

# Comprehensive Benchmark of Association (Free) Energy Complexes

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Citation Report

#	ARTICLE	IF	CITATIONS
8	Benchmarking Ground-State Geometries and Vertical Excitation Energies of a Selection of P-Type Semiconducting Molecules with Different Polarity. <i>Journal of Physical Chemistry A</i> , 2015, 119, 12876-12891.	1.1	25
9	Consistent structures and interactions by density functional theory with small atomic orbital basis sets. <i>Journal of Chemical Physics</i> , 2015, 143, 054107.	1.2	605
10	Assessment of semiempirical enthalpy of formation in solution as an effective energy function to discriminate native-like structures in protein decoy sets. <i>Journal of Computational Chemistry</i> , 2016, 37, 1962-1972.	1.5	9
11	Converging ligand-binding free energies obtained with free-energy perturbations at the quantum mechanical level. <i>Journal of Computational Chemistry</i> , 2016, 37, 1589-1600.	1.5	46
12	Halogen bonded supramolecular capsules: a challenging test case for quantum chemical methods. <i>Chemical Communications</i> , 2016, 52, 9893-9896.	2.2	26
13	Planetary Orbital Systems Composed of Cycloparaphenylenes. <i>Journal of Organic Chemistry</i> , 2016, 81, 4559-4565.	1.7	22
14	Comment on "Theoretical studies on a carbonaceous molecular bearing: association thermodynamics and dual-mode rolling dynamics" by H. Isobe, K. Nakamura, S. Hitosugi, S. Sato, H. Tokoyama, H. Yamakado, K. Ohno and H. Kono, <i>Chem. Sci.</i> , 2015, 6, 2746. <i>Chemical Science</i> , 2016, 7, 2924-2928.	3.7	4
15	Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. <i>Chemical Reviews</i> , 2016, 116, 5301-5337.	23.0	312
16	Prebiotic synthesis of nucleic acids and their building blocks at the atomic level – merging models and mechanisms from advanced computations and experiments. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20047-20066.	1.3	48
17	Ligand-Binding Affinity Estimates Supported by Quantum-Mechanical Methods. <i>Chemical Reviews</i> , 2016, 116, 5520-5566.	23.0	216
18	Dispersion-Corrected Mean-Field Electronic Structure Methods. <i>Chemical Reviews</i> , 2016, 116, 5105-5154.	23.0	1,032
19	Noncovalent Interactions by Quantum Monte Carlo. <i>Chemical Reviews</i> , 2016, 116, 5188-5215.	23.0	114
20	Organic crystal polymorphism: a benchmark for dispersion-corrected mean-field electronic structure methods. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 502-513.	0.5	53
21	QM/MM Calculations on Proteins. <i>Methods in Enzymology</i> , 2016, 577, 119-158.	0.4	75
22	Small Atomic Orbital Basis Set First-Principles Quantum Chemical Methods for Large Molecular and Periodic Systems: A Critical Analysis of Error Sources. <i>ChemistryOpen</i> , 2016, 5, 94-109.	0.9	57
23	Assessment of DFT Functionals for QTAIM Topological Analysis of Halogen Bonds with Benzene. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9071-9080.	1.1	37
24	Double helicenes. <i>Chemical Physics Letters</i> , 2016, 666, 13-18.	1.2	3
25	Theoretical investigation of the interactions between the $\pi$ -systems of molecular organic semiconductors and an analysis of the contributions of repulsion and electrostatics. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1138-1152.	1.0	5

