

Comprehensive Benchmark Results for the Domain Based Coupled Cluster Method (DLPNO-CCSD(T)) for Closed-Shell

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Insight into the synthesis of N-methylated polypeptides. <i>Polymer Chemistry</i> , 2020, 11, 6919-6927.	1.9	3
2	Chalcogen-mercury bond formation and disruption in model Rabenstein's reactions: A computational analysis. <i>Journal of Computational Chemistry</i> , 2020, 41, 2045-2054.	1.5	13
3	Kinetic modeling of methyl pentanoate pyrolysis based on <i>ab initio</i> calculations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 17978-17986.	1.3	8
4	A case study of density functional theory and domain-based local pair natural orbital coupled cluster for vibrational effects on EPR hyperfine coupling constants: vibrational perturbation theory versus <i>ab initio</i> molecular dynamics. <i>Molecular Physics</i> , 2020, 118, e1797916.	0.8	9
5	Explicitly correlated coupled cluster method for accurate treatment of open-shell molecules with hundreds of atoms. <i>Journal of Chemical Physics</i> , 2020, 153, 094105.	1.2	22
6	Efficient Synthesis of β -Lactones by Cobalt-Catalyzed Carbonylative Ring Expansion of Oxetanes under Syngas Atmosphere. <i>ChemCatChem</i> , 2020, 12, 5898-5902.	1.8	12
7	Reversible switching between housane and cyclopentanediyli isomers: an isonitrile-catalysed thermal reverse reaction. <i>Dalton Transactions</i> , 2020, 49, 13986-13992.	1.6	8
8	Bond Dissociation Energies in the Gas Phase for Large Molecular Ions by Threshold Collision-Induced Dissociation Experiments: Stretching the Limits. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8692-8707.	1.1	11
9	How Big is the Pinacol Boronic Ester as a Substituent?. <i>Angewandte Chemie</i> , 2020, 132, 22589-22593.	1.6	7
10	How Big is the Pinacol Boronic Ester as a Substituent?. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 22403-22407.	7.2	32
11	Extrapolation to the Limit of a Complete Pair Natural Orbital Space in Local Coupled-Cluster Calculations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6142-6149.	2.3	45
12	Hindered rotor benchmarks for the transition states of free radical additions to unsaturated hydrocarbons. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 27241-27254.	1.3	2
13	Mechanistic Insights into the <i>ortho</i> -Defluorination-Hydroxylation of 2-Halophenolates Promoted by a Bis($\frac{1}{4}$ -oxo)dicopper(III) Complex. <i>Inorganic Chemistry</i> , 2020, 59, 17018-17027.	1.9	8
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15	Hydration of Atmospheric Molecular Clusters III: Procedure for Efficient Free Energy Surface Exploration of Large Hydrated Clusters. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5253-5261.	1.1	16
16	The ORCA quantum chemistry program package. <i>Journal of Chemical Physics</i> , 2020, 152, 224108.	1.2	1,915
17	Assessment of the DLPNO Binding Energies of Strongly Noncovalent Bonded Atmospheric Molecular Clusters. <i>ACS Omega</i> , 2020, 5, 7601-7612.	1.6	38
18	Computational study on the mechanism of CBT-Cys click reaction. <i>Computational and Theoretical Chemistry</i> , 2020, 1185, 112874.	1.1	3

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24	Double hybrid $\langle \text{scp} \rangle \text{DFT} \langle /scp \rangle$ calculations with Slater type orbitals. <i>Journal of Computational Chemistry</i> , 2020, 41, 1660-1684.	1.5	16
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26	Assessing conformer energies using electronic structure and machine learning methods. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26381.	1.0	40
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30	Reactivity of Undissociated Molecular Nitric Acid at the Air-Water Interface. <i>Journal of the American Chemical Society</i> , 2021, 143, 453-462.	6.6	14
31	Strong bases behave as weak bases in nanoscale chemical environments: implication in humidity-swing CO ₂ air capture. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 14811-14817.	1.3	7
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33	Accurate Reduced-Cost CCSD(T) Energies: Parallel Implementation, Benchmarks, and Large-Scale Applications. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 860-878.	2.3	32
34	Canonical and explicitly-correlated coupled cluster correlation energies of sub-kJ mol ⁻¹ accuracy via cost-effective hybrid-post-CBS extrapolation. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 9571-9584.	1.3	12
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93	Amino Acids Compete with Ammonia in Sulfuric Acid-Based Atmospheric Aerosol Prenucleation: The Case of Glycine and Serine. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5195-5206.	1.1	10
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