Ibon Alkorta

List of Publications by Year in Descending Order

931 papers	27,090 citations	69 h-index	125 g-index
992 ext. papers	29,477 ext. citations	3.1 avg, IF	7.6 L-index

#	Paper	IF	Citations
931	Density functional theory studies on C with substitutional TiN impurities.. *Journal of Molecular Modeling*, **2022**, 28, 62	2	0
930	Determination of the tautomerism of albendazole desmotropes using solution and solid state NMR together with DFT theoretical calculations, both energies and chemical shifts. *Journal of Molecular Structure*, **2022**, 1261, 132883	3.4	0
929	A DFT study of the tautomerism of 1H-benzo[de]cinnolines and their protonated forms. *Theoretical Chemistry Accounts*, **2022**, 141, 1	1.9	0
928	Strategies for the direct oxidative esterification of thiols with alcohols. *RSC Advances*, **2022**, 12, 14521-14534	3.7	0
927	Methods for Direct Reductive N-Methylation of Nitro Compounds. *Topics in Current Chemistry*, **2022**, 380,	7.2	
926	Substitution effects via aromaticity, polarizability, APT, AIM, IR analysis, and hydrogen adsorption in CTi nanostructures: a DFT survey. *Journal of Molecular Modeling*, **2021**, 27, 348	2	0
925	Recent trends in dehydroxylative trifluoro-methylation, -methoxylation, -methylthiolation, and -methylselenylation of alcohols.. *RSC Advances*, **2021**, 11, 39593-39606	3.7	4
924	Direct halosulfonylation of alkynes: an overview.. *RSC Advances*, **2021**, 11, 33447-33460	3.7	6
923	IR and NMR properties of N-base:PH2F:BeX2 ternary and corresponding binary complexes stabilised by pnicogen and beryllium bonds. *Molecular Physics*, **2021**, 119, e1905191	1.7	4
922	A 13C chemical shifts study of iodopyrazoles: experimental results and relativistic and non-relativistic calculations. *Structural Chemistry*, **2021**, 32, 925-937	1.8	0
921	A Density Functional Theory Study of Optical Rotation in Some Aziridine and Oxirane Derivatives. *ChemPhysChem*, **2021**, 22, 764-774	3.2	0
920	Carboranes as Lewis Acids: Tetrel Bonding in CB11H11 Carbonium Ylide. *Crystals*, **2021**, 11, 391	2.3	2
919	Transition-metal-catalyzed dehydrogenative coupling of alcohols and amines: A novel and atom-economical access to amides. *Journal of the Chinese Chemical Society*, **2021**, 68, 723-737	1.5	18
918	The Electrophilicities of XCF and XCl (X=H, Cl, Br, I) and the Propensity of These Molecules To Form Hydrogen and Halogen Bonds with Lewis Bases: An Ab Initio Study. *ChemPlusChem*, **2021**, 86, 778-784	2.8	2
917	Evaluation of Electron Density Shifts in Noncovalent Interactions. *Journal of Physical Chemistry A*, **2021**, 125, 4741-4749	2.8	3
916	Reactivity of Coinage Metal Hydrides for the Production of H Molecules. *ChemistryOpen*, **2021**, 10, 724-730	2.3	1
915	Alkylammonium Cation Affinities of Nitrogenated Organobases: The Roles of Hydrogen Bonding and Proton Transfer. *ChemPlusChem*, **2021**, 86, 1097-1105	2.8	

914	A DFT quest for effects of fused rings on the stability of remote N-heterocyclic carbenes. *Structural Chemistry*, **2021**, 32, 787-798	1.8	4
913	Multinuclear magnetic resonance studies of five silver(I) trinuclear pyrazolate complexes. *Structural Chemistry*, **2021**, 32, 215-224	1.8	1
912	A static and dynamic NMR study of 10-hydrazino-BODIPY. *Magnetic Resonance in Chemistry*, **2021**, 59, 454-464	2.1	1
911	Computational study of a B36 borophene as an electronic sensor for the anti-cancer drug cisplatinum. *Journal of Computational Electronics*, **2021**, 20, 635-642	1.8	5
910	A structural analysis of 2,5-diaryl-4H-2,4-dihydro-3H-1,2,4-triazol-3-ones: NMR in the solid state, X-ray crystallography, and GIPAW calculations. *Magnetic Resonance in Chemistry*, **2021**, 59, 423-438	2.1	2
909	A new strategy for the synthesis of 2-mercaptobenzazole derivatives by green chemistry metrics. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2021**, 196, 1-5	1	1
908	Ultrasound Assisted Chromatography-Free Synthesis of Triazolo [1,2-a]Indazole-Triones in the Presence of 1,4-Diazabicyclo[2.2.2] Octanium Diacetate as an Environmentally Friendly Green Media. *Polycyclic Aromatic Compounds*, **2021**, 41, 963-973	1.3	2
907	Hexa-cata-hexabenzocoronene nanographene as a promising anode material for Mg-ion batteries. *Journal of Molecular Modeling*, **2021**, 27, 45	2	
906	Intermolecular difunctionalization of alkenes: synthesis of β-hydroxy sulfides.. *RSC Advances*, **2021**, 11, 13138-13151	3.7	21
905	Vicinal halo-trifluoromethylation of alkenes.. *RSC Advances*, **2021**, 11, 14941-14955	3.7	19
904	The recent development of donepezil structure-based hybrids as potential multifunctional anti-Alzheimer's agents: highlights from 2010 to 2020.. *RSC Advances*, **2021**, 11, 30781-30797	3.7	2
903	On the 3D -> 2D Isomerization of Hexaborane(12). *Chemistry*, **2021**, 3, 28-38	2.1	0
902	Progress and recent trends in the direct selenocyanation of (hetero)aromatic C-H bonds.. *RSC Advances*, **2021**, 11, 22305-22316	3.7	5
901	Recent progress in application of nanocatalysts for carbonylative Suzuki cross-coupling reactions.. *RSC Advances*, **2021**, 11, 2112-2125	3.7	7
900	Spontaneous bond dissociation cascades induced by Be clusters (n = 2,4). *Physical Chemistry Chemical Physics*, **2021**, 23, 6448-6454	3.6	1
899	Non-Covalent Interactions of the Lewis Acids CuX, AgX, and AuX (X = F and Cl) with Nine Simple Lewis Bases B: A Systematic Investigation of Coinage-Metal Bonds by Ab Initio Calculations. *Inorganics*, **2021**, 9, 13	2.9	4
898	A theoretical study of inversion barriers and NMR chemical shifts of 3-pyrazolines (2,3-dihydro-1H-pyrazoles). *Journal of Heterocyclic Chemistry*, **2021**, 58, 1015-1028	1.9	1
897	An efficient one-pot synthesis of novel 6-hydroxy-14-aryl-8H-dibenzo[a,i]xanthene-8,13(14H)-diones derived from lawsone. *Research on Chemical Intermediates*, **2021**, 47, 2207	2.8	3

896	Adsorption of syn-propanethial S-oxide on the Zn12O12 cluster: insights from ab-initio modelling. *Journal of Sulfur Chemistry*, **2021**, 42, 308-321	2.3	
895	Conformational analysis of 2,5-diaryl-4-methyl-2,4-dihydro-3H-1,2,4-triazol-3-ones: Multinuclear NMR and DFT calculations. *Journal of Heterocyclic Chemistry*, **2021**, 58, 1130-1140	1.9	
894	The SN2 reaction and its relationship with the Walden inversion, the Finkelstein and Menshutkin reactions together with theoretical calculations for the Finkelstein reaction. *Structural Chemistry*, **2021**, 32, 1755-1761	1.8	3
893	Clustering of Electron Deficient B- and Be-Containing Analogues: In the Fight for Tetracoordination, Beryllium Takes the Lead. *European Journal of Inorganic Chemistry*, **2021**, 2021, 4393	2.3	0
892	Sequestration of Carbon Dioxide with Frustrated Lewis Pairs Based on N-Heterocycles with Silane/Germane Groups. *Journal of Physical Chemistry A*, **2021**, 125, 6976-6984	2.8	0
891	Investigation of fused remote N-heterocyclic silylenes (frNHSis), at DFT. *Journal of Molecular Modeling*, **2021**, 27, 299	2	
890	The mechanism of the reaction of hydrazines with α,β-unsaturated carbonyl compounds to afford hydrazones and 2-pyrazolines (4,5-dihydro-1H-pyrazoles): Experimental and theoretical results. *Tetrahedron*, **2021**, 97, 132413	2.4	3
889	Stationary states of systems with intermolecular interactions dominated by electrostatics: Structure of trimethylammonium and tetramethylammonium chlorides and bromides in the gas phase, monomers and dimers. *Chemical Physics Letters*, **2021**, 778, 138809	2.5	0
888	How Aromatic Fluorination Exchanges the Interaction Role of Pyridine with Carbonyl Compounds: The Formaldehyde Adduct. *Chemistry - A European Journal*, **2021**, 27, 13870-13878	4.8	2
887	Direct synthesis of sulfenamides, sulfinamides, and sulfonamides from thiols and amines.. *RSC Advances*, **2021**, 11, 32394-32407	3.7	4
886	Alkoxysulfenylation of alkenes: development and recent advances.. *RSC Advances*, **2021**, 11, 32513-32525	3.7	3
885	Hydroxysulfonylation of alkenes: an update.. *RSC Advances*, **2021**, 11, 21651-21665	3.7	8
884	Tetranuclear copper(II) cubane complexes derived from self-assembled 1,3-dimethyl-5-(o-phenolate-azo)-6-aminouracil: structures, non-covalent interactions and magnetic property. *New Journal of Chemistry*, **2021**, 45, 2742-2753	3.6	4
883	Recent advances in intermolecular 1,2-difunctionalization of alkenes involving trifluoromethylthiolation.. *RSC Advances*, **2021**, 11, 24474-24486	3.7	7
882	Anion Complexation Strongly Influences the Reactivity of Octafluorocyclooctatetraene. *ChemistrySelect*, **2021**, 6, 13897-13905	1.8	
881	Interaction between Trinuclear Regium Complexes of Pyrazolate and Anions, a Computational Study. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	1
880	Hybrid Boron-Carbon Chemistry. *Molecules*, **2020**, 25,	4.8	1
879	Perimidines: a unique amphoteric heteroaromatic system. *Russian Chemical Reviews*, **2020**, 89, 1204-1260	6.8	8

878	Cavity-trapped electrons: lithium doped tetracyano-2,6-naphthoquinodimethane (TNAP) systems. *Journal of Molecular Modeling*, **2020**, 26, 118	2	
877	Hydrogen vs. Halogen Bonds in 1-Halo--Carboranes. *Materials*, **2020**, 13,	3.5	5
876	-Fluorobenzenesulfonimide: a useful and versatile reagent for the direct fluorination and amination of (hetero)aromatic C-H bonds.. *RSC Advances*, **2020**, 10, 16756-16768	3.7	24
875	Spodium Bonds: Noncovalent Interactions Involving Group 12 Elements. *Angewandte Chemie*, **2020**, 132, 17635-17640	3.6	14
874	Spodium Bonds: Noncovalent Interactions Involving Group 12 Elements. *Angewandte Chemie - International Edition*, **2020**, 59, 17482-17487	16.4	70
873	Bonding between electron-deficient atoms: strong Lewis-acid character preserved in XYX (X = B, Al; Y = Be, Mg) bridges. *New Journal of Chemistry*, **2020**, 44, 11870-11878	3.6	1
872	Environment-Sensitive Probes for Illuminating Amyloid Aggregation and in Zebrafish. *ACS Sensors*, **2020**, 5, 2792-2799	9.2	11
871	Mutual Influence of Pnicogen Bonds and Beryllium Bonds: Energies and Structures in the Spotlight. *Journal of Physical Chemistry A*, **2020**, 124, 5871-5878	2.8	9
870	Anion-Anion Complexes Established between Aspartate Dimers. *ChemPhysChem*, **2020**, 21, 1052-1059	3.2	12
869	Not Only Hydrogen Bonds: Other Noncovalent Interactions. *Crystals*, **2020**, 10, 180	2.3	169
868	Supramolecular lead(II) architectures engineered by tetrel bonds. *CrystEngComm*, **2020**, 22, 2389-2396	3.3	20
867	Direct Amination of Aromatic C-H Bonds with Free Amines. *Topics in Current Chemistry*, **2020**, 378, 37	7.2	22
866	Complexes Between Adamantane Analogues BX -X = {CH, NH, O ; SiH, PH, S} - and Dihydrogen, BX:H (= 1-4). *Molecules*, **2020**, 25,	4.8	2
865	An Interacting Quantum Atoms (IQA) and Relative Energy Gradient (REG) Study of the Halogen Bond with Explicit Analysis of Electron Correlation. *Molecules*, **2020**, 25,	4.8	8
864	A GIPAW versus GIAO-ZORA-SO study of C and N CPMAS NMR chemical shifts of aromatic and heterocyclic bromo derivatives. *Solid State Nuclear Magnetic Resonance*, **2020**, 108, 101676	3.1	5
863	Unusual Complexes of P(CH) with FH, ClH, and ClF. *Molecules*, **2020**, 25,	4.8	1
862	Hydrogen bonds and halogen bonds in complexes of carbones L->C<-L as electron donors to HF and ClF, for L = CO, N, HNC, PH, and SH. *Physical Chemistry Chemical Physics*, **2020**, 22, 15966-15975	3.6	4
861	From Very Strong to Inexistent Be-Be Bonds in the Interactions of Be with Systems. *ChemPhysChem*, **2020**, 21, 2701-2708	3.2	2

860	Regium Bonds between Silver(I) Pyrazolates Dinuclear Complexes and Lewis Bases (N2, OH2, NCH, SH2, NH3, PH3, CO and CNH). *Crystals*, **2020**, 10, 137	2.3	11
859	Oxidative carboxylation of olefins with CO: environmentally benign access to five-membered cyclic carbonates.. *RSC Advances*, **2020**, 10, 9103-9115	3.7	15
858	Complexes H CO:PXH and HCO H : PXH for X=NC, F, Cl, CN, OH, CCH, CH , and H: Pnicogen Bonds and Hydrogen Bonds. *ChemPhysChem*, **2020**, 21, 741-748	3.2	6
857	A Conceptual DFT Study of Phosphonate Dimers: Dianions Supported by H-Bonds. *Journal of Physical Chemistry A*, **2020**, 124, 2207-2214	2.8	18
856	Borophene as an electronic sensor for metronidazole drug: A computational study. *Journal of Molecular Graphics and Modelling*, **2020**, 96, 107539	2.8	44
855	Are Anions of Cyclobutane Beryllium Derivatives Stabilized through Four-Center One-Electron Bonds?. *Journal of Physical Chemistry A*, **2020**, 124, 1515-1521	2.8	2
854	An experimental and computational NMR study of organometallic nine-membered rings: Trinuclear silver(I) complexes of pyrazolate ligands. *Magnetic Resonance in Chemistry*, **2020**, 58, 319-328	2.1	9
853	Calculated coupling constants J(X-Y) and K(X-Y), and fundamental relationships among the reduced coupling constants for molecules H X-YH , with X, Y ? H, Li, Be, B, C, N, O, F, P, S, and Cl. *Magnetic Resonance in Chemistry*, **2020**, 58, 727-732	2.1	
852	Metastable Dianions and Dications. *ChemPhysChem*, **2020**, 21, 1597-1607	3.2	10
851	Stabilisation of dianion dimers trapped inside cyanostar macrocycles. *Physical Chemistry Chemical Physics*, **2020**, 22, 11348-11353	3.6	9
850	A DFT study on the sulfanilamide interaction with graphyne-like boron nitride nanosheet. *Journal of Sulfur Chemistry*, **2020**, 41, 483-497	2.3	8
849	Theoretical and Spectroscopic Characterization of API-Related Azoles in Solution and in Solid State. *Current Pharmaceutical Design*, **2020**, 26, 4847-4857	3.3	1
848	Recent Advances in the Application of Nanometal Catalysts for Glaser Coupling. *Current Organic Chemistry*, **2020**, 23, 2489-2503	1.7	17
847	Complexes between bicyclic boron derivatives and dihydrogen: the importance of strain. *Structural Chemistry*, **2020**, 31, 1273-1279	1.8	0
846	Theoretical calculations of the chemical shifts of cyclo[n]phosphazenes for n = 2, 3, 4 and 5 (X2PN)n with X = CH3, F, Cl and Br: the effect of relativistic corrections. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2020**, 195, 307-313	1	5
845	Fluorescence mechanism switching from ICT to PET by substituent chemical manipulation: Macrophage cytoplasm imaging probes. *Dyes and Pigments*, **2020**, 175, 108172	4.6	5
844	Aryl sulfonyl chlorides and sodium aryl sulfinates: non-volatile, non-stench, and non-toxic aryl thiol surrogates for direct aryl-sulfenylation of C H bonds. *Journal of Sulfur Chemistry*, **2020**, 41, 210-228	2.3	12
843	A theoretical and spectroscopic (NMR and IR) study of indirubin in solution and in the solid state. *Journal of Physical Organic Chemistry*, **2020**, 33, e4043	2.1	3

842	A density functional theory outlook on the possible sensing ability of boron nitride nanotubes and their Al- and Si-doped derivatives for sulfonamide drugs. *Journal of Sulfur Chemistry*, **2020**, 41, 82-95	2.3	9
841	Theoretical studies of perimidine and its derivatives: structures, energies, and spectra. *Structural Chemistry*, **2020**, 31, 25-35	1.8	4
840	Cross-dehydrogenative Coupling Reactions Between Formamidic C(sp)-H and X-H (X = C, O, N) Bonds. *Topics in Current Chemistry*, **2020**, 378, 46	7.2	7
839	Rivalry between Regium and Hydrogen Bonds Established within Diatomic Coinage Molecules and Lewis Acids/Bases. *ChemPhysChem*, **2020**, 21, 2557-2563	3.2	10
838	A relative energy gradient (REG) study of the nitrogen inversion in N-substituted aziridines. *Chemical Physics Letters*, **2020**, 758, 137927	2.5	1
837	Direct sulfonamidation of (hetero)aromatic C-H bonds with sulfonyl azides: a novel and efficient route to -(hetero)aryl sulfonamides.. *RSC Advances*, **2020**, 10, 37299-37313	3.7	31
836	A C(□hole)?Cl□n tetrel interaction driving a metal□rganic supramolecular assembly. *CrystEngComm*, **2020**, 22, 6979-6982	3.3	1
835	A Computational Study of Metallacycles Formed by Pyrazolate Ligands and the Coinage Metals M = Cu(I), Ag(I) and Au(I): (pzM) for = 2, 3, 4, 5 and 6. Comparison with Structures Reported in the Cambridge Crystallographic Data Center (CCDC). *Molecules*, **2020**, 25,	4.8	2
834	Diborane Concatenation Leads to New Planar Boron Chemistry. *ChemPhysChem*, **2020**, 21, 2460-2467	3.2	7
833	The Lewis acidities of gold(I) and gold(III) derivatives: a theoretical study of complexes of AuCl and AuCl3. *Structural Chemistry*, **2020**, 31, 1909-1918	1.8	6
832	An ab initio investigation of alkali-metal non-covalent bonds BLiR and BNaR (R = F, H or CH) formed with simple Lewis bases B: the relative inductive effects of F, H and CH. *Physical Chemistry Chemical Physics*, **2020**, 22, 16421-16430	3.6	6
831	Probing the structures, binding energies, and spin-spin coupling constants of halogen-bonded Azine:ClF complexes. *Chemical Physics Letters*, **2020**, 761, 137916	2.5	3
830	Regiospecific Synthesis and Structural Studies of 3,5-Dihydro-4-pyrido[2,3-][1,4]diazepin-4-ones and Comparison with 1,3-Dihydro-2-benzo[][1,4]diazepin-2-ones. *ACS Omega*, **2020**, 5, 25408-25422	3.9	5
829	The Importance of Strain (Preorganization) in Beryllium Bonds. *Molecules*, **2020**, 25,	4.8	1
828	Methods for the direct synthesis of thioesters from aldehydes: a focus review. *Journal of Sulfur Chemistry*, **2020**, 41, 96-115	2.3	23
827	Recent trends in the direct oxyphosphorylation of C-C multiple bonds.. *RSC Advances*, **2020**, 11, 470-483	3.7	12
826	The synergy of different solid-state techniques to elucidate the supramolecular assembly of two 1H-benzotriazole polymorphs. *Physical Chemistry Chemical Physics*, **2019**, 21, 19879-19889	3.6	4
825	NC and SS Interactions in Complexes, Molecules, and Transition Structures HN(CH)SX:SCO, for X = F, Cl, NC, CCH, H, and CN. *Molecules*, **2019**, 24,	4.8	3

824	Theoretical studies of conformational analysis and intramolecular dynamic phenomena. *Structural Chemistry*, **2019**, 30, 2029-2055	1.8	0
823	Recent advances in direct trifluoromethylation of olefinic C-H bonds.. *RSC Advances*, **2019**, 9, 27625-27639	3.7	29
822	The strange case of achiral compounds which were reported to always crystallize in the same chiral group. *Structural Chemistry*, **2019**, 30, 633-636	1.8	2
821	Cooperative Effects in Weak Interactions: Enhancement of Tetrel Bonds by Intramolecular Hydrogen Bonds. *Molecules*, **2019**, 24,	4.8	8
820	The beryllium bond. *Advances in Inorganic Chemistry*, **2019**, 73, 73-121	2.1	27
819	A DFT study on nanocones, nanotubes (4,0), nanosheets and fullerene C as anodes in Mg-ion batteries.. *RSC Advances*, **2019**, 9, 853-862	3.7	17
818	Modulating the intrinsic reactivity of molecules through non-covalent interactions. *Physical Chemistry Chemical Physics*, **2019**, 21, 2222-2233	3.6	10
817	Solvent-free incorporation of CO into 2-oxazolidinones: a review.. *RSC Advances*, **2019**, 9, 19465-19482	3.7	29
816	Assignment of H and C NMR data for three pairs of diastereomers of 4'-X benzo[1,3]cyclopropa[1,2-b]chromene-4,5-diones (X□=□H, OCH , and Cl). *Magnetic Resonance in Chemistry*, **2019**, 57, 512-521	2.1	3
815	Exploring N C tetrel and O S chalcogen bonds in HN(CH)SX:OCS systems, for X = F, NC, Cl, CN, CCH, and H. *Chemical Physics Letters*, **2019**, 730, 466-471	2.5	20
814	Ternary Complexes Stabilized by Chalcogen and Alkaline-Earth Bonds: Crucial Role of Cooperativity and Secondary Noncovalent Interactions. *Chemistry - A European Journal*, **2019**, 25, 11688-11695	4.8	13
813	Bond Length Alternation Observed Experimentally: The Case of 1H-Indazole. *Chemistry - A European Journal*, **2019**, 25, 10172-10178	4.8	4
812	Non-Covalent Interactions Involving Alkaline-Earth Atoms and Lewis Bases B: An ab Initio Investigation of Beryllium and Magnesium Bonds, B□□MR2 (M = Be or Mg, and R = H, F or CH3). *Inorganics*, **2019**, 7, 35	2.9	14
811	Can a Cl-H□□F Hydrogen Bond Replace a Cl□□F Halogen Bond? HXP:ClY:ZH versus HXP:ClY:HZ for Y, Z = F, Cl. *Journal of Physical Chemistry A*, **2019**, 123, 3992-3999	2.8	1
810	The extraordinary richness of the reaction between diazomethane and tetracyanoethylene: can computational calculations shed light on old papers?. *New Journal of Chemistry*, **2019**, 43, 7831-7838	3.6	1
809	Gas-phase reactivity tuned through the interaction with alkaline-earth derivatives. *Theoretical Chemistry Accounts*, **2019**, 138, 1	1.9	5
808	Recent developments in decarboxylative cross-coupling reactions between carboxylic acids and N-H compounds.. *RSC Advances*, **2019**, 9, 8964-8976	3.7	46
807	The structure of the anti-aging agent J147 used for treating Alzheimer's disease. *Acta Crystallographica Section C, Structural Chemistry*, **2019**, 75, 271-276	0.8	3

