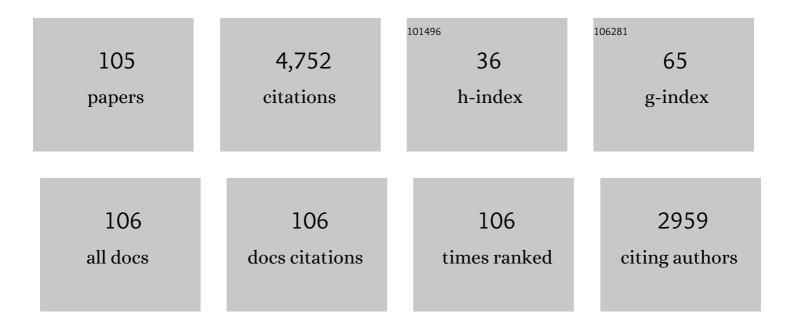
List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/1052591/publications.pdf Version: 2024-02-01



ALEYANDDE FALLDE

#	Article	IF	CITATIONS
1	A KINETIC DATABASE FOR ASTROCHEMISTRY (KIDA). Astrophysical Journal, Supplement Series, 2012, 199, 21.	3.0	436
2	THE 2014 KIDA NETWORK FOR INTERSTELLAR CHEMISTRY. Astrophysical Journal, Supplement Series, 2015, 217, 20.	3.0	291
3	Detection of complex organic molecules in a prestellar core: a new challenge for astrochemical models. Astronomy and Astrophysics, 2012, 541, L12.	2.1	269
4	BASECOL2012: A collisional database repository and web service within the Virtual Atomic and Molecular Data Centre (VAMDC). Astronomy and Astrophysics, 2013, 553, A50.	2.1	193
5	R12-calibrated H2O–H2 interaction: Full dimensional and vibrationally averaged potential energy surfaces. Journal of Chemical Physics, 2008, 129, 134306.	1.2	134
6	Refractory and semi-volatile organics at the surface of comet 67P/Churyumov-Gerasimenko: Insights from the VIRTIS/Rosetta imaging spectrometer. Icarus, 2016, 272, 32-47.	1.1	127
7	THE CHEMISTRY OF VIBRATIONALLY EXCITED H ₂ IN THE INTERSTELLAR MEDIUM. Astrophysical Journal, 2010, 713, 662-670.	1.6	119
8	Quasi-classical rate coefficient calculations for the rotational (de)excitation of H2O by H2. Astronomy and Astrophysics, 2007, 472, 1029-1035.	2.1	118
9	Ammonium salts are a reservoir of nitrogen on a cometary nucleus and possibly on some asteroids. Science, 2020, 367, .	6.0	115
10	Improved low-temperature rate constants for rotational excitation of CO by H\$_mathsf{2}\$. Astronomy and Astrophysics, 2006, 446, 367-372.	2.1	94
11	Interstellar chemistry of nitrogen hydrides in dark clouds. Astronomy and Astrophysics, 2014, 562, A83.	2.1	93
12	Rotational excitation of HC3N by H2and He at low temperatures. Astronomy and Astrophysics, 2007, 464, 1147-1154.	2.1	87
13	Nitrogen hydrides and the H ₂ ortho-to-para ratio in dark clouds. Astronomy and Astrophysics, 2012, 537, A20.	2.1	83
14	A full nine-dimensional potential-energy surface for hydrogen molecule-water collisions. Journal of Chemical Physics, 2005, 122, 221102.	1.2	82
15	Collisional excitation of water in warm astrophysical media. Astronomy and Astrophysics, 2008, 492, 257-264.	2.1	82
16	Charge-Transfer Energy in the Waterâ^'Hydrogen Molecular Aggregate Revealed by Molecular-Beam Scattering Experiments, Charge Displacement Analysis, and ab Initio Calculations. Journal of the American Chemical Society, 2010, 132, 13046-13058.	6.6	80
17	On the robustness of the ammonia thermometer. Monthly Notices of the Royal Astronomical Society, 2009, 399, 425-431.	1.6	77
18	The impact of collisional rate coefficients on molecular hyperfine selective excitation. Monthly Notices of the Royal Astronomical Society, 2012, 425, 740-748.	1.6	73

#	Article	IF	CITATIONS
19	Influence of a new potential energy surface on the rotational (de)excitation of H\$_{mathsf 2}\$O by H\$_{mathsf 2}\$ at low temperature. Astronomy and Astrophysics, 2006, 460, 323-329.	2.1	70
20	Electron-impact rotational excitation of water. Monthly Notices of the Royal Astronomical Society, 2004, 347, 323-333.	1.6	64
