

Supporting Information-I

Catalytically Active Lead-Imidazolium Coordination Assemblies with Diversified Lead(II) Coordination Environments

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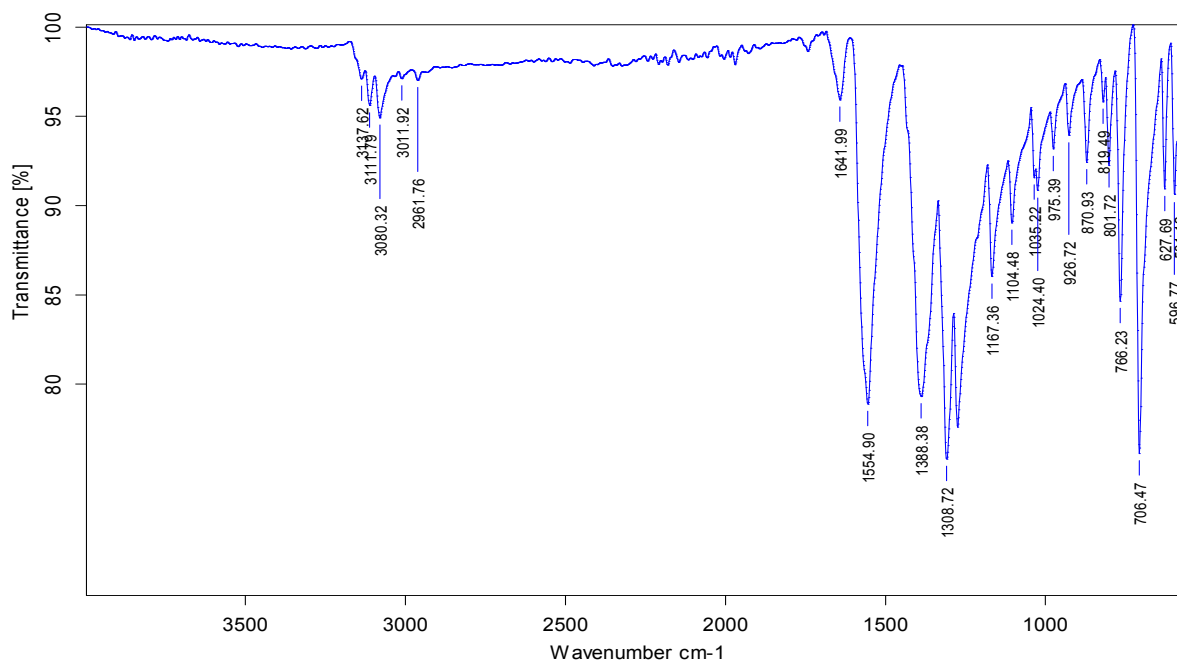


Figure S1. FT-IR spectrum of **1**

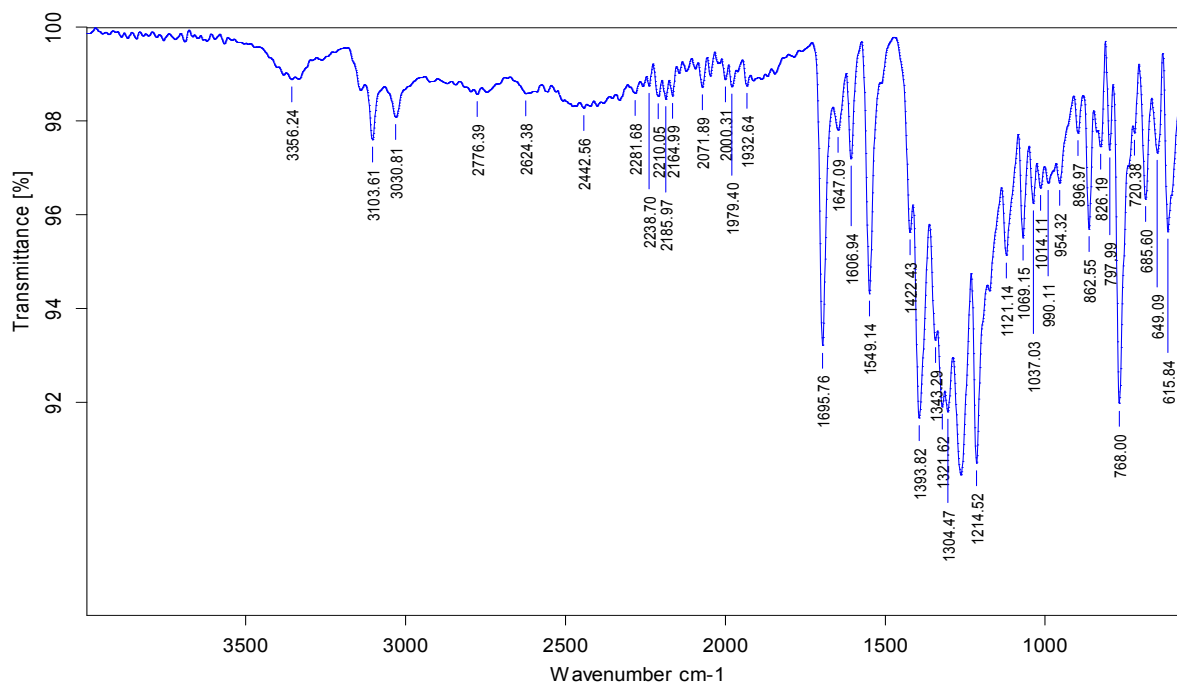


Figure S2. FT-IR spectrum of **2**.

