Devesh Kumar

List of Publications by Year in Descending Order

122 papers	7,637 citations	48 h-index	86 g-index
131 ext. papers	8,184 ext. citations	7.8 avg, IF	5.88 L-index

#	Paper	IF	Citations
122	Biotransformation of BPA via epoxidation catalyzed by Cytochrome P450. *Inorganic Chemistry Communication*, **2022**, 139, 109321	3.1	0
121	A theoretical investigation of nonlinear optical and electronic molecular parameters of hexabutyloxytryphenylene and halogenated hexabutyloxytryphenylene molecules using density functional theory (DFT) for nonlinear device applications. *Physica Scripta*, **2022**, 97, 065808	2.6	1
120	Interplay Between Theory and Experiment: A Future Approach for Biomedical Research **2022**, 41-67		
119	Ferromagnetic Coupling in Oxidovanadium(IV)-Porphyrin Radical Dimers. *Inorganic Chemistry*, **2021**, 60, 16492-16506	5.1	0
118	Metabolism of 8-aminoquinoline (8AQ) Primaquine via aromatic hydroxylation step mediated by Cytochrome P450 enzyme using Density Functional Theory. *Journal of Organometallic Chemistry*, **2021**, 957, 122154	2.3	0
117	Scavenging of OH and OOH radicals by polyradicals of small polycyclic aromatic hydrocarbons. *Journal of Molecular Modeling*, **2021**, 27, 112	2	
116	DFT-based numerical study of the re-entrant phase and optical parameters of the homologous series of MBC liquid crystal molecules studied under the influence of an electric field. *Bulletin of Materials Science*, **2021**, 44, 1	1.7	
115	Modeling the hydroxylation of estragole via human liver cytochrome P450. *Journal of Molecular Modeling*, **2021**, 27, 199	2	
114	Molecular spectroscopy and electro-optical effect of I52 liquid crystal molecules studied under the influence of an external electric field (THz): a theoretical approach. *Journal of Molecular Modeling*, **2021**, 27, 11	2	1
113	Interplay between two degenerate spin state determines the hydroxylation of 4-nitrophenol catalyzed via Cytochrome P450. *Inorganic Chemistry Communication*, **2021**, 132, 108857	3.1	0
112	Electro-optical odd-even effect of APAPA liquid crystal molecules studied under the influence of an extraneous electric field (THz): A theoretical approach. *Journal of Molecular Liquids*, **2020**, 318, 114254	6	1
111	Molecular spectroscopy and adverse optical properties of N-(p-hexyloxy-benzylidene)-p-toluidine (HBT) liquid crystal molecule studied by DFT methodology. *IOP SciNotes*, **2020**, 1, 015202	1.2	6
110	Interplay between two spin states determines the hydroxylation catalyzed by P monooxygenase from Trichoderma brevicompactum. *Journal of Computational Chemistry*, **2020**, 41, 1330-1336	3.5	1
109	Odd–even effect of 7O.m liquid crystal compound series studied under the effect of the electric field by density functional theory (DFT) methods. *European Physical Journal Plus*, **2020**, 135, 1	3.1	5
108	Effect of annealing temperature on the spectroscopic and photoluminescence properties of CdO-ZnO nanocomposites. *Journal of Modern Optics*, **2020**, 67, 1410-1415	1.1	
107	Even–odd effect of the homologous series of nCHBT liquid crystal molecules under the influence of an electric field: A theoretical approach **2020**, 94, 1		6
106	Interaction of modified nucleic bases with graphene and doped graphenes: a DFT study. *Bulletin of Materials Science*, **2020**, 43, 1	1.7	0

105	Interplay Between Steric and Electronic Effects: A Joint Spectroscopy and Computational Study of Nonheme Iron(IV)-Oxo Complexes. *Chemistry - A European Journal*, **2019**, 25, 5086-5098	4.8	25
104	Hydrogen by Deuterium Substitution in an Aldehyde Tunes the Regioselectivity by a Nonheme Manganese(III)Peroxo Complex. *Angewandte Chemie*, **2019**, 131, 10749-10753	3.6	13
103	Hydrogen by Deuterium Substitution in an Aldehyde Tunes the Regioselectivity by a Nonheme Manganese(III)-Peroxo Complex. *Angewandte Chemie - International Edition*, **2019**, 58, 10639-10643	16.4	27
