Nicola Tasinato

List of Publications by Year
in descending order

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69 papers	1,577 citations	279798 23 h-index	361022 35 g-index
71 all docs	71 docs citations	71 times ranked	780 citing authors

#	Article	IF	Citations
1	The Spectroscopic Characterization of Halogenated Pollutants through the Interplay between Theory and Experiment: Application to R1122. Molecules, 2022, 27, 748.	3.8	8
2	Accurate Quantum Chemical Spectroscopic Characterization of Glycolic Acid: A Route Toward its Astrophysical Detection. Journal of Physical Chemistry A, 2022, 126, 2373-2387.	2.5	16
3	Gliding on Ice in Search of Accurate and Cost-Effective Computational Methods for Astrochemistry on Grains: The Puzzling Case of the HCN Isomerization. Journal of Chemical Theory and Computation, 2022, 18, 3111-3121.	5.3	4
4	Dipolar 1,3â€cycloaddition of thioformaldehyde S â€methylide (<scp> CH ₂ SCH) Tj ETQq0 0 0 rgBT /Overlock 10 T ₃ </scp> , <scp> SO ₂ </scp> , <scp>. Journal of Computational Chemistry, 2022, 43, 1420-1433.	3.3	6
5	Isomerization and Fragmentation Reactions on the [C₂SH₄] Potential Energy Surface: The Metastable Thione S-Methylide Isomer. Journal of Organic Chemistry, 2021, 86, 2941-2956.	3.2	11
6	A computational insight into the relationship between side chain IR line shapes and local environment in fibril-like structures. Journal of Chemical Physics, 2021, 154, 084105.	3.0	1
7	Looking for the Elusive Imine Tautomer of Creatinine: Different States of Aggregation Studied by Quantum Chemistry and Molecular Spectroscopy. ChemPlusChem, 2021, 86, 1374-1386.	2.8	14
8	Development and Validation of a Parameter-Free Model Chemistry for the Computation of Reliable Reaction Rates. Journal of Chemical Theory and Computation, 2021, 17, 4913-4928.	5.3	34
9	Accurate Biomolecular Structures by the Nano-LEGO Approach: Pick the Bricks and Build Your Geometry. Journal of Chemical Theory and Computation, 2021, 17, 7290-7311.	5.3	45
10	A Computational Journey across Nitroxide Radicals: From Structure to Spectroscopic Properties and Beyond. Molecules, 2021, 26, 7404.	3.8	5
11	Unraveling the role of additional OH-radicals in the Hâ€“Abstraction from Dimethyl sulfide using quantum chemical computations. Chemical Physics Letters, 2020, 739, 136963.	2.6	9
12	Accuracy Meets Interpretability for Computational Spectroscopy by Means of Hybrid and Double-Hybrid Functionals. Frontiers in Chemistry, 2020, 8, 584203.	3.6	50
13	Reinvestigation of the Deceptively Simple Reaction of Toluene with OH and the Fate of the Benzyl Radical: The â€œHiddenâ€•Routes to Cresols and Benzaldehyde. Journal of Physical Chemistry A, 2020, 124, 5917-5930.	2.5	18
14	A twist on the reaction of the CN radical with methylamine in the interstellar medium: new hints from a state-of-the-art quantum-chemical study. Monthly Notices of the Royal Astronomical Society, 2020, 496, 4298-4310.	4.4	24
15	Sextic centrifugal distortion constants: interplay of density functional and basis set for accurate yet feasible computations. Molecular Physics, 2020, 118, e1734678.	1.7	12
16	Exploring the Maze of C₂N₂H₅ Radicals and Their Fragments in the Interstellar Medium with the Help of Quantum-Chemical Computations. ACS Earth and Space Chemistry, 2020, 4, 774-782.	2.7	13
17	The Role of State-of-the-Art Quantum-Chemical Calculations in Astrochemistry: Formation Route and Spectroscopy of Ethanimine as a Paradigmatic Case. Molecules, 2020, 25, 2873.	3.8	20
18	DFT meets the segmented polarization consistent basis sets: Performances in the computation of molecular structures, rotational and vibrational spectroscopic properties. Journal of Molecular Structure, 2020, 1208, 127886.	3.6	23

