

# François Fillaux

## List of Publications by Year in descending order

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105  
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1,942  
citations

236612

25  
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315357

38  
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107  
all docs

107  
docs citations

107  
times ranked

992  
citing authors

#	ARTICLE	IF	CITATIONS
1	A New Look at Proton Transfer Dynamics Along the Hydrogen Bonds in Amides and Peptides. <i>Science</i> , 1994, 264, 1285-1289.	6.0	130
2	Inelastic-neutron-scattering study of methyl tunneling and the quantum sine-Gordon breather in isotopic mixtures of 4-methyl-pyridine at low temperature. <i>Physical Review B</i> , 1990, 42, 5990-6006.	1.1	76
3	Proton dynamics in the hydrogen bond. The inelastic neutron scattering spectrum of potassium hydrogen carbonate at 5 K. <i>Chemical Physics</i> , 1988, 124, 425-437.	0.9	62
4	Structure and dynamics of the symmetric hydrogen bond in potassium hydrogen maleate: a neutron scattering study. <i>Chemical Physics</i> , 1999, 244, 387-403.	0.9	61
5	Proton transfer dynamics in the hydrogen bond. Inelastic neutron scattering, infrared and Raman spectra of Na3H(SO4)2, K3H(SO4)2 and Rb3H(SO4)2. <i>Chemical Physics</i> , 1991, 154, 135-144.	0.9	60
6	Calculations of infrared and Raman band profiles of strong hydrogen bonds, OH stretching bands and proton dynamics in crystalline potassium hydrogen carbonate. <i>Chemical Physics</i> , 1983, 74, 405-412.	0.9	58
7	Inelastic neutron-scattering study of the proton dynamics in N-methylacetamide at 20 K. <i>Chemical Physics</i> , 1993, 176, 249-278.	0.9	54
8	Quantum proton transfer and interconversion in the benzoic acid crystal: vibrational spectra, mechanism and theory. <i>Chemical Physics</i> , 2002, 276, 181-210.	0.9	50
9	Incoherent elastic-neutron-scattering study of the vibrational dynamics and spin-related symmetry of protons in the KHCO3 crystal. <i>Physical Review B</i> , 1999, 59, 4134-4145.	1.1	48
10	Inelastic-neutron-scattering study at low temperature of the quantum sine-Gordon breather in 4-methyl-pyridine with partially deuterated methyl groups. <i>Physical Review B</i> , 1991, 44, 12280-12293.	1.1	46
11	Inelastic Neutron Scattering Study of the Proton Dynamics in Manganese Oxides: I. and Manganite. <i>Journal of the Electrochemical Society</i> , 1993, 140, 585-591.	1.3	43
12	Vibrational spectra and dynamics of conformation and hydrogen bonding of n-methylacetamide. I. Conformational dynamics of the CH3CONHCH3 molecule and NH out of plane band splitting. <i>Chemical Physics</i> , 1981, 62, 275-285.	0.9	39
13	An inelastic neutron scattering study of the proton dynamics in $\hat{I}^3$ -MnO2. <i>Chemical Physics</i> , 1991, 149, 459-469.	0.9	38
14	The anisotropy of the proton momentum distribution in KHCO3: A deep inelastic neutron scattering study. <i>Journal of Chemical Physics</i> , 1991, 94, 4411-4415.	1.2	37
15	Vibrational force field of solid imidazole from inelastic neutron scattering. <i>Journal of Chemical Physics</i> , 1995, 103, 8444-8455.	1.2	35
16	Theoretical model for calculations of infrared and Raman band profiles of strong hydrogen bonds in ordered media. <i>Chemical Physics</i> , 1983, 74, 395-404.	0.9	32
17	Structure of matrix isolated N-methylacetamide. <i>Chemical Physics Letters</i> , 1976, 39, 547-551.	1.2	31
18	Inelastic neutron-scattering study of the proton dynamics in coals. <i>Fuel</i> , 1995, 74, 865-873.	3.4	31

