Alberto Requena

List of Publications by Year
in descending order

139 papers	2,190 citations	201385 27 h-index	329751 37 g-index
149 all docs	149 docs citations	149 times ranked	1837 citing authors

#	Article	IF	Citations
1	Assessing the Importance of Proton Transfer Reactions in DNA. Accounts of Chemical Research, 2014, 47, 2467-2474.	7.6	98
2	Intermolecular Proton Transfer in Microhydrated Guanineâ˜'Cytosine Base Pairs: a New Mechanism for Spontaneous Mutation in DNA. Journal of Physical Chemistry A, 2009, 113, 10549-10556.	1.1	77
3	Effects of Hydration on the Proton Transfer Mechanism in the Adenineâ˜'Thymine Base Pair. Journal of Physical Chemistry A, 2009, 113, 7892-7898.	1.1	71
4	Harmonic Models in Cartesian and Internal Coordinates to Simulate the Absorption Spectra of Carotenoids at Finite Temperatures. Journal of Chemical Theory and Computation, 2013, 9, 4947-4958.	2.3	62
5	Combined effect of stacking and solvation on the spontaneous mutation in DNA. Physical Chemistry Chemical Physics, 2011, 13, 14584.	1.3	52
6	The wavefunction of the complex coordinate method. Molecular Physics, 1980, 40, 1107-1115.	0.8	44
7	A modified Ehrenfest method that achieves Boltzmann quantum state populations. Chemical Physics Letters, 2006, 417, 53-57.	1.2	44
8	A Theoretical Study of the Reaction of Î²-Carotene with the Nitrogen Dioxide Radical in Solution. Journal of Physical Chemistry B, 2010, 114, 4366-4372.	1.2	41
9	A theoretical study of the HgAr2(3P1â†1S0) vibronic spectrum. Journal of Chemical Physics, 1993, 98, 1007-1017.	1.2	40
10	The Ehrenfest method with quantum corrections to simulate the relaxation of molecules in solution: Equilibrium and dynamics. Journal of Chemical Physics, 2007, 126, 014503.	1.2	40
11	Si-BEARING MOLECULES TOWARD IRC+10216: ALMA UNVEILS THE MOLECULAR ENVELOPE OF CWLeo. Astrophysical Journal Letters, 2015, 805, L13.	3.0	40
12	Rotational predissociation of triatomic van der Waals molecules. Journal of Chemical Physics, 1980, 72, 3018-3026.	1.2	39
13	Vibrational predissociation of the I2â‹¯Ne2 cluster: A molecular dynamics with quantum transitions study. Journal of Chemical Physics, 1998, 109, 6320-6328.	1.2	37
14	Optimal generalized internal vibrational coordinates and potential energy surface for the ground electronic state of SO2. Journal of Chemical Physics, 2001, 115, 139-148.	1.2	35
15	A Density Functional Theory Study of the Structure and Vibrational Spectra of Î²-Carotene, Capsanthin, and Capsorubin. Journal of Physical Chemistry A, 2008, 112, 4815-4825.	1.1	34
16	Double proton transfer mechanism in the adenineâ€“uracil base pair and spontaneous mutation in RNA duplex. Chemical Physics Letters, 2009, 484, 64-68.	1.2	34
17	Instantaneous normal modes, resonances, and decay channels in the vibrational relaxation of the amide I mode of N-methylacetamide-D in liquid deuterated water. Journal of Chemical Physics, 2010, 132, 224501.	1.2	33
18	Optimization of vibrational coordinates. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 1681.	1.7	32

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19	Theoretical study of the low-lying excited states of -carotene isomers by a multireference configuration interaction method. Chemical Physics, 2010, 373, 98-103.	0.9	32
20	Theoretical Study of the Tautomerism in the One-Electron Oxidized Guanineâ"Cytosine Base Pair. Journal of Physical Chemistry B, 2010, 114, 13439-13445.	1.2	32
21	Competition between electronic and vibrational predissociation in Arâ€"I2(B): a molecular dynamics with quantum transitions study. Chemical Physics, 1999, 240, 229-239.	0.9	30
22	Molecular dynamics simulation of the I2(X)â‹¯Ar isomers population in a free-jet expansion: Thermodynamics versus kinetic control. Journal of Chemical Physics, 2002, 116, 1944-1953.	1.2	30
