9 0

642 From the gas phase to the solid state: The chemical bonding in the superheavy element flerovium. 1

641 Strategies for Controlling the Spatial Orientation of Single Molecules Tethered on DNA Origami Templates Physisorbed on Glass Substrates: Intercalation and Stretching. **2022**, 23, 7690 2

640 Rotational spectroscopic studies of the tetrel bonded CH3CN-CO2 complex. **2022**, 111671 0

639 Hydrocarbon Soluble Alkali-Metal-Aluminium Hydride Surrog[ATES]. 0

638 Gas adsorption effects of monolayer GeSe in terms of anisotropic transport properties.

637 First-principles study of the adsorption of flavonoids on graphene oxide.

636 A DFT theoretical investigation on the interplay effects between cation-□and intramolecular hydrogen bond interactions in the mesalazine?Fe2+ binary complex. **2022**, 141, 0

635 Dissecting Noncovalent Interactions in Carboxyl-Functionalized Ionic Liquids Exhibiting Double and Single Hydrogens Bonds Between Ions of Like Charge.

634 The impact of the size of acetylated cyclodextrin on the stability of amorphous metronidazole. **2022**, 122025 0

633 Density functional theory study of the hydrogen evolution reaction in haeckelite boron nitride quantum dots. **2022**, 1

632 Quantum Inelastic Scattering of ArHAr+, HeHHe+, and NeHNe+ with He on New Potential Energy Surfaces. 0

631 Structural and thermodynamics properties of pure phase alkanes, monoamides and alkane/monoamide mixtures with an ab initio based force-field model. **2022**, 119797

630 The Interaction of Deep Eutectic Solvents with Pristine Carbon Nanotubes and Their Associated Defects: A Density Functional Theory Study. **2022**, 119855 0

629 The influence of a single water molecule on the reaction of BrO + HONO. **2022**, 108261

628 DFT study on CH?O, CH□SCN and S□□nteraction energies in three dinuclear mixed valence cobalt(III/II) complexes with secondary diamine ligands having inner N2O2 and outer O4 compartments. **2022**, 116039 0

627 Singlet O2 Oxidation of the Radical Cation versus the Dehydrogenated Neutral Radical of 9-Methylguanine in a Watson□rick Base Pair. Consequences of Structural Context. 0

626 Oxacalix[4]arene based dual-signalling fluorimetric and electrochemical chemosensor for the selective detection of nitroaromatic compounds. **2022**, 362, 119791 1

625	Hydrogen bonds in aqueous choline chloride solutions by DFT calculations and X-ray scattering. **2022**, 362, 119742		1
624	Cooperative strengthening of the halogen bond in cyclic clusters of iodine monofluoride, (IF)n (n□=□3□8): From a closed-shell interaction, F-I□F, to a symmetric partly covalent interaction, F□I□F. **2022**, 803, 139825		1
623	Experimental studies on thermophysical properties of protic ionic liquids for thermal energy storage systems. **2022**, 54, 105251		0
622	Insights on the enhanced nitrogen dioxide sensing using doped boron nitride nanosheets through the quantum chemical studies. **2022**, 562, 111629		0
621	Enhanced interlayer coupling in twisted bilayer graphene quantum dots. **2022**, 600, 154148		
620	Adsorption of toxic and non-toxic metals with new model of CX[4]: Experimental and computational investigation, Spectroscopic, QTAIM, and Antibacterial activity analyses. **2022**, 1268, 133618		0
619	Chirality transfer observed in Raman optical activity spectra. **2022**, 281, 121604		
618	Quantum chemistry study of the multiphoton absorption□in enhanced green fluorescent protein□at the single amino acid residue level.		1
617	Tuning the Topological Band Gap of Bismuthene with Silicon-based Substrates.		
616	Hydrogen and halogen bonds formed by MCO3 (M = Zn, Cd) and their enhancement by a spodium bond. *Molecular Physics*,	1.7	1
615	A comparative computational study of binary complexes of the structural isomers, propargylimine and acrylonitrile, with small molecules in the interstellar medium (ism). **2022**, 113827		
614	Theoretical investigation on the mechanisms and kinetics of the reactions of hydroperoxy radical with dimethyl sulphide and ethyl methyl sulphide. *Molecular Physics*,	1.7	
613	DFT□Assisted Structure Determination from Powder X-ray Diffraction Data of a New Zonisamide/?-Caprolactam Cocrystal. **2022**, 12, 1020		1
612	Demarcating Noncovalent and Covalent Bond Territories: Imine-CO2 Complexes and Cooperative CO2 Capture.		0
611	Photo-Induced Reactions between Glyoxal and Hydroxylamine in Cryogenic Matrices. **2022**, 27, 4797		
610	Fragment Localized Molecular Orbitals.		0
609	Computational Modeling for the Oxidation Reactions of the Cysteine Residues with the Superoxide and the Organic Radical Species.		
608	Rational truncation, mutation, and halogenation of bradykinin neuropeptides as potent ACEII inhibitors by integrating molecular dynamics simulations, quantum mechanics calculations, and in vitro assays.		0

607	Muscimol hydration and vibrational spectroscopy The impact of explicit and implicit water. **2022**, 363, 119870	
606	Aqueous microsolvation of 4-hydroxy-2-butanone: competition between intra- and inter-molecular hydrogen bonds. **2022**, 24, 19919-19926	1
605	A Quantum Chemical Deep-Dive into the Interactions of 3-Methylindole and Its Halogenated Derivatives owards an Improved Ligand Design and Tryptophan Stacking. **2022**, 15, 935	1
604	Gas-Sensing Properties of B/N-Modified SnS2 Monolayer to Greenhouse Gases (NH3, Cl2, and C2H2). **2022**, 15, 5152	0
603	Importance of Sugar Phosphate Backbone and Counterions to First-Principles Modeling of Nucleobases. **2022**, 126, 5744-5751	
602	Adsorption of Polycyclic Aromatic Hydrocarbons and C60 onto Forsterite: CH Bond Activation by the Schottky Vacancy. **2022**, 6, 2009-2023	0
601	Ring-Opening Polymerization of L-Lactide Catalyzed by Potassium-Based Complexes: Mechanistic Studies. **2022**, 14, 2982	1
600	A Density Functional Theory and Information-Theoretic Approach Study of Interaction Energy and Polarizability for Base Pairs and Peptides. **2022**, 15, 938	0
599	The tetrel bonding role in supramolecular aggregation of lead(II) acetate and a thiosemicarbazide derivative. **2022**, 78, 685-694	0
598	Noble Gas Silicon Cations: Theoretical Insights into the Nature of the Bond. **2022**, 27, 4592	0
597	Theoretical study on the kinetics of the reactions of hydrogen atom, methyl radical with methanethiol and ethanethiol.	
596	Cation- Interaction-Mediated Tumour Drug Delivery for Deep Intratumoral Penetration and Treatment. 2205043	1
595	Stacked supramolecular junctions.	3
594	Noncovalent interactions in model molecular clusters containing the tetrel atoms Si and Ge.	
593	Electron in a cube: Synthesis and characterization of perfluorocubane as an electron acceptor. **2022** , 377, 756-759	3
592	Theoretical Investigations of the OH-Initialized Oxidation of 4-Methyl-3-Penten-2-One in the Atmosphere.	0
591	Tailoring the hydrogen storage performance of the Cr-, Mn-, and Fe-doped circumcoronenes by the presence of N and B co-dopants: Computational study. **2022**,	
590	A new potential energy surface and rovibrational spectra of the CO CO2 complex: Dependence on the antisymmetric stretching vibration of CO2. **2022**, 157, 084310	

589	Binding Energy Evaluation Platform: A Database of Quantum Chemical Binding Energy Distributions for the Astrochemical Community. **2022**, 262, 17	0
588	Quantum mechanical study of interactions between sunscreen ingredients and nucleotide bases. **2022**, 28,	
587	Noncovalent interactions between benzochalcogenadiazoles and nitrogen bases. **2022**, 28,	1
586	Weakly bound complexes of selenophene with water as seen in matrix isolation FTIR. **2022**, 111689	
585	Carbonyl sulfide gas detection by pure, Zn- and Cd-decorated AlP nano-sheet.	4
584	Hyperfine resolved rate coefficients of HC17O+ with H2 (j = 0).	0
583	Perception of Mg adsorption on the BC2N nanotube as a anode for rechargeable Mg ion batteries. **2022**, 47, 29006-29013	
582	Cyclized oligomer of tetracyanoquinodimethane-tetrathiafulvalene (TCNQ-TTF): a versatile macrocyclic molecule by DFT calculations.	
581	Halogen□Halogen and □Hole Interactions in Supramolecular Aggregates and Electrical Conductivity Properties of Cu(II)-Based 1D Coordination Polymers.	4
580	Binding propensity and selectivity of cationic, anionic, and neutral guests with model hydrophobic hosts: A first principles study.	0
579	Gaseous transport properties of the ground and excited Cr, Co and Ni cations in He: Ab initio study of electronic state chromatography.	0
578	Diaminopyridine Hg(II)-based 1D supramolecular polymer: Crystallographic and computational insights into spodium bonding. **2022**, 123517	
577	Al-, Ga-, and In-decorated BP nanotubes as chemical sensors for 2-chloroethanol. **2022**, 153, 589-596	1
576	The Binding Behavior of Peptide Ligands to Human Osteoclast-stimulating Factor SH3 Domain can be Shifted by a Rationally Designed □Stacking System.	
575	Calculation of the intermolecular potential energy surfaces of $${mathbf{H}mathbf{e}mathbf{H}}_{3}^{+}$$ by means of ab initio methods. **2022**, 141,	
574	Neural network interaction potentials for para-hydrogen with flexible molecules. **2022**, 157, 074302	1
573	Experimental and theoretical characterization of chelidonic acid structure.	1
572	Explaining the interaction of mangiferin with MMP-9 and NF-□a computational study. **2022**, 28,	

571	Hydrogen Bonds of Coordinated Ethylenediamine and a Water Molecule: Joint Crystallographic and Computational Study of Second Coordination Sphere.	0
570	Computational investigation of isoeugenol transformations on a platinum cluster : Direct deoxygenation to propylcyclohexane. **2022**, 529, 112541	1
569	Ground-State Properties of Metallic Solids from Ab Initio Coupled-Cluster Theory. **2022**, 13, 7497-7503	1
568	Pursuing the basis set limit of CCSD(T) non-covalent interaction energies for medium-sized complexes: case study on the S66 compilation.	2
567	Influence of 5-Halogenation on the Base-Pairing Energies of Protonated Cytidine Nucleoside Analogue Base Pairs: Implications for the Stabilities of Synthetic i-Motif Structures for DNA Nanotechnology Applications.	
566	Microhydration of Phenyl Formate: Gas-Phase Laser Spectroscopy, Microwave Spectroscopy, and Quantum Chemistry Calculations.	1
565	Physical mechanisms of intermolecular interactions from symmetry-adapted perturbation theory. **2022**, 28,	2
564	Improved Estimates of Host-Guest Interaction Energies for Endohedral Fullerenes Containing Rare Gas Atoms, Small Molecules, and Cations.	2
563	Theoretical study on L-H+-L with identical donors: short strong hydrogen bond or not?.	
562	Photoinduced Charge Transfer in the Zn-Methanol Cation Studied with Selected-Ion Photofragment Imaging.	2
561	Upcycling Mask Waste to Carbon Capture Sorbents: A Combined Experimental and Computational Study.	1
560	A polarizable fragment density model and its applications. **2022**, 157, 084108	
559	Molecular design and rational optimization of synergistic effect between the two wings of a roughly orthogonal cation- stacking system at nasopharyngeal carcinoma YAP1-TEAD4 parallel Helix-Helix interaction interface.	
558	Quaternary diammonium reagents hosted on polymer nanofibers for hexachloridoiridate(IV) specificity: Experimental and theoretical studies. **2022**, 187, 107810	
557	Dynamic Investigations of Rare Gas-NO+ Interactions. 1518-1528	
556	Co-amorphous systems using epigallocatechin-3-gallate as a co-former: Stability, in vitro dissolution, in vivo bioavailability and underlying molecular mechanisms. **2022**, 178, 82-93	
555	Adsorption of glyphosate on graphene and functionalized graphenes: A DFT study. **2022**, 1215, 113840	
554	Bromochlorodifluoromethane interaction with pristine and doped BN nanosheets: A DFT study. **2022**, 10, 108367	1

