## Proper basis set for quantum mechanical studies of pote carbohydrates

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**Citation Report** 

#	Article	IF	CITATIONS
1	Crystal structure of penta-O-acetyl-β-d-galactopyranose with modeling of the conformation of the acetate groups. Carbohydrate Research, 2002, 337, 2301-2310.	2.3	13
2	Studies on aliphatic polyesters. Part III. Ab initio, density functional and force field studies of esters with tartaric units. Computational and Theoretical Chemistry, 2003, 624, 287-307.	1.5	0
3	Studies on aliphatic polyesters. Part III. Ab initio, density functional and force field studies of esters with tartaric units. Computational and Theoretical Chemistry, 2003, 636, 243-263.	1.5	0
4	Thermometer ions for matrix-enhanced laser desorption/ionization internal energy calibration. Rapid Communications in Mass Spectrometry, 2003, 17, 1847-1854.	1.5	50
5	Effectiveness of Diffuse Basis Functions for Calculating Relative Energies by Density Functional Theory. Journal of Physical Chemistry A, 2003, 107, 1384-1388.	2.5	688
6	Advanced conformational energy surfaces for cellobiose**. Cellulose, 2004, 11, 449-462.	4.9	41
7	B3LYP/6-311++G** study of α- and β-d-glucopyranose and 1,5-anhydro-d-glucitol: 4C1 and 1C4 chairs, 3,OB and B3,O boats, and skew-boat conformations. Carbohydrate Research, 2004, 339, 537-551.	2.3	120
8	Evaluation of carbohydrate molecular mechanical force fields by quantum mechanical calculations. Carbohydrate Research, 2004, 339, 937-948.	2.3	61
9	Theoretical Study of the Relative Stability of Rotational Conformers of α and β-d-Glucopyranose in Gas Phase and Aqueous Solution. Journal of the American Chemical Society, 2004, 126, 7311-7319.	13.7	75
10	Modeling ring puckering in strained systems: application to 3,6-anhydroglycosides. Carbohydrate Research, 2005, 340, 2030-2038.	2.3	10
11	Comparative performance of MM3(92) and two TINKER? MM3 versions for the modeling of carbohydrates. Journal of Computational Chemistry, 2005, 26, 471-483.	3.3	35
12	Proper Gaussian Basis Sets for Density Functional Studies of Water Dimers and Trimers. Journal of Physical Chemistry B, 2005, 109, 21471-21475.	2.6	36
13	Circular Hydrogen Bond Networks on the Surface of β-Ribofuranose in Aqueous Solution. Journal of Physical Chemistry B, 2005, 109, 12603-12611.	2.6	10
14	Density Functional Study of the Conformational Space of4C1d-Glucuronic Acid. Journal of Physical Chemistry A, 2005, 109, 892-897.	2.5	24
15	Binding Energy Curves from Nonempirical Density Functionals II. van der Waals Bonds in Rare-Gas and Alkaline-Earth Diatomics. Journal of Physical Chemistry A, 2005, 109, 11015-11021.	2.5	82
16	Quantum mechanics studies of cellobiose conformations. Canadian Journal of Chemistry, 2006, 84, 603-612.	1.1	59
17	A theoretical study of glucose mutarotation in aqueous solution. Carbohydrate Research, 2006, 341, 1029-1040.	2.3	69
18	Computational Study of the Conformational Space of Methyl 2,4-Diacetyl·l²-d-xylopyranoside:Â4C1and1C4Chairs, Skew-Boats (2SO,1S3), and B3,OBoat Forms. Journal of Physical Chemistry A, 2006, 110, 7477-7484.	2.5	15

#	Article	IF	CITATIONS
19	The SPASIBA Force Field for Chondroitin Sulfate:  Vibrational Analysis of d-Glucuronic and N-acetyl-d-Galactosamine 4-Sulfate Sodium Salts. Journal of Physical Chemistry A, 2006, 110, 11359-11370.	2.5	26