102	Effective optical properties of the one-dimensional periodic structure of (hbox {TiO}_{{2}}) and (hbox {SiO}_{2 }) layers with a defect layer of nanocomposite consisting of silver nanoparticle and E7 liquid crystal **2019**, 93, 1		4
101	Effect of Reaction Temperature on Shape Evolution of Palladium Nanoparticles and Their Cytotoxicity against A-549 Lung Cancer Cells. *ACS Omega*, **2019**, 4, 21839-21847	3.9	2
100	Tunable transmission of a nematic liquid crystal as defect in a 1D periodic structure of dielectric materials by orientation and re-orientation of liquid crystal molecules. *European Physical Journal E*, **2018**, 41, 100	1.5	2
99	Dramatic rate-enhancement of oxygen atom transfer by an iron(iv)-oxo species by equatorial ligand field perturbations. *Dalton Transactions*, **2018**, 47, 14945-14957	4.3	21
98	Diheme Cytochrome c: Structure-Function Correlation and Effect of Heme-Heme Interactions. *Inorganic Chemistry*, **2018**, 57, 11498-11510	5.1	15
97	Assessing therapeutic potential of molecules: molecular property diagnostic suite for tuberculosis ((mathbf{MPDS}^{mathbf{TB}})). *Journal of Chemical Sciences*, **2017**, 129, 515-531	1.8	12
96	Adsorption of small gas molecules on pure and Al-doped graphene sheet: a quantum mechanical study. *Bulletin of Materials Science*, **2017**, 40, 1263-1271	1.7	16
95	A comparative ab intio study on structural evolution, stability and electronic properties of undoped and Al-doped GaxNy (x + y = 4-25 clusters. *European Physical Journal Plus*, **2017**, 132, 1	3.1	2
94	Keto-Enol Tautomerization Triggers an Electrophilic Aldehyde Deformylation Reaction by a Nonheme Manganese(III)-Peroxo Complex. *Journal of the American Chemical Society*, **2017**, 139, 18328-18338	16.4	51
93	Correlation of mesogenic properties with intermolecular interaction energy for homologous series of HnCBP. *Molecular Crystals and Liquid Crystals*, **2017**, 652, 51-66	0.5	1
92	Origin of the Enhanced Reactivity of Nitrido-Bridged Diiron(IV)-Oxo Porphyrinoid Complexes over Cytochrome P450 Compound I. *ACS Catalysis*, **2016**, 6, 2230-2243	13.1	75
91	Deformylation Reaction by a Nonheme Manganese(III)Peroxo Complex via Initial Hydrogen-Atom Abstraction. *Angewandte Chemie*, **2016**, 128, 11257-11261	3.6	17
90	A Systematic Account on Aromatic Hydroxylation by a Cytochrome P450 Model Compound I: A Low-Pressure Mass Spectrometry and Computational Study. *Chemistry - A European Journal*, **2016**, 22, 18608-18619	4.8	54
89	Deformylation Reaction by a Nonheme Manganese(III)-Peroxo Complex via Initial Hydrogen-Atom Abstraction. *Angewandte Chemie - International Edition*, **2016**, 55, 11091-5	16.4	55
88	Polarizability study of nematic liquid crystal 4-cyano-4?-pentylbiphenyl (5CB) and its nitrogen derivatives. *Chemical Physics*, **2015**, 456, 41-46	2.3	8

87	A copper(II) complex with a Cu-S bond. Attenuated total reflectance, electron paramagnetic resonance, resonance Raman and atoms-in-molecule calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 151, 96-9	4.4	5
86	On copper copper bond in hydrated cupric acetate. *Computational and Theoretical Chemistry*, **2015**, 1061, 1-5	2	10
85	Pyrazolo[3,4-d]pyrimidines as novel inhibitors of O-acetyl-L-serine sulfhydrylase of Entamoeba histolytica: an in silico study. *Journal of Molecular Modeling*, **2015**, 21, 96	2	22
84	Drug metabolism by cytochrome p450 enzymes: what distinguishes the pathways leading to substrate hydroxylation over desaturation?. *Chemistry - A European Journal*, **2015**, 21, 9083-92	4.8	100
83	A Trimetal Carbene with Reactivity Reminiscent of Fischer Tropsch Catalysis. *Organometallics*, **2015** , 34, 1651-1660	3.8	4