553	Opto-electronic properties of isomers of azobispyridine. **2022**, 805, 139956	
552	Use of tetraphenyl (hydroxyl) imidazole for colorimetric detection of iodide: Optical properties, computational characterizations, NBO, QTAIM, and NCI-RDG analyses. **2022**, 144, 109917	1
551	Interaction of CO2 with TiO2/reduced graphene oxide as superior catalysts: Dispersion-corrected density functional theory simulation. **2022**, 128, 109279	
550	Electronic structure calculations of the fundamental interactions in solvent extraction desalination. **2022**, 364, 119986	0
549	DFT-based modeling of polypyrole/B12N12 nanocomposite for the photocatalytic applications. **2022**, 170, 110949	
548	Nonlinear optical (NLO) response of boron phosphide nanosheet by alkali metals doping: A DFT study. **2022**, 151, 107007	1
547	New complexes of indium(III) diaryldithiophosphates: Structural characterization and insight into supramolecular interactions. **2022**, 226, 116094	
546	The molecular species in saturated and overheated vapors of Sc(acac)3: A first structural study of bis-acetylacetonate scandium Sc(acac)2 radical. **2022**, 806, 139989	
545	Rotational spectrum of anisole-CO2: Cooperative C⋯O tetrel bond and C H⋯O hydrogen bond. **2022**, 282, 121677	0
544	Dual modification to stabilize Non-IPR C72 fullerene: A new theoretical strategy. **2022**, 117, 108289	
543	Exploring dithiolate-amine binary ligand systems for the supramolecular assemblies of Ni(II) coordination compounds: Crystal structures, theoretical studies, cytotoxicity studies, and molecular docking studies. **2022**, 543, 121157	0
542	Unfurling Anion-π Interactions Involving Graphynes.	0
541	Density Functional Theory Study of the Regioselectivity in Copolymerization of bis-Styrenic Molecules with Propylene Using Zirconocene Catalyst. **2022**, 12, 1039	1
540	Thermodynamics and Spectroscopy of Halogen- and Hydrogen-Bonded Complexes of Haloforms with Aromatic and Aliphatic Amines. **2022**, 27, 6124	0
539	The first principle study of chalcogen bonds, pnicogen bond and their mutual effects in a set of complexes between the triazine with SHF and PH2F ligands. **2022**, 1216, 113867	0
538	Experimental and DFT investigation on the role of aromaticity on the stability of hydrogen bonded complexes of cyclohexanone with amines and hydroxyl compounds. **2022**, 366, 120221	0
537	Helicene adsorption on graphene, hexagonal boron nitride, graphane, and fluorographane. **2022**, 806, 139998	1
536	Chlorine trifluoride gas adsorption on the Fe, Ru, Rh, and Ir decorated gallium nitride nanotubes. **2022**, 356, 114945	0

535	Metal-decorated BN monolayer as potential chemical sensors for detection of purinethol drug. **2022**, 145, 109919	0
534	Sarin chemical warfare agent detection by Sc-decorated XN nanotubes (X = Al or Ga). **2022**, 145, 109941	0
533	Reaction of the thallium(I) cation with [2.2]paracyclophane: Experimental and theoretical study. **2022**, 543, 121205	0
532	Adsorption of trivalent and pentavalent arsenic ions from the aqueous stream using natural Bombax ceiba fibers: Insights from density functional theory calculations. **2022**, 3-4, 100012	0
531	Nitrogenated Holey Graphene (C2N-h2D): An excellent sensor for neurotransmitter amino acids. **2022**, 606, 154740	0
530	Sensing cyclosarin (a chemical warfare agent) by Cucurbit[n]urils: A DFT/TD-DFT study. **2023**, 1272, 134163	0
529	Design and synthesis of pyrazole, pyrazolone and 1,3,4-oxadiazole derivatives having pyrrole motif as a source of new antimicrobial and anticancer agents. **2023**, 1272, 134087	1
528	Experimental and theoretical study of the physicochemical properties of the novel imidazole-based eutectic solvent. **2023**, 118, 108319	0
527	The Molecular Nature of the Eliminating Azeotrope in Extractive Distillation by Ionic Liquid Entrainer.	0
526	The role of phosphoric acid in the crystallization of lenalidomide form DH water system. **2022**, 24, 6357-6366	0
525	Recognition and mechanistic investigation of anion sensing by ruthenium(ii) arene complexes and bio-imaging application. **2022**, 51, 13071-13084	0
524	Molecular strategy towards ROMP-derived hyperbranched poly(olefin)s featuring various bridged perylene diimides.	0
523	Density Functional Theory on the CO2 Absorption Process with Ionic Liquids. **2022**, 967-972	0
522	Comprehending radicals, diradicals and their bondings in aggregates of imide-fused polycyclic aromatic hydrocarbons. **2022**, 13, 9985-9992	0
521	The role of attractive and repulsive interactions in the stabilization of ammonium salts structures.	0
520	New theoretical investigation of rotational inelastic (de)-excitation of calcium isocyanide CaNC(2) in collision with He(1S).	0
519	Importance of Cu and Ag Regium bonds in supramolecular chemistry and biology: A combined crystallographic and ab initio study..	0
518	Aggregation and support effects in the oxidation of fluxional atomic metal clusters. The paradigmatic Cu5 case.	2

517	Computational investigation of the increased virulence and pathogenesis of SARS-CoV-2 lineage B.1.1.7. **2022**, 24, 20371-20380	0
516	Modelling the strength of mineral□organic binding: organic molecules on the □Al2O3(0001) surface. **2022**, 12, 27604-27615	0
515	Binding of saturated and unsaturated C6-hydrocarbons to the electrophilic anion [B12Br11]□a systematic mechanistic study. **2022**, 24, 21759-21772	0
514	A high polarity poly(vinylidene fluoride-co-trifluoroethylene) random copolymer with an all-trans conformation for solid-state LiNi0.8Co0.1Mn0.1O2/lithium metal batteries. **2022**, 10, 18061-18069	3
513	An Ab Initio Computational Study of Binding Energies of Interstellar Complex Organic Molecules on Crystalline Water Ice Surface Models. **2022**, 281-292	0
512	Coronene-based quantum dots for the delivery of the doxorubicin anticancer drug: a computational study. **2022**, 46, 18518-18534	0
511	Uncovering the origins of supramolecular similarity in a series of benzimidazole structures. **2022**, 24, 6600-6610	0
510	Photo-induced reversible nitric oxide capture by Fe□M(CO2H)4 (M = Co, Ni, Cu) as a building block of mixed-metal BTC-based MOFs. **2022**, 24, 22859-22870	0
509	Structural systematics in isomorphous binary co-crystal solvates comprising 2,2?-dithiodibenzoic acid, 4-halobenzoic acid and dimethylformamide (1 : 1 : 1), for halide = chloride, bromide and iodide. **2022**, 24, 5907-5921	0
508	Crystal engineering of molecules with through-space □effect hydrogen bonds: 3a,6 : 7,9a-diepoxybenzo[de]isoquinolines possessing a free amino group. **2022**, 24, 6093-6100	0
507	Structure and IR spectroscopic properties of complexes of 1,2,4-triazole and 3-amino-1,2,4-triazole with dinitrogen isolated in solid argon. **2023**, 285, 121901	1
506	Analysis of Radial Cross Sections of the Potential Energy of the Interacting □□2 Complex. **2022**, 65, 403-409	0
505	Investigation of Non-Covalent Interactions of Copper (II) Complexes with Small Biomolecules.	0
504	Gallium (III) Complexes with 5-Bromosalicylaldehyde Benzoylhydrazones: In Silico Studies and In Vitro Cytotoxic Activity. **2022**, 27, 5493	1
503	Understanding the Interaction between Polybutadiene and Alumina via Density Functional Theory Calculations and Machine-Learned Atomistic Simulations. **2022**, 126, 16792-16803	1
502	Immobilized magnetic copper hydrazone complexes for oxidation of styrene to benzaldehyde by tert-butylhydroxyperoxide: an experimental and theoretical approach.	0
501	Theoretical study on the interaction between 3,4-dinitropyrazole and cyclotetramethylene tetranitramine.	0
500	Theoretical study of the interaction of fullerenes with the emerging contaminant carbamazepine for detection in aqueous environments. **2022**, 12,	0

499	Triel Bond Formed by Malondialdehyde and Its Influence on the Intramolecular H-Bond and Proton Transfer. **2022**, 27, 6091	0
498	Sensing of Acetaminophen Drug Using Silicon-Doped Graphdiyne: a DFT Inspection.	0
497	Probing the Directionality of S⋯O/N Chalcogen Bond and Its Interplay with Weak C–H⋯O/N/S Hydrogen Bond Using Molecular Electrostatic Potential.	0
496	Enantiomeric resolution of pidotimod and its isomers in pidotimod oral solutions by using HPLC QDa.	0
495	Thermodynamic and Computational (DFT) Study of Non-Covalent Interaction Mechanisms of Charge Transfer Complex of Linagliptin with 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) and Chloranilic acid (CHA). **2022**, 27, 6320	1
494	Exploring of spacer fluorination effect on the characteristics and physicochemical properties of the newly designed task specific dicationic imidazolium-based ionic liquids: A quantum chemical approach. **2022**, 261-262, 110026	0
493	Flipping Kinetics of the Water Trimer on Acenaphthylene: Persistence of a Highly Dipolar ddd Configuration at Interstellar Temperatures.	0
492	Intermolecular Interactions of Nucleoside Antibiotic Tunicamycin with On-Target MraYCB-TUN and Off-Target DPAGT1-TUN in the Active Sites Delineated by Quantum Mechanics/Molecular Mechanics Calculations. **2022**, 7, 32970-32987	0
491	Carbonaceous-Material-Induced Gelation of Concentrated Electrolyte Solutions for Application in Lithium–Sulfur Battery Cathodes.	0
490	Structural, vibrational and electronic properties of some tetrel-bonded complexes of the fluorinated methanes methyl fluoride, difluoromethane and fluoroform: an ab initio study. **2022**, 28,	0
489	A computational study on acetaminophen drug complexed with Mn+, Fe2+, Co+, Ni2+, and Cu+ ions: structural analysis, electronic properties, and solvent effects. **2022**, 28,	0
488	Enhancing Effects of the Cyano Group on the C-X⋯N Hydrogen or Halogen Bond in Complexes of X-Cyanomethanes with Trimethyl Amine: CH3–(CN)n–X⋯NMe3, (n = 0–3; X = H, Cl, Br, I). **2022**, 23, 11289	1
487	Weak interactions between epinephrine and thymine. **2022**, 19,	0
486	Explicitly Correlated Double-Hybrid DFT: A Comprehensive Analysis of the Basis Set Convergence on the GMTKN55 Database.	3
485	Size-dependent adsorption performance of ZnO nanoclusters for drug delivery applications.	0
484	Spectroscopy of Retinoic Acid at the Air–Water Interface. **2022**, 126, 6908-6919	1
483	Monolayer Silicon Carbide as an Efficient Adsorbent for Volatile Organic Compounds: An Ab Initio Approach.	0
482	Ar-Matrix Studies of the Photochemical Reaction between CS2 and ClF: Prereactive Complexes and Bond Isomerism of the Photoproducts. **2022**, 2, 765-778	0

