

JOURNAL ARTICLES

CHEMISTRY

244. Venkatesh V., Mishra N.K., Romero-Canelón I., Vernooij R.R., Shi H., Coverdale J.P.C., Habtemariam A., Verma S., Sadler P.J., Supramolecular Photoactivatable Anticancer Hydrogels, *Journal of the American Chemical Society*, Vol. 139, 5656-5659 (2017).
245. Sarbajna A., Pandey P., Rahaman S.M.W., Singh K., Tyagi A., Dixneuf P.H., Bera J.K., A Triflamide-Tethered N-Heterocyclic Carbene–Rhodium(I) Catalyst for Hydroalkoxylation Reactions: Ligand-Promoted Nucleophilic Activation of Alcohols, *ChemCatChem*, Vol. 9, 1397-1401 (2017).
246. Singh G., Nandi A., Gadre S.R., Chiba T., Fujii A., A combined theoretical and experimental study of phenol-(acetylene)_n ($n \leq 7$) clusters, *Journal of Chemical Physics*, Vol. 146, - (2017).
247. Gupta A.K., De D., Katoch R., Garg A., Bharadwaj P.K., Synthesis of a NbO Type Homochiral Cu(II) Metal-Organic Framework: Ferroelectric Behavior and Heterogeneous Catalysis of Three-Component Coupling and Pechmann Reactions, *Inorganic Chemistry*, Vol. 56, 4697-4705 (2017).
248. Guchhait T., Sasmal S., Khan F.S.T., Rath S.P., Oxo- and hydroxo-bridged diiron(III) porphyrin dimers: Inorganic and bio-inorganic perspectives and effects of intermacrocylic interactions, *Coordination Chemistry Reviews*, Vol. 337, 112-144 (2017).
249. Sarbajna A., Dutta I., Daw P., Dinda S., Rahaman S.M.W., Sarkar A., Bera J.K., Catalytic Conversion of Alcohols to Carboxylic Acid Salts and Hydrogen with Alkaline Water, *ACS Catalysis*, Vol. 7, 2786-2790 (2017).
250. Penke Y.K., Anantharaman G., Ramkumar J., Kar K.K., Aluminum Substituted Cobalt Ferrite (Co–Al–Fe) Nano Adsorbent for Arsenic Adsorption in Aqueous Systems and Detailed Redox Behavior Study with XPS, *ACS Applied Materials and Interfaces*, Vol. 9, 11587-11598 (2017).
251. Saravanan R.K., Saha P., Venkatesh V., Gopakumar T.G., Verma S., Coordination-Controlled One-Dimensional Molecular Chains in Hexapodal Adenine-Silver Ultrathin Films, *Inorganic Chemistry*, Vol. 56, 3976-3982 (2017).
252. Saha B., Iqbal S.A., Petrovic A.G., Berova N., Rath S.P., Complexation of Chiral Zinc-Porphyrin Tweezer with Achiral Diamines: Induction and Two-Step Inversion of Interporphyrin Helicity Monitored by ECD, *Inorganic Chemistry*, Vol. 56, 3849-3860 (2017).
253. Tripathi K.M., Bhati A., Singh A., Sonker A.K., Sarkar S., Sonkar S.K., Sustainable Changes in the Contents of Metallic Micronutrients in First Generation Gram Seeds Imposed by Carbon Nano-onions: Life Cycle Seed to Seed Study, *ACS Sustainable Chemistry and Engineering*, Vol. 5, 2906-2916 (2017).
254. Chu X., Xu X., Su H., Raje S., Angamuthu R., Tung C.-H., Wang W., Heteronuclear assembly of Ni-Cu dithiolato complexes: Synthesis, structures, and reactivity studies, *Inorganic Chemistry Frontiers*, Vol. 4, 706-711 (2017).

