
LIST OF FIGURES / SCHEMES

CHAPTER 1

Figure 1.1:	Analogy between molecular and supramolecular chemistry	1
Figure 1.2:	Categorization of non-covalent interactions	3
Figure 1.3:	Comparison between IUPAC definition and basic definition	4
Figure 1.4:	Strength of various interactions	5
Figure 1.5:	(a) Three conformers of benzene dimer for different π - π stackings, (b) Quadrupole moment of benzene	6
Figure 1.6:	(a) π ••• π interaction in adjacent pyrene moiety in 1D CP (CCDC No. 1536824), (b) 2D network extending to 3D network through π ••• π interaction in a MOF of a pyrazole ligand (CCDC No. 925250)	6
Figure 1.7:	Coordination bond interaction: CPs and MOFs	7
Figure 1.8:	(a) Schematic representation of first-generation porous network MOFs, (b) third-generation porous network MOFs	9
Figure 1.9:	Different architecture of 1D CPs/MOFs (Paddle-wheel: CCDC No. 1850472)	10
Figure 1.10:	Overview of different types of geometries in 1D, 2D, and 3D networks	12
Figure 1.11:	(a) 1D Linear chain CP (CCDC No. 1108424), (b) 1D Linear chain CP with hugging helical type conformation (CCDC No. 163024), (c) Crisscross pattern in 1D Linear chain CP (CCDC No. 179774)	13
Figure 1.12:	(a) 1D Zigzag CP (CCDC No. 629972), (b) 1D Zigzag CP with 2 Over and 2 Under type packing (CCDC No. 207401), (c) 1D Molecular Ladder CP (CCDC No. 1248145)	14
Figure 1.13:	(a) Represents the sidewise extension of 1D molecular railroad (CCDC No. 1222031), (b) Pink color single chain represents 1D molecular antenna; where red dotted lines are shown noncovalent interaction (CCDC No. 836453)	16
Figure 1.14:	(a) and (b) two different geometrical with (6,3) representation in 2D infinite nets, (c) (4,4) representation in 2D infinite nets	16
Figure 1.15:	2D Rectangular grid network by 4,4'-bpy and its analogue where the cavities are encapsulated with benzene molecules (represented in space-fill model) (CCDC No. 156766)	17
Figure 1.16:	The net view of a 2D molecular bilayer of $[\text{Co}(\text{NO}_3)(\text{L})_{1.5}]_n$, (CCDC No. 120532)	18
Figure 1.17:	2D herringbone network from mixed ligand (CCDC No. 614666)	19
Figure 1.18:	2D honeycomb network from (a) pyrazine (CCDC No. 1206001), and (b) 4,4'-bpy (CCDC No. 1302600) ligands	19

Figure 1.19:	(a) Three -connected T-shaped geometry, (b) 3D Lincoln Log networks by Zaworotko group (CCDC No. 1321203), (c) Three-connected Cu(II) center with 4,4'-bpy, (d) Rectangular shape of three different size channels in 3D networks with nitrate anions (CCDC No. 1311992), (e) Adamantanoid cage of 4,4'-bpy with Ag(I) by Ciani group (CCDC No. 1302198)	20
Figure 1.20:	Classification of interpenetration in CPs/MOFs networks	21
Figure 1.21:	Bis(pyridyl)-mono-imine directed zigzag and helical chain (HgI ₂ CCDC No. 835329 and HgCl ₂ CCDC No. 835327)	23
Figure 1.22:	Different geometry in CPs (T-shaped Cd CP: CCDC No. 154668, distorted T-shaped Cd CP: CCDC No. 154667, F-joint: CCDC No. 154667, Propeller-shape: CCDC No. 166629)	24
Scheme 1.1:	Different hydrogen bonding motifs	26
Scheme 1.2:	Different bis(pyridyl) moieties with amide spacer and their conformation	27
Figure 1.23:	Left-/right handed helical CPs by bis(pyridyl)-diamide as co-ligand (CCDC No. 954315)	28
Figure 1.24:	Two types of SBUs from the same ligand with β sheet recognition (CCDC No. 253152 and 253151)	29
Figure 1.25:	Possible types of PSM	30
Figure 1.26:	SC-SC leads the 2D to 3D transformation by removable of I ₂ molecules	31
Figure 1.27:	Representation of two different routes of transmetalation	31
Figure 1.28:	Insertion of naphthalene guest molecules (CCDC No. 630422)	32
Figure 1.29:	Application of MOFs by using their properties with few examples	33
Figure 1.30:	Jablonski diagram	35

