Elangannan Arunan

List of Publications by Year
in descending order

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125 papers	5,607 citations	159358 30 h-index	79541 73 g-index
135 all docs	135 docs citations	135 times ranked	5179 citing authors

#	Article	IF	Citations
1	Measurement of Donor-Acceptor Interchange Tunnelling in Ar(H2O)2 using Rotational Spectroscopy and a Re-look at Its Structure and Bonding. Journal of Molecular Structure, 2022, 1252, 132094.	1.8	1
2	Rotational spectroscopic studies of the tetrel bonded CH3CN-CO2 complex. Journal of Molecular Spectroscopy, 2022, 388, 111671.	0.4	3
3	A review on hydroxyapatite coatings for the biomedical applications: experimental and theoretical perspectives. Journal of Materials Chemistry B, 2021, 9, 228-249.	2.9	91
4	Effects of Multiple OH/SH Substitution on the Hâ€Bonding/Stability versus Aromaticity of Benzene Rings: From Computational Insights. ChemistrySelect, 2021, 6, 5120-5139.	0.7	6
5	Structure and Internal Motions of a Multifunctional Alcoholâ€“Water Complex: Rotational Spectroscopy of the Propargyl AlcoholÂ·Â·Â·H₂O Dimer. Journal of Physical Chemistry A, 2021, 125, 7138-7150.	1.1	4
6	Volume 100 of the Journal of the Indian Institute of Science and 100ÂYears of the Latimer and Rodebush Paper on Hydrogen Bonding. Journal of the Indian Institute of Science, 2020, 100, 3-4.	0.9	0
7	One Hundred Years After the Latimer and Rodebush Paper, Hydrogen Bonding Remains an Elephant!. Journal of the Indian Institute of Science, 2020, 100, 249-255.	0.9	6
8	A Detailed Classification of Three-Centre Two-Electron Bonds. Australian Journal of Chemistry, 2020, 73, 767.	0.5	3
9	Coriolis Interactions in benzene-water and related molecular complexes. Journal of Molecular Spectroscopy, 2020, 370, 111277.	0.4	4
10	Reply to â€œComments on â€˜Inter/Intramolecular Bonds in TH₅⁺ (T = C/Si/Ge): H₂ as Tetrel Bond Acceptor and the Uniqueness of Carbon Bondsâ€™â€•. Journal of Physical Chemistry A, 2019, 123, 9244-9245.	1.1	0
11	Isolation of a Halogen-Bonded Complex Formed between Methane and Chlorine Monofluoride and Characterisation by Rotational Spectroscopy and Ab Initio Calculations. Molecules, 2019, 24, 4257.	1.7	1
12	Chemical bonding in Period 2 homonuclear diatomic molecules: a comprehensive relook. Journal of Chemical Sciences, 2019, 131, 1.	0.7	6
13	Inter/Intramolecular Bonds in TH₅⁺ (T = C/Si/Ge): H₂ as Tetrel Bond Acceptor and the Uniqueness of Carbon Bonds. Journal of Physical Chemistry A, 2019, 123, 1168-1176.	1.1	26
14	Interstellar hydrogen bonding. Advances in Space Research, 2018, 61, 2870-2880.	1.2	18
15	Theoretical investigation of interstellar Câ€“Câ€“O and Câ€“Oâ€“C bonding backbone molecules. Astrophysics and Space Science, 2018, 363, 1.	0.5	13
16	The H₂S Dimer is Hydrogenâ€Bonded: Direct Confirmation from Microwave Spectroscopy. Angewandte Chemie, 2018, 130, 15419-15423.	1.6	2
17	The H₂S Dimer is Hydrogenâ€Bonded: Direct Confirmation from Microwave Spectroscopy. Angewandte Chemie - International Edition, 2018, 57, 15199-15203.	7.2	47
18	Theoretical investigation of reaction kinetics and thermodynamics of the keto-enol tautomerism of 1, 3, 5-triazin-2, 4(1H, 3H)-dione and its substituted systems utilizing density functional theory and transition state theory methods. Computational and Theoretical Chemistry, 2018, 1141, 15-40.	1.1	4