20	A comparative study of the influence of some protecting groups on the reactivity of d-glucosamine acceptors with a galactofuranosyl donor. Carbohydrate Research, 2006, 341, 1096-1104.	2.3	21
21	An investigation of the pyranose ring interconversion path of α-l-idose calculated using density functional theory. Carbohydrate Research, 2006, 341, 2565-2574.	2.3	36
22	Efficient synthesis and structural analysis of new dioxopiperazine isoquinolines. Tetrahedron, 2006, 62, 4408-4418.	1.9	8
23	Carbohydrates and quantum chemistry: how useful is this combination?. Theoretical Chemistry Accounts, 2006, 116, 137-147.	1.4	18
24	Computational studies of the interactions between emeraldine and palladium atom. Surface Science, 2006, 600, 1679-1683.	1.9	4
25	Experimental and Computational Studies of the Recognition of Amino Acids by Galactosyl-imine and -amine Derivatives:Â An Attempt to Understand the Lectinâ^'Carbohydrate Interactions. Journal of Organic Chemistry, 2007, 72, 3430-3442.	3.2	35
26	Correlatedab initioquantum chemical calculations of di- and trisaccharide conformations. Journal of Computational Chemistry, 2007, 28, 1965-1973.	3.3	10
27	Calculating gas phase energies of an α(1–4) linked disaccharide: electronic structure theory and classical atomistic simulation. Computational and Theoretical Chemistry, 2007, 806, 9-22.	1.5	1
28	DFT study of α- and β-d-allopyranose at the B3LYP/6-311++Gâ^—â^— level of theory. Carbohydrate Research, 200 342, 196-216.	)7 <sub>,2.3</sub>	48
29	Metal Binding Induced Conformational Interconversions in Methyl ß-D-xylopyranoside. Theoretical Chemistry Accounts, 2007, 117, 223-229.	1.4	6
30	Conformational and electronic effects on the regioselectivity of the glycosylation of different anomers of N-dimethylmaleoyl-protected glucosamine acceptors. Organic and Biomolecular Chemistry, 2008, 6, 554-561.	2.8	13
31	Interaction of Methyl β- <scp>d</scp> -Xylopyranoside with Metal Ions:  Density Functional Theory Study of Cationic and Neutral Bridging and Pendant Complexes. Journal of Physical Chemistry A, 2008, 112, 1823-1831.	2.5	6
32	Sugars. , 2008, , 297-307.		0
33	Conformational Analysis of Thioether Musks Using Density Functional Theory. International Journal of Molecular Sciences, 2009, 10, 3488-3501.	4.1	4
34	Interaction energy and the shift in OH stretch frequency on hydrogen bonding for the H <sub>2</sub> O → H <sub>2</sub> O, CH <sub>3</sub> OH → H <sub>2</sub> O, and H <sub>2</sub> O → CH <sub>3</sub> OH dimers. Journal of Computational Chemistry, 2010, 31, 963-972.	3.3	17
35	Systematic probing of an atomic charge set of sialic acid disaccharides for the rational molecular modeling of avian influenza virus based on molecular dynamics simulations. Carbohydrate Research, 2009, 344, 541-544.	2.3	3
36	The (α-1,6) glycosidic bond of isomaltose: a tricky system for theoretical conformational studies. Carbohydrate Research, 2009, 344, 1235-1247.	2.3	11

#	Article	IF	CITATIONS
37	Comparative DFT study on the α-glycosidic bond in reactive species of galactosyl diphosphates. Chemical Papers, 2009, 63, .	2.2	25
38	Evaluation of Density Functionals and Basis Sets for Carbohydrates. Journal of Chemical Theory and Computation, 2009, 5, 679-692.	5.3	183
39	Chapter 4 Computational Studies of the Role of Glycopyranosyl Oxacarbenium Ions in Glycobiology and Glycochemistry. Advances in Carbohydrate Chemistry and Biochemistry, 2009, 62, 83-159.	0.9	77
40	Assessing the performance of recent density functionals for bulk solids. Physical Review B, 2009, 79, .	3.2	740