255. Chandrasekhar P., Savitha G., Moorthy J.N., Robust MOFs of “tsg” Topology Based on Trigonal Prismatic Organic and Metal Cluster SBUs: Single Crystal to Single Crystal Postsynthetic Metal Exchange and Selective CO₂ Capture, *Chemistry - A European Journal*, Vol. 23, 7297-7305 (2017).
256. Mandal R., Sundararaju B., Cp*Co(III)-Catalyzed Annulation of Carboxylic Acids with Alkynes, *Organic Letters*, Vol. 19, 2544-2547 (2017).
257. López R., Rico J.F., Ramírez G., Ema I., Zorrilla D., Kumar A., Yeole S.D., Gadre S.R., Topology of molecular electron density and electrostatic potential with DAMQT, *Computer Physics Communications*, Vol. 214, 207-215 (2017).
258. Kumar Shahi C., Pradhan S., Bhattacharyya A., Kumar R., Ghorai M.K., Accessing Quinoxalines by Ring-Opening/Cyclization/Detosylation/Aromatization of Activated Aziridines with 2-Bromoanilines: Synthesis of Tyrphostin AG 1296, *European Journal of Organic Chemistry*, Vol. 2017, 3487-3495 (2017).
259. Bhatt G., Kant R., Mishra K., Yadav K., Singh D., Gurunath R., Bhattacharya S., Impact of surface roughness on Dielectrophoretically assisted concentration of microorganisms over PCB based platforms, *Biomedical Microdevices*, Vol. 19, - (2017).
260. Sen M., Dahiya P., Premkumar J.R., Sundararaju B., Dehydrative Cp*Co(III)-Catalyzed C-H Bond Allenylation, *Organic Letters*, Vol. 19, 3699-3702 (2017).
261. Mondal P., Rath S.P., A Tunable Cyclic Container: Guest-Induced Conformational Switching, Efficient Guest Exchange, and Selective Isolation of C₇₀ from a Fullerene Mixture, *Chemistry - An Asian Journal*, Vol. 12, 1824-1835 (2017).
262. Biswas S., Bejoymohandas K.S., Das S., Kalita P., Reddy M.L.P., Oyarzabal I., Colacio E., Chandrasekhar V., Mononuclear Lanthanide Complexes: Energy-Barrier Enhancement by Ligand Substitution in Field-Induced Dy^{III} SIMs, *Inorganic Chemistry*, Vol. 56, 7985-7997 (2017).
263. Gupta S., Mukherjee P., Sengupta B., Sen P., Dynamical response in methanol-chloroform binary solvent mixture over fs-μs time regime, *Physics and Chemistry of Liquids*, Vol. , 1-12 (2017).
264. Singh S.P., Guha S., Bose P., Kunnikuruvaan S., Mechanism of the Hydrolysis of Endosulfan Isomers, *Journal of Physical Chemistry A*, Vol. 121, 5156-5163 (2017).
265. Pradhan S., Shahi C.K., Bhattacharyya A., Chauhan N., Ghorai M.K., Syntheses of Tetrahydrobenzoazepinoindoles and Dihydrobenzodiazepinoindoles via Ring-Opening Cyclization of Activated Aziridines with 2-(2-Bromophenyl)-1H-indoles, *Organic Letters*, Vol. 19, 3438-3441 (2017).
266. Fatma S., Bishnoi A., Verma A.K., Singh R., Srivastava A., Synthesis, crystal structure, spectroscopic and quantum chemical studies of novel 3-((2-chlorophenyl)(piperidin-1-yl)methyl)-4-hydroxy-1-phenylquinolin-2(1H)-one, *Journal of Molecular Structure*, Vol. 1139, 338-352 (2017).
267. Rajasekaran P., Mallikharjunarao Y., Vankar Y.D., Synthesis of 1 C -Aryl/Alkyl 2 C - Branched Sugar-Fused Isochroman Derivatives by Sequential Prins and Friedel-

- Crafts Cyclizations on a Perlin Aldehyde Derived Substrate, *Synlett*, Vol. 28, 1346-1352 (2017).
268. Mehrotra S., Raje S., Jain A.K., Angamuthu R., Benzimidazolines Convert Sulfur Dioxide to Bisulfate at Room Temperature and Atmospheric Pressure Utilizing Aerial Oxygen, *ACS Sustainable Chemistry and Engineering*, Vol. 5, 6322-6328 (2017).
269. Ojha D., Chandra A., Vibrational echo spectral observables and frequency fluctuations of hydration shell water around a fluoride ion from first principles simulations, *Journal of Chemical Sciences*, Vol. 129, 1069-1080 (2017).
270. Agarwal R.A., One step hydrothermal synthesis of transition metal based coordination polymers along with magnetic and electrical conductive Ag and Au nanospheres and rods, *Journal of Solid State Chemistry*, Vol. 251, 116-121 (2017).
271. Shukla A., Keshavamurthy S., Controlling the quantum rotational dynamics of a driven planar rotor by rebuilding barriers in the classical phase space, *Journal of Chemical Sciences*, Vol. 129, 1005-1016 (2017).
272. Maurya S.K., Dutta C., Goswami D., Concentration Dependent Approach for Accurate Determination of Two-Photon Absorption Cross-Section of Fluorescent dye Molecule, *Journal of Fluorescence*, Vol. 27, 1399-1403 (2017).
273. Ghosh S., Abbas Z., Dasari S., Patra A.K., Luminescent Eu³⁺ and Tb³⁺ complexes of 4-aminophenyl terpyridine (ptpy): Photophysical aspects, DNA and serum protein binding properties, *Journal of Luminescence*, Vol. 187, 46-52 (2017).
274. Eqbal A., Srinivasan S., Sathyamurthy N., Stabilisation of the [6]-prismane structure by silicon substitution, *Journal of Chemical Sciences*, Vol. 129, 911-917 (2017).
275. Debnath J., Kunnikuruvan S., Sinha N., Parandekar P.V., Prakash O., Tsotsis T.K., Nair N.N., A database-based approach for predicting coupled cascade reaction kinetics in polymers: application to oxidative degradation kinetics of high-performance polymers, *Molecular Simulation*, Vol. 44, 582-589 (2018).
276. Gupta S., Kumar A., Joshi K.B., Study of electron transfer process in aqueous methanol system by using tryptophan based short peptide – Amino acid pairs, *Journal of Photochemistry and Photobiology A: Chemistry*, Vol. 356, 556-564 (2018).
277. Roy S., Saswati, Lima S., Dhaka S., Maurya M.R., Acharyya R., Eagle C., Dinda R., Synthesis, structural studies and catalytic activity of a series of dioxidomolybdenum(VI)-thiosemicarbazone complexes, *Inorganica Chimica Acta*, Vol. 474, 134-143 (2018).
278. Rao G.H.M., A Novel Diazomethane-Mediated Synthesis of Azetidine-Embedded Tetracyclic Ketal Systems, *Synthesis (Germany)*, Vol., - (2018).
279. Roy B.C., Debnath S., Chakrabarti K., Paul B., Maji M., Kundu S., Ortho -Amino group functionalized 2,2'-bipyridine based Ru(II) complex catalysed alkylation of secondary alcohols, nitriles and amines using alcohols, *Organic Chemistry Frontiers*, Vol. 5, 1008-1018 (2018).
280. Dethe D.H., Dherange B.D., Total Synthesis of Adunctin B, *Journal of Organic Chemistry*, Vol. 83, 3392-3396 (2018).