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19	Molecules In Space: Physics, Chemistry And Biology. , 2018, , .		0
20	Is Indian Science Ready to Tackle Conflict of Interest in a Rational Way?. Current Science, 2018, 114, 1385.	0.4	0
21	Hydrogen Bonding: From Biological Systems To Interstellar Medium. , 2018, , .		0
22	Partition function and astronomical observation of interstellar isomers: Is there a link?. Advances in Space Research, 2017, 59, 1161-1171.	1.2	11
23	Shock-wave processing of C₆₀ in hydrogen. Astronomy and Astrophysics, 2017, 599, A42.	2.1	15
24	C5H9N isomers: pointers to possible branched chain interstellar molecules. European Physical Journal D, 2017, 71, 1.	0.6	9
25	Interstellar protonated molecular species. Advances in Space Research, 2017, 60, 709-721.	1.2	18
26	Accurate rotational constants for linear interstellar carbon chains: achieving experimental accuracy. Astrophysics and Space Science, 2017, 362, 1.	0.5	13
27	Shock Tube Ignition Delay Studies of Dicyclopentadiene. , 2017, , 333-336.		0
28	SYSTEMATIC THEORETICAL STUDY ON THE INTERSTELLAR CARBON CHAIN MOLECULES. Astrophysical Journal, 2016, 832, 144.	1.6	34
29	Interstellar isomeric species: Energy, stability and abundance relationship. European Physical Journal Plus, 2016, 131, 1.	1.2	19
30	One hundred years of Lewis Chemical Bond!. Journal of Chemical Sciences, 2016, 128, 1517-1518.	0.7	4
31	Chemical Education in India: Addressing Current Challenges and Optimizing Opportunities. Journal of Chemical Education, 2016, 93, 1731-1736.	1.1	9
32	Why are Hydrogen Bonds Directional?. Journal of Chemical Sciences, 2016, 128, 1571-1577.	0.7	29
33	Pyrolysis of 3-carene: Experiment, Theory and Modeling. Journal of Chemical Sciences, 2015, 127, 2119-2135.	0.7	5
34	Microwave Spectrum of Hexafluoroisopropanol and Torsional Behavior of Molecules with a CF₃â€“Câ€“CF₃ Group. Journal of Physical Chemistry A, 2015, 119, 5650-5657.	1.1	18
35	Dynamics of chemical bond: general discussion. Faraday Discussions, 2015, 177, 121-154.	1.6	8
36	Inter molecular azideâ€“diisocyanate coupling: new insights for energetic solid propellants. RSC Advances, 2015, 5, 50478-50482.	1.7	6

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37	Local and Global Dynamics: general discussion. Faraday Discussions, 2015, 177, 381-403.	1.6	0
38	Intramolecular hydrogen bond: Can it be part of the basis set of valence internal coordinates in normal mode analysis?. Journal of Chemical Sciences, 2015, 127, 1127-1134.	0.7	8
39	Three centered hydrogen bonds of the type Cî€Oâ‹¯H(N)â‹¯Xâ€“C in diphenyloxamide derivatives involving halogens and a rotating CF‹sub›3‹/sub› group: NMR, QTAIM, NCI and NBO studies. Physical Chemistry Chemical Physics, 2015, 17, 7528-7536.	1.3	16
40	Study of structures, energies and vibrational frequencies of (O2)n+ (n=2â€“5) clusters by GGA and meta-GGA density functional methods. Computational and Theoretical Chemistry, 2015, 1056, 24-36.	1.1	4
41	Time and Space resolved Methods: general discussion. Faraday Discussions, 2015, 177, 263-292.	1.6	1