481	CO2 Adsorption over 3d Transition-Metal Nanoclusters Supported on Pyridinic N3-Doped Graphene: A DFT Investigation. **2022**, 15, 6136	2
480	Computational Exploration of a Metal(II) Catecholate-Functionalized UiO-66 Nanoporous Metal□Organic Framework for Effective NOx Capture.	0
479	Structure of ethylammonium hydrogen sulfate protic ionic liquid through DFT calculations and MD simulations: the role of hydrogen bonds.	0
478	A theoretical investigation on the interaction mechanism between 1-methyl-3,4,5-trinitropyrazole and 1,3,5,7-Tetranitro-1,3,5,7-tetrazocane.	0
477	Computation of the Binding Energies between Human ACE2 and Spike RBDs of the Original Strain, Delta and Omicron Variants of the SARS-CoV-2: A DFT Simulation Approach. 2200337	0
476	Novel grafted hydrogel for Iron and ammonia removal from ground water, synthesis and computational chemistry study.	0
475	Sandwich, Triple-Decker and Other Sandwich-like Complexes of Cyclopentadienyl Anions with Lithium or Sodium Cations. **2022**, 27, 6269	0
474	Structural and Energetic Properties of Weak Noncovalent Interactions in Two Closely Related 3,6-Disubstituted-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole Derivatives: In Vitro Cyclooxygenase Activity, Crystallography, and Computational Investigations. **2022**, 7, 34506-34520	0
473	Unique Dispersion-Induced Tetrel Bond with Co-operative □hole-Induced Pnicogen Bond in the POCl3-Acetone Heterodimer: Experimental Confirmation at Low Temperatures. **2022**, 126, 6637-6647	0
472	Silicon-doped Boron Nitride Nanosheets for Enhanced Toxic Gas Sensing: An ab initio Approach.	0
471	An insight into interaction of the uracil, thymine and cytosine biomolecules with methimazole anti-thyroid drug: DFT and GD3-DFT approaches.	0
470	A full-dimensional ab initio potential energy surface and rovibrational spectra for the Ar□O2 complex. **2022**, 141,	0
469	Experimental and theoretical study of the effect of different functionalities of graphene oxide/polymer composites on selective CO2 capture. **2022**, 12,	0
468	DFT calculations, structural analysis, solvent effects, and non-covalent interaction study on the para-aminosalicylic acid complex as a tuberculosis drug: AIM, NBO, and NMR analyses. **2022**, 28,	0
467	Antioxidation activity of molecular hydrogen via protoheme catalysis in vivo: an insight from ab initio calculations. **2022**, 28,	0
466	Benchmarking PES-Learn's machine learning models predicting accurate potential energy surface for quantum scattering.	2
465	Properties and Stabilities of Cyclic and Open Chains of Halogen Bonds. **2022**, 126, 6443-6455	1
464	Theoretical Investigation on the Selective Hydroxyl Radical□nduced Decolorization of Methylene-Blue-Dyed Polymer Films. **2022**, 10, 169	0

463	Accurate Reproduction of Quantum Mechanical Many-Body Interactions in Peptide Main-Chain Hydrogen-Bonding Oligomers by the Polarizable Gaussian Multipole Model.	0
462	4-component relativistic Hamiltonian with effective QED potentials for molecular calculations.	0
461	Excitations and spectra from equilibrium real-time Green's functions. **2022**, 106,	0
460	Expanding the Knowledge of the Selective-Sensing Mechanism of Nitro Compounds by Luminescent Terbium Metal□Organic Frameworks through Multiconfigurational ab Initio Calculations. **2022**, 126, 7040-7050	0
459	Role of Metal Selection in the Radiation Stability of Isostructural M-UiO-66 Metal□Organic Frameworks. **2022**, 34, 8403-8417	2
458	The Effect of Surface Composition on the Selective Capture of Atmospheric CO2 by ZIF Nanoparticles: The Case of ZIF-8.	2
457	Tracking Topological and Electronic Effects on the Folding and Stability of Guanine-Deficient RNA G-Quadruplexes, Engineered with a New Computational Tool for De Novo Quadruplex Folding. **2022**, 23, 10990	0
456	Adsorption of Thiotepa anticancer drugs on the BC3 nanotube as a promising nanocarriers for drug delivery. **2022**,	0
455	-Comparison of □-hole aerogen-bonding interactions based on C2H4□NgOX2 (Ng = Kr, Xe; X = F, Cl, Br) complexes. **2022**, 28,	0
454	Theoretical probing into complexation of Si-5LIO-1-Cm-3,2-HOPO with Uranyl. **2022**, 141,	0
453	New task-specific ionic liquids based on phenyl diazenyl methyl pyridinium cation: Energetic, electronic and optical properties exploration based on DFT calculations. **2022**, 108352	0
452	Experimental and Theoretical Study on the Interactions between Dopamine Hydrochloride and Vitamin B6 Hydrochloride. **2022**, 96, 2299-2306	0
451	Alternating 1-Phenyl-2,2,2-Trifluoroethanol Conformational Landscape With the Addition of One Water: Conformations and Large Amplitude Motions.	1
450	Theoretical Study of the Structure and Binding Energies of Dimers of Zn(II)-Porphyrin Derivatives.	0
449	Supramolecular and theoretical investigation of copper(II) complexes containing 2,2?-bipyridine and substituted chalcone ligands: Estimation of non-covalent interactions. **2022**, 134271	0
448	Paracetamol adsorption on C60 fullerene and its derivatives: In silico insights. **2022**, 100769	0
447	Experimental and Theoretical Studies on the Interaction of Dopamine Hydrochloride with Nicotinic Acid.	0
446	Structures of the (Imidazole)nH+ ... Ar (n=1,2,3) complexes determined from IR spectroscopy and quantum chemical calculations.	0

445	Theoretical investigation for the reactions of hydrogen atom with dimethyl sulfide, ethyl methyl sulfide: Mechanism and kinetics properties. **2022**, 1217, 113893	0
444	Modelling the octanol-air partition coefficient of aromatic pollutants based on the solvation free energy and the dimer effect. **2022**, 309, 136608	0
443	I?N halogen bonding in 1 : 1 co-crystals formed between 1,4-diiodotetrafluorobenzene and the isomeric n-pyridinealdazines (n = 2, 3 and 4): assessment of supramolecular association and influence upon solid-state photoluminescence properties.	1
442	Highly stable and isomorphic donor□cceptor stacking in a family of n-type organic semiconductors of BTBT□□CNQ derivatives.	0
441	S66x8 noncovalent interactions revisited: new benchmark and performance of composite localized coupled-cluster methods. **2022**, 24, 25555-25570	1
440	Intermolecular amide and aldehyde interactions: rotational spectroscopy of the complexes of formaldehyde with 2-azetidinone and formamide.	1
439	Hydrogen bond networks in gas-phase complex anions. **2022**, 12, 29137-29142	0
438	Interplay of unique N...□pnicogen and H...□H...O hydrogen bonding interactions in the heterodimers of nitromethane with acetylene and benzene as □electron donors: Experimental characterization at low temperatures under isolated conditions with computational corroboration.	0
437	Coordination Polymers and molecular complexes of Group 13 Metal Halides with Bis-pyridylethane: comparison with rigid N-containing ligands.	0
436	Metalloborospherenes with a Stabilized Classical Fullerene-Like Borospherene B36 as Electric Field Manipulated Second-Order Nonlinear Optical Switches.	0
435	Enhancement of tetrel bond involving tetrazole-TtR3 (Tt = C, Si; R = H, F). Promotion of SiR3 transfer by a triel bond. **2022**, 24, 25895-25903	0
434	Reduced nucleophilicity: an intrinsic property of the Lewis base atom interacting with H in hydrogen-bonds with Lewis acids HX (X = F, Cl, Br, I, CN, CCH, CP). **2022**, 24, 25822-25833	1
433	Involvement of Arsenic Atom of AsF3 in Five Pnicogen Bonds: Differences between X-ray Structure and Theoretical Models. **2022**, 27, 6486	1
432	Dual-Ligand Strategy Employing Rigid 2,5-Thiophenedicarboxylate and 1,10-Phenanthroline as Coligands for Solvothermal Synthesis of Eight Lanthanide(III) Coordination Polymers: Structural Diversity, DFT Study, and Exploration of the Luminescent Tb(III) Coordination Polymer as an Efficient Chemical Sensor for Nitroaromatic Compounds.	1
431	Probing the Structure□Property Relationships of Na+□□Cl@C50N5H5 under the External Electric Field.	0
430	The Bonding Nature of Fe□O Complexes in Heme Proteins.	0
429	Electronic fingerprint mechanism of NOx sensor based on single-material SnP3 logical junction. **2022**, 8,	0
428	Crystal Structure Survey and Theoretical Analysis of Bifurcated Halogen Bonds. **2022**, 22, 6521-6530	1

427	Why Is β-d-Glucose Monomorphic? Insights from Accurate Experimental Charge Density at 90 K. **2022**, 22, 6627-6638	0
426	Systematic Evaluation of Counterpoise Correction in Density Functional Theory.	3
425	Insight into the nature of the noncovalent interactions of furan, pyridine and pyrazine with AtX.	0
424	Hydrogen Bonding in Crystals of Pyrrol-2-yl Chloromethyl Ketone Derivatives and Methyl Pyrrole-2-Carboxylate. **2022**, 12, 1523	0
423	Structural properties of Hachimoji nucleic acids and their building blocks: Comparison of genetic systems with four, six and eight alphabets.	0
422	Efficient synthesis of new azo-sulfonamide derivatives and investigation of their molecular docking and cytotoxicity results. **2022**, 104383	1
421	Effects of Lewis Basicity and Acidity on π-Hole Interactions in Carbon-Bearing Complexes: A Comparative Ab Initio Study. **2022**, 23, 13023	0
420	Does DFT work for H□2O and H2S dimers?.	0
419	Be2C monolayer as an efficient adsorbent of toxic volatile organic compounds: theoretical investigation.	0
418	Interaction of the Silver(I) Cation with [2.2]Paracyclophane: Experimental and Theoretical Study. **2022**, 7,	0
417	Zigzag direction nanoarchitectonics of monolayer GeSe for SO2 gas sensors with high sensitivity and selectivity: a first-principles study. **2022**, 128,	0
416	Structural modeling, energetic analysis and molecular design of a π-stacking system at the complex interface of pediatric respiratory syncytial virus nucleocapsid with the C-terminal peptide of phosphoprotein. **2022**, 106916	0
415	Dicationic ionic liquids (DILs) based on the phenyl and perfluoro-phenyl π-spacer-linked triazolium cations: a quantum chemical comparative study. **2022**, 141,	0
414	Binding Energies of Interstellar Relevant S-bearing Species on Water Ice Mantles: A Quantum Mechanical Investigation. **2022**, 938, 158	0
413	Presentation of the simple and accurate models for estimating the individual hydrogen bond energies of Watson□rick base pairs.	0
412	Structure-Directing Interplay between Tetrel and Halogen Bonding in Co-Crystal of Lead(II) Diethyldithiocarbamate with Tetraiodoethylene. **2022**, 23, 11870	0
411	Selectively Identifying Exposed-over-Unexposed C□+ Pairs in Human Telomeric i-Motif Structures with Length-Dependent Polymorphism. **2022**, 94, 14994-15001	0
410	Sulfur/Polyacrylonitrile-Based N-Terminated Graphene Nanoribbon Cathodes for Li-S Batteries. **2022**, 18,	0