23	Aerosol Lidar Intercomparison in the Framework of SPALINETâ€"The Spanish Lidar Network: Methodology and Results. IEEE Transactions on Geoscience and Remote Sensing, 2009, 47, 3547-3559.	2.7	30
24	Antioxidant Properties of Î²-Carotene Isomers and Their Role in Photosystems: Insights from Ab Initio Simulations. Journal of Physical Chemistry A, 2012, 116, 3498-3506.	1.1	30
25	About the overestimation of the basis set superposition error on interaction energy calculations for van der Waals systems. Journal of Chemical Physics, 1986, 84, 5077-5080.	1.2	29
26	A new fluorescence turn-on chemosensor for nanomolar detection of Al³⁺ constructed from a pyridineâ€"pyrazole system. New Journal of Chemistry, 2018, 42, 2933-2941.	1.4	29
27	Rotational effects in the vibrational predissociation of Xâ‹…â‹…â‹…H2 van der Waals molecules. Journal of Chemical Physics, 1980, 73, 4347-4352.	1.2	27
28	Hybrid quantum/classical simulation and kinetic study of the vibrational predissociation of Cl2â‹¯Nen (n=2,â€Š3). Journal of Chemical Physics, 1999, 111, 4577-4588.	1.2	27
29	Determination of highly excited rovibrational states for N2O using generalized internal coordinates. Journal of Chemical Physics, 1999, 110, 6339-6352.	1.2	26
30	Application of trajectory surface hopping to vibrational predissociation. Chemical Physics Letters, 1997, 280, 185-188.	1.2	25
31	Time evolution of reactants, intermediates, and products in the vibrational predissociation of Br2â‹¯Ne: A theoretical study. Journal of Chemical Physics, 2000, 113, 10130-10142.	1.2	24
32	Variational Calculations of Rovibrational Energies for CO2. Journal of Molecular Spectroscopy, 2001, 205, 62-72.	0.4	24
33	Density Functional Theory Study of the Stability and Vibrational Spectra of the Î²-Carotene Isomers. Journal of Physical Chemistry A, 2009, 113, 9899-9907.	1.1	24
34	Labelling Herceptin with a novel oxaliplatin derivative: a computational approach towards the selective drug delivery. Journal of Molecular Modeling, 2014, 20, 2401.	0.8	24
35	HINTS OF A ROTATING SPIRAL STRUCTURE IN THE INNERMOST REGIONS AROUND IRC +10216. Astrophysical Journal, 2016, 818, 192.	1.6	24
36	Determination of a Potential Energy Surface for CO2Using Generalized Internal Vibrational Coordinates. Journal of Molecular Spectroscopy, 1999, 195, 137-146.	0.4	23

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37	Impact of DFT functionals on the predicted magnesiumâ€“DNA interaction: an ONIOM study. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	23
38	Curvilinear Jacobi and Radau normal coordinates for linear triatomic molecules. Application to CO2. Chemical Physics, 1993, 175, 255-264.	0.9	21
39	Atomistic Molecular Dynamics Simulations of the Interactions of Oleic and 2-Hydroxyoleic Acids with Phosphatidylcholine Bilayers. Journal of Physical Chemistry B, 2011, 115, 11727-11738.	1.2	21
40	Conformational changes of Î²-carotene and zeaxanthin immersed in a model membrane through atomistic molecular dynamics simulations. Physical Chemistry Chemical Physics, 2013, 15, 6527.	1.3	21
41	DFT Simulation of Structural and Optical Properties of 9-Aminoacridine Half-Sandwich Ru(II), Rh(III), and Ir(III) Antitumoral Complexes and Their Interaction with DNA. Journal of Chemical Theory and Computation, 2017, 13, 3898-3910.	2.3	21
42	Full quantum vibrational simulation of the relaxation of the cyanide ion in water using the Ehrenfest method with quantum corrections. Journal of Chemical Physics, 2008, 129, 154501.	1.2	20
43	Hybrid Quantum/Classical Simulations of the Vibrational Relaxation of the Amide I Mode of N-Methylacetamide in D₂O Solution. Journal of Physical Chemistry B, 2012, 116, 2969-2980.	1.2	20