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19	Quantum entanglement and nonlocal proton transfer dynamics in dimers of formic acid and analogues. <i>Chemical Physics Letters</i> , 2005, 408, 302-306.	1.2	31
20	Hydrogen bonding and quantum dynamics in the solid state. <i>International Reviews in Physical Chemistry</i> , 2000, 19, 553-564.	0.9	29
21	Observation of the dynamical structure arising from spatially extended quantum entanglement and long-lived quantum coherence in the KHCO <sub>3</sub> crystal. <i>Physical Review B</i> , 2003, 67, .	1.1	29
22	Inelastic neutron-scattering study of the proton dynamics in carbons and coals. <i>Carbon</i> , 1994, 32, 1325-1331.	5.4	28
23	The Pauli principle and the vibrational dynamics of protons in solids: A new spin-related symmetry. <i>Physica D: Nonlinear Phenomena</i> , 1998, 113, 172-183.	1.3	28
24	Inelastic neutron scattering study of proton dynamics in carbon blacks. <i>Carbon</i> , 1996, 34, 903-908.	5.4	27
25	Inelastic-neutron-scattering study of the sine-Gordon breather interactions in isotopic mixtures of 4-methyl-pyridine. <i>Physical Review B</i> , 1998, 58, 11416-11419.	1.1	27
26	Neutron spectroscopic investigations on different grades of modified furnace blacks and gas blacks. <i>Carbon</i> , 1999, 37, 437-444.	5.4	26
27	Collective rotation of methyl groups in isotopic mixtures of 4-methylpyridine at low temperature. Inelastic neutron scattering spectra. <i>Chemical Physics Letters</i> , 1989, 162, 188-195.	1.2	25
28	Inelastic neutron scattering study of the proton dynamics in HNO <sub>3</sub> graphite intercalation compounds. <i>Chemical Physics</i> , 1999, 242, 273-281.	0.9	25
29	Butterfly motion of isolated perylene in its ground and first excited singlet states. <i>Chemical Physics Letters</i> , 1985, 114, 384-387.	1.2	24
30	Spectroscopic studies of the monosubstituted amides. VI. Neutron inelastic scattering spectra of N-methyl acetamide. <i>Chemical Physics</i> , 1977, 26, 295-300.	0.9	22
31	Raman OH stretching band shape of and proton dynamics in CsH <sub>2</sub> PO <sub>4</sub> . <i>Chemical Physics</i> , 1984, 86, 127-136.	0.9	22
32	Inelastic neutron scattering study of free proton dynamics in coal. <i>Journal of Non-Crystalline Solids</i> , 1995, 188, 161-168.	1.5	22
33	Proton-transfer dynamics in the hydrogen bond. Inelastic neutron scattering, infrared and Raman spectra of KH(CF <sub>3</sub> COO) <sub>2</sub> and CsH(CF <sub>3</sub> COO) <sub>2</sub> . <i>Chemical Physics</i> , 1991, 158, 113-127.	0.9	21
34	Proton transfer in malonaldehyde: From reaction path to Schrödinger's Cat. <i>Chemical Physics Letters</i> , 2005, 415, 357-361.	1.2	21
35	Extended tunnelling states in the benzoic acid crystal: Infrared and Raman spectra of the OH and OD stretching modes. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 4327.	1.3	21
36	Inelastic neutron-scattering study of the proton transfer dynamics in polyglycine I at 20 K. <i>Biophysical Chemistry</i> , 1994, 53, 155-168.	1.5	20