409	Enhancing NO Uptake in Metal-Organic Frameworks via Linker Functionalization. A Multi-Scale Theoretical Study. **2022**, 4, 1300-1311	1
408	Research on the adsorption of environmentally friendly insulating gas C 4 F 7 N decomposed components on the surface of Al 2 O 3.	0
407	Polychlorinated Biphenyls Interactions with Water Characterization Based on the Analysis of Non-Covalent Interactions and Energy Partitioning. **2022**, 14, 12529	0
406	Scissor-like Face to Face Stacking: A Surprising Preference Induced by the Isocyano Group in the Self-Assembled Dimer of Phenyl Isocyanide. **2022**, 13, 9934-9940	1
405	Molecular Recognition of FDA-Approved Small Molecule Protein Kinase Drugs in Protein Kinases. **2022**, 27, 7124	0
404	Hydrogen-Bonding Motifs in Adducts of Allylamine with the 10 Simplest n-Alcohols: Single-Crystal X-ray Diffraction Studies and Computational Analysis. **2022**, 22, 6405-6417	0
403	Sugar-Based Phase-Selective Supramolecular Self-Assembly System for Dye Removal and Selective Detection of Cu2+ Ions. **2022**, 7, 39310-39324	0
402	Open-cage Fullerene as Molecular Container for F-, Cl-, Br- and I-.	2
401	Open-cage Fullerene as Molecular Container for F-, Cl-, Br- and I-.	0
400	Complexes of carbon dioxide with methanol and its monohalogen-substituted: beyond the tetrel bond. **2022**, 140158	0
399	Experimental and theoretical investigation into the response to shock wave for booster explosives JO9C, JH14, JH6, and insensitive RDX. **2022**, 28,	0
398	Hydration Structure of Na+ and K+ Ions in Solution Predicted by Data-Driven Many-Body Potentials.	0
397	Continuous absorption and emission of light by the heteronuclear rare gas (ArXe)+ and (KrXe)+ ions.	1
396	Ab initio studies on complexes of ozone with triatomic and larger molecules.	0
395	Prediction of Multiple Hydrogen Ligation at a Vanadium(II) Site in a Metal Organic Framework. 10471-10478	2
394	The role of water and acid catalysis in the reaction of acetone with hydrogen peroxide: A DFT study. **2022**, 1217, 113908	0
393	A NMR hybrid J-coupling alternation (hJCA) parameter linearly correlated to properties of intermolecular H-bonded chains. **2022**, 1217, 113913	0
392	A stability analysis of choline chloride: urea deep eutectic solvent using density functional theory. **2022**, 1217, 113921	0

391	Harnessing molecular isomerization in polymer gels for sequential logic encryption and anticounterfeiting. **2022**, 8,	1
390	How to Stabilize Carbenes in Enzyme Active Sites without Metal Ions.	1
389	Computational Investigation of the conformer selective complexes of 1,2,3,4-tetrahydroisoquinoline: ammonia (THIQ: NH3) in S0. **2022**, 134475	0
388	Liquid-liquid equilibrium and insights of intermolecular interactions for separation of isopropyl acetate + isopropanol by imidazolium-based ionic liquids. **2022**, 140, 104571	0
387	Structural microheterogeneity and hydrogen bonding properties in the mixtures of two ionic liquids with a common imidazolium cation. **2022**, 368, 120594	0
386	A novel sustained-release formulation of 5-fluorouracil-phenylalanine cocrystal self-assembled by cocrystal-entrapped micelle strategy displays enhanced antitumor efficacy. **2022**, 368, 120665	0
385	Functionalized maghemite nanoparticles for enhanced adsorption of uranium from simulated wastewater and magnetic harvesting. **2023**, 216, 114569	0
384	Investigation of non-covalent interactions in Polypyrrole/Polyaniline/Carbon black ternary complex for enhanced thermoelectric properties via interfacial carrier scattering and π-stacking. **2023**, 630, 46-60	0
383	Integrated in silico-in vitro molecular modeling and design of halogenated phenylalanine-containing antihypertensive peptide inhibitors with halogen bonds to target human angiotensin-I-converting enzyme. **2023**, 565, 111732	0
382	The molecular nature of the eliminating azeotropy of dimethyl carbonate–ethanol system by ionic liquid entrainer. **2023**, 305, 122420	0
381	Efficient separation of methane, ethane and propane on mesoporous metal-organic frameworks. **2023**, 453, 139642	1
380	Spectroscopic and molecular simulation studies on the interaction of imazaquin herbicide with cucurbiturils (n = 6, 8). **2023**, 1274, 134444	0
379	Comparative DFT-D3 assessment of fluorogenic supramolecular interaction of naphthalene moiety location on new dibenzodiaza-crown ether macrocycles with C60. **2023**, 1273, 134343	0
378	The organic co-crystal formed by naphthalenediimide-based triangular macrocycle and coronene: intermolecular charge transfers and nonlinear optical properties.	1
377	Molecular Self-Assembly of DBBA on Au(111) at Room Temperature.	0
376	Non-covalent Bonds in Group 1 and Group 2 Elements: The "Alkalene bond"	0
375	Examining the gas-phase homodimers of 3,3,3-trifluoro-1,2-epoxypropane using quantum chemistry and microwave spectroscopy.	0
374	Modular Synthesis, Host-Guest Complexation and Solvation-Controlled Relaxation of Nanohoops with Donor-Acceptor Structures.	0

373	Accuracy of quantum chemistry structures of chiral tag complexes and the assignment of absolute configuration.	0
372	Impacts of noncovalent interactions involving sulfur atoms on protein stability, structure, folding, and bioactivity.	1
371	Adjusting the Balance between Hydrogen and Chalcogen Bonds.	1
370	Mitigating cerium migration for perfluorosulfonic acid membranes using organic ligands. **2023**, 554, 232320	0
369	Ab initio study on the singlet states of Zn-RG (RG□=□He, Ne, Ar, Kr, Xe, Rn) molecules. **2023**, 287, 122091	0
368	A Computational Characterization of 2,2?-bis(trifluoromethyl)-[1,1?-biphenyl]-4,4?-diamine Iodine Dopant for Improving Power-Conversion Efficiency of Perovskite Solar Cells. **2022**, 11, 111001	0
367	Solvent effects on the photooxidation of indolepyrazines.	0
366	Functionalized electrodes embedded in nanopores: read-out enhancement?.	0
365	Crystal structure, vibration spectra, antibacterial and non-linear optical properties of a picrate based on triphenylphosphinium dication. **2022**, 134552	0
364	Elastic and glancing-angle rate coefficients for heating of ultracold Li and Rb atoms by collisions with room-temperature noble gases, H2, and N2.	1
363	Comparative study on adsorption of volatile organic compounds on graphene, boron nitride and boron carbon nitride nanosheets. **2022**, 115021	0
362	The Influence of the Halide in the Crystal Structures of 1-(2,3,5,6-Tetrafluoro-4-pyridyl)-3-benzylimidazolium Halides. **2022**, 27, 7634	0
361	Chalcogen Bond as a Factor Stabilizing Ligand Conformation in the Binding Pocket of Carbonic Anhydrase IX Receptor Mimic. **2022**, 23, 13701	2
360	Alkali-Metal-Free Coinage Metalides: Specific Pairing and Location of Doping Atoms Bring Forth High Stability and Considerable Nonlinear Optical Response.	0
359	Study on Gas Chromatography Retention Time Variation of Acetic Acid Combined with Quantum Chemical Calculation.	0
358	Oligomer formation from the gas-phase reactions of Criegee intermediates with hydroperoxide esters: mechanism and kinetics. **2022**, 22, 14529-14546	1
357	Superefficient separation of HFC-245fa/HF using extractive distillation: from computational thermodynamics to process assessment. **2022**, 122663	0
356	Ab initio relativistic potential energy surface with analytical long-range part of benzene-Rn complex and its application to intermolecular vibrations. **2022**, 111756	0

355	Association Complexes of Calix[6]arenes with Amino Acids Explained by Energy-Partitioning Methods. **2022**, 27, 7938	1
354	Quantum Chemical Investigation on Hydrolysis of Orally Active Organometallic Ruthenium(II) and Osmium(II) Anticancer Drugs and Their Interaction with Histidine.	0
353	Perfluoropropionic Acid-Driven Nucleation of Atmospheric Molecules under Ambient Conditions. **2022**, 126, 8449-8458	0
352	Torsional Tunneling Splitting in a Water Trimer.	0
351	Adsorption behavior and sensing properties of toxic gas molecules onto PtnBe (n=5, 7, 10) clusters: A DFT benchmark study. **2022**, 33, 104851	0
350	Sensing behavior of porous B6N6 boron nitride covalent organic framework toward cathinone drugs: A DFT study. **2022**, 146, 110205	0
349	Order versus Disorder in the Cocrystals of m-Halogenopyridines with m-Halogenobenzoic Acids: The Effects of the I···O Halogen Bond.	0
348	In-silico and in-detail experimental interaction studies of new antitumor Zn(II) complex with CT-DNA and serum albumin. 1-18	0
347	Controlling the Polymorphism of Indomethacin with Poloxamer 407 in a Gas Antisolvent Crystallization Process.	0
346	Chelidamic acid tautomers in copper(II) compounds. One-pot synthesis, crystal structure, spectroscopic and DFT studies. **2022**, 116210	0
345	The binding affinity of human pediatric respiratory syncytial virus Phosphoprotein's C-terminal tail to nucleocapsid can be improved by a rationally designed halogen-bonded system. **2023**, 118, 108374	0
344	Sebaceous gland-inspired self-lubricated de-icing coating by continuously secreting lubricants. **2023**, 174, 107311	0
343	Design of a Zr-based metal□organic framework as an efficient fosfomycin carrier: a combined experimental and DFT study.	0
342	Theoretical investigations of functionalization of graphene and ZnO monolayers with mercaptopurine at aqueous media: A dispersion-corrected DFT calculations and molecular dynamic simulations. **2023**, 369, 120865	1
341	Role of OH?O/S conventional hydrogen bonds in considerable Csp2H blue-shift in the binary systems of acetaldehyde and thioacetaldehyde with substituted carboxylic and thiocarboxylic acids. **2022**, 12, 35309-35319	0
340	A critical comparison of CH versus interactions in the benzene dimer: obtaining benchmarks at the CCSD(T) level and assessing the accuracy of lower scaling methods.	0
339	Theoretical investigation of C1C4 hydrocarbons adsorption and separation in a porous metallocavitand. **2022**, 12, 34053-34065	0
338	Exploration of Cl l and stacking contacts along with conductivity properties of a Cu-MOF featured with paddle-wheel SBUs.	0

337	Polymorphism in carboxamide compounds with high-Z? crystal structures.	0
336	Predicting adsorption behavior of Triacanthine anticancer drug with pure B12N12 nano-cage: A theoretical study. **2023**, 100, 100812	0
335	Modified lithium metal anode via anions-planting protection mechanisms for dendrite-free long-life lithium metal batteries.	0
334	Theoretical investigation on intermolecular interactions, co-crystal structure, thermal decomposition mechanism, and shock properties of 3-nitro-1,2,4-triazol-5-one (NTO) and ammonium perchlorate.	0
333	Revealing the supramolecular features of two Zn(II) complexes derived from a new hydrazone ligand: A combined crystallographic, theoretical and antibacterial study.	0
332	Thermophysical modelling of transport and optical properties of 1-propanol+1,3-diaminopropane or 1,2-diaminopropane or 1-amino-2-propanol binary liquid mixture at T=298.15-318.15 K: Molecular interaction analysis by density functional theory (DFT) and graph theoretical approach (GTA). **2023**, 142, 104641	0
331	Synthesis, structural characterization and DFT study of N-(pyrimidyl)-□amino acids/peptide: □alanine, □aminobutyric acid, 5-aminovaleric acid, 6-aminohexanoic acid and glycylglycine.	0
330	Guanidinium□mino acid hydrogen-bonding interactions in protein crystal structures: implications for guanidinium-induced protein denaturation. **2022**, 25, 857-869	0
329	Atoms in molecules theory, electrostatic potential surface and frontier molecular orbital analyses on water multimers and pyridine □Water hydrogen bonded complexes. **2023**, 1219, 113960	0
328	Theoretical investigation of intermolecular interactions between CNT, SiCNT and SiCGeNT nanomaterials with vinyl chloride molecule: A DFT, NBO, NCI, and QTAIM study. **2023**, 131, 109602	0
327	Enclathration of Mn(II)(H2O)6 guests and unusual Cu?O bonding contacts in supramolecular assemblies of Mn(II) Co-crystal hydrate and Cu(II) Pyridinedicarboxylate: Antiproliferative evaluation and theoretical studies. **2023**, 230, 116243	0
326	Large 31P-NMR enhancements in liquid state dynamic nuclear polarization through radical/target molecule non-covalent interaction. **2022**, 25, 822-828	0
325	Character of intermolecular vibrations in the benzene□eon complex based on CCSD(T) and SAPT potential energy surfaces. **2022**, 25, 419-427	0
324	Spodium bonding to anticrown-Hg3 boosts phosphorescence of cyclometalated-PtII complexes.	0
323	Theoretical study of hydrogen bond interactions of methanesulfonic acid with eugenol/methyleugenol. **2023**, 1219, 113977	0
322	Electronic structures of zwitterionic and protonated forms of glycine betaine in water: Insights into solvent effects from ab initio simulations. **2023**, 369, 120871	0
321	Microcrystal Electron Diffraction (MicroED) Structure Determination of a Mechanochemically Synthesized Co-crystal not Affordable from Solution Crystallization.	0
320	The van der Waals interactions in systems involving superheavy elements: the case of oganesson (Z = 118). **2022**, 25, 633-645	0

