Judith MillÃ¡n Moneo

List of Publications by Year
in descending order

33 papers	567 citations	623734 14 h-index	642732 23 g-index
36 all docs	36 docs citations	36 times ranked	473 citing authors

#	Article	IF	Citations
1	Ab initio ground potential energy surface, VTST and QCT study of the O(3P)+CH4(Xâ€‰1A1)â†'OH(Xâ€‰2Î)+CH3(Xâ€‰2A2â€³) reaction. Journal of Chemical Physics, 1999, 110, 7326-7338.	3.0	73
2	Ab initiopotential energy surface, variational transition state theory, and quasiclassical trajectory studies of the F+CH4â†'HF+CH3 reaction. Journal of Chemical Physics, 2004, 120, 5181-5191.	3.0	46
3	Ab initio analytical potential energy surface and quasiclassical trajectory study of the O+(4S)+H2(Xâ€Š1Î£g+)â†'OH+(Xâ€Š3Î£â^')+H(2S) reaction and isotopic variants. Journal of Chemical Physics, 2004, 120, 4705-4714.	3.0	42
4	Ab initio, kinetics, and dynamics study of Cl+CH4â†'HCl+CH3. Journal of Chemical Physics, 2002, 117, 5730-5741.	3.0	40
5	Exploring microsolvation of the anesthetic propofol. Physical Chemistry Chemical Physics, 2012, 14, 4398.	2.8	40
6	Unravelling Proteinâ€“DNA Interactions at Molecular Level: A DFT and NCI Study. Journal of Chemical Theory and Computation, 2016, 12, 523-534.	5.3	35
7	Shaping Micelles: The Interplay Between Hydrogen Bonds and Dispersive Interactions. Angewandte Chemie - International Edition, 2013, 52, 7772-7775.	13.8	31
8	Mimicking anaestheticâ€“receptor interaction: a combined spectroscopic and computational study of propofolâ¯phenol. Physical Chemistry Chemical Physics, 2012, 14, 8956.	2.8	25
9	A Spectroscopic and Computational Study of Propofol Dimers and Their Hydrated Clusters. ChemPhysChem, 2012, 13, 3819-3826.	2.1	23
10	Ab initiostudy of the O(1D)+CH4(Xâ€Š1A1)â†'OH(Xâ€Š2Î)+CH3(Xâ€Š2A2â€³) reaction: Ground and excited potential energy surfaces. Journal of Chemical Physics, 2003, 119, 9504-9512.	3.0	21
11	Isomerism of the Aniline Trimer. Angewandte Chemie - International Edition, 2018, 57, 15112-15116.	13.8	19
12	Calculation of traces ofp-order replacement operators overN-electron spin-adapted spaces. Physical Review A, 1993, 47, 923-928.	2.5	18
13	A combined spectroscopic and theoretical study of propofolÂ·(H2O)3. Journal of Chemical Physics, 2012, 137, 074303.	3.0	18
14	Formation of water polyhedrons in propofolâ€“water clusters. Physical Chemistry Chemical Physics, 2013, 15, 568-575.	2.8	16
15	Water Encapsulation by Nanomicelles. Angewandte Chemie - International Edition, 2014, 53, 12480-12483.	13.8	14
16	Discriminating the structure ofexo-2-aminonorbornane using nuclear quadrupole coupling interactions. Journal of Chemical Physics, 2011, 134, 164311.	3.0	12
17	Unraveling the Benzocaineâ€“Receptor Interaction at Molecular Level Using Mass-Resolved Spectroscopy. Journal of Physical Chemistry B, 2013, 117, 13472-13480.	2.6	11
18	Mimicking anestheticâ€“receptor interactions in jets: the propofolâ€“isopropanol cluster. Physical Chemistry Chemical Physics, 2014, 16, 16968.	2.8	9

#	Article	IF	Citations
19	Competition between stacked and hydrogen bonded structures of cytosine aggregates. Physical Chemistry Chemical Physics, 2017, 19, 8826-8834.	2.8	9
20	Magic Numbers in the Solvation of the Propofol Dimer. ChemPhysChem, 2013, 14, 1558-1562.	2.1	8
21	Vibrational predissociation dynamics of methaneâ€“Ar: an ab initio approach. Faraday Discussions, 2001, 118, 143-158.	3.2	6
22	Single Hydration of the Peptide Bond: The Case of the Vince Lactam. Journal of Physical Chemistry A, 2012, 116, 10099-10106.	2.5	6
23	Isomerism of the Aniline Trimer. Angewandte Chemie, 2018, 130, 15332-15336.	2.0	6
24	Molecular hydration of propofol dimers in supersonic expansions: formation of active centre-like structures. Physical Chemistry Chemical Physics, 2014, 16, 23301-23307.	2.8	4
25	A formal construction of theN-electron Hamiltonian matrix and its blocks factorization. Societa Italiana Di Fisica Nuovo Cimento B-General Physics, Relativity Astronomy and Mathematical Physics and Methods, 1991, 106, 1079-1084.	0.2	3
26	Calculation of the dimension of full configuration interaction spaces: application to the determination of spectroscopic terms. Computational and Theoretical Chemistry, 1993, 287, 63-66.	1.5	3
27	Transition from Planar to Nonplanar Hydrogen Bond Networks in the Solvation of Aromatic Dimers: Propofol2-(H2O)2â€“4. Journal of Physical Chemistry A, 2013, 117, 3396-3404.	2.5	3
28	Behind the Reactivity of Lactones: A Computational and Spectroscopic Study of PhenolÂ·Î³-Butyrolactone. Journal of Physical Chemistry A, 2014, 118, 2568-2575.	2.5	3
29	Conformational landscape of isolated capped amino acids: on the nature of non-covalent interactions. European Physical Journal D, 2017, 71, 1.	1.3	3
30	Structural Distortion of the Epoxy Groups in Norbornanes: A Rotational Study of exoâ€2,3â€Epoxynorbornane. ChemPhysChem, 2015, 16, 2609-2614.	2.1	2
31	Exploring Epigenetic Marks by Analysis of Noncovalent Interactions. ChemBioChem, 2021, 22, 408-415.	2.6	2
32	Contraction algorithms for third-order reduced density matrices: Symmetric group approach. Journal of Mathematical Chemistry, 1993, 13, 177-189.	1.5	0
33	Analysis of several methods in the direct approximation of reduced density matrices. Societa Italiana Di Fisica Nuovo Cimento B-General Physics, Relativity Astronomy and Mathematical Physics and Methods, 1993, 108, 491-498.	0.2	0