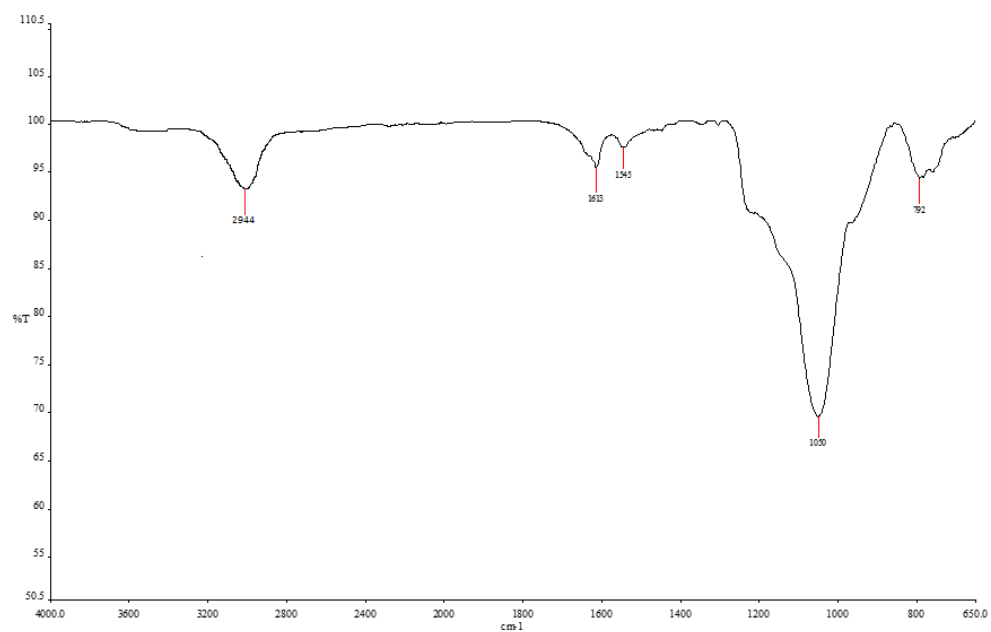


SUPPLEMENTARY INFORMATION

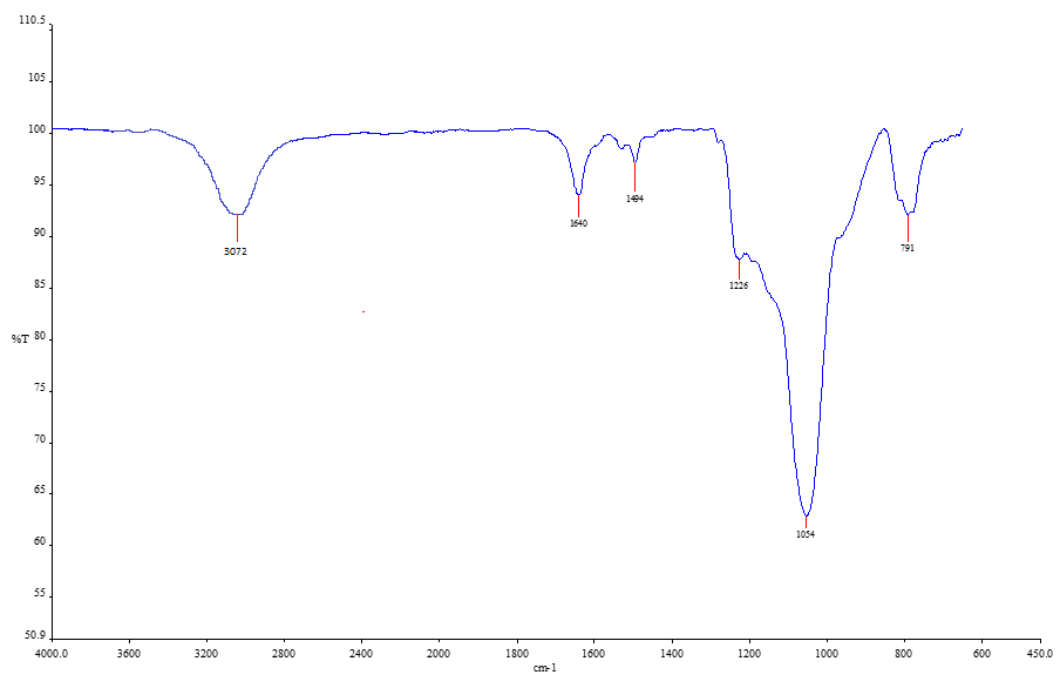
**Synthesis of MCM-41 Immobilized (Phenoxy)Imine Palladium(II) Complexes as Recyclable Catalysts in the Methoxycarbonylation of 1-Hexene**

