Berta FernÃ¡ndez

List of Publications by Year
in descending order

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116	3,404	236612	161609
papers	citations	25 h-index	54 g-index

117	117	117	2863
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
2	The benzeneâ€“argon complex: A ground and excited state ab initio study. Journal of Chemical Physics, 1998, 108, 2784-2790.	1.2	144
3	Ground state benzeneâ€“argon intermolecular potential energy surface. Journal of Chemical Physics, 1999, 111, 198-204.	1.2	86
4	The heliumâ€“, neonâ€“, and argonâ€“cyclopropane van der Waals complexes: Ab initio ground state intermolecular potential energy surfaces and intermolecular dynamics. Journal of Chemical Physics, 2001, 115, 8431-8439.	1.2	84
5	Gauge invariant coupled cluster response theory using optimized nonorthogonal orbitals. Journal of Chemical Physics, 2001, 114, 6983-6993.	1.2	82
6	The effect of intermolecular interactions on the electric properties of helium and argon. I. Ab initio calculation of the interaction induced polarizability and hyperpolarizability in He2 and Ar2. Journal of Chemical Physics, 1999, 111, 10099-10107.	1.2	75
7	Coupled cluster calculations of the ground state potential and interaction induced electric properties of the mixed dimers of helium, neon and argon. Molecular Physics, 2004, 102, 101-110.	0.8	65
8	The effect of intermolecular interactions on the electric properties of helium and argon. III. Quantum statistical calculations of the dielectric second virial coefficients. Journal of Chemical Physics, 2002, 117, 2609-2618.	1.2	60
9	The effect of intermolecular interactions on the electric properties of helium and argon. II. The dielectric, refractivity, Kerr, and hyperpolarizability second virial coefficients. Journal of Chemical Physics, 1999, 111, 10108-10118.	1.2	48
10	Rovibrational structure of the Arâ€“CO complex based on a novel three-dimensional ab initio potential. Journal of Chemical Physics, 2002, 117, 6562-6572.	1.2	47
11	Spin polarization in restricted electronic structure theory: Multiconfiguration selfâ€consistentâ€field calculations of hyperfine coupling constants. Journal of Chemical Physics, 1992, 97, 3412-3419.	1.2	46
12	Ab initiocalculation of the frequency-dependent interaction induced hyperpolarizability of Ar2. Journal of Chemical Physics, 1999, 110, 2872-2882.	1.2	46
13	Benzene-argon S1 intermolecular potential energy surface. Journal of Chemical Physics, 1999, 111, 5922-5928.	1.2	44
14	Predicting the Helical Sense of Poly(phenylacetylene)s from their Electron Circular Dichroism Spectra. Angewandte Chemie - International Edition, 2018, 57, 3666-3670.	7.2	44
15	Ab Initio Ground- and Excited-State Intermolecular Potential Energy Surfaces for the NOâ€“Ne and NOâ€“Ar van der Waals Complexes. Journal of Physical Chemistry A, 2012, 116, 7319-7328.	1.1	40
16	Influence of Multiple Conformations and Paths on Rate Constants and Product Branching Ratios. Thermal Decomposition of 1-Propanol Radicals. Journal of Physical Chemistry A, 2018, 122, 4790-4800.	1.1	37
17	Accurate intermolecular ground state potential of the Arâ€“N2 complex. Journal of Chemical Physics, 1999, 110, 8525-8532.	1.2	35
18	Interaction-induced electric properties and cooperative effects in model systems. Physical Chemistry Chemical Physics, 2010, 12, 852-862.	1.3	34