42	Dynamics of the chemical bond: inter- and intra-molecular hydrogen bond. Faraday Discussions, 2015, 177, 51-64.	1.6	24
43	Conformational Stability and Intramolecular Hydrogen Bonding in 1,2-Ethanediol and 1,4-Butanediol. Journal of Physical Chemistry A, 2015, 119, 3710-3720.	1.1	48
44	H‹sub›2‹/sub›Oâ€“CH‹sub›4‹/sub›and H‹sub›2‹/sub›Sâ€“CH‹sub›4‹/sub›complexes: a direct comparison through molecular beam experiments and ab initio calculations. Physical Chemistry Chemical Physics, 2015, 17, 30613-30623.	1.3	22
45	X-Hâ‹¯C hydrogen bonds in n-alkane-HX (X = F, OH) complexes are stronger than C-Hâ‹¯X hydrogen bonds. Journal of Chemical Sciences, 2015, 127, 1035-1045.	0.7	10
46	Microwave spectroscopic and theoretical investigations of the strongly hydrogen bonded hexafluoroisopropanolâ‹¯water complex. Physical Chemistry Chemical Physics, 2015, 17, 24774-24782.	1.3	20
47	Future challenges: general discussion. Faraday Discussions, 2015, 177, 517-545.	1.6	3
48	The X-Câ€¦Y Carbon Bond. Challenges and Advances in Computational Chemistry and Physics, 2015, , 323-356.	0.6	9
49	Shock Tube Studies on Thermal Decomposition of 2-Chloroethylbenzene. , 2015, , 191-196.		0
50	Rotational spectra of propargyl alcohol dimer: A dimer bound with three different types of hydrogen bonds. Journal of Chemical Physics, 2014, 141, 164311.	1.2	14
51	Thermal Decomposition of Propargyl Alcohol: Single Pulse Shock Tube Experimental and ab Initio Theoretical Study. Journal of Physical Chemistry A, 2014, 118, 5927-5938.	1.1	10
52	Azide and Alkyne Terminated Polybutadiene Binders: Synthesis, Cross-linking, and Propellant Studies. Industrial & Engineering Chemistry Research, 2014, 53, 16612-16620.	1.8	31
53	Hydrogen bonding, halogen bonding and lithium bonding: an atoms in molecules and natural bond orbital perspective towards conservation of total bond order, inter- and intra-molecular bonding. Physical Chemistry Chemical Physics, 2014, 16, 22935-22952.	1.3	149
54	Do identical polar diatomic molecules form stacked or linear dimers?. Resonance, 2014, 19, 704-712.	0.2	1

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55	The Xâ€“CÂ·Â·Â·Ï€ (X = F, Cl, Br, CN) Carbon Bond. Journal of Physical Chemistry A, 2014, 118, 10081-10089.	1.1	113
56	The Xâ€“Câ‹¯Y (X = O/F, Y = O/S/F/Cl/Br/N/P) â€˜carbon bondâ€™ and hydrophobic interactions. Physical Chemistry Chemical Physics, 2013, 15, 14377.	1.3	289
57	Microwave, infrared-microwave double resonance, and theoretical studies of C2H4â‹¯H2S complex. Journal of Chemical Physics, 2013, 139, 104303.	1.2	18
58	Microwave Spectroscopic and Atoms in Molecules Theoretical Investigations on the Arâ‹…â‹…â‹…Propargyl Alcohol Complex: Arâ‹…â‹…â‹…Hï£¿O, Arâ‹…â‹…â‹…Ï€, and Arâ‹…â‹…â‹…C Interactions. ChemPhysChem, 2013, 14, 754-763.	1.0	34
59	Chemistry in India: Unlocking the Potential. Angewandte Chemie - International Edition, 2013, 52, 114-117.	7.2	8
60	Comprehensive investigations on DNaâ‹¯A (D=H/F) complexes show why â€˜sodium bondingâ€™ is not commonly observed. Chemical Physics Letters, 2013, 568-569, 63-69.	1.2	5
61	Investigations on high enthalpy shock wave exposed graphitic carbon nanoparticles. Diamond and Related Materials, 2013, 35, 53-57.	1.8	30