82	Drug Metabolism by Cytochrome P450 Enzymes: What Distinguishes the Pathways Leading to Substrate Hydroxylation Over Desaturation?. *Chemistry - A European Journal*, **2015**, 21, 8973-8973	4.8	3
81	Structure and mechanism leading to formation of the cysteine sulfinate product complex of a biomimetic cysteine dioxygenase model. *Chemistry - A European Journal*, **2015**, 21, 7470-9	4.8	19
80	A comprehensive test set of epoxidation rate constants for iron(iv)-oxo porphyrin cation radical complexes. *Chemical Science*, **2015**, 6, 1516-1529	9.4	88
79	A Hemilabile Palladium Carbon Bond: Characterization and Its Implication in Catalysis. *Organometallics*, **2014**, 33, 3243-3246	3.8	13
78	Properties and reactivities of nonheme iron(IV)-oxo versus iron(V)-oxo: long-range electron transfer versus hydrogen atom abstraction. *Physical Chemistry Chemical Physics*, **2014**, 16, 22611-22	3.6	5
77	Quantum mechanics/molecular mechanics study on the oxygen binding and substrate hydroxylation step in AlkB repair enzymes. *Chemistry - A European Journal*, **2014**, 20, 435-46	4.8	104
76	Long-range electron transfer triggers mechanistic differences between iron(IV)-oxo and iron(IV)-imido oxidants. *Journal of the American Chemical Society*, **2014**, 136, 17102-15	16.4	93
75	Synthesis and ligand non-innocence of thiolate-ligated (N4S) Iron(II) and nickel(II) bis(imino)pyridine complexes. *Inorganic Chemistry*, **2013**, 52, 10467-80	5.1	20
74	Inversion of enantioselectivity of a mononuclear non-heme iron(II)-dependent hydroxylase by tuning the interplay of metal-center geometry and protein structure. *Angewandte Chemie - International Edition*, **2013**, 52, 9677-81	16.4	45
73	Mechanistic insight into halide oxidation by non-heme iron complexes. Haloperoxidase versus halogenase activity. *Chemical Communications*, **2013**, 49, 10926-8	5.8	36
72	Comparison of the reactivity of nonheme iron(IV)-oxo versus iron(IV)-imido complexes: which is the better oxidant?. *Angewandte Chemie - International Edition*, **2013**, 52, 12288-92	16.4	79
71	Rationalization of the barrier height for p-Z-styrene epoxidation by iron(IV)-oxo porphyrin cation radicals with variable axial ligands. *Inorganic Chemistry*, **2013**, 52, 7968-79	5.1	63
70	Generation of a high-valent iron imido corrolazine complex and NR group transfer reactivity. *Inorganic Chemistry*, **2013**, 52, 4668-82	5.1	49

69	Inversion of Enantioselectivity of a Mononuclear Non-Heme Iron(II)-dependent Hydroxylase by Tuning the Interplay of Metal-Center Geometry and Protein Structure. *Angewandte Chemie*, **2013**, 125, 9859-9863	3.6	13
68	Comparison of the Reactivity of Nonheme Iron(IV)Oxo versus Iron(IV)Imido Complexes: Which is the Better Oxidant?. *Angewandte Chemie*, **2013**, 125, 12514-12518	3.6	23
67	An antimony(V) substituted Keggin heteropolyacid, H4PSbMo11O40: Why is its catalytic activity in oxidation reactions so different from that of H4PVMo11O40?. *Journal of Molecular Catalysis A*, **2012**, 356, 152-157		12
66	Mechanism of S-oxygenation by a cysteine dioxygenase model complex. *Journal of Physical Chemistry A*, **2012**, 116, 582-91	2.8	33
65	Axial ligand effect on the rate constant of aromatic hydroxylation by iron(IV)-oxo complexes mimicking cytochrome P450 enzymes. *Journal of Physical Chemistry B*, **2012**, 116, 718-30	3.4	55
64	Axial and equatorial ligand effects on biomimetic cysteine dioxygenase model complexes. *Organic and Biomolecular Chemistry*, **2012**, 10, 5401-9	3.9	16
63	Theoretical study on the mechanism of the oxygen activation process in cysteine dioxygenase enzymes. *Journal of the American Chemical Society*, **2011**, 133, 3869-82	16.4	174
62	Water as biocatalyst in cytochrome P450. *Faraday Discussions*, **2011**, 148, 373-83; discussion 421-41	3.6	27
61	Comparison of computational methods to model DNA minor groove binders. *Journal of Chemical Information and Modeling*, **2011**, 51, 558-71	6.1	57