806	Direct C□H bond sulfenylation of (Het)arenes using sulfonyl hydrazides as thiol surrogate: a review. *Journal of Sulfur Chemistry*, **2019**, 40, 289-311	2.3	33
805	Multinuclear NMR spectra and GIAO/DFT calculations of N-benzylazoles and N-benzylbenzazoles. *Structural Chemistry*, **2019**, 30, 1729-1735	1.8	9
804	A chalcogen-bonded complex HN?S=C=S formed by ammonia and carbon disulfide characterised by chirped-pulse, broadband microwave spectroscopy. *Journal of Chemical Physics*, **2019**, 150, 084307	3.9	15
803	Understanding Regium Bonds and their Competition with Hydrogen Bonds in Au :HX Complexes. *ChemPhysChem*, **2019**, 20, 1572-1580	3.2	27
802	Recent trends in direct mono-, di-, and tri-fluoromethyl(thiol)ation of S-H bonds. *Journal of Sulfur Chemistry*, **2019**, 40, 565-585	2.3	17
801	Probing C?S chalcogen bonds in complexes SC:SHX, for X = NO2, NC, F, Cl, CN, CCH, and NH2. *Chemical Physics Letters*, **2019**, 721, 86-90	2.5	7
800	An Example of Polynomial Expansion: The Reaction of 3(5)-Methyl-1-Pyrazole with Chloroform and Characterization of the Four Isomers. *Molecules*, **2019**, 24,	4.8	3
799	Cations brought together by hydrogen bonds: the protonated pyridine-boronic acid dimer explained. *Physical Chemistry Chemical Physics*, **2019**, 21, 5796-5802	3.6	25
798	Methods for direct C(sp)-H bonds azidation.. *RSC Advances*, **2019**, 9, 25199-25215	3.7	25
797	Potential Energy Surfaces of HN(CH)SX:CO for X = F, Cl, NC, CN, CCH, and H: N□□C Tetrel Bonds and O□□S Chalcogen Bonds. *Journal of Physical Chemistry A*, **2019**, 123, 7270-7277	2.8	19
796	Prototropic tautomerism of the addition products of N-heterocyclic carbenes to CO2, CS2, and COS. *Structural Chemistry*, **2019**, 30, 1971-1979	1.8	3
795	Systematic behaviour of electron redistribution on formation of halogen-bonded complexes BXY, as determined via XY halogen nuclear quadrupole coupling constants. *Physical Chemistry Chemical Physics*, **2019**, 21, 16914-16922	3.6	2
794	Theoretical study of some □phosphinines and their NMR spectra. *Magnetic Resonance in Chemistry*, **2019**, 57, 975-981	2.1	4
793	Weak Interactions Get Strong: Synergy between Tetrel and Alkaline-Earth Bonds. *Journal of Physical Chemistry A*, **2019**, 123, 7124-7132	2.8	22
792	Understanding Regium Bonds and their Competition with Hydrogen Bonds in Au2:HX Complexes. *ChemPhysChem*, **2019**, 20, 1552-1552	3.2	2
791	Cross-Dehydrogenative Coupling Reactions Between C(sp)-H and X-H (X = N, P, S, Si, Sn) Bonds: An Environmentally Benign Access to Heteroatom-Substituted Alkynes. *Topics in Current Chemistry*, **2019**, 377, 20	7.2	25
790	A structural study of new tetrakis(1H-pyrazol-1-yl)methanes. *Tetrahedron*, **2019**, 75, 130690	2.4	2
789	Sequestration of CO by Phosphatrane Molecules. *ChemPhysChem*, **2019**, 20, 3195-3200	3.2	3

788	What Types of Noncovalent Bonds Stabilize Dimers (XCP), for X = CN, Cl, F, and H?. *Journal of Physical Chemistry A*, **2019**, 123, 10086-10094	2.8	3
787	Modulating intramolecular chalcogen bonds in aromatic (thio)(seleno)phene-based derivatives. *Physical Chemistry Chemical Physics*, **2019**, 21, 23645-23650	3.6	8
786	Relativistic Effects on NMR Parameters of Halogen-Bonded Complexes. *Molecules*, **2019**, 24,	4.8	5
785	A walk around the application of nanocatalysts for cross-dehydrogenative coupling of C-H bonds.. *RSC Advances*, **2019**, 9, 41684-41702	3.7	21
784	Immobilized TiO nanoparticles on carbon nanotubes: an efficient heterogeneous catalyst for the synthesis of chromeno[]pyridine derivatives under ultrasonic irradiation.. *RSC Advances*, **2019**, 9, 41868-41876	3.7	26
783	Pnicogen bonds in complexes with CO and CS: differentiating properties. *Molecular Physics*, **2019**, 117, 1117-1127	1.7	10
782	Interaction of N-Heterocyclic Carbenes and Simple Carbenes with Small Molecules (One to Three Atoms) Excluding Metals: Formation of Covalent C□ Bonds. *Journal of Heterocyclic Chemistry*, **2019**, 56, 359-370	1.9	3
781	Energetic, Topological and Electric Field Analyses of Cation-Cation Nucleic Acid Interactions in Watson-Crick Disposition. *ChemPhysChem*, **2019**, 20, 148-158	3.2	8
780	Transition metal-catalyzed intramolecular cyclization of N-Boc-protected propargyl/ethynyl amines: a novel and convenient access to 2-oxazolidinone/oxazolone derivatives. *Journal of the Iranian Chemical Society*, **2019**, 16, 617-627	2	9
779	Lin@Tetracyanoethylene (n = 1□4) systems: Lithium salt vs lithium electride. *Computational and Theoretical Chemistry*, **2019**, 1149, 17-23	2	6
778	A theoretical NMR study of polymorphism in crystal structures of azoles and benzazoles. *Magnetic Resonance in Chemistry*, **2019**, 57, 275-284	2.1	7
777	Adsorption sensitivity of pristine and Al- or Si-doped boron nitride nanoflake to COCl2: a DFT study. *Molecular Physics*, **2019**, 117, 626-634	1.7	9
776	Reaction of ClF and Cl2 with PH2X: The oxidation of P(III) to P(V). *Chemical Physics Letters*, **2019**, 715, 190-194	2.5	3
775	Electronic and Work Function-Based Sensors for Acetylsalicylic Acid Based on the AlN and BN Nanoclusters: DFT Studies. *Journal of Cluster Science*, **2019**, 30, 151-159	3	6
774	A relative energy gradient (REG) study of the planar and perpendicular torsional energy barriers in biphenyl. *Theoretical Chemistry Accounts*, **2019**, 138, 12	1.9	23
773	Complexes between H2 and neutral oxyacid beryllium derivatives. The role of angular strain. *Molecular Physics*, **2019**, 117, 1142-1150	1.7	5
772	S-arylation of 2-mercaptobenzazoles: a comprehensive review. *Journal of Sulfur Chemistry*, **2018**, 39, 443-463	2.3	26
771	Hydrogen and Halogen Bonding in Cyclic FH:FCl Complexes, for n = 0-4. *Journal of Physical Chemistry A*, **2018**, 122, 2587-2597	2.8	12

770	Recent advantages in the metal (bulk and nano)-catalyzed S-arylation reactions of thiols with aryl halides in water: a perfect synergy for eco-compatible preparation of aromatic thioethers. *Journal of Sulfur Chemistry*, **2018**, 39, 332-349	2.3	37
769	The structure of fosfomycin salts in solution and in the solid state by nuclear magnetic resonance spectroscopy and DFT calculations. *Tetrahedron*, **2018**, 74, 3937-3942	2.4	8
768	Weak interactions and cooperativity effects on disiloxane: a look at the building block of silicones. *Molecular Physics*, **2018**, 116, 1539-1550	1.7	8
767	Strengths of non-covalent interactions in hydrogen-bonded complexes B?HX and halogen-bonded complexes B?XY (X, Y = F, Cl): an ab initio investigation. *New Journal of Chemistry*, **2018**, 42, 10548-10554	3.6	12
766	Be- and Mg-Based Electron and Anion Sponges. *ChemPhysChem*, **2018**, 19, 1701-1706	3.2	5
765	The structures of 1,4-diaryl-5-trifluoromethyl-1H-1,2,3-triazoles related to J147, a drug for treating Alzheimer's disease. *Acta Crystallographica Section C, Structural Chemistry*, **2018**, 74, 513-522	0.8	5
764	Complexes of O=C=S with Nitrogen Bases: Chalcogen Bonds, Tetrel Bonds, and Other Secondary Interactions. *ChemPhysChem*, **2018**, 19, 1886	3.2	21
763	Synthesis, Structure and Anion Sensing Properties of a Dicationic Bis(imidazolium)-Based Cyclophane. *ChemistrySelect*, **2018**, 3, 3855-3859	1.8	5
762	Remote modulation of singlet□triplet gaps in carbenes. *Chemical Physics Letters*, **2018**, 694, 48-52	2.5	2
761	A vibrational circular dichroism (VCD) methodology for the measurement of enantiomeric excess in chiral compounds in the solid phase and for the complementary use of NMR and VCD techniques in solution: the camphor case. *Analyst, The*, **2018**, 143, 1406-1416	5	12
760	Trapping One Electron between Three Beryllium Atoms: Very Strong One-Electron Three-Center Bonds. *ChemPhysChem*, **2018**, 19, 1068-1074	3.2	5
759	Hydrogen-Bonding Acceptor Character of Be, the Beryllium Three-Membered Ring. *Journal of Physical Chemistry A*, **2018**, 122, 1472-1478	2.8	9
758	Alkaline-earth (Be, Mg and Ca) bonds at the origin of huge acidity enhancements. *Physical Chemistry Chemical Physics*, **2018**, 20, 2413-2420	3.6	25
757	Nanocatalysts for C□e cross-coupling reactions. *RSC Advances*, **2018**, 8, 291-301	3.7	32
756	Fostering the Basic Instinct of Boron in Boron-Beryllium Interactions. *Journal of Physical Chemistry A*, **2018**, 122, 3313-3319	2.8	5
755	The structure of 2,4,6-tris(1H□pyrazol-1-yl)-1,3,5-triazine in the solid state: on polymorphs, pseudopolymorphs and co-crystals. *Structural Chemistry*, **2018**, 29, 15-21	1.8	3
754	Molecular structure in the solid state by X-ray crystallography and SSNMR and in solution by NMR of two 1,4-diazepines. *Journal of Molecular Structure*, **2018**, 1155, 205-214	3.4	6
753	A LFER analysis of the singlet-triplet gap in a series of sixty-six carbenes. *Chemical Physics Letters*, **2018**, 691, 33-36	2.5	14

752	Intramolecular magnesium bonds in malonaldehyde-like systems: a critical view of the resonance-assisted phenomena. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	2
751	Decarboxylative cross-coupling reactions for P(O)-C bond formation.. *RSC Advances*, **2018**, 8, 26383-26398	3.7	35
750	The effect of electric field and Al doping on the sensitivity of hexa-peri-hexabenzocoronene nanographene to chloropicrin. *Applied Organometallic Chemistry*, **2018**, 32, e4486	3.1	9
749	Predicted Gas-Phase and Liquid-Phase Acidities of Carborane Carboxylic and Dicarboxylic Acids. *ChemistrySelect*, **2018**, 3, 4344-4353	1.8	3
748	Complexes of CO with the Azoles: Tetrel Bonds, Hydrogen Bonds and Other Secondary Interactions. *Molecules*, **2018**, 23,	4.8	26
747	Binding indirect greenhouse gases OCS and CS by nitrogen heterocyclic carbenes (NHCs). *Physical Chemistry Chemical Physics*, **2018**, 20, 19552-19559	3.6	10
746	A theoretical study of perovskites related to CH3NH3PbX3 (X = F, Cl, Br, I). *New Journal of Chemistry*, **2018**, 42, 13889-13898	3.6	10
745	Recent Advances in Synthesis of Functionalized Lactams through Cyclization of N-Propargyl Amine/Amide Derivatives. *Current Organic Chemistry*, **2018**, 22, 199-205	1.7	17
744	Intramolecular ipso-Cyclization of N-Arylpropiolamides: A Novel and Straightforward Synthetic Approach for Azaspiro[4.5]decatrien-2-ones. *Current Organic Chemistry*, **2018**, 22, 286-297	1.7	18
743	Nano-structured Catalytic Systems in Cyanation of Aryl Halides with K4[Fe(CN)6]. *Current Organic Chemistry*, **2018**, 22, 1862-1874	1.7	5
742	The Hydrogen-bond Basicity of Carbenes. *Croatica Chemica Acta*, **2018**, 91,	0.8	2
741	The Structure of N-phenyl-pyrazoles and Indazoles: Mononitro, Dinitro, and Trinitro Derivatives. *Journal of Heterocyclic Chemistry*, **2018**, 55, 44-64	1.9	7
740	A theoretical NMR study of selected benzazoles: Comparison of GIPAW and GIAO-PCM (DMSO) calculations. *Magnetic Resonance in Chemistry*, **2018**, 56, 164-171	2.1	13
739	Large Proton-Affinity Enhancements Triggered by Noncovalent Interactions. *Chemistry - A European Journal*, **2018**, 24, 1971-1977	4.8	14
738	Application of switchable solvent-based liquid phase microextraction for preconcentration and trace detection of cadmium ions in baby food samples. *Journal of the Iranian Chemical Society*, **2018**, 15, 491-498	2	15
737	An interacting quantum atom study of model S 2 reactions (X CH X, X = F, Cl, Br, and I). *Journal of Computational Chemistry*, **2018**, 39, 546-556	3.5	26
736	A Facile and Promising Synthetic Strategy toward Functionalized 2H-Chromenes from Aryl Propargyl Ethers. A Review. *Organic Preparations and Procedures International*, **2018**, 50, 544-564	1.1	2
735	Chemical Fixation of CO2 to Allylic (Allenylic) Amines: A Green Route to Synthesis of Functionalized 2-Oxazolidones. *Mini-Reviews in Organic Chemistry*, **2018**, 15, 315-323	1.7	18

734	Intramolecular Cyclization of Aryl Propargyl Ethers: A Straightforward and Convenient Approach to Benzofuran Derivatives. *Current Organic Synthesis*, **2018**, 15, 972-981	1.9	5
733	Metal Catalyzed Carboxylative Coupling of Terminal Alkynes, Organohalides and Carbon Dioxide: A Novel and Promising Synthetic Strategy Toward 2-Alkynoates (A Review). *Current Organic Chemistry* , **2018**, 22, 315-322	1.7	20
732	Competing Dispersive Interactions: From Small Energy Differences to Large Structural Effects in Methyl Jasmonate and Zingerone. *Journal of Physical Chemistry Letters*, **2018**, 9, 5906-5914	6.4	16
731	Cross-Dehydrogenative C-H/S-H Coupling Reactions. *Topics in Current Chemistry*, **2018**, 376, 39	7.2	55
730	Solvent and Substituent Effects on the Phosphine + CO2 Reaction. *Inorganics*, **2018**, 6, 110	2.9	4
729	A theoretical study of the properties of ninety-two aromatic six-membered rings including benzene, azines, phosphinines and azaphosphinines. *Heteroatom Chemistry*, **2018**, 29, e21441	1.2	4
728	The structure of four thallium tris(1H-pyrazol-1-yl)hydroborates in the solid state by X-ray crystallography and in solution by NMR and DFT-GIAO calculations. *Inorganica Chimica Acta*, **2018**, 483, 402-410	2.7	5
727	An Ab Initio Investigation of the Geometries and Binding Strengths of Tetrel-, Pnictogen-, and Chalcogen-Bonded Complexes of CO_2, NO, and CS_2 with Simple Lewis Bases: Some Generalizations. *Molecules*, **2018**, 23,	4.8	37
726	Using protonation to change a Cl?N halogen bond in N-Base:ClOH complexes to a Cl?O halogen bond. *Chemical Physics Letters*, **2018**, 710, 123-128	2.5	7
725	Cross-Dehydrogenative Coupling Reactions Between P(O)-H and X-H (X = S, N, O, P) Bonds. *Topics in Current Chemistry*, **2018**, 376, 23	7.2	49
724	Complexes between neutral oxyacid beryllium salts and dihydrogen: a possible way for hydrogen storage?. *Dalton Transactions*, **2018**, 47, 12516-12520	4.3	6
723	Recent advances in sulfur-nitrogen bond formation cross-dehydrogenative coupling reactions.. *RSC Advances*, **2018**, 8, 18456-18469	3.7	45
722	Diaryl ethers synthesis: nano-catalysts in carbon-oxygen cross-coupling reactions.. *RSC Advances*, **2018**, 8, 19125-19143	3.7	31
721	Libration of phenyl groups detected by VT-SSNMR: Comparison with X-ray crystallography. *Magnetic Resonance in Chemistry*, **2018**, 56, 1083-1088	2.1	2
720	Advancements in six-membered cyclic carbonate (1,3-dioxan-2-one) synthesis utilizing carbon dioxide as a C1 source.. *RSC Advances*, **2018**, 8, 17976-17988	3.7	39
719	Transition-metal-catalyzed C–N cross-coupling reactions of N-unsubstituted sulfoximines: a review. *Journal of Sulfur Chemistry*, **2018**, 39, 674-698	2.3	48
718	Enhancement of Thermodynamic Gas-Phase Acidity and Basicity of Water by Means of Secondary Interactions. *ChemPhysChem*, **2018**, 19, 2486-2491	3.2	2
717	Analysis of the interactions in FCCF:(H2O) and FCCF:(H2O)2 complexes through the study of their indirect spin–spin coupling constants. *Molecular Physics*, **2018**, 116, 2396-2405	1.7	6

716	Synthesis and characterization of a Ni nanoparticle stabilized on Ionic liquid-functionalized magnetic Silica nanoparticles for tandem oxidative reaction of primary alcohols. *Applied Organometallic Chemistry*, **2018**, 32, e4452	3.1	14
715	Green and recyclable sulfonated graphene and graphene oxide nanosheet catalysts for the syntheses of 3,4-dihydropyrimidinones. *Monatshefte F□ Chemie*, **2017**, 148, 321-326	1.4	14
714	New protocols to access imidazoles and their ring fused analogues: synthesis from N-propargylamines. *RSC Advances*, **2017**, 7, 7079-7091	3.7	56
713	Lone-Pair Hole on P: P□□N Pnicogen Bonds Assisted by Halogen Bonds. *Journal of Physical Chemistry A*, **2017**, 121, 1362-1370	2.8	26
712	Borylene as an electron-pair donor for P□ pnicogen bonds. *Structural Chemistry*, **2017**, 28, 1419-1427	1.8	14
711	A theoretical study of the H n F4□ Si:N-base (n = 1□) tetrel-bonded complexes. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	22
710	The structure of N-arylindazoles and their aza-derivatives in the solid state: A systematic analysis of the Cambridge Structural Database coupled with DFT calculations. *Journal of Molecular Structure*, **2017**, 1137, 186-192	3.4	3
709	N-Propargylic □enaminocarbonyls: powerful and versatile building blocks in organic synthesis. *RSC Advances*, **2017**, 7, 13198-13211	3.7	61
708	Eco-friendly synthesis of 3,4-dihydroquinoxalin-2-amine, diazepine-tetrazole and benzodiazepine-2-carboxamide derivatives with the aid of MCM-48/H5PW10V2O40. *Applied Organometallic Chemistry*, **2017**, 31, e3729	3.1	9
707	Is it possible to use the 31P chemical shifts of phosphines to measure hydrogen bond acidities (HBA)? A comparative study with the use of the 15N chemical shifts of amines for measuring HBA. *Journal of Physical Organic Chemistry*, **2017**, 30, e3690	2.1	5
706	Hydrogen-bonded complexes with carbenes as electron-pair donors. *Chemical Physics Letters*, **2017**, 675, 46-50	2.5	16
705	Trapping CO by Adduct Formation with Nitrogen Heterocyclic Carbenes (NHCs): A Theoretical Study. *Chemistry - A European Journal*, **2017**, 23, 10604-10609	4.8	31
704	Carbenes as Electron-Pair Donors To CO for C□□C Tetrel Bonds and C-C Covalent Bonds. *Journal of Physical Chemistry A*, **2017**, 121, 4039-4047	2.8	38
703	Curcumin Related 1,4-Diazepines: Regioselective Synthesis, Structure Analysis, Tautomerism, NMR Spectroscopy, X-ray Crystallography, Density Functional Theory and GIAO Calculations. *ChemistrySelect*, **2017**, 2, 3732-3738	1.8	5
702	Supramolecular organization of perfluorinated 1H-indazoles in the solid state using X-ray crystallography, SSNMR and sensitive (VCD) and non sensitive (MIR, FIR and Raman) to chirality vibrational spectroscopies. *Physical Chemistry Chemical Physics*, **2017**, 19, 1632-1643	3.6	14
701	A theoretical study on the electronic sensitivity of the pristine and Al-doped B24N24 nanoclusters to F2CO and Cl2CO gases. *Structural Chemistry*, **2017**, 28, 1919-1926	1.8	5
700	Intramolecular cyclization of N-allyl propiolamides: a facile synthetic route to highly substituted □lactams (a review). *RSC Advances*, **2017**, 7, 28407-28418	3.7	35
699	Carbenes as Electron-Pair Donors for P???C Pnicogen Bonds. *ChemPhysChem*, **2017**, 18, 1597-1610	3.2	21