21	display="inline"> <mml:mi>O</mml:mi> <mml:mi>r</mml:mi> <mml:mi>t</mml:mi> <mml:mi><mml:mi>h</mml:mi><mml:ri>mathvariant="normal">â^²<mml:mi>P</mml:mi><mml:mi>a</mml:mi><mml:mi>r</mml:mi><mml:mi> xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>a</mml:mi> mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn>Conversion by</mml:ri></mml:mi>	ni>omi>a2.9	:mi> <mml:mi ıl:mi> 62</mml:mi
22	Proton Exchange at Low Temperature: An Accu. Physical Review Letters, 2011, 107, 023201. Low-energy electron collisions with water: elastic and rotationally inelastic scattering. Journal of Physics B: Atomic, Molecular and Optical Physics, 2004, 37, 801-807.	0.6	61
23	Constraining the ortho-to-para ratio of H ₂ with anomalous H ₂ CO absorption. Astronomy and Astrophysics, 2009, 506, 1243-1247.	2.1	59
24	The Leiden Atomic and Molecular Database (LAMDA): Current Status, Recent Updates, and Future Plans. Atoms, 2020, 8, 15.	0.7	59
25	The IRAM-30 m line survey of the Horsehead PDR. Astronomy and Astrophysics, 2013, 557, A101.	2.1	58
26	Nitrogen hydrides in the cold envelope of IRASÂ16293-2422. Astronomy and Astrophysics, 2010, 521, L52.	2.1	56
27	ORTHO-PARA SELECTION RULES IN THE GAS-PHASE CHEMISTRY OF INTERSTELLAR AMMONIA. Astrophysical Journal Letters, 2013, 770, L2.	3.0	53
28	The origin of gas-phase HCO and CH ₃ O radicals in prestellar cores. Astronomy and Astrophysics, 2016, 587, A130.	2.1	51
29	Electron and positron collisions with polar molecules: studies with the benchmark water molecule. Physica Scripta, 2009, 80, 015301.	1.2	50
30	Rotational excitation of mono- and doubly-deuterated water by hydrogen molecules. Monthly Notices of the Royal Astronomical Society, 2012, 420, 699-704.	1.6	42
31	First detection of ND in the solar-mass protostar IRAS16293-2422. Astronomy and Astrophysics, 2010, 521, L42.	2.1	41
32	Ortho-to-para ratio of interstellar heavy water. Astronomy and Astrophysics, 2010, 521, L31.	2.1	40
33	On the importance of full-dimensionality in low-energy molecular scattering calculations. Scientific Reports, 2016, 6, 28449.	1.6	40
34	History of the solar-type protostar IRAS 16293–2422 as told by the cyanopolyynes. Astronomy and Astrophysics, 2017, 597, A40.	2.1	40
35	Collisional excitation of sulfur dioxide in cold molecular clouds. Astronomy and Astrophysics, 2011, 531, A103.	2.1	40
36	Collisional excitation of HC ₃ N by para- and ortho-H ₂ . Monthly Notices of the Royal Astronomical Society, 2016, 460, 2103-2109.	1.6	39

#	Article	IF	CITATIONS
37	Chemical complexity induced by efficient ice evaporation in the Barnard 5 molecular cloud. Astronomy and Astrophysics, 2017, 607, A20.	2.1	38
38	The rotational excitation of the HCN and HNC molecules by H2 revisited. Monthly Notices of the Royal Astronomical Society, 2017, 468, 1084-1091.	1.6	37
39	Communication: Rotational excitation of interstellar heavy water by hydrogen molecules. Journal of Chemical Physics, 2010, 133, 231105.	1.2	36
40	Electron-impact excitation of diatomic hydride cations – I. HeH ⁺ , CH ⁺ , ArH ⁺ . Monthly Notices of the Royal Astronomical Society, 2016, 455, 3281-3287.	1.6	36
41	Deuteration of ammonia in the starless core Ophiuchus/H-MM1. Astronomy and Astrophysics, 2017, 600, A61.	2.1	36
42	The Dense Gas Fraction in Galactic Center Clouds. Astrophysical Journal, 2018, 868, 7.	1.6	35