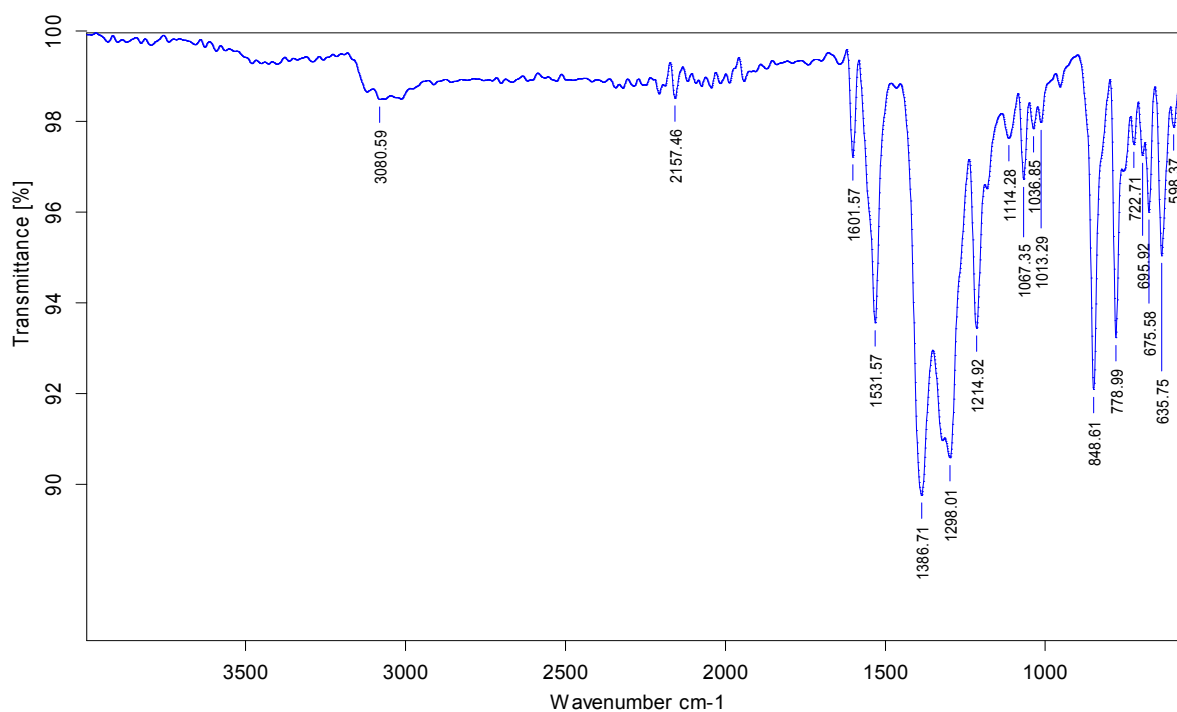


Figure S3. FT-IR spectrum of **3**.

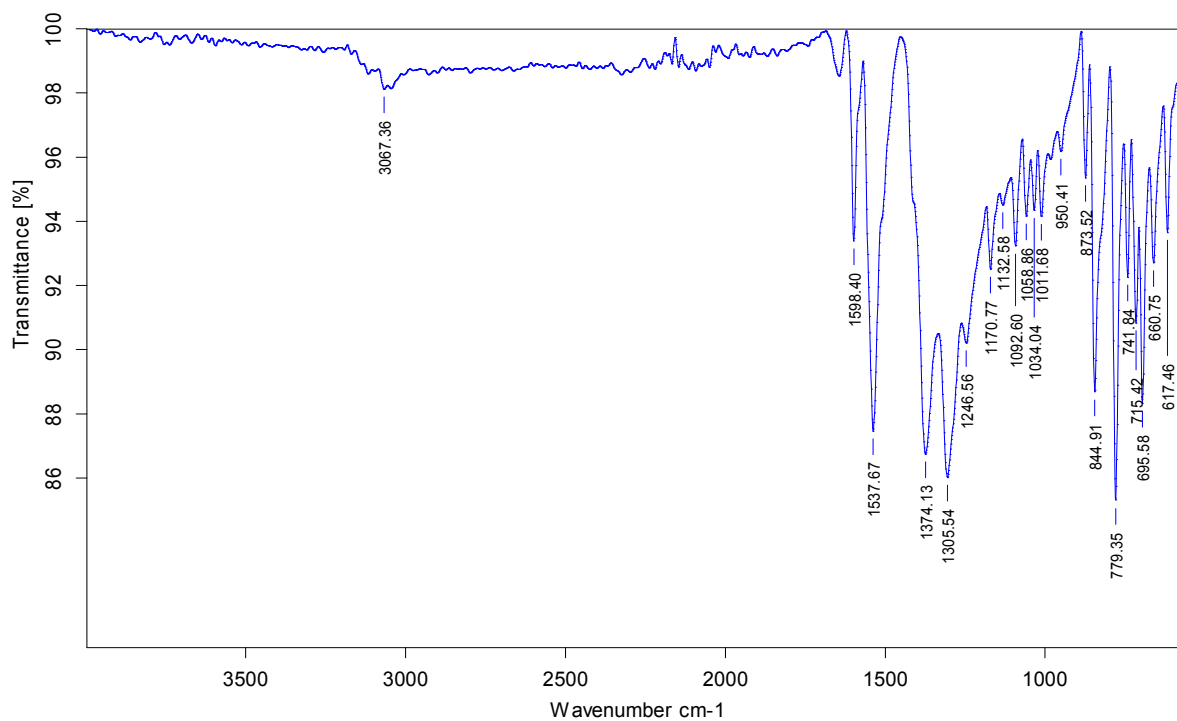


Figure S4. FT-IR spectrum of **4**.