62	Glycidyl Azide Polymer Crosslinked Through Triazoles by Click Chemistry: Curing, Mechanical and Thermal Properties. Propellants, Explosives, Pyrotechnics, 2013, 38, 525-532.	1.0	32
63	Fe as Hydrogen/Halogen Bond Acceptor in Square Pyramidal Fe(CO)₅. Inorganic Chemistry, 2013, 52, 9153-9161.	1.9	11
64	Towards a broadband chirped pulse Fourier transform microwave spectrometer. Indian Journal of Physics, 2012, 86, 225-235.	0.9	2
65	Infrared Spectra of Dimethylphenanthrenes in the Gas phase. Journal of Physical Chemistry A, 2012, 116, 5769-5778.	1.1	4
66	Highâ€temperature kinetics of the reaction between CN and hydrocarbons using a novel highâ€enthalpy flow tube. International Journal of Chemical Kinetics, 2012, 44, 753-766.	1.0	10
67	Computational investigations on covalent dimerization/oligomerization of polyacenes: Is it relevant to soot formation?. Journal of Computational Chemistry, 2012, 33, 1762-1772.	1.5	15
68	Getting Fundamental Molecular Properties from Shock Tubes. , 2012, , 59-66.		0
69	Direct Infrared Absorption Spectroscopy of Benzene Dimer. Journal of Physical Chemistry A, 2011, 115, 11263-11268.	1.1	36
70	Microwave spectroscopic and theoretical studies on the phenylacetyleneâ‹¯H2O complex: Câ€“Hâ‹¯O and Oâ€“Hâ‹¯Ï€ hydrogen bonds as equal partners. Physical Chemistry Chemical Physics, 2011, 13, 14153.	1.3	28
71	Definition of the hydrogen bond (IUPAC Recommendations 2011). Pure and Applied Chemistry, 2011, 83, 1637-1641.	0.9	1,449
72	Defining the hydrogen bond: An account (IUPAC Technical Report). Pure and Applied Chemistry, 2011, 83, 1619-1636.	0.9	856

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73	Microwave spectrum and structure of C6H5CCHâ‹¯H2S complex. Journal of Molecular Spectroscopy, 2011, 268, 147-156.	0.4	22
74	van der Waals. Resonance, 2010, 15, 584-587.	0.2	7
75	Molecule matters van der Waals molecules. Resonance, 2010, 15, 667-674.	0.2	2
76	Peter Debye. Resonance, 2010, 15, 1056-1059.	0.2	0
77	Crystalline ethane-1,2-diol does not have intra-molecular hydrogen bonding: Experimental and theoretical charge density studies. Journal of Molecular Structure, 2010, 964, 126-133.	1.8	66
78	Infrared Spectra of Dimethylquinolines in the Gas Phase: Experiment and Theory. Journal of Physical Chemistry A, 2010, 114, 8351-8358.	1.1	7
79	Molecule matters van der Waals molecules. Resonance, 2009, 14, 346-356.	0.2	4
80	Molecule Matters van der Waals Molecules. Resonance, 2009, 14, 1210-1222.	0.2	5
81	Characterization of circumstellar carbonaceous dust analogues produced by pyrolysis of acetylene in a porous graphite reactor. Carbon, 2009, 47, 3295-3305.	5.4	32
82	The hydrogen bond: a molecular beam microwave spectroscopistâ€™s view with a universal appeal. Physical Chemistry Chemical Physics, 2009, 11, 8974.	1.3	48
83	Spectroscopic studies of micro-explosions. , 2009, , 377-382.		3
84	Ignition delay studies on hydrocarbon fuel with and without additives. , 2009, , 745-750.		0
85	Hydrogen bonding with a hydrogen bond: The methaneâ€“water complex and the penta-coordinate carbon. Chemical Physics Letters, 2008, 467, 37-40.	1.2	68
86	Infrared spectra of dimethylnaphthalenes in the gas phase. Vibrational Spectroscopy, 2008, 47, 1-9.	1.2	21