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19	Decoding the ECD Spectra of Poly(phenylacetylene)s: Structural Significance. ACS Omega, 2019, 4, 5233-5240.	1.6	32
20	Accurate ab initio rovibronic spectrum of the Xâ€‰1Î£g+ and Bâ€‰1Î£u+ states in Ar2. Journal of Chemical Physics, 1998, 109, 10255-10262.	1.2	31
21	Importance of electron correlation effects and basis set superposition error in calculations of interaction energies and interaction-induced electric properties in hydrogen-bonded complexes: a model study. Theoretical Chemistry Accounts, 2011, 128, 555-561.	0.5	31
22	Synthesis, antimicrobial evaluation and theoretical prediction of NMR chemical shifts of thiazole and selenazole derivatives with high antifungal activity against Candida spp.. Journal of Molecular Structure, 2016, 1108, 427-437.	1.8	31
23	The Competitive Aggregation Pathway of an Asymmetric Chiral Oligo(pâ€phenyleneethynylene) Towards the Formation of Individual P and M Supramolecular Helical Polymers. Angewandte Chemie - International Edition, 2021, 60, 9919-9924.	7.2	31
24	Ab initio calculation of the refractivity and hyperpolarizability second virial coefficients of neon gas. Molecular Physics, 2003, 101, 1983-1995.	0.8	30
25	Computational and experimental investigation of intermolecular states and forces in the benzeneâ€“helium van der Waals complex. Journal of Chemical Physics, 2003, 119, 12956-12964.	1.2	30
26	Accurate intermolecular ground-state potential-energy surfaces of the HCCHâ€“He, Ne, and Ar van der Waals complexes. Journal of Chemical Physics, 2005, 123, 014309.	1.2	28
27	Chiral information harvesting in helical poly(acetylene) derivatives using oligo(p-phenyleneethynylene)s as spacers. Chemical Science, 2020, 11, 7182-7187.	3.7	28
28	Molecular mechanics (MM2) and conformational analysis of compounds with Nï£¿Cï£¿O units. Parametrization of the force field and anomeric effect. Journal of Computational Chemistry, 1991, 12, 78-90.	1.5	25
29	Merging Supramolecular and Covalent Helical Polymers: Four Helices Within a Single Scaffold. Journal of the American Chemical Society, 2021, 143, 20962-20969.	6.6	25
30	Dissociation of a Strong Acid in Neat Solvents: Diffusion Is Observed after Reversible Proton Ejection Inside the Solvent Shell. Journal of Physical Chemistry B, 2013, 117, 14065-14078.	1.2	24
31	Comment on â€œThe importance of high-order correlation effects for the COâ€“CO interaction potentialâ€• [Chem. Phys. Lett. 314 (1999) 326]. Chemical Physics Letters, 2001, 334, 419-423.	1.2	23
32	Fluorobenzeneâ€“argon ground-state intermolecular potential energy surface. Journal of Chemical Physics, 2004, 120, 8582-8586.	1.2	23
33	Calculation of hyperfine coupling constants of the CN and CP ground state radicals. Journal of Chemical Physics, 1993, 98, 7012-7019.	1.2	22
34	The water-nitric oxide intermolecular potential-energy surface revisited. Journal of Chemical Physics, 2009, 130, 104303.	1.2	22
35	The Benzeneâ‹¯Argon Ground-State Intermolecular Potential Energy Surface Revisited. Journal of Physical Chemistry A, 2009, 113, 5212-5216.	1.1	22
36	Polymeric Helical Structures Ã la Carte by Rational Design of Monomers. Macromolecules, 2020, 53, 3182-3193.	2.2	22