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37	Vibrational spectra and dynamics of conformation and hydrogen bonding of N-methylacetamide. II. Dynamics of the NH...O Hydrogen bond and NH (ND) stretching band structure. <i>Chemical Physics</i> , 1981, 62, 287-302.	0.9	19
38	Proton-transfer dynamics in the hydrogen bond. Inelastic neutron scattering spectra of sodium, rubidium and caesium hydrogen carbonates at low temperature. <i>Journal of Molecular Structure</i> , 1992, 270, 339-349.	1.8	19
39	Vibrational study of various crystalline phases of thallium dihydrogen phosphate TH <sub>2</sub> PO <sub>4</sub> and its deuterated analog TID <sub>2</sub> PO <sub>4</sub> . <i>Chemical Physics</i> , 1993, 171, 203-220.	0.9	19
40	Crystal structure and low-temperature methyl-group dynamics of cobalt and nickel acetates. <i>Journal of Chemical Physics</i> , 1998, 109, 9062-9074.	1.2	19
41	Proton transfer in the KHCO <sub>3</sub> and benzoic acid crystals: A quantum view. <i>Journal of Molecular Structure</i> , 2007, 844-845, 308-318.	1.8	18
42	Spectroscopic study of monosubstituted amides. VII-low frequency Raman spectra of crystallized N-methylacetamide. <i>Journal of Raman Spectroscopy</i> , 1978, 7, 244-248.	1.2	17
43	Proton dynamics in the hydrogen bond. Inelastic neutron scattering by single crystals of CsH <sub>2</sub> PO <sub>4</sub> at 20 K. <i>Chemical Physics</i> , 1989, 130, 257-270.	0.9	17
44	Inelastic Neutron Scattering Study of the Proton Dynamics in Manganese Oxides: II . Proton Insertion in Electrodeposited. <i>Journal of the Electrochemical Society</i> , 1993, 140, 592-598.	1.3	17
45	Inelastic neutron scattering study of the localized dynamics of protons in KHCO <sub>3</sub> single crystals. <i>Physical Review B</i> , 2002, 66, .	1.1	17
46	Comment on "Quantum correlations between protons in potassium bicarbonate". <i>Journal of Physics Condensed Matter</i> , 2004, 16, 1007-1010.	0.7	16
47	Macroscopic quantum entanglement and "super-rigidity" of protons in the KHCO <sub>3</sub> crystal from 30 to 300 K. <i>Journal of Physics Condensed Matter</i> , 2006, 18, 3229-3249.	0.7	16
48	The Crystal Structure and Methyl Group Dynamics in the Room-Temperature and Low-Temperature Phases of Lithium Acetate Dihydrate. <i>Journal of Solid State Chemistry</i> , 1996, 126, 184-188.	1.4	15
49	Proton transfer across hydrogen bonds: From reaction path to Schrödinger's cat. <i>Pure and Applied Chemistry</i> , 2007, 79, 1023-1039.	0.9	15
50	Inelastic neutron scattering study of <sup>55</sup> MnO <sub>2</sub> : the dynamics of (H <sup>+</sup> ) <sub>4</sub> entities in Mn <sup>4+</sup> vacancies. <i>Chemical Physics</i> , 1992, 164, 311-319.	0.9	14
51	The effects of NH <sub>3</sub> free rotation on the inelastic neutron scattering spectrum of Ni(NH <sub>3</sub> ) <sub>2</sub> Ni(CN) <sub>4</sub> ·2C <sub>6</sub> D <sub>6</sub> at 20 K. <i>Chemical Physics</i> , 1993, 176, 279-287.	0.9	14
52	Inelastic neutron scattering study of proton dynamics in Ca(OH) <sub>2</sub> at 20 K. <i>Chemical Physics</i> , 1995, 197, 81-90.	0.9	14
53	Neutron Compton scattering study of proton-transfer dynamics in partially deuterated N-methylacetamide: CD <sub>3</sub> CONHCD <sub>3</sub> . <i>Chemical Physics Letters</i> , 1995, 240, 114-118.	1.2	13
54	Inelastic neutron scattering study of methyl tunnelling in an oriented single-crystal of 2,6-dimethylpyrazine at low temperature and rotational "potential" calculations. <i>Chemical Physics</i> , 1998, 226, 1-13.	0.9	13