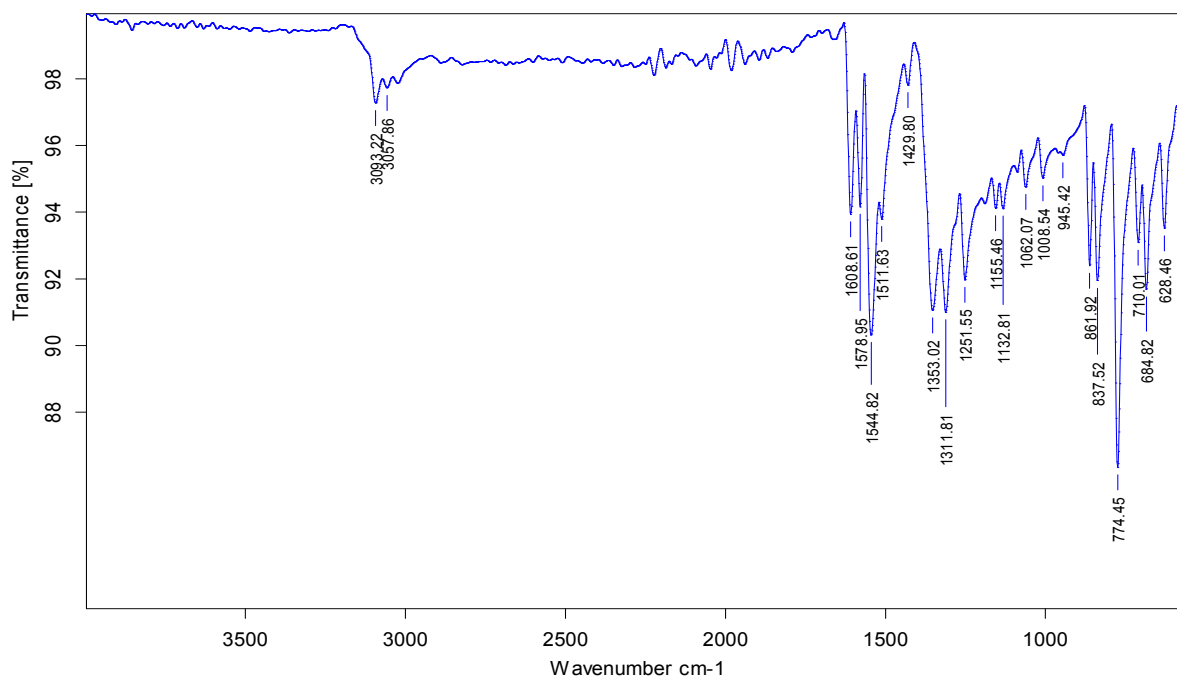


Figure S5. FT-IR spectrum of **5**.

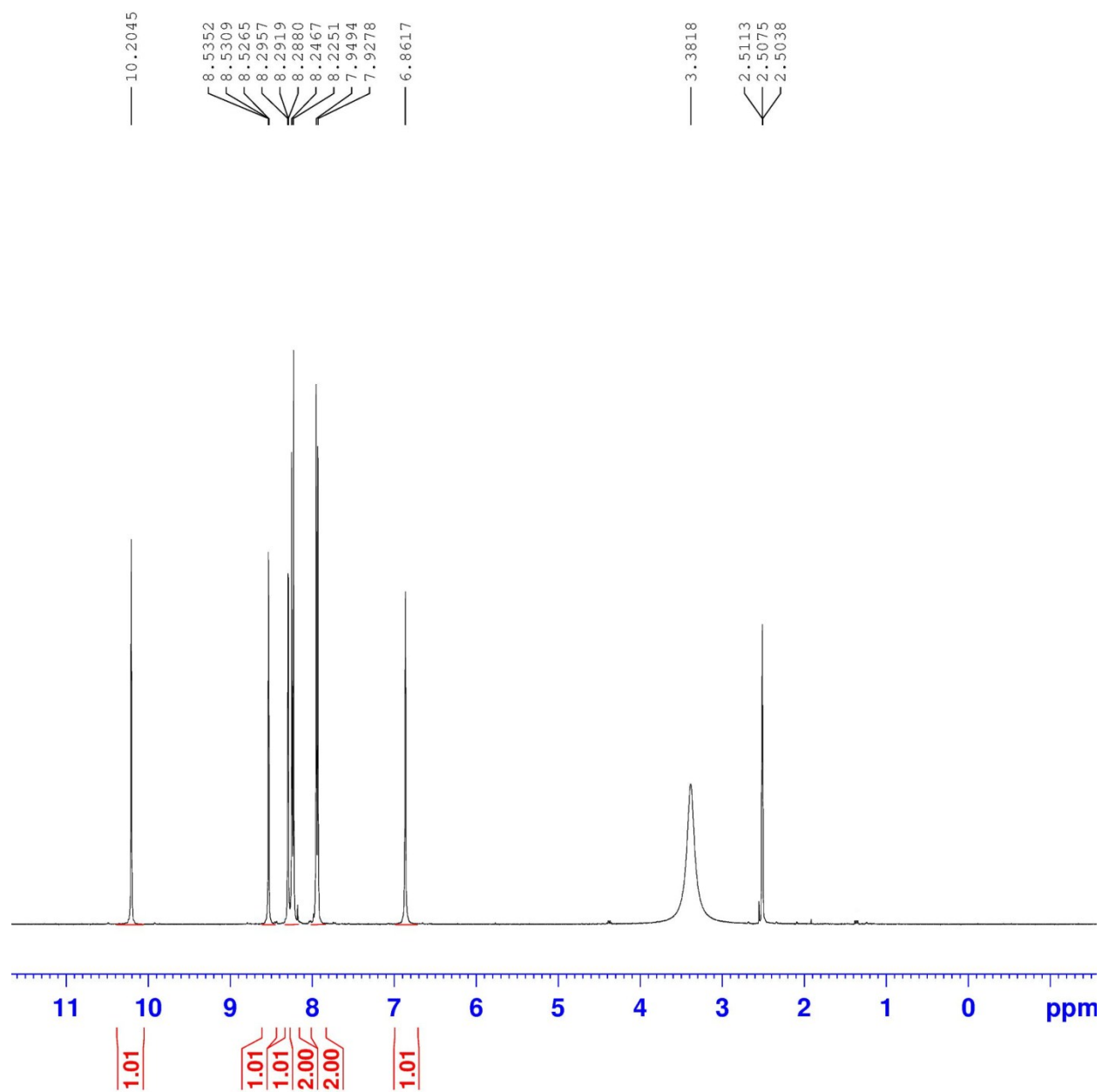


Figure S6. ¹H NMR spectrum of **2**.