319	High drug carrying efficiency of boron-doped Triazine based covalent organic framework toward anti-cancer tegafur; a theoretical perspective. **2023**, 1220, 113990	0
318	Density functional theory study of the sensing of ozone gas molecules by using fullerene-like Group-III nitride nanostructures. **2023**, 650, 414553	0
317	Selective sensing of DNA/RNA nucleobases by metal-functionalized silicon nanowires: A DFT approach. **2023**, 36, 102529	0
316	A comparative study on the physicochemical properties of the nanostructured triazolium based ionic liquids composed of [5F-PhMTZ]+ cation and various anions with their non-fluorinated cation analogues. **2023**, 1220, 113984	0
315	The Cd-decorated AlN nanotube as a potential chemical sensor for chloropicrin: DFT studies. **2023**, 1220, 113982	0
314	Effects of mesylate-/tartrate-based ionic liquids-water mixtures on the phase transition behaviors and stability of corn starch: A comparative study. **2023**, 303, 120456	0
313	Molecular simulation investigations on interaction properties of the teriflunomide□chitosan complex in aqueous solution. **2023**, 174, 111171	1
312	Adsorption behavior of methylene blue on graphene and hexagonal boron nitride monolayers in aqueous solution: A first-principles treatment. **2023**, 174, 111151	0
311	Hydrogen bond interactions between thioethers and amides: A joint rotational spectroscopic and theoretical study of the formamide?dimethyl sulfide adduct. **2023**, 288, 122199	0
310	Fragmentation modeling of gas-phase ionic liquid clusters in high-voltage electric field. **2023**, 335, 126919	0
309	S66 noncovalent interactions benchmark re-examined: Composite localized coupled cluster approaches. **2022**,	1
308	Hydrogermylation initiated by trialkylborohydrides: a living anionic mechanism. **2022**, 58, 13979-13982	1
307	Self-diffusion and molecular association in the binary systems dimethyl sulfoxide □chloroform and acetone □chloroform. **2022**, 4, 100673	0
306	The importance of tetrel bonding interactions with carbon in two arrestive iso-structural Cd(ii)Salen coordination complexes: a comprehensive DFT overview in crystal engineering. **2022**, 12, 35860-35872	0
305	DFT and COSMO-RS studies on dicationic ionic liquids (DILs) as potential candidates for CO2 capture: the effects of alkyl side chain length and symmetry in cations. **2022**, 12, 35418-35435	0
304	Solvent effects on catechol□ binding af□ity: investigating the role of the intra-molecular hydrogen bond through a computational multi-level approach..	0
303	Alkali metal□methyl short contacts in aluminates: more than agostic interactions.	0
302	Cu(II)-Based Molecular Hexagons Forming Honeycomb-like Networks Exhibit High Electrical Conductivity. **2022**, 61, 19828-19837	0

301	Influence of the metal□support and metal□metal interactions on Pd nucleation and NO adsorption in a Pd4/□Al2O3 (110D) model. **2022**, 28,	0
300	Synthesis and Computational and X-ray Structure of 2, 3, 5-Triphenyl Tetrazolium, 5-Ethyl-5-phenylbarbituric Acid Salt. **2022**, 12, 1706	1
299	How Does Spin Play with the Cycloaddition to Paramagnetic Endohedral Metallofullerenes? The Curious Case of TiSc2N@C80. **2022**, 61, 19183-19192	0
298	Structural, electronic, and nonlinear optical properties of small silver clusters doped graphyne and pyrazine-modified graphyne: A computational and comparative study.	0
297	[3 + 2]-Cycloadditions with Porphyrin π-Bonds: Theoretical Basis of the Counterintuitive meso-Aryl Group Influence on the Rates of Reaction. **2022**, 87, 16473-16482	0
296	The interaction mechanism of polystyrene microplastics with pharmaceuticals and personal care products. **2022**, 160632	0
295	Spin-Polarized Resonant Tunneling in Antiferromagnetic Heterojunctions of Graphene Nanoribbons with 3d Adatoms. **2022**, 18,	0
294	Theoretical insight into the acidity and cooperativity effect of the LLM-105□(HNO3)2 system. **2022**, 28,	0
293	QUANTUM CHEMICAL SIMULATION OF 2,4,7-TRINITRO-9H-FLUORENE-9-ONE CHARGE-TRANSFER COMPLEXES WITH NONLINEAR POLYCYCLIC AROMATIC HYDROCARBONS. CRYSTAL AND MOLECULAR STRUCTURE OF THE (1:1) 2,4,7-TRINITRO-9H- FLUORENE-9-ONE COMPLEX WITH PHENANTHRENE. **2022**, 63, 1758-1769	0
292	Quantum mechanical study on complexation phenomenon of pillar[5]arene towards neutral dicyanobutane. 1-13	0
291	Efficient Computation of the Interaction Energies of Very Large Non-covalently Bound Complexes.	0
290	Occurrence and stability of anion□interactions between phosphate and nucleobases in functional RNA molecules. **2022**, 50, 11455-11469	0
289	A Theoretical Study of the Halogen Bond between Heteronuclear Halogen and Benzene. **2022**, 27, 8078	1
288	An Embedded Fragment Method for Molecules in Strong Magnetic Fields. **2022**, 18, 7412-7427	0
287	Gold(I)⋯Lanthanide(III) Bonds in Discrete Heterobimetallic Compounds: A Combined Computational and Topological Study. **2022**, 61, 20308-20315	0
286	Supramolecular Diversity, Theoretical Investigation and Antibacterial Activity of Cu, Co and Cd Complexes Based on the Tridentate N,N,O-Schiff Base Ligand Formed In Situ. **2022**, 27, 8233	0
285	Ability of Peripheral H Bonds to Strengthen a Halogen Bond.	1
284	Enantiomeric Resolution of Pidotimod and Its Isomers in Pidotimod Oral Solutions Using Chiral RP-HPLC with Quadrupole Dalton Analyzer Detection.	0

283	Energy property and covalency of H2S□X (X = N2, CO, CS and SiO) hydrogen bond. **2023**, 98, 015407	0
282	Adsorption of thioindole as a biologically active anti-cancer to C 20 fullerene in different reaction media using density functional theory.	0
281	Weak Interactions between Poly(ether imide) and Carbon Dioxide: A Multiscale Investigation Combining Experiments, Theory, and Simulations. **2022**, 55, 10773-10787	1
280	Development of accurate potentials for the physisorption of water on graphene.	0
279	Role of Different Solvents and Tailor-Made Additives in Asymmetry in Growth Rates along the Opposite Ends of the Polar Axis: The Riddle of □Resorcinol.	0
278	Tetrafluorosubstituted Metal Phthalocyanines: Study of the Effect of the Position of Fluorine Substituents on the Chemiresistive Sensor Response to Ammonia. **2022**, 10, 515	1
277	One-dimensional nanospace confinement effects on the chemical properties of organic molecules in carbon nanotubes: Quantum chemical calculation analyses. **2022**, 1, 175-187	0
276	Can the Fluxionality in Borospherene Influence the Confinement-Induced Bonding between Two Noble Gas Atoms?. **2022**, 27, 8683	0
275	Suppressing Deep Oxidation by Detached Nano-sized Boron Oxide in Oxidative Dehydrogenation of Propane Revealed by the Density Functional Theory Study. **2022**, 126, 21263-21271	0
274	Effects of Atypical Hydrogen Bonds and □Interactions on Nonlinear Optical Properties: Dimers of Triangular Structures Based on Perylene, Naphthalene, and Pyromellitic Diimides.	1
273	Tetrel Bonding in Anion Recognition: A First Principles Investigation. **2022**, 27, 8449	1
272	Polarizable Molecular Block Model: Toward the Development of an Induced Dipole Force Field for DNA. **2022**, 126, 10646-10661	0
271	Triel Bonds with Au Atoms as Electron Donors.	0
270	A first principles study of nonlinear optical properties of a quinoline derivative.	0
269	Separation of ethyl acetate and ethanol by imidazole ionic liquids based on mechanism analysis and liquid-liquid equilibrium experiment. **2022**, 121108	0
268	S□□O Hydrogen Bond Can Win over O□□S Hydrogen Bond: Gas-Phase Spectroscopy of 2-Fluorothiophenol□□H2O Complex. **2022**, 126, 9178-9189	0
267	A Cost Effective Scheme for the Highly Accurate Description of Intermolecular Binding in Large Complexes. **2022**, 23, 15773	0
266	Investigating the effect of structural antisite defects on the adsorption and detection of ozone gas by AlP nanotubes.	0

265	Abnormalities of the Halogen Bonds in the Complexes between Y2CTe (Y = H, F, CH3) and XF (X = F, Cl, Br, I). **2022**, 27, 8523	0
264	Accurate geometry and non-covalent interactions in 1-phenylethanol and its monohydrate: A rotational study.	0
263	On structure and properties of tripropylammonium-based protic ionic liquids with bis(trifluoromethylsulfonyl)imide and hydrogen sulfate anions.	0
262	The intermolecular interactions of ammonia with chlorine and bromine oxides: a theoretical study. **2023**, 29,	0
261	Metal chelation ability of Protocatechuic acid anion with 210Po84; A theoretical insight. **2022**, 113996	1
260	Exploring the Dynamical Nature of Intermolecular Hydrogen Bonds in Benzamide, Quinoline and Benzoic Acid Derivatives. **2022**, 27, 8847	1
259	Metallocenes and Beyond for Propene Polymerization: Energy Decomposition of Density Functional Computations Unravels the Different Interplay of Stereoelectronic Effects. **2022**, 41, 3872-3883	0
258	Theoretical and experimental exploration for efficient separation of carbazole from anthracene oil with quaternary ammonium salts via forming deep eutectic solvents. **2022**, 368, 120831	0
257	MoBioTools : A toolkit to setup quantum mechanics/molecular mechanics calculations.	0
256	Behavior of HF and (HF) 2 inside a fullerene cage: An in silico study using different density functionals.	0
255	A Computational Perspective on the Chemical Reaction of HFO-1234zc with the OH Radical in the Gas Phase and in the Presence of Mineral Dust.	0
254	Interaction of CH3CN and CH3NC with He: Potential Energy Surfaces and Low-Energy Scattering.	0
253	Reactions of Thorium Oxide Clusters with Water: the Effects of Oxygen Content.	0
252	Quantum-Chemical Study of Acid□Base Interaction between Alkylamines and Different Br□sted Acids. **2022**, 96, 2704-2711	0
251	Cross Second Virial Coefficients of the H2O□H2S and H2O□SO2 Systems from First Principles.	0
250	From Induced-Fit Assemblies to Ternary Inclusion Complexes with Fullerenes in Corannulene-Based Molecular Tweezers. **2022**, 87, 16691-16706	0
249	X-ray Structures and Computational Studies of Two Bioactive 2-(Adamantane-1-carbonyl)-N-substituted Hydrazine-1-carbothioamides. **2022**, 27, 8425	0
248	Insight into the nature of the noncovalent interactions of furan, pyridine, and pyrazine with AtX. **2023**, 29,	0