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37	Synthesis and In Vitro Antiproliferative Activity of Thiazole-Based Nitrogen Mustards: The Hydrogen Bonding Interaction between Model Systems and Nucleobases. Anti-Cancer Agents in Medicinal Chemistry, 2014, 14, 1271-1281.	0.9	22
38	MCSCF polarizability and hyperpolarizabilities of HCl and HBr. Chemical Physics Letters, 1998, 288, 677-688.	1.2	21
39	Argon broadening of the 13CO R(0) and R(7) transitions in the fundamental band at temperatures between 80 and 297K: comparison between experiment and theory. Journal of Molecular Spectroscopy, 2003, 222, 131-141.	0.4	21
40	The chlorobenzene-argon ground state intermolecular potential energy surface. Journal of Chemical Physics, 2004, 121, 1390-1396.	1.2	21
41	New basis sets for the evaluation of interaction energies: an ab initio study of the Heâ€“He, Neâ€“Ne, Arâ€“Ar, Heâ€“Ne, Heâ€“Ar and Neâ€“Ar van der Waals complex internuclear potentials and ro-vibrational spectra. Physical Chemistry Chemical Physics, 2010, 12, 13586.	1.3	21
42	Benzeneâ€“argon triplet intermolecular potential energy surface. Journal of Chemical Physics, 2003, 119, 4762-4767.	1.2	19
43	The COâ€“Ne van der Waals complex: ab initio intermolecular potential energy, interaction induced electric dipole moment and polarizability surfaces, and second virial coefficients. Physical Chemistry Chemical Physics, 2009, 11, 9871.	1.3	19
44	Dissymmetric Chiral Poly(diphenylacetylene)s: Secondary Structure Elucidation and Dynamic Luminescence. Angewandte Chemie - International Edition, 2022, , .	7.2	18
45	Calculation of hyperfine coupling constants of the ground state Xâ€‰3Î£â¯ of NH and B2. Journal of Chemical Physics, 1993, 99, 5995-6003.	1.2	17
46	Comment on â€œGround-state geometry of small Ni-C clustersâ€• Physical Review B, 2003, 68, .	1.1	17
47	Conformation and charge distribution of bicyclic Î²-lactams: Structure-activity relationships. Biopolymers, 1992, 32, 97-106.	1.2	16
48	Hyperfine and nuclear quadrupole coupling in chlorine and fluorine dioxides. Journal of Chemical Physics, 1997, 106, 1847-1855.	1.2	16
49	Study of the benzeneâ‹…N2 intermolecular potential-energy surface. Journal of Chemical Physics, 2003, 118, 1230-1241.	1.2	16
50	Predicting the Helical Sense of Poly(phenylacetylene)s from their Electron Circular Dichroism Spectra. Angewandte Chemie, 2018, 130, 3728-3732.	1.6	16
51	Theory of hyperfine coupling constants of solvated molecules: Applications involving methyl and ClO2 radicals in different solvents. Journal of Chemical Physics, 1996, 104, 629-635.	1.2	15
52	A coupled cluster response study of the electric dipole polarizability, first and second hyperpolarizabilities of HCl. Physical Chemistry Chemical Physics, 2002, 4, 2884-2890.	1.3	15
53	Accurate intermolecular ground state potential of the Ar-N2 van der Waals complex. Journal of Chemical Physics, 2004, 121, 10419-10425.	1.2	15
54	Accurate intermolecular ground state potential of the Ne-HCl van der Waals complex. Journal of Chemical Physics, 2004, 121, 4599-4604.	1.2	14

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55	Accurate intermolecular ground state potential of the Neâ€“N2 van der Waals complex. Journal of Chemical Physics, 2004, 120, 9104-9112.	1.2	14
56	Coupled cluster calculations of interaction energies in benzeneâ€“fluorobenzene van der Waals complexes. Chemical Physics Letters, 2007, 441, 332-335.	1.2	14
57	Refined ab initio intermolecular ground-state potential energy surface for the Heâ€“C₂H₂ van der Waals complex. Molecular Physics, 2013, 111, 1173-1177.	0.8	14
58	Ab initio study of the COâ€“N2 complex: a new highly accurate intermolecular potential energy surface and rovibrational spectrum. Physical Chemistry Chemical Physics, 2018, 20, 12624-12636.	1.3	14
59	Conformational analysis of bicyclic systems including the Nî—¸Cî—¸O unit by molecular mechanics. Journal of Molecular Structure, 1991, 245, 53-67.	1.8	13
60	Ab initio potential-energy surface and rovibrational states of the HCNâ€“HCl complex. Journal of Chemical Physics, 2006, 124, 204315.	1.2	13
61	New basis sets for the evaluation of interactionâ€induced electric properties in hydrogenâ€bonded complexes. Journal of Computational Chemistry, 2013, 34, 275-283.	1.5	13
62	p-Difluorobenzeneâ^'Argon Ground State Intermolecular Potential Energy Surfaceâ€. Journal of Physical Chemistry A, 2005, 109, 11602-11608.	1.1	12
63	Density dependence of electric properties of binary mixtures of inert gases. Molecular Physics, 2006, 104, 305-318.	0.8	12
64	Rotational Structure of Small ⁴He Clusters Seeded with HF, HCl, and HBr Molecules. Journal of Physical Chemistry A, 2007, 111, 12275-12288.	1.1	12
65	Towards an understanding of the heliumâ€“acetylene van der Waals complex. Molecular Physics, 2012, 110, 2743-2750.	0.8	12
66	Dissecting the concaveâ€“convex Ï€â€Ï€ interaction in corannulene and sumanene dimers: SAPT(DFT) analysis and performance of DFT dispersionâ€corrected methods. Journal of Computational Chemistry, 2018, 39, 93-104.	1.5	12
67	The CCSD(T) model with Cholesky decomposition of orbital energy denominators. International Journal of Quantum Chemistry, 2011, 111, 349-355.	1.0	11
68	Fluorescence quenching of the N-methylquinolinium cation by pairs of water or alcohol molecules. Physical Chemistry Chemical Physics, 2018, 20, 307-316.	1.3	11
69	Interpretation of the hyperfine coupling constants of the boron trimer in rareâ€gas matrices. Journal of Chemical Physics, 1993, 98, 3060-3065.	1.2	10
70	Accurate computations of the rovibrational spectrum of the Heâ€“HF van der Waals complex. Molecular Physics, 2006, 104, 1413-1420.	0.8	10
71	Ab initio studies of molecules with N-C-O units. Computational and Theoretical Chemistry, 1990, 205, 235-244.	1.5	9
72	Theoretical absorption spectrum of the Arâ€“CO van der Waals complex. Journal of Chemical Physics, 2003, 118, 9596-9607.	1.2	9