43	A Monte Carlo error estimator for the expansion of rigid-rotor potential energy surfaces. Journal of Mathematical Chemistry, 2012, 50, 588-601.	0.7	34
44	The role of rotation in the vibrational relaxation of water by hydrogen molecules. Journal of Chemical Physics, 2005, 123, 104309.	1.2	33
45	Fine and hyperfine excitation of NH and ND by He: On the importance of calculating rate coefficients of isotopologues. Journal of Chemical Physics, 2012, 137, 114306.	1.2	33
46	The rotational excitation of HCN and HNC by He: new insights on the HCN/HNC abundance ratio in molecular clouds. Monthly Notices of the Royal Astronomical Society, 2010, , .	1.6	32
47	EXPERIMENTAL AND THEORETICAL ANALYSIS OF LOW-ENERGY CO + H ₂ INELASTIC COLLISIONS. Astrophysical Journal Letters, 2015, 799, L9.	3.0	32
48	State-to-state chemistry and rotational excitation of CH+ in photon-dominated regions. Monthly Notices of the Royal Astronomical Society, 2017, 469, 612-620.	1.6	31
49	<i>Ab initio</i> computation of the broadening of water rotational lines by molecular hydrogen. Physical Review A, 2010, 82, .	1.0	30
50	Communication: Mapping water collisions for interstellar space conditions. Journal of Chemical Physics, 2010, 133, 131103.	1.2	28
51	Potential energy surface and rotational cross sections for methyl formate colliding with helium. Journal of Chemical Physics, 2011, 135, 024301.	1.2	28
52	Overtone vibrational spectroscopy in H2-H2O complexes: A combined high level theoretical <i>ab initio</i> , dynamical and experimental study. Journal of Chemical Physics, 2012, 137, 084301.	1.2	27
53	WEAK MASER EMISSION OF METHYL FORMATE TOWARD SAGITTARIUS B2(N) IN THE GREEN BANK TELESCOPE PRIMOS SURVEY. Astrophysical Journal, 2014, 783, 72.	1.6	27
54	Collisional excitation of NH3 by atomic and molecular hydrogen. Monthly Notices of the Royal Astronomical Society, 2017, 470, 2204-2211.	1.6	27

#	Article	IF	CITATIONS
55	Rate coefficients for electron-impact rotational excitation of H3+ and H3O+. Monthly Notices of the Royal Astronomical Society, 2003, 340, 468-472.	1.6	25
56	Modelling the molecular composition and nuclear-spin chemistryof collapsing pre-stellar sourcesâ~ Monthly Notices of the Royal Astronomical Society, 2018, 477, 4454-4472.	1.6	25
57	Rotational excitation of HC ₃ N by H ₂ and He at low temperatures. Astronomy and Astrophysics, 2007, 475, 391-391.	2.1	24
58	Interaction of H ₂ 0 with CO: potential energy surface, bound states and scattering calculations. Physical Chemistry Chemical Physics, 2018, 20, 5469-5477.	1.3	24
59	Cross Sections for Electron Collisions with H2O. Journal of Physical and Chemical Reference Data, 2021, 50, .	1.9	24
60	An Efficient Statistical Method to Compute Molecular Collisional Rate Coefficients. Astrophysical Journal Letters, 2018, 853, L5.	3.0	23
61	The nitrogen isotopic ratio of HC3N towards the L1544 prestellar core. Monthly Notices of the Royal Astronomical Society, 2018, 480, 1174-1186.	1.6	23
62	Scattering of CO with H2O: Statistical and classical alternatives to close-coupling calculations. Journal of Chemical Physics, 2018, 148, 244308.	1.2	21
63	Isomerism Effects in the Collisional Excitation of Cyanoacetylene by Molecular Hydrogen. ACS Earth and Space Chemistry, 2019, 3, 1151-1157.	1.2	21