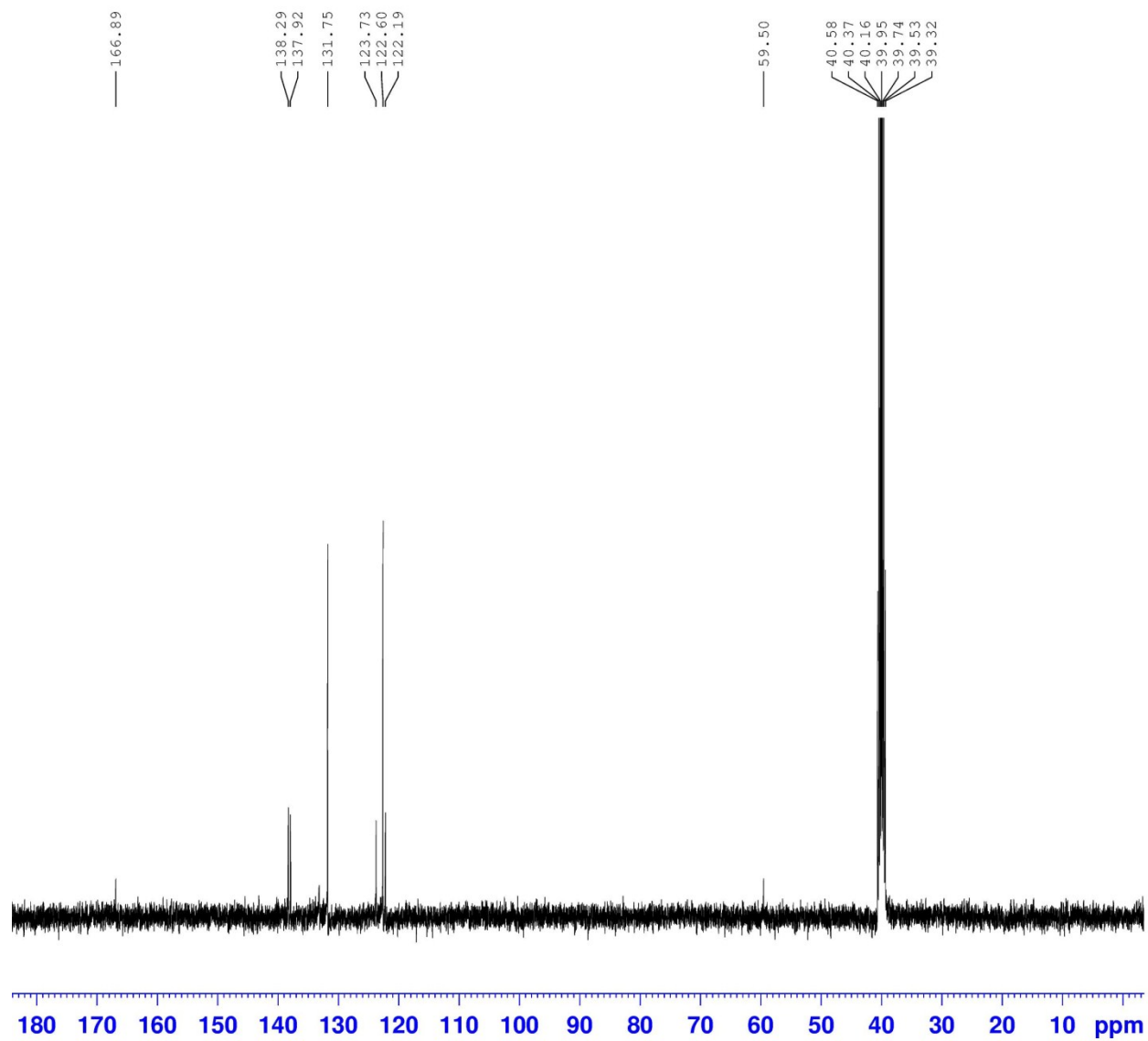


Figure S7. ¹³C NMR spectrum of **2**.