CHAPTER 2

Figure 2.1:	Purchased chemicals which were used as precursors for the synthesis of organic ligands	48
Scheme 2.1:	Aryl based imine spacer ligands	50
Scheme 2.2:	Pyrene based imine spacer ligands	51
Scheme 2.3:	Synthesis of ligands-based on amide spacers	51
Scheme 2.4:	Synthesis of ligands based on sulfonamide spacers	52
Figure 2.2:	Synthesis of CPs in crystalline form through slow diffusion	52
Figure 2.3:	High pressure autoclave reactor for solvothermal synthesis of MOFs	53
Figure 2.4:	Yoe-Jones Method	57
Figure 2.5:	Mathematical calculation for Yoe-Jones Method	57
Figure 2.6:	Schematic representation of instrumentation part of spectrofluorometer	58

Figure 2.7: Representation of impedance complex quantity 62

CHAPTER 3A

- Figure 3A.1:** Energy diagram for H- and J-aggregates based on Kasha's excitation theory model 64
- Figure 3A.2:** Three types of molecule array in face-to-face stacking in **L1d** 66
- Scheme 3A.1:** Bis(aryl)-di-imine ligands with (CH₂)_n spacer backbone 66
- Figure 3A.3:** C-H...N interactions of butylene spacer resulted in corrugated layers of head-to-tail interaction 66
- Figure 3A.4:** Illustration of crystal structure of **L1a**: (a) Asymmetric unit of **L1a**; (b) Arrangement of adjacent molecules; (c) Packing of the molecules (figures were generated from the data obtained from CCDC No. 1118104) 71
- Figure 3A.5:** Illustration of crystal structure of **L1b**: (a) Asymmetric unit of **L1b** showing the non-planar geometry of the molecule; (b) Centroid-to-centroid distance between the adjacent aromatic rings; (c) Packing of the molecules (figures were generated from the data obtained from CCDC No. 1207284) 71
- Figure 3A.6:** Illustration of crystal structure of **L1d**: (a) Packing of the molecules (hydrogen atoms are removed for clarity); (b) Three types of molecules of **L1d** are present in the asymmetric unit, which is shown in different colours. (figures were generated from the data obtained from CCDC No. 963345) 72
- Figure 3A.7:** Illustration of crystal structure of **L2b**: (a) Asymmetric unit; (b) 1D arrangement of the molecules: notice that the aromatic centroid-to-centroid distance is more than 5 Å; (c) Herringbone arrangement of **L2b** molecules in crystal packing (figures were generated from the data obtained from CCDC No. 608471) 72
- Figure 3A.8:** Illustration of crystal structure of **L2d**: (a) Asymmetric unit; (b) Offset arrangement of the molecules to form a 1D network; (c) Herringbone arrangement of the molecules of **L2d** (hydrogen atoms were removed for clarity) (figures were generated from the data obtained from CCDC No. 962823) 73
- Figure 3A.9:** Illustration of crystal structure of **L2c** and **L3c**: (a) Asymmetric unit in **L2c**; (b) Packing of the molecules of **L2c** via C-H...N interactions to form non-covalent macrocyclic moiety; (c) Asymmetric unit in **L3c**; (d) Non-covalent "macrocyclic" moiety in **L3c**; (e) Offset packing of the corrugated layers in **L3c** (hydrogen atoms are removed for clarity) (figures were generated from the data obtained from CCDC No. 721559 (**L2c**) and 930055(**L3c**)) 74
- Figure 3A.10:** (a) Calculated PXRD of **L1a**; generated from crystal data CCDC No. 1118104; (b) Experimental PXRD of **L1a**; (c) Calculated PXRD of **L1b**; generated from crystal data CCDC No. 1207284; (d) Experimental PXRD of **L1b**; (e) Calculated PXRD of **L2b**; generated from crystal data CCDC No. 608471; (f) Experimental PXRD of **L2b** 74