698	The organic chemistry of poly(1 H -pyrazol-1-yl)methanes. *Coordination Chemistry Reviews*, **2017**, 339, 153-182	23.2	27
697	Yolk-Shell Fe3O4-Polyaniline Decorated Pd-Ni Nanoparticles with Enhanced Performance for Direct Formic Acid Fuel Cell. *Nano*, **2017**, 12, 1750016	1.1	3
696	Azines as Electron-Pair Donors to CO for N⋯C Tetrel Bonds. *Journal of Physical Chemistry A*, **2017**, 121, 8017-8025	2.8	25
695	Carbon-Carbon Bonding between Nitrogen Heterocyclic Carbenes and CO. *Journal of Physical Chemistry A*, **2017**, 121, 8136-8146	2.8	34
694	Intramolecular Cyclization of N-Arylpropiolamides: A New Strategy for the Synthesis of Functionalized 2-Quinolones. *Current Organic Chemistry*, **2017**, 21,	1.7	10
693	Theoretical Study of Intramolecular Interactions in Peri-Substituted Naphthalenes: Chalcogen and Hydrogen Bonds. *Molecules*, **2017**, 22,	4.8	16
692	Are beryllium-containing biphenyl derivatives efficient anion sponges?. *Journal of Molecular Modeling*, **2017**, 24, 16	2	6
691	Intramolecular cyclization of N-propargyl anilines: a new synthetic entry into highly substituted indoles. *Journal of the Iranian Chemical Society*, **2017**, 14, 2339-2353	2	15
690	Simultaneous Occurrence of Quadruple Lewis Acid-Base Interactions between Selenium Atoms in Selenocarbonyl Dimers. *ChemPhysChem*, **2017**, 18, 3498-3503	3.2	5
689	Modulating the Proton Affinity of Silanol and Siloxane Derivatives by Tetrel Bonds. *Journal of Physical Chemistry A*, **2017**, 121, 7424-7431	2.8	14
688	Transition metal-catalyzed [2 + 2 + 2] cycloaddition of nitrogen-linked 1,6-diynes: a straightforward route to fused pyrrolidine systems. *RSC Advances*, **2017**, 7, 43716-43736	3.7	35
687	Nanocomposite of ZIF-67 metal□rganic framework with reduced graphene oxide nanosheets for high-performance supercapacitor applications. *Journal of Materials Science: Materials in Electronics*, **2017**, 28, 18040-18048	2.1	47
686	Hydrogen Bond versus Halogen Bond in Cation-Cation Complexes: Effect of the Solvent. *ChemPhysChem*, **2017**, 18, 3462-3468	3.2	28
685	The Curious Case of 2-Propyl-1H-benzimidazole in the Solid State: An Experimental and Theoretical Study. *Journal of Physical Chemistry A*, **2017**, 121, 5665-5674	2.8	9
684	Using one halogen bond to change the nature of a second bond in ternary complexes with PCl and FCl halogen bonds. *Faraday Discussions*, **2017**, 203, 29-45	3.6	15
683	Halogen bonding with carbene bases. *Chemical Physics Letters*, **2017**, 685, 338-343	2.5	11
682	Activation of Dinitrogen as A Dipolarophile in 1,3-Dipolar Cycloadditions: A Theoretical Study Using Nitrile Imines as "Octet" 1,3-Dipoles. *Scientific Reports*, **2017**, 7, 6115	4.9	7
681	Modulation of in:out and out:out conformations in [X.X'.X''] phosphatranes by Lewis acids. *Physical Chemistry Chemical Physics*, **2017**, 19, 20647-20656	3.6	2

680	Beryllium-based fluorenes as efficient anion sponges. *Physical Chemistry Chemical Physics*, **2017**, 19, 23052-23059	3.6	10
679	Adsorption and decomposition of formaldehyde on the B12N12 nanostructure: a density functional theory study. *Monatshefte F□ Chemie*, **2017**, 148, 1727-1731	1.4	16
678	Enhancing Intramolecular Chalcogen Interactions in 1-Hydroxy-8-YH-naphthalene Derivatives. *Journal of Physical Chemistry A*, **2017**, 121, 8995-9003	2.8	8
677	A Density Functional Theory Study on the Interaction Between 5-Fluorouracil Drug and C24 Fullerene. *Journal of Cluster Science*, **2017**, 28, 2681-2692	3	14
676	Nitroxide stable radicals interacting as Lewis bases in hydrogen bonds: A search in the Cambridge structural data base for intermolecular contacts. *Journal of Molecular Structure*, **2017**, 1148, 150-161	3.4	4
675	Selective sensing of ozone and the chemically active gaseous species of the troposphere by using the C fullerene and graphene segment. *Talanta*, **2017**, 162, 505-510	6.2	43
674	Environmentally friendly and highly efficient synthesis of benzoxazepine and malonamide derivatives using HPA/TPI-Fe3O4 nanoparticles as recoverable catalyst in aqueous media. *Applied Organometallic Chemistry*, **2017**, 31, e3603	3.1	8
673	A DFT study on electronic and optical properties of aspirin-functionalized B12N12 fullerene-like nanocluster. *Structural Chemistry*, **2017**, 28, 735-748	1.8	53
672	An insight on the aromatic changes in closed shell icosagen, tetrel, and pnictogen phenalenyl derivatives. *Structural Chemistry*, **2017**, 28, 345-355	1.8	5
671	An ab initio study on substituent and cooperative effects in bifurcated fluorine bonds. *Molecular Physics*, **2017**, 115, 278-287	1.7	4
670	Nucleophilicities of Lewis Bases B and Electrophilicities of Lewis Acids A Determined from the Dissociation Energies of Complexes B?A Involving Hydrogen Bonds, Tetrel Bonds, Pnictogen Bonds, Chalcogen Bonds and Halogen Bonds. *Molecules*, **2017**, 22,	4.8	21
669	Halogen Bonding Involving CO and CS with Carbon as the Electron Donor. *Molecules*, **2017**, 22,	4.8	12
668	F-NMR Diastereotopic Signals in Two N-CHF□Derivatives of (4S,7R)-7,8,8-Trimethyl-4,5,6,7-tetrahydro-4,7-methano-2H-indazole. *Molecules*, **2017**, 22,	4.8	7
667	Properties of cationic pnicogen-bonded complexes F4-nHnP+:N-base with H□□□N linear and n = 1□. *Molecular Physics*, **2016**, 114, 102-117	1.7	11
666	A computational study on [(PH2X)2]□+ homodimers involving intermolecular two-center three-electron bonds. *Structural Chemistry*, **2016**, 27, 753-762	1.8	9
665	A theoretical evidence for cooperative enhancement in aerogen-bonding interactions: Open-chain clusters of KrOF2 and XeOF2. *Chemical Physics Letters*, **2016**, 662, 80-85	2.5	30
664	The strengthening effect of a hydrogen or lithium bond on the Z□□N aerogen bond (Z = Ar, Kr and Xe): a comparative study. *Molecular Physics*, **2016**, 114, 3265-3276	1.7	15
663	Cation-cation and anion-anion complexes stabilized by halogen bonds. *Physical Chemistry Chemical Physics*, **2016**, 18, 27939-27950	3.6	40

662	The Thermodynamic Stability of Adamantylideneadamantane and Its Proton- and Electron-Exchanges. Comparison with Simple Alkenes. *Bulletin of the Chemical Society of Japan*, **2016**, 89, 762-769	5.1	4
661	Maximizing the solar energy storage of the four substituted norbornadiene-quadricyclane system: DFT calculations. *Russian Journal of Physical Chemistry A*, **2016**, 90, 136-143	0.7	10
660	Structure, binding energy and chiral discrimination in oxathiirane homodimers. *Computational and Theoretical Chemistry*, **2016**, 1090, 171-179	2	7
659	Boron as an Electron-Pair Donor for B???Cl Halogen Bonds. *ChemPhysChem*, **2016**, 17, 3112-3119	3.2	21
658	New page to access pyridine derivatives: synthesis from N-propargylamines. *RSC Advances*, **2016**, 6, 71662-71676	3.7	66
657	The structures of two scorpionates: thallium tetrakis(3-phenyl-1H-pyrazol-1-yl)borate and potassium tetrakis(3-cyclopropyl-1H-pyrazol-1-yl)borate. *Acta Crystallographica Section C, Structural Chemistry*, **2016**, 72, 819-825	0.8	3
656	The structure of 4,5,6,7-tetrafluoro-1H-benzotriazole in solid state and in solution. *Journal of Fluorine Chemistry*, **2016**, 192, 98-104	2.1	5
655	Is there theoretical evidence for mutual influence between halogen and pnicogen-hydride bonds? An ab initio study. *Journal of Chemical Sciences*, **2016**, 128, 1905-1912	1.8	1
654	Unusual acid-base properties of the P molecule in hydrogen-, halogen-, and pnicogen-bonded complexes. *Physical Chemistry Chemical Physics*, **2016**, 18, 32593-32601	3.6	16
653	Platinum nanoparticles supported on polymeric ionic liquid functionalized magnetic silica: effective and reusable heterogeneous catalysts for the selective oxidation of alcohols in water. *RSC Advances*, **2016**, 6, 106769-106777	3.7	10
652	Beryllium-Based Anion Sponges: Close Relatives of Proton Sponges. *Chemistry - A European Journal*, **2016**, 22, 18322-18325	4.8	21
651	Essential versus accidental isochrony of diastereotopic nuclei in NMR spectroscopy. *Structural Chemistry*, **2016**, 27, 671-679	1.8	2
650	A computational study of azaphospholes: anions and neutral tautomers. *Structural Chemistry*, **2016**, 27, 1531-1542	1.8	5
649	Aromatic changes in isoelectronic derivatives of phenalenyl radicals by central carbon replacement. *Tetrahedron*, **2016**, 72, 4690-4699	2.4	7
648	Charged versus Neutral Hydrogen-Bonded Complexes: Is There a Difference in the Nature of the Hydrogen Bonds?. *Chemistry - A European Journal*, **2016**, 22, 9226-34	4.8	66
647	Fullerene and corannulene derivatives acting as insulators of Cl(-) and BeH2. *Physical Chemistry Chemical Physics*, **2016**, 18, 6059-68	3.6	5
646	Cooperativity in Tetrel Bonds. *Journal of Physical Chemistry A*, **2016**, 120, 648-56	2.8	88
645	The structure of β-diketones related to curcumin determined by X-ray crystallography, NMR (solution and solid state) and theoretical calculations. *Structural Chemistry*, **2016**, 27, 705-730	1.8	16

644	Interaction of beryllium derivatives with N-methylated DNA bases: 9-methylguanine and 1-methylcytosine. *Tetrahedron*, **2016**, 72, 1978-1983	2.4	4
643	Theoretical studies on the conformation of large carbocyclic rings. I. 5,6,11,12,17,18-Hexahydrotribenzo[a,e,i]cyclododecane (1,2;5,6;9,10-tribenzododeca-1,5,8-triene). *Tetrahedron Letters*, **2016**, 57, 1838-1842	2	1
642	Halogen bonding. The role of the polarizability of the electron-pair donor. *Physical Chemistry Chemical Physics*, **2016**, 18, 7300-9	3.6	38
641	The structure and properties of 5,6-dinitro-1H-benzotriazole. *Journal of Molecular Structure*, **2016**, 1113, 153-161	3.4	7
640	Modulating intramolecular P□□N pnictogen interactions. *Physical Chemistry Chemical Physics*, **2016**, 18, 9148-60	3.6	26
639	A novel multicomponent reaction between amino acids, aromatic aldehydes and p-toluenesulfonylmethyl isocyanide: an efficient and green one-pot synthesis using nanosilica. *Green Chemistry Letters and Reviews*, **2016**, 9, 13-19	4.7	4
638	Aromaticity of benzenoid hydrocarbons with inserted B=B□and B□HB□H□groups: a comparison. *Structural Chemistry*, **2016**, 27, 91-99	1.8	3
637	The effect of cytosine methylation on its halogen-bonding properties. *Computational and Theoretical Chemistry*, **2016**, 1076, 101-108	2	11
636	A new avenue to the synthesis of highly substituted pyrroles: synthesis from N-propargylamines. *RSC Advances*, **2016**, 6, 18619-18631	3.7	88
635	A Proof of Concept: 2-Pyrazolines (4,5-Dihydro-1H-pyrazoles) Can Be Used as Organocatalysts via Iminium Activation. *Letters in Organic Chemistry*, **2016**, 13, 414-419	0.6	1
634	H2XP:OH2 Complexes: Hydrogen vs. Pnicogen Bonds. *Crystals*, **2016**, 6, 19	2.3	16
633	B4H4 and B4(CH3)4 as Unique Electron Donors in Hydrogen-Bonded and Halogen-Bonded Complexes. *Journal of Physical Chemistry A*, **2016**, 120, 5745-51	2.8	15
632	Exergonic and Spontaneous Production of Radicals through Beryllium Bonds. *Angewandte Chemie - International Edition*, **2016**, 55, 8736-9	16.4	21
631	Saddle-Shaped Cyclic Indole Tetramers: 3D Electroactive Molecules. *Chemistry - A European Journal*, **2016**, 22, 10651-60	4.8	4
630	The Conformational Map of Volatile Anesthetics: Enflurane Revisited. *Chemistry - A European Journal*, **2016**, 22, 9804-11	4.8	4
629	The (1) H NMR spectrum of pyrazole in a nematic phase. *Magnetic Resonance in Chemistry*, **2016**, 54, 637-40	2.2	5
628	On the existence of intramolecular one-electron Be-Be bonds. *Chemical Communications*, **2016**, 52, 9656-9	5.8	25
627	Highly solvatochromic and tunable fluorophores based on a 4,5-quinolimide scaffold: novel CDK5 probes. *Chemical Communications*, **2016**, 52, 9652-5	5.8	18

626	Host-Guest Chemistry: Oxoanion Recognition Based on Combined Charge-Assisted C-H or Halogen-Bonding Interactions and Anion???Anion Interactions Mediated by Hydrogen Bonds. *Chemistry - A European Journal*, **2016**, 22, 7533-44	4.8	37
625	Using (FH)2 and (FH)3 to Bridge the Hole and the Lone Pair at P in Complexes with H2 XP, for X=CH3 , OH, H, CCH, F, Cl, NC, and CN. *ChemPhysChem*, **2016**, 17, 1475-85	3.2	2
624	Exergonic and Spontaneous Production of Radicals through Beryllium Bonds. *Angewandte Chemie*, **2016**, 128, 8878-8881	3.6	8
623	A theoretical and experimental NMR study of BODIPY 493/503: difluoro{2-[1-(3,5-dimethyl-2H-pyrrol-2-ylidene-N)ethyl]-3,5-dimethyl-1H-pyrrolato-N}boron. *Magnetic Resonance in Chemistry*, **2016**, 54, 684-8	2.1	7
622	Symmetric bifurcated halogen bonds: substituent and cooperative effects. *Molecular Physics*, **2016**, 114, 3610-3619	1.7	4
621	Oxime ethers as useful synthons in the synthesis of a number of key medicinal heteroaromatic compounds. *Journal of the Iranian Chemical Society*, **2016**, 13, 1235-1256	2	25
620	Anionic complexes of F and Cl with substituted methanes: Hydrogen, halogen, and tetrel bonds. *Chemical Physics Letters*, **2016**, 655-656, 115-119	2.5	35
619	An ab initio study on the nature of hole interactions in pnicogen-bonded complexes with carbene as an electron donor. *Molecular Physics*, **2016**, 114, 2115-2122	1.7	15
618	Insight into the intermolecular interactions in the NF3HSO system: a computational study. *Journal of Sulfur Chemistry*, **2016**, 37, 674-682	2.3	
617	Competition between intramolecular hydrogen and pnictogen bonds in protonated systems. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	5
616	Novel routes to quinoline derivatives from N-propargylamines. *RSC Advances*, **2016**, 6, 49730-49746	3.7	66
615	New route to 1,4-oxazepane and 1,4-diazepane derivatives: synthesis from N-propargylamines. *RSC Advances*, **2016**, 6, 99781-99793	3.7	44
614	Comparative Study of Charge-Assisted Hydrogen- and Halogen-Bonding Capabilities in Solution of Two-Armed Imidazolium Receptors toward Oxoanions. *Journal of Organic Chemistry*, **2016**, 81, 7448-58	4.2	29
613	(15)N NMR Spectroscopy, X-ray and Neutron Diffraction, Quantum-Chemical Calculations, and UV/vis-Spectrophotometric Titrations as Complementary Techniques for the Analysis of Pyridine-Supported Bicyclic Guanidine Superbases. *Journal of Organic Chemistry*, **2016**, 81, 7612-25	4.2	25
612	Possibility of sensing, adsorbing, and destructing the Tabun-2D-skeletal (Tabun nerve agent) by C20 fullerene and its boron and nitrogen doped derivatives. *Synthetic Metals*, **2016**, 220, 606-611	3.6	49
611	Static and Dynamic Properties of Fluorinated 4-Aryl-1,5-Benzodiazepinones. *ChemistrySelect*, **2016**, 1, 861-870	1.8	7
610	Weak interactions within nitryl halide heterodimers. *New Journal of Chemistry*, **2016**, 40, 9060-9072	3.6	6
609	Chalcogen bonds in complexes of SOXY (X, Y = F, Cl) with nitrogen bases. *Journal of Physical Chemistry A*, **2015**, 119, 535-41	2.8	52

608	Ab initio study in the hydration process of metaphosphoric acid: the importance of the pnictogen interactions. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	6
607	P□□N pnicogen bonds in cationic complexes of F□+ and F□P+ with nitrogen bases. *Journal of Physical Chemistry A*, **2015**, 119, 3125-33	2.8	35
606	Theoretical study of the geometrical, energetic and NMR properties of atranes. *Journal of Organometallic Chemistry*, **2015**, 794, 206-215	2.3	24
605	Synthesis, structure and biological activity of 3(5)-trifluoromethyl-1H-pyrazoles derived from hemicurcuminoids. *Journal of Molecular Structure*, **2015**, 1100, 518-529	3.4	13
604	The influence of intermolecular halogen bonds on the tautomerism of nucleobases. I. Guanine. *Tetrahedron*, **2015**, 71, 5260-5266	2.4	6
603	Halogen, chalcogen and pnictogen interactions in (XNO2)2 homodimers (X = F, Cl, Br, I). *New Journal of Chemistry*, **2015**, 39, 6791-6802	3.6	42
602	Interplay between Beryllium Bonds and Anion-□Interactions in BeR2:C6X6:Y- Complexes (R = H, F and Cl, X = H and F, and Y = Cl and Br). *Molecules*, **2015**, 20, 9961-76	4.8	10
601	The influence of halogen bonds on tautomerism: the case of 3-mercapto-1,2-azoles (pyrazoles, isoxazoles, isothiazoles). *Structural Chemistry*, **2015**, 26, 639-645	1.8	7
600	The interaction energies between glycoluril clip and thiophenol derivatives using density functional theory calculations. *Journal of Sulfur Chemistry*, **2015**, 36, 351-357	2.3	7
599	Adding Only One Priority Rule Allows Extending CIP Rules to Supramolecular Systems. *Chirality*, **2015**, 27, 339-43	2.1	6
598	Double Hole-Lump Interaction between Halogen Atoms. *Journal of Physical Chemistry A*, **2015**, 119, 3746-52	2.8	26
597	Can HN[double bond, length as m-dash]NH, FN[double bond, length as m-dash]NH, or HN[double bond, length as m-dash]CHOH bridge the □hole and the lone pair at P in binary complexes with H2XP, for X = F, Cl, NC, OH, CN, CCH, CH3, and H?. *Physical Chemistry Chemical Physics*, **2015**, 17, 30729-35	3.6	14
596	Lowering the pKa of a bisimidazoline lead with halogen atoms results in improved activity and selectivity against Trypanosoma brucei in vitro. *European Journal of Medicinal Chemistry*, **2015**, 101, 806-17	6.8	20
595	Dual Role of the 1,2,3-Triazolium Ring as a Hydrogen-Bond Donor and Anion-□Receptor in Anion-Recognition Processes. *Chemistry - A European Journal*, **2015**, 21, 9797-808	4.8	41
594	Exploring the PX3:NCH and PX3:NH3 potential surfaces, with X = F, Cl, and Br. *Chemical Physics Letters*, **2015**, 641, 84-89	2.5	24
593	Exploring the (H2C?PH2)(+):N-Base Potential Surfaces: Complexes Stabilized by Pnicogen, Hydrogen, and Tetrel Bonds. *Journal of Physical Chemistry A*, **2015**, 119, 11701-10	2.8	24
592	Linear free-energy relationships between a single gas-phase ab initio equilibrium bond length and experimental pKa values in aqueous solution. *ChemPhysChem*, **2015**, 16, 465-9	3.2	11
591	Using beryllium bonds to change halogen bonds from traditional to chlorine-shared to ion-pair bonds. *Physical Chemistry Chemical Physics*, **2015**, 17, 2259-67	3.6	45