87	Aerodynamic drag reduction by heat addition into the shock layer for a large angle blunt cone in hypersonic flow. Physics of Fluids, 2008, 20, .	1.6	36
88	Unpaired and Ïƒ Bond Electrons as H, Cl, and Li Bond Acceptors:â€‰ An Anomalous One-Electron Blue-Shifting Chlorine Bond. Journal of Physical Chemistry A, 2007, 111, 9699-9706.	1.1	78
89	Ab initio and AIM theoretical analysis of hydrogen-bond radius of HD (D = F, Cl, Br, CN, HO, HS and) Tj ETQq1 1 0.784314 rgBT /Overlo	1.3	53
90	Rotational spectra of mono-substituted asymmetric C6H6â€“H2O dimers. Journal of Molecular Spectroscopy, 2005, 232, 308-314.	0.4	9

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91	Rotational spectra and structure of the Ar2â€“H2S complex: pulsed nozzle Fourier transform microwave spectroscopic and ab initio studies. Physical Chemistry Chemical Physics, 2005, 7, 2740.	1.3	10
92	Is there a hydrogen bond radius? Evidence from microwave spectroscopy, neutron scattering and X-ray diffraction results. New Journal of Chemistry, 2005, 29, 371.	1.4	50
93	Thermal decomposition of haloethanols: single pulse shock tube and ab initio studies. , 2005, , 621-626.		2
94	Chlorine bond distances in ClF and Cl2 complexes. Journal of Molecular Structure, 2004, 688, 203-205.	1.8	11
95	Rotational spectra and structure of the floppy C2H4â€“H2S complex: bridging hydrogen bonding and van der Waals interactions. Chemical Physics Letters, 2004, 393, 22-27.	1.2	25
96	Pulsed Nozzle Fourier Transform Microwave Spectrometer: Advances and Applications. Applied Spectroscopy Reviews, 2004, 39, 131-181.	3.4	31
97	Thermal Decomposition of 2-Fluoroethanol:â€‰ Single Pulse Shock Tube and ab Initio Studies. Journal of Physical Chemistry A, 2003, 107, 9782-9793.	1.1	18
98	Ab initio, DFT and transition state theory calculations on 1,2-HF, HCl and ClF elimination reactions from CH2Fâ€“CH2Cl. Physical Chemistry Chemical Physics, 2003, 5, 3897-3904.	1.3	34
99	Rotational spectrum of the weakly bonded C6H6â€“H2S dimer and comparisons to C6H6â€“H2O dimer. Journal of Chemical Physics, 2002, 117, 9766-9776.	1.2	52
100	Rotational spectra, structures, and dynamics of small Ar[sub m]â€“(H[sub 2]O)[sub n] clusters: The Arâ€“(H[sub 2]O)[sub 2] trimer. Journal of Chemical Physics, 2002, 116, 4886.	1.2	14
101	Infrared chemiluminescence: Evidence for adduct formation in the Hâ€‰+â€‰CH2XI reaction and studies of the Nâ€‰+â€‰CH2X (Xâ€‰=â€‰Cl/F/I/H) reactions. Physical Chemistry Chemical Physics, 2002, 4, 51-59.	1.3	5
102	Unimolecular HCl Elimination from 1,2-Dichloroethane:â€‰ A Single Pulse Shock Tube and ab Initio Study. Journal of Physical Chemistry A, 2002, 106, 8366-8373.	1.1	24
103	Chlorofluoroamines: Ab Initio and DFT Studies on Their Structure, Enthalpies of Formation, and Unimolecular Reaction Pathways. Journal of Physical Chemistry A, 2001, 105, 8533-8540.	1.1	12
104	Rotational spectra and structures of the Ar3â€“H2O and Ar3â€“H2S symmetric tops. Journal of Chemical Physics, 2001, 114, 1242-1248.	1.2	20
105	Hydrogen bond radii for the hydrogen halides and van der Waals radius of hydrogen. Journal of Chemical Physics, 2001, 114, 3880-3882.	1.2	31
