Quantum Chemical Strain Analysis For Mechanochemic

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Citation Report

#	Article	IF	Citations
1	Force-induced retro-click reaction of triazoles competes with adjacent single-bond rupture. Chemical Science, 2017, 8, 5567-5575.	3.7	20
2	An algorithm to locate optimal bond breaking points on a potential energy surface for applications in mechanochemistry and catalysis. Journal of Chemical Physics, 2017, 147, 152710.	1.2	22
3	Theoretical simulation of the infrared signature of mechanically stressed polymer solids. Beilstein Journal of Organic Chemistry, 2017, 13, 1710-1716.	1.3	6
5	Toward a theory of mechanochemistry: Simple models from the very beginnings. International Journal of Quantum Chemistry, 2018, 118, e25775.	1.0	18
6	Mechanochemistry of nucleosides, nucleotides and related materials. Beilstein Journal of Organic Chemistry, 2018, 14, 955-970.	1.3	68
7	Twist and Returnâ^'Induced Ring Strain Triggers Quick Relaxation of a (Z)-Stabilized Cyclobisazobenzene. Journal of Physical Chemistry Letters, 2018, 9, 4776-4781.	2.1	17
8	Mechanochemically Gated Photoswitching: Expanding the Scope of Polymer Mechanochromism. Synlett, 2019, 30, 1725-1732.	1.0	19
9	Ultrafast dynamics of highly constrained azobenzene macrocycles. EPJ Web of Conferences, 2019, 205, 09002.	0.1	0
10	Implementing the mechanical force into the conceptual DFT framework: understanding and predicting molecular mechanochemical properties. Physical Chemistry Chemical Physics, 2019, 21, 7378-7388.	1.3	25
11	Reaction milling for scalable synthesis of N, P-codoped covalent organic polymers for metal-free bifunctional electrocatalysts. Chemical Engineering Journal, 2019, 358, 427-434.	6.6	44
12	The hunt for reactive alkynes in bio-orthogonal click reactions: insights from mechanochemical and conceptual DFT calculations. Chemical Science, 2020, 11, 1431-1439.	3.7	21
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16	Strain visualization for strained macrocycles. Chemical Science, 2020, 11, 3923-3930.	3.7	62
17	Tuning the Mechanical Properties of Metallopolymers via Ligand Interactions: A Combined Experimental and Theoretical Study. Macromolecules, 2020, 53, 2021-2030.	2.2	18
18	Quantum chemical modeling of molecules under pressure. International Journal of Quantum Chemistry, 2021, 121, e26208.	1.0	14
19	Mechanochemically Triggered Topology Changes in Expanded Porphyrins. Chemistry - A European Journal, 2021, 27, 3397-3406.	1.7	14

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20	Modeling Molecules under Pressure with Gaussian Potentials. Journal of Chemical Theory and Computation, 2021, 17, 583-597.	2.3	17
21	The activation efficiency of mechanophores can be modulated by adjacent polymer composition. RSC Advances, 2021, 11, 7391-7396.	1.7	4
22	The many flavours of mechanochemistry and its plausible conceptual underpinnings. Nature Reviews Chemistry, 2021, 5, 148-167.	13.8	176
23	Mechanical degradation estimation of thermosets by peak shift assessment: General approach using infrared spectroscopy. Polymer, 2021, 221, 123585.	1.8	5
24	Designing Force Probes Based on Reversible 6Ï€-Electrocyclizations in Polyenes Using Quantum Chemical Calculations. Journal of Organic Chemistry, 2021, 86, 7477-7489.	1.7	5
25	Understanding the Mechanochemistry of Ladder-Type Cyclobutane Mechanophores by Single Molecule Force Spectroscopy. Journal of the American Chemical Society, 2021, 143, 12328-12334.	6.6	26
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34	Mechanochemical synthesis of halogenated heterocyclic compounds. Chemistry of Heterocyclic Compounds, 2023, 59, 525-533.	0.6	0
35	Wandering through quantum-mechanochemistry: from concepts to reactivity and switches. Physical Chemistry Chemical Physics, 0, , .	1.3	0