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	Dissymmetric Chiral Poly(diphenylacetylene)s: Secondary Structure Elucidation and Dynamic Luminescence. Angewandte Chemie - International Edition, 2022, , .	7.2	18
2	Dissymmetric Chiral Poly(diphenylacetylene)s: Secondary Structure Elucidation and Dynamic Luminescence. Angewandte Chemie, 2022, 134, .	1.6	5
3	The PM6-FGC Method: Improved Corrections for Amines and Amides. Molecules, 2022, 27, 1678.	1.7	2
4	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
5	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
6	From Oligo(Phenyleneethynylene) Monomers to Supramolecular Helices: The Role of Intermolecular Interactions in Aggregation. Molecules, 2021, 26, 3530.	1.7	2
7	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
8	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
9	Chiral information harvesting in helical poly(acetylene) derivatives using oligo(p-phenyleneethynylene)s as spacers. Chemical Science, 2020, 11, 7182-7187.	3.7	28
10	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
11	Polymeric Helical Structures Ã la Carte by Rational Design of Monomers. Macromolecules, 2020, 53, 3182-3193.	2.2	22
12	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
13	Decoding the ECD Spectra of Poly(phenylacetylene)s: Structural Significance. ACS Omega, 2019, 4, 5233-5240.	1.6	32
14	Theoretical calculation of NMR shifts in newly developed antibacterial 4-formylbenzoic acid-based thiazoles. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	4
15	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
16	Predicting the Helical Sense of Poly(phenylacetylene)s from their Electron Circular Dichroism Spectra. Angewandte Chemie, 2018, 130, 3728-3732.	1.6	16
17	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
18	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

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19	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
20	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
21	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
22	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
23	Theoretical evaluation of NMR shifts in polycyclic aromatic hydrocarbons. Molecular Physics, 2017, 115, 2201-2208.	0.8	1
24	New basis set for the prediction of the specific rotation in flexible biological molecules. RSC Advances, 2016, 6, 19897-19902.	1.7	9
25	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
26	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
27	The infrared spectrum of the Neâ€“C2D2 complex. Journal of Chemical Physics, 2015, 143, 204307.	1.2	2
28	Theoretical Study of the Pyridineâ€“Helium van der Waals Complexes. Journal of Physical Chemistry A, 2015, 119, 10999-11006.	1.1	2
29	Applicability of medium-size basis sets in calculations of molecular dynamic polarisabilities. Molecular Physics, 2015, 113, 1786-1793.	0.8	1
30	The infrared spectrum of the Heâ€“C2D2 complex. Journal of Chemical Physics, 2015, 142, 084312.	1.2	5
31	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
32	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
33	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
34	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
35	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
36	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

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37	Heâ€“, Neâ€“, and Arâ€“Phosgene Intermolecular Potential Energy Surfaces. Journal of Physical Chemistry A, 2013, 117, 3835-3843.	1.1	1
38	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
39	A high-accuracy theoretical study of the CH_nP Systemsnâ€‰=â€‰1-3. Journal of Computational Chemistry, 2013, 34, 2020-2031.	1.5	6
40	Accurate calculation of the intensity dependence of the refractive index using polarized basis sets. Journal of Chemical Physics, 2012, 136, 024302.	1.2	7
41	Ab initio ground state phenylacetyleneâ€“argon intermolecular potential energy surface and rovibrational spectrum. Journal of Chemical Physics, 2012, 137, 074305.	1.2	9
42	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
43	Towards an understanding of the heliumâ€“acetylene van der Waals complex. Molecular Physics, 2012, 110, 2743-2750.	0.8	12
44	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
45	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
46	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
47	The CCSD(T) model with Cholesky decomposition of orbital energy denominators. International Journal of Quantum Chemistry, 2011, 111, 349-355.	1.0	11
48	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
49	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
50	Interaction-induced electric properties and cooperative effects in model systems. Physical Chemistry Chemical Physics, 2010, 12, 852-862.	1.3	34
51	The water-nitric oxide intermolecular potential-energy surface revisited. Journal of Chemical Physics, 2009, 130, 104303.	1.2	22
52	The Benzeneâ‹¯Argon Ground-State Intermolecular Potential Energy Surface Revisited. Journal of Physical Chemistry A, 2009, 113, 5212-5216.	1.1	22
53	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
54	Theoretical pressure and dielectric second virial coefficients of CO-Ar. Molecular Physics, 2008, 106, 881-892.	0.8	6