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73	The Fluorobenzeneâ^'Argon S₁ Excited-State Intermolecular Potential Energy Surface. Journal of Physical Chemistry A, 2007, 111, 7876-7881.	1.1	9
74	New bases for the evaluation of interaction energies: An ab initio study of the COâ€"Ne van der Waals complex intermolecular potential and ro-vibrational spectrum. Chemical Physics, 2011, 386, 88-94.	0.9	9
75	Ab initio ground state phenylacetyleneâ€"argon intermolecular potential energy surface and rovibrational spectrum. Journal of Chemical Physics, 2012, 137, 074305.	1.2	9
76	New basis sets for the evaluation of the COâ€"Ne van der Waals complex interaction induced electric dipole moment and polarizability surfaces. Molecular Physics, 2012, 110, 2503-2512.	0.8	9
77	New basis set for the prediction of the specific rotation in flexible biological molecules. RSC Advances, 2016, 6, 19897-19902.	1.7	9
78	Ab initio gradient conformational analysis of polyazocyclohexanes:1,4-diazocyclohexane, 1,3-diazocyclohexane and 1,3,5-triazocyclohexane. Computational and Theoretical Chemistry, 1990, 205, 223-234.	1.5	8
79	Conformational analysis of bicyclic systems including the Nî—¸Cî—¸O unit by molecular mechanics. Journal of Molecular Structure, 1991, 263, 157-166.	1.8	7
80	Theoretical study of some nitriles: Intramolecular hydrogen bonds and anomeric effect. Journal of Computational Chemistry, 1992, 13, 722-729.	1.5	7
81	Evaluation of hyperfine coupling tensors of the BeH and BeF radicals. Chemical Physics Letters, 1995, 232, 463-471.	1.2	7
82	Thep-Difluorobenzeneâ^'Argon S1Excited State Intermolecular Potential Energy Surface. Journal of Physical Chemistry A, 2006, 110, 13259-13263.	1.1	7
83	Accurate calculation of the intensity dependence of the refractive index using polarized basis sets. Journal of Chemical Physics, 2012, 136, 024302.	1.2	7
84	Small and Efficient Basis Sets for the Evaluation of Accurate Interaction Energies: Aromatic Moleculeâ€"Argon Ground-State Intermolecular Potentials and Rovibrational States. Journal of Physical Chemistry A, 2014, 118, 10288-10297.	1.1	7
85	Conformational analysis of bicyclic systems including the Nî—¸Cî—¸O unit by molecular mechanics Part II. 4,5- and 5,6- Tetramethylene perhydro-1,3-oxazines. Journal of Molecular Structure, 1991, 246, 301-319.	1.8	6
86	An ab initio 4-21G gradient study of clavulanic acid. Structural Chemistry, 1992, 3, 321-327.	1.0	6
87	Accurate intermolecular ground state potential of the Heâ€"HCl van der Waals complex. Chemical Physics Letters, 2006, 419, 55-58.	1.2	6
88	Theoretical pressure and dielectric second virial coefficients of CO-Ar. Molecular Physics, 2008, 106, 881-892.	0.8	6
89	A high-accuracy theoretical study of the CH_nP Systemsnâ€‰=â€‰1-3. Journal of Computational Chemistry, 2013, 34, 2020-2031.	1.5	6
90	The Role of Substituents in Optical Rotation of Oxiranes, Oxetanes, and Oxathietanes. Journal of Chemical Information and Modeling, 2019, 59, 2103-2109.	2.5	6