590	The paradox of hydrogen-bonded anion-anion aggregates in oxoanions: a fundamental electrostatic problem explained in terms of electrophilic□□nucleophilic interactions. *Journal of Physical Chemistry A*, **2015**, 119, 183-94	2.8	79
589	Substituent effects on the properties of pnicogen-bonded complexes H□P:PYH□for X, Y = F, Cl, OH, NC, CCH, CH□CN, and H. *Journal of Physical Chemistry A*, **2015**, 119, 224-33	2.8	35
588	An NMR and Computational Study of Azolo[a]pyrimidines with Special Emphasis on Pyrazolo[1,5-a]pyrimidines. *Journal of Heterocyclic Chemistry*, **2015**, 52, 336-345	1.9	10
587	Theoretical study of cyanophosphines: Pnicogen vs. dipole□dipole interactions. *Computational and Theoretical Chemistry*, **2015**, 1053, 305-314	2	18
586	Simultaneous aromatic-beryllium bonds and aromatic-anion interactions: naphthalene and pyrene as models of fullerenes, carbon single-walled nanotubes, and graphene. *ChemPhysChem*, **2015**, 16, 2680-6	3.2	8
585	A theoretical and experimental study of the NMR spectra of 4,5,6,7-tetrafluorobenzazoles with special stress on PCM calculations of chemical shifts. *Magnetic Resonance in Chemistry*, **2015**, 53, 353-62	2.1	15
584	Observation of diastereotopic signals in (15) N NMR spectroscopy. *Angewandte Chemie - International Edition*, **2015**, 54, 3997-4000	16.4	4
583	Creating □holes through the formation of beryllium bonds. *Chemistry - A European Journal*, **2015**, 21, 12676-82	4.8	32
582	Observation of Diastereotopic Signals in 15N NMR Spectroscopy. *Angewandte Chemie*, **2015**, 127, 4069-4072	5.6	
581	Understanding the Aldo-Enediolate Tautomerism of Glycolaldehyde in Basic Aqueous Solutions. *ChemPhysChem*, **2015**, 16, 2226-36	3.2	6
580	Computational Study of Proton Transfer in Tautomers of 3- and 5-Hydroxypyrazole Assisted by Water. *ChemPhysChem*, **2015**, 16, 2140-50	3.2	12
579	A multinuclear magnetic resonance study of fluoro derivatives of hydroxybenzaldehydes. *Magnetic Resonance in Chemistry*, **2015**, 53, 624-31	2.1	2
578	Application of Si-doped graphene as a metal-free catalyst for decomposition of formic acid: A theoretical study. *International Journal of Quantum Chemistry*, **2015**, 115, 1153-1160	2.1	22
577	THE TAUTOMERISM OF PYRAZOLINES (DIHYDROPYRAZOLES). *Journal of the Chilean Chemical Society*, **2015**, 60, 2966-2970	2.5	5
576	The intermolecular interaction studies in the complexes of isothiocyanic acid (HNCS) and its derivatives with H2S: a computational study. *Journal of Sulfur Chemistry*, **2015**, 36, 207-215	2.3	2
575	Crystal and molecular structures of two 1H-2-substituted benzimidazoles. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2015**, 230,	1	7
574	Influence of fluoro and cyano substituents in the aromatic and antiaromatic characteristics of cyclooctatetraene. *Physical Chemistry Chemical Physics*, **2015**, 17, 14961-71	3.6	9
573	The Pnicogen Bond in Review: Structures, Binding Energies, Bonding Properties, and Spin-Spin Coupling Constants of Complexes Stabilized by Pnicogen Bonds. *Challenges and Advances in Computational Chemistry and Physics*, **2015**, 191-263	0.7	50

572	Properties of Cationic Pnicogen-Bonded Complexes F(4-n)H(n)P(+):N-Base with F-P□□N Linear and n = 0-3. *Journal of Physical Chemistry A*, **2015**, 119, 5853-64	2.8	42
571	Pnicogen and hydrogen bonds: complexes between PH3X(+) and PH2X systems. *Physical Chemistry Chemical Physics*, **2015**, 17, 3261-72	3.6	68
570	Diazole-based powdered cocrystal featuring a helical hydrogen-bonded network: structure determination from PXRD, solid-state NMR and computer modeling. *Solid State Nuclear Magnetic Resonance*, **2015**, 65, 49-63	3.1	22
569	A theoretical study of the gas phase (proton affinity) and aqueous (pKa) basicity of a series of 150 pyrazoles. *New Journal of Chemistry*, **2015**, 39, 2861-2871	3.6	16
568	Cooperative interaction between hydrogen bond and N□□Y interactions (Y = H, Li, F, Cl, and Br): a comparative study. *Canadian Journal of Chemistry*, **2015**, 93, 626-631	0.9	
567	Sensing and catalytic decomposition of hydrogen peroxide by silicon carbide nanotubes: A DFT study. *International Journal of Quantum Chemistry*, **2015**, 115, 471-476	2.1	6
566	Experimental and theoretical studies on the rearrangement of 2-oxoazepane □-amino acids into 2'-oxopiperidine □(2,3,3) -amino acids: an example of intramolecular catalysis. *Chemistry - A European Journal*, **2015**, 21, 2489-500	4.8	3
565	An experimental and theoretical study of the structure of Lamotrigine in its neutral and protonated forms: evidence of Lamotrigine enantiomers. *Tetrahedron*, **2014**, 70, 2784-2795	2.4	13
564	□ and □ pnicogen bonds in complexes H2XP:PCX, for X = F, Cl, OH, NC, CN, CCH, CH3, and H. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	24
563	A theoretical study of the structure and protonation of Palbociclib (PD 0332991). *Journal of Molecular Structure*, **2014**, 1056-1057, 209-215	3.4	8
562	Cooperativity in beryllium bonds. *Physical Chemistry Chemical Physics*, **2014**, 16, 4305-12	3.6	32
561	Spontaneous proton transfers induced by beryllium bondsView all notes. *Molecular Physics*, **2014**, 112, 592-600	1.7	27
560	A theoretical study of the thermodynamic and hydrogen-bond basicity of TEMPO radical and related nitroxides. *Structural Chemistry*, **2014**, 25, 1873-1880	1.8	6
559	On the transferability of atomic contributions to the optical rotatory power of hydrogen peroxide, methyl hydroperoxide and dimethyl peroxide. *Molecular Physics*, **2014**, 112, 1624-1632	1.7	3
558	Open bis(triazolium) structural motifs as a benchmark to study combined hydrogen- and halogen-bonding interactions in oxoanion recognition processes. *Journal of Organic Chemistry*, **2014**, 79, 6959-69	4.2	72
557	Carbohydrates in the gas phase: conformational preference of D-ribose and 2-deoxy-D-ribose. *New Journal of Chemistry*, **2014**, 38, 529-538	3.6	21
556	Discovery of anion-□ interactions in the recognition mechanism of inorganic anions by 1,2,3-triazolium rings. *Chemical Communications*, **2014**, 50, 4680-2	5.8	26
555	Ramsey terms for two-, three-, and four-bond coupling involving 15N and 17O in hydrogen-bonded and nonhydrogen-bonded systems: are coupling constants sensitive to RAHBs?. *Molecular Physics*, **2014**, 112, 107-116	1.7	12

554	On the intermolecular interactions of isothiocyanic acid (HNCS) with disulfur monoxide (SSO): a first principles approach. *Journal of Sulfur Chemistry*, **2014**, 35, 484-492	2.3	5
553	Static and dynamic properties of 1,1'-bi-2-naphthol and its conjugated acids and bases. *Chemistry - A European Journal*, **2014**, 20, 14816-25	4.8	9
552	A computational study on 3-azonia-, 3-phosphonia-, and 3-arsoniaspiro[2.2]pentanes and related three-membered heterocycles. *ChemPhysChem*, **2014**, 15, 3493-501	3.2	1
551	Arene□Ruthenium Chemistry and Brønsted Acid Catalysis of a Chiral Phosphane-Hydroxyl Ligand. *Organometallics*, **2014**, 33, 616-619	3.8	16
550	Pnicogen-bonded anionic complexes. *Journal of Physical Chemistry A*, **2014**, 118, 3386-92	2.8	66
549	Characterizing traditional and chlorine-shared halogen bonds in complexes of phosphine derivatives with ClF and Cl2. *Journal of Physical Chemistry A*, **2014**, 118, 4222-31	2.8	32
548	The origin of the splitting of 13C and 15N NMR signals of 3(5)-phenyl-5(3)-methylpyrazolium chloride and bromide in the solid state: Quantum Espresso calculations. *Journal of Molecular Structure*, **2014**, 1075, 551-558	3.4	8
547	A theoretical and experimental study of the racemization process of hexaaza[5]helicenes. *Tetrahedron*, **2014**, 70, 8750-8757	2.4	3
546	Pnicogen bonds between X?PH3 (X = O, S, NH, CH2) and phosphorus and nitrogen bases. *Journal of Physical Chemistry A*, **2014**, 118, 1527-37	2.8	73
545	Traditional and ion-pair halogen-bonded complexes between chlorine and bromine derivatives and a nitrogen-heterocyclic carbene. *Journal of Physical Chemistry A*, **2014**, 118, 9552-60	2.8	33
544	Synthesis of the glycoluril derivatives by the HZSM-5 nanozeolite as a catalyst. *Green Chemistry Letters and Reviews*, **2014**, 7, 119-125	4.7	8
543	Heteroatom effects in XC5H5C Arduengo-type carbenes (X = CH, N, P, and As) in singlet and triplet states. *Russian Journal of Physical Chemistry A*, **2014**, 88, 1138-1141	0.7	
542	Neutral alkaline-metal and alkaline-earth-metal derivatives of imidazole and benzimidazole. *Journal of Physical Chemistry A*, **2014**, 118, 4195-204	2.8	5
541	Aromaticity and Magnetic Properties of 1- and 2-Indenones and Their Aza Derivatives. *European Journal of Organic Chemistry*, **2014**, 2014, 5370-5377	3.2	4
540	Single electron pnicogen bonded complexes. *Journal of Physical Chemistry A*, **2014**, 118, 947-53	2.8	78
539	Chiral self-assembly of enantiomerically pure (4S,7R)-campho[2,3-c]pyrazole in the solid state: a vibrational circular dichroism (VCD) and computational study. *Tetrahedron: Asymmetry*, **2014**, 25, 507-515		10
538	Intramolecular pnicogen interactions in phosphorus and arsenic analogues of proton sponges. *Physical Chemistry Chemical Physics*, **2014**, 16, 15900-9	3.6	53
537	Influence of substituent effects on the formation of P□□Cl pnicogen bonds or halogen bonds. *Journal of Physical Chemistry A*, **2014**, 118, 2360-6	2.8	67

536	Adamantyl analogues of paracetamol as potent analgesic drugs via inhibition of TRPA1. *PLoS ONE*, **2014**, 9, e113841	3.7	11
535	Noncovalent interactions in dimers and trimers of SO3 and CO. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	56
534	Nanostructured Poly (2,2?-bithiophene)-co-(3-dodecylthiophene): Preparation, Investigation of the Electroactivity, Conductivity, and Morphology. *International Journal of Polymeric Materials and Polymeric Biomaterials*, **2014**, 63, 323-329	3	2
533	Some Interesting Features of Non-Covalent Interactions. *Croatica Chemica Acta*, **2014**, 87, 291-306	0.8	11
532	An exploration of the ozone dimer potential energy surface. *Journal of Chemical Physics*, **2014**, 140, 2443[illegible]	3.1	7
531	Strongly bound noncovalent (SO3)n:H2CO complexes (n = 1, 2). *Physical Chemistry Chemical Physics*, **2014**, 16, 18974-81	3.6	40
530	Chiral discrimination in dimers of diphosphines PH□PH□ and PH□PHF. *ChemPhysChem*, **2014**, 15, 3663-70	3.2	10
529	A Spectroscopic Study of Colchicine in the Solid State and in Solution by Multinuclear Magnetic Resonance and Vibrational Circular Dichroism. *Helvetica Chimica Acta*, **2014**, 97, 471-490	2	10
528	Pnicogen-bonded complexes H(n)F(5-n)P:N-base, for n = 0-5. *Journal of Physical Chemistry A*, **2014**, 118, 10144-54	2.8	33
527	An experimental and theoretical NMR study of NH-benzimidazoles in solution and in the solid state: proton transfer and tautomerism. *Beilstein Journal of Organic Chemistry*, **2014**, 10, 1620-9	2.5	30
526	Insight into detailed mechanism of the atmospheric reaction of imidogen with hydroxyl: a computational study. *Structural Chemistry*, **2014**, 25, 169-175	1.8	4
525	Tautomerism, structure in solution and in the solid state of 1:9,5:10-anthradipyrazole. *Structural Chemistry*, **2014**, 25, 683-690	1.8	3
524	Can conventional bases and unsaturated hydrocarbons be converted into gas-phase superacids that are stronger than most of the known oxyacids? The role of beryllium bonds. *Chemistry - A European Journal*, **2013**, 19, 11637-43	4.8	47
523	Characterizing complexes with pnicogen bonds involving sp2 hybridized phosphorus atoms: (H2C?PX)2 with X = F, Cl, OH, CN, NC, CCH, H, CH3, and BH2. *Journal of Physical Chemistry A*, **2013**, 117, 6893-903	2.8	63
522	Orthogonal interactions between nitryl derivatives and electron donors: pnictogen bonds. *Physical Chemistry Chemical Physics*, **2013**, 15, 14310-8	3.6	69
521	A theoretical study of the conformation and dynamic properties of 1,5-benzodiazepines and their derivatives. *Computational and Theoretical Chemistry*, **2013**, 1019, 108-115	2	16
520	One-pot synthesis, FT-IR and density functional method (DFT) studies on N-benzyl-N-ethyl-N-[5-nitro-2-(1,1,3,3-Tetramethylbutylamino)-1-benzofuran-3-yl]amine. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 116, 65-73	4.4	13
519	The structures of two aldazines: [1,1'-(1E,1'E)-hydrazine-1,2-diylidenebis(methan-1-yl-1-ylidene)dinaphthalen-2-ol] (Lumogen) and 2,2'-(1E,1'E)-hydrazine-1,2-diylidenebis(methan-1-yl-1-ylidene)diphenol (salicylaldazine) in the solid state and in solution. *Magnetic Resonance in Chemistry*, **2013**, 51, 530-40	2.1	5

518	Relationship between experimental pKa values in aqueous solution and a gas phase bond length in bicyclo[2.2.2]octane and cubane carboxylic acids. *Journal of Physical Organic Chemistry*, **2013**, 26, 791-796	2.1	9
517	HRgCN and HRgNC as halogen bond acceptors (Rg=Kr and Xe): A theoretical study upon strength and nature of halogen?nitrogen and halogen?carbon interactions. *Computational and Theoretical Chemistry*, **2013**, 1020, 1-6	2	6
516	Modeling the mechanism of glycosylation reactions between ethanol, 1,2-ethanediol and methoxymethanol. *Physical Chemistry Chemical Physics*, **2013**, 15, 14026-36	3.6	6
515	Comparative study on the stabilities and properties of heterodimers containing the intermolecular interactions of CF2Cl2 with the isoelectronic and isostructure species of N2O and CO2. *Structural Chemistry*, **2013**, 24, 1737-1745	1.8	10
514	A theoretical investigation of the mechanism of formation of a simplified analog of the green fluorescent protein (GFP) from a peptide model. *Structural Chemistry*, **2013**, 24, 1145-1151	1.8	5
513	Theoretical studies of parent 1-, 2-, 3-pyrazolines and their methylated derivatives. *Structural Chemistry*, **2013**, 24, 421-432	1.8	9
512	HOMA parameters for the boron□boron bond: How the introduction of a BB bond influences the aromaticity of selected hydrocarbons. *Structural Chemistry*, **2013**, 24, 543-548	1.8	17
511	Enhancing and modulating the intrinsic acidity of imidazole and pyrazole through beryllium bonds. *Journal of Molecular Modeling*, **2013**, 19, 4139-45	2	31
510	On the Reliability of Pure and Hybrid DFT Methods for the Evaluation of Halogen, Chalcogen, and Pnicogen Bonds Involving Anionic and Neutral Electron Donors. *Journal of Chemical Theory and Computation*, **2013**, 9, 5201-10	6.4	204
509	Conformational preference and chiroptical response of carbohydrates D-ribose and 2-deoxy-D-ribose in aqueous and solid phases. *Journal of Physical Chemistry B*, **2013**, 117, 14599-614	3.4	15
508	Pnicogen bonded complexes of PO2X (X = F, Cl) with nitrogen bases. *Journal of Physical Chemistry A* , **2013**, 117, 10497-503	2.8	124
507	A facile method to determine the absolute structure of achiral molecules: supramolecular-tilt structures. *Chemistry - A European Journal*, **2013**, 19, 6044-51	4.8	5
506	Non-covalent interactions: complexes of guanidinium with DNA and RNA nucleobases. *Journal of Physical Chemistry B*, **2013**, 117, 11608-16	3.4	28
505	A theoretical study of the limits of the acidity of carbon acids in phase transfer catalysis in water and in liquid ammonia. *Open Chemistry*, **2013**, 11, 1711-1722	1.6	2
504	Exploring (NH2F)2, H2FP:NFH2, and (PH2F)2 potential surfaces: hydrogen bonds or pnicogen bonds?. *Journal of Physical Chemistry A*, **2013**, 117, 183-91	2.8	78
503	Spontaneous ion-pair formation in the gas phase induced by Beryllium bonds. *Chemical Physics Letters*, **2013**, 590, 22-26	2.5	27
502	The location of stationary points in the reaction of fluoroformyloxyl radical (FCO2(C2V)) with atomic hydrogen: A computational study on the pathways of the singlet and triplet reaction and intersystem crossing. *Computational and Theoretical Chemistry*, **2013**, 1022, 86-93	2	2
501	Intermolecular spin□spin coupling constants between 31P atoms. *Comptes Rendus Chimie*, **2013**, 16, 937-944	2.7	11

500	A silver complex of chloroquine: synthesis, characterization and structural properties. *New Journal of Chemistry*, **2013**, 37, 1391	3.6	5
499	The structure of azines derived from C-formyl-1H-imidazoles in solution and in the solid state: tautomerism, configurational and conformational studies. *Magnetic Resonance in Chemistry*, **2013**, 51, 203-21	2.1	16
498	Synthesis and structural study of 2-arylbenzotriazoles related to Tinuvins. *Tetrahedron*, **2013**, 69, 3027-3038	2.4	18
497	Complexes between dihydrogen and amine, phosphine, and arsine derivatives. Hydrogen bond versus pnictogen interaction. *Journal of Physical Chemistry A*, **2013**, 117, 3243-51	2.8	44
496	Phosphorus as a simultaneous electron-pair acceptor in intermolecular P□□N pnicogen bonds and electron-pair donor to Lewis acids. *Journal of Physical Chemistry A*, **2013**, 117, 3133-41	2.8	63
495	Theoretical study of the mutarotation of erythrose and threose: acid catalysis. *Carbohydrate Research*, **2013**, 372, 1-8	2.9	13
494	Linear free energy relationships in halogen bonds. *CrystEngComm*, **2013**, 15, 3178	3.3	27
493	Ab Initio Study of Cooperative Effects in Complexes X:HBO:Z, with X, Z=LiH, HNC, HF, HCN, HCl, ClF, and HBO: Structures, Binding Energies, and Spin-Spin Coupling Constants across Intermolecular Bonds. *Zeitschrift Fur Physikalische Chemie*, **2013**, 227, 821-839	3.1	2
492	Tracing environment effects that influence the stability of anion□anion complexes: The case of phosphate□phosphate interactions. *Chemical Physics Letters*, **2013**, 555, 106-109	2.5	54
491	Theoretical and Experimental NMR Study of a Series of Five Nitrobenzene-1,2-Diamines. *Spectroscopy Letters*, **2013**, 46, 91-99	1.1	5
490	Solvent effects on guanidinium-anion interactions and the problem of guanidinium Y-aromaticity. *Journal of Physical Organic Chemistry*, **2013**, 26, 378-385	2.1	17
489	Ab initio study of water clustering in the presence of a methyl radical. *Structural Chemistry*, **2013**, 24, 491-497	1.8	3
488	The reaction of NH-indazoles with 1-fluoro-2,4-dinitrobenzene: the unusual formation of benzotriazole-N-oxides. *New Journal of Chemistry*, **2013**, 37, 2384	3.6	4
487	Pnicogen-bonded cyclic trimers (PH2X)3 with X = F, Cl, OH, NC, CN, CH3, H, and BH2. *Journal of Physical Chemistry A*, **2013**, 117, 4981-7	2.8	89
486	Resonance assisted hydrogen bonds in open-chain and cyclic structures of malonaldehyde enol: A theoretical study. *Journal of Molecular Structure*, **2013**, 1048, 138-151	3.4	25
485	Substituent effects on the cooperativity of halogen bonding. *Journal of Physical Chemistry A*, **2013**, 117, 5551-7	2.8	69
484	Structure of NH-benzazoles (1H-benzimidazoles, 1H- and 2H-indazoles, 1H- and 2H-benzotriazoles). *Chemistry of Heterocyclic Compounds*, **2013**, 49, 177-202	1.4	21
483	Predicting pKa Values in Aqueous Solution for the Guanidine Functional Group from Gas Phase Ab Initio Bond Lengths. *Molecular Informatics*, **2013**, 32, 363-76	3.8	20

482	Properties of complexes H2C?(X)P:PXH2, for X = F, Cl, OH, CN, NC, CCH, H, CH3, and BH2: P⋯P pnicogen bonding at σholes and πholes. *Journal of Physical Chemistry A*, **2013**, 117, 11592-604	2.8	65
481	Atropisomerization in N-aryl-2(1H)-pyrimidin-(thi)ones: a ring-opening/rotation/ring-closure process in place of a classical rotation around the pivot bond. *Journal of Organic Chemistry*, **2013**, 78, 12577-84	4.2	9
480	A tris(pyrazol-1-yl)methane bearing carboxylic acid groups at position 4: {1-[bis(4-carboxy-3,5-dimethyl-1H-pyrazol-1-yl)methyl]-3,5-dimethyl-1H-pyrazole-4-carboxylato}sodium dihydrate. *Acta Crystallographica Section C: Crystal Structure Communications*, **2013**, 69, 972-6		5
479	Self-assembly structures of 1H-indazoles in the solution and solid phases: a vibrational (IR, FIR, Raman, and VCD) spectroscopy and computational study. *ChemPhysChem*, **2013**, 14, 3355-60	3.2	11
478	Intramolecular pnicogen interactions in PHF-(CH2)(n)-PHF (n=2-6) systems. *ChemPhysChem*, **2013**, 14, 1656-65	3.2	44
477	Structure of 1,5-benzodiazepinones in the solid state and in solution: Effect of the fluorination in the six-membered ring. *Beilstein Journal of Organic Chemistry*, **2013**, 9, 2156-67	2.5	10
476	Variations in the structures and binding energies of binary complexes with HBO. *Chemical Physics Letters*, **2012**, 538, 5-9	2.5	5
475	Homo- and heterochiral dimers (PHFX)2, X = Cl, CN, CH3, NC: To what extent do they differ?. *Chemical Physics Letters*, **2012**, 538, 14-18	2.5	56
474	Tautomerism of hydroxychromenopyrazoles. *Journal of Molecular Structure*, **2012**, 1015, 162-165	3.4	1
473	Two polymorphs of 8-hydroxycarbostyril: X-ray crystallography, solid-state NMR and DFT calculations. *Journal of Molecular Structure*, **2012**, 1008, 88-94	3.4	7
472	The tautomeric structures of 3(5),3?(5?)-azopyrazole [(E)-1,2-di(1H-pyrazol-3(5)-yl)diazene)]: The combined use of NMR and electronic spectroscopies with DFT calculations. *Journal of Molecular Structure*, **2012**, 1015, 138-146	3.4	10
471	Intermolecular weak interactions in HTeXH dimers (X=O, S, Se, Te): hydrogen bonds, chalcogen-chalcogen contacts and chiral discrimination. *ChemPhysChem*, **2012**, 13, 496-503	3.2	92
470	Calculation of the HOMA model parameters for the carbon–boron bond. *Structural Chemistry*, **2012**, 23, 595-600	1.8	29
469	Weak interactions between hypohalous acids and dimethylchalcogens. *Physical Chemistry Chemical Physics*, **2012**, 14, 9880-9	3.6	36
468	Multinuclear NMR Characterization of Cyanuric Fluoride (2,4,6-Trifluoro-1,3,5-triazine). *Journal of Heterocyclic Chemistry*, **2012**, 49, 1257-1259	1.9	24
467	Interplay of F-H⋯F hydrogen bonds and P⋯N pnicogen bonds. *Journal of Physical Chemistry A*, **2012**, 116, 9205-13	2.8	85
466	Strong interactions between copper halides and unsaturated systems: new metallocycles? Or the importance of deformation. *Physical Chemistry Chemical Physics*, **2012**, 14, 11468-77	3.6	20
465	Structures, binding energies, and spin-spin coupling constants of geometric isomers of pnicogen homodimers (PHFX)2, X = F, Cl, CN, CH3, NC. *Journal of Physical Chemistry A*, **2012**, 116, 3056-60	2.8	75