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19	Modeling amino-acid side chain infrared spectra: the case of carboxylic residues. Physical Chemistry Chemical Physics, 2020, 22, 3008-3016.	2.8	10
20	State-of-the-art computation of the rotational and IR spectra of the methyl-cyclopropyl cation: hints on its detection in space. Physical Chemistry Chemical Physics, 2019, 21, 3431-3439.	2.8	17
21	Molecular synthons for accurate structural determinations: the equilibrium geometry of 1-chloro-1-fluoroethene. Physical Chemistry Chemical Physics, 2019, 21, 3615-3625.	2.8	15
22	Accuracy and Interpretability: The Devil and the Holy Grail. New Routes across Old Boundaries in Computational Spectroscopy. Chemical Reviews, 2019, 119, 8131-8191.	47.7	167
23	Tailorâ€made computational protocols for precise characterization of small biological building blocks using QM and MM approaches. Biopolymers, 2018, 109, e23109.	2.4	10
24	A Bit of Sugar on TiO₂: Quantum Chemical Insights on the Interfacial Interaction of Glycolaldehyde over Titanium Dioxide. Journal of Physical Chemistry C, 2018, 122, 6041-6051.	3.1	7
25	Line-by-line spectroscopic parameters of HFC-32 ro-vibrational transitions within the atmospheric window around 8.2â€Î¼m. Journal of Molecular Spectroscopy, 2018, 348, 57-63.	1.2	4
26	Rotational and Infrared Spectroscopy of Ethanimine: A Route toward Its Astrophysical and Planetary Detection. Astrophysical Journal, 2018, 855, 123.	4.5	35
27	Towards the SMART workflow system for computational spectroscopy. Physical Chemistry Chemical Physics, 2018, 20, 26034-26052.	2.8	16
28	Theory Meets Experiment for Noncovalent Complexes: The Puzzling Case of Pnicogen Interactions. Angewandte Chemie, 2018, 130, 14049-14053.	2.0	7
29	Unveiling the Sulfurâ€“Sulfur Bridge: Accurate Structural and Energetic Characterization of a Homochalcogen Intermolecular Bond. Angewandte Chemie - International Edition, 2018, 57, 15822-15826.	13.8	49
30	Theory Meets Experiment for Noncovalent Complexes: The Puzzling Case of Pnicogen Interactions. Angewandte Chemie - International Edition, 2018, 57, 13853-13857.	13.8	60
31	Noncovalent Interactions and Internal Dynamics in Pyridineâ€“Ammonia: A Combined Quantumâ€Chemical and Microwave Spectroscopy Study. Chemistry - A European Journal, 2017, 23, 4876-4883.	3.3	39
32	Accurate Vibrationalâ€“Rotational Parameters and Infrared Intensities of 1-Bromo-1-fluoroethene: A Joint Experimental Analysis and Ab Initio Study. Journal of Physical Chemistry A, 2017, 121, 3305-3317.	2.5	18
33	Development and Implementation of Advanced Fitting Methods for the Calculation of Accurate Molecular Structures. Journal of Chemical Theory and Computation, 2017, 13, 3060-3075.	5.3	50
34	Collision induced broadening of Î½1 band and ground state spectral lines of sulfur dioxide perturbed by N2 and O2. Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 198, 155-163.	2.3	3
35	On the competition between weak O Hâ‹¯F and C Hâ‹¯F hydrogen bonds, in cooperation with C Hâ‹¯O contacts, in the difluoromethane â€“ tert-butyl alcohol cluster. Journal of Molecular Spectroscopy, 2017, 337, 90-95.	1.2	26
36	Computing sextic centrifugal distortion constants by DFT: A benchmark analysis on halogenated compounds. Journal of Molecular Spectroscopy, 2017, 335, 117-125.	1.2	24

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37	CO2-, He- and H2-broadening coefficients of SO2 for Î½1 band and ground state transitions for astrophysical applications. Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 203, 367-376.	2.3	18
38	Correct Modeling of Cisplatin: a Paradigmatic Case. Angewandte Chemie, 2017, 129, 14026-14029.	2.0	0
39	Correct Modeling of Cisplatin: a Paradigmatic Case. Angewandte Chemie - International Edition, 2017, 56, 13838-13841.	13.8	24
40	VMS-ROT: A New Module of the Virtual Multifrequency Spectrometer for Simulation, Interpretation, and Fitting of Rotational Spectra. Journal of Chemical Theory and Computation, 2017, 13, 4382-4396.	5.3	34
41	Study of the Vibrational Spectra and Absorption Cross Sections of 1-Chloro-1-fluoroethene by a Joint Experimental and Ab Initio Approach. Journal of Physical Chemistry A, 2016, 120, 8369-8386.	2.5	17
42	Structural features of the carbonâ€“sulfur chemical bond: a semi-experimental perspective. Canadian Journal of Chemistry, 2016, 94, 1065-1076.	1.1	40
43	FTIR spectra of CH2F2 in the 1000â€“1300 cmâ^'1 region: Rovibrational analysis and modeling of the Coriolis and anharmonic resonances in the Î½3, Î½5, Î½7, Î½9 and 2Î½4 polyad. Journal of Quantitative Spectroscopy and Radiative Transfer, 2016, 175, 8-16.	2.3	14
44	The energetic of (CH2F2)2 investigated by TDL IR spectroscopy and DFT computations: From collision induced relaxation of ro-vibrational transitions to non-covalent interactions. Journal of Chemical Physics, 2015, 142, 134310.	3.0	14
45	Unveiling the non-covalent interactions of molecular homodimers by dispersion-corrected DFT calculations and collision-induced broadening of ro-vibrational transitions: application to (CH2F2)2 and (SO2)2. Physical Chemistry Chemical Physics, 2015, 17, 5659-5669.	2.8	36
46	Adsorption of F2CCFCl on TiO2 nano-powder: Structures, energetics and vibrational properties from DRIFT spectroscopy and periodic quantum chemical calculations. Applied Surface Science, 2015, 353, 986-994.	6.1	28
47	Insights into the interaction between CH2F2 and titanium dioxide: DRIFT spectroscopy and DFT analysis of the adsorption energetics. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 1614-1620.	3.9	6
48	Self-, N₂-, O₂-broadening coefficients and line parameters of HFC-32 for Î½₇ band and ground state transitions from infrared and microwave spectroscopy. Molecular Physics, 2014, 112, 2384-2396.	1.7	15
49	What are the spectroscopic properties of HFC-32? Answers from DFT. International Journal of Quantum Chemistry, 2014, 114, 1472-1485.	2.0	16
50	N2-, O2- and He-collision-induced broadening of sulfur dioxide ro-vibrational lines in the 9.2Î¼m atmospheric window. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 118, 373-379.	3.9	20
51	Anharmonic theoretical simulations of infrared spectra of halogenated organic compounds. Journal of Chemical Physics, 2013, 139, 074310.	3.0	72
52	Investigation of CHBrF2 adsorbed on TiO2 through IR spectroscopy and DFT calculations. Vibrational Spectroscopy, 2013, 65, 142-146.	2.2	3
53	A complete listing of sulfur dioxide self-broadening coefficients for atmospheric applications by coupling infrared and microwave spectroscopy to semiclassical calculations. Journal of Quantitative Spectroscopy and Radiative Transfer, 2013, 130, 233-248.	2.3	17
54	An integrated experimental and quantum-chemical investigation on the vibrational spectra of chlorofluoromethane. Journal of Chemical Physics, 2013, 139, 164302.	3.0	36