247	Highly sensitive amphetamine drug detection based on silicon nanowires: Theoretical investigation. **2022**, 102584	0
246	Diffuse Basis Functions for Relativistic s and d Block Gaussian Basis Sets.	0
245	Chitosan Dextran phosphate carbamate hydrogels for locally controlled co-delivery of doxorubicin and indomethacin: From computation study to in vivo pharmacokinetics. **2022**,	0
244	Atomically precise binding conformations of adenine and its variants on gold using single molecule conductance signatures. **2022**, 157, 234201	0
243	A Tetranuclear Ni(II)-Cubane Cluster Molecule Build by Four μ3-O-Methanolate (MeO) Ligands, Externally Cohesive by Four Unprecedented Bridging μ2-N7,O6-Acyclovirate (acv-H) Anions. **2023**, 13, 7	0
242	CO2 Capture Using Dicationic Ionic Liquids (DILs): Molecular Dynamics and DFT-IR Studies on the Role of Cations.	0
241	Rotational State-to-State Rate Coefficients of HeHNe+ by Collision with He at Low Temperatures.	0
240	Influence of adsorption of gold and silver nanoclusters on structural, electronic, and nonlinear optical properties of pentacene-5,12-dione: a DFT study. **2023**, 55,	0
239	Understanding the impact of halogen functional group (Br, Cl, F, OH) in amprenavir ligand of the HIV protease. 1-14	0
238	Modeling coarse-grained van der Waals interactions using dipole-coupled anisotropic quantum Drude oscillators.	0
237	Quantitative Descriptions of Dewar-Chatt-Duncanson Bonding Model: A Case Study of Zeise and Its Family Ions.	0
236	Periodic trends in the hydration energies and critical sizes of alkaline earth and transition metal dication water complexes.	0
235	Factors contributing to halogen bond strength and stretch or contraction of internal covalent bond.	1
234	Structural and Energetic Features of BaseBase Stacking Contacts in RNA.	0
233	Insights into the interactions between cellulose and biological molecules. **2023**, 523, 108738	0
232	Benchmarking Two-Body Contributions to Crystal Lattice Energies and a Range-Dependent Assessment of Approximate Methods.	0
231	Explicitly correlated six-dimensional potential energy surface for the SiCSi+H2 complex.	0
230	Computational insight into a mechanistic overview of water exchange kinetics and thermodynamic stabilities of bis and tris-aquated complexes of lanthanides. **2023**, 13, 1516-1529	0

229	Deciphering electronic and structural effects in Copper Corrole/Graphene Hybrids.	0
228	Fine-structure excitation of CCS by He: Potential energy surface and scattering calculations.	0
227	Enhanced hydrogen storage performance of Li and Co functionalized h-GaN nanosheets: DFT study. **2023**, 108415	0
226	Structural, electronic and nonlinear optical properties, reactivity and solubility of the drug dihydroartemisinin functionalized on the carbon nanotube. **2023**, 9, e12663	1
225	Molecular insights into the functionalization of Au13 nanocluster with mercaptopurine anti-cancer drug. **2023**, 414547	0
224	Collective stabilization through n-π and P□phosphorous bonding with cooperative halogen and hydrogen bonding in POCl3-Nitrile dimers: Matrix isolation infrared spectroscopic and ab initio computational studies. **2023**, 134916	0
223	Cocrystals assembled from iodoperfluorobenzene and flexible NTPO via halogen and □hole bonds. **2023**, 79,	0
222	Accurate calculation of the interaction of a barium monofluoride molecule with an argon atom: A step towards using matrix isolation of BaF for determining the electron electric dipole moment. **2023**, 391, 111736	0
221	Conformational Landscape and Hydrogen Bonding Pattern of Psilocin: Computational Insights. **2023**, 8,	0
220	MP2 study of the adsorption of CO2 onto the water monomer, dimer and trimer. **2023**, 142,	0
219	Stepwise Hydrations of Anhydride Tuned by Hydrogen Bonds: Rotational Study on Maleic Anhydride-(H2O)1-3.	0
218	Hydrogen-bonding interactions involving the Imidazol-2-ylidene and its Heavy-atom analogues. **2023**, 1220, 114020	1
217	The role of nature of aromatic ring on cooperativity between □stacking and ion□interactions: A computational study. **2023**, 1220, 114022	0
216	Structural analysis and electronic properties of transition metal ions (Ni2+, Fe2+, Mn+ and Co+) with psoralen biomolecule as an anticancer drug. **2023**, 986, 122606	0
215	An ab initio study of the structural, vibrational and electronic properties of some tetrel-bonded complexes of methane and tetrafluoromethane. **2023**, 1220, 114021	0
214	Exploring the adsorption behavior of pyrazinamide on the surface of X12Y12(X□=□B, Al; Y□=□N, P) nanocages: A in-silico study. **2023**, 372, 121211	0
213	Simultaneous square wave voltammetry detection of azo dyes using silver nanoparticles assembled on carbon nanofibers. **2023**, 441, 141782	0
212	Mechanistic insights into the adsorption of endocrine disruptors onto polystyrene microplastics in water. **2023**, 319, 121017	0

211	Helical coordination complex of Hg(ClO4)2 with bulky hydrazone derivative: A Möbius-like discrete metal chelate. **2023**, 149, 110393	0
210	The spectroscopic and transition properties of ZnHe: MRCI+Q study including spin-orbit coupling. **2023**, 297, 108482	0
209	Synthesis of phenazone based carboxamide under thiourea reaction conditions. Molecular and crystal structure, Hirshfeld surface analysis and intermolecular interaction energies. **2023**, 1278, 134948	0
208	Application of facilitated transfer mechanisms of SEBS/[P(14)666][TMPP] composite membrane on CH4/N2 separation. **2023**, 11, 109243	0
207	Bacterial nanocellulose and long-chain fatty acids interaction. **2022**, 10, 218-249	0
206	Interaction energy of Cl 2 and Br 2 with H 2 O : Exchange, dispersion and density the crucial ingredients.	0
205	The Pincer Ligand Supported Ruthenium Catalysts for Acetylene Hydrochlorination: Molecular Mechanisms from Theoretical Insights. **2023**, 13, 31	0
204	Origin of Catalysis by Nitroalkane Oxidase. **2023**, 127, 151-162	0
203	Theoretical Strategies for Functionalisation and Encapsulation of Nanotubes. **2011**, 225-278	0
202	Calculation of the Transport and Relaxation Properties of the Ar–HCl van der Waals Complex Using a New Potential Energy Surface: Comparison of the Classical and Full Quantum Mechanical Kinetic Theory Results with Molecular Dynamics Simulations. **2023**, 127, 1053-1067	0
201	Graphene oxide and flavonoids as potential inhibitors of the spike protein of SARS-CoV-2 variants and interaction between ligands: a parallel study of molecular docking and DFT.	0
200	Rotational Excitation of NCCN by p-H2(jc = 0) at Low Temperatures.	0
199	The Effect of Counterions on the Detection of Cu2+ Ions in Aqueous Solutions Using Quartz Tuning Fork (QTF) Sensors Modified with L-Cysteine Self-Assembled Monolayers: Experimental and Quantum Chemical DFT Study. **2023**, 11, 88	0
198	Selective and Efficient Synthesis of Pine Sterol Esters Catalyzed by Deep Eutectic Solvent. **2023**, 28, 993	0
197	A Formulation of the Many-Body Expansion (MBE) for Periodic Systems: Application to Several Ice Phases. **2023**, 14, 989-999	0
196	Open-Cage Fullerene as a Selective Molecular Trap for LiF/[BeF]+.	0
195	Intermolecular interactions between the heavy-atom analogues of acetylene T2H2 (T = Si, Ge, Sn, Pb) and HCN. **2023**, 29,	1
194	Computational and experimental studies on the micellar morphology and emission mechanisms of AIE and H-bonding fluorescent composites. **2023**, 13, 4612-4622	0

193	Two- and Three-Directional Synthesis by 3-7MCRs of Novel (Imidazolidine/Thiazolidine)-2,4-Diones: Characterization, Antibacterial, Anticonvulsant and Molecular Docking Investigation.	0
192	The Origin of Amphipathic Nature of Short and Thin Pristine Carbon Nanotubes Fully Recyclable 1D Water-in-Oil Emulsion Stabilizers. 2202407	1
191	Hydrogen bonds of a water molecule in the second coordination sphere of amino acid metal complexes: Influence of amino acid coordination. **2023**, 112151	0
190	Theoretical exploration of noncovalent interactions in Sc2C2@C2n (n = 40, 41, and 42)?[12]CPP, PF[12]CPP. **2023**, 13, 4553-4563	0
189	Effect of the QM Size, Basis Set, and Polarization on QM/MM Interaction Energy Decomposition Analysis.	1
188	Sensing Bisphenol A by Means of Surface-Enhanced Raman Spectroscopy and DFT Calculations to Elucidate the Enhancement Mechanism That Dominates the Spectrum. **2023**, 11, 78	0
187	Extracting Quantitative Information at Quantum Mechanical Level from Noncovalent Interaction Index Analyses.	0
186	Digging on the Mechanism of Some Diels-Alder Reactions. The Role of the Reaction Electronic Flux.	0
185	Computational study of the interaction of the psychoactive amphetamine with 1,2-indanedione and 1,8-diazafluoren-9-one as fingerprinting reagents. **2023**, 13, 4077-4088	0
184	Chemical Stabilization of [4]Cycloparaphenylene via Encapsulation of Alkaline-earth Metals.	0
183	Recent advances on halogen bonds within the quantum theory of atoms-in-molecules. **2023**, 469-490	0
182	Molecular Structure. **2023**, 487-506	0
181	Combining multi-scale simulations and experiments to unveil the adsorption of methylene blue in graphene tridimensional-based materials.	0
180	Electronic structure and density functional theory. **2023**, 3-35	0
179	Molecular Dynamics with Chemical Accuracy-Alkane Adsorption in Acidic Zeolites. **2023**, 13, 2011-2024	0
178	On the concentration polarisation in molten Li salts and borate-based Li ionic liquids.	0
177	Two-Step ONIOM Method for the Accurate Estimation of Individual Hydrogen Bond Energy in Large Molecular Clusters. **2023**, 127, 1219-1232	0
176	TFRegNCI: Interpretable Noncovalent Interaction Correction Multimodal Based on Transformer Encoder Fusion.	0

175	Accuracy of Intermolecular interaction Energies, Particularly Those of Hetero Atom Containing Molecules Obtained by van der Waals DFT Calculations. **2023**, 8,	0
174	Structural and quantitative analysis of intermolecular solid-state interactions in cocrystals obtained from nucleobases and methylxanthines with gallic acid. **2023**, 1280, 135074	0
173	Experimental FTIR-MI and Theoretical Studies of Isocyanic Acid Aggregates. **2023**, 28, 1430	0
172	A comparative DFT study on Al- and Si- doped single-wall carbon nanotubes (SWCNTs) for Ribavirin drug sensing and detection. **2023**, 158, 107360	0
171	A DFT study of hydrogen adsorption on Pt modified carbon nanocone structures: Effects of modification and inclination of angles. **2023**,	0
170	Phenolic compounds extraction from propolis using imidazole based ionic liquids: a theoretical and experimental study.	0
169	Revisiting the BODIPY-borane dyad for the design of efficient aqueous phase molecular probes for anion recognition: A DFT/TD-DFT study. **2023**, 439, 114603	0
168	Using Stationary Points on Potential Energy Surfaces to Model Intermolecular Interactions and Retention in Gas Chromatography. **2004**, 59, 329-334	0
167	The $${text{NH}}_{4}^{ + }$$(H2O)n Reagent Ion: Calculations of the Structure, Thermodynamic Parameters of Hydration, Equilibrium Composition, and Mobility. **2022**, 77, 1770-1783	0
166	Multiscale quantum algorithms for quantum chemistry. **2023**, 14, 3190-3205	0
165	Effects of aggregation on the structures and excited-state absorption for zinc phthalocyanine. **2023**, 25, 10278-10287	0
164	Selective and efficient detection of Pb2+ in aqueous solution by lanthanoid-organic frameworks bearing pyridine-3,4-dicarboxylic acid and glutaric acid.	0
163	Comparison of three cyclodextrins to optimize bisphenol A extraction from source water: Computational, spectroscopic, and analytical studies. 2300012	0
162	Unveiling the thermodynamic and molecular mechanisms for the separation of diethoxymethane and ethanol azeotrope by deep eutectic solvents. **2023**, 376, 121451	0
161	Molecular-level understanding of the rovibrational spectra of N2O in gaseous, supercritical, and liquid SF6 and Xe. **2023**, 158, 144302	0
160	Electrostatic interactions, binding energies and structures of the Be+2 **2023**, 1222, 114070	0
159	Computational Study of Driving Forces in ATSP, PDIQ, and P53 Peptide Binding: C?O C?O Tetrel Bonding Interactions at Work.	0
158	Theoretical and Experimental Study for Cross-Coupling Aldol Condensation over Mono- and Bimetallic UiO-66 Nanocatalysts. **2023**, 6, 5422-5433	0