60	Effect of the axial ligand on substrate sulfoxidation mediated by iron(IV)-oxo porphyrin cation radical oxidants. *Chemistry - A European Journal*, **2011**, 17, 6196-205	4.8	79
59	Nonheme ferric hydroperoxo intermediates are efficient oxidants of bromide oxidation. *Chemical Communications*, **2011**, 47, 11044-6	5.8	63
58	Oxidative properties of a nonheme Ni(II)(O2) complex: Reactivity patterns for C-H activation, aromatic hydroxylation and heteroatom oxidation. *Chemical Communications*, **2011**, 47, 10674-6	5.8	22
57	What factors influence the rate constant of substrate epoxidation by compound I of cytochrome P450 and analogous iron(IV)-oxo oxidants?. *Journal of the American Chemical Society*, **2010**, 132, 7656-67	16.4	155
56	Steric factors override thermodynamic driving force in regioselectivity of proline hydroxylation by prolyl-4-hydroxylase enzymes. *Journal of Physical Chemistry A*, **2010**, 114, 13234-43	2.8	36
55	P450 enzymes: their structure, reactivity, and selectivity-modeled by QM/MM calculations. *Chemical Reviews*, **2010**, 110, 949-1017	68.1	791
54	Coupling and uncoupling mechanisms in the methoxythreonine mutant of cytochrome P450cam: a quantum mechanical/molecular mechanical study. *Journal of Biological Inorganic Chemistry*, **2010**, 15, 361-72	3.7	12
53	Effect of porphyrin ligands on the regioselective dehydrogenation versus epoxidation of olefins by oxoiron(IV) mimics of cytochrome P450. *Journal of Physical Chemistry A*, **2009**, 113, 11713-22	2.8	66
52	QM/MM study of the second proton transfer in the catalytic cycle of the D251N mutant of cytochrome P450cam. *Journal of Physical Chemistry B*, **2009**, 113, 9577-88	3.4	13

51	How is the reactivity of cytochrome P450cam affected by Thr252X mutation? A QM/MM study for X = serine, valine, alanine, glycine. *Journal of the American Chemical Society*, **2009**, 131, 4755-63	16.4	50
50	Electronic properties of pentacoordinated heme complexes in cytochrome P450 enzymes: search for an Fe(I) oxidation state. *Physical Chemistry Chemical Physics*, **2009**, 11, 10219-26	3.6	27
49	A valence bond modeling of trends in hydrogen abstraction barriers and transition states of hydroxylation reactions catalyzed by cytochrome P450 enzymes. *Journal of the American Chemical Society*, **2008**, 130, 10128-40	16.4	213
48	Multireference ab initio quantum mechanics/molecular mechanics study on intermediates in the catalytic cycle of cytochrome P450(cam). *Journal of Physical Chemistry A*, **2008**, 112, 12904-10	2.8	42
47	A tribute to Sason Shaik. *Journal of Physical Chemistry A*, **2008**, 112, 12721-3	2.8	
46	Reactivity of high-valent iron-oxo species in enzymes and synthetic reagents: a tale of many states. *Accounts of Chemical Research*, **2007**, 40, 532-42	24.3	454
45	Theoretical study of N-demethylation of substituted N,N-dimethylanilines by cytochrome P450: the mechanistic significance of kinetic isotope effect profiles. *Journal of Physical Chemistry B*, **2007**, 111, 7700-10	3.4	103
44	Formation of the active species of cytochrome p450 by using iodosylbenzene: a case for spin-selective reactivity. *Chemistry - A European Journal*, **2007**, 13, 4103-15	4.8	42
43	Singlet diradical character of an oxidized ruthenium trithiolate: electronic structure and reactivity. *Angewandte Chemie - International Edition*, **2007**, 46, 4085-8	16.4	20
42	Singlet Diradical Character of an Oxidized Ruthenium Trithiolate: Electronic Structure and Reactivity. *Angewandte Chemie*, **2007**, 119, 4163-4166	3.6	4
41	A Density Functional Study of the Factors That Influence the Regioselectivity of Toluene Hydroxylation by Cytochrome P450 Enzymes. *European Journal of Inorganic Chemistry*, **2007**, 2007, 2966-2974	2.2	27