- Figure 3A.11:** UV-Visible absorption spectra of (a) **L1a**, (b) **L1b**, (c) **L2a**, (d) **L2b**, (e) **L3a**, (f) **L3b**, (g) **L4a**, (h) **L4b** in solid-state and in 1×10^{-4} M solution 76
- Figure 3A.12:** PL spectra of **L2a** (a) $\lambda_{\text{ex}} = 300$ nm, (b) $\lambda_{\text{ex}} = 450$ nm and **L2b** (c) $\lambda_{\text{ex}} = 300$ nm, (d) $\lambda_{\text{ex}} = 420$ nm at different concentrations 77
- Figure 3A.13:** PL spectra of **L3a** (a) $\lambda_{\text{ex}} = 320$ nm, (b) $\lambda_{\text{ex}} = 440$ nm and **L3b** (c) $\lambda_{\text{ex}} = 300$ nm, (d) $\lambda_{\text{ex}} = 420$ nm at different concentrations 78
- Figure 3A.14:** PL spectra of **L4a** (a) $\lambda_{\text{ex}} = 280$ nm, (b) $\lambda_{\text{ex}} = 450$ nm and **L4b** (c) $\lambda_{\text{ex}} = 320$ nm, (d) $\lambda_{\text{ex}} = 420$ nm at different concentrations 79
- Figure 3A.15:** Solid-state PL spectra of (a) **L2b**, (b) **L2a**, (c) **L3b**, (d) **L3a**, (e) **L4b** and (f) **L4a** 80
- Figure 3A.16:** Normalized absorption and emission spectra (at excitation $\lambda = 300$ nm) of (a) **L2a** and (b) **L2b** 81
- Figure 3A.17:** TCSPC decay profiles of **L2b** in different concentration in MeOH with excitation at 375 nm 81
- Scheme 3A.2:** Arrangement of the molecules of **L1a**, **L1b** and **L1d** in the solid state; notice the face-to-face stacking of the molecules. Although it is inclined in the case of **L1a** and **L1b**, no fluorescence is observed in solid-state 84
- Scheme 3A.3:** The face-to-face stacking arrangement of **L2b** molecules 84
- Scheme 3A.4:** Arrangement of the molecules of **L2d** and **L3d** in the solid state; Notice the offset stacking of molecules 84
- Scheme 3A.5:** Arrangement of the molecules of **L2c** and **L3c** in the solid-state; notice the formation of new "chromophore" on aggregation and in the solid-state 85
- Figure 3A.18:** ^1H NMR spectra of **L1a** at different concentrations taken in CDCl_3 85
- Figure 3A.19:** ^1H NMR spectra of **L3b** at different concentrations taken in CDCl_3 86
- Scheme 3A.6:** Arrangement of the molecules in **L2b** and **L3b** resulted in deshielded aromatic proton and shielded methyl protons 87
- Figure 3A.20:** ^1H NMR spectra of **L2d** at different concentrations taken in CDCl_3 87
- Figure 3A.21:** NOESY of **L2b** in CDCl_3 at a concentration of 2 M 88

CHAPTER 3B

- Scheme 3B.1:** Approaches to remove thorny ACQ effect of pyrene 92
- Figure 3B.1:** Effective substitution positions in pyrene which may prevent ACQ. The red circles represent the more active position on the periphery of pyrene 93
- Figure 3B.2:** Illustrations of crystal structure of **L5a**: (a) Molecular geometry of **L5a**; (b) Non-covalent interactions present between the molecules of **L5a**; (c) Benzene C-H $\cdots\pi$ interactions between two **L5a** molecules; (d) Pyrene C-H $\cdots\pi$ interactions between two **L5a** molecules 99