464	A theoretical NMR study of the structure of benzynes and some of their carbocyclic and heterocyclic analogs. *Tetrahedron*, **2012**, 68, 6548-6556	2.4	24
463	The tautomerism of fluorinated indazolinones in the solid state. *Journal of Molecular Structure*, **2012**, 1022, 139-146	3.4	5
462	Electron density shift description of non-bonding intramolecular interactions. *Computational and Theoretical Chemistry*, **2012**, 991, 124-133	2	34
461	Thermodynamic and hydrogen-bond basicity of phosphine oxides: Effect of the ring strain. *Computational and Theoretical Chemistry*, **2012**, 994, 81-90	2	6
460	Conformational study of the open-chain and furanose structures of D-erythrose and D-threose. *Carbohydrate Research*, **2012**, 358, 96-105	2.9	23
459	Regioselectivity in the intramolecular Heck reaction of a series of cyclic sulfonamides: an experimental and computational study. *Chemistry - A European Journal*, **2012**, 18, 13379-87	4.8	11
458	A theoretical study of hemiacetal formation from the reaction of methanol with derivatives of CX3CHO (X = H, F, Cl, Br and I). *Journal of Physical Organic Chemistry*, **2012**, 25, 1286-1292	2.1	5
457	Atropisomerism and Axial Chirality in Heteroaromatic Compounds. *Advances in Heterocyclic Chemistry*, **2012**, 1-188	2.4	78
456	Mechanisms of formation of hemiacetals: intrinsic reactivity analysis. *Journal of Physical Chemistry A* , **2012**, 116, 8250-9	2.8	23
455	Analysis of the interactions between difluoroacetylene and one or two hydrogen fluoride molecules based on calculated spin□spin coupling constants. *Computational and Theoretical Chemistry*, **2012**, 998, 98-105	2	14
454	New C2-symmetry diols accumulating one stereogenic axis and two stereogenic centers. *Tetrahedron*, **2012**, 68, 9645-9651	2.4	6
453	Influence of Hydrogen Bonds on the P□□P Pnicogen Bond. *Journal of Chemical Theory and Computation*, **2012**, 8, 2320-7	6.4	94
452	The chiral structure of 1H-indazoles in the solid state: a crystallographic, vibrational circular dichroism and computational study. *New Journal of Chemistry*, **2012**, 36, 749	3.6	27
451	Modulating the Strength of Hydrogen Bonds through Beryllium Bonds. *Journal of Chemical Theory and Computation*, **2012**, 8, 2293-300	6.4	73
450	Prototropic tautomerism of 5-aryloxy-1(2)H-tetrazoles. *Magnetic Resonance in Chemistry*, **2012**, 50, 193-5	2.1	1
449	The structure of glibenclamide in the solid state. *Magnetic Resonance in Chemistry*, **2012**, 50, 246-55	2.1	20
448	Competition and interplay between □hole and □hole interactions: a computational study of 1:1 and 1:2 complexes of nitryl halides (O2NX) with ammonia. *Journal of Physical Chemistry A*, **2012**, 116, 5199-206	2.8	78
447	Electrostatics at the origin of the stability of phosphate-phosphate complexes locked by hydrogen bonds. *ChemPhysChem*, **2012**, 13, 1421-4	3.2	81

446	FCl:PCX complexes: old and new types of halogen bonds. *Journal of Physical Chemistry A*, **2012**, 116, 2300-8	2.8	48
445	A theoretical study of 1:1 and 1:2 complexes of acetylene with nitrosyl hydride. *Structural Chemistry*, **2012**, 23, 847-856	1.8	7
444	A theoretical reappraisal of the cyclol hypothesis. *Structural Chemistry*, **2012**, 23, 873-877	1.8	3
443	A theoretical study of six-membered rings containing the N=S=N motif. *Structural Chemistry*, **2012**, 23, 1245-1252	1.8	10
442	A theoretical study of the parent NH-benzazoles (benzimidazoles, indazoles and benzotriazoles): geometries, energies, acidity and basicity, NMR properties and molecular electrostatic potentials. *Arkivoc*, **2012**, 2012, 85-107	0.9	17
441	An ab initio study of cooperative effects in ternary complexes X:CNH:Z with X, Z = CNH, FH, ClH, FCl, and HLi: structures, binding energies, and spin-spin coupling constants across intermolecular bonds. *Physical Chemistry Chemical Physics*, **2011**, 13, 13951-61	3.6	38
440	Theoretical study of the HXYH dimers (X, Y = O, S, Se). Hydrogen bonding and chalcogen–chalcogen interactions. *Molecular Physics*, **2011**, 109, 2543-2552	1.7	75
439	Unprecedented 1,3-diaza[3]ferrocenophane scaffold as molecular probe for anions. *Inorganic Chemistry*, **2011**, 50, 4212-20	5.1	26
438	TDDFT study of the UV-vis spectra of subporphyrazines and subphthalocyanines. *Journal of Porphyrins and Phthalocyanines*, **2011**, 15, 1220-1230	1.8	18
437	Tuning the interaction energy of hydrogen bonds: the effect of the substituent. *Journal of Physical Chemistry A*, **2011**, 115, 12561-71	2.8	19
436	Synthesis and structural characterization of 1,2,4-diazaphospholide complexes of titanium(IV) and titanium(III). *Inorganic Chemistry*, **2011**, 50, 12408-10	5.1	16
435	Atropisomerism and conformational aspects of meso-tetraarylporphyrins and related compounds. *Journal of Porphyrins and Phthalocyanines*, **2011**, 15, 1-28	1.8	52
434	A theoretical study of the conformation of 2,2?-bifuran, 2,2?-bithiophene, 2,2?-bitellurophene and mixed derivatives: Chalcogen–chalcogen interactions or dipole–dipole effects?. *Computational and Theoretical Chemistry*, **2011**, 974, 37-42	2	19
433	Definition of the hydrogen bond (IUPAC Recommendations 2011). *Pure and Applied Chemistry*, **2011**, 83, 1637-1641	2.1	1111
432	Defining the hydrogen bond: An account (IUPAC Technical Report). *Pure and Applied Chemistry*, **2011**, 83, 1619-1636	2.1	738
431	Isomerization barriers in bis(4H-thiopyran) and in bithioxanthenes. *Tetrahedron*, **2011**, 67, 7316-7320	2.4	2
430	A theoretical study of the effect of copper(I) chloride on the azido/tetrazole isomerism. *Tetrahedron*, **2011**, 67, 8724-8730	2.4	8
429	Oxazolidinone cross-alkylation during Evans' asymmetric alkylation reaction. *Tetrahedron*, **2011**, 67, 9104-9111	2.4	5

428	Determination of the absolute configuration of 1,3,5-triphenyl-4,5-dihydropyrazole enantiomers by a combination of VCD, ECD measurements, and theoretical calculations. *Tetrahedron: Asymmetry*, **2011**, 22, 1120-1124		10
427	Rates of enantiomerization in axially chiral 2,2?-bipyridines with restricted rotation: an ab initio study. *Tetrahedron: Asymmetry*, **2011**, 22, 1180-1183		7
426	31P□31P spin□spin coupling constants for pnicogen homodimers. *Chemical Physics Letters*, **2011**, 512, 184-187	2.5	125
425	Multiple 3c2e bonding of methane with metal cations. *Chemical Physics Letters*, **2011**, 515, 210-213	2.5	1
424	Computational study of mutarotation in erythrose and threose. *Carbohydrate Research*, **2011**, 346, 2933-9	2.9	17
423	Dihydrogen bonding vs metal-□interaction in complexes between H2 and metal hydride. *Journal of Physical Chemistry A*, **2011**, 115, 201-10	2.8	26
422	Modeling the allosteric effect: modification of the tautomerism by intermolecular interactions and extension to molecular wires. *Structural Chemistry*, **2011**, 22, 707-715	1.8	3
421	Conformational analysis of N,N?-dinaphthyl heterocyclic carbenes: imidazol-2-ylidenes and imidazolin-2-ylidenes. *Structural Chemistry*, **2011**, 22, 1087-1094	1.8	6
420	An experimental NMR and computational study of 4-quinolones and related compounds. *Monatshefte F□ Chemie*, **2011**, 142, 731-742	1.4	15
419	An ab initio study of the proton transfer and tautomerization processes in hydroxycarbene. *Theoretical Chemistry Accounts*, **2011**, 128, 563-567	1.9	4
418	Crystal and molecular structure of three biologically active nitroindazoles. *Journal of Molecular Structure*, **2011**, 985, 75-81	3.4	9
417	Relationships between interaction energy, intermolecular distance and electron density properties in hydrogen bonded complexes under external electric fields. *Chemical Physics Letters*, **2011**, 507, 185-189	2.5	255
416	Thermodynamic and kinetic effects of Lewis acid complexation on a Schiff base present in two tautomeric forms. *Journal of Physical Organic Chemistry*, **2011**, 24, 744-750	2.1	5
415	Glyoxal oligomers: A computational study. *International Journal of Quantum Chemistry*, **2011**, 111, 3057-3069	2.1	9
414	A theoretical study of the interactions of NF(3) with neutral ambidentate electron donor and acceptor molecules. *Physical Chemistry Chemical Physics*, **2011**, 13, 674-83	3.6	35
413	[1,2,3]Triazolo[1,5-a]pyridyl phosphines reflecting the influence of phosphorus lone pair orientation on spectroscopic properties. *Dalton Transactions*, **2011**, 40, 1387-95	4.3	7
412	The boron-boron single bond in diborane(4) as a non-classical electron donor for hydrogen bonding. *Physical Chemistry Chemical Physics*, **2011**, 13, 14026-32	3.6	29
411	Simultaneous interactions of anions and cations with cyclohexane and adamantane: aliphatic cyclic hydrocarbons as charge insulators. *Journal of Physical Chemistry A*, **2011**, 115, 13124-32	2.8	18

410	Structures, energies, bonding, and NMR properties of pnicogen complexes H2XP:NXH2 (X ? H, CH3, NH2, OH, F, Cl). *Journal of Physical Chemistry A*, **2011**, 115, 13724-31	2.8	153
409	Ab initio study of ternary complexes X:(HCNH)(+):Z with X, Z = NCH, CNH, FH, ClH, and FCl: diminutive cooperative effects on structures, binding energies, and spin-spin coupling constants across hydrogen bonds. *Journal of Physical Chemistry A*, **2011**, 115, 12677-87	2.8	20
408	Structures, energies, and spin-spin coupling constants of methyl-substituted 1,3-diborata-2,4-diphosphoniocyclobutanes: four-member B-P-B-P rings B2P2(CH3)(n)H(8-n), with n = 0, 1, 2, 4. *Journal of Physical Chemistry A*, **2011**, 115, 10502-10	2.8	1
407	Structures, energies, and spin-spin coupling constants of fluoro-substituted 1,3-diborata-2,4-diphosphoniocyclobutanes: four-member B-P-B-P rings B2P2F(n)H(8-n) with n = 0, 1, 2, 4. *Journal of Physical Chemistry A*, **2011**, 115, 4511-20	2.8	5
406	Cooperativity between the hydrogen bonding and halogen bonding in F3CX ⋯NCH(CNH) ⋯NCH(CNH) complexes (X=Cl, Br). *Molecular Physics*, **2011**, 109, 1641-1648	1.7	38
405	Theoretical study of the 1:1 and 2:1 (homo- and heterochiral) complexes of XOOX' (X, X' = H, CH3) with lithium cation. *Journal of Physical Chemistry A*, **2011**, 115, 7805-10	2.8	6
404	A computational study of the conformation of heterocyclic systems related to biphenyl. *Computational and Theoretical Chemistry*, **2011**, 964, 25-31	2	8
403	A theoretical study of the conformation, basicity and NMR properties of 2,2?-, 3,3?- and 4,4?-bipyridines and their conjugated acids. *Computational and Theoretical Chemistry*, **2011**, 966, 334-339	2	21
402	A theoretical study of the hydrogen bonding properties of H2BNH2: Some considerations on the basis set superposition error issue. *Computational and Theoretical Chemistry*, **2011**, 967, 147-151	2	33
401	Do nitrogen bases form chlorine-shared and ion-pair halogen bonds?. *Chemical Physics Letters*, **2011**, 508, 6-9	2.5	23
400	Cation⋯ interactions: Complexes of guanidinium and simple aromatic systems. *Chemical Physics Letters*, **2011**, 511, 129-134	2.5	29
399	Synthesis and biological evaluation of indazole derivatives. *European Journal of Medicinal Chemistry*, **2011**, 46, 1439-47	6.8	19
398	Synthesis of [1,2,4]-triazolo[1,5-a]pyrimidines by Dimroth rearrangement of [1,2,4]-triazolo[4,3-a]pyrimidines: A theoretical and NMR study. *Journal of Molecular Structure*, **2011**, 987, 13-24	3.4	23
397	A 13C and 15N experimental NMR and theoretical study of the structure of linear primary aliphatic amines and ammonium salts: from C1 to C18. *Tetrahedron*, **2011**, 67, 4633-4639	2.4	13
396	Electric field effects on nuclear magnetic shielding of the 1:1 and 2:1 (homo and heterochiral) complexes of XOOX' (X, X' = H, CH3) with lithium cation and their chiral discrimination. *Journal of Chemical Physics*, **2011**, 135, 104116	3.9	8
395	Silica Gel Promotes Cascade Synthesis of 2-(Heteroaryl)acetamide Derivatives from Isocyanides, Dialkylamines, and Heteroarylcarbaldehydes. *Synthetic Communications*, **2011**, 41, 1444-1454	1.7	8
394	A theoretical study of the conformation of meso-tetraphenylporphyrin (TPPH2), its anions, cations and metal complexes (Mg2+, Ca2+ and Zn2+). *Journal of Porphyrins and Phthalocyanines*, **2010**, 14, 630-638	1.8	3
393	A theoretical multinuclear NMR study of pyrazolylborates. *Heterocyclic Communications*, **2010**, 16,	1.7	8

392	Do traditional, chlorine-shared, and ion-pair halogen bonds exist? An ab initio investigation of FCl:CNX complexes. *Journal of Physical Chemistry A*, **2010**, 114, 12958-62	2.8	77
391	Cooperative and diminutive unusual weak bonding in F3CX···HMgH···Y and F3CX···Y···HMgH trimers (X = Cl, Br; Y = HCN, and HNC). *Journal of Physical Chemistry A*, **2010**, 114, 12106-11	2.8	72
390	Probing (1)J(C-F) and (n)J(F-F) spin-spin coupling constants for fluoroazines: an ab initio theoretical investigation. *Journal of Physical Chemistry A*, **2010**, 114, 2637-43	2.8	18
389	Dihydrogen bond cooperativity in aza-borane derivatives. *Journal of Physical Chemistry A*, **2010**, 114, 8457-62	2.8	41
388	Crystallization of an achiral cyclohexanone ethylene ketal in enantiomorphs and determination of the absolute structure. *Journal of the American Chemical Society*, **2010**, 132, 7862-3	16.4	12
387	Two-, three-, and four-bond NF spinSpin coupling constants in fluoroazines. *Molecular Physics*, **2010**, 108, 1367-1373	1.7	8
386	A computational study of the potential energy surface of peroxyformic acid dimers. *Journal of Physical Chemistry A*, **2010**, 114, 9388-93	2.8	5
385	Ab initio study of nonadditivity effects: spin-spin coupling constants for tetrafluoroethene in ternary pi complexes. *Journal of Physical Chemistry A*, **2010**, 114, 3713-7	2.8	4
384	A theoretical comparison of the chemical shifts of three related heterocycles: 1H-pyrazoles, 1H-1,2,4-triazoles and 1H-1,2,4-diazaphospholes. *Computational and Theoretical Chemistry*, **2010**, 942, 1-6		18
383	Prediction of the basicities of pyridines in the gas phase and in aqueous solution. *Journal of Chemical Information and Modeling*, **2010**, 50, 87-96	6.1	23
382	Ab initio study of ternary complexes A...NCH...C with A,C = HCN, HF, HCl, ClF, and LiH: energetics and spin-spin coupling constants across intermolecular bonds. *Journal of Physical Chemistry A*, **2010**, 114, 8463-73	2.8	23
381	Structural and electronic effects on one-bond spin-spin coupling constants 1J(B-N), 1J(B-H), and 1J(B-F) for complexes of nitrogen bases with BH3 and its fluoro-substituted derivatives. *Journal of Physical Chemistry A*, **2010**, 114, 12775-9	2.8	5
380	Fast degenerate double proton transfer in the solid state between two indazolinone tautomers. *CrystEngComm*, **2010**, 12, 4052	3.3	7
379	On the electronic structure and stability of icosahedral r-X2Z10H12 and Z12H(12)(2-) clusters; r = {ortho, meta, para}, X = {C, Si}, Z = {B, Al}. *Physical Chemistry Chemical Physics*, **2010**, 12, 5101-8	3.6	14
378	Do corresponding coupling constants in hydrogen-bonded homo- and hetero-chiral dimers differ?. *Canadian Journal of Chemistry*, **2010**, 88, 694-699	0.9	6
377	Ab initio EOM-CCSD investigation of one-bond C-C, N-C, and N-N spin-spin coupling constants in fluoroazines. *Journal of Physical Chemistry A*, **2010**, 114, 5205-10	2.8	5
376	Cooperativity in multiple unusual weak bonds. *Theoretical Chemistry Accounts*, **2010**, 126, 1-14	1.9	242
375	A theoretical study of the stationary structures of the methane surface with special emphasis on NMR properties. *Chemical Physics Letters*, **2010**, 489, 35-38	2.5	4

374	An ab initio investigation of the properties of H2:HX hydrogen-bonded complexes. *Chemical Physics Letters*, **2010**, 489, 159-163	2.5	22
373	The azido-tetrazole and diazo-1,2,3-triazole tautomerism in six-membered heteroaromatic rings and their relationships with aromaticity: Azines and perimidine. *Tetrahedron*, **2010**, 66, 2863-2868	2.4	49
372	Distinction between homochiral and heterochiral dimers of 1-aza[n]helicenes (n=17) with alkaline cations. *Tetrahedron: Asymmetry*, **2010**, 21, 962-968		20
371	A SOPPA theoretical study of the spin–spin coupling constants of all fluorobenzenes C6HnF6−n (n=05). *Journal of Molecular Structure*, **2010**, 964, 119-125	3.4	13
370	The structures of chiral and racemate campho[2,3-c]pyrazole: A combined crystallographic, solid-state NMR and computational study. *Journal of Molecular Structure*, **2010**, 965, 74-81	3.4	13
369	Influence of the basis set on the calculation of the absolute 13C shieldings of methyl derivatives (CH3X with X = CH3, CN, NH2, NO2, OH, F) with special emphasis in the cases of X = Cl, Br, SH, SeH, and PH2. *Structural Chemistry*, **2010**, 21, 755-759	1.8	7
368	Conformational analysis of dibenzo[a,e]cyclooctadiene and three related heterocyclic compounds. *Structural Chemistry*, **2010**, 21, 885-891	1.8	9
367	Computational NMR Spectroscopy **2010**, 37-61		10
366	Universal features of the electron density distribution in hydrogen-bonding regions: a comprehensive study involving H...X (X=H, C, N, O, F, S, Cl, pi) interactions. *Chemistry - A European Journal*, **2010**, 16, 2442-52	4.8	204
365	New insights into factors influencing B-N bonding in X:BH(3-n)F(n) and X:BH(3-n)Cl(n) for X=N2, HCN, LiCN, H2CNH, NF3, NH3 and n=0-3: the importance of deformation. *Chemistry - A European Journal*, **2010**, 16, 11897-905	4.8	37
364	Structural studies of 2-methyl-7-substituted pyrazolo[1,5-a]pyrimidines. *Journal of Heterocyclic Chemistry*, **2010**, 47, 1259-1268	1.9	17
363	Difluorobenzenes revisited: an experimental and theoretical study of spin-spin coupling constants for 1,2-, 1,3-, and 1,4-difluorobenzene. *Magnetic Resonance in Chemistry*, **2010**, 48, 68-73	2.1	11
362	A theoretical NMR study of ortho and para-substituted benzenes compared with silabenzenes, pyridines and phosphabenzenes. *Magnetic Resonance in Chemistry*, **2010**, 48 Suppl 1, S32-7	2.1	21
361	The solid-state structure of primary fatty amines: True amines or ammonium amides?. *Journal of Molecular Structure*, **2010**, 969, 106-110	3.4	2
360	15N-15N spin-spin coupling constants through intermolecular hydrogen bonds in the solid state. *Journal of Magnetic Resonance*, **2010**, 206, 274-9	3	10
359	The interplay of hydrogen bonds and halogen bonds in the structure of NH-pyrazoles bearing C-aryl and C-halogen substituents. *Inorganica Chimica Acta*, **2010**, 363, 1332-1342	2.7	22
358	An experimental and theoretical study of 1J(13C–14N) coupling constants in nitro-aromatic and nitro-heteroaromatic compounds. *Journal of Molecular Structure*, **2010**, 979, 180-185	3.4	4
357	The azido-tetrazole tautomerism in azoles and its relationships with aromaticity and NMR properties. *Tetrahedron*, **2010**, 66, 5071-5081	2.4	37