64	Rigid-Bender Close-Coupling Treatment of the Inelastic Collisions of H ₂ 0 with <i>para</i> -H ₂ . Journal of Physical Chemistry A, 2019, 123, 5704-5712.	1.1	19
65	Ortho–para-H2 conversion by hydrogen exchange: Comparison of theory and experiment. Journal of Chemical Physics, 2012, 137, 154303.	1.2	18
66	Interaction of Chiral Propylene Oxide (CH ₃ CHCH ₂ O) with Helium: Potential Energy Surface and Scattering Calculations. ACS Earth and Space Chemistry, 2019, 3, 964-972.	1.2	18
67	The ortho-to-para ratio of water in interstellar clouds. Monthly Notices of the Royal Astronomical Society, 2019, 487, 3392-3403.	1.6	17
68	Efficient Methanol Production on the Dark Side of a Prestellar Core. Astrophysical Journal, 2020, 895, 101.	1.6	17
69	Nuclear-Spin Selection Rules in the Chemistry of Interstellar Nitrogen Hydrides. Journal of Physical Chemistry A, 2013, 117, 9800-9806.	1.1	16
70	Collisional excitation of water by hydrogen atoms. Monthly Notices of the Royal Astronomical Society, 2015, 446, 2312-2316.	1.6	15
71	Comparative experimental and theoretical study of the rotational excitation of CO by collision with ortho- and para-D ₂ molecules. Physical Chemistry Chemical Physics, 2017, 19, 189-195.	1.3	15
72	Collisional Excitation and Weak Maser Action of Interstellar Methanimine. Journal of Physical Chemistry Letters, 2018, 9, 3199-3204.	2.1	15

#	Article	IF	CITATIONS
73	Rotationally inelastic collisions of SiO with H2. Monthly Notices of the Royal Astronomical Society, 2018, 479, 2692-2701.	1.6	15
74	Rotational excitation of H2O by <i>para</i> -H2 from an adiabatically reduced dimensional potential. Journal of Chemical Physics, 2012, 136, 094109.	1.2	14
75	Ortho-to-para ratio of NH ₂ . Astronomy and Astrophysics, 2016, 586, A128.	2.1	14
76	Rotational excitation of water by hydrogen molecules: Comparison of results from classical and quantum mechanics. Journal of Chemical Physics, 2006, 124, 214310.	1.2	13
77	Note: Second virial coefficient of the water-hydrogen complex from an explicitly correlated potential energy surface. Journal of Chemical Physics, 2011, 135, 116101.	1.2	13
78	Potential energy surface and bound states of the H2O–HF complex. Journal of Chemical Physics, 2020, 153, 214301.	1.2	13
79	The effect of COâ^'H2O collisions in the rotational excitation of cometary CO. Monthly Notices of the Royal Astronomical Society, 2020, 493, 776-782.	1.6	13
80	Sulfur gas-phase abundance in dense cores. Astronomy and Astrophysics, 2022, 658, A168.	2.1	13
81	Influence of collisional rate coefficients on water vapour excitation. Astronomy and Astrophysics, 2012, 547, A81.	2.1	12
82	CN excitation and electron densities in diffuse molecular clouds. Monthly Notices of the Royal Astronomical Society, 2013, 435, 3541-3546.	1.6	12
83	The NH ₂ D hyperfine structure revealed by astrophysical observations. Astronomy and Astrophysics, 2016, 586, L4.	2.1	12
84	Rotational excitation of the interstellar NH2 radical by H2. Journal of Chemical Physics, 2017, 146, 064309.	1.2	12
85	SOFIA/GREAT Discovery of Terahertz Water Masers ^{â^—} . Astrophysical Journal, 2017, 843, 94.	1.6	12
86	Depletion and fractionation of nitrogen in collapsing cores. Astronomy and Astrophysics, 2020, 643, A76.	2.1	12