Figure 3B.3: Illustrations of crystal structure of L5a : Packing of L5a molecules in three dimensions	100
Figure 3B.4: UV-Visible spectra in DMF and solid-state (in BaSO ₄): (a) L5a ; (b) L6a ; (c) L7a ; (d) L8a ; (e) L9a	101
Figure 3B.5: PL spectra of (a) L5a (excitation wavelength 420 nm) and (b) L6a (excitation wavelength 370 nm) in DMF at different concentrations (slit width 10 nm)	102
Figure 3B.6: PL spectra of (a) L7a (excitation wavelength 420 nm), (b) L8a (excitation wavelength 400 nm) and (c) L9a (excitation wavelength 420 nm) in DMF at different concentrations and in solid state	103
Scheme 3B.2: Length of alkyl spacer and its effect on aggregate concentration for maximum AIE	104
Figure 3B.7: Aggregation induced emission in THF: Water	104
Scheme 3B.3: (a) ACQ observed on L6a due to stacking of aromatic rings; (b) AIE observed in L7a-L9a due to the presence of flexible alkyl chain in the spacer	105

CHAPTER 3C

Scheme 3C.1: Various types of H-bonding synthon of amide	111
Figure 3C.1: Sulfonamide featuring as anion receptors	112
Scheme 3C.2: Schematic correlation between the non-covalent interactions and emission properties	113
Figure 3C.2: Benzenesulfonamides tuned with various substituents to extract photophysical properties	114
Scheme 3C.3: Bis(pyridyl)-disulfonamides and their amidic counter parts	115
Figure 3C.3: ORTEP (showing thermal ellipsoid at 50% probability) of asymmetric unit of L10b	118
Figure 3C.4: Illustrations of crystal structure of L10b : (a) Geometry of a molecule of L10b ; (b) N-H...N hydrogen bonded interactions resulting in 1D hydrogen bonded chains; (c) packing of the molecules via various non-covalent interactions	119
Figure 3C.5: ORTEP (showing thermal ellipsoid at 50% probability) of asymmetric unit of L11b	119
Figure 3C.6: Illustrations of crystal structure of L11b : (a) Geometry of a molecule of L11b ; (b) N-H...N hydrogen bonded interactions resulting packing of L11b ; (c) N-H...N hydrogen bonded interactions between the L11b molecules	120
Figure 3C.7: (a) Experimental and simulated powder XRD of L10b ; (b) Experimental and simulated powder XRD of L11b	121
Scheme 3C.4: (a) Arrangement of the molecules of L16b ; notice the prevention of self-complimentary amide to amide hydrogen bonds, (b) arrangement of the molecules of L11b ; notice the formation of N-H-N hydrogen bond due to tetrahedral sulfur centre	121

- Figure 3C.8:** Illustrations of crystal structure of **L16b**: (a) Molecular geometry (b) packing of molecules via N–H•••N hydrogen bond interactions to form 1D network; Structures are generated from CCDC no. 259256 122
- Figure 3C.9:** Illustrations of crystal structure of **L15b**: (a) Molecular geometry (b) packing of molecules via N–H•••N hydrogen bond interactions to form 2D network; Structures are generated from CCDC no. 694503 122
- Figure 3C.10:** UV-Visible spectra of **L10b-L12b** in methanol and solid state: (a) **L10b** (b) **L11b** and (c) **L12b** 123
- Figure 3C.11:** Concentration dependent emission spectra: (a) **L10b**; (b) **L11b** and (c) **L12b** 124
- Scheme 3C.5:** Arrangement of the molecules of **L10b** in solid state and in solution state (a) & (b); observe face to face stacking in solid state (a); notice the prevention of ACQ in lower concentration (b), no fluorescence observe in solid state due to non-planarity (c); non-planarity of **L11b** diminished in solution state (d) 126