356	A theoretical analysis of the conformational space of tris(2-methylbenzimidazol-1-yl)methane. *Tetrahedron: Asymmetry*, **2010**, 21, 437-442		9
355	Theoretical study of the halogen–hydride complexes between XeH2 and carbon halogenated derivatives. *Computational and Theoretical Chemistry*, **2010**, 955, 140-144		12
354	Chiral recognition in self-complexes of diketopiperazine derivatives. *Journal of Physical Organic Chemistry*, **2010**, 23, 1155-1172	2.1	11
353	A theoretical study of the sulfenate–sulfoxide rearrangement. Effect of the hydrogen bond complexation. *International Journal of Quantum Chemistry*, **2010**, 110, 2391-2397	2.1	1
352	N-substituted-1,2,3-triazoles: synthesis, characterization and evaluation as cannabinoid ligands. *Arkivoc*, **2010**, 2010, 127-147	0.9	3
351	1,2,4-Diazaphospholide complexes of tin(II): from nitride stannylene to stannylenated ammonium ions. *Chemistry - A European Journal*, **2009**, 15, 6581-5	4.8	19
350	3-(Pyridin-2-yl)[1,2,3]triazolo[1,5-a]quinoline: A Theoretical and Experimental Analysis of Ring-Chain Isomerisation. *European Journal of Organic Chemistry*, **2009**, 2009, 5765-5778	3.2	10
349	13C and 15N NMR spectra of aminobenzimidazoles in solution and in the solid state. *Magnetic Resonance in Chemistry*, **2009**, 47, 100-4	2.1	18
348	A theoretical structural analysis of the factors that affect (1)J(NH), (1h)J(NH) and (2h)J(NN) in N-H...N hydrogen-bonded complexes. *Magnetic Resonance in Chemistry*, **2009**, 47, 249-56	2.1	11
347	The behavior of Gliclazide in solution and in the solid state: a case of organic compound presenting a solid-solution structure. *Magnetic Resonance in Chemistry*, **2009**, 47, 472-7	2.1	8
346	A DFT and AIM analysis of the spin-spin couplings across the hydrogen bond in the 2-fluorobenzamide and related compounds. *Magnetic Resonance in Chemistry*, **2009**, 47, 585-92	2.1	42
345	Molecular complexes between pi-excedent heterocycles (indoles and carbazole) and pi-deficient polynitrobenzenes. *Magnetic Resonance in Chemistry*, **2009**, 47, 917-24	2.1	5
344	A theoretical and experimental NMR study of (+)-biotin methyl ester. *Journal of Molecular Structure* , **2009**, 920, 323-326	3.4	15
343	The structure of two pyrazole esters related to Rimonabant. *Journal of Molecular Structure*, **2009**, 937, 10-15	3.4	2
342	A computational study of the cooperativity in clusters of interhalogen derivatives. *Structural Chemistry*, **2009**, 20, 63-71	1.8	66
341	Chiral distinction in square planar Pt and Pd complexes of 2,2?-bipyridine derivatives. *Structural Chemistry*, **2009**, 20, 557-563	1.8	6
340	A theoretical study of diborenes HLB=BLH for L=CO, NH3, OH2, PH3, SH2, ClH: structures, energies, and spin–spin coupling constants. *Theoretical Chemistry Accounts*, **2009**, 124, 187-195	1.9	9
339	N- versus -configuration in mono- and bis-pyrrole and imidazole derivatives of alkaline earth metals. *Journal of Physical Organic Chemistry*, **2009**, 22, 747-755	2.1	4

338	Double proton transfer in crystals of 1,3,4,6,7,8-hexahydro-2H-pyrimido[1,2-a] pyrimidine (hppH): 13C and 15N CPMAS NMR study of (hppH)2. *Journal of Physical Organic Chemistry*, **2009**, 23, 526-535	2.1	9
337	Structural study of diarylazoles related to Rimonabant. *Journal of Molecular Structure*, **2009**, 920, 82-89	3.4	10
336	Theoretical studies of azapentalenes. Part 4: Theoretical study of the properties of 3a,6a-diazapentalene. *Tetrahedron*, **2009**, 65, 5760-5766	2.4	7
335	Theoretical studies of azapentalenes. Part 5: Bimanes. *Tetrahedron*, **2009**, 65, 6244-6250	2.4	7
334	Does 7-norcaranone (bicyclo[4.1.0]heptan-7-one) exist?. *Computational and Theoretical Chemistry*, **2009**, 896, 92-95		4
333	A theoretical and NMR experimental study of N1,N3-di(3-aminoacridin-6-yl)-isophthalamide and N2,N6-di(3-aminoacridin-6-yl)-2,6-dicarboxamide. *Journal of Molecular Structure*, **2009**, 928, 132-137	3.4	3
332	A computational study of dimers and trimers of nitrosyl hydride: Blue shift of NH bonds that are involved in H-bond and orthogonal interactions. *Chemical Physics*, **2009**, 362, 1-7	2.3	16
331	Stabilities and properties of ozone–nitrosyl hydride (O3HNO) complexes: A computational study. *Chemical Physics Letters*, **2009**, 474, 253-257	2.5	13
330	The structure of Rimonabant in the solid state and in solution: an experimental and theoretical study. *European Journal of Medicinal Chemistry*, **2009**, 44, 1864-9	6.8	10
329	Theoretical calculations of a model of NOS indazole inhibitors: interaction of aromatic compounds with Zn-porphyrins. *Bioorganic and Medicinal Chemistry*, **2009**, 17, 8027-31	3.4	16
328	How Aromaticity Affects the Chemical and Physicochemical Properties of Heterocycles: A Computational Approach. *Topics in Heterocyclic Chemistry*, **2009**, 155-202	0.2	15
327	A theoretical study of the neutral and the double-charged cation of cyclo[8]pyrrole and its interaction with inorganic anions. *Open Chemistry*, **2009**, 7, 683-689	1.6	7
326	An Ab Initio Study of the Structures and Selected Properties of 1,2-Dihydro-1,2-azaborine and Related Molecules. *Journal of Chemical Theory and Computation*, **2009**, 5, 2239-47	6.4	39
325	Beryllium Bonds, Do They Exist?. *Journal of Chemical Theory and Computation*, **2009**, 5, 2763-71	6.4	140
324	Characterizing complexes with F-Li...N, H-Li...N, and CH3Li...N lithium bonds: structures, binding energies, and spin-spin coupling constants. *Journal of Physical Chemistry A*, **2009**, 113, 10327-34	2.8	17
323	Characterizing complexes with F-Li+-F lithium bonds: structures, binding energies, and spin-spin coupling constants. *Journal of Physical Chemistry A*, **2009**, 113, 8359-65	2.8	7
322	Simultaneous Interaction of Tetrafluoroethene with Anions and Hydrogen-Bond Donors: A Cooperativity Study. *Journal of Chemical Theory and Computation*, **2009**, 5, 1186-94	6.4	50
321	The effect of perfluorination on the aromaticity of benzene and heterocyclic six-membered rings. *Journal of Physical Chemistry A*, **2009**, 113, 6789-94	2.8	38

320	Systematic Comparison of Second-Order Polarization Propagator Approximation (SOPPA) and Equation-of-Motion Coupled Cluster Singles and Doubles (EOM-CCSD) Spin-Spin Coupling Constants for Molecules with C, N, and O Double and Triple Bonds and Selected F-Substituted Derivatives. *Journal of Chemical Theory and Computation*, **2009**, 5, 208-16	6.4	41
319	A systematic comparison of second-order polarization propagator approximation and equation-of-motion coupled cluster singles and doubles C-C, C-N, N-N, C-H, and N-H spin-spin coupling constants. *Journal of Physical Chemistry A*, **2009**, 113, 12411-20	2.8	28
318	Energetic vs synergetic stability: a theoretical study. *Journal of Physical Chemistry A*, **2009**, 113, 3266-73	2.8	49
317	Theoretical study of the 1:1 complexes between carbon monoxide and hypohalous acids. *Journal of Physical Chemistry A*, **2009**, 113, 3237-44	2.8	44
316	Effect of an external electric field on the dissociation energy and the electron density properties: The case of the hydrogen bonded dimer HF...HF. *Journal of Chemical Physics*, **2009**, 130, 044104	3.9	53
315	Carbon...carbon weak interactions. *Journal of Physical Chemistry A*, **2009**, 113, 8387-93	2.8	61
314	Chiral recognition in bicyclic guanidines. *Collection of Czechoslovak Chemical Communications*, **2009**, 74, 299-312		5
313	Chirality and Chiral Recognition **2009**, 37-86		4
312	Spin-spin coupling across intermolecular F-Cl...N halogen bonds. *Journal of Physical Chemistry A*, **2008**, 112, 7925-9	2.8	40
311	Ab initio EOM-CCSD spin-spin coupling constants for hydrogen-bonded formamide complexes: bridging complexes with NH3, (NH3)2, H2O, (H2O)2, FH, and (FH)2. *Journal of Physical Chemistry A*, **2008**, 112, 6338-43	2.8	18
310	A theoretical and experimental NMR study of the tautomerism of two phenylene-bis-C-substituted pyrazoles. *New Journal of Chemistry*, **2008**, 32, 2225	3.6	19
309	A Systematic Comparison of Second-Order Polarization Propagator Approximation (SOPPA) and Equation-of-Motion Coupled Cluster Singles and Doubles (EOM-CCSD) Spin-Spin Coupling Constants for Selected Singly Bonded Molecules, and the Hydrides NH3, H2O, and HF and Their Protonated and Deprotonated Ions and Hydrogen-Bonded Complexes. *Journal of Chemical Theory*	6.4	47
308	How to determine whether intramolecular H...H interactions can be classified as dihydrogen bonds. *Journal of Physical Chemistry A*, **2008**, 112, 2721-7	2.8	68
307	Structures, Bonding, and One-Bond B-N and B-H Spin-Spin Coupling Constants for a Series of Neutral and Anionic Five-Membered Rings Containing BN Bonds. *Journal of Chemical Theory and Computation*, **2008**, 4, 1869-76	6.4	4
306	Competition of hydrogen bonds and halogen bonds in complexes of hypohalous acids with nitrogenated bases. *Journal of Physical Chemistry A*, **2008**, 112, 10856-63	2.8	159
305	The structure of alkali metal derivatives of azoles: N-sigma versus pi structures. *Journal of Physical Chemistry A*, **2008**, 112, 7682-8	2.8	19
304	Molecular complexes of pentazolo[1,2-a]pentazole, N8. *Journal of Physical Chemistry A*, **2008**, 112, 1817-23	2.8	14
303	The Boat Conformation in Pyrazaboles. A Theoretical and Experimental Study *Crystal Growth and Design*, **2008**, 8, 838-847	3.5	25

302	Structure of N,N'-bis(amino acids) in the solid state and in solution. A 13C and 15N CPMAS NMR study. *Journal of Organic Chemistry*, **2008**, 73, 8575-8	4.2	8
301	Pi-systems as simultaneous hydride and hydrogen bond acceptors. *Journal of Physical Chemistry A*, **2008**, 112, 6753-9	2.8	22
300	Dihydrogen bond cooperativity in (HCCBeH)n clusters. *Journal of Chemical Physics*, **2008**, 129, 064115	3.9	26
299	Atomic partition of the optical rotatory power of methylhydroperoxide. *Journal of Chemical Physics*, **2008**, 128, 064318	3.9	9
298	The use of a molecular balance derived from 5,5?-bipyrazole to calculate [illegible]stacking interactions. *Tetrahedron Letters*, **2008**, 49, 7246-7249	2	12
297	Proton transfer in C-halogen pyrazole cyclamers. A theoretical study. *Structural Chemistry*, **2008**, 19, 191-198	1.8	15
296	Substitution effects on neutral and protonated pyridine derivatives along the periodic table. *Structural Chemistry*, **2008**, 19, 339-352	1.8	17
295	A computational study of the effect of C-lithiation on the NMR properties (chemical shifts and coupling constants) of aziridines. *Structural Chemistry*, **2008**, 19, 785-792	1.8	11
294	Hydrogen bonds and ionic interactions in Guanidine/Guanidinium complexes: a computational case study. *Structural Chemistry*, **2008**, 19, 923-933	1.8	27
293	Inverse hydrogen bonds between XeH2 and hydride and fluoride derivatives of Li, Be, Na and Mg. *Theoretical Chemistry Accounts*, **2008**, 121, 181-186	1.9	12
292	Theoretical study of racemization in chiral alkenylidene truxenes. *Journal of Physical Organic Chemistry*, **2008**, 21, 381-386	2.1	4
291	A computational study of 2J(HH)(gem) indirect spin-spin coupling constants in simple hydrides of the second and third periods. *Magnetic Resonance in Chemistry*, **2008**, 46, 356-61	2.1	16
290	Spin-spin coupling across intramolecular N-H(+)-N hydrogen bonds in models for proton sponges: an ab initio investigation. *Magnetic Resonance in Chemistry*, **2008**, 46, 457-63	2.1	16
289	A review with comprehensive data on experimental indirect scalar NMR spin-spin coupling constants across hydrogen bonds. *Magnetic Resonance in Chemistry*, **2008**, 46, 599-624	2.1	68
288	Experimental measurements and theoretical calculations of the chemical shifts and coupling constants of three azines (benzalazine, acetophenoneazine and cinnamaldazine). *Magnetic Resonance in Chemistry*, **2008**, 46, 859-64	2.1	106
287	Resolving an apparent discrepancy between theory and experiment: spin-spin coupling constants for FCCF. *Magnetic Resonance in Chemistry*, **2008**, 46, 1003-6	2.1	24
286	Synthesis, characterization, molecular structure and theoretical studies of axially fluoro-substituted subazaporphyrins. *Chemistry - A European Journal*, **2008**, 14, 1342-50	4.8	86
285	Synthesis and preferred all-syn conformation of C3-symmetrical N-(hetero)arylmethyl triindoles. *Chemistry - A European Journal*, **2008**, 14, 8555-61	4.8	25

284	A computational study of dimers and trimers of hypohalous acids. *Chemical Physics Letters*, **2008**, 454, 201-206	2.5	29
283	Interaction of positively and negatively charged aromatic hydrocarbons with benzene and triphenylene: Towards a model of pure organic insulators. *Chemical Physics Letters*, **2008**, 460, 406-410	2.5	33
282	A study in desmotropy. *Solid State Nuclear Magnetic Resonance*, **2008**, 34, 68-76	3.1	25
281	Cation dinitrogen complexes [N(2)...X...N(2)]+, X+=H+, Li+, Na+, Be(2+), Mg(2+). *Solid State Nuclear Magnetic Resonance*, **2008**, 34, 105-9	3.1	2
280	Application of Free-Wilson matrices to the analysis of the tautomerism and aromaticity of azapentalenes: a DFT study. *Tetrahedron*, **2008**, 64, 3826-3836	2.4	32
279	A study of the tautomerism of β-dicarbonyl compounds with special emphasis on curcuminoids. *Tetrahedron*, **2008**, 64, 8089-8094	2.4	58
278	[1,2,3]Triazolo[1,5-a]pyridines. A theoretical (DFT) study of the ring–chain isomerization. *Tetrahedron*, **2008**, 64, 11150-11158	2.4	15
277	The relative stability of pyridinium and 1,7-diaza[12]annulenium quaternary salts. *Tetrahedron Letters*, **2008**, 49, 2060-2062	2	
276	Heteropentalenes aromaticity: A theoretical study. *Computational and Theoretical Chemistry*, **2008**, 851, 75-83		25
275	Desmotropy in reduced plumbagins: α- and β-Dihydroplumbagins. *Journal of Molecular Structure*, **2008**, 891, 325-328	3.4	10
274	Atropisomerism in the 2-arylimino-N-(2-hydroxyphenyl)thiazoline series: influence of hydrogen bonding on the racemization process. *Journal of Organic Chemistry*, **2008**, 73, 403-11	4.2	43
273	Acid properties of porphyrins and related systems. *Russian Journal of General Chemistry*, **2008**, 78, 784-792	0.7	5
272	The molecular structure of 1,3-dimethyl-4-phenyl-1H-pyrazole-5-carboxylic acid. *Arkivoc*, **2008**, 2008, 74-84	0.9	3
271	How Aromaticity Affects the Chemical and Physicochemical Properties of Heterocycles: A Computational Approach. *Topics in Heterocyclic Chemistry*, **2008**, 155	0.2	1
270	A theoretical and experimental study of the fluxional behaviour of molybdenum dihydrobis- and hydrotris-pyrazolylborates. *Dalton Transactions*, **2007**, 3995-9	4.3	9
269	Spin-Spin Coupling Constants for Iminoboranes RBNH, HBNR, and RBNR and Comparisons with Corresponding Isoelectronic Acetylenes RCCH and RCCR, for R = H, CH3, NH2, OH, and F. *Journal of Chemical Theory and Computation*, **2007**, 3, 549-56	6.4	7
268	Cocrystals of 3,5-Dimethyl-1H-pyrazole and Salicylic Acid: Controlled Formation of Trimers via O–H···N Hydrogen Bonds. *Crystal Growth and Design*, **2007**, 7, 1176-1184	3.5	27
267	Weakly bound complexes of N2O: an ab initio theoretical analysis toward the design of N2O receptors. *Journal of Physical Chemistry A*, **2007**, 111, 2077-83	2.8	10

266	Chiral recognition in diaziridine clusters and the problem of racemization waves. *Journal of Physical Chemistry A*, **2007**, 111, 1096-103	2.8	14
265	Theoretical study of complexes and fluoride cation transfer between N2F+ and electron donors. *Journal of Physical Chemistry A*, **2007**, 111, 7154-61	2.8	41
264	Probing P-H+-P hydrogen bonds: structures, binding energies, and spin-spin coupling constants. *Journal of Physical Chemistry A*, **2007**, 111, 3416-22	2.8	21
263	Attacking boron nucleophiles: NMR properties of five-membered diazaborole rings. *Journal of Physical Chemistry A*, **2007**, 111, 419-21	2.8	13
262	The structure of fluorinated indazoles: the effect of the replacement of a H by a F atom on the supramolecular structure of NH-indazoles. *New Journal of Chemistry*, **2007**, 31, 936-946	3.6	32
261	Topological properties of the electrostatic potential in weak and moderate N...H hydrogen bonds. *Journal of Physical Chemistry A*, **2007**, 111, 6425-33	2.8	56
260	Unusual substituent effects on the bonding of iminoboranes. *Physical Chemistry Chemical Physics*, **2007**, 9, 3970-7	3.6	29
259	Bonding Properties Related with Chiral Discrimination in Dinuclear Metal Complexes of Group 10. *European Journal of Inorganic Chemistry*, **2007**, 2007, 324-332	2.3	7
258	Pyrazolo[1,5-a]pyrimidines. A combined multinuclear magnetic resonance (1H, 13C, 15N, 19F) and DFT approach to their structural assignment. *Magnetic Resonance in Chemistry*, **2007**, 45, 513-7	2.1	29
257	Statistical analysis of (13)C and (15)N NMR chemical shifts from GIAO/B3LYP/6-311 + + G** calculated absolute shieldings. *Magnetic Resonance in Chemistry*, **2007**, 45, 797-800	2.1	178
256	Structure and tautomerism of 4-bromo substituted 1H-pyrazoles. *Tetrahedron*, **2007**, 63, 8104-8111	2.4	42
255	The structural and theoretical study of 1H-3,5-di-phenyl-1,2,4-diazaphosphole in the solid state. *Tetrahedron*, **2007**, 63, 9129-9133	2.4	26
254	Enantiodifferentiation in protonation processes: A theoretical study. *Computational and Theoretical Chemistry*, **2007**, 811, 37-44		2
253	A comparative ab initio study of SF6?X and CF4?X complexes (X = H, F, Cl, CN, NC, N3 and NCO). *Computational and Theoretical Chemistry*, **2007**, 819, 136-141		1
252	Computational studies of the structure of aldazines and ketazines: Part 2. Halogen and unsaturated derivatives. *Computational and Theoretical Chemistry*, **2007**, 847, 25-31		8
251	Ab initio study of complexes pairing HRgX and H2 (Rg = Ar, Kr and X = F, Cl, CN). *Chemical Physics Letters*, **2007**, 439, 284-287	2.5	15
250	Stabilities and properties of O3HOCl complexes: A computational study. *Chemical Physics Letters*, **2007**, 449, 23-27	2.5	39
249	The intrinsic (gas-phase) acidities of bridgehead alcohols. *International Journal of Mass Spectrometry*, **2007**, 267, 302-307	1.9	14