40	Reactivity patterns of cytochrome P450 enzymes: multifunctionality of the active species, and the two states-two oxidants conundrum. *Natural Product Reports*, **2007**, 24, 533-52	15.1	89
39	The Electronic Structure of Reduced Phosphovanadomolybdates and the Implications on Their Use in Catalytic Oxidation Initiated by Electron Transfer. *Journal of Physical Chemistry C*, **2007**, 111, 7711-7719	3.8	19
38	On the identity and reactivity patterns of the "second oxidant" of the T252A mutant of cytochrome P450cam in the oxidation of 5-methylenenylcamphor. *Journal of Inorganic Biochemistry*, **2006**, 100, 2054-68	4.2	26
37	Characterization of manganese(V)-oxo polyoxometalate intermediates and their properties in oxygen-transfer reactions. *Journal of the American Chemical Society*, **2006**, 128, 15451-60	16.4	89
36	Gauging the relative oxidative powers of compound I, ferric-hydroperoxide, and the ferric-hydrogen peroxide species of cytochrome P450 toward C-H hydroxylation of a radical clock substrate. *Journal of the American Chemical Society*, **2006**, 128, 473-84	16.4	60
35	Proton-shuffle mechanism of O-O activation for formation of a high-valent oxo-iron species of bleomycin. *Journal of the American Chemical Society*, **2006**, 128, 16148-58	16.4	41
34	Ferromagnetic bonding: high spin copper clusters (n+1)Cu(n); n = 2-14) devoid of electron pairs but possessing strong bonding. *Journal of Physical Chemistry A*, **2006**, 110, 8510-8	2.8	24

33	In silico design of a mutant of cytochrome P450 containing selenocysteine. *Journal of the American Chemical Society*, **2006**, 128, 2649-53	16.4	35
32	Kinetic isotope effect is a sensitive probe of spin state reactivity in C-H hydroxylation of N,N-dimethylaniline by cytochrome P450. *Journal of the American Chemical Society*, **2006**, 128, 394-5	16.4	75
31	Two-state reactivity in alkane hydroxylation by non-heme iron-oxo complexes. *Journal of the American Chemical Society*, **2006**, 128, 8590-606	16.4	308
30	Catalysts for monooxygenations made from polyoxometalate: an iron(V)-oxo derivative of the Lindqvist anion. *Inorganic Chemistry*, **2006**, 45, 8655-63	5.1	29
29	New features in the catalytic cycle of cytochrome P450 during the formation of compound I from compound 0. *Journal of Physical Chemistry B*, **2005**, 109, 19946-51	3.4	50
28	Sulfoxidation mechanisms catalyzed by cytochrome P450 and horseradish peroxidase models: spin selection induced by the ligand. *Biochemistry*, **2005**, 44, 8148-58	3.2	68
27	Theory favors a stepwise mechanism of porphyrin degradation by a ferric hydroperoxide model of the active species of heme oxygenase. *Journal of the American Chemical Society*, **2005**, 127, 8204-13	16.4	74
26	Theoretical investigation of C--H hydroxylation by (N4Py)Fe(IV)=O(2+): an oxidant more powerful than P450?. *Journal of the American Chemical Society*, **2005**, 127, 8026-7	16.4	172
25	Two states and two more in the mechanisms of hydroxylation and epoxidation by cytochrome P450. *Journal of the American Chemical Society*, **2005**, 127, 13007-18	16.4	146
24	The high-valent iron-oxo species of polyoxometalate, if it can be made, will be a highly potent catalyst for C-H hydroxylation and double-bond epoxidation. *Journal of the American Chemical Society*, **2005**, 127, 17712-8	16.4	87
23	Theoretical perspective on the structure and mechanism of cytochrome P450 enzymes. *Chemical Reviews*, **2005**, 105, 2279-328	68.1	999
22	Multistate reactivity in styrene epoxidation by compound I of cytochrome p450: mechanisms of products and side products formation. *Chemistry - A European Journal*, **2005**, 11, 2825-35	4.8	101
21	Theoretical Perspective on the Structure and Mechanism of Cytochrome P450 Enzymes. *ChemInform*, **2005**, 36, no		2
20	The intrinsic axial ligand effect on propene oxidation by horseradish peroxidase versus cytochrome P450 enzymes. *Journal of Biological Inorganic Chemistry*, **2005**, 10, 181-9	3.7	56