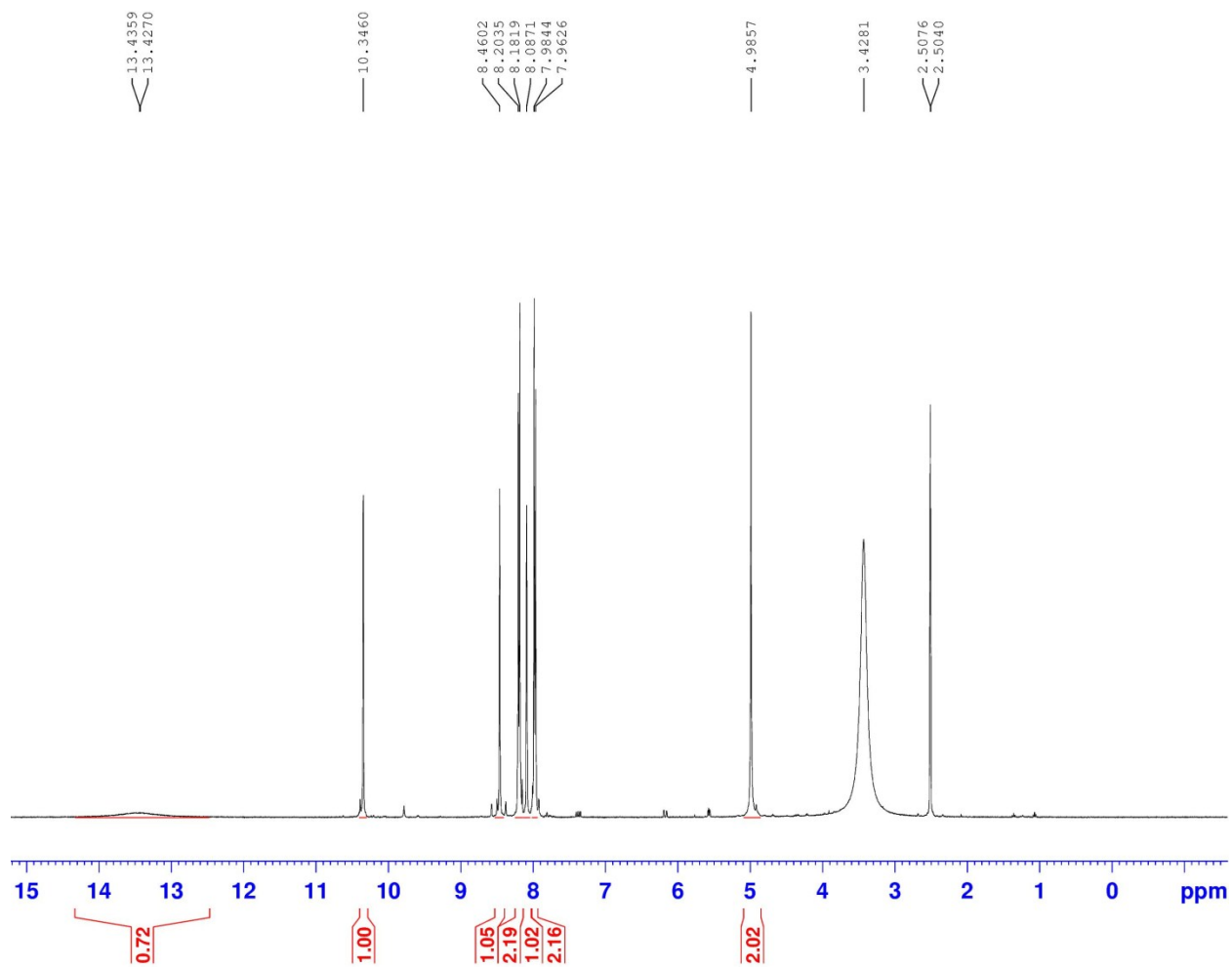


Figure S8. 1H NMR spectrum of $L^2H_2Br_2$.

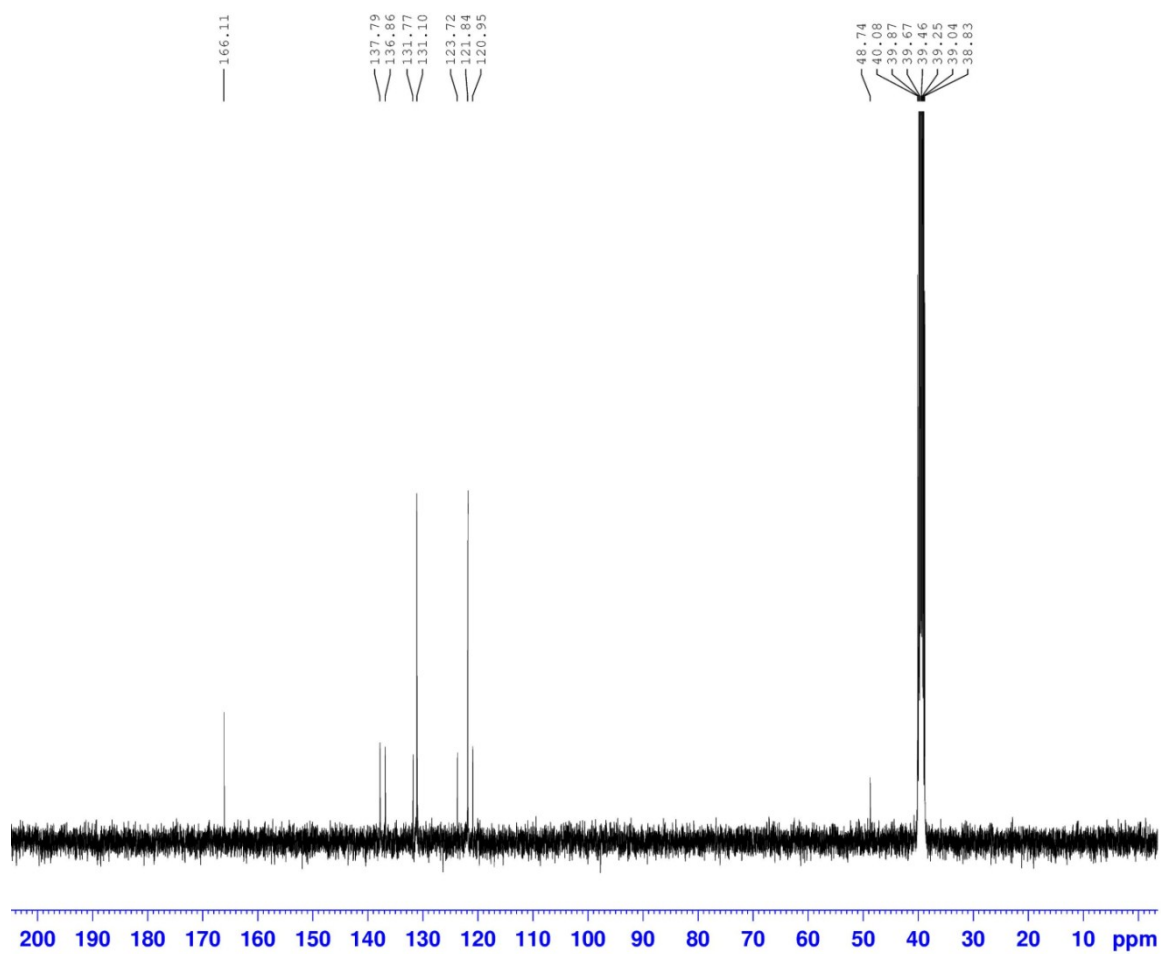


Figure S9. ^{13}C NMR spectrum of $L^2H_2Br_2$.