41	27 ps DFT molecular dynamics simulation of αâ€maltose: A reduced basis set study. Journal of Computational Chemistry, 2010, 31, 2087-2097.	3.3	9
42	DFTMD studies of glucose and epimers: anomeric ratios, rotamer populations, and hydration energies. Carbohydrate Research, 2010, 345, 503-511.	2.3	50
43	Trends in the frequencies of ν(AsO <i><sub><i>x</i></sub></i> H <sub><i>x</i>–1</sub> ) [ <i>x</i> = 2–4] in selected As(V)-containing compounds investigated using quantum chemical calculations. Canadian Journal of Chemistry, 2010, 88, 65-77.	1.1	15
44	Ring Puckering: A Metric for Evaluating the Accuracy of AM1, PM3, PM3CARB-1, and SCC-DFTB Carbohydrate QM/MM Simulations. Journal of Physical Chemistry B, 2010, 114, 17142-17154.	2.6	83
45	Theoretical investigation of some <i>N</i> -nitrosodiphenylamine biological molecules — A natural bond orbital (NBO) study. Canadian Journal of Chemistry, 2011, 89, 1230-1235.	1.1	1
46	Local Site Selectivity and Conformational Structures in the Glycosidic Bond Scission of Cellobiose. Journal of Physical Chemistry B, 2011, 115, 10682-10691.	2.6	29
47	Accurate Conformational Energy Differences of Carbohydrates: A Complete Basis Set Extrapolation. Journal of Chemical Theory and Computation, 2011, 7, 988-997.	5.3	26
48	A comparative study of the O-3 reactivity of isomeric N-dimethylmaleoyl-protected d-glucosamine and d-allosamine acceptors. Carbohydrate Research, 2011, 346, 569-576.	2.3	9
49	A reoptimized GROMOS force field for hexopyranoseâ€based carbohydrates accounting for the relative free energies of ring conformers, anomers, epimers, hydroxymethyl rotamers, and glycosidic linkage conformers. Journal of Computational Chemistry, 2011, 32, 998-1032.	3.3	147
50	Quantum chemical calculations on solvation effects for selected photoreactive aromatic organic molecules of atmospheric relevance. Computational and Theoretical Chemistry, 2011, 965, 346-352.	2.5	4
51	Obtención de DÃmeros por Termólisis de 1,2-Propanodiol. Informacion Tecnologica (discontinued), 2012, 23, 3-12.	0.3	2
52	On the path to glycan conformer identification: Gas-phase study of the anomers of methyl glycosides of N-acetyl-d-glucosamine and N-acetyl-d-galactosamine. International Journal of Mass Spectrometry, 2012, 330-332, 285-294.	1.5	26
53	Correction to DFT interaction energies by an empirical dispersion term valid for a range of intermolecular distances. Physical Chemistry Chemical Physics, 2012, 14, 3414.	2.8	10
54	Specific rotation as a property to validate monosaccharide conformations. Carbohydrate Research, 2012, 350, 62-67.	2.3	6

#	Article	IF	Citations
55	Conformational analysis of cellobiose by electronic structure theories. Carbohydrate Research, 2012, 350, 68-76.	2.3	55
56	Barrierless Inter and Intramolecular Proton Transfer; A DFT Study of Tautomerism in Microsolvated and Protonated Systems. Journal of Physical Chemistry A, 2013, 117, 6809-6816.	2.5	9
57	A DFT study on the reaction mechanisms of isocyanide-based multicomponent synthesis of polysubstituted cyclopentenes. Computational and Theoretical Chemistry, 2013, 1018, 85-90.	2.5	3
58	The anomeric effect: the dominance of exchange effects in closed-shell systems. Organic and Biomolecular Chemistry, 2013, 11, 299-308.	2.8	49
59	Conformational studies of diosgenyl 2-amino-2-deoxy-β-d-glucopyranosides at the PM3 and DFT levels of theory. Carbohydrate Research, 2013, 377, 4-13.	2.3	2