281. Tripathi G., Ramanathan G., Crystallographic studies on complexes of potassium iodide and copper perchlorate with N, N'-dicyclohexylurea tethered to a benzo-12-crown-4, *Journal of Molecular Structure*, Vol. 1156, 273-279 (2018).
282. Bertocchi M.J., Zhang X.-F., Bajpai A., Moorthy J.N., Weiss R.G., Fluorescence quenching of sterically-graded pyrene molecules by N,N-dialkylanilines. Exciplexes or locally excited states?, *Journal of Photochemistry and Photobiology A: Chemistry*, Vol. 355, 467-478 (2018).
283. Rajesh N., Barsu N., Sundararaju B., Recent advances in C(sp³)-H bond carbonylation by first row transition metals, *Tetrahedron Letters*, Vol. 59, 862-868 (2018).
284. Bar A.K., Kalita P., Sutter J.-P., Chandrasekhar V., Pentagonal-Bipyramid Ln(III) Complexes Exhibiting Single-Ion-Magnet Behavior: A Rational Synthetic Approach for a Rigid Equatorial Plane, *Inorganic Chemistry*, Vol. 57, 2398-2401 (2018).
285. Garg P., Singh A., Unmasking Dipole Character of Acyl Ketene Dithioacetals via a Cascade Reaction with Arynes: Synthesis of Benzo[b]thiophenes, *Organic Letters*, Vol. 20, 1320-1323 (2018).
286. Singh A., Badi-Uz-Zama K., Ramanathan G., Protonation of the imino nitrogen deactivates the excited state of imidazolin-5-one in the solid state, *Journal of Chemical Sciences*, Vol. 130, - (2018).
287. Sudarkodi V., Sooraj K., Nair N.N., Basu S., Parandekar P.V., Sinha N.K., Prakash O., Tsotsis T., Mechanical response of two polyimides through coarse-grained molecular dynamics simulations, *Modelling and Simulation in Materials Science and Engineering*, Vol. 26, - (2018).
288. Sharma B., Chandra A., Born-Oppenheimer Molecular Dynamics Simulations of a Bromate Ion in Water Reveal Its Dual Kosmotropic and Chaotropic Behavior, *Journal of Physical Chemistry B*, Vol. 122, 2090-2101 (2018).
289. Kalsi D., Barsu N., Sundararaju B., CoIII-Catalyzed Isonitrile Insertion/Acyl Group Migration Between C-H and N-H bonds of Arylamides, *Chemistry - A European Journal*, Vol. 24, 2360-2364 (2018).
290. Saha A., Bhattacharyya A., Talukdar R., Ghorai M.K., Stereospecific syntheses of enamionitriles and β -Enaminoesters via Domino Ring-Opening Cyclization (DROC) of Activated Cyclopropanes with Pronucleophilic Malononitriles, *Journal of Organic Chemistry*, Vol. 83, 2131-2144 (2018).
291. Ray S.K., Biswas R.G., Suneja A., Sadhu M.M., Singh V.K., (R)-DM-SEGPHOS-Ag(I)-Catalyzed Enantioselective Synthesis of Pyrrolidines and Pyrrolizidines via (1,3)- and Double (1,3)-Dipolar Cycloaddition Reactions, *Journal of Organic Chemistry*, Vol. 83, 2293-2308 (2018).
292. Maji M., Chakrabarti K., Paul B., Roy B.C., Kundu S., Ruthenium(II)-NNN-Pincer-Complex-Catalyzed Reactions Between Various Alcohols and Amines for Sustainable C-N and C-C Bond Formation, *Advanced Synthesis and Catalysis*, Vol. 360, 722-729 (2018).
293. Saswati, Roy S., Dash S.P., Acharyya R., Kaminsky W., Ugone V., Garribba E., Harris C., Lowe J.M., Dinda R., Chemistry of oxidomolybdenum(IV) and -(VI)

