Analysis of the core-repulsion functions used in AM1 and PM3 semiempirical calculations: Conformational analysis of ring systems

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#	Paper	IF	Citations
46	Supramolecular complexes based on calixarenes: force field calculations and applications for chemical sensors. *Supramolecular Science*, **1994**, 1, 11-19		28
45	Relative stability of alternative chair forms and hydroxymethyl conformations of □d-glucopyranose. *Carbohydrate Research*, **1995**, 276, 219-251	2.9	174
44	Theoretical structure investigations of N-acetyl-l-proline amide. *Journal of Molecular Structure*, **1995**, 352-353, 59-70	3.4	23
43	Solvent effects on Diels-Alder reactions. A semi-empirical study. *Computational and Theoretical Chemistry*, **1995**, 331, 37-50		26
42	MNDO/AM1/PM3 quantum mechanical semiempirical and molecular mechanics barriers to internal rotation: a comparative study. *Computational and Theoretical Chemistry*, **1995**, 335, 129-139		23
41	Model for Aqueous Solvation Based on Class IV Atomic Charges and First Solvation Shell Effects. *The Journal of Physical Chemistry*, **1996**, 100, 16385-16398		335
40	A pseudrotation model and ring-puckering of cyclopentane. *Computational and Theoretical Chemistry*, **1996**, 362, 243-255		35
39	Quantum mechanical investigation of cyclic 3?,5?-adenosine monophosphate, the second hormonal messenger. *Computational and Theoretical Chemistry*, **1996**, 362, 297-304		8
38	Conformational equilibria of 5-substituted-1,3-dithianes. Study of solvent effects. *Computational and Theoretical Chemistry*, **1997**, 418, 113-118		2
37	The origin of the problems with the PM3 core repulsion function. *Computational and Theoretical Chemistry*, **1997**, 393, 31-38		80
36	NMR and semiempirical conformational analysis of the 2-aryl-1,3-dihydroxy-4,4,5,5-tetramethylimidazolidines. *Tetrahedron*, **1997**, 53, 16911-16922	2.4	7
35	Ab initio and density functional study of the conformational space of 1C4 □L-fucose. *Journal of Computational Chemistry*, **1997**, 18, 330-342	3.5	37
34	Combined AM1/MM3 computations on organic systems: the Diels□Alder reaction as a test case. *Chemical Physics Letters*, **1998**, 296, 239-244	2.5	6
33	Quantum mechanical/molecular mechanical self-consistent Madelung potential method for treatment of polar molecular crystals. *Journal of Computational Chemistry*, **1998**, 19, 38-50	3.5	23
32	Vibrational analysis of stilbene and its isotopomers on the ground state potential energy surface. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **1998**, 54, 1017-1039	4.4	27
31	The Role of Menthyl Group in Catalyzed Asymmetric Diels□Alder Reactions. A Combined Quantum Mechanics/Molecular Mechanics Study. *Journal of Organic Chemistry*, **1998**, 63, 4664-4670	4.2	11
30	Computational study of solvation and stereoselectivity in deprotonation of cyclohexene oxide by a chiral lithium amide. *Tetrahedron: Asymmetry*, **1999**, 10, 265-279		19