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55	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
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	The Fluorobenzeneâ¯Argon S₁ Excited-State Intermolecular Potential Energy Surface. Journal of Physical Chemistry A, 2007, 111, 7876-7881.	1.1	9
58	Thep-Difluorobenzeneâ¯Argon S1Excited State Intermolecular Potential Energy Surface. Journal of Physical Chemistry A, 2006, 110, 13259-13263.	1.1	7
59	Ab initio potential-energy surface and rovibrational states of the HCNâ€“HCl complex. Journal of Chemical Physics, 2006, 124, 204315.	1.2	13
60	Density dependence of electric properties of binary mixtures of inert gases. Molecular Physics, 2006, 104, 305-318.	0.8	12
61	Accurate intermolecular ground state potential of the Heâ€“HCl van der Waals complex. Chemical Physics Letters, 2006, 419, 55-58.	1.2	6
62	Accurate computations of the rovibrational spectrum of the Heâ€“HF van der Waals complex. Molecular Physics, 2006, 104, 1413-1420.	0.8	10
63	p-Difluorobenzeneâ¯Argon Ground State Intermolecular Potential Energy Surfaceâ€. Journal of Physical Chemistry A, 2005, 109, 11602-11608.	1.1	12
64	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
65	Accurate intermolecular ground state potential of the Ne-HCl van der Waals complex. Journal of Chemical Physics, 2004, 121, 4599-4604.	1.2	14
66	Fluorobenzeneâ€“argon ground-state intermolecular potential energy surface. Journal of Chemical Physics, 2004, 120, 8582-8586.	1.2	23
67	The chlorobenzene-argon ground state intermolecular potential energy surface. Journal of Chemical Physics, 2004, 121, 1390-1396.	1.2	21
68	Accurate intermolecular ground state potential of the Neâ€“N2 van der Waals complex. Journal of Chemical Physics, 2004, 120, 9104-9112.	1.2	14
69	Accurate intermolecular ground state potential of the Ar-N2 van der Waals complex. Journal of Chemical Physics, 2004, 121, 10419-10425.	1.2	15
70	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
71	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
72	Ab initio calculation of the refractivity and hyperpolarizability second virial coefficients of neon gas. Molecular Physics, 2003, 101, 1983-1995.	0.8	30

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73	Study of the benzeneâ‹…N2 intermolecular potential-energy surface. Journal of Chemical Physics, 2003, 118, 1230-1241.	1.2	16
74	Benzeneâ€“argon triplet intermolecular potential energy surface. Journal of Chemical Physics, 2003, 119, 4762-4767.	1.2	19
75	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
76	Theoretical absorption spectrum of the Arâ€“CO van der Waals complex. Journal of Chemical Physics, 2003, 118, 9596-9607.	1.2	9
77	Comment on â€œGround-state geometry of small Ni-C clustersâ€• Physical Review B, 2003, 68, .	1.1	17
78	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
79	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
80	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
81	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
82	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
83	Gauge invariant coupled cluster response theory using optimized nonorthogonal orbitals. Journal of Chemical Physics, 2001, 114, 6983-6993.	1.2	82
84	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
85	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
86	Ab initiocalculation of the frequency-dependent interaction induced hyperpolarizability of Ar2. Journal of Chemical Physics, 1999, 110, 2872-2882.	1.2	46
87	Accurate intermolecular ground state potential of the Arâ€“N2 complex. Journal of Chemical Physics, 1999, 110, 8525-8532.	1.2	35
88	Ground state benzeneâ€“argon intermolecular potential energy surface. Journal of Chemical Physics, 1999, 111, 198-204.	1.2	86
89	Benzene-argon S1 intermolecular potential energy surface. Journal of Chemical Physics, 1999, 111, 5922-5928.	1.2	44
90	MCSCF polarizability and hyperpolarizabilities of HCl and HBr. Chemical Physics Letters, 1998, 288, 677-688.	1.2	21

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91	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
92	The benzeneâ€“argon complex: A ground and excited state ab initio study. Journal of Chemical Physics, 1998, 108, 2784-2790.	1.2	144
93	Hyperfine and nuclear quadrupole coupling in chlorine and fluorine dioxides. Journal of Chemical Physics, 1997, 106, 1847-1855.	1.2	16
94	Evaluation of the BeOH and MgOH hyperfine coupling tensors. Chemical Physics Letters, 1996, 259, 635-640.	1.2	5
95	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
96	Evaluation of hyperfine coupling tensors of the BeH and BeF radicals. Chemical Physics Letters, 1995, 232, 463-471.	1.2	7
97	Parametrization of a force field for studying some beta-lactams. Journal of Computational Chemistry, 1994, 15, 455-465.	1.5	4
98	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
99	Calculation of hyperfine coupling constants of the CN and CP ground state radicals. Journal of Chemical Physics, 1993, 98, 7012-7019.	1.2	22
100	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
101	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
102	A theoretical study of 1-amino-3-butene and 3-butene-1-thiol. Structural Chemistry, 1992, 3, 225-229.	1.0	1
103	An ab initio 4-21G gradient study of clavulanic acid. Structural Chemistry, 1992, 3, 321-327.	1.0	6
104	Structure-activity relationships in verapamil and analogues using molecular mechanics calculations. International Journal of Pharmaceutics, 1992, 79, 199-203.	2.6	4
105	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
106	Conformation and charge distribution of bicyclic Î²-lactams: Structure-activity relationships. Biopolymers, 1992, 32, 97-106.	1.2	16
107	Theoretical study of some nitriles: Intramolecular hydrogen bonds and anomeric effect. Journal of Computational Chemistry, 1992, 13, 722-729.	1.5	7
108	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

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109	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
110	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
111	An ab initio study of proton transfer in triose reductone. Computational and Theoretical Chemistry, 1991, 226, 181-196.	1.5	4
112	An ab initio conformational analysis of isobutylamine and diisopropylamine. Computational and Theoretical Chemistry, 1991, 251, 319-326.	1.5	1
113	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
114	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
115	Ab initio studies of molecules with N-C-O units. Computational and Theoretical Chemistry, 1990, 205, 235-244.	1.5	9
116	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