- complexes with ONS donor ligands: Synthesis, computational evaluation and oxo-transfer reactions, *Polyhedron*, Vol. 141, 322-336 (2018).
294. Singh H., Singh S., Agarwal P., Tandon P., Erande R.D., Dethe D.H., Structural and spectroscopic analysis of indole alkaloids: Molecular docking and DFT approach, *Journal of Molecular Structure*, Vol. 1153, 262-274 (2018).
 295. Chandra Maji R., Mishra S., Bhandari A., Singh R., Olmstead M.M., Patra A.K., A Copper(II) Nitrite That Exhibits Change of Nitrite Binding Mode and Formation of Copper(II) Nitrosyl Prior to Nitric Oxide Evolution, *Inorganic Chemistry*, Vol. 57, 1550-1561 (2018).
 296. Dethe D.H., Sau S.K., Biomimetic Enantioselective Total Synthesis of (-)-Petromindole, *Organic Letters*, Vol. 20, 632-635 (2018).
 297. Veeraswamy V., Goswami G., Mukherjee S., Ghosh K., Saha M.L., Sengupta A., Ghorai M.K., Memory of Chirality Concept in Asymmetric Intermolecular Michael Addition of α -Amino Ester Enolates to Enones and Nitroalkenes, *Journal of Organic Chemistry*, Vol. 83, 1106-1115 (2018).
 298. Dethe D.H., Dherange B.D., Das S., Biomimetic Total Syntheses of Callistrilones A, B, and D, *Organic Letters*, Vol. 20, 680-683 (2018).
 299. Sengupta B., Das N., Sen P., Monomerization and aggregation of β -lactoglobulin under adverse condition: A fluorescence correlation spectroscopic investigation, *Biochimica et Biophysica Acta - Proteins and Proteomics*, Vol. 1866, 316-326 (2018).
 300. Yadav S., Chandra A., Structural and Dynamical Nature of Hydration Shells of the Carbonate Ion in Water: An Ab Initio Molecular Dynamics Study, *Journal of Physical Chemistry B*, Vol. 122, 1495-1504 (2018).
 301. Gupta M., De D., Tomar K., Bharadwaj P.K., From Zn(II)-Carboxylate to Double-Walled Zn(II)-Carboxylate Phosphate MOF: Change in the Framework Topology, Capture and Conversion of CO₂, and Catalysis of Strecker Reaction, *Inorganic Chemistry*, Vol. 56, 14605-14611 (2017).
 302. Dey A., Das S., Kundu S., Mondal A., Rouzières M., Mathonière C., Clérac R., Suriya Narayanan R., Chandrasekhar V., Heterometallic Heptanuclear [Cu₅Ln₂] (Ln = Tb, Dy, and Ho) Single-Molecule Magnets Organized in One-Dimensional Coordination Polymeric Network, *Inorganic Chemistry*, Vol. 56, 14612-14623 (2017).
 303. Sen M., Mandal R., Das A., Kalsi D., Sundararaju B., Cp*Co(III)-Catalyzed Bis-isoquinolone Synthesis by C-H Annulation of Arylamide with 1,3-Diyne, *Chemistry - A European Journal*, Vol. 23, 17454-17457 (2017).
 304. Dhamija A., Saha B., Rath S.P., Metal-Center-Driven Supramolecular Chirogenesis in Tweezer Amino Alcohol Complexes: Structural, Spectroscopic, and Theoretical Investigations, *Inorganic Chemistry*, Vol. 56, 15203-15215 (2017).
 305. Yadav S., Chandra A., Preferential solvation, ion pairing, and dynamics of concentrated aqueous solutions of divalent metal nitrate salts, *Journal of Chemical Physics*, Vol. 147, - (2017).

306. Srivastav S.K., Johari A., Patel S.K.S., Gajbhiye N.S., Presence of glassy state and large exchange bias in nanocrystalline BiFeO₃, *Journal of Magnetism and Magnetic Materials*, Vol. 441, 503-510 (2017).
307. Wani M.A., Pandey M.D., Pandey R., Maurya S.K., Goswami D., A Dual-Signaling Ferrocene-Pyrene Dyad: Triple-Mode Recognition of the Cu(II) Ions in Aqueous Medium, *Journal of Fluorescence*, Vol. 27, 2279-2286 (2017).
308. Srivastava A.K., Pandey S.K., Misra N., Structure, electronic properties and electronic excitation analyses of Si₆₀[sbnd]Si₆₀ dimer and Si₅₉Al[sbnd]Si₅₉P complex, *Current Applied Physics*, Vol. 17, 1376-1381 (2017).
309. Mukherjee P., Das A., Sen P., Ultrafast excited state deactivation channel of thioflavin T adsorbed on SDS micelle: A combined femtosecond fluorescence and transient absorption study, *Journal of Photochemistry and Photobiology A: Chemistry*, Vol. 348, 287-294 (2017).
310. Dutta I., De S., Yadav S., Mondol R., Bera J.K., Aerobic oxidative coupling of alcohols and amines towards imine formation by a dicopper(I,I) catalyst, *Journal of Organometallic Chemistry*, Vol. 849-850, 117-124 (2017).
311. Agarwal R.A., Gupta N.K., Developing multifunctional nanoparticles in a 1-D coordination polymer of Cd(II), *Journal of Solid State Chemistry*, Vol. 255, 206-214 (2017).
312. Mudsainiyan R.K., Pandey S.K., A Combined Theoretical Calculation and Hirshfeld Surface Analysis of Cooperative Non-covalent Interactions in the Crystal Packing in [Cu(L1)₂(EDA)], *Zeitschrift fur Anorganische und Allgemeine Chemie*, Vol. 643, 1245-1252 (2017).
313. Dubbu S., Vankar Y.D., Diversity-Oriented Synthesis of Carbohydrate Scaffolds through the Prins Cyclization of Differently Protected d-Mannitol-Derived Homoallylic Alcohols, *European Journal of Organic Chemistry*, Vol. 2017, 5986-6002 (2017).
314. Chugh M., Ranganathan M., Lattice kinetic Monte Carlo simulation study of the early stages of epitaxial GaN(0001) growth, *Applied Surface Science*, Vol. 422, 1120-1128 (2017).
315. Singh G., Verma R., Wagle S., Gadre S.R., Explicit hydration of ammonium ion by correlated methods employing molecular tailoring approach, *Molecular Physics*, Vol. 115, 2708-2720 (2017).
316. Verma K., Viswanathan K.S., Majumder M., Sathyamurthy N., How different is the borazine-acetylene dimer from the benzene-acetylene dimer? A matrix isolation infrared and ab initio quantum chemical study, *Molecular Physics*, Vol. 115, 2637-2648 (2017).
317. Goura J., Colacio E., Herrera J.M., Suturina E.A., Kuprov I., Lan Y., Wernsdorfer W., Chandrasekhar V., Heterometallic Zn₃Ln₃ Ensembles Containing (μ₆-CO₃) Ligand and Triangular Disposition of Ln³⁺ ions: Analysis of Single-Molecule Toroid (SMT) and Single-Molecule Magnet (SMM) Behavior, *Chemistry - A European Journal*, Vol. 23, 16621-16636 (2017).

