

Francisco Partal Ureña

List of Publications by Year in descending order

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949
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#	ARTICLE	IF	CITATIONS
1	Electronic structure of kaempferol-Cu ²⁺ coordination compounds: a DFT, QAIM and NBO study in the gas phase. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	1.4	5
2	Hydrogen bonding network in a chiral alcohol: (1R,2S,5R)- α -menthol. Conformational preference studied by IR-Raman-VCD spectroscopies and quantum chemical calculations. <i>Structural Chemistry</i> , 2013, 24, 671-680.	2.0	11
3	L-Serine in aqueous solutions at different pH: Conformational preferences and vibrational spectra of cationic, anionic and zwitterionic species. <i>Journal of Molecular Structure</i> , 2013, 1046, 136-146.	3.6	23
4	Study of the Photoinduced Supramolecular Chirality in Columnar Liquid Crystals by Infrared and VCD Spectroscopies. <i>Journal of Physical Chemistry B</i> , 2012, 116, 5090-5096.	2.6	18
5	Conformational landscape and hydrogen bonding in (S)- α -perillyl acid: experimental VCD, IR, Raman, and theoretical DFT studies. <i>Tetrahedron: Asymmetry</i> , 2012, 23, 780-788.	1.8	10
6	Conformational preference of short aromatic amino acids from the FT-IR, FT-Raman and Far-IR spectroscopies, and quantum chemical calculations: L-phenylalanine and L-tyrosine. <i>Tetrahedron: Asymmetry</i> , 2012, 23, 1084-1092.	1.8	23
7	The chiral structure of 1H-indazoles in the solid state: a crystallographic, vibrational circular dichroism and computational study. <i>New Journal of Chemistry</i> , 2012, 36, 749.	2.8	32
8	Terpenes in the gas phase: The Far-IR spectrum of perillaldehyde. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2012, 113, 1261-1265.	2.3	14
9	Conformational landscape of a chiral crown ether: a vibrational circular dichroism spectroscopy and computational study. <i>Tetrahedron: Asymmetry</i> , 2012, 23, 294-299.	1.8	11
10	Characterization of H-bonding networks in chiral alcohols using Infrared, Raman and Vibrational Circular Dichroism spectroscopies, and density functional calculations: (S)- α -perillyl alcohol. <i>Tetrahedron: Asymmetry</i> , 2012, 23, 515-525.	1.8	6
11	Chiral terpenes in different phases: R- α -camphorquinone studied by IR-Raman-VCD spectroscopies and theoretical calculations. <i>Structural Chemistry</i> , 2011, 22, 67-76.	2.0	12
12	IR-Raman-VCD study of R-(+)-Pulegone: Influence of the solvent. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 767-776.	3.9	24
13	Rotational strength sign and normal modes description: A theoretical and experimental comparative study in bicyclic terpenes. <i>Chirality</i> , 2010, 22, E123-9.	2.6	6
14	Conformational study of (R)-(+)-limonene in the liquid phase using vibrational spectroscopy (IR, Tj ETQq0 0 0 rgBT /Qverlock 10 Tf 50 2	1.8	47
15	Conformational landscape in chiral terpenes from vibrational spectroscopy and quantum chemical calculations: S-(+)-carvone. <i>Vibrational Spectroscopy</i> , 2009, 51, 318-325.	2.2	31
16	Terpenes in the gas phase: The structural conformation of S- α -perillaldehyde investigated by microwave spectroscopy and quantum chemical calculations. <i>Chemical Physics Letters</i> , 2009, 473, 17-20.	2.6	21
17	Conformational preference of a chiral terpene: vibrational circular dichroism (VCD), infrared and Raman study of S- α -limonene oxide. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 2459.	2.8	21
18	Raman and IR spectra of the unstable ionic species potassium trimethylsilylanolate: The role of the counterion in its theoretical interpretation. <i>Journal of Raman Spectroscopy</i> , 2008, 39, 460-467.	2.5	4

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19	Triethylsilanol: Molecular Conformations and Role of the Hydrogen-Bonding Oligomerization in Its Vibrational Spectra. <i>Journal of Physical Chemistry A</i> , 2008, 112, 1545-1551.	2.5	6
20	Conformational Flexibility in Terpenes: Vibrational Circular Dichroism (VCD), Infrared and Raman Study of <i>S</i> -Perillaldehyde. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7887-7893.	2.5	38
21	Conformations, Structures, and Vibrational Spectra of Triethylchloro- and Triethylbromosilane Using Theoretical Methods, Gas Phase Electron Diffraction, and IR and Raman Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2870-2878.	2.5	5
22	Validation of the Existence of Tetrameric Species of Potassium Trimethylsilanolate in the Gas Phase with a Theoretical Cluster Model: A Role of the Counterion as Charge Localizer in the Structure. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2629-2633.	2.5	2
23	Photoinduced Chiral Nematic Organization in an Achiral Glassy Nematic Azopolymer. <i>Advanced Functional Materials</i> , 2007, 17, 3486-3492.	14.9	82
24	Structure and vibrational spectra of vinyl ether conformers. The comparison of B3LYP and MP2 predictions. <i>Chemical Physics</i> , 2007, 333, 148-156.	1.9	11
25	An experimental and theoretical study of the molecular structure and vibrational spectra of iodotrimethylsilane (SiI ₃ Me ₃). <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 477-485.	2.8	9
26	Vibrational spectra and structure of methoxysilanes and products of their hydrolysis. <i>Vibrational Spectroscopy</i> , 2006, 40, 1-9.	2.2	19
27	Vibrational spectrum of chlorotrimethylsilane. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2005, 62, 293-301.	3.9	12
28	The vibrational spectra of (CH ₃) ₃ SiX (S=H, F, Br) molecules, revisited. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2005, 62, 1058-1069.	3.9	11
29	Vibrational spectrum of methoxytrimethylsilane. <i>Journal of Molecular Structure</i> , 2005, 744-747, 331-338.	3.6	13
30	Structure and vibrational spectra of dimethylsilanediol and methylsilanetriol dimers. <i>Chemical Physics Letters</i> , 2005, 412, 359-364.	2.6	6
31	Anharmonic spectra of methanol and silanol: A comparative study. <i>Journal of Molecular Spectroscopy</i> , 2005, 233, 203-209.	1.2	6
32	Intramolecular hydrogen bonding in silanediols. <i>Computational and Theoretical Chemistry</i> , 2004, 678, 249-256.	1.5	16
33	Vibrational spectra of trimethylsilanol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2004, 60, 1169-1178.	3.9	26
34	Hydrogen bonding and structure of silanediol dimers and tetramers. <i>Chemical Physics Letters</i> , 2004, 384, 326-331.	2.6	16
35	Condensation reactions in silanol-water clusters. <i>Chemical Physics Letters</i> , 2003, 368, 616-624.	2.6	13
36	A new insight into the vibrational analysis of pyridine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2003, 59, 2815-2839.	3.9	121

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37	Effect of the Silyl Substitution on Structure and Vibrational Spectra of Hydrogen-Bonded Networks in Dimers, Cyclic Trimers, and Tetramers. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11644-11652.	2.5	21
38	Vibrational analysis of the inelastic neutron scattering spectrum of pyridine. <i>Chemical Physics</i> , 2000, 261, 239-247.	1.9	13
39	Astrophysical Molecules AlD and CaH: Transition Probabilities and Dissociation Energy. <i>Astrophysics and Space Science</i> , 2000, 272, 345-352.	1.4	21