CHAPTER 4A

- Figure 4A.1:** Classification of metal ion detection techniques 128
- Scheme 4A.1:** Metal ion sensing property of **L3c** 131
- Figure 4A.2:** (a) UV-Visible absorption spectra of **L3c** with different metal salts in 1:1 ratio, IR spectrum of (a) **L3c**, (b) 1: 1 (**L3c**: Ni⁺²), (c) 1: 1 (**L3c**: Cd⁺²) 135
- Figure 4A.3:** (a) UV-Visible absorption spectra of 1 mL of 0.5×10^{-4} M **L3c** on adding different volume of 10^{-3} M of Ni(II) solution (Total solution volume = 2 mL), (b) Absorbance (of n \rightarrow π^* peak) vs. Volume of Ni(II) solution in overall volume of 2 mL solution 136
- Figure 4A.4:** (a) UV-Visible absorption spectra of 1 mL of 0.5×10^{-4} M **L3c** on adding different volume of 10^{-3} M of Cd(II) solution (Total solution volume = 2 mL), (b) Absorbance (of n \rightarrow π^* peak) vs. Volume of Cd(II) solution in overall volume of 2 mL solution 137
- Figure 4A.6:** Binding constant calculation of Ni(II)-**L3c** complex 138
- Figure 4A.5:** (a) Determination of binding constant of Ni⁺² with **L3c** from Yoe Jones method using non-linear least square fit analysis method at 281 nm 138
- Figure 4A.7:** Linear fit of Absorbance (\sim 281nm) vs. Concentration of Ni(II) in 1×10^{-5} M of **L3c** 139
- Figure 4A.8:** Selectivity of **L3c** towards Ni(II) and Cd(II): (a) Absorbance (281 nm) profile of **L3c** and Ni(II) in presence of four equivalents of interfering M⁺²; (b) Absorbance (280 nm) profile of **L3c** and Cd(II) in presence of four equivalents of interfering M⁺² 139
- Figure 4A.9:** UV-Visible absorption spectra of **L2'c** and **L4c** with different metal ions 141
- Figure 4A.10:** Schematically diagram of possible structure of different di-imines 141

- Figure 4A.11:** (a) The pH study of Ni(II)-**L3c** complex at 281 nm and inside image represents their corresponding spectra (b) Stability of Ni(II)-**L3c** complex with various anions at 281 nm and their absorbance profile 142
- Figure 4A.12:** PXRD of Ni(II)-**L3c** complex; Simulated PXRD generated from crystal data CCDC no. 1043600 (blue line); Experimental PXRD of synthesized **L3c**-Ni(II) complex (red line) 142
- Figure 4A.13:** ¹H NMR spectra (a) **L3c**, (b) 1:1 (**L3c**:Cd(II)), (c) at t = 0 h, 1:2 (**L3c**: Cd(II)) and (d) at t = 24 h, (**L3c**:Cd) 143
- Figure 4A.14:** (a) Illustration of crystal structure of **L3c**; Notice the gauche-anti-gauche conformation of butyl chain and C–H•••N interactions to form non-covalent chromophore moiety; Figures were generated from the data obtained from CCDC no. 930055 (b): Illustration of crystal structure of **L3c**-Ni(II): (p) Asymmetric unit; (q) O–H•••Cl⁻ and N=C–H•••Cl⁻ hydrogen bond interactions between the **L3c**-Ni(II) molecules; (r) 3D packing of the molecules; Notice the arrangement of the aromatic rings; Figures were generated from CCDC no. 1043600 144
- Figure 4A.15:** SEM analysis of (a) Ni(II)-**L3c**, (b) **L3c** and (d) Cd(II)-**L3c** and (c) EDS analysis of Cd(II)-**L3c** 145
- Figure 4A.16:** Some other Imine and Azo based Ni²⁺ sensor with their detection limit reported in literature 146