318. Verma A., Tomar K., Bharadwaj P.K., Chiral Cadmium(II) Metal-Organic Framework from an Achiral Ligand by Spontaneous Resolution: An Efficient Heterogeneous Catalyst for the Strecker Reaction of Ketones, *Inorganic Chemistry*, Vol. 56, 13629-13633 (2017).
319. Sharma B., Chandra A., Ab Initio Molecular Dynamics Simulation of the Phosphate Ion in Water: Insights into Solvation Shell Structure, Dynamics, and Kosmotropic Activity, *Journal of Physical Chemistry B*, Vol. 121, 10519-10529 (2017).
320. Shee S., Paul B., Panja D., Roy B.C., Chakrabarti K., Ganguli K., Das A., Das G.K., Kundu S., Tandem Cross Coupling Reaction of Alcohols for Sustainable Synthesis of β -Alkylated Secondary Alcohols and Flavan Derivatives, *Advanced Synthesis and Catalysis*, Vol. 359, 3888-3893 (2017).
321. Mukhopadhyay A., Mishra A.K., Jana K., Moorthy J.N., A new MediaChrom (fluorosolvatochromic and acidochromic) based on bipolar donor-acceptor conjoined carbazolo-phenazine, *Journal of Photochemistry and Photobiology A: Chemistry*, Vol. 347, 199-208 (2017).
322. Khorwal V., Sen P., Ultrafast excited state intermolecular proton transfer dynamics of 2-(4'-Pyridyl)benzimidazole inside the nanocavity of reverse micelles, *Journal of Photochemistry and Photobiology A: Chemistry*, Vol. 347, 86-92 (2017).
323. Agarwal R.A., Flexible porous coordination polymer of Ni(II) for developing nanoparticles through acid formation and redox activity of the framework, *Journal of Solid State Chemistry*, Vol. 254, 119-125 (2017).
324. Pratibha, Singh S., Sivakumar S., Verma S., Purine-Based Fluorescent Sensors for Imaging Zinc Ions in HeLa Cells, *European Journal of Inorganic Chemistry*, Vol. 2017, 4202-4209 (2017).
325. Bertocchi M.J., Lupicki A., Bajpai A., Moorthy J.N., Weiss R.G., Influence of Cations on the Fluorescence Quenching of an Ionic, Sterically Congested Pyrenyl Moiety by Iodide in Water, *Journal of Physical Chemistry A*, Vol. 121, 7588-7596 (2017).
326. Mandal D., Dolai R., Chrysochos N., Kalita P., Kumar R., Dhara D., Maiti A., Narayanan R.S., Rajaraman G., Schulzke C., Chandrasekhar V., Jana A., Stepwise Reversible Oxidation of N-Peralkyl-Substituted NHC-CAAC Derived Triazaalkenes: Isolation of Radical Cations and Dications, *Organic Letters*, Vol. 19, 5605-5608 (2017).
327. Mukhopadhyay A., Hossen T., Ghosh I., Koner A.L., Nau W.M., Sahu K., Moorthy J.N., Helicity-Dependent Regiodifferentiation in the Excited-State Quenching and Chiroptical Properties of Inward/Outward Helical Coumarins, *Chemistry - A European Journal*, Vol. 23, 14797-14805 (2017).
328. Jadhav S.D., Singh A., Oxidative Annulations Involving DMSO and Formamide: K₂S₂O₈ Mediated Syntheses of Quinolines and Pyrimidines, *Organic Letters*, Vol. 19, 5673-5676 (2017).
329. Kayal A., Chandra A., Infrared Spectral and Dynamical Properties of Water Confined in Nanobubbles at Hybrid Interfaces of Diamond and Graphene: A Molecular Dynamics Study, *Journal of Physical Chemistry C*, Vol. 121, 23455-23462 (2017).

330. Kayal A., Chandra A., Orientational order and dynamics of interfacial water near a hexagonal boron-nitride sheet: An ab initio molecular dynamics study, *Journal of Chemical Physics*, Vol. 147, - (2017).
331. Kalsi D., Barsu N., Dahiya P., Sundararaju B., C-H and N-H Bond Annulation of Benzamides with Isonitriles Catalyzed by Cobalt(III), *Synthesis (Germany)*, Vol. 49, 3937-3944 (2017).
332. Rao M.L.N., Ramakrishna B.S., Rhodium-Catalyzed Directing-Group-Assisted Aldehydic C-H Arylations with Aryl Halides, *European Journal of Organic Chemistry*, Vol. 2017, 5080-5093 (2017).
333. Chakrabarti K., Maji M., Panja D., Paul B., Shee S., Das G.K., Kundu S., Utilization of MeOH as a C1 Building Block in Tandem Three-Component Coupling Reaction, *Organic Letters*, Vol. 19, 4750-4753 (2017).
334. De D., Bhattacharyya A., Bharadwaj P.K., Enantioselective Aldol Reactions in Water by a Proline-Derived Cryptand and Fixation of CO₂ by Its Exocyclic Co(II) Complex, *Inorganic Chemistry*, Vol. 56, 11443-11449 (2017).
335. Raj A.M., Porel M., Mukherjee P., Ma X., Choudhury R., Galoppini E., Sen P., Ramamurthy V., Ultrafast Electron Transfer from Upper Excited State of Encapsulated Azulenes to Acceptors across an Organic Molecular Wall, *Journal of Physical Chemistry C*, Vol. 121, 20205-20216 (2017).
336. Pandit Y.A., Sanfui S., Rath S.P., Intermacrocyclic Interaction Triggers Facile One-Pot Synthesis of a Chlorin-Porphyrin Heterodimer, *Chemistry - A European Journal*, Vol. 23, 13415-13422 (2017).
337. Yadav S., Choudhary A., Chandra A., A First-Principles Molecular Dynamics Study of the Solvation Shell Structure, Vibrational Spectra, Polarity, and Dynamics around a Nitrate Ion in Aqueous Solution, *Journal of Physical Chemistry B*, Vol. 121, 9032-9044 (2017).
338. Garg P., Jadhav S.D., Singh A., Oxidation State Dichotomy in Copper-Catalyzed Intramolecular Cyclization of α -Diazoanilides: An Integrated Synthetic Platform for Oxindoles and Isatins Enabled by Oxygenase-Type Reactivity, *Asian Journal of Organic Chemistry*, Vol. 6, 1019-1023 (2017).
339. Fiscaro G., Genovese L., Andreussi O., Mandal S., Nair N.N., Marzari N., Goedecker S., Soft-Sphere Continuum Solvation in Electronic-Structure Calculations, *Journal of Chemical Theory and Computation*, Vol. 13, 3829-3845 (2017).
340. Sharma V., De D., Pal S., Saha P., Bharadwaj P.K., A 2D Coordination Network That Detects Nitro Explosives in Water, Catalyzes Baylis-Hillman Reactions, and Undergoes Unusual 2D \rightarrow 3D Single-Crystal to Single-Crystal Transformation, *Inorganic Chemistry*, Vol. 56, 8847-8855 (2017).
341. Dixit G.K., Ranganathan M., Modeling elastic anisotropy in strained heteroepitaxy, *Journal of Physics Condensed Matter*, Vol. 29, - (2017).
342. Pandey S.K., Manogaran D., Manogaran S., Schaefer H.F., Quantification of Hydrogen Bond Strength Based on Interaction Coordinates: A New Approach, *Journal of Physical Chemistry A*, Vol. 121, 6090-6103 (2017).