Saphan Akiri and Stephen Ojwach \*

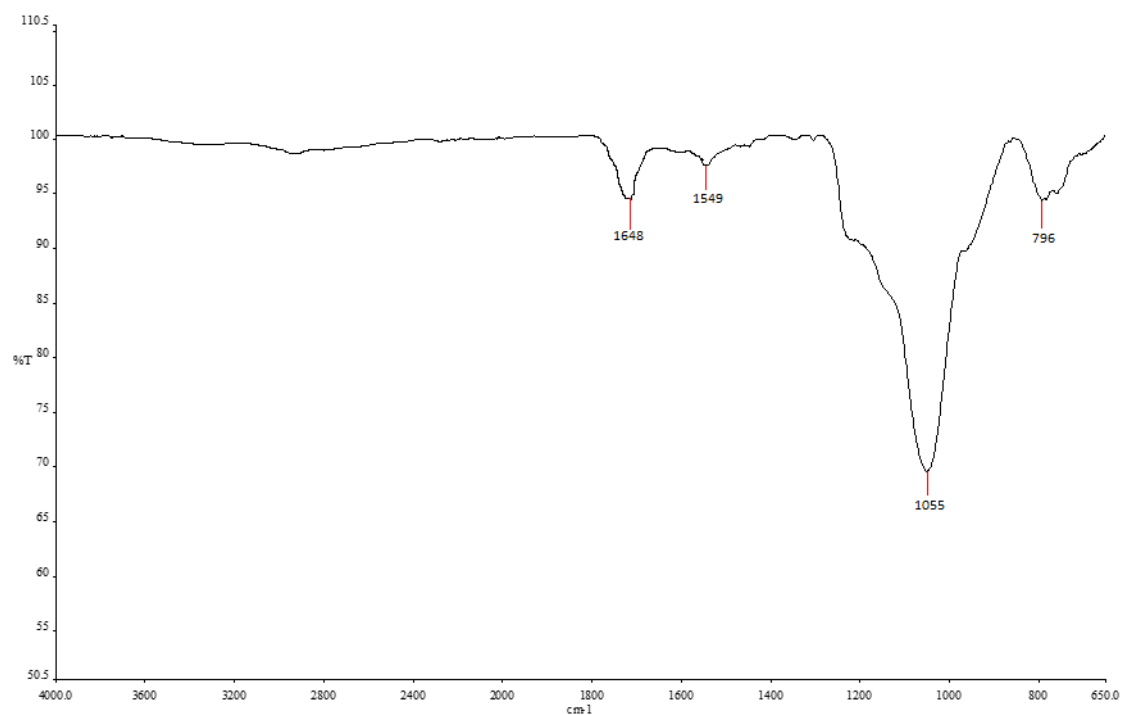
<sup>a</sup>School of Chemistry and Physics, University of KwaZulu-Natal, Private Bag X01,  
Scottsville, Pietermaritzburg 3209, South Africa



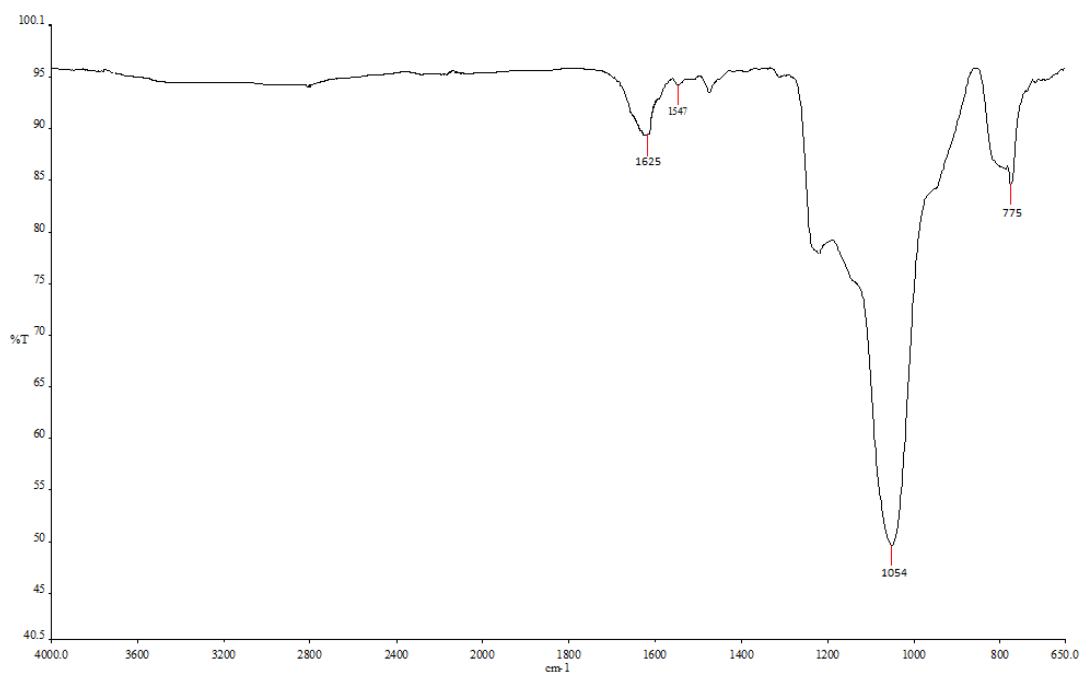
**Figure S1.** The IR spectrum of ligand **HL3** showing  $\nu(\text{C}=\text{N})$  at 1614 and  $\nu(\text{Si-O-Si})$  at 1061.