CHAPTER 4B

- Figure 4B.1:** Different Schiff base moieties used for complexation through DFT calculation 152
- Scheme 4B.1:** (Proposed) Metal ion sensing property of **L2c** 153
- Figure 4B.2:** UV-Visible absorption spectra of **L2c** with different metal salts in 1:2 ratio 154
- Figure 4B.3:** (a and b) PL spectra of **L2c** with different metal ions at two different excitation wavelengths. (c) Under UV-visible light (365 nm) and (d) Visible light 155
- Figure 4B.4:** (a) UV-Visible absorption spectra for titration of **L2c** (1 mL; 0.5 x 10⁻⁴ M) with of Fe(II) solution of solution (1 x 10⁻³ M) in 10 μL steps (Total volume of solution = 2mL), (b) Piece wise linear fit plot of Absorbance (at 595 nm peak) vs. Volume of Fe(II) solution plot 156
- Figure 4B.5:** Determination of binding constant of Fe(II) with **L2c** from Yoe Jones method using non-linear least square fit analysis method at 595 nm 156
- Figure 4B.6:** Variation of absorbance at wavelength 278 nm by adding different metal ions 157
- Figure 4B.7:** (a) The UV-visible spectra and the bar diagram represents the Reversibility of Fe(II)-**L2c** towards anions at 595 nm (b) Absorbance (at 595 nm) for probe-Fe²⁺ complex solution at different pH values taken in the MeOH/ aqueous HEPES buffer solution (1:1, v/v, 1 mM, pH = 7.3) 158

Figure 4B.8: NMR spectra of Fe(II)- L2c complex and L2c receptor	159
Figure 4B.9: (a) Crystal structure of L2c and (b) Optimized structure of L2c	159
Figure 4B.10: (a) Optimized geometry of Fe(II)- L2c complex (b) Two Fe(II) are lying in two different planes	161
Figure 4B.11: Contour molecular orbitals of receptor and Fe(II)- L2c with HOMO-LUMO gap	162
Figure 4B.12: (a) Theoretical UV-visible spectra of receptor L2c and (b) Fe(II)- L2c complex	162
Figure 4B.13: The UV-visible spectra represents the determination of spike Fe(II) ion in river water sample by L2c	163

CHAPTER 5

Scheme 5.1: Pyridyl based exo-bidentate ligands equipped with groups for coordinate bond as well as hydrogen bond interactions	166
Scheme 5.2: Synthesis of CP1 and CP2 : Analysis of adsorption-desorption of iodine, solvochromism, photocatalytic dye degradation and impedance measurement	174
Figure 5.1: Transmetalation reaction of CP1 with Cu(II): (a) Reaction kinetics monitored by EDX and (b) Images of single crystal to single crystal transformation of CP1 to CP2	176
Figure 5.2: Illustration for crystal structure of CP1 : (a) 1D looped chain in CP1	176
Figure 5.3: Illustration for crystal structure of CP1 : (a) Geometry of L15b in CP1 , (b) Hydrogen bond interaction of N-H groups in CP1 with the DMF molecules (Hydrogen atoms are removed for clarity), (c) Offset packing of the 1D chains (Chains are shown in different colours for clarity)	177
Figure 5.4: Illustration for crystal structure of CP2 : (a) Asymmetric unit in CP2 , (b) Geometry of two types of L15b in CP2 , (c) 1D looped chain, (d) Hydrogen bond interaction of N-H groups in CP2 with the DMF molecules (Hydrogen atoms are removed for clarity), (e) Offset packing of the 1D chains (Chains are shown in different colours for clarity)	179
Figure 5.5: Temperature dependence molar magnetic susceptibility of CP1 per formula unit: $\chi_m T$ vs T plot of CP1 fits the Curie-Weiss law	180
Figure 5.6: TGA derivative plot of weight% of (a) (CP1 and CP1*) and (b) (CP2 and CP2*)	181
Figure 5.7: Solid state UV-visible spectrum of L15b	181
Figure 5.8: Solid state UV-visible spectra of (a) (CP1 and CP1*) and (b) (CP2 and CP2*)	182
Figure 5.9: Tauc plot for band gap determination in CP1 and CP2	182
Figure 5.10: Dye degradation studies of CP2 under UV light	183