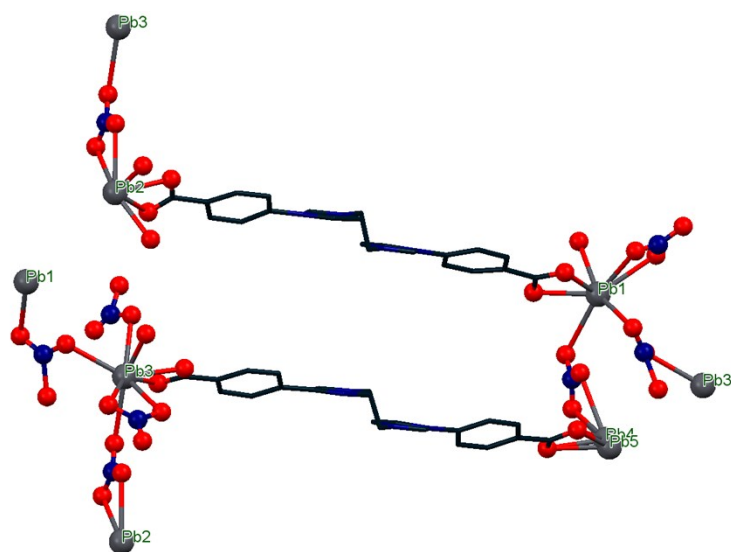
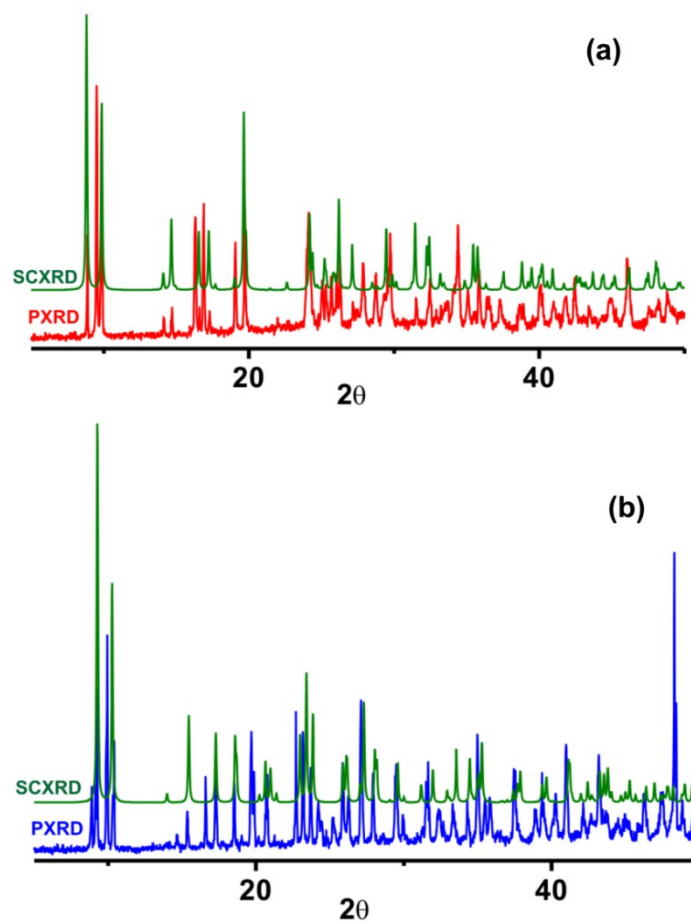
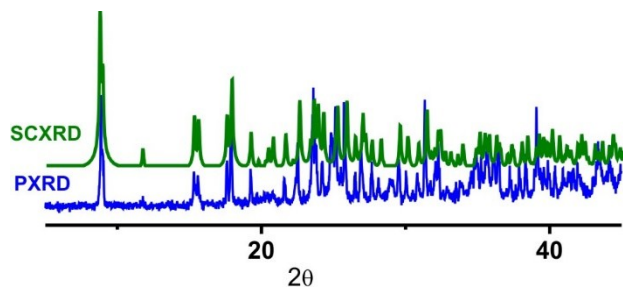


Figure S10. Coordination mode of lead centres in **3**.



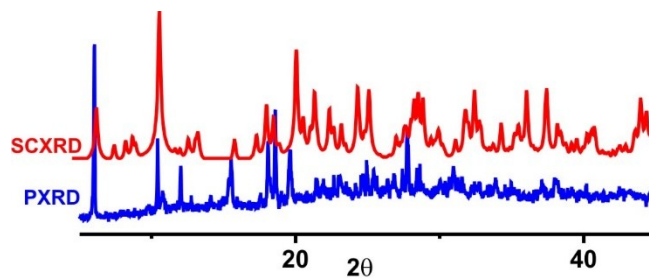
Although complexes **4** and **5** were isolated from same starting materials, **4** was isolated after 12 h and **5** was isolated after 48 h. We never isolated **4** and **5** together under any of these (vide supra) reactions. In order to prove this, we have performed the PXRD for the bulk sample and compared with simulated PXRD peaks of single crystal X-ray data (using mercury software). The experimental PXRD matches very well with simulated PXRD, which clearly supports the purity of bulk sample (purity is on par with single crystal). We assume that the comparison of PXRD is more appropriate than elemental analysis (as reported in MOF chemistry).

Figure S11. (a) PXRD of **4** (simulated in green, experimental in red); (b) PXRD of **5** (simulated in green, experimental in blue).



Similarly, as shown below the experimental PXRD of **1** matches very well with its simulated PXRD.

Figure S12. PXRD of **1** (simulated in green, experimental in red)



In addition, the experimental PXRD of **3** matches very well with its simulated PXRD.