44	Vibrational dynamics of polyatomic molecules in solution: assignment, time evolution and mixing of instantaneous normal modes. Theoretical Chemistry Accounts, 2011, 128, 769-782.	0.5	19
45	Rovibrational energy levels and expectation values for perturbed Kratzer oscillators. Journal of Chemical Physics, 1986, 85, 3939-3944.	1.2	18
46	Hypervirial calculations of Morse oscillator matrix elements. Journal of Chemical Physics, 1983, 78, 4792-4793.	1.2	17
47	Self-consistent-field calculation of vibrational bound states for triatomic molecules using transformed Jacobi coordinates. The Journal of Physical Chemistry, 1991, 95, 2292-2297.	2.9	17
48	Excited vibrational states and potential energy function for OCS determined using generalized internal coordinates. Journal of Chemical Physics, 2000, 113, 5695-5704.	1.2	17
49	Surface hopping simulation of the vibrational relaxation of I2 in liquid xenon using the collective probabilities algorithm. Journal of Chemical Physics, 2004, 121, 10611-10622.	1.2	16
50	Molecular Dynamics Simulations and Instantaneous Normal-Mode Analysis of the Vibrational Relaxation of the Cå^'H Stretching Modes ofN-methylacetamide-din Liquid Deuterated Water. Journal of Physical Chemistry A, 2010, 114, 11450-11461.	1.1	16
51	A method for analyzing the vibrational energy flow in biomolecules in solution. Journal of Chemical Physics, 2011, 135, 204106.	1.2	16
52	Twoâ€¢center matrix elements for Kratzer oscillators. Journal of Chemical Physics, 1990, 93, 3408-3412.	1.2	15
53	On the use of optimal internal vibrational coordinates for symmetrical bent triatomic molecules. Journal of Chemical Physics, 2005, 122, 224319.	1.2	15
54	Hybrid quantum/classical simulation of the vibrational relaxation of the bend fundamental in liquid water. Journal of Chemical Physics, 2009, 131, 204505.	1.2	15

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55	Ab initiocalculations of intermolecular potentials. The ground state of the Arï£¿H2van der Waals molecule. Journal of Computational Chemistry, 1985, 6, 39-45.	1.5	14
56	Rotationalâ€“vibrational matrix elements for Kratzer oscillators. Journal of Chemical Physics, 1989, 90, 5536-5540.	1.2	14
57	Variational calculation of vibrational energies of triatomic molecules usingSCFoptimized modes. International Journal of Quantum Chemistry, 1991, 40, 685-694.	1.0	14
58	Hyperspherical Kinematic Vibrational Coordinates for Linear Triatomic Molecules. The Journal of Physical Chemistry, 1995, 99, 11051-11060.	2.9	14
59	Matrix elements for rotating Morse oscillators. Physical Review A, 1986, 34, 4380-4386.	1.0	13
60	Use of rotated Jacobi coordinates to calculate vibrational levels of hydrogen cyanide. The Journal of Physical Chemistry, 1992, 96, 9691-9696.	2.9	13
61	Generalized hyperspherical coordinates for molecular vibrations. The Journal of Physical Chemistry, 1993, 97, 5831-5835.	2.9	13
62	Global potential energy surfaces for the CO2 and CS2 molecules. Chemical Physics Letters, 1999, 313, 670-678.	1.2	13
63	A theoretical study of the vibrational spectrum of the CS2 molecule. Journal of Chemical Physics, 2002, 116, 7495-7508.	1.2	13
64	Theoretical Study of the Temperature Dependence of the Vibrational Relaxation of the H₂O Bend Fundamental in Liquid Water and the Subsequent Distortion of the Hydrogen Bond Network. Journal of Physical Chemistry B, 2014, 118, 9427-9437.	1.2	13
65	Structure, Spectra, and DFT Simulation of Nickel Benzazolate Complexes with Tris(2-aminoethyl)amine Ligand. Inorganic Chemistry, 2017, 56, 3663-3673.	1.9	13
66	Energy levels for perturbed Morse oscillators. International Journal of Quantum Chemistry, 1980, 17, 931-942.	1.0	12
67	Improved analytic potential models for bent AB2 molecules. Journal of Molecular Spectroscopy, 1989, 136, 185-196.	0.4	12