- Figure 5.11:** (a) % dye degradation by **CP1** and **CP2** under UV and CFL light (b) (i) ^1H NMR spectrum of **MB** in D_2O and (ii) ^1H NMR spectrum of **MB** after degradation by **CP2** under UV light 184
- Figure 5.12:** Schematic representation of charge transfer for photocatalytic degradation in CPs 184
- Figure 5.13:** Microscope Images of Iodine adsorption in **CP1** over time 185
- Figure 5.14:** Adsorption of iodine by **CP1**, (b) Desorption of iodine from **CP1**, (c) Adsorption of iodine by **CP2**, (d) Desorption of iodine from **CP2** 186
- Figure 5.15:** (a) Nyquist plot, (b) Conductivities vs. frequency plot, (c) Modulus vs. frequency plot, (d) Dielectric vs. frequency plot 187

CHAPTER 6

- Figure 6.1:** (a) ORTEP of asymmetric unit of **Zn(II)-MOF** showing thermal ellipsoids at 50% probability level; (b) Coordination environment of Zn(II) center and the resultant secondary building unit (SBU) 196
- Figure 6.2:** Illustrations of crystal structure of **Zn(II)-MOF**: (a) A triangle-tessellated hexagonal net; (b) Interpenetrated 3 hexagonal net; (c) Showing different topologies in one complete pinwheel hex net with pillar; (d) Side view of interpenetrated network in ac plane 197
- Figure 6.3:** Extended the core moiety of **Zn(II)-MOF** 197
- Figure 6.4:** Thermogravimetric analysis of the **Zn-MOF** 198
- Figure 6.5:** (a) Phase purity comparison between calculated PXRD and experimental PXRD of **Zn-MOF**; (b) Represents changing crystallinity after water wash of **Zn-MOF** 198
- Scheme 6.1:** **Zn(II)-MOF** catalysed Knoevenagel condensation between active methylene and aldehyde substrate 199
- Figure 6.6:** Stacked IR spectra compared structural integrity of **Zn(II)-MOF** catalyst (before catalysis) (a) & after catalysis; first cycle (b) second cycle; (c) third cycle 200
- Figure 6.7:** Recyclability of Zn(II)-MOF catalyst 200
- Figure 6.8:** Proposed mechanism of Knoevenagel condensation from the catalyst viewpoint 201
- Figure 6.9:** Representation of the pores in **Zn-MOF** 201
- Figure 6.10:** SEM results proposed the structural integrity and pore diameter (a), (b) and (c), BET-plot (d) 202

CHAPTER 7

- Figure 7.1:** Packing of molecules in **L1a** and **L2b** 205

Figure 7.2:	$\pi\cdots\pi$ interactions with head to tail arrangement in L5a	206
Figure 7.3:	Macrocyclic chromophore species in L10b	206
Figure 7.4:	Channels in a 1D looped chain of CP1	207
Figure 7.5:	Bifunctional acid base centre in Zn-MOF	208
Scheme 7.1:	Possible CPs from L11b	209
Figure 7.6:	Pinwheel structure of Zn(II)-MOF	209