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55	Interpretation of the vibrational spectra of methylglyoxal and biacetyl in their first singlet excited electronic states. <i>Chemical Physics</i> , 1984, 87, 117-123.	0.9	12
56	Rotational dynamics of the methyl group in the 4-methyl pyridine crystal. <i>Chemical Physics Letters</i> , 1986, 125, 41-46.	1.2	12
57	Inelastic neutron-scattering study of free proton dynamics in $\hat{1}^3$ -MnO <sub>2</sub> . <i>Chemical Physics</i> , 1996, 209, 111-125.	0.9	12
58	Interplay of quantum methyl rotation and crystal structure in the lithium acetate dihydrate: neutron diffraction, inelastic neutron scattering and theory. <i>Chemical Physics</i> , 2003, 290, 101-120.	0.9	12
59	A neutron scattering study of strong-symmetric hydrogen bonds in potassium and cesium hydrogen bistrifluoroacetates: Determination of the crystal structures and of the single-well potentials for protons. <i>Journal of Chemical Physics</i> , 2008, 128, 204502.	1.2	12
60	Neutron inelastic scattering of the methyl torsional mode in hydrogenated and deuterated 4-methylpyridine crystals at 5 K. <i>Chemical Physics Letters</i> , 1988, 146, 549-552.	1.2	11
61	Methyl group tunnelling studies in calixarenes. <i>Physica B: Condensed Matter</i> , 1994, 202, 279-286.	1.3	10
62	Inelastic neutron scattering study of proton dynamics in polyanilines. <i>Synthetic Metals</i> , 1996, 81, 211-214.	2.1	10
63	Comment on: "A symmetric hydrogen bond revisited: potassium hydrogen maleate by variable temperature, variable pressure neutron diffraction and plane-wave DFT methods" [Chem. Phys. Lett. 381 (2003) 102]. <i>Chemical Physics Letters</i> , 2004, 399, 289-291.	1.2	10
64	A new class of compounds suited to study the torsional dynamics in the quantum regime: the calixarenes. <i>Chemical Physics Letters</i> , 1993, 201, 427-432.	1.2	9
65	Inelastic neutron-scattering study of methyl tunnelling and the quantum sine-Gordon breather mode in isotopic mixtures of 2,6-dimethyl-pyridine at low temperature. <i>Physica B: Condensed Matter</i> , 1994, 202, 302-310.	1.3	9
66	Molecular tunnelling in p-tert-butylcalix[4]arene(2:1)p-xylene. <i>Molecular Physics</i> , 1994, 81, 609-619.	0.8	9
67	Collective rotational tunneling of methyl groups and quantum solitons in 4-methylpyridine: Neutron scattering studies of single crystals. <i>Physical Review B</i> , 2003, 68, .	1.1	9
68	Neutron scattering studies of K <sub>3</sub> H(SO <sub>4</sub> ) <sub>2</sub> and K <sub>3</sub> D(SO <sub>4</sub> ) <sub>2</sub> : The particle-in-a-box model for the quantum phase transition. <i>Journal of Chemical Physics</i> , 2012, 137, 074504.	1.2	9
69	Infrared band-shape analysis and hydrogen-bonding dynamics of the HCOOH low-temperature crystal. <i>Chemical Physics</i> , 1985, 100, 355-363.	0.9	8
70	The impact of vibrational spectroscopy with neutrons on our view of quantum dynamics in hydrogen bonds and proton transfer. <i>Journal of Molecular Structure</i> , 2002, 615, 45-59.	1.8	8
71	Synchrotron and neutron diffraction study of 4-methylpyridine-N-oxide at low temperature. <i>Acta Crystallographica Section B: Structural Science</i> , 2006, 62, 627-633.	1.8	8
72	Vibrational spectra and structure of N-methylacetamide in some solid complexes with neutral salts. <i>Canadian Journal of Chemistry</i> , 1985, 63, 1473-1476.	0.6	7

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73	Vibrational study of metal-substituted MPS3 layered compounds: $MII1 \times MI2 \times PS3$ with $MI1 = Mn, Cd$ , and $MI2 = Cu$ ( $x = 0.13$ ) or $Ag$ ( $x = 0.50$ ). <i>Journal of Solid State Chemistry</i> , 1988, 72, 283-292.	1.4	7
74	NH3 free rotors in Hofmann clathrates. <i>Physica B: Condensed Matter</i> , 1996, 226, 199-201.	1.3	7
75	Structure of manganese diacetate tetrahydrate and low-temperature methyl-group dynamics. <i>Acta Crystallographica Section B: Structural Science</i> , 2001, 57, 36-44.	1.8	7
76	Observation and interpretation of the fluorescence excitation spectrum of hexafluorobiacetyl under free jet expansion. <i>Chemical Physics</i> , 1985, 95, 293-298.	0.9	6
77	Inelastic neutron scattering study of isotopic mixtures of lithium acetate with partially deuterated CH2D groups and sine-Gordon dynamics. <i>Physica B: Condensed Matter</i> , 1996, 226, 241-243.	1.3	6
78	Étude spectroscopique des amides modélés. III. Spectres et conformations de deux amides substitués par des modèles de chaînes latérales. Le n-isopropylacétamide et le n(1,2-diméthyl)butylamide. <i>Journal De Chimie Physique Et De Physico-Chimie Biologique</i> , 1975, 72, 42-50.	0.2	6
79	Proton transfer: Recent results from neutron vibrational spectroscopy. <i>Physica B: Condensed Matter</i> , 1996, 226, 213-217.	1.3	5
80	A neutron diffraction study of macroscopically entangled proton states in the high temperature phase of the KHCO3 crystal at 340 K. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 015225.	0.7	5
81	A neutron diffraction study of the crystal of benzoic acid from 6 to 293 K and a macroscopic-scale quantum theory of the lattice of hydrogen-bonded dimers. <i>Chemical Physics</i> , 2016, 479, 26-35.	0.9	5
82	CH(CID) stretching band shape analysis in isolated 1:1 complexes of hydrochloric acid with ethers. <i>Chemical Physics</i> , 1986, 106, 447-458.	0.9	4
83	Proton tunnelling in the intramolecular hydrogen bond of 9-Hydroxyphenalenone. <i>Journal of Molecular Structure</i> , 2004, 700, 147-149.	1.8	4
84	VIBRATIONAL SPECTROSCOPY AND QUANTUM LOCALIZATION. <i>Advanced Series in Nonlinear Dynamics</i> , 2004, , 73-148.	0.4	4
85	Inelastic neutron scattering studies of polypyrroles and partially deuterated analogues. <i>Solid State Ionics</i> , 2001, 145, 451-457.	1.3	3
86	The vibrational spectroscopy of hydrogen bonds. <i>Physica B: Condensed Matter</i> , 1991, 174, 246-250.	1.3	2
87	Inelastic Neutron Scattering Studies of the Proton Dynamics in Bi-Doped Manganese Oxides. <i>Journal of the Electrochemical Society</i> , 2000, 147, 4184.	1.3	2
88	2,6-Dimethylpyrazine at 5 K: a neutron-diffraction study. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2001, 57, o1116-o1117.	0.2	2
89	Evidence of macroscopically entangled protons in a mixed isotope crystal of $KH_{1-x}D_xCO_3$ . <i>Journal of Physics Condensed Matter</i> , 2010, 22, 045402.	0.7	2
90	Quantum interferences revealed by neutron diffraction accord with a macroscopic-scale quantum-theory of ferroelectrics $KH_2(1-x)D_2xPO_4$ . <i>European Physical Journal B</i> , 2016, 89, 1.	0.6	2