157	Theoretical evaluation of boron carbide nanotubes as non-enzymatic glucose sensors. **2023**, 140510	0
156	Development of solid dispersions based on 3- (2,6-difluorobenzyl) -5- (5-bromo-1H-indol-3-ylmethylene) thiazolidine-2,4-dione for schistosomicidal treatment. **2023**, 248, 108455	0
155	Competition and interplay between Hydrogen, Tetrel, and Halogen bonds from interactions of COCl2 and HX (X□=□F, Cl, Br, and I). **2023**, 1223, 114099	0
154	Conformers of 1,4-dioxane and their hydrogen bond complexation with methanol. **2023**, 126, 103519	0
153	Nonlinear optical properties of superalkali@teetotum boron clusters with potential applications on the electro-optic modulator. **2023**, 1223, 114078	0
152	Study on intermolecular hydrogen bond of uric acid water-clusters. **2023**, 818, 140424	0
151	H□Bond interactions in water multimers and water multimers□Pyridine complexes: Natural bond orbital and reduced density gradient isosurface analyses. **2023**, 377, 121524	0
150	Density, viscosity, and H2S solubility of N-butylmorpholine bromide iron-based ionic liquids. **2023**, 378, 121592	0
149	Effective enantioselective recognition by steady-state fluorescence spectroscopy: Towards a paradigm shift to optical sensors with unusual chemical architecture. **2023**, 294, 122526	0
148	Cooperativity effects in a new pterostilbene/phenanthroline cocrystal. **2023**, 1282, 135227	0
147	Hydrogen bonding to graphene surface: A comparative computational study. **2023**, 551, 121454	0
146	Atmospheric degradation mechanism of anthracene initiated by OH□A DFT prediction. **2023**, 121, 108426	0
145	Oxygen-containing functional groups enhance uranium adsorption by aged polystyrene microplastics: Experimental and theoretical perspectives. **2023**, 465, 142730	0
144	Sulfido-bridged 1,2-bis(diphenylphosphino)ethane (dppe) appended trinuclear nickel(II) clusters: Crystallographic and computational analyses. **2023**, 551, 121471	0
143	Combined experimental and theoretical studies of bis-chalcone: Estimation of non-covalent interactions. **2023**, 1282, 135189	0
142	Study on the structural characteristics and interaction mechanisms of ionic liquid mixtures with a common imidazolium cation. **2023**, 380, 121743	0
141	Insight into the role of pseudo-halides as multiple hydrogen bond acceptors in the formation of supramolecular 1D assembly of di and trinuclear zinc complexes. **2023**, 553, 121516	0
140	Micro-mechanism insights into the adsorption of anionic dyes using quaternary ammonium-functionalised chitosan aerogels. **2023**, 313, 120855	1

139	Cu-loaded MOF-303 for iodine adsorption: The roles of Cu species and pyrazole ligands. **2023**, 619, 156819	0
138	A computational study on the potential application of metal-doped AlN nanotubes for chloroform detection. **2023**, 1222, 114047	0
137	Highly furosemide uptake employing magnetic graphene oxide: DFT modeling combined to experimental approach. **2023**, 379, 121652	0
136	A density functional theory investigation on norepinephrine interaction with amino acids and alcohols. **2023**, 1283, 135305	0
135	Competition of hydrogen, tetrel, and halogen bonds in COCl2-HOX (X=F, Cl, Br, I) complexes. **2023**, 122, 108482	0
134	Computational investigations on the 4‐cyanopyridine adsorbed on ZnO‐graphene oxide nanocomposite toward the efficient performance of surface‐enhanced Raman scattering. **2023**, 133, 109693	0
133	Analysis of non-covalent interactions in the acetone-chloroform system by MP2/CBS quantum chemical calculations.	0
132	Effect of Polydopamine Coating of Cellulose Nanocrystals on Performance of PCL/PLA Bio-Nanocomposites. **2023**, 16, 1087	0
131	Comparative study of the efficiency of silicon carbide, boron nitride and carbon nanotube to deliver cancerous drug, azacitidine: A DFT study. **2023**, 154, 106593	0
130	Open-Cage Fullerene as a Selective Molecular Trap for LiF/[BeF] +. **2023**, 135,	0
129	Characterization of competing halogen-bonding and hydrogen-bonding motifs in the acetonitrile/hydrogen iodide dimer. **2023**, 568, 111843	0
128	Insight into the stabilization mechanism of imidazole-based ionic liquids at the interface of the carbon nanotubes: A computational study. **2023**, 375, 121320	0
127	Understanding lead and mercury adsorption by post-synthetically modified linkers in UiO-66 MOF. A computational theoretical study. **2023**, 49, 481-488	0
126	Collisional excitation of HCNH+ by He and H2: New potential energy surfaces and inelastic rate coefficients. **2023**, 158, 074304	0
125	Pyridinecarboxaldehydes: Structures, Vibrational Assignments and Molecular Characteristics Using Experimental and Theoretical Methods. **2023**, 53,	0
124	Self-Healing, Robust, Liquid-Repellent Coatings Exploiting the Donor‐Acceptor Self-Assembly. **2023**, 15, 8699-8708	0
123	A New Motif in Halogen Bonding: Cooperative Intermolecular S‐Br???O, O???F, and F???F Associations in the Crystal Packing of α,ω-Di(sulfonyl bromide) Perfluoroalkanes. **2023**, 18,	0
122	Reduced Nucleophilicities σ‐B of Lewis Bases B: Is σ‐B Independent of Whether B is Involved in a Hydrogen Bond or a Halogen Bond?. **2023**, 88,	0

121	Dynamic Construction and Maintenance of Confined Nanoregions via Hydrogen-Bond Networks between Acetylene Reactants and a Polyoxometalate-Based Metal□Organic Framework. **2023**, 15, 8275-8285	1
120	Laser-induced Coulomb explosion imaging of alkali-metal dimers on helium nanodroplets. **2023**, 107,	0
119	Boron nitride nanocage as drug delivery systems for chloroquine, as an effective drug for treatment of coronavirus disease: A DFT study. **2023**, 150, 110482	0
118	Competition Between the Two □Holes in the Formation of a Chalcogen Bond.	0
117	Making and Breaking□nsight into the Symmetry of Salen Analogues. **2023**, 15, 424	0
116	Torsional Rotation in Ditopic Receptor Host and its Complex Formation with Resorcinol Guest: A Computational Study.	0
115	Molecular dynamics simulation studies of 1,3-dimethyl imidazolium nitrate ionic liquid with water. **2023**, 158, 084505	0
114	Insights into interactions of N-ethylpentylone drug with water and biomacromolecules.	0
113	Single-electron spodium bonds: Substituent effects. **2023**, 37,	0
112	Assessment of three-body dispersion models against coupled-cluster benchmarks for crystalline benzene, carbon dioxide, and triazine. **2023**, 158, 094110	0
111	Computational and theoretical investigation of the geometrical structures, vibrational spectra and thermodynamic properties of the ionic and molecular clusters existing in vapours over strontium diiodide. **2023**, 121,	0
110	Two Crystal Forms of 4?-Methyl-2,4-dinitrodiphenylamine: Polymorphism Governed by Conformational Flexibility of a Supramolecular Synthon. **2023**, 13, 296	0
109	Hydroxyl-initiated oxidation processes of phenylenediamines treated by the atmospheric plasma: A theoretical study in gas phase.	0
108	Cyclophosphamide drug sensing characteristics by using pure and Ti-doped graphyne-like BN-yne. **2023**, 150, 110535	0
107	High-precision cavity-enhanced spectroscopy for studying the H2□Ar collisions and interactions. **2023**, 158, 094303	0
106	A theoretical adsorption study of the inner-core and outer-core hydrated alkali metal cation□ircumcoronene complexes.	0
105	Exploring alkali metal cation?hydrogen interaction in the formation half sandwich complexes with cycloalkanes: a DFT approach. **2023**,	0
104	Stability Mechanism of Menthol and Fatty Acid Based Hydrophobic Eutectic Solvents: Insights from Nonbonded Interactions. **2023**, 11, 3539-3556	0

103	Theoretical understanding of stability of mechanically interlocked carbon nanotubes and their precursors. **2023**, 25, 7527-7539	0
102	Centrosymmetric Nickel(II) Complexes Derived from Bis-(Dithiocarbamato)piperazine with 1,1?-Bis-(Diphenylphosphino)ferrocene and 1,2-Bis-(Diphenylphosphino)ethane as Ancillary Ligands: Syntheses, Crystal Structure and Computational Studies. **2023**, 13, 343	0
101	Does a halogen bond require positive potential on the acid and negative potential on the base?. **2023**, 25, 7184-7194	0
100	Halogen Bond-Involving Supramolecular Assembly Utilizing Carbon as a Nucleophilic Partner of I???C Non-covalent Interaction. **2023**, 18,	0
99	Collision-induced three-body polarizability of helium. **2023**, 158, 114303	0
98	A Density Functional Study on Adrucil Drug Sensing Based on the Rh-Decorated Gallium Nitride Nanotube. **2023**, 52, 3156-3164	0
97	The Electron Density. **2023**, 31-101	0
96	Site of the Hydroxyl Group Determines the Surface Behavior of Bipolar Chain-Oxidized Cholesterol Derivatives-Langmuir Monolayer Studies Supplemented with Theoretical Calculations. **2023**, 127, 2011-2021	0
95	Accurate non-covalent interaction energies on noisy intermediate-scale quantum computers via second-order symmetry-adapted perturbation theory. **2023**, 14, 3587-3599	0
94	Radical Pairing Interactions and Donor–Acceptor Interactions in Cyclobis(paraquat-p-phenylene) Inclusion Complexes. **2023**, 28, 2057	0
93	Temperature-induced transformation between layered herringbone polymorphs in molecular bilayer organic semiconductors. **2023**, 7,	0
92	Introducing a New Type of Drug Delivery System Based on the Silicon Carbide Monolayer.	0
91	Inclusion complexation and liposomal encapsulation of an isoniazid hydrazone derivative in cyclodextrin for pH-dependent controlled release. **2023**, 81, 104302	0
90	Green corrosion inhibitors of steel based on peptides and their constituents: a combination of experimental and computational approach.	0
89	Delivery of Cisplatin Anti-cancer Drug by Si-Decorated Al24N24 Nanocage: DFT Evaluation of Electronic and Structural Features. **2023**, 52, 3281-3290	0
88	Trapping of Small Molecules within Single or Double Cyclo[18]carbon Rings. **2023**, 28, 2157	0
87	Structures and stabilities of PAH clusters solvated by water aggregates: The case of the pyrene dimer. **2023**, 158, 114308	0
86	Complexes of LiF and LiCl with LiF, LiCl, LiH, HF, HCl, H2, Li2, F2, Cl2, FCl, H2O and NH3. Structures, energies and vibrational frequencies. **2023**, 121,	0