68	Rovibrational energies, partition functions and equilibrium fractionation of the CO2 isotopologues. Journal of Quantitative Spectroscopy and Radiative Transfer, 2014, 147, 233-251.	1.1	12
69	A Pyreneâ€Pyrazoleâ€Based Rotamer Senses Hg2+on the Nanomolar Scale. ChemistrySelect, 2017, 2, 2512-2519.	0.7	12
70	Energy eigenvalues for Lennard-Jones potentials using the hypervirial perturbative method. Journal of Physics B: Atomic, Molecular and Optical Physics, 1990, 23, 2771-2781.	0.6	11
71	Variational calculations of vibrational states of N2O using hyperspherical normal coordinates. Journal of Chemical Physics, 1996, 105, 6099-6110.	1.2	11
72	Optimal internal coordinates, vibrational spectrum, and effective Hamiltonian for ozone. Journal of Chemical Physics, 2007, 126, 244305.	1.2	11

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73	Semiclassical model for accidental predissociation in diatomic molecules. Journal of Molecular Spectroscopy, 1980, 82, 364-378.	0.4	10
74	Vibrational levels of water by the self-consistent-field method using Radau coordinates. The Journal of Physical Chemistry, 1992, 96, 4341-4346.	2.9	10
75	Optimal generalized internal vibrational coordinates for symmetrical linear triatomic molecules. Chemical Physics Letters, 1998, 298, 36-42.	1.2	10
76	Could the addition of hp-hMG and GnRH antagonists modulate the response in IVF-ICSI cycles?. Human Fertility, 2010, 13, 41-49.	0.7	10
77	On the stabilization angle of the complex rotation method. Chemical Physics Letters, 1981, 78, 13-15.	1.2	9
78	Perturbation for a rigid rotator in an electric field. International Journal of Quantum Chemistry, 1982, 22, 1263-1270.	1.0	9
79	Analytical expressions for vibrational matrix elements of Morse oscillators. Physical Review A, 1988, 38, 4205-4212.	1.0	9
80	Size evolution of the vibrational predissociation process in Br2Â·Â·Â·Nen clusters: Simulation and kinetic study. Faraday Discussions, 2001, 118, 257-268.	1.6	9
81	Theoretical calculations of vibrational frequencies and rotational constants of the N2O isotopomers. Journal of Molecular Spectroscopy, 2003, 217, 43-58.	0.4	9
82	Collective probabilities algorithm for surface hopping calculations. Journal of Chemical Physics, 2003, 119, 6489-6499.	1.2	9
83	Molecular dynamics with quantum transitions study of the vibrational relaxation of the HOD bend fundamental in liquid D2O. Journal of Chemical Physics, 2012, 136, 234507.	1.2	9
84	Conformational Changes of Trialanine in Water Induced by Vibrational Relaxation of the Amide I Mode. Journal of Physical Chemistry B, 2016, 120, 348-357.	1.2	9
85	Experimental and theoretical study of the photofragmentation process: Ar3++hÎ½â†'Ar2++Ar. Journal of Chemical Physics, 2000, 113, 2175-2181.	1.2	8
86	Using the Screened Coulomb Potential To Illustrate the Variational Method. Journal of Chemical Education, 2012, 89, 1152-1158.	1.1	8
87	Structure and Spectroscopic Properties of Nickel Benzazolate Complexes with Hydrotris(pyrazolyl)borate Ligand. Inorganic Chemistry, 2014, 53, 5502-5514.	1.9	8
88	Antibodies as Carrier Molecules: Encapsulating Anti-Inflammatory Drugs inside Herceptine. Journal of Physical Chemistry B, 2018, 122, 2064-2072.	1.2	8
89	On the Role of Entropy in the Stabilization of Î±-Helices. Journal of Chemical Information and Modeling, 2020, 60, 6523-6531.	2.5	8
90	Mutagenic effects induced by the attack of NO2 radical to the guanine-cytosine base pair. Frontiers in Chemistry, 2015, 3, 13.	1.8	7

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91	Vibrational self-consistent-field approximation for triatomic molecules using hyperspherical modes with application to H2O. International Journal of Quantum Chemistry, 1992, 42, 475-488.	1.0	6