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91	Macroscopic quantum tunnelling of protons in the KHCO <sub>3</sub> crystal. Journal of Molecular Structure, 2006, 790, 122-128.	1.8	1
92	Nonlocal protons and deuterons opposed to disorder: a single-crystal neutron diffraction study of KH <sub>0.76</sub> D <sub>0.24</sub> CO <sub>3</sub> and a theoretical framework. Journal of Physics Condensed Matter, 2008, 20, 252202.	0.7	1
93	The quantum phase-transitions of water. Europhysics Letters, 2017, 119, 40008.	0.7	1
94	The Macroscopic Quantum Behavior of Protons in the KHCO <sub>3</sub> Crystal: Theory and Experiments. Progress in Theoretical Chemistry and Physics, 2008, , 319-340.	0.2	1
95	Rotational tunnelling and the rotational potential of methyl groups in the zinc, manganese and cobalt chloride salts of 4-methylpyridine. Molecular Physics, 1993, 80, 671-683.	0.8	0
96	Nsutite, proton dynamics and momentum distributions. Ferroelectrics, 1995, 167, 43-51.	0.3	0
97	2,6-Dimethylpyrazine at 20â€¦K: a neutron-diffraction study. Acta Crystallographica Section E: Structure Reports Online, 2001, 57, o1113-o1115.	0.2	0
98	Proton dynamics in an extended array of hydrogen bonds: normal coordinates, proton transfer and macroscopic quantum entanglement in the ground state. Journal of Molecular Structure, 2004, 700, 133-145.	1.8	0
99	Proton Dynamics in Solids: Vibrational Spectroscopy with Neutrons. , 2005, , 267-304.		0
100	Where are Protons and Deuterons in KH <sub>p</sub> D <sub>1</sub> CO <sub>3</sub> ? A Neutron Diffraction Study. Zeitschrift Fur Physikalische Chemie, 2008, 222, 1279-1290.	1.4	0
101	EXPERIMENTAL STUDIES AND THEORY OF NONLINEAR ROTATIONAL DYNAMICS IN THE QUANTUM REGIME: THE INTERPLAY OF STRUCTURE, DYNAMICS AND LOCALIZATION IN CRYSTALS. , 2003, , .		0
102	COLLECTIVE ROTATIONAL TUNNELLING AND QUANTUM SINE-GORDON SOLITONS. , 2003, , .		0
103	Introduction to Vibrational Spectroscopy â€” From the Normal Mode to the Local Mode: Infrared, Raman and Inelastic Neutron Scattering. , 1989, , 79-91.		0
104	Nonlinear Coupling and Vibrational Dynamics. , 1989, , 93-102.		0
105	Inelastic Neutron Scattering Study of the Quantum Sine-Gordon Breather in 4-Methyl-Pyridine. NATO ASI Series Series B: Physics, 1993, , 465-468.	0.2	0