19	One oxidant, many pathways: a theoretical perspective of monooxygenation mechanisms by cytochrome P450 enzymes. *Journal of Biological Inorganic Chemistry*, **2004**, 9, 661-8	3.7	81
18	How do aldehyde side products occur during alkene epoxidation by cytochrome P450? Theory reveals a state-specific multi-state scenario where the high-spin component leads to all side products. *Journal of Inorganic Biochemistry*, **2004**, 98, 1183-93	4.2	57
17	Porphyrin traps its terminator! Concerted and stepwise porphyrin degradation mechanisms induced by heme-oxygenase and cytochrome p450. *Angewandte Chemie - International Edition*, **2004**, 43, 1129-32	16.4	55
16	Computer-generated high-valent iron--oxo and manganese--oxo species with polyoxometalate ligands: how do they compare with the iron--oxo active species of heme enzymes?. *Angewandte Chemie - International Edition*, **2004**, 43, 5661-5	16.4	63

15	Porphyrin Traps Its Terminator! Concerted and Stepwise Porphyrin Degradation Mechanisms Induced by Heme-Oxygenase and Cytochrome P450. *Angewandte Chemie*, **2004**, 116, 1149-1152	3.6	10
14	Computer-Generated High-Valent Iron□Oxo and Manganese□Oxo Species with Polyoxometalate Ligands: How do they Compare with the Iron□Oxo Active Species of Heme Enzymes?. *Angewandte Chemie*, **2004**, 116, 5779-5783	3.6	9
13	The Rebound Controversy□An Overview and Theoretical Modeling of the Rebound Step in C□H Hydroxylation by Cytochrome P450. *European Journal of Inorganic Chemistry*, **2004**, 2004, 207-226	2.3	138
12	Radical clock substrates, their C-H hydroxylation mechanism by cytochrome P450, and other reactivity patterns: what does theory reveal about the clocks' behavior?. *Journal of the American Chemical Society*, **2004**, 126, 1907-20	16.4	138
11	External electric field will control the selectivity of enzymatic-like bond activations. *Journal of the American Chemical Society*, **2004**, 126, 11746-9	16.4	201
10	Oxygen economy of cytochrome P450: what is the origin of the mixed functionality as a dehydrogenase-oxidase enzyme compared with its normal function?. *Journal of the American Chemical Society*, **2004**, 126, 5072-3	16.4	67
9	A predictive pattern of computed barriers for C-h hydroxylation by compound I of cytochrome p450. *Journal of the American Chemical Society*, **2004**, 126, 8362-3	16.4	195
8	How does product isotope effect prove the operation of a two-state "rebound" mechanism in C-H hydroxylation by cytochrome P450?. *Journal of the American Chemical Society*, **2003**, 125, 13024-5	16.4	86
7	Active species of horseradish peroxidase (HRP) and cytochrome P450: two electronic chameleons. *Journal of the American Chemical Society*, **2003**, 125, 15779-88	16.4	153
6	Molecular Ordering of a Nematogen at Phase Transition Temperature - A Theoretical Study. *Phase Transitions*, **2002**, 75, 621-629	1.3	
5	Odd-even Effect in a Homologous Series of 4-n-Alkylbenzoic Acids: Role of Anisotropic Pair Potential. *Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences*, **2002**, 57, 189-193	1.4	5
4	Order of a Thermotropic Mesogen: HCCPP-A Statistical Study Based on Quantum Mechanics and Computer Simulation. *Molecular Crystals and Liquid Crystals*, **2002**, 378, 65-75	0.5	3
3	Molecular Organization in a Nematogen: PBPCN -A Computational Analysis Based on Quantum Mechanics. *Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences*, **2001**, 56, 730-734	1.4	2
2	Smectogenic Behaviour of 7O.6 at it's Phase Transition Temperature: A Computational Analysis Reprint request to. *Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences*, **2001**, 56, 873-878	1.4	
1	A comparative study of crystal packing vs. conformational energy of N-acetyl-2,3-didehydroproline. *International Journal of Quantum Chemistry*, **1995**, 55, 71-74	2.1	