LIST OF TABLES

Table 2.1: Instrumentation details	47
Table 2.2: List of synthesised organic ligands	50
Table 3A.1: UV-Visible absorption maxima for compounds L1a , L1b , L2a , L2b , L3a , L3b , L4a and L4b	76
Table 3A.2: λ_{\max} in the PL spectra of the compounds (Figure A-26)	79
Table 3A.3: Molar extinction coefficient of UV-visible spectra of L2a in wavelengths near 300 nm	80
Table 3A.4: Fluorescence lifetime data for L2a , L2b , L3a , L3b , L4a and L4b	82
Table 3A.5: Absolute quantum yields in solution and solid states	83
Table 3B.1: Crystallographic data of L5a	97
Table 3C.1: Crystallographic data of L10b , and L11b	118
Table 3C.2: Comparison of λ_{\max} values of solution and solid state spectra	123
Table 4A.1: Determination of Ni ⁺² ion	146
Table 4B.1: DFT calculation table for receptor and Fe(II)- L2c complexes	160
Table 4B.2: The bond lengths and bond angles of Fe(II)- L2c 12	161
Table 4B.3: Spike Fe(II) ion determination in river water	163
Table 5.1: Crystal structure data and refinement parameters for CP1 and CP2	175
Table 5.2: Orientations of aromatic planes of L15b in CP1 & CP2 [Planes are labelled in Figure 5.3a]	178
Table 6.1: Crystal data of Zn(II)-MOF	195
Table 6.2: Knoevenagel condensation of benzaldehydes and malononitrile	199

LIST OF ABBREVIATIONS / SYMBOLS

Abbreviation/Symbol	Description
%	percentage
°	degree
∠	angle
Å	angstrom
α	alpha
β	beta
χ	chi
δ	delta
ε	epsilon
γ	gamma
φ	phi
λ	lambda
μ	mu
ν	nu
θ	theta
ρ	rho
σ	sigma
τ	tau
ω	omega
1D	one dimensional
2D	two dimensional
3D	three dimensional
AAS	Atomic Absorption Spectroscopy
ACN/MeCN	acetonitrile
ATR	Attenuated Total Reflection
bipy	4,4'-bipyridine
CAU	Christian-Albrechts-University

° C	degree centigrade
Calcd	Calculated
cm	centimetre
conc.	concentrated
CDCl ₃	deuterated chloroform
CPs	Coordination Polymers
COF	Covalent Organic Framework
<i>d</i>	doublet
DCM	dichloromethane
DMF	<i>N,N</i> -dimethylformamide
dil.	diluted
DMSO	dimethylsulfoxide
DMSO- <i>d</i> ₆	deuterated dimethylsulfoxide
DTA	Differential Thermal Analysis
ε	molar extinction coefficient
EDX	Energy Dispersive X-Ray
EtOH	ethanol
ESI-MS	Electron Spray Ionization Mass Spectrometry
FID	Flame Ionisation Detector
FTIR	Fourier Transform Infrared
FWHM	Full width at half maximum
GC	Gas Chromatography
h	hour
HPRA	High Pressure Reactor Autoclave
HRMS	High Resolution Mass Spectrometry
HKUST	Hong Kong University of Science and Technology
ISO	International Organisation for Standardisation
IRMOF	Isorecticular Metal-Organic-Framework
<i>J</i>	coupling constant
L	ligand
MB	methylene blue
MeOH	methanol
<i>m</i>	multiplet

mp	melting point
mg	milligram
MHz	Mega Hertz
MG	malachite green
MOFs	Metal-Organic-Frameworks
MO	methyl orange
min	minute
mL	milliliter
mmol	millimole
MIL	Materials of Institute Lavoisier
NMR	Nuclear Magnetic Resonance
ORTEP	Oak Ridge Thermal Ellipsoid Plot
ppm	parts per million
PSM	Post-synthetic Modification
PSD	Post-synthetic deprotection
RB	Rhodamine B
SCSC	single crystal to single crystal
<i>s</i>	singlet
SQUID	Superconducting Quantum Interference Device
SEM	Scanning Electron Microscope
<i>t</i>	triplet
<i>t</i> -Bu	tertiary butyl
TEA	triethylamine
TGA	Thermo Gravimetric Analysis
THF	tetrahydrofuran
TLC	Thin Layer Chromatography
TCSPC	Time Correlated Single Photon Count
TMS	tetramethylsilane
TMU	Tarbiat Modares University
UV	UltraViolet
UiO	University of Oslo
XRD	X-ray diffraction
μM	micromolar

δ	delta
<i>o</i> -	ortho
<i>m</i> -	meta
<i>p</i> -	para
<i>br</i>	broad
<i>q</i>	quartet