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91	Firefly luciferin precursor 2-cyano-6-hydroxybenzothiazole: Fluorescence Ã la carte controlled by solvent and acidity. Dyes and Pigments, 2020, 177, 108285.	2.0	6
92	New Approach for Correcting Noncovalent Interactions in Semiempirical Quantum Mechanical Methods: The Importance of Multiple-Orientation Sampling. Journal of Chemical Theory and Computation, 2021, 17, 5556-5567.	2.3	6
93	Evaluation of the BeOH and MgOH hyperfine coupling tensors. Chemical Physics Letters, 1996, 259, 635-640.	1.2	5
94	The infrared spectrum of the Heâ€“C2D2 complex. Journal of Chemical Physics, 2015, 142, 084312.	1.2	5
95	New Basis Set for the Evaluation of Specific Rotation in Flexible Biological Molecules in Solution. Journal of Physical Chemistry A, 2018, 122, 5477-5483.	1.1	5
96	Dissymmetric Chiral Poly(diphenylacetylene)s: Secondary Structure Elucidation and Dynamic Luminescence. Angewandte Chemie, 2022, 134, .	1.6	5
97	An ab initio study of proton transfer in triose reductone. Computational and Theoretical Chemistry, 1991, 226, 181-196.	1.5	4
98	Structure-activity relationships in verapamil and analogues using molecular mechanics calculations. International Journal of Pharmaceutics, 1992, 79, 199-203.	2.6	4
99	Conformational analysis of tricyclic systems including the Nî—¸Cî—¸O unit by molecular mechanics IV. Perhydrocycloalkane [e] pyrido[1,2-c]-1,3-oxazines. Journal of Molecular Structure, 1992, 274, 259-275.	1.8	4
100	Parametrization of a force field for studying some beta-lactams. Journal of Computational Chemistry, 1994, 15, 455-465.	1.5	4
101	Small and efficient basis sets for the evaluation of accurate interaction-induced linear and non-linear electric properties in model hydrogen-bonded complexes. Molecular Physics, 2015, 113, 3362-3369.	0.8	4
102	Theoretical calculation of NMR shifts in newly developed antibacterial 4-formylbenzoic acid-based thiazoles. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	4
103	The infrared spectrum of the Neâ€“C2D2 complex. Journal of Chemical Physics, 2015, 143, 204307.	1.2	2
104	Theoretical Study of the Pyridineâ€“Helium van der Waals Complexes. Journal of Physical Chemistry A, 2015, 119, 10999-11006.	1.1	2
105	Accurate calculation of optically induced birefringences in chiral systems using efficient polarized basis sets. Physical Chemistry Chemical Physics, 2018, 20, 29717-29723.	1.3	2
106	From Oligo(Phenyleneethynylene) Monomers to Supramolecular Helices: The Role of Intermolecular Interactions in Aggregation. Molecules, 2021, 26, 3530.	1.7	2
107	The PM6-FGC Method: Improved Corrections for Amines and Amides. Molecules, 2022, 27, 1678.	1.7	2
108	Study of the geometric trends and rotational constants of 1-fluoro-2-propanol and 2-fluoropropanol by Ab Initio calculations. Tetrahedron Computer Methodology, 1989, 2, 85-92.	0.2	1

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109	An ab initio conformational analysis of isobutylamine and diisopropylamine. Computational and Theoretical Chemistry, 1991, 251, 319-326.	1.5	1
110	A theoretical study of 1-amino-3-butene and 3-butene-1-thiol. Structural Chemistry, 1992, 3, 225-229.	1.0	1
111	Heâ€“, Neâ€“, and Arâ€“Phosgene Intermolecular Potential Energy Surfaces. Journal of Physical Chemistry A, 2013, 117, 3835-3843.	1.1	1
112	Basis sets for the evaluation of van der Waals complex interaction energies: Ne-N2 intermolecular potential and microwave spectrum. Journal of Computational Chemistry, 2014, 35, 199-203.	1.5	1
113	Applicability of medium-size basis sets in calculations of molecular dynamic polarisabilities. Molecular Physics, 2015, 113, 1786-1793.	0.8	1
114	Theoretical evaluation of NMR shifts in polycyclic aromatic hydrocarbons. Molecular Physics, 2017, 115, 2201-2208.	0.8	1
115	Systematic Analysis of the Role of Substituents in Oxiranes, Oxetanes, and Oxathietanes Chemical Shifts. Journal of Physical Chemistry A, 2021, 125, 2077-2087.	1.1	1
116	A Semi-empirical Study of some Clavulanic Acid Derivatives in Relation to their Activity as Î²-Lactamase Inhibitors. Journal of Pharmacy and Pharmacology, 2011, 45, 25-29.	1.2	0