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26	Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Benchmarks for Ground-State Properties. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1097-1120.	2.3	74
27	Benchmark Calculations of Interaction Energies in Noncovalent Complexes and Their Applications. <i>Chemical Reviews</i> , 2016, 116, 5038-5071.	23.0	346
28	Towards full Quantum-Mechanics-Based Protein-Ligand Binding Affinities. <i>ChemPhysChem</i> , 2017, 18, 898-905.	1.0	46
29	First-Principles Models for van der Waals Interactions in Molecules and Materials: Concepts, Theory, and Applications. <i>Chemical Reviews</i> , 2017, 117, 4714-4758.	23.0	408
30	Noncovalent Interactions and Internal Dynamics in Pyridine-Ammonia: A Combined Quantum-Chemical and Microwave Spectroscopy Study. <i>Chemistry - A European Journal</i> , 2017, 23, 4876-4883.	1.7	39
31	Revealing the Intermolecular Interactions of Asphaltene Dimers by Quantum Chemical Calculations. <i>Energy &amp; Fuels</i> , 2017, 31, 2488-2495.	2.5	59
32	Theoretical Investigation of the Binding of Nucleobases to Cucurbiturils by Dispersion Corrected DFT Approaches. <i>Journal of Physical Chemistry B</i> , 2017, 121, 4733-4744.	1.2	40
33	A Robust and Accurate Tight-Binding Quantum Chemical Method for Structures, Vibrational Frequencies, and Noncovalent Interactions of Large Molecular Systems Parametrized for All spd-Block Elements ( $Z = 1-86$ ). <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1989-2009.	2.3	1,072
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37	Enantiomerically pure tetraphenylene-based homochiral macrocyclic tetramer and its recognition property towards $C_{76}$ fullerene. <i>Tetrahedron</i> , 2017, 73, 3606-3611.	1.0	1
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40	Quantum Chemical Dissection of the Shortest P=O...I Halogen Bond: The Decisive Role of Crystal Packing Effects. <i>Chemistry - A European Journal</i> , 2017, 23, 5687-5691.	1.7	20
41	Bidirectional Photomodulation of Surface Tension in Langmuir Films. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 291-296.	7.2	13
42	Bidirectional Photomodulation of Surface Tension in Langmuir Films. <i>Angewandte Chemie</i> , 2017, 129, 297-302.	1.6	8
43	Influence of size, shape, heteroatom content and dispersive contributions on guest binding in a coordination cage. <i>Chemical Communications</i> , 2017, 53, 11933-11936.	2.2	27

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44	Toward the Accurate Prediction of Liquid Phase Oxidation of Aromatics: A Detailed Kinetic Mechanism for Toluene Autoxidation. <i>Energy &amp; Fuels</i> , 2017, 31, 12893-12913.	2.5	15
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53	A Comprehensive Overview of the DFT-D3 London-Dispersion Correction. , 2017, , 195-219.		57
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69	A Simple Correction for Nonadditive Dispersion within Extended Symmetry-Adapted Perturbation Theory (XSAPT). <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5128-5142.	2.3	19
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81	Accurate and Efficient <i>ab Initio</i> Calculations for Supramolecular Complexes: Symmetry-Adapted Perturbation Theory with Many-Body Dispersion. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2706-2714.	2.1	51
82	A generally applicable atomic-charge dependent London dispersion correction. <i>Journal of Chemical Physics</i> , 2019, 150, 154122.	1.2	697
83	Analytical gradient for the domain-based local pair natural orbital second order Møller-Plesset perturbation theory method (DLPNO-MP2). <i>Journal of Chemical Physics</i> , 2019, 150, 164102.	1.2	35
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85	Evaluation of DFT Methods and Implicit Solvation Models for Anion-Guest Systems. <i>Helvetica Chimica Acta</i> , 2019, 102, e1900032.	1.0	13
86	Semiempirical Quantum-Chemical Methods with Orthogonalization and Dispersion Corrections. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1743-1760.	2.3	45
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91	Structure, stability, and nature of bonding between high energy water clusters confined inside cucurbituril: A computational study. <i>Computational and Theoretical Chemistry</i> , 2019, 1148, 44-54.	1.1	13
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95	Recent developments in symmetry-adapted perturbation theory. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2020, 10, e1452.	6.2	102
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100	Self-Assembly of Hollow Organic Nanotubes Driven by Arene Regioisomerism. <i>ChemPlusChem</i> , 2020, 85, 2372-2375.	1.3	4
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112	Clamlike Cyclotricatechylene-based Capsules: Identifying the Roles of Protonation State and Guests as well as the Drivers for Stability and (Anti-)Cooperativity. <i>Chemistry - an Asian Journal</i> , 2020, 15, 1301-1314.	1.7	4
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114	Extended <i>tight-binding</i> quantum chemistry methods. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1493.	6.2	596
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141	Third-Order Many-Body Expansion of OSV-MP2 Wave Function for Low-Order Scaling Analytical Gradient Computation. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6841-6860.	2.3	5
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143	Perylene Bisimide Cyclophanes as Biaryl Enantiomerization Catalystsâ€Explorations into Î€â€Î€ Catalysis and Hostâ€Guest Chirality Transfer. <i>Journal of Organic Chemistry</i> , 2022, 87, 5485-5496.	1.7	7
144	A density-functional benchmark of vibrational free-energy corrections for molecular crystal polymorphism. <i>Journal of Chemical Physics</i> , 2022, 156, 114108.	1.2	7
145	The PM6-FGC Method: Improved Corrections for Amines and Amides. <i>Molecules</i> , 2022, 27, 1678.	1.7	2
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