343. Barsu N., Emayavaramban B., Sundararaju B., Linear Selective C–H Bond Alkylation with Activated Olefins Catalyzed by Cp*CoIII, *European Journal of Organic Chemistry*, Vol. 2017, 4370-4374 (2017).
344. Verma A., De D., Tomar K., Bharadwaj P.K., An Amine Functionalized Metal-Organic Framework as an Effective Catalyst for Conversion of CO₂ and Biginelli Reactions, *Inorganic Chemistry*, Vol. 56, 9765-9771 (2017).
345. Kunnikuruvan S., Parandekar P.V., Prakash O., Tsotsis T.K., Nair N.N., Polymerization Mechanism and Cross-Link Structure of Nadic End-Capped Polymers: A Quantum Mechanical and Microkinetic Investigation, *Macromolecules*, Vol. 50, 6081-6087 (2017).
346. Zhang A., Raje S., Liu J., Li X., Angamuthu R., Tung C.-H., Wang W., Nickel-Mediated Stepwise Transformation of CO to Acetaldehyde and Ethanol, *Organometallics*, Vol. 36, 3135-3141 (2017).
347. Mishra N.K., Jain A., Peter C., Verma S., Combining Experimental and Simulation Techniques to Understand Morphology Control in Pentapeptide Nanostructures, *Journal of Physical Chemistry B*, Vol. 121, 8155-8161 (2017).
348. Chandrasekhar V., Mahanti B., Pandey M.D., Narayanan R.S., Cyclometalated Ir(III) Complex as a Metalloligand and a Selective Cu(II) Sensor: Synthesis and Structural Characterization of a Heterometallic Tetranuclear Ir(III)/Cu(II) Complex, *ACS Omega*, Vol. 3, 2786-2792 (2018).
349. Bais V.S., Mohapatra B., Ahamad N., Boggaram S., Verma S., Prakash B., Investigating the inhibitory potential of 2-Aminopurine metal complexes against serine/threonine protein kinases from *Mycobacterium tuberculosis*, *Tuberculosis*, Vol. 108, 47-55 (2018).
350. Srivastava A.K., Pandey S.K., Misra N., A computational study on semiconducting Si60, Si59Al and Si59P nanocages, *Chemical Physics Letters*, Vol. 691, 82-86 (2018).
351. Dey A., Das S., Palacios M.A., Colacio E., Chandrasekhar V., Single-Molecule Magnet and Magnetothermal Properties of Two-Dimensional Polymers Containing Heterometallic [Cu5Ln2] (Ln = GdIII and DyIII) Motifs, *European Journal of Inorganic Chemistry*, Vol. , - (2018).
352. Rana N.K., Shukla K., Mahto P., Jha R.K., Singh V.K., A facile and highly diastereoselective synthesis of carbocyclic spiro-pyrazolones via DABCO catalyzed Michael-Michael domino reaction, *Tetrahedron*, Vol. , - (2018).
353. Ugwu D.I., Okoro U.C., Mishra N.K., Synthesis, characterization and in vitro antitrypanosomal activities of new carboxamides bearing quinoline moiety, *PLoS ONE*, Vol. 13, - (2018).
354. Ugwu D.I., Okoro U.C., Ukoha P.O., Gupta A., Okafor S.N., Novel anti-inflammatory and analgesic agents: synthesis, molecular docking and in vivo studies, *Journal of Enzyme Inhibition and Medicinal Chemistry*, Vol. 33, 405-415 (2018).