92	On the interaction of a beam of polar molecules with a static and a resonant RF field as a source of molecular interferences. European Physical Journal D, 2008, 49, 297-303.	0.6	6
93	Instantaneous normal mode analysis of the vibrational relaxation of the amide I mode of alanine dipeptide in water. Journal of Chemical Physics, 2013, 138, 205102.	1.2	6
94	Quantum solution of coupled harmonic oscillator systems beyond normal coordinates. Journal of Mathematical Chemistry, 2017, 55, 1964-1984.	0.7	6
95	Tuning the Optical Properties of Novel Antitumoral Drugs Based on Cyclometalated Iridium(III) Complexes. Journal of Physical Chemistry A, 2019, 123, 8644-8649.	1.1	6
96	Self-consistent field vibrational energies for a system of coupled oscillators using the hypervirial and the Hellmann-Feynman theorems. Journal of Quantitative Spectroscopy and Radiative Transfer, 1983, 29, 471-475.	1.1	5
97	Charge distribution analysis on Arâ€”H2 system. Computational and Theoretical Chemistry, 1986, 136, 99-110.	1.5	5
98	Excited state dynamics in HgAr2: statistical analysis of vibrational state distribution. Faraday Discussions, 1994, 97, 131-142.	1.6	5
99	Relaxation pathways of the OD stretch fundamental of HOD in liquid H2O. Journal of Chemical Physics, 2016, 145, 244502.	1.2	5
100	HIGH-RESOLUTION ROTATIONAL SPECTRUM, DUNHAM COEFFICIENTS, AND POTENTIAL ENERGY FUNCTION OF NaCl. Astrophysical Journal, 2016, 825, 150.	1.6	5
101	A vibrational Hamiltonian model for triatomic molecules based on the Kratzer and Poschl Teller potentials. International Journal of Quantum Chemistry, 1994, 52, 165-175.	1.0	4
102	An analytical perturbation treatment of the rotating Morse oscillator. Journal of Physics B: Atomic, Molecular and Optical Physics, 2008, 41, 105102.	0.6	4
103	A spectroscopic potential energy surface for FCN. Journal of Quantitative Spectroscopy and Radiative Transfer, 2012, 113, 1155-1169.	1.1	4
104	Energetic Self-Folding Mechanism in Î±-Helices. Journal of Physical Chemistry B, 2019, 123, 8186-8194.	1.2	4
105	Vibrational and rotational predissociation of triatomic van der Waals molecules. Societa Italiana Di Fisica Nuovo Cimento B-General Physics, Relativity Astronomy and Mathematical Physics and Methods, 1981, 63, 46-49.	0.2	3
106	Microcomputer-based question bank for training and assessment in biochemistry. Biochemical Education, 1984, 12, 108-111.	0.1	3
107	Hypervirial calculation of perturbedâ€”Morse-oscillator potentials for diatomic molecules. Journal of Quantitative Spectroscopy and Radiative Transfer, 1985, 34, 233-242.	1.1	3
108	Efficient parabolic evaluation of coupling terms in hybrid quantum/classical simulations. Chemical Physics, 2009, 358, 57-60.	0.9	3

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109	Host-pathogen interaction of root-knot nematode Meloidogyne incognita on pepper in the southeast of Spain. European Journal of Plant Pathology, 2011, 131, 511-518.	0.8	3
110	Theoretical vibrational terms and rotational constants for the 15N substituted isotopologues of N2O calculated using normal hyperspherical coordinates. Journal of Quantitative Spectroscopy and Radiative Transfer, 2012, 113, 26-46.	1.1	3
111	Quantum treatment of HÃ©nonâ€“Heiles systems using oblique coordinates. Journal of Physics B: Atomic, Molecular and Optical Physics, 2017, 50, 025101.	0.6	3
112	Quantum solutions of identical linearly coupled harmonic oscillators using oblique coordinates. Journal of Physics B: Atomic, Molecular and Optical Physics, 2019, 52, 055101.	0.6	3
113	Quantum description of linearly coupled harmonic oscillator systems using oblique coordinates. Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 53, 025101.	0.6	3