106	Unimolecular Reaction Dynamics of CH3COCl and FCH2COCl:â€‰ An Infrared Chemiluminescence and ab Initio Study. Journal of Physical Chemistry A, 1998, 102, 6412-6420.	1.1	17
107	Rotational spectra, structure, and internal dynamics of Arâ€“H2S isotopomers. Journal of Chemical Physics, 1997, 106, 5309-5315.	1.2	34
108	The Câ”C Bond Is Stronger than the Câ”Cl Bond in CH3COCl. Journal of Physical Chemistry A, 1997, 101, 4838-4839.	1.1	21

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109	Rotational spectra, structures, and dynamics of small Armâ€“(H2O)n clusters: The Ar2â€“H2O trimer. Journal of Chemical Physics, 1996, 105, 8495-8501.	1.2	27
110	Rotational spectra and structures of the C6H6â€“HCN dimer and Ar3â€“HCN tetramer. Journal of Chemical Physics, 1995, 103, 3917-3927.	1.2	31
111	Excited Î½3vibrational state of the Arâ€“HCN and Krâ€“HCN dimers. Journal of Chemical Physics, 1995, 103, 493-496.	1.2	7
112	Rotational spectra and van der Waals potentials of Neâ€“Ar. Journal of Chemical Physics, 1995, 102, 1181-1187.	1.2	58
113	Infrared chemiluminescence studies of the atomic hydrogen + chlorofluoroamine (H + NFCl2) and H + NFCl reactions. The Journal of Physical Chemistry, 1994, 98, 494-501.	2.9	18
114	Rotational spectra and structures of Rgâ€“C6H6â€“H2O trimers and the Neâ€“C6H6 dimer (Rg=Ne, Ar, or Kr). Journal of Chemical Physics, 1994, 101, 861-868.	1.2	53
115	Infrared chemiluminescence studies of the reactions of H atoms with CCl3, CF2Cl, and CH2CH2Cl radicals at 300 and 475â€‚K: recombinationâ€“elimination vs. abstraction mechanisms. Canadian Journal of Chemistry, 1994, 72, 568-576.	0.6	30
116	Rotational Spectra, Structure, and Dynamics of Arm-(H2O)n Clusters: Ar2-H2O, Ar3-H2O, Ar-(H2O)2, and Ar-(H2O)3. Journal of the American Chemical Society, 1994, 116, 8418-8419.	6.6	35
117	Infrared chemiluminescence studies of H + BrCN and H abstraction by CN reactions. Importance of the HNC channel. Chemical Physics Letters, 1993, 207, 81-87.	1.2	28
118	Rotational spectrum and structure of Neâ€“C6H6â€“H2O, an aromatic sandwich. Journal of Chemical Physics, 1993, 99, 6208-6210.	1.2	29
119	The rotational spectrum, structure and dynamics of a benzene dimer. Journal of Chemical Physics, 1993, 98, 4294-4296.	1.2	314
120	Lowâ€rotational spectra, internal rotation, and structures of several benzeneâ€“water dimers. Journal of Chemical Physics, 1993, 99, 4883-4893.	1.2	184
121	Vibrationâ€“rotational Einstein coefficients for HF/DF and HCl/DCl. Journal of Chemical Physics, 1992, 97, 1734-1741.	1.2	67
122	Vibrational relaxation rate constants for HF(v=1â€“4) by CO, CO2, and HCN with product identification by infrared emission. Journal of Chemical Physics, 1992, 97, 6348-6362.	1.2	10
123	Hydrogen cyanide infrared chemiluminescence from the hydrogen atom + iodine cyanide reaction. The Journal of Physical Chemistry, 1991, 95, 4190-4193.	2.9	13
124	Hydrogen fluoride/hydrogen chloride vibrational and rotational distributions from three- and four-centered unimolecular elimination reactions. The Journal of Physical Chemistry, 1991, 95, 1539-1547.	2.9	64
125	Sequence Determination in Acrylic Acid-Methyl Methacrylate Copolymers by 13C and 1H NMR Spectroscopy. Polymer Journal, 1989, 21, 689-695.	1.3	18