355. Srivastava A.K., Misra N., Pandey S.K., DFT Study on Planar (CaO)_n Rings (n = 1–5) and Their Hydrogen Storage Behavior: Ca–O Versus Mg–O Clusters, *Journal of Cluster Science*, Vol. 29, 57-65 (2018).
356. Ranjan R., Prakash A., Singh A., Singh A., Garg A., Gupta R.K., Effect of tantalum doping in a TiO₂ compact layer on the performance of planar spiro-OMeTAD free perovskite solar cells, *Journal of Materials Chemistry A*, Vol. 6, 1037-1047 (2018).
357. Gupta A.K., De D., Tomar K., Bharadwaj P.K., A Cu(II) metal-organic framework with significant H₂ and CO₂ storage capacity and heterogeneous catalysis for the aerobic oxidative amination of C(sp³)-H bonds and Biginelli reactions, *Dalton Transactions*, Vol. 47, 1624-1634 (2018).
358. Karmakar A., Chandra A., Dynamics of vibrational spectral diffusion in water: Effects of dispersion interactions, temperature, density, system size and fictitious orbital mass, *Journal of Molecular Liquids*, Vol. 249, 169-178 (2018).
359. Patra S., Keshavamurthy S., Detecting reactive islands using Lagrangian descriptors and the relevance to transition path sampling, *Physical Chemistry Chemical Physics*, Vol. 20, 4970-4981 (2018).
360. Mukhopadhyay A., Mandal K.J., Moorthy J.N., Anionic merocyanine dyes based on thiazol-2-hydrazides: Reverse solvatochromism, preferential solvation and multiparametric approaches to spectral shifts, *Physical Chemistry Chemical Physics*, Vol. 20, 4149-4159 (2018).
361. Panday P., Garg P., Singh A., Manganese-Dioxide-Catalyzed Trifluoromethylation and Azidation of Styrenyl Olefins via Radical Intermediates, *Asian Journal of Organic Chemistry*, Vol. 7, 111-115 (2018).
362. Maddali L.N.R., Meka S., Cross-coupling reactivity of 1,1-dichloroalkenes under palladium catalysis: Domino synthesis of diarylalkynes, *New Journal of Chemistry*, Vol. 42, 4412-4418 (2018).
363. Sen M., Rajesh N., Emayavaramban B., Premkumar J.R., Sundararaju B., Isolation of Cp*CoIII–Alkenyl Intermediate in Efficient Cobalt-Catalyzed C–H Alkenylation with Alkynes, *Chemistry - A European Journal*, Vol. 24, 342-346 (2018).
364. Roy Choudhuri J., Chandra A., Effects of dispersion interactions on the structure, polarity, and dynamics of liquid-vapor interface of an aqueous NaCl solution: Results of first principles simulations at room temperature, *Journal of Chemical Physics*, Vol. 148, - (2018).
365. Sahana S., Mishra G., Sivakumar S., Bharadwaj P.K., 2-(2'-Hydroxyphenyl)-benzothiazole (HBT)-terpyridine conjugate: A highly specific ICT based fluorescent probe for Zn²⁺ ions and its application in confocal cell imaging, *Journal of Photochemistry and Photobiology A: Chemistry*, Vol. 351, 231-239 (2018).
366. Sahana S., Mishra G., Sivakumar S., Bharadwaj P.K., Rhodamine – Cyclohexane diamine based “turn-on” fluorescence chemosensor for Cr³⁺: Photophysical & confocal cell imaging studies, *Journal of Photochemistry and Photobiology A: Chemistry*, Vol. 351, 42-49 (2018).
367. Srivastava P., Singh K., Verma M., Sivakumar S., Patra A.K., Photoactive platinum(II) complexes of nonsteroidal anti-inflammatory drug naproxen: Interaction

- with biological targets, antioxidant activity and cytotoxicity, *European Journal of Medicinal Chemistry*, Vol. 144, 243-254 (2018).
368. Agarwal R.A., Synthesis of non-toxic As and Cr nanoparticles through redox activity of highly flexible layered coordination polymer of Ni(II), *Nanotechnology*, Vol. 29, - (2018).
369. Mangeswara Rao G.H., Khan F.A., Synthesis of γ -butyrolactone fused cyclooctene, *Synthetic Communications*, Vol. 48, 318-322 (2018).
370. Vithani N., Jagtap P.K.A., Verma S. K., Tripathi R., Awasthi S., Nair N. N., Prakash, B. Mechanism of Mg^{2+} -Accompanied Product Release in Sugar Nucleotidyltransferases, *Structure*, Vol. 26, 459-466 (2018).
371. Sudarkodi V., Sooraj K. Nair N. N., Basu S., Parandekar P. V., Sinha N. K., Prakash O., Tsotsis T. Mechanical response of two polyimides through coarse-grained molecular dynamics simulations, *Modelling and Simulation in Materials Science and Engineering*, Vol. 26, 025013 (2018).
372. Awasthi S., Nair N. N., Exploring high dimensional free energy landscapes: Temperature accelerated sliced sampling, *Journal of Chemical Physics*, Vol. 146, 094108 (2017).
373. Das C. K., Nair N. N., Hydrolysis of Cephalexin and Meropenem by New Delhi Metallo β -Lactamase: Substrate Protonation Mechanism is Drug Dependent, *Physical Chemistry Chemical Physics*, Vol. 19, 13111-13121 (2017).
374. Awasthi A., Gupta S., Tripathi, R., Nair, N. N., Mechanism and Kinetics of Aztreonam Hydrolysis Catalyzed by Class-C β -Lactamase: A Temperature-Accelerated Sliced Sampling Study, *Journal of Physical Chemistry B*, Vol. 122, 4299-4308 (2018).
375. Sengupta, Rajput, A., Barman, S.K., and Mukherjee, R.N., "Low-spin $[M^II(L)_2]$ and $[M^III(L)_2]^+$ (M = Fe and Co) Complexes of Tridentate Azo-Containing Pyridine/Pyrazine Amide Ligands: Structures, Properties and Redox Potential Correlations", *Dalton Trans.*, 46, 11291-11305(2017).
376. Barman, S.K., Mondal, T., Koley, D., Lloret, F., and Mukherjee, R.N., "A Phenoxo-bridged Dicopper(II) Complex as a Model for Phosphatase Activity: Mechanistic Insights from Combined Experimental and Computational study", *Dalton Trans.*, 46, 4038-4054 (2017).
377. Mukhopadhyay, A., Maka, V.K., Savitha, G., Moorthy, J.N., "Photochromic 2D metal-organic framework nanosheets (MONs): Design, synthesis, and functional MON-ormosil composite", *Chem* 4 (5), 1059-1079 (2018).
378. Jhulki, S., Seth, S., Rafiq, S., Ghosh, A., Chow, T.J., Moorthy, J.N., "Nitrogen-Free Bifunctional Biantryl Leads to Stable White-Light Emission in Bilayer and Multilayer OLED Devices", *ACS Omega* 3 (2), 1416-1424 (2018).
379. Seth, S., Savitha, G., Moorthy, J.N. "Metal-Mediated Self-Assembly of a Twisted Biphenyl-Tetraacid Linker with Semi-rigid Core and Peripheral Flexibility: Concomitant Formation of Compositionally Distinct MOFs" *Crystal Growth & Design* 18 (4), 2129-2137 (2018).