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55	Anharmonic force field and vibrational dynamics of CH2F2 up to 5000 cmâ¯1 studied by Fourier transform infrared spectroscopy and state-of-the-art ab initio calculations. Journal of Chemical Physics, 2012, 136, 214302.	3.0	37
56	Quantum-chemical ab initio investigation of the vibrational spectrum of halon 1113 and its anharmonic force field: A joint experimental and computational approach. Chemical Physics, 2012, 397, 55-64.	1.9	22
57	Modelling the anharmonic and Coriolis resonances within the six level polyad involving the Î½4 fundamental in the ro-vibrational spectrum of vinyl fluoride. Journal of Quantitative Spectroscopy and Radiative Transfer, 2012, 113, 1240-1249.	2.3	16
58	Microwave, High-Resolution Infrared, and Quantum Chemical Investigations of CHBrF₂: Ground and v₄ = 1 States. Journal of Physical Chemistry A, 2011, 115, 453-459.	2.5	25
59	Toward a Complete Understanding of the Vinyl Fluoride Spectrum in the Atmospheric Region. ChemPhysChem, 2011, 12, 356-363.	2.1	20
60	Anharmonic resonances in the CH chromophore overtone spectra of CHBrF₂. Molecular Physics, 2011, 109, 2163-2172.	1.7	12
61	Collisional Effects On Quantum Cascade Laser Induced Molecular Alignment. AIP Conference Proceedings, 2010, , .	0.4	7
62	Time dependent measurements of nitrous oxide and carbon dioxide collisional relaxation processes by a frequency down-chirped quantum cascade laser: Rapid passage signals and the time dependence of collisional processes. Journal of Chemical Physics, 2010, 132, 164301.	3.0	20
63	Spectroscopic measurements of SO2 line parameters in the 9.2â€,Î¼m atmospheric region and theoretical determination of self-broadening coefficients. Journal of Chemical Physics, 2010, 132, 044315.	3.0	26
64	Spectroscopic study of CHBrF2 up to 9500â€,cmâ¯1: Vibrational analysis, integrated band intensities, and ab initio calculations. Journal of Chemical Physics, 2010, 133, 044310.	3.0	19
65	An investigation of collisional processes in a Dicke narrowed transition of water vapor in the 7.8â€,Î¼m spectral region by frequency down-chirped quantum cascade laser spectroscopy. Journal of Chemical Physics, 2010, 132, 044316.	3.0	16
66	Determination of the vinyl fluoride line intensities by TDL spectroscopy: the object oriented approach of Visual Line Shape Fitting Program to line profile analysis. Molecular Physics, 2010, 108, 677-685.	1.7	17
67	Quantum cascade laser spectroscopy: diagnostics to non-linear optics. Journal of Modern Optics, 2009, 56, 2034-2048.	1.3	22
68	Infrared Spectra, Integrated Band Intensities, and Anharmonic Force Field of H2C=CHF. Journal of Physical Chemistry A, 2009, 113, 1497-1504.	2.5	26
69	High-Resolution Infrared Study of Vinyl Fluoride in the 750â¯1050 cm-1 Region:â€‰ Rovibrational Analysis and Resonances Involving the Î½8, Î½10, and Î½11 Fundamentals. Journal of Physical Chemistry A, 2006, 110, 13412-13418.	2.5	12