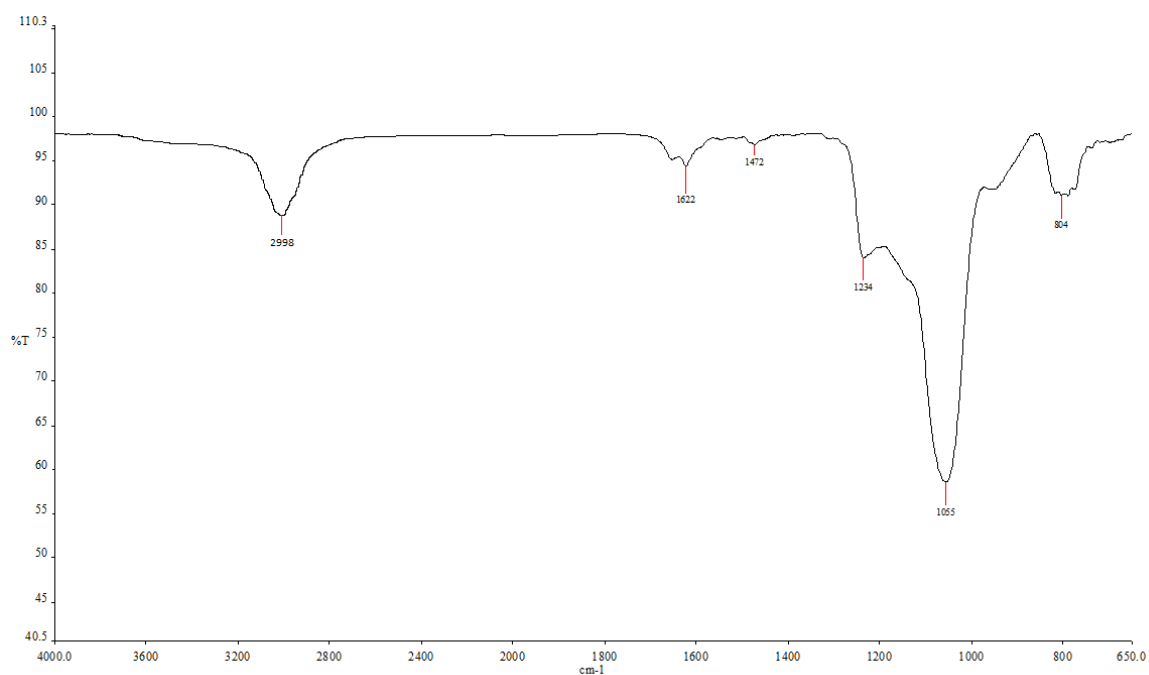
**Figure S2.** The IR spectrum of ligand **HL4** showing  $\nu(\text{C}=\text{N})$  at 1611 and  $\nu(\text{Si-O-Si})$  at 1031.