248	An experimental and DFT analysis of coupling constants in [31P(CH3)nH(4□)]+ systems where n = 0□4 with a note on [14N(C2H5)4]+ and [31P(C2H5)4]+. *Journal of Molecular Structure*, **2007**, 837, 147-152	3.4	3
247	Tailor-made naphthyridines: Self-assembling multiple hydrogen-bonded supramolecular architectures from dimer to helix. *Journal of Molecular Structure*, **2007**, 846, 97-107	3.4	31
246	Theoretical study of neutral and protonated triple bonded molecules formed between C, N, Si, P, B and Al. *Theoretical Chemistry Accounts*, **2007**, 118, 533-539	1.9	3
245	Substitution effects in N-pyrazole and N-imidazole derivatives along the periodic table. *Structural Chemistry*, **2007**, 18, 965-975	1.8	13
244	Substitution effects in phenyl and N-pyrrole derivatives along the periodic table. *Structural Chemistry*, **2007**, 18, 797-805	1.8	22
243	Benzyl group conformation in 4-benzyl-4-hydroxypiperidines. *Journal of Structural Chemistry*, **2007**, 48, 1036-1045	0.9	3
242	Synthesis of 4-Aryl-3(5)-(2-hydroxyphenyl)pyrazoles by Reaction of Isoflavones and their 4-Thio Analogues with Hydrazine Derivatives. *Australian Journal of Chemistry*, **2007**, 60, 905	1.2	14
241	The use of chemical shifts vs. coupling constants for studying tautomerism: a combined experimental and theoretical approach. *Structural Chemistry*, **2007**, 18, 703-708	1.8	11
240	HC[triple bond]P and H3C-C[triple bond]P as proton acceptors in protonated complexes containing two phosphorus bases: structures, binding energies, and spin-spin coupling constants. *Journal of Physical Chemistry A*, **2007**, 111, 9924-30	2.8	14
239	Dual cation and anion acceptor molecules. The case of the (eta6-C6H6)(eta6C6F6)Cr0 complex. *Journal of Physical Chemistry A*, **2007**, 111, 3137-42	2.8	28
238	Double addition of azoles to glyoxal: characterization of the bis-adducts and theoretical study of their structure. *Arkivoc*, **2007**, 2007, 55-66	0.9	4
237	Computational studies of the structure of aldazines and ketazines. Part 1. Simple compounds. *Arkivoc*, **2007**, 2008, 48-56	0.9	2
236	Theoretical study of dihydrogen bonds in HnMH?HArF and HnMH?HKrF complexes (n=1□; M=Be, Al, Ga, Si, Ge). *Chemical Physics*, **2006**, 324, 459-464	2.3	25
235	Synthesis of Pyrazoles by Treatment of 3-Benzylchromones, 3-Benzylflavones and Their 4-Thio Analogues with Hydrazine. *European Journal of Organic Chemistry*, **2006**, 2006, 2825-2832	3.2	35
234	A 1H, 13C and 15N NMR study in solution and in the solid state of six N-substituted pyrazoles and indazoles. *Magnetic Resonance in Chemistry*, **2006**, 44, 566-70	2.1	24
233	Computed coupling constants in X(CH3)nH(4-n) moieties where X = 13C and 15N+, and n = 0-4: comparisons with experimental data. *Magnetic Resonance in Chemistry*, **2006**, 44, 698-707	2.1	14
232	The structure of ammonium pyrazolates in the solid state. *Magnetic Resonance in Chemistry*, **2006**, 44, 1067-72	2.1	8
231	Theoretical models of directional proton molecular transport. *Organic and Biomolecular Chemistry*, **2006**, 4, 3096-101	3.9	14

230	Theoretical study of dihydrogen bonds between (XH)2, X = Li, Na, BeH, and MgH, and weak hydrogen bond donors (HCN, HNC, and HCCH). *Journal of Physical Chemistry A*, **2006**, 110, 10279-86	2.8	80
229	Stereoisomer discrimination in complexes of halogen-substituted difuranes and Li or Na cations. *Journal of Physical Chemistry A*, **2006**, 110, 13310-6	2.8	5
228	Chiral recognition in self-complexes of tetrahydroimidazo[4,5-d]imidazole derivatives: from dimers to heptamers. *Journal of Physical Chemistry A*, **2006**, 110, 2259-68	2.8	28
227	On the Existence of Agostic Bonds: Bonding Analyses of Titanium Alkyl Complexes. *Organometallics*, **2006**, 25, 5638-5647	3.8	56
226	An ab initio study of 15N-11B spin-spin coupling constants for borazine and selected derivatives. *Journal of Physical Chemistry A*, **2006**, 110, 9959-66	2.8	45
225	Competition between nonclassical hydrogen-bonded acceptor sites in complexes of neutral AH2 Radicals (A = B, Al, and Ga): A theoretical investigation. *Journal of Physical Chemistry A*, **2006**, 110, 10817-21	2.8	24
224	Effect of dimerization and racemization processes on the electron density and the optical rotatory power of hydrogen peroxide derivatives. *Journal of Physical Chemistry A*, **2006**, 110, 7247-52	2.8	12
223	Theoretical Studies on Chiral Discrimination. *Current Organic Chemistry*, **2006**, 10, 695-714	1.7	16
222	Structural-activity relationship study on C-4 carbon atom of the CB1 antagonist SR141716: synthesis and pharmacological evaluation of 1,2,4-triazole-3-carboxamides. *European Journal of Medicinal Chemistry*, **2006**, 41, 114-20	6.8	20
221	Chiral discrimination in binuclear square planar metal complexes of group 10. *Inorganic Chemistry Communication*, **2006**, 9, 712-715	3.1	9
220	An Atoms in Molecules analysis of the differences between meso and chiral forms of oxirane and cyclobutene derivatives. *Chemical Physics Letters*, **2006**, 417, 367-370	2.5	7
219	XeH2 as a proton-accepting molecule for dihydrogen bonded systems: A theoretical study. *Chemical Physics Letters*, **2006**, 422, 226-229	2.5	20
218	The carbon carbon bond dissociation energy as a function of the chain length. *Chemical Physics Letters*, **2006**, 425, 221-224	2.5	26
217	Self-aggregation as a source of chiral discrimination. *Chemical Physics Letters*, **2006**, 427, 289-294	2.5	17
216	The structure of protonated HCP: A classical or non-classical ion?. *Chemical Physics Letters*, **2006**, 429, 23-26	2.5	7
215	Theoretical study of the bond energy in n-silanes and n-germanes: Comparison with n-alkanes. *Chemical Physics Letters*, **2006**, 429, 58-61	2.5	10
214	Regioselectivity in the formation of norbornene-fused pyrazoles: preparation of 1-substituted derivatives of 4,5,6,7-tetrahydro-1H-4,7-methanoindazole. *Tetrahedron*, **2006**, 62, 3362-3369	2.4	7
213	The calculated enthalpies of the nine pyrazole anions, cations, and radicals: a comparison with experiment. *Tetrahedron*, **2006**, 62, 8683-8686	2.4	16

212	A DFT study of the geometric, magnetic NMR chemical shifts and optical rotation properties of Tröger's bases. *Tetrahedron: Asymmetry*, **2006**, 17, 191-198		16
211	Phosphole, pyrrole, and their tetrahydro derivatives: A theoretical study of their properties. *Structural Chemistry*, **2006**, 17, 13-17	1.8	14
210	The annular tautomerism of imidazoles and pyrazoles: The possible existence of nonaromatic forms. *Structural Chemistry*, **2006**, 17, 439-444	1.8	38
209	Classification of hydrogen-bond motives in crystals of NH-pyrazoles: a mixed empirical and theoretical approach. *Arkivoc*, **2006**, 2006, 15-30	0.9	2
208	The structure of 2,3-dihydro-3-(2,4-dioxo-6-methylpyran-3-ylidene)-2-(2-nitrobenzyl)-1,4-benzothiazine and the problem of orthogonal interactions. *Arkivoc*, **2006**, 2006, 136-142	0.9	5
207	Periodic trends in bond dissociation energies. A theoretical study. *Journal of Physical Chemistry A*, **2005**, 109, 4359-65	2.8	56
206	3-(2-Pyridyl)-[1,2,3]triazolo[1,5-a]pyridines. An experimental and theoretical (DFT) study of the ring-chain isomerization. *Organic and Biomolecular Chemistry*, **2005**, 3, 3905-10	3.9	43
205	The X-Ray Molecular Structure of 1-(2?,4?-Dinitrophenyl)-1,2,3-triazole and the Problem of the Orthogonal Interaction Between a 'Pyridine-Like' Nitrogen and a Nitro Group. *Australian Journal of Chemistry*, **2005**, 58, 817	1.2	18
204	Theoretical study of HCN and HNC neutral and charged clusters. *Journal of Physical Chemistry B*, **2005**, 109, 18189-94	3.4	52
203	Chiral discrimination in lithium complexes of bis(5H-pyrroles) and bis(oxazolines). *Journal of Physical Chemistry A*, **2005**, 109, 9573-7	2.8	8
202	Chiral recognition in cyclic alpha-hydroxy carbonyl compounds: a theoretical study. *Journal of Physical Chemistry A*, **2005**, 109, 3262-6	2.8	10
201	Modelling protein-RNA interactions: an electron density study of the guanidinium and formate complexes with RNA bases. *Organic and Biomolecular Chemistry*, **2005**, 3, 366-71	3.9	23
200	A theoretical study of the influence of nitrogen angular constraints on the properties of amides: rotation/inversion barriers and hydrogen bond accepting abilities of N-formylaziridine and -azirine. *New Journal of Chemistry*, **2005**, 29, 1450	3.6	14
199	Ab initio study of the influence of trimer formation on one- and two-bond spin-spin coupling constants across an X-H-Y hydrogen bond: AH:XH:YH3 complexes for A, X = 19F, 35Cl and Y = 15N, 31P. *Journal of Physical Chemistry A*, **2005**, 109, 2350-5	2.8	10
198	Interaction energies and NMR indirect nuclear spin-spin coupling constants in linear HCN and HNC complexes. *Journal of Physical Chemistry A*, **2005**, 109, 6555-64	2.8	48
197	Topological analysis of the electron density distribution in perturbed systems. I. Effect of charge on the bond properties of hydrogen fluoride. *Journal of Physical Chemistry A*, **2005**, 109, 6532-9	2.8	21
196	Study of the reaction of chalcone analogs of dehydroacetic acid and o-aminothiophenol: synthesis and structure of 1,5-benzothiazepines and 1,4-benzothiazines. *Tetrahedron*, **2005**, 61, 6642-6651	2.4	68
195	Effect of HB complexation on the optical rotatory power of oxiranes. *Chemical Physics Letters*, **2005** , 409, 163-166	2.5	6

194	Are resonance-assisted hydrogen bonds resonance assisted? A theoretical NMR study. *Chemical Physics Letters*, **2005**, 411, 411-415	2.5	101
193	A theoretical investigation of NH?OP hydrogen bonds through 15N31P and 1H31P coupling constants. *Chemical Physics Letters*, **2005**, 412, 97-100	2.5	11
192	Barriers to the intramolecular N- to N-transfer of different groups in pyrazoles: Prototropy vs. Elementotropy. *Heteroatom Chemistry*, **2005**, 16, 628-636	1.2	14
191	Solid-State NMR Study of the Tautomerism of Acetylacetone Included in a Host Matrix. *Helvetica Chimica Acta*, **2005**, 88, 1931-1942	2	15
190	Cooperativity and proton transfer in hydrogen-bonded triads. *ChemPhysChem*, **2005**, 6, 1411-8	3.2	47
189	The tautomerism of 1H-pyrazole-3(5)-(N-tert-butyl)carboxamide in the solid state and in solution. *Magnetic Resonance in Chemistry*, **2005**, 43, 89-91	2.1	27
188	Theoretical study of 31P, 31P coupling constants in cyclotriphosphazenes. *Magnetic Resonance in Chemistry*, **2005**, 43, 471-4	2.1	7
187	A theoretical study of multinuclear coupling constants in pyrazoles. *Magnetic Resonance in Chemistry*, **2005**, 43, 985-91	2.1	18
186	Structure of the products of condensation of hydroxylamine with trifluoromethyl-beta-diketones: assignments of the diastereotopic protons of the 4-methylene group in 5-hydroxy-5-trifluoromethyl-delta2-isoxazolines. *Magnetic Resonance in Chemistry*, **2005**, 43, 1040-3	2.1	11
185	Effect of fluoro substituents and central atom nature on chiral derivatives of bisdiphenylborates and isoelectronic structures. *Tetrahedron: Asymmetry*, **2005**, 16, 755-760		10
184	Polyynes vs. Cumulenes: Their Possible Use as Molecular Wires. *Structural Chemistry*, **2005**, 16, 77-79	1.8	17
183	Dimers of 1,8a-Dihydro-1,8-Naphthyridine Derivatives as Models of Chiral Self-Recognition. *Structural Chemistry*, **2005**, 16, 339-345	1.8	7
182	A Theoretical Study on the Tautomerism of C-Carboxylic and Methoxycarbonyl Substituted Azoles. *Structural Chemistry*, **2005**, 16, 507-514	1.8	27
181	Chiral recognition in phosphinic acid dimers. *Journal of Physical Organic Chemistry*, **2005**, 18, 491-497	2.1	13
180	Theoretical estimation of the annular tautomerism of indazoles. *Journal of Physical Organic Chemistry*, **2005**, 18, 719-724	2.1	48
179	Influence of protonation on the electron density derived properties. *Arkivoc*, **2005**, 2005, 305-320	0.9	59
178	The structure of 1,1,3-trimethyl-2- pyrazolinium perchlorate: An X-ray crystallographic and GIAO/DFT multinuclear NMR study. *Spectroscopy*, **2004**, 18, 605-611		8
177	19F-19F spin-spin coupling constant surfaces for (HF)2 clusters: the orientation and distance dependence of the sign and magnitude of J(F-F). *Journal of Chemical Physics*, **2004**, 120, 3237-43	3.9	30

176	Fluorine–fluorine Interactions: NMR and AIM Analysis. *Structural Chemistry*, **2004**, 15, 117-120	1.8	92
175	Paradigms and Paradoxes: The Position of the Lone Pair in Amines: A Comparison Between Bader's AIM Approach and Pure Geometrical Considerations. *Structural Chemistry*, **2004**, 15, 599-604	1.8	5
174	Karplus-type relationships between scalar coupling constants: 3 J HH molecular versus 4h J HH supramolecular coupling constants. *Theoretical Chemistry Accounts*, **2004**, 111, 31-35	1.9	13
173	Synthesis of Pyrazolyl-2-pyrazolines by Treatment of 3-(3-Aryl-3-oxopropenyl)chromen-4-ones with Hydrazine and Their Oxidation to Bis(pyrazoles). *European Journal of Organic Chemistry*, **2004**, 2004, 4672-4679	3.2	41
172	The tautomerism of Omeprazole in solution: a 1H and 13C NMR study. *Magnetic Resonance in Chemistry*, **2004**, 42, 712-4	2.1	52
171	A GIAO/DFT study of 1H, 13C and 15N shieldings in amines and its relevance in conformational analysis. *Magnetic Resonance in Chemistry*, **2004**, 42, 955-61	2.1	50
170	Study of the structure of 1-hydroxymethylindazole and 1-hydroxymethylbenzotriazole by X-ray crystallography, multinuclear NMR in solution and DFT calculations. *Journal of Heterocyclic Chemistry*, **2004**, 41, 285-289	1.9	10
169	The structure of 1-formyl-3-phenyl-2-pyrazoline in the gas phase (DFT calculations), in solution (NMR) and in the solid state (X-ray crystallography). *Journal of Molecular Structure*, **2004**, 689, 251-254	3.4	15
168	The structure of p-nitrophenylhydrazones of aldehydes: the case of the p-nitrophenylhydrazone of 2-diethylamino-5-methoxy-2H-indazole-3-carboxaldehyde. *Journal of Molecular Structure*, **2004**, 699, 17-21	3.4	9
167	Chiral discrimination and isomerization processes in monomers, dimers and trimers of sulfoxides and thioperoxides. *Tetrahedron: Asymmetry*, **2004**, 15, 1391-1399		13
166	Classical versus redox tautomerism: substituent effects on the keto/enol and sulfoxide/sulfenic acid equilibria. *Tetrahedron Letters*, **2004**, 45, 4127-4129	2	10
165	A theoretical study of the tautomerism and ionization of 5-substituted NH-tetrazoles. *Computational and Theoretical Chemistry*, **2004**, 668, 123-132		57
164	Theoretical study of peptide model dimers. Homo versus heterochiral complexes. *Computational and Theoretical Chemistry*, **2004**, 680, 191-198		7
163	Influence of the H/F replacement on the homoaromaticity of homotropylium ion: a GIAO/DFT theoretical study. *Tetrahedron*, **2004**, 60, 2259-2265	2.4	9
162	Synthesis, experimental and theoretical NMR study of 2?-hydroxychalcones bearing a nitro substituent on their B ring. *Tetrahedron*, **2004**, 60, 6513-6521	2.4	24
161	On the tautomerism of pyrazolones: the geminal 2J[pyrazole C-4,H-3(5)] spin coupling constant as a diagnostic tool. *Tetrahedron*, **2004**, 60, 6791-6805	2.4	44
160	Tetrahydroacridin-9-ones, 9-chlorotetrahydroacridines, 9-amino-tetrahydroacridines and 9-(pyrazol-1-yl)-tetrahydroacridines derived from chiral cyclanones. *European Journal of Medicinal Chemistry*, **2004**, 39, 37-48	6.8	20
159	The enormous apparent gas-phase acidity of cubylamine. *Chemical Physics Letters*, **2004**, 398, 560-563	2.5	6

158	Multiple hydrogen bonds and tautomerism in naphthyridine derivatives. *New Journal of Chemistry*, **2004**, 28, 700-707	3.6	40
157	Modeling Protein–RNA Interactions: An Electron-Density Study of the Formamide and Formic Acid Complexes with RNA Bases. *Journal of Physical Chemistry B*, **2004**, 108, 3335-3341	3.4	37
156	The Structure of Two 1-(Nitrophenyl)-2-pyrazolines: a Crystallographic and Theoretical Study. *Australian Journal of Chemistry*, **2004**, 57, 1103	1.2	14
155	Discovery of 5-(4-chlorophenyl)-1-(2,4-dichlorophenyl)-3-hexyl-1h-1,2,4-triazole, a novel in vivo cannabinoid antagonist containing a 1,2,4-triazole motif. *Journal of Medicinal Chemistry*, **2004**, 47, 2939-42	8.3	67
154	Computed Spin–Spin Coupling Constants (1JX-Y) in Molecules HmXYHn for X and Y = 13C, 15N, and 31P: Comparisons with Experiment and Insights into the Signs of 1JX-Y. *Journal of Physical Chemistry A*, **2004**, 108, 3662-3667	2.8	32
153	Do coupling constants and chemical shifts provide evidence for the existence of resonance-assisted hydrogen bonds?. *Molecular Physics*, **2004**, 102, 2563-2574	1.7	119
152	Homoheteroaromaticity: the case study of azepine and dibenzazepine. *Organic and Biomolecular Chemistry*, **2004**, 2, 1587-91	3.9	25
151	Protic Acidity of Some Aliphatic and Alicyclic Hydrocarbons in the Gas Phase and in Solution. An Empirical and Computational Link. *Collection of Czechoslovak Chemical Communications*, **2004**, 69, 2134-2146		1
150	Hydrogen bond acceptor properties of two radicals: nitric oxide molecule and hydrogen atom. *Arkivoc*, **2004**, 2003, 31-36	0.9	2
149	The behavior of 5H-dibenz[b,f]azepine in sulfuric acid solution. *Arkivoc*, **2004**, 2004, 206-212	0.9	6
148	Theoretical study of cyameluric acid and related compounds. *Arkivoc*, **2004**, 2004, 130-136	0.9	13
147	Fentanyl and its analogue N-(1-phenylpyrazol-3-yl)-N-[1-(2-phenylethyl)-4-piperidyl]propanamide: 1H- and 13C-NMR spectroscopy, X-ray crystallography, and theoretical calculations. *Chemical and Pharmaceutical Bulletin*, **2003**, 51, 929-34	1.9	9
146	Computed EOM-CCSD 19F-19F Spin-Spin Coupling Constants in Small Organic Molecules. *Zeitschrift Fur Physikalische Chemie*, **2003**, 217, 1565-1576	3.1	18
145	Review on DFT and ab initio Calculations of Scalar Coupling Constants. *International Journal of Molecular Sciences*, **2003**, 4, 64-92	6.3	69
144	GIAO Calculations of Chemical Shifts in Heterocyclic Compounds. *Structural Chemistry*, **2003**, 14, 377-389	1.8	71
143	The Molecular Structure and NMR Properties of P-Phosphinoylmethyl Aminophosphonium Salts. *Structural Chemistry*, **2003**, 14, 391-397	1.8	6
142	The Structure of N1-Hydroxylophine N3-Oxide (=1-Hydroxy-2,4,5- triphenyl-1H-imidazole 3-Oxide) in the Solid State. *Helvetica Chimica Acta*, **2003**, 86, 1026-1039	2	9
141	Comparison of electron density properties in frozen and relaxed electronic distributions. *Journal of Computational Chemistry*, **2003**, 24, 416-21	3.5	6

140	Stereoelectronic, strain, and medium effects on the protonation of cubylamine, a Janus-like base. *Angewandte Chemie - International Edition*, **2003**, 42, 2281-4	16.4	17
139	Hydrogen bonding properties of krypton derivatives. *Chemical Physics Letters*, **2003**, 381, 505-511	2.5	14
138	A theoretical study of (old and new) non-classical carbocations derived from cyclic saturated hydrocarbons. *Journal of Physical Organic Chemistry*, **2003**, 16, 546-554	2.1	14
137	Protonation and phase effects on the NMR chemical shifts of imidazoles and pyrazoles: experimental results and GIAO calculations. *New Journal of Chemistry*, **2003**, 27, 734-742	3.6	37
136	Structure of a 4-nitroso-5-aminopyrazole and its salts: tautomerism, protonation, and E/Z isomerism. *Journal of Organic Chemistry*, **2003**, 68, 8831-7	4.2	21
135	Aromatic Systems as Charge Insulators: Their Simultaneous Interaction with Anions and Cations. *Journal of Physical Chemistry A*, **2003**, 107, 9428-9433	2.8	50
134	Interaction of Protein Backbone with Nucleic Acid Bases. *Journal of Physical Chemistry B*, **2003**, 107, 5306-5310	3.4	20
133	Two-Bond 15N–19F Spin–Spin Coupling Constants (2hJN-F) across NH+...F Hydrogen Bonds. *Journal of Physical Chemistry A*, **2003**, 107, 3126-3131	2.8	20
132	Two-Bond 19F–15N Spin–Spin Coupling Constants (2hJF-N) across FH···N Hydrogen Bonds. *Journal of Physical Chemistry A*, **2003**, 107, 3121-3125	2.8	34
131	DNA Triplexes: A Study of Their Hydrogen Bonds. *Journal of Physical Chemistry B*, **2003**, 107, 323-330	3.4	26
130	Influence of carbocation stability in the gas phase on solvolytic reactivity: beyond bridgehead derivatives. *Journal of Organic Chemistry*, **2003**, 68, 3786-96	4.2	33
129	Two-Bond 13C–15N Spin–Spin Coupling Constants (2hJC-N) Across CH···N Hydrogen Bonds. *Journal of Physical Chemistry A*, **2003**, 107, 3222-3227	2.8	22
128	The influence of chain elongation on Karplus-type relationships: a DFT study of scalar coupling constants in polyacetylene derivatives. *Organic and Biomolecular Chemistry*, **2003**, 1, 585-7	3.9	6
127	Large chiral recognition in hydrogen-bonded complexes and proton transfer in pyrrolo[2,3-b]pyrrole dimers as model compounds. *Journal of Organic Chemistry*, **2003**, 68, 7485-9	4.2	65
126	A theoretical study of the origin of rotational barriers in push–pull ethylenes. *Computational and Theoretical Chemistry*, **2002**, 585, 27-34		21
125	Theoretical study of the SiH group as potential hydrogen bond donor. *International Journal of Quantum Chemistry*, **2002**, 86, 122-129	2.1	8
124	An experimental (NMR) and theoretical (GIAO) study of the tautomerism of benzotriazole in solution. *Tetrahedron*, **2002**, 58, 9089-9094	2.4	43
123	1-Benzoylazoles: an experimental (NMR and crystallography) and theoretical study. *Journal of Molecular Structure*, **2002**, 605, 199-212	3.4	17