85	DENSITY FUNCTIONAL THEORY INVESTIGATION ON DRUG-DRUG INTERACTIONS: ESCITALOPRAM AND SALICYLIC ACID.	0
84	DFT CALCULATIONS IN MONOMERIC AND DIMERIC FORMS OF N-BENZYLMALEIMIDE (NBM) COMBINED WITH VIBRATIONAL SPECTROSCOPIC PARAMETERS.	0
83	Pyridine Ionic Liquid-Based Deep Eutectic Solvents Selectively Separating Toluene from Alkanes. **2023**, 37, 4233-4243	0
82	Synthesis of 4-Amino-N-[2 (diethylamino)Ethyl]Benzamide Tetraphenylborate Ion-Associate Complex: Characterization, Antibacterial and Computational Study. **2023**, 28, 2256	0
81	Strong reactivity and electronic sensitivity of Au-decorated BC3 nanotubes toward the phenylpropanolamine drug. **2023**, 129,	0
80	Synthesis, X-ray characterization and DFT calculations of a series of 3-substituted 4,5-dichloroisothiazoles. **2023**, 25, 1976-1985	0
79	Exploring the Relationship between Reactivity and Electronic Structure in Isorhodanine Derivatives Using Computer Simulations. **2023**, 28, 2360	0
78	Performance of Density Functionals and Semiempirical 3c Methods for Small Gold□thiolate Clusters. **2023**, 127, 2242-2257	0
77	Solvation Effects on Polarizability of Aromatic Fluids. **2023**, 127, 2237-2249	0
76	Tetrel bond involving -CH3 group in HnXCH3 (X = F, Cl, and Br, n = 0; X = O, S, and Se, n = 1; X = N, P, and As, n = 2). Cooperativity with triel bond and beryllium bond. **2023**, 121,	0
75	Synthesis and conformational preferences of peptides and proteins with cysteine sulfonic acid. **2023**, 21, 2779-2800	0
74	Modeling Catalyzed Reactions on Metal-Doped Amorphous Silicates: The Case of Niobium-Catalyzed Ethylene Epoxidation. **2023**, 127, 4984-4997	0
73	First-principles study of nitrogen-doped porous graphene for Na+, K+, Mg2+, and Ca2+ cations adsorption.	0
72	Cocrystallization of Antifungal Compounds Mediated by Halogen Bonding. **2023**, 23, 2932-2940	0
71	New insights into the alkoxy effects on auxiliary adsorption and inhibiting charge recombination in dye-sensitized solar cells with high open circuit voltage: a theoretical investigation. **2023**, 25, 8532-8543	0
70	A dispersion-corrected DFT calculations on encapsulation of Favipiravir drug used as antiviral against COVID-19 into carbon-, boron-, and aluminum-nitride nanotubes for optimal drug delivery systems combined with molecular docking simulations.	0
69	An investigation of Solid-State Emission of Halogenated Diphenyl Phosphanyl Anthracenes. 2202753	0
68	Speciation of Hexavalent Chromium in Aqueous Solutions Using a Magnetic Silica-Coated Amino-Modified Glycidyl Methacrylate Polymer Nanocomposite. **2023**, 16, 2233	0

67	Evaluation of an electrochemical sensor based on gold nanoparticles supported on carbon nanofibers for detection of tartrazine dye.	0
66	Halogen-Bonded Mono-, Di-, and Tritopic N-Alkyl-3-iodopyridinium Salts. **2023**, 23, 2361-2374	0
65	Hole intermolecular interactions between carbon oxides and dihalogens: Ab-initio investigations.	0
64	DFT and TD-DFT study of hydrogen bonded complexes of aspartic acid and n water (n = 1 and 2). **2023**, 29,	0
63	Research on separation sulfides from fuel oil using sulfolane: Liquid-liquid equilibrium and mechanism exploration. **2023**, 182, 107036	0
62	Tetrel-Bond Interactions Involving Metallylenes TH2 (T = Si, Ge, Sn, Pb): Dual Binding Behavior. **2023**, 28, 2577	0
61	Polycyclic Aromatic Hydrocarbons as Anode Materials in Lithium-Ion Batteries: A DFT Study. **2023**, 127, 2511-2522	0
60	Structure and stability of the sH binary hydrate cavity and host-guest versus guest-guest interactions therein: A DFT approach.	0
59	DFT insights into competing mechanisms of guaiacol hydrodeoxygenation on a platinum cluster. **2023**, 25, 10460-10471	0
58	Interpretable Machine Learning Model for Predicting Interaction Energies between Dimethyl Sulfide and Potential Absorbing Solvents. **2023**, 62, 5274-5285	0
57	A Comprehensive Ab Initio Study of Halogenated A U and G C Base Pair Geometries and Energies. **2023**, 24, 5530	0
56	H2O HF@C70: Encapsulation Energetics and Thermodynamics. **2023**, 11, 123	0
55	Compatibility and Interaction Mechanism between the C4F7N/CO2/O2 Gas Mixture and FKM and NBR. **2023**, 8, 11414-11424	0
54	A Computational Insight on the Effect of Encapsulation and Li Functionalization on Si12C12 Heterofullerene for H2 Adsorption: A Strategy for Effective Hydrogen Storage. **2023**, 6, 3374-3389	0
53	5-fluorouracil-caffeic acid cocrystal delivery agent with long-term and synergistic high-performance antitumor effects. **2022**, 17, 2215-2229	0
52	Cooperativity and intermolecular hydrogen bonding in donor-acceptor complexes of phenol and polyhydroxybenzenes.	0
51	Interactions between Paracetamol and Formaldehyde: Theoretical Investigation and Topological Analysis. **2023**, 8, 11725-11735	0
50	Semiclassical Vibrational Spectroscopy of Real Molecular Systems by Means of Cross-Correlation Filter Diagonalization. **2023**, 127, 2902-2911	0

49	Tuning the odd–even effect on two-dimensional assemblies of curcumin derivatives by alkyl chain substitution: a scanning tunnelling microscopy study. **2023**, 25, 10917-10924	0
48	Computational Investigation of Deoxyribose and Phosphate Substitutions Effects on the Hydrogen Bond Strength of Adenine–Thymine Base Pair in the Gas Phase and Water Solution. **2022**, 96, 3290-3302	0
47	Collision excitation of nitrous acid (HONO) by helium: isomerization effect. **2023**, 521, 4162-4172	0
46	Role of Non-Covalent Interactions in Carbonic Anhydrase II–Topiramate Complex Based on QM/MM Approach. **2023**, 16, 479	0
45	Hydrogen bonding guest-water interactions in pinacolone, tert-butyl amine, and tert-butylmethyl ether: a theoretical study on energetics, structure, and topological +. **2023**, 29,	0
44	Ibuprofen and Paracetamol when They Meet: Quantum Theory of Atoms in Molecules Perspective. **2023**, 44, 188-196	0
43	Application of Pure and Au-Decorated YN (Y = B, Al, and Ga) Nanotubes as Good Media for Toxic Phosgene Oxime Gas Adsorption.	0
42	Imidazolin-2-imine and Imidazolin-2-methylidene Substitutions to Benzene, Pyridine, Phosphine, and N-Heterocyclic Carbene Predict Highly Electron-rich Ligands. **2023**, 42, 571-580	0
41	Hydrogen bonds of OC ? NH motif in rings in drugs: A molecular electrostatic potential analysis.	0
40	Square-planar and octahedral nickel complexes of an acylhydrazone ligand and the serendipitous isolation of a potential octahedral nickel acylhydrazone precursor.	0
39	Supported Pt Nanoclusters on Single-Layer MoS2 for the Detection of Cortisol: From Atomistic Scale to Device Modeling.	0
38	Preferential Crystallization of tert-Butyl-calix[6]arene Chlorobenzene Solvate from a Solvent Mixture.	0
37	Analysis of intermolecular interactions of n-perfluoroalkanes with circumcoronene using dispersion-corrected DFT calculations: comparison with those of n-alkanes.	0
36	Engineering supramolecular helical assemblies via interplay between carbon(sp) tetrel and halogen bonding interactions.	0
35	Hydrogen bond properties of Se in [ROH–Se(CH3)2] complexes (R = H, CH3, C2H5): matrix-isolation infrared spectroscopy and theoretical calculations.	0
34	Quantum state–resolved molecular dipolar collisions over four decades of energy. **2023**, 379, 1031-1036	0
33	Structure of choline chloride-carboxylic acid deep eutectic solvents by wide-angle X-ray scattering and DFT calculations. **2023**, 25, 10481-10494	0
32	Computational Insights on Solvation and Hydrogen Bonding Studies of Indomethacin. **2023**, 35, 861-868	0

31	Complexes of hydrogen peroxide molecules with DNA nucleic bases. 1-6	0
30	Bibliography. **2023**, 431-464	0
29	Multiscale Theoretical Study of Sulfur Dioxide (SO2) Adsorption in Metal□Organic Frameworks. **2023**, 28, 3122	0
28	The Tetrel Bond and Tetrel Halide Perovskite Semiconductors. **2023**, 24, 6659	0
27	Molecular modeling for sensing of cisplatin drug by graphdiyne: electronic study via DFT. **2023**, 29,	0
26	Three-in-one: exploration of co-encapsulation of cabazitaxel, bicalutamide and chlorin e6 in new mixed cyclodextrin-crosslinked polymers. **2023**, 13, 10923-10939	0
25	Photoabsorption of Microhydrated Naphthalene and Its Cyano-Substituted Derivatives: Probing Prereactive Models for Photodissociation in Molecular Clouds.	0
24	Accurate Interaction Energies of CO2 with the 20 Naturally Occurring Amino Acids.	0
23	Hydrogen Bonding with Hydridic Hydrogen□Experimental Low-Temperature IR and Computational Study: Is a Revised Definition of Hydrogen Bonding Appropriate?.	0
22	Physicochemical properties of the N-methyl-6-hydroxyquinolinium□based protic ionic liquids in the gas and solution media: M062□X-GD3/6□311 + + G(d,p) study.	0
21	Encapsulation of Astatide by a water cage.	0
20	Metalloporphyrin reduced C70 fullerenes as adsorbents and detectors of ethenone; A DFT, NBO, and TD-DFT study. **2023**, 108481	0
19	Theoretical Study on the Interaction between Cis-2 Bis(benzofuro) [60]fullerene Derivative and NO Dominated Double Gas Molecule. **2023**,	0
18	Quantum Mechanical and Classical Calculation of the Transport and Relaxation Properties of He...CO2 Complex Using a New PES.	0
17	Prediction, Application, and Mechanism Exploration of Liquid□Liquid Equilibrium Data in the Extraction of Aromatics Using Sulfolane. **2023**, 11, 1228	0
16	Sulfur□rene interactions: the S?□and SH?□interactions in the dimers of benzofuran?sulfur dioxide and benzofuran?hydrogen sulfide.	0
15	Theoretical FRET Efficiency of an Antenna Material Containing Natural Dyes and Zeolite L.	0
14	Theoretical Study on CO₂/SO₂ Absorption Using <i>N</i>- Alkylethylenediaminium Protic Ionic Liquid. 5, 49-62	0

13	The Microwave Spectra and Molecular Structures of (Z)-1-Chloro-3,3,3-Trifluoropropene and Its Gas-Phase Heterodimer with the Argon Atom. **2023**, 111779	0
12	2D silicene nanosheets for the detection of DNA nucleobases for genetic biomarker: a DFT study.	0
11	Halogen bonding: a designer strategy for graphyne-like two-dimensional architectures. **2023**, 142,	0
10	Mechanical Bonding as a Promoter of Crystalline Diversity in Halogenated [2]Rotaxanes.	0
9	A Theoretical Study of Tris-(<i>o</i>-benzoquinonediimine)-First-Row Divalent Transition Metal Complexes. **2023**, 13, 172-188	0
8	Meta-GGA Density Functional Calculations on Atoms with Spherically Symmetric Densities in the Finite Element Formalism.	0
7	De-excitation rates of the newly discovered C5H+ in collision with He.	0
6	Static and Dynamical Quantum Studies of CX3-AlX2 and CSiX3-BX2 (X = F, Cl, Br) Complexes with Hydrocyanic Acid: Unusual Behavior of Strong Hole at Triel Center. **2023**, 24, 7881	0
5	Advances in understanding the phosphate binding to soil constituents: A Computational Chemistry perspective. **2023**, 887, 163692	0
4	Designing a promising sensor for SF6 decomposed gases by using platinum doped-aluminum nitride nanotubes. **2023**, 153, 110743	0
3	Potential energy surface of LiD2 system for cold collisions. **2023**,	0
2	Collisional excitation of N+(3P) in interstellar clouds. **2023**, 522, 6251-6257	0
1	Characterization of Thymoquinone-Sulfobutylether- Cyclodextrin Inclusion Complex for Anticancer Applications. **2023**, 28, 4096	0