Figure S13. PXRD of **3** (simulated in red, experimental in blue)

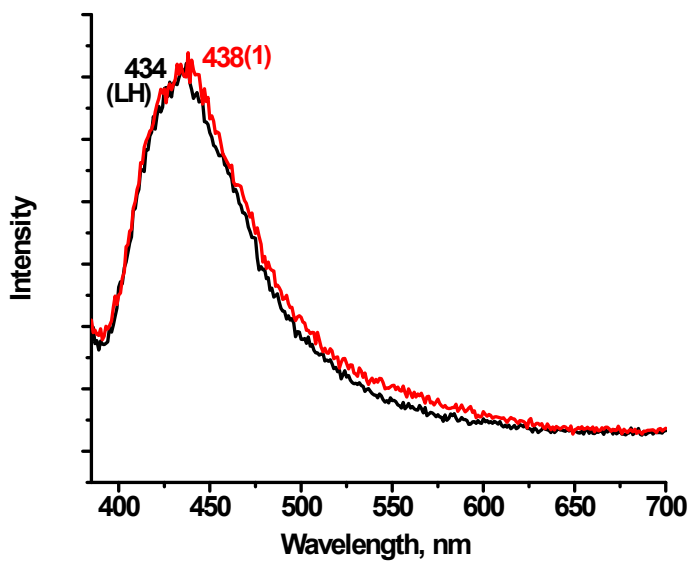


Figure S14. Solid state emission spectrum of **1** compared with **LH**

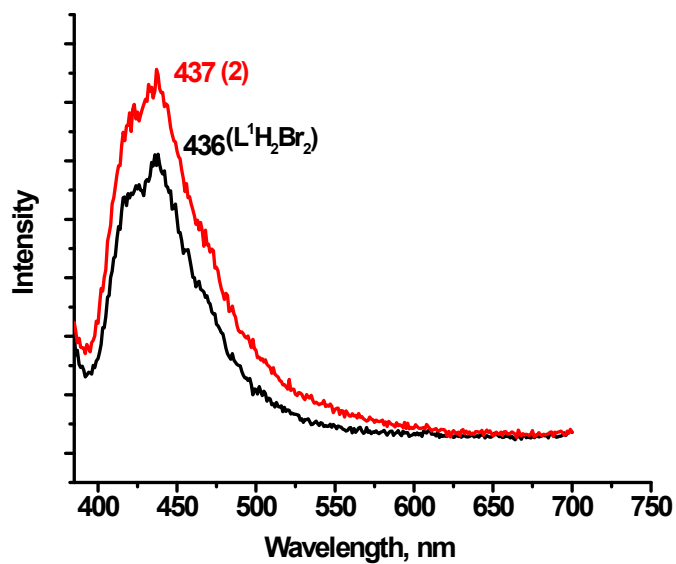


Figure S15. Solid state emission spectrum of **2** compared with $L^1H_2Br_2$.

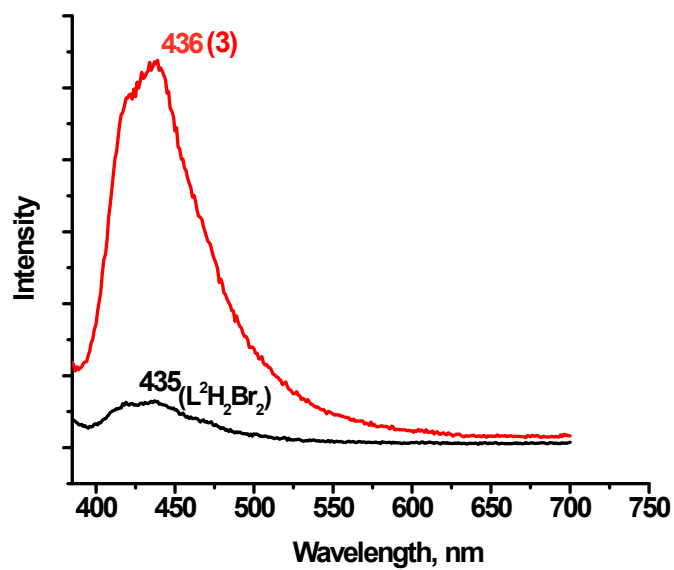


Figure S16. Solid state emission spectrum of **3** compared with $L^2H_2Br_2$.

