# Halima Mouhib

List of Publications by Year
in descending order



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|---|---|---|---|
| 38 papers | 584 citations | 567281 15 h-index | 642732 23 g-index |
| 38 all docs | 38 docs citations | 38 times ranked | 568 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | The furan microsolvation blind challenge for quantum chemical methods: First steps. Journal of Chemical Physics, 2018, 148, 014301. | 3.0 | 44 |
| 2 | The microwave spectrum of allyl acetate. Molecular Physics, 2010, 108, 763-770. | 1.7 | 37 |
| 3 | Cassis Odor through Microwave Eyes: Olfactory Properties and Gas-Phase Structures of all the Cassyrane Stereoisomers and its Dihydro Derivatives. Angewandte Chemie - International Edition, 2011, 50, 5576-5580. | 13.8 | 35 |
| 4 | Methyl Internal Rotation in the Microwave Spectrum of oâ€Methyl Anisole. ChemPhysChem, 2017, 18, 1855-1859. | 2.1 | 35 |
| 5 | Conformational ensemble of human Î±-synuclein physiological form predicted by molecular simulations. Physical Chemistry Chemical Physics, 2016, 18, 5702-5706. | 2.8 | 32 |
| 6 | A touch of lavender: gas-phase structure and dynamics of the monoterpene linalool validated by microwave spectroscopy. Physical Chemistry Chemical Physics, 2013, 15, 10012. | 2.8 | 29 |
| 7 | The hydrophobic effect characterises the thermodynamic signature of amyloid fibril growth. PLoS Computational Biology, 2020, 16, e1007767. | 3.2 | 29 |
| 8 | Efficient Macrocyclization by a Novel Oxyâ€Oxoniaâ€Cope Reaction: Synthesis and Olfactory Properties of New Macrocyclic Musks. Chemistry - A European Journal, 2012, 18, 7010-7015. | 3.3 | 28 |
| 9 | Conformational Analysis of Green Apple Flavour: The Gasâ€Phase Structure of Ethyl Valerate Validated by Microwave Spectroscopy. ChemPhysChem, 2012, 13, 1297-1301. | 2.1 | 28 |
| 10 | The first microsolvation step for furans: New experiments and benchmarking strategies. Journal of Chemical Physics, 2020, 152, 164303. | 3.0 | 28 |
| 11 | Structural Studies on Ethyl Isovalerate by Microwave Spectroscopy and Quantum Chemical Calculations. Journal of Physical Chemistry A, 2011, 115, 118-122. | 2.5 | 26 |
| 12 | The Conformation of Odorants in Different States of Aggregation: A Joint Venture in Microwave Spectroscopy and X-ray Diffraction. ChemPhysChem, 2011, 12, 761-764. | 2.1 | 21 |
| 13 | Mechanical Unfolding of an Autotransporter Passenger Protein Reveals the Secretion Starting Point and Processive Transport Intermediates. ACS Nano, 2016, 10, 5710-5719. | 14.6 | 21 |
| 14 | Competing Dispersive Interactions: From Small Energy Differences to Large Structural Effects in Methyl Jasmonate and Zingerone. Journal of Physical Chemistry Letters, 2018, 9, 5906-5914. | 4.6 | 18 |
| 15 | Two conformers of ethyl pivalate studied by microwave spectroscopy. Journal of Molecular Spectroscopy, 2010, 261, 59-62. | 1.2 | 17 |
| 16 | Laboratory microwave, millimeter wave and far-infrared spectra of dimethyl sulfide. Astronomy and Astrophysics, 2016, 589, A127. | 5.1 | 17 |
| 17 | Molecular structure and ring tunneling of phenyl formate as observed by microwave spectroscopy and quantum chemistry. Journal of Molecular Spectroscopy, 2017, 337, 59-64. | 1.2 | 14 |
| 18 | Communication through the furan ring: the conformational effect on the internal rotation of 5-methyl furfural studied by microwave spectroscopy. Physical Chemistry Chemical Physics, 2018, 20, 25577-25582. | 2.8 | 14 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | The heavy atom structures and <sup>33</sup>S quadrupole coupling constants of 2-thiophenecarboxaldehyde: insights from microwave spectroscopy. Molecular Physics, 2020, 118, e1728406. | 1.7 | 12 |