60	Acetylated methyl 1,2-dideoxyhex-1-enopyranuronates in density functional theory conformational studies. Carbohydrate Research, 2013, 371, 1-7.	2.3	21
61	Quantum chemical approach toward the electronic, photophysical and charge transfer properties of the materials used in organic field-effect transistors. Materials Chemistry and Physics, 2013, 138, 468-478.	4.0	26
62	Carbohydrate–Protein Interactions. Advances in Carbohydrate Chemistry and Biochemistry, 2014, 71, 9-136.	0.9	60
63	Polarimetry as a Tool for the Study of Solutions of Chiral Solutes. ChemPhysChem, 2014, 15, 195-207.	2.1	25
64	Effect of Neighbors on the Conformational Preferences of Glycosidic Linkages in Glycyrrhizic Acid and Its Mono- and Dideprotonated Forms: X-ray, NMR, and Computational Studies. Crystal Growth and Design, 2014, 14, 5871-5880.	3.0	8
65	DFT, QTAIM, and NBO Study of Adsorption of Rare Gases into and on the Surface of Sulfur-Doped, Single-Wall Carbon Nanotubes. Journal of Physical Chemistry C, 2015, 119, 6502-6510.	3.1	45
66	Regioselective Acylation of Diols and Triols: The Cyanide Effect. Journal of the American Chemical Society, 2016, 138, 6002-6009.	13.7	51
67	Diastereomeric Glycosyl Sulfoxides Display Different Recognition Features versus <i>E. coli</i> βâ€Galactosidase. European Journal of Organic Chemistry, 2016, 2016, 5117-5122.	2.4	9
68	DFT/PCM theoretical study of the conversion of methyl 4-O-methyl-α-d-galactopyranoside 6-sulfate and its 2-sulfated derivative into their 3,6-anhydro counterparts. Carbohydrate Research, 2016, 426, 15-25.	2.3	3
69	Testing the CP-correction procedure with different DFT methods on H-bonding complexes of $\hat{I}^{e}$ -carrabiose with water molecules. Journal of Molecular Modeling, 2017, 23, 31.	1.8	8
70	Adsorption of thiophene on the surfaces of X 12 Y 12 (X = Al, B, and Y = N,P) nanoclusters; A DFT study. Journal of Molecular Liquids, 2017, 238, 303-309.	4.9	88
71	Mechanistic Insights and Kinetic Modeling of Cellobiose Decomposition in Hot Compressed Water. Energy & Fuels, 2017, 31, 2203-2216.	5.1	11
72	The long-range convergence of the energetic properties of the water monomer in bulk water at room temperature. Physical Chemistry Chemical Physics, 2017, 19, 20941-20948.	2.8	9

#	Article	IF	CITATIONS
73	Adsorption of rare gases on the C <sub>20</sub> nanocage: a theoretical investigation. Materials Research Express, 2018, 5, 035006.	1.6	12
74	A DFT study on the catalytic ability of aluminum doped graphene for the initial steps of the conversion of methanol to gasoline. Computational and Theoretical Chemistry, 2018, 1127, 8-15.	2.5	9
75	Comparative conformational studies of 3,4,6-tri- O -acetyl-1,5-anhydro-2-deoxyhex-1-enitols at the DFT level. Carbohydrate Research, 2018, 462, 13-27.	2.3	23
76	The concern of emergence of multi-station reaction pathways that might make stepwise the mechanism of the 1,3-dipolar cycloadditions of azides and alkynes. Journal of Molecular Structure, 2018, 1155, 58-64.	3.6	13
77	Performance of Density-Functional Tight-Binding in Comparison to Ab Initio and First-Principles Methods for Isomer Geometries and Energies of Glucose Epimers in Vacuo and Solution. ACS Omega, 2018, 3, 16899-16915.	3.5	12
78	DFT Optimization of Isolated Molecular Chain Sheet Models Constituting Native Cellulose Crystal Structures. ACS Omega, 2018, 3, 8050-8058.	3.5	21
