A quantitative quantum-chemical analysis tool for the c molecules

Journal of Chemical Physics

140, 134107

DOI: 10.1063/1.4870334

Citation Report

#	Article	IF	Citations
1	On the calculation of internal forces in mechanically stressed polyatomic molecules. Journal of Chemical Physics, 2014, 141, 134115.	1.2	10
2	A General Quantum Mechanically Derived Force Field (QMDFF) for Molecules and Condensed Phase Simulations. Journal of Chemical Theory and Computation, 2014, 10, 4497-4514.	2.3	154
3	Some studies on generalized coordinate sets for polyatomic molecules. Journal of Chemical Physics, 2015, 143, 224103.	1.2	8
4	On the use of different coordinate systems in mechanochemical force analyses. Journal of Chemical Physics, 2015, 143, 074118.	1.2	18
5	Finding mechanochemical pathways and barriers without transition state search. Journal of Chemical Physics, 2015, 142, 174106.	1.2	20
7	Perspective: Mechanochemistry of biological and synthetic molecules. Journal of Chemical Physics, 2016, 144, 030901.	1.2	82
8	Stiff-stilbene photoswitch ruptures bonds not by pulling but by local heating. Physical Chemistry Chemical Physics, 2016, 18, 15848-15853.	1.3	12
9	Bond breaking in stretched molecules: multi-reference methods versus density functional theory. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	25
10	Can Strained Hydrocarbons Be â€œForcedâ€•To Be Stable?. Journal of Physical Chemistry A, 2016, 120, 7198-7204.	1.1	9
11	Response to Comment on T. Stauch, A. Dreuw, â€œStiff-stilbene photoswitch ruptures bonds not by pulling but by local heatingâ€; Phys. Chem. Chem. Phys., 2016, 18, 15848. Physical Chemistry Chemical Physics, 2016, 18, 26994-26997.	1.3	3
12	Advances in Quantum Mechanochemistry: Electronic Structure Methods and Force Analysis. Chemical Reviews, 2016, 116, 14137-14180.	23.0	140
13	Knots â€œChoke Offâ€•Polymers upon Stretching. Angewandte Chemie - International Edition, 2016, 55, 811-814.	7.2	30
14	Predicting the Efficiency of Photoswitches Using Force Analysis. Journal of Physical Chemistry Letters, 2016, 7, 1298-1302.	2.1	11
15	Force-induced retro-click reaction of triazoles competes with adjacent single-bond rupture. Chemical Science, 2017, 8, 5567-5575.	3.7	20
16	Quantum Chemical Strain Analysis For Mechanochemical Processes. Accounts of Chemical Research, 2017, 50, 1041-1048.	7.6	35
17	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
18	Franckâ€“Condon Theory of Quantum Mechanochemistry. Journal of Physical Chemistry A, 2017, 121, 5758-5762.	1.1	9
19	Theoretical simulation of the infrared signature of mechanically stressed polymer solids. Beilstein Journal of Organic Chemistry, 2017, 13, 1710-1716.	1.3	6

#	Article	IF	Citations
21	Exploring Potential Energy Surface with External Forces. Journal of Chemical Theory and Computation, 2018, 14, 6306-6316.	2.3	7
22	Theoretical studies of the pyranose ring under mechanical stress. Carbohydrate Research, 2018, 470, 64-72.	1.1	7
23	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
24	The Mechanism of Flexâ€Activation in Mechanophores Revealed By Quantum Chemistry. ChemPhysChem, 2020, 21, 2402-2406.	1.0	7
25	The rupture mechanism of rubredoxin is more complex than previously thought. Chemical Science, 2020, 11, 6036-6044.	3.7	1
26	Mechanochemically Triggered Topology Changes in Expanded Porphyrins. Chemistry - A European Journal, 2021, 27, 3397-3406.	1.7	14
27	The role of polymer mechanochemistry in responsive materials and additive manufacturing. Nature Reviews Materials, 2021, 6, 84-98.	23.3	151
28	Modeling Molecules under Pressure with Gaussian Potentials. Journal of Chemical Theory and Computation, 2021, 17, 583-597.	2.3	17
29	The activation efficiency of mechanophores can be modulated by adjacent polymer composition. RSC Advances, 2021, 11, 7391-7396.	1.7	4
30	Mechanical degradation estimation of thermosets by peak shift assessment: General approach using infrared spectroscopy. Polymer, 2021, 221, 123585.	1.8	5
31	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
32	A Two-Step Baromechanical Cycle for Repeated Activation and Deactivation of Mechanophores. Journal of Physical Chemistry Letters, 2021, 12, 9470-9474.	2.1	5
33	Mechanophores in polymer mechanochemistry: Insights from single-molecule experiments and computer simulations. , 2021, , 113-139.		1
34	Modern Plant Metabolomics for the Discovery and Characterization of Natural Products and Their Biosynthetic Genes. , 2020, , 156-188.		1
36	Influence of an external electric field on the rupture force of decane, 4-decanone, and dicumyl peroxide molecules: Computational insight. Materials Today Communications, 2022, 32, 103928.	0.9	0
38	Wandering through quantum-mechanochemistry: from concepts to reactivity and switches. Physical Chemistry Chemical Physics, 0, , .	1.3	0