

Table of Contents

	Page No.
Abstract	i-vi
Declaration	vii
Certificate from Supervisor	viii
Certificate of the External Examiner and ODEC	ix
Acknowledgements	x-xii
List of Schemes	xvii-xix
List of Figures	xx-xxi
List of Tables	xxii
General Experimental Information	xxiii
Abbreviations and Symbols	xxiv-xxv
Chapter 1. Introduction	1-55
1.1 General Introduction	1-2
1.1.1 Indole-based functionalization reactions	2-4
1.1.1.1 Palladium (Pd) catalyzed C-2 functionalization of indole	5-11
1.1.1.2 Transition metal-free C-3 functionalization of indole	11-14
1.1.2 Oxidative coupling reactions	14
1.1.2.1 Heterogeneous catalyst-based Suzuki-Miyaura cross-coupling reaction	15-16
1.1.2.2 Advantages of nanocatalyst	16
1.1.2.3 Solid-Supported Pd-nanocatalyst	16
1.1.2.3.1 Pd-catalyst supported on silica	16-18
1.1.2.3.2 Pd-catalyst supported on metal oxides and layered double hydroxides	18-19
1.1.2.3.3 Pd-catalyst supported on graphitic carbon nitride (g-C ₃ N ₄)	19-20
1.1.2.3.4 Pd-catalyst supported on polymer	20-21
1.1.2.3.5 Pd-catalyst supported on dendrimer	21-23
1.1.2.3.6 Pd-catalyst supported on cyclodextrin	23-24
1.1.2.4 General mechanism for nanocatalyst-based Suzuki-Miyaura cross-coupling reaction	25
1.1.2.5 Decarboxylative coupling of cinnamic acid	25-28
1.1.2.5.1 Decarboxylative coupling incorporating carbon radical	28-31
1.1.2.5.2 Decarboxylative coupling incorporating nitrogen radical	31-32

1.1.2.5.3 Decarboxylative coupling incorporating silicon, phosphorus, and sulfur radicals	32-34
1.2 The Thesis	34
1.3 Objectives of the present work	34
1.4 Bibliography	35-55
Chapter 2. Potassium Peroxodisulfate Catalyzed Convenient Synthesis of Bis(indolyl)methane <i>via</i> Radical Path	56-73
2.1 Introduction	56-57
2.2 Experimental section	57
2.2.1 General procedure for the synthesis of BIM	57
2.3 Results and Discussion	58
2.3.1 Optimization of reaction conditions	58-59
2.3.2 Substrate scope study	59-60
2.3.3 Control experiment	60-61
2.3.4 Plausible mechanism	61-62
2.4 Conclusion	62-63
2.5 ¹ H and ¹³ C NMR analytical data	63-70
2.6 Bibliography	71-73
Chapter 3. Pd/C catalyzed C-2 Selective Direct Functionalization of Indoles with Aryl Iodides	74-92
3.1 Introduction	74-75
3.2 Experimental section	75
3.2.1 General procedure for the synthesis of C-2 arylated indole	75
3.3 Results and Discussion	76
3.3.1 Optimization of reaction conditions	76-77
3.3.2 Substrate scope study	77-79
3.3.3 Heterogeneity test	79
3.3.4 Reusability test	79
3.3.5 Control experiment	79-80
3.3.6 Plausible mechanism	80-81
3.4 Conclusion	81
3.5 ¹ H and ¹³ C NMR analytical data	81-88
3.6 Bibliography	89-92
Chapter 4. Halogen Bonding Assisted C-3 Benzylolation of Indoles and N-	93-120

Benzylation of Imidazoles at Room Temperature	
4.1 Introduction	93-95
4.2 Experimental Section	96
4.2.1 General procedure for the synthesis of C-3 benzylated indoles	96
4.3 Results and Discussion	96
4.3.1 Optimization of reaction conditions	96-97
4.3.2 Substrate scope study	97-100
4.3.3 Mechanism study	100-101
4.3.4 Plausible mechanism	101-102
4.4 Conclusion	102
4.5 ¹ H and ¹³ C NMR analytical data	102-115
4.6 Bibliography	116-120
Chapter 5. Exploring Pd(0)/g-C₃N₄O Catalyzed Suzuki-Miyaura Cross-	121-151
Coupling Reaction with Minimal Base-Stoichiometry	
5.1 Introduction	121-123
5.2 Experimental Section	123
5.2.1 Synthesis of g-C ₃ N ₄ O	123
5.2.2 Synthesis of Pd(0)/g-C ₃ N ₄ O	124
5.2.3 General procedure for synthesis of biaryls	124
5.3 Results and Discussion	124
5.3.1 Characterization of synthesized materials	124-129
5.3.2 Catalytic activity of Pd(0)/g-C ₃ N ₄ O	130
5.3.2.1 Optimization of reaction conditions	130-131
5.3.2.2 Substrate scope study	131-133
5.3.2.3 Heterogeneity test	134
5.3.2.4 Reusability test	134
5.3.2.5 Control experiment	135-136
5.3.2.6 Plausible Mechanism	136-137
5.4 Conclusion	137-138
5.5 ¹ H and ¹³ C NMR analytical data	138-144
5.6 Bibliography	145-151
Chapter 6. CuO/C Catalyzed Decarboxylative Alkenylation of Cyclic Ethers	152-176
6.1 Introduction	152-153

6.2 Experimental Section	153
6.2.1 Catalyst preparation	153
6.2.2 General procedure for decarboxylative C-H functionalization	154
6.3 Results and Discussion	154
6.3.1 Catalyst characterization	154-158
6.3.2 Catalytic activity of CuO/C	158
6.3.2.1 Optimization of reaction conditions	158-159
6.3.2.2 Substrate scope study	160-161
6.3.2.3 Heterogeneity test	161
6.3.2.4 Reusability test	161-162
6.3.2.5 Control experiment	162
6.3.2.6 Plausible mechanism	162-163
6.4 Conclusion	164
6.5 ¹ H and ¹³ C NMR analytical data	164-170
6.6 Bibliography	170-176
Chapter 7. Conclusion and Future Scope	177-179
7.1 General Conclusion	177-178
7.2 Future Scope	178-179
Annexure A & B	a-b
List of Publications	a
List of Conferences	b