79	Experiment and Modeling Study of Glucose Pyrolysis: Formation of 3-Hydroxy-Î <sup>3</sup> -butyrolactone and 3-(2 <i>H</i> )-Furanone. Energy & Fuels, 2018, 32, 9519-9529.	5.1	18
80	Raman and surfaceâ€enhanced Raman spectroscopy for the analysis of Mexican yellow dyestuff. Journal of Raman Spectroscopy, 2019, 50, 1546-1554.	2.5	12
81	Mechanism of oligosaccharide synthesis <i>via</i> a mutant GH29 fucosidase. Reaction Chemistry and Engineering, 2019, 4, 402-409.	3.7	10
82	Study of the structure, the electronic and spectral properties of D-glucaro-dilactones. Journal of King Saud University - Science, 2019, 31, 427-433.	3.5	0
83	Appraisal of the Role of In silico Methods in Pyrazole Based Drug Design. Mini-Reviews in Medicinal Chemistry, 2021, 21, 204-216.	2.4	9
84	Spectroscopic (FT-IR, Raman) analysis and computational study on conformational geometry, AIM and biological activity of cephalexin from DFT and molecular docking approach. Journal of Molecular Structure, 2021, 1240, 130594.	3.6	14
85	Diastereomers and Low-Temperature Oxidation. Journal of Physical Chemistry A, 2021, 125, 8064-8073.	2.5	11
86	Non-Boltzmann Effects in Chain Branching and Pathway Branching for Diethyl Ether Oxidation. Energy & Fuels, 2021, 35, 17890-17908.	5.1	16
87	The importance of orientation of exocyclic groups in a naphthoxyloside: A specific rotation calculation study. Journal of Physical Organic Chemistry, 2017, 30, e3708.	1.9	0
88	Electronic structures and properties of small \$\$(hbox {BCN})_{x}\$\$ (x =1–5) clusters and \$\$(hbox) Tj ETQq1	1 9.78431	4 ggBT /Over
89	Theoretical Studies on Sensing of Transition Metals Using C2n Surface. SSRN Electronic Journal, 0, , .	0.4	0
90	Computational Spectroscopic Investigation of the Effect of Nitrosyl Bonding Type on Molecular Properties in Iron Tetracarbonyl Nitrosyl Complex. SSRN Electronic Journal, 0, , .	0.4	0

#	Article	IF	CITATIONS
91	Structural Features Governing the Metabolic Stability of Tetraethyl-Substituted Nitroxides in Rat Liver Microsomes. Antioxidants, 2023, 12, 402.	5.1	5
92	Transition Metal Sensing with Nitrogenated Holey Graphene: A First-Principles Investigation. Molecules, 2023, 28, 4060.	3.8	7
93	Syntheses and Electrochemical and EPR Studies of Porphyrins Functionalized with Bulky Aromatic Amine Donors. Molecules, 2023, 28, 4405.	3.8	1
94	A density functional theory study on the adsorption of different organic sulfides on boron nitride nanosheet. RSC Advances, 2023, 13, 31622-31631.	3.6	0
95	DFT mechanistic study of [4+2] cycloaddition reactions of 1-methyl-1H-pyrrole-2,5-dione with furoic acid, anticancer Activity, molecular modeling and ADMET properties of new products from the Norcantharimide family substituted by a carboxylic acid. Computational and Theoretical Chemistry, 2023, 1230, 114384.	2.5	0
96	In vitro and in silico evaluation of the antimicrobial and antioxidant activities of spiropyrazoline oxindole congeners. Arabian Journal of Chemistry, 2024, 17, 105465.	4.9	1
97	Exploring Acceptor Modification in Heliceneâ€Phenylamineâ€Based Small Molecules for Organic and Perovskite Solar Cells. Energy Technology, 2024, 12, .	3.8	0
98	V-shaped naphthalene diimide-based chromophores: First theoretical framework for designing high efficacy of organic solar cells. Synthetic Metals, 2024, 303, 117548.	3.9	0
99	Theoretical investigation of substituted end groups in thiopheneâ€phenylâ€ŧhiophene (TPT) derivatives for high efficiency organic solar cells. Journal of Physical Organic Chemistry, 0, , .	1.9	0