29	Stereoselective Diamine Chelates of a Chiral Lithium Amide Dimer: New Insights into the Coordination Chemistry of Chiral Lithium Amides. *Journal of the American Chemical Society*, **1999**, 121, 1883-1887	16.4	40
28	Performance of the semiempirical PM3 (tm) method in the geometry optimization of transition metal complexes. *Journal of Computational Chemistry*, **2000**, 21, 562-571	3.5	28
27	Improving description of hydrogen bonds at the semiempirical level: water–water interactions as test case. *Journal of Computational Chemistry*, **2000**, 21, 572-581	3.5	69
26	Basic ideas for the correction of semiempirical methods describing H-bonded systems. *Chemical Physics Letters*, **2000**, 330, 118-124	2.5	65
25	Computational, ReactIR-, and NMR-spectroscopic investigations on the chiral formyl anion equivalent N-(alpha-lithiomethylthiomethyl)-4-isopropyl-5,5-diphenyloxazolidin-2-one and related compounds. *Chemistry - A European Journal*, **2001**, 7, 4117-25	4.8	26
24	A novel mixed dimer of a norephedrine-derived chiral lithium amide and 2-lithium-1-methylimidazole, and catalytic enantioselective deprotonation of cyclohexene oxide. *Chemistry - A European Journal*, **2001**, 7, 4368-77	4.8	30
23	Quantum Chemical Calculations on Alkali Metal Complexes. **2001**, 334-345		
22	PDDG/PM3 and PDDG/MNDO: improved semiempirical methods. *Journal of Computational Chemistry*, **2002**, 23, 1601-22	3.5	268
21	Asymmetric addition of n-butyllithium to aldehydes: new insights into the reactivity and enantioselectivity of the chiral amino ether accelerated reaction. *Tetrahedron*, **2002**, 58, 4717-4725	2.4	39
20	Testing electronic structure methods for describing intermolecular H...H interactions in supramolecular chemistry. *Journal of Computational Chemistry*, **2004**, 25, 99-105	3.5	29
19	Composition and structure of activated complexes in stereoselective deprotonation of cyclohexene oxide by a mixed dimer of chiral lithium amide and lithiated imidazole. *Tetrahedron: Asymmetry*, **2004**, 15, 1607-1613		12
18	A model for double asymmetric induction in the stereocontrolled reduction of glycosyl alpha-ketoesters with oxazaborolidines. *Journal of the American Chemical Society*, **2004**, 126, 6996-7008	16.4	12
17	1:2 Formic Acid/Acetylene Complexes: Ab Initio and Matrix Isolation Studies of Weakly Interacting Systems. *Journal of Physical Chemistry A*, **2004**, 108, 11846-11854	2.8	26
16	Benchmark Results for Hydrogen Atom Transfer between Carbon Centers and Validation of Electronic Structure Methods for Bond Energies and Barrier Heights. *Journal of Physical Chemistry A* , **2004**, 108, 2475-2486	2.8	63
15	Simulation of liquid water using semiempirical Hamiltonians and the divide and conquer approach. *Journal of Physical Chemistry A*, **2005**, 109, 3425-32	2.8	58
14	Application of combined thermoanalytical techniques in the investigation of cyclodextrin inclusion complexes. *Journal of Thermal Analysis and Calorimetry*, **2006**, 84, 693-701	4.1	23
13	Specific Reaction Parametrization of the AM1/d Hamiltonian for Phosphoryl Transfer Reactions: H, O, and P Atoms. *Journal of Chemical Theory and Computation*, **2007**, 3, 486-504	6.4	131
12	Mechanism for intein C-terminal cleavage: a proposal from quantum mechanical calculations. *Biophysical Journal*, **2007**, 92, 847-53	2.9	36

11	Self-consistent polarization neglect of diatomic differential overlap: application to water clusters. *Journal of Chemical Physics*, **2008**, 128, 164111	3.9	24
10	Combining a genetic algorithm with a linear scaling semiempirical method for protein–ligand docking. *Computational and Theoretical Chemistry*, **2009**, 898, 31-41		12
9	Are current semiempirical methods better than force fields? A study from the thermodynamics perspective. *Journal of Physical Chemistry A*, **2009**, 113, 11938-48	2.8	47
8	Simulation of the (H2O)8 cluster with the SCC-DFTB electronic structure method. *Chemical Physics Letters*, **2012**, 543, 45-49	2.5	23
7	Application of the SCC-DFTB method to hydroxide water clusters and aqueous hydroxide solutions. *Journal of Physical Chemistry B*, **2013**, 117, 5165-79	3.4	50
6	Water interactions with hydrophobic groups: assessment and recalibration of semiempirical molecular orbital methods. *Journal of Chemical Physics*, **2014**, 141, 034106	3.9	15
5	Conformational studies of dammarane-type triterpenoids using computational and NMR spectroscopic methods. *Magnetic Resonance in Chemistry*, **2015**, 53, 1035-42	2.1	2
4	Novel quantitative structure-activity relationship model to predict activities of natural products against COVID-19. *Chemical Biology and Drug Design*, **2021**, 97, 978-983	2.9	2
3	Building A Bridge Between AB Initio and Semiempirical Theories of Molecular Electronic Structure. **1995**, 25-67		3
2	Quantum Chemical Descriptors in Structure-Activity Relationships Calculation, Interpretation, and Comparison of Methods. **2004**,		1
1	QSAR Model Study of 2,3,4,5-tetrahydro-1H-pyrido[4,3-b]indole of Cystic-brosis-transmembrane Conductance-regulator Gene Potentiators. *Letters in Drug Design and Discovery*, **2021**, 18,	0.8	0