122	Interaction of anions with perfluoro aromatic compounds. *Journal of the American Chemical Society*, **2002**, 124, 8593-8	16.4	460
121	From weak to strong interactions: A comprehensive analysis of the topological and energetic properties of the electron density distribution involving XH?FY systems. *Journal of Chemical Physics*, **2002**, 117, 5529-5542	3.9	1196
120	Molecular Versus Supramolecular Chemistry: The Rotational Barriers About Covalent Bonds and Hydrogen Bonds. *Structural Chemistry*, **2002**, 13, 97-98	1.8	6
119	Discrimination of hydrogen-bonded complexes with axial chirality. *Journal of Chemical Physics*, **2002**, 117, 6463-6468	3.9	62
118	Thermodynamic Stabilities of Carbocations. *Advances in Physical Organic Chemistry*, **2002**, 37, 57-135	0.3	16
117	Synthesis, 1H and 13C NMR Study of Pyrazoles Derived from Chiral Cyclohexanones (3-Methylcyclohexanone, Menthone, Pulegone, Dihydrocarvone and Carvone). *Heterocycles*, **2002**, 57, 307	0.8	12
116	(3h)J((15)N-(31)P) spin-spin coupling constants across N[bond]H....O[bond]P hydrogen bonds. *Journal of the American Chemical Society*, **2002**, 124, 6393-7	16.4	29
115	Ab Initio Study of the Structural, Energetic, Bonding, and IR Spectroscopic Properties of Complexes with Dihydrogen Bonds. *Journal of Physical Chemistry A*, **2002**, 106, 9325-9330	2.8	85
114	Influence of intermolecular hydrogen bonds on the tautomerism of pyridine derivatives. *Journal of Organic Chemistry*, **2002**, 67, 1515-9	4.2	61
113	One-Bond (1dJH-H) and Three-Bond (3dJX-M) SpinSpin Coupling Constants Across XHHHM Dihydrogen Bonds. *Journal of Physical Chemistry A*, **2002**, 106, 9331-9337	2.8	28
112	Self-discrimination of enantiomers in hydrogen-bonded dimers. *Journal of the American Chemical Society*, **2002**, 124, 1488-93	16.4	76
111	Interaction of adenine with synthetic receptors: a theoretical study. *Perkin Transactions II RSC*, **2002**, 894-898		11
110	Triaziridine and tetrazetidine vs. cyclic water trimer and tetramer: A computational approach to the relationship between molecular and supramolecular conformational analysis. *Physical Chemistry Chemical Physics*, **2002**, 4, 2123-2129	3.6	10
109	An ab initio study of the NMR properties (absolute shieldings and NICS) of a series of significant aromatic and antiaromatic compounds. *Tetrahedron*, **2001**, 57, 6043-6049	2.4	36
108	A 13C NMR study of the structure of four cinnamic acids and their methyl esters. *Journal of Molecular Structure*, **2001**, 595, 1-6	3.4	19
107	Ab initio study of azolides: Energetic and spectroscopic properties. *Journal of Heterocyclic Chemistry*, **2001**, 38, 443-450	1.9	20
106	A density functional theoretical study of the influence of cavities and water molecules on tautomerism: The case of pyridones and 1,2,4-triazoles linked to crown ethers and esters. *Journal of Heterocyclic Chemistry*, **2001**, 38, 1387-1391	1.9	18
105	Basicity of N-H- and N-Methyl-1,2,3-triazoles in the Gas Phase, in Solution, and in the Solid State An Experimental and Theoretical Study. *European Journal of Organic Chemistry*, **2001**, 2001, 3013	3.2	107

104	About the evaluation of the local kinetic, potential and total energy densities in closed-shell interactions. *Chemical Physics Letters*, **2001**, 336, 457-461	2.5	349
103	Strained systems as hydrogen bond acceptors: the case of benzyne. *Chemical Physics Letters*, **2001**, 350, 325-330	2.5	11
102	A Theoretical and Experimental Study of the Interaction of C6F6 with Electron Donors. *Structural Chemistry*, **2001**, 12, 459-464	1.8	26
101	Aminopropylsilanes versus silatranes: an experimental and theoretical study. *Journal of Organometallic Chemistry*, **2001**, 625, 148-153	2.3	33
100	A theoretical study of the addition reactions of HF, H2O, H2S, NH3 and HCN to carbodiimide and related heterocumulenes. *Computational and Theoretical Chemistry*, **2001**, 544, 5-23		6
99	Transition metals as hydrogen bond acceptors: a theoretical study. *Computational and Theoretical Chemistry*, **2001**, 537, 139-150		13
98	Intramolecular Hydrogen Bonds inortho-Substituted Hydroxybenzenes and in 8-Susbtituted 1-Hydroxynaphthalenes:Can a Methyl Group Be an Acceptor of Hydrogen Bonds?. *Journal of Physical Chemistry A*, **2001**, 105, 10462-10467	2.8	119
97	The structure of halogeno-1,2,4-triazoles in the solid state and in solution. *New Journal of Chemistry* , **2001**, 25, 1061-1068	3.6	53
96	A solid-state NMR, X-ray diffraction, and ab initio computational study of hydrogen-bond structure and dynamics of pyrazole-4-carboxylic acid chains. *Journal of the American Chemical Society*, **2001**, 123, 7898-906	16.4	79
95	Hydrogen Bond vs Proton Transfer between Neutral Molecules in the Gas Phase. *Journal of Physical Chemistry A*, **2001**, 105, 7481-7485	2.8	53
94	Molecular Complexes between Silicon Derivatives and Electron-Rich Groups. *Journal of Physical Chemistry A*, **2001**, 105, 743-749	2.8	166
93	A Multinuclear NMR Spectral Study of Parent Azoles and Benzazoles: Experimental Results and GIAO Ab initio Calculations. *Heterocycles*, **2001**, 55, 2109	0.8	24
92	13C and15N NMR shieldings of 1,2,4-diazaphospholes in the solid state and in solution. *Spectroscopy*, **2001**, 15, 27-32		10
91	Water Clusters: Towards an Understanding Based on First Principles of Their Static and Dynamic Properties. *Angewandte Chemie - International Edition*, **2000**, 39, 717-721	16.4	213
90	Basicity of 1-nitroaryl-4,5-dihydropyrazoles: pK a measurements and theoretical calculations. *Journal of Physical Organic Chemistry*, **2000**, 13, 372-381	2.1	7
89	Supramolecular structure of 1H-pyrazoles in the solid state: a crystallographic and ab initio study. *Acta Crystallographica Section B: Structural Science*, **2000**, 56 (Pt 6), 1018-28		85
88	Effects of fluorine substitution on hydrogen bond interactions. *Journal of Fluorine Chemistry*, **2000**, 101, 233-238	2.1	67
87	Vibrational spectra of 3,5-dimethylpyrazole and deuterated derivatives. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2000**, 56A, 1469-98	4.4	40

86	Comparison of models to correlate electron density at the bond critical point and bond distance. *Computational and Theoretical Chemistry*, **2000**, 496, 131-137		113
85	Basicity and Proton Transfer in Proton Sponges and Related Compounds: An Ab Initio Study. *Structural Chemistry*, **2000**, 11, 335-340	1.8	21
84	Solution and solid state (CPMAS) NMR studies of the tautomerism of six-membered heterocyclic compounds related to 2-pyridones. *Spectroscopy*, **2000**, 14, 121-126		18
83	Behavior of Ylides Containing N, O, and C Atoms as Hydrogen Bond Acceptors. *Journal of the American Chemical Society*, **2000**, 122, 11154-11161	16.4	1021
82	Novel bronchodilators: synthesis, transamination reactions, and pharmacology of a series of pyrazino[2,3-c][1,2,6]thiadiazine 2, 2-dioxides. *Journal of Medicinal Chemistry*, **2000**, 43, 4219-27	8.3	15
81	The P4□Li+ Ion in the Gas Phase: A Planetary System. *Journal of the American Chemical Society*, **2000**, 122, 4451-4454	16.4	37
80	4hJ(31P□31P) Coupling Constants through N□H+□N Hydrogen Bonds:□A Comparsion of Computed ab Initio and Experimental Data. *Journal of Physical Chemistry A*, **2000**, 104, 7165-7166	2.8	36
79	Synthesis and structural studies of some [14]paracyclo-bis-(1,2)pyrazolium- and (1,3)imidazolium-phanes. *Tetrahedron*, **1999**, 55, 2327-2340	2.4	17
78	How strong are the complexes between methane radical cation and noble gas atoms?. *Chemical Physics Letters*, **1999**, 311, 281-291	2.5	5
77	A General Equation Holds for the Geometry of Hydrogen Bonds with O and N Acceptors. *Structural Chemistry*, **1999**, 10, 157-159	1.8	9
76	Can aromaticity be described with a single parameter? Benzene vs. cyclohexatriene. *New Journal of Chemistry*, **1999**, 23, 951-954	3.6	27
75	The structure of 3,5-bis(trifluoromethyl)pyrazole in the gas phase and in the solid state. *New Journal of Chemistry*, **1999**, 23, 1231-1237	3.6	31
74	Theoretical Study of Strong Hydrogen Bonds between Neutral Molecules: The Case of Amine Oxides and Phosphine Oxides as Hydrogen Bond Acceptors. *Journal of Physical Chemistry A*, **1999**, 103, 272-279	2.8	143
73	Monohydride and Monofluoride Derivatives of B, Al, N and P. Theoretical Study of Their Ability as Hydrogen Bond Acceptors. *Journal of Physical Chemistry A*, **1999**, 103, 8861-8869	2.8	24
72	Fluoropyrazoles: An Ab initio Study. *Heterocycles*, **1999**, 51, 355	0.8	11
71	Ab Initio (GIAO) Calculations of Absolute Nuclear Shieldings for Representative Compounds Containing 1(2)H, 6(7)Li, 11B, 13C, 14(15)N, 17O, 19F, 29Si, 31P, 33S, and 35Cl Nuclei. *Structural Chemistry*, **1998**, 9, 187-202	1.8	78
70	Bond Length□Electron Density Relationships: From Covalent Bonds to Hydrogen Bond Interactions. *Structural Chemistry*, **1998**, 9, 243-247	1.8	131
69	Dissociation Energies and Rotational Barriers About CC Single, Double, and Triple Bonds: A Hybrid HF-DFT Approach (Becke3LYP/6-311++G**). *Structural Chemistry*, **1998**, 9, 59-63	1.8	9

68	Solvent effect on the tautomerism of 4-aminopyrazino[2,3-c][1,2,6]thiadiazine 2,2-dioxides. *Journal of the Chemical Society Perkin Transactions II*, **1998**, 1889-1892		11
67	Radicals as hydrogen bond acceptors. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1998**, 102, 429-435		43
66	Bifurcated Hydrogen Bonds: Three-Centered Interactions. *Journal of Physical Chemistry A*, **1998**, 102, 9925-9932	2.8	198
65	Similarity studies on guanidinium, imidazolinium, and imidazolium cations: toward new bradykinin antagonists. *Journal of Molecular Graphics and Modelling*, **1998**, 16, 150-6, 166-7	2.8	9
64	The additive properties of the electron density at the bond critical points in hydrogen-bonded complexes. *Computational and Theoretical Chemistry*, **1998**, 452, 227-232		17
63	Isocyanides as hydrogen bond acceptors. *Theoretical Chemistry Accounts*, **1998**, 99, 116-123	1.9	42
62	A theoretical study of epibatidine. *Journal of the Chemical Society Perkin Transactions II*, **1998**, 2665-2670		14
61	Conformation of 5,6,11,12-tetrahydrodibenzo[a,e]cyclooctene: an experimental and theoretical NMR study. *New Journal of Chemistry*, **1998**, 22, 1079-1083	3.6	16
60	1,2-Proton shifts in pyrazole and related systems: a computational study of [1,5]-sigmatropic migrations of hydrogen and related phenomena *Journal of the Chemical Society Perkin Transactions II*, **1998**, 2497-2504		50
59	Ring Strain and Hydrogen Bond Acidity. *Journal of Organic Chemistry*, **1998**, 63, 7759-7763	4.2	25
58	Charge-Transfer Complexes between Dihalogen Compounds and Electron Donors. *Journal of Physical Chemistry A*, **1998**, 102, 9278-9285	2.8	175
57	Ab initio hybrid DFT GIAO calculations of the shielding produced by carbon arbon bonds and aromatic rings in 1H NMR spectroscopy. *New Journal of Chemistry*, **1998**, 22, 381-385	3.6	67
56	Non-conventional hydrogen bonds. *Chemical Society Reviews*, **1998**, 27, 163	58.5	476
55	A computational approach to intermolecular proton transfer in the solid state: assistance by proton acceptor molecules. *Journal of the Chemical Society Perkin Transactions II*, **1998**, 2671-2676		30
54	Inverse Hydrogen-Bonded Complexes. *Journal of Physical Chemistry A*, **1997**, 101, 4236-4244	2.8	91
53	Theoretical Study of the Influence of Electric Fields on Hydrogen-Bonded Acid Base Complexes. *Journal of Physical Chemistry A*, **1997**, 101, 9791-9800	2.8	101
52	An Attractive Interaction between the Cloud of C6F6 and Electron-Donor Atoms. *Journal of Organic Chemistry*, **1997**, 62, 4687-4691	4.2	168
51	Carbon acidity and ring strain: A hybrid HF-DFT approach (Becke3LYP/6 11++G**). *Tetrahedron*, **1997**, 53, 9741-9748	2.4	29

50	Unusual Hydrogen Bonds: H□□□Interactions. *Journal of Physical Chemistry A*, **1997**, 101, 9457-9463	2.8	173
49	Tautomerism and the Mills-Nixon-like effect in pyrazoles. *Structural Chemistry*, **1997**, 8, 189-195	1.8	18
48	The Mills-Nixon effect on enol-enol tautomerism in ß-dicarbonyl compounds and on annular tautomerism in NH-pyrazoles: A semi-empirical study. *Tetrahedron*, **1997**, 53, 1403-1410	2.4	23
47	Field effects on dihydrogen bonded systems. *Chemical Physics Letters*, **1997**, 275, 423-428	2.5	63
46	A 3D model of the delta opioid receptor and ligand-receptor complexes. *Protein Engineering, Design and Selection*, **1996**, 9, 573-83	1.9	39
45	Carbenes and Silylenes as Hydrogen Bond Acceptors. *The Journal of Physical Chemistry*, **1996**, 100, 19367-19370		74
44	Synthesis, hydrolysis reactions and conformational study of 2-substituted 3,5-diamino-4-nitroso-2H-1,2,6-thiadiazine 1,1-dioxides. *Journal of the Chemical Society Perkin Transactions II*, **1996**, 293-297		7
43	Dihydrogen bonds (A–H?H–B). *Chemical Communications*, **1996**, 1633-1634	5.8	84
42	Similarity Study on Peptide ß-turn Conformation Mimetics. *Journal of Molecular Modeling*, **1996**, 2, 16-25	2	10
41	Theoretical and experimental analysis of properties in heterocycles containing the aminosulphonylamino moiety. *Journal of Physical Organic Chemistry*, **1996**, 9, 203-211	2.1	15
40	Molecular polarization potential maps of the nucleic acid bases. *International Journal of Quantum Chemistry*, **1996**, 57, 123-135	2.1	124
39	A statistical survey of the Cambridge structural database concerning density and packing. *Journal of Molecular Structure*, **1996**, 382, 205-213	3.4	12
38	Similarity Study on Peptide >-turn Conformation Mimetics. *Journal of Molecular Modeling*, **1996**, 2, 16-25	2	12
37	. *International Journal of Quantum Chemistry*, **1996**, 57, 123	2.1	63
36	Constrained C-terminal hexapeptide neurotensin analogues containing a 3-oxoindolizidine skeleton. *International Journal of Peptide Research and Therapeutics*, **1995**, 1, 269-276		3
35	2-Amino-3-oxohexahydroindolizino[8,7-b]indole-5-carboxylate derivatives as new scaffolds for mimicking ß-turn secondary structures. Molecular dynamics and stereoselective synthesis. *Tetrahedron*, **1995**, 51, 7841-7856	2.4	33
34	Approximations in the computation of molecular polarization maps **1995**, 1, 26-37		5
33	Theoretical Study of CH.cntdot..cntdot..cntdot.O Hydrogen Bonds in H2O-CH3F, H2O-CH2F2, and H2O-CHF3. *The Journal of Physical Chemistry*, **1995**, 99, 6457-6460		67

32	Sequence divergence analysis for the prediction of seven-helix membrane protein structures: II. A 3-D model of human rhodopsin. *Protein Engineering, Design and Selection*, **1994**, 7, 1231-8	1.9	23
31	Sequence divergence analysis for the prediction of seven-helix membrane protein structures: I. Comparison with bacteriorhodopsin. *Protein Engineering, Design and Selection*, **1994**, 7, 1221-9	1.9	10
30	Imidazole and benzimidazole addition to quinones. Formation of meso and d,l isomers and crystal structure of the d,l isomer of 2,3-Bis(benzimidazol-1'-yl)-1,4-dihydroxybenzene. *Tetrahedron*, **1994**, 50, 12489-12510	2.4	18
29	Comparison of methods to estimate geometric and electronic properties on sulfur containing compounds. *Theoretica Chimica Acta*, **1994**, 89, 1-12		25
28	The induced polarization of the water molecule. *Chemical Physics Letters*, **1994**, 224, 160-165	2.5	21
27	Molecular polarization maps as a tool for studies of intermolecular interactions and chemical reactivity. *Journal of Molecular Graphics*, **1994**, 12, 3-13		25
26	Molecular electrostatic potential of D1 and D2 dopamine agonists. *Journal of Medicinal Chemistry*, **1994**, 37, 210-3	8.3	16
25	Comparative study between ab initio and semiempirical electrostatic potentials on molecular surfaces. *Journal of Computational Chemistry*, **1993**, 14, 530-540	3.5	17
24	Conformational analysis of 2,3,6,7-tetrahydroazepines with implications for D1-selective benzazepines. *Journal of Computational Chemistry*, **1993**, 14, 571-578	3.5	7
23	Comparison of methods to estimate the free energy of solvation:Importance in the modulation of the affinity of 3-benzazepines for the D1receptor. *Journal of Computational Chemistry*, **1993**, 14, 620-626	3.5	19
22	Considerations on the recognition of the D1 receptor by agonists. *Journal of Computer-Aided Molecular Design*, **1993**, 7, 659-670	4.2	8
21	Strategies for indirect computer-aided drug design. *Pharmaceutical Research*, **1993**, 10, 475-86	4.5	51
20	Effect of the basis set on the computation of molecular polarization. *The Journal of Physical Chemistry*, **1993**, 97, 9113-9119		20
19	N-substituted pyrazino[2,3-c][1,2,6]thiadiazine 2,2-dioxides. A new class of diuretics. *Journal of Medicinal Chemistry*, **1992**, 35, 3977-83	8.3	12
18	Quantum mechanical parametrization of a conformationally dependent hydrophobic index. *International Journal of Quantum Chemistry*, **1992**, 44, 203-218	2.1	20
17	Theoretical studies of aza analogues of platonic hydrocarbons.. *Computational and Theoretical Chemistry*, **1991**, 228, 47-60		19
16	Selective Bromination of Pyrido[2,3-c][1,2,6]thiadiazine 2,2-Dioxides. *Synthetic Communications*, **1991**, 21, 827-831	1.7	3
15	Synthesis and E/Z Stereoisomerism of 6-Carbaldoxime Derivatives of Pyrazino[2,3-c]-1,2,6-thiadiazine 2,2-Dioxide. *Heterocycles*, **1991**, 32, 279	0.8	3

14	Theoretical studies of aza analogues of platonic hydrocarbons. *Computational and Theoretical Chemistry*, **1990**, 206, 67-75		32
13	Theoretical studies on aza-analogs of platonic hydrocarbons. *Computational and Theoretical Chemistry*, **1990**, 208, 63-77		16
12	Synthesis and Physico-Chemical Properties of 6- and 7-Monosubstituted Pyrazino|2,3-c |-1,2,6-thiadiazine 2,2-Dioxides. *Pteridines*, **1990**, 2, 3-21	0.6	9
11	Energy calculations and computer modeling of chromatographic separations on microcrystalline cellulose triacetate. *Chromatographia*, **1989**, 27, 77-81	2.1	7
10	Reactivity of Cyanogen towards N-Substituted Sulfamides: Synthesis of 1,2,5-Thiadiazole 1,1-Dioxide Derivatives. *Liebigs Annalen Der Chemie*, **1989**, 1989, 1135-1137		6
9	A molecular orbital study of the conformation (inversion and rotational barriers) and electronic properties of sulfamide. *Canadian Journal of Chemistry*, **1989**, 67, 2227-2236	0.9	15
8	Synthesis and reactivity of some amino-substituted 1,2,5-thiadiazole 1,1-dioxides. *Liebigs Annalen Der Chemie*, **1988**, 1988, 337-341		9
7	Reactivity of malononitrile towards sulphamide and N-substituted sulphamides: synthesis and hydrolysis reactions of 3,5-diamino-1,2,6-thiadiazine 1,1-dioxides. *Journal of the Chemical Society Perkin Transactions 1*, **1988**, 1271-1275		10
6	Topological Properties of the Electron Distribution in Hydrogen-bonded Systems425-451		9
5	The effect of the hybrid multi-layered Graphene oxide/Talc as a hydrophobic agent in epoxy coating. *Plastics, Rubber and Composites*,1-22	1.5	0
4	Microsolvation of the Be-F bond in complexes of BeF2, BeF3−1, and BeF4−2 with nH2O, for n = 1–6. *Molecular Physics*,e1933637	1.7	1
3	Substituent effects of fused Hammick silylenes via density functional theory survey. *Journal of Physical Organic Chemistry*,e4264	2.1	1
2	The interaction between ethionamide and pristine, Si-, Ga-, and Al-doped boron nitride nanoflakes: A computational study. *Journal of Sulfur Chemistry*,1-17	2.3	0
1	Hydro-trifluoromethyl(thiol)ation of alkenes: a review*. *Journal of Sulfur Chemistry*,1-21	2.3	