Damian Moran

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Impact of Hydrogen Bonding on the Susceptibility of Peptides to Oxidation. Chemistry - an Asian Journal, 2017, 12, 1485-1489.	1.7	11
2	Bond Dissociation Energies and Radical Stabilization Energies:  An Assessment of Contemporary Theoretical Procedures. Journal of Physical Chemistry A, 2007, 111, 13638-13644.	1.1	101
3	Carbene Stabilization by Aryl Substituents. Is Bigger Better?. Journal of the American Chemical Society, 2007, 129, 3763-3770.	6.6	56
4	Ab Initio Modeling of Glycosyl Torsions and Anomeric Effects in a Model Carbohydrate: 2-Ethoxy Tetrahydropyran. Biophysical Journal, 2007, 93, 1-10.	0.2	48
5	An Evaluation of Harmonic Vibrational Frequency Scale Factors. Journal of Physical Chemistry A, 2007, 111, 11683-11700.	1.1	2,264
6	Thermochemistry and Kinetics of Hydrogen Abstraction by Methyl Radical from Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry A, 2006, 110, 13624-13631.	1.1	41
7	Metal-Mediated Formation of Gas-Phase Amino Acid Radical Cationsâ€,#. Journal of Physical Chemistry A, 2006, 110, 8304-8315.	1.1	64
8	Gas-phase regiocontrolled generation of charged amino acid and peptide radicals. Chemical Communications, 2006, , 4233.	2.2	52
9	Popular Theoretical Methods Predict Benzene and Arenes To Be Nonplanar. Journal of the American Chemical Society, 2006, 128, 9342-9343.	6.6	238
10	The oxidation states of copper and iron in mineral sulfides, and the oxides formed on initial exposure of chalcopyrite and bornite to air. Geochimica Et Cosmochimica Acta, 2006, 70, 2210-2228.	1.6	202
11	An Assessment of Theoretical Procedures for Predicting the Thermochemistry and Kinetics of Hydrogen Abstraction by Methyl Radical from Benzene. Journal of Physical Chemistry A, 2006, 110, 8942-8951.	1.1	70
12	An Experimental and Theoretical Investigation of Gas-Phase Reactions of Ca2+ with Glycine. Chemistry - A European Journal, 2006, 12, 6787-6796.	1.7	57
13	Rearrangements in Model Peptide-Type Radicalsvia Intramolecular Hydrogen-Atom Transfer. Helvetica Chimica Acta, 2006, 89, 2254-2272.	1.0	39
14	On the Origin ofCis/TransStereoselectivity in Intramolecular Dielsâ^'Alder Reactions of Substituted Pentadienyl Acrylates: A Comprehensive Density Functional Study. Journal of Organic Chemistry, 2005, 70, 10841-10853.	1.7	22
15	Bond Dissociation Energies and Radical Stabilization Energies Associated with Model Peptide-Backbone Radicals. Journal of Physical Chemistry A, 2005, 109, 6318-6325.	1.1	72
16	σ-Aromaticity and σ-Antiaromaticity in Saturated Inorganic Rings. Journal of Physical Chemistry A, 2005, 109, 3711-3716.	1.1	60
17	Intramolecular Dielsâ^'Alder Reactions of Ester-Linked 1,3,8-Nonatrienes. Journal of Organic Chemistry, 2005, 70, 5561-5570.	1.7	33
18	Theoretical Study of Complexes of Closo-Borane, Alane, and Gallane Anions with Cations of Light Metals Inside and Outside of Icosahedral Clusters [A12H122-] (A: B, Al, and Ga) ChemInform, 2003, 34, no.	0.1	0

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19	Molecular structures and energetics of the neutral aluminum–trimethylaluminum complex: an Al–Al bonded global minimum?. Chemical Physics Letters, 2003, 378, 65-70.	1.2	2
20	Aromatic stabilization in heterofullerenes C48X12(X = N, P, B, Si). Journal of Physical Organic Chemistry, 2003, 16, 726-730.	0.9	35
21	Towards Graphite:  Magnetic Properties of Large Polybenzenoid Hydrocarbons. Journal of the American Chemical Society, 2003, 125, 6746-6752.	6.6	158
22	Increased Reactivity of the•Cr(CO)3(C5Me5) Radical with Thiones versus Thiols: A Theoretical and Experimental Investigation. Inorganic Chemistry, 2003, 42, 8494-8503.	1.9	19
23	A Theoretical and Structural Investigation of Thiocarbon Anions. Journal of Organic Chemistry, 2003, 68, 8808-8814.	1.7	23
24	On the Viability of Small Endohedral Hydrocarbon Cage Complexes:Â X@C4H4, X@C8H8, X@C8H14, X@C10H16, X@C12H12, and X@C16H16. Journal of the American Chemical Society, 2003, 125, 11442-11451.	6.6	45
25	Ïf-Antiaromaticity in Cyclobutane, Cubane, and Other Molecules with Saturated Four-Membered Rings. Organic Letters, 2003, 5, 23-26.	2.4	108
26	Structures and Stabilities of Endo- and Exohedral Dodecahedrane Complexes (X@C20H20 and) Tj ETQq0 0 0 rgBT	/Overlock 1.1	10 Tf 50 46
27	On the Stability of Large [4n]Annulenes. Organic Letters, 2003, 5, 2983-2986.	2.4	118
28	Aromaticity of the Bergman, Myersâ ´`Saito, Schmittel, and Directly Related Cyclizations of Enediynes. Journal of Organic Chemistry, 2002, 67, 1453-1461.	1.7	80
29	Theoretical Study of Complexes of Closo-Borane, Alane, and Gallane Anions with Cations of Light Metals Inside and Outside of Icosahedral Clusters [A12H122-] (A = B, Al, and Ga). Journal of Physical Chemistry A, 2002, 106, 11594-11602.	1.1	23

30	2-Pyridinethiol/2-Pyridinethione Tautomeric Equilibrium. A Comparative Experimental and Computational Study. Journal of Organic Chemistry, 2002, 67, 9061-9069.	1.7	78

31	Structures, Stabilities, and Ionization Potentials of Dodecahedrane Endohedral Complexes. Journal of Physical Chemistry A, 2002, 106, 5144-5154.	1.1	64	
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Theoretical Study of Icosahedralcloso-Borane, -Alane, and -Gallane Dianions (A12H122-; A = B, Al, Ga) with Endohedral Noble Gas Atoms (Ng = He, Ne, Ar, and Kr) and Their Lithium Salts (Li[Ng@A12H12]-and) Tj ETQqQ@0 rgBT Øverlock 1

33	Th-Symmetrical N8(CC)6and P8(CC)6; an Extraordinary Contrast in Heterofullerene Stability. Organic Letters, 2001, 3, 3233-3236.	2.4	18
34	The Almost Bottleable Triplet Carbene: 2,6-dibromo-4-tert-butyl-2â€~,6â€~-bis(trifluoromethyl)-4â€~-isopropyldiphenylcarbene. Journal of the American Chemical Society, 2001, 123, 4331-4335.	6.6	25