114	Ab Initio Partition Functions and Thermodynamic Quantities for the Molecular Hydrogen Isotopologues. Journal of Physical Chemistry A, 2021, 125, 9226-9241.	1.1	3
115	Rotational predissociation of the Ar-H2 van der Waals molecule. Journal of Quantitative Spectroscopy and Radiative Transfer, 1986, 35, 127-130.	1.1	2
116	HypervirialSCFtreatment for vibrational energy levels of triatomic molecules. International Journal of Quantum Chemistry, 1987, 32, 511-516.	1.0	2
117	Perturbative virtualSCF CItreatment for energy levels of coupled oscillator systems. International Journal of Quantum Chemistry, 1989, 36, 49-60.	1.0	2
118	The Rotating Morseâ€“Pekeris Oscillator Revisited. Journal of Chemical Education, 2008, 85, 1675.	1.1	2
119	Understanding the connection between conformational changes of peptides and equilibrium thermal fluctuations. Physical Chemistry Chemical Physics, 2017, 19, 3459-3463.	1.3	2
120	Intraresidual Correlated Motions in Peptide Chains. Journal of Chemical Information and Modeling, 2019, 59, 4524-4527.	2.5	2
121	Approximated Eigenenergy for doubly perturbed oscillators. Computational and Theoretical Chemistry, 1983, 93, 227-230.	1.5	1
122	Vibrational-rotational levels of diatomicRKRpotentials. International Journal of Quantum Chemistry, 1984, 25, 677-686.	1.0	1
123	Calculation of the absolute infrared frequencies and intensities of a diatomic molecule or of local diatomic groups. Computers & Chemistry, 1985, 9, 115-120.	1.2	1
124	Perturbed morse oscillator in diatomic molecules: an hypervirial treatment. Computational and Theoretical Chemistry, 1985, 120, 157-162.	1.5	1
125	Perturbative calculation of energy levels for coupled oscillators using the adiabatic approximation. Molecular Physics, 1987, 61, 1513-1518.	0.8	1
126	Perturbed Morse expansion for triatomic molecules. Computational and Theoretical Chemistry, 1988, 166, 357-362.	1.5	1

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127	Analytical perturbation treatment of vibrational stretch-bend couplings. Journal of Quantitative Spectroscopy and Radiative Transfer, 1989, 42, 149-155.	1.1	1
128	Vibrational Bound States of the He2Ne+ Cation. Journal of Physical Chemistry A, 2009, 113, 14896-14903.	1.1	1
129	Energy levels for a system of coupled oscillators. Computational and Theoretical Chemistry, 1983, 93, 221-226.	1.5	0
130	Perturbative treatment of anharmonic diatomic oscillators in the generator coordinate description. Computational and Theoretical Chemistry, 1985, 120, 41-45.	1.5	0
131	Predissociation in van der Waals molecules. Computational and Theoretical Chemistry, 1985, 120, 47-62.	1.5	0
132	Hypervirial treatment of centrifugal distortion of 2Î energy levels. Journal of Quantitative Spectroscopy and Radiative Transfer, 1986, 35, 29-37.	1.1	0
133	SCF calculations of excited vibrational energy levels for normal modes. Computational and Theoretical Chemistry, 1988, 166, 339-344.	1.5	0
134	Perturbative multi-step adiabatic treatment for energy levels of multidimensional coupled systems. Computational and Theoretical Chemistry, 1988, 166, 345-350.	1.5	0
135	Variational HEG calculation of vibration rotation transition moments for diatomic molecules.. Computational and Theoretical Chemistry, 1988, 166, 351-356.	1.5	0
136	The adiabatic multi-step separation method for vibrational states: application to SO2. Computational and Theoretical Chemistry, 1992, 254, 91-98.	1.5	0
137	Mixed quantum classical steps: a DVR hopping method. PhysChemComm, 2000, 3, 29-35.	0.8	0
138	A rotating spiral structure in the innermost regions around IRC+10216. Journal of Physics: Conference Series, 2016, 728, 022005.	0.3	0
139	Impact of DFT functionals on the predicted magnesiumâ€“DNA interaction: an ONIOM study. Highlights in Theoretical Chemistry, 2013, , 271-279.	0.0	0