87	Cold and Yet Complex: Detection of Ethylene Oxide in a Prestellar Core. ACS Earth and Space Chemistry, 2019, 3, 1000-1013.	1.2	11
88	Low-Energy Water–Hydrogen Inelastic Collisions. Journal of Physical Chemistry A, 2020, 124, 259-264.	1.1	11
89	Deuterium fractionation of nitrogen hydrides: detections of NHD and ND2. Monthly Notices of the Royal Astronomical Society, 2020, 499, 1795-1804.	1.6	9
90	Non-LTE modelling of cyanoacetylene: evidence for isomer-specific excitation. Monthly Notices of the Royal Astronomical Society, 2020, 501, 1911-1919.	1.6	9

#	Article	IF	CITATIONS
91	The excitation of OH by H2 revisited – II. Hyperfine resolved rate coefficients. Monthly Notices of the Royal Astronomical Society, 2020, 493, 3491-3495.	1.6	9
92	Observations and Analysis of CH ⁺ Vibrational Emissions from the Young, Carbon-rich Planetary Nebula NGC 7027: A Textbook Example of Chemical Pumping. Astrophysical Journal, 2021, 917, 15.	1.6	9
93	The excitation of OH by H2 revisited – I: fine-structure resolved rate coefficients. Monthly Notices of the Royal Astronomical Society, 2017, 471, 4249-4255. Angle-Resolved Electron Scattering from <mml:math< td=""><td>1.6</td><td>8</td></mml:math<>	1.6	8
94	xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"> <mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">H</mml:mi </mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow>mathvariant="normal">O</mml:msub></mml:mrow> near 0°. Physical Review Letters, 2019,	≥29 ≷mml:mi	8
95	123, 033401. Rate constants for the H+ + H2 reaction from 5 K to 3000 K with a statistical quantum method. Journal of Chemical Physics, 2021, 154, 054310.	1.2	8
96	Probing Low-Energy Resonances in Water-Hydrogen Inelastic Collisions. Physical Review Letters, 2020, 125, 143402.	2.9	7
97	Note: On the inclusion of a diagonal Born-Oppenheimer correction in the reduced dimensional treatment of the H2O–para-H2 complex. Journal of Chemical Physics, 2017, 146, 226102.	1.2	6
98	Rotational non-LTE in HCN in the thermosphere of Titan: Implications for the radiative cooling. Astronomy and Astrophysics, 2013, 555, A122.	2.1	5
99	An accurate 5D potential energy surface for H3O+–H2 interaction. Journal of Chemical Physics, 2020, 153, 094301.	1.2	5
100	Cross Sections and Rate Coefficients for Vibrational Excitation of H2O by Electron Impact. Atoms, 2021, 9, 62.	0.7	5
101	Collisional cooling of primordial and interstellar media by H2. Monthly Notices of the Royal Astronomical Society, 2021, 507, 3564-3571.	1.6	4
102	Rotational excitation of H3O+ cations by <i>para-</i> H2: improved collisional data at low temperatures. Monthly Notices of the Royal Astronomical Society, 2021, 509, 1252-1261.	1.6	4
103	Collisional Excitation and Non-LTE Modeling of Interstellar Chiral Propylene Oxide. Astrophysical Journal, 2022, 926, 3.	1.6	4
104	The excitation of NH2 in the interstellar medium. Monthly Notices of the Royal Astronomical Society, 2019, 490, 2178-2182.	1.6	3
105	Absolute measurements of state-to-state rotational energy transfer between CO and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">H<mml:mn>2</mml:mn></mml:mi </mml:msub> at interstellar temperatures. Physical Review A. 2022. 105</mml:math 	1.0	2