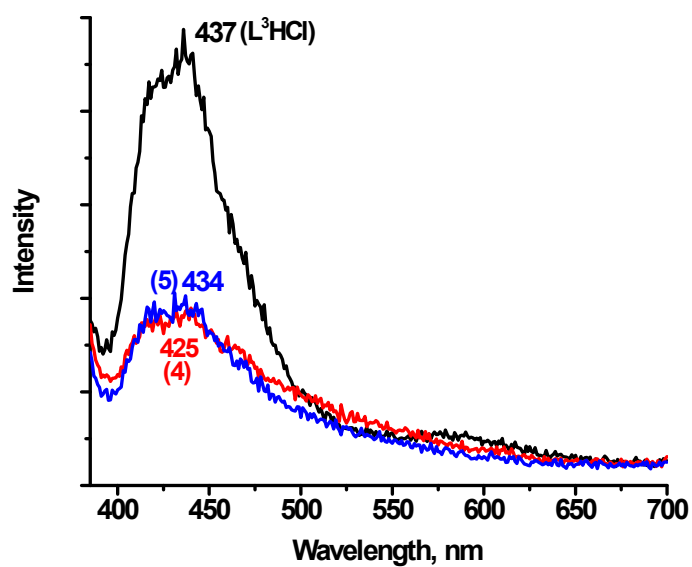
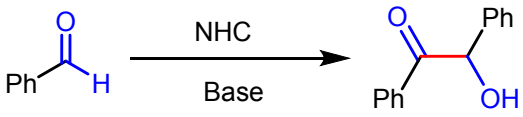
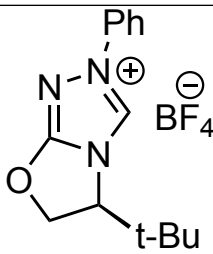
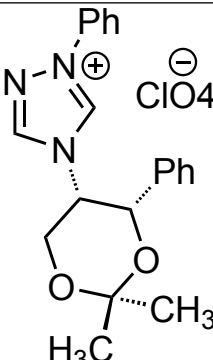
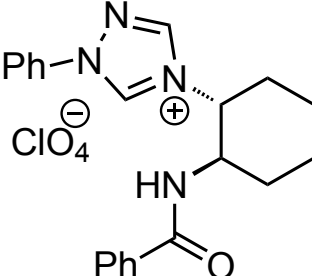
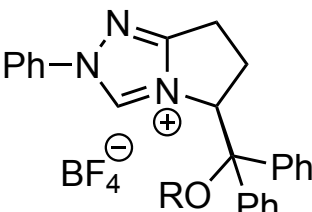
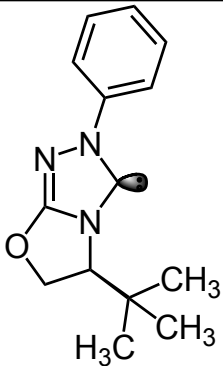
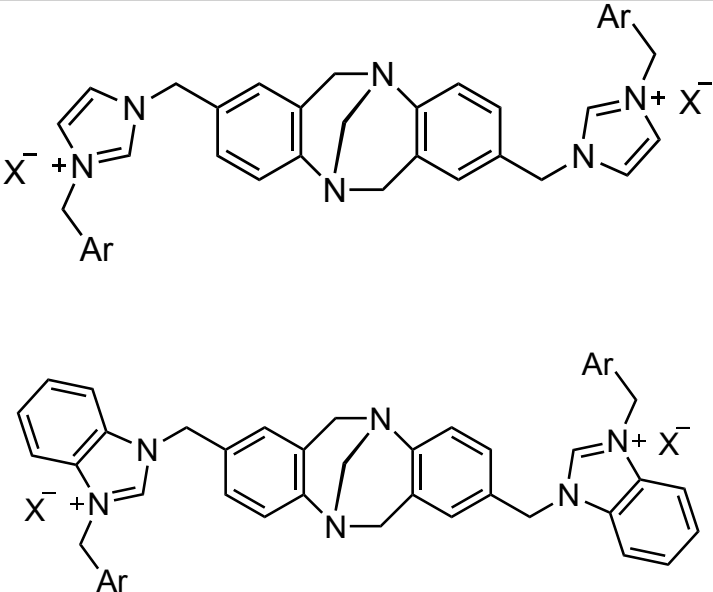
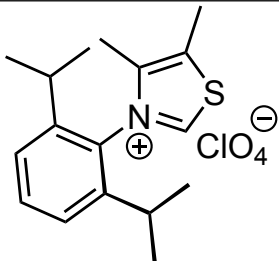
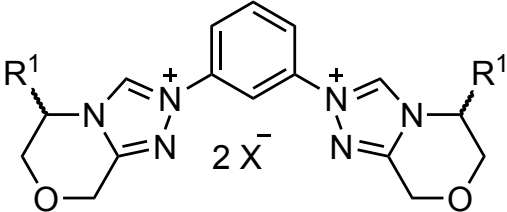


Figure S17. Solid state emission spectrum of **4**, **5** compared with L³HCl.

Table S1: Selected examples of NHC (organocatalyst) mediated benzoin condensation reaction

				
Entry	Isolated yield	Time	Catalyst	Reference
1	33-83%	16 h		Enders D, Niemeier O and Henseler A <i>Chem. Rev.</i> , 2007, 107 , 5606-5655
2	22-72 %	60 h		Enders D, Niemeier O and Henseler A <i>Chem. Rev.</i> , 2007, 107 , 5606-5655
3	0-33%	48 h	 	Louise Baragwanath, Christopher A. Rose, Kirsten Zeitler, and Stephen J. Connon, <i>J. Org. Chem.</i> 2009, 74 , 9214–9217

4	33-90 %	16 h		Dieter Enders and Ulrike Kallfass, <i>Angew. Chem. Int. Ed.</i> 2002, 41 , 1743-1745
5	72-95 %	20 h		Satyanarayana A and Prabusankar G, <i>J. Chem. Sci.</i> , 2015, 127 , No. 5, pp. 821–831
6	72-82 %	22 h		Isabel Piel, Marius D. Pawelczyk, Keiichi Hirano, Roland Fröhlich, and Frank Glorius, <i>Eur. J. Org. Chem.</i> 2011, 5475–5484
7	27-98 %	20 h		Yajun Ma, Siping Wei, Jie Wu, Fei Yang, Bo Liu, Jingbo Lan, Shengyong Yang, and Jingsong You, <i>Adv. Synth. Catal.</i> 2008, 350, 2645 – 2651

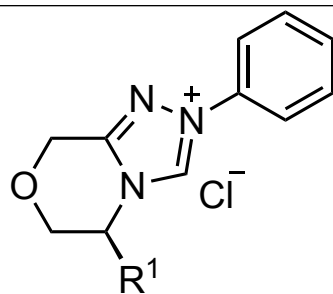
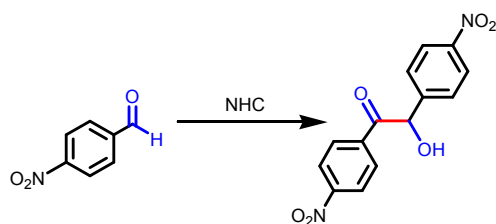


Table S2: Catalysts **1-5** mediated benzoin condensation of 4-nitrobenzaldehyde in 12 h.

Entry	Catalyst	Isolated Yield(%)		
		First run	Second run	Third run
1	1	98.75	96.88	97.21
2	2	94.90	96.10	96.74
3	3	91.25	93.43	89.78
4	4	95.10	97.95	94.76
5	5	89.87	87.65	90.65

Table S3: Selected examples of insitu N-Heterocyclic Carbene mediated benzoin condensation of 4-nitrobenzaldehyde.



Entry	Isolated Yield, %	Time	Catalyst	Reference
1	27	24 h		Hernandez, Karel et al <i>Chemistry - A European Journal</i> , 2015, 21(8) , 3335-3346.
2	34	20 sec		Bag, Seema et al, <i>Journal of Chemical Research.</i> , 2006, 4 , 267-269.
3	85	12 h		Mohanazadeh, Farajollah and Aghvami, Majid, <i>Phosphorus, Sulfur and Silicon and the Related Elements.</i> , 2007, 182(10) , 2467-2475.
4	0	20 h		Iwamoto, Ken-ichi et al <i>Tetrahedron Letters.</i> , 2006, 47(40) , 7175-7177.