380. Chandrasekhar, P., Bajpai, A., Savitha, G., Moorthy, J.N., "Concomitant Formation of Compositionally Distinct Coordination Polymers Based on a Triacid Linker: Solvent-Mediated Metamorphosis", *European Journal of Inorganic Chemistry* 2017 (8), 1163-1170 (2017).
381. Jhulki, S., Mishra, A.K., Chow, T.J., Moorthy, J.N., "Carbo [5] helicene versus planar phenanthrene as a scaffold for organic materials in OLEDs: the electroluminescence of anthracene-functionalized emissive materials" *New Journal of Chemistry*, 2017 41 (23), 14730-14737 (2017).
382. Singh A. K., Khan F. S. T., Rath S P, Silver(III)···Silver(III) Interaction Stabilizes the Syn-form in a Porphyrin Dimer Upon Oxidation, *Angew. Chem. Int. Ed. Vol. 56*, 8849-8854 (2017).
383. Khan F. S. T., Guchhait, T., Sasmal S., Rath S. P. , Hydroxo-Bridged Diiron(III) and Dimanganese(III) Bisporphyrins: Modulation of Metal Spins by Counter Anions, *Dalton Trans. Vol. 46*, 1012-1037 (2017).
384. Guchhait T. , Sarkar S., Pandit Y. A., Rath S. P., Probing Bis-Fe^{IV} MauG: Isolation of Highly Reactive Radical Intermediates, *Chem. Eur. J. (Communication) Vol. 23*, 10270-10275 (2017).
385. Mondal P., Sarkar S., Rath S. P., Cyclic Bisporphyrin Based Flexible Molecular Containers: Controlling Guest Arrangements and Supramolecular Catalysis by Tuning Cavity Size, *Chem. Eur. J. Vol. 23*, 7093-7103 (2017).
386. Singhal, S., Dinda, S., Goswami, D., "Measurement of pure optical nonlinearity in carbon disulfide with a high-repetition-rate femtosecond laser", *Applied Optics* **56**(3), 644-648 (2017).
387. Makhal, K. and Goswami, D., "pH Effect on two-photon cross section of highly fluorescent dyes using femtosecond two-photon induced fluorescence", *Journal of Fluorescence* **17**(1) 339-356 (2017).
388. Bhattacharyya, I. and Goswami, D., "Two-dimensional imaging of a second order nonlinear optical process", *Current Science* **112**(4), 830-834 (2017).
389. Makhal, K., Mathur, P., Maurya, S.K., and Goswami, D., "Extracting third order optical nonlinearities of Mn (III)Phthalocyanine chloride using high repetition rate femtosecond pulses", *Journal of Applied Physics* **121**(5), 053103 (2017).
390. Mishra, S., Awasthi, P., Singh, J., Gupta, R.K., Singh, V., Kant, R., Jeet, R., Goswami, D., and Goel, A., "White Light Induced E/Z-Photoisomerization of Diphenylamine-Tethered Fluorescent Stilbene Derivatives: Synthesis, Photophysical, and Electrochemical Investigation", *The Journal of Organic Chemistry*, **DOI: 10.1021/acs.joc.8b00033** (2018).
391. Paul, B.; Shee, S.; Panja, D.; Chakrabarti, K.; Kundu, S. "Direct Synthesis of N,N-Dimethylated and β -Methyl N,N-Dimethylated Amines from Nitriles Using Methanol: Experimental and Computational Studies." *ACS Catal.*, 2018, 8, 2890 (2018).
392. Shee, S.; Paul, B.; Panja, D.; Roy, B. C.; Chakrabarti, K.; Ganguli, K.; Das, A.; Das, G. K.; Kundu, S. "Tandem Cross Coupling Reaction of Alcohols for Sustainable

Synthesis of β -Alkylated Secondary Alcohols and Flavan Derivatives" *Adv. Synth. Catal.*, 2017, 359, 3888 (2017).

393. Paul, B.; Shee, S.; Chakrabarti, K.; Kundu, S. "Tandem Transformation of Nitro Compounds to N-methylated Amines: Greener Strategy for the Utilization of Methanol as a Methylating Agent" *ChemSusChem*, 2017, 9, 2370 (2017).
394. Gupta, D.; Mishra, A.; Kundu, S. "Cu (II)- β -CD as Water-Loving Catalyst for One-Pot Synthesis of Triazoles and Biofuels Intermediate at Room Temperature without any other Additive" *ChemistrySelect*, 2017, 2, 2997 (2017).