| 20 | Sulfur-Containing Flavors: Gas Phase Structures of Dihydro-2-methyl-3-thiophenone. Journal of Physical Chemistry A, 2013, 117, 6652-6656. | 2.5 | 10 |
| 21 | The microwave spectrum of allyl acetone. Journal of Molecular Spectroscopy, 2015, 312, 46-50. | 1.2 | 10 |
| 22 | Understanding the structure and dynamic of odorants in the gas phase using a combination of microwave spectroscopy and quantum chemical calculations. Journal of Physics B: Atomic, Molecular and Optical Physics, 2014, 47, 143001. | 1.5 | 9 |
| 23 | Conformational analysis of tert-butyl acetate using a combination of microwave spectroscopy and quantum chemical calculations. Journal of Molecular Spectroscopy, 2016, 322, 38-42. | 1.2 | 9 |
| 24 | Favored Conformations of Carbonyl Compounds: A Structural Study ofnâ€Octanal. ChemPhysChem, 2017, 18, 2631-2636. | 2.1 | 9 |
| 25 | Challenging the Molecular Parameters of Vetiver: Can 4,5â€Dimethylâ€3â€(3â€²â€methylbutâ€1â€²â€enâ€2â€²â€yl)â€4â€phenylcyclopentâ€2â€enâ€1â€one Mimic Zizanenes in Structur European Journal of Organic Chemistry, 2019, 2019, 2643-2652. | 2.4 | 9 |
| 26 | Conformational Landscape of Diisopropyl Ketone: Quantum Chemical Calculations Validated by Microwave Spectroscopy. Journal of Physical Chemistry A, 2013, 117, 311-314. | 2.5 | 6 |
| 27 | From Cats and Blackcurrants: Structure and Dynamics of the Sulfurâ€Containing Cassis Odorant Cat Ketone. Chemistry and Biodiversity, 2014, 11, 1554-1566. | 2.1 | 6 |
| 28 | The Conformation of Pentanoates in the Solid and in the Gas Phase. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2014, 69, 303-312. | 1.5 | 6 |
| 29 | Quantum-Chemical Ab Initio Calculations on Ala-(C<sub>5</sub>H<sub>5</sub>Al) and Galabenzene (C<sub>5</sub>H<sub>5</sub>Ga). Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2014, 69, 349-359. | 1.5 | 5 |
| 30 | Conformational dimorphism ino-nitrobenzoic acid: alternative ways to avoid the O...O clash. Acta Crystallographica Section C, Structural Chemistry, 2016, 72, 566-571. | 0.5 | 5 |
| 31 | Charge density of the biologically active molecule (2-oxo-1,3-benzoxazol-3(2H)-yl)acetic acid. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 142-150. | 1.1 | 4 |
| 32 | Molecules in confinement in clusters, quantum solvents and matrices: general discussion. Faraday Discussions, 2018, 212, 569-601. | 3.2 | 4 |
| 33 | Large Amplitude Motions in Fruit Flavors: The Case of Alkyl Butyrates. ChemPhysChem, 2020, 21, 20-25. | 2.1 | 3 |
| 34 | Structural insight from intermolecular interactions and energy framework analyses of 2-substituted 6,7,8,9-tetrahydro-11H-pyrido[2,1-b]quinazolin-11-ones. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2021, 77, 416-426. | 1.1 | 2 |
| 35 | Quantifying soft degrees of freedom in volatile organic compounds: insight from quantum chemistry and focused single molecule experiments. Physical Chemistry Chemical Physics, 2020, 22, 27850-27860. | 2.8 | 2 |
| 36 | Highlights from the Faraday Discussion 296: quantum effects in small molecular systems, 10â€“12 September 2018, Edinburgh, United Kingdom. Chemical Communications, 2018, 54, 13620-13625. | 4.1 | 0 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Copperâ€“Chalcogen Bonds in Olfaction: Accurate ab Initio Characterization of CuSH and CuOH. Journal of Physical Chemistry A, 2019, 123, 1177-1185. | 2.5 | 0 |
| 38 | Impact of pathogenic mutations of the GLUT1 glucose transporter on channel dynamics using ConsDYN enhanced sampling. F1000Research, 0, 8, 322. | 1.6 | 0 |