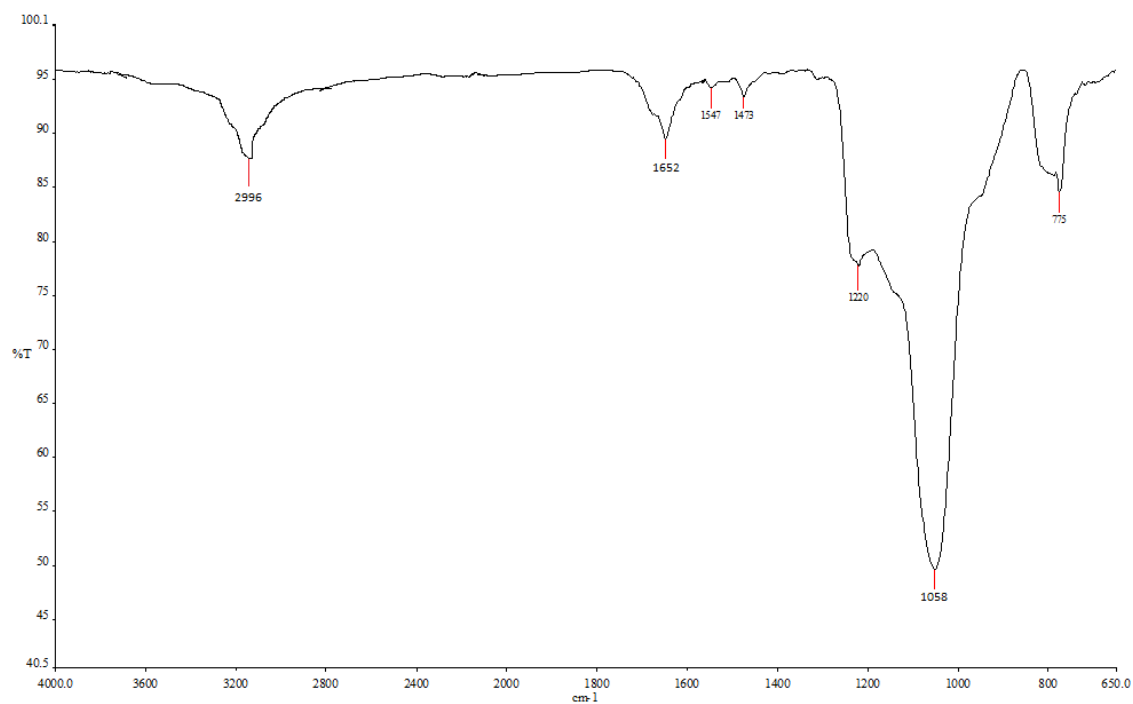
**Figure S3.** The IR spectrum of complex **1** showing  $\nu(\text{C}=\text{N})$  at 1648 and  $\nu(\text{Si}-\text{O}-\text{Si})$  at 1055.



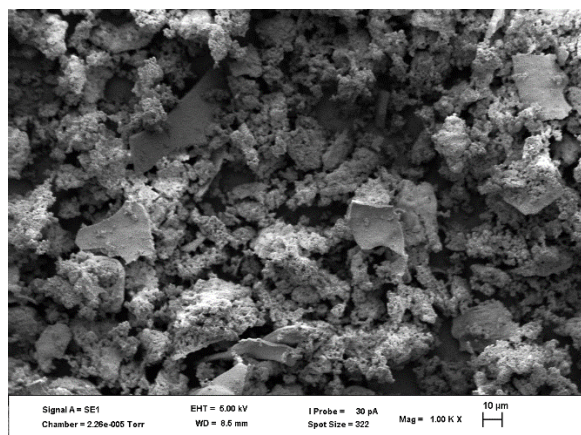
**Figure S4.** The IR spectrum of complex **2** showing  $\nu(\text{C}=\text{N})$  at 1625 and  $\nu(\text{Si}-\text{O}-\text{Si})$  at 1054.



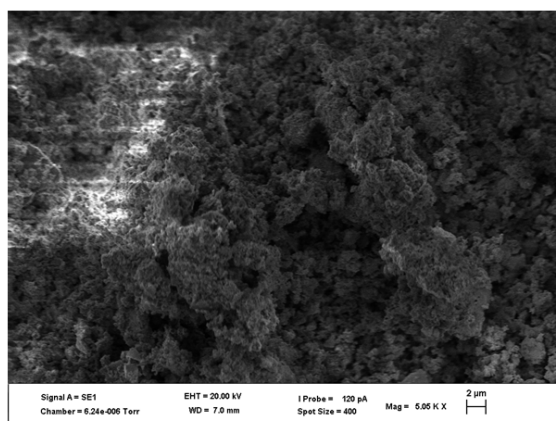
**Figure S5.** The IR spectrum of complex **3** showing  $\nu(\text{C}=\text{N})$  at 1622 and  $\nu(\text{Si-O-Si})$  at 1055.



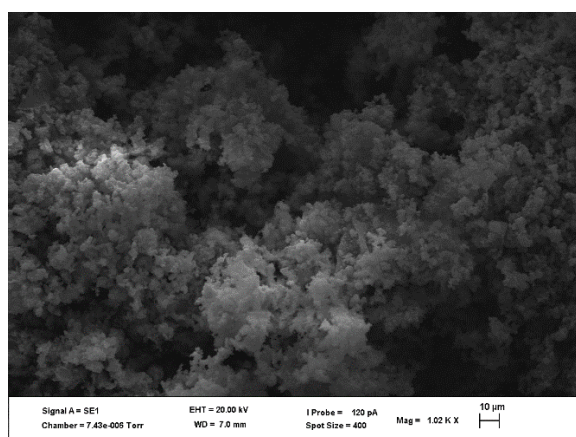
**Figure S6.** The IR spectrum of complex **4** showing  $\nu(\text{C}=\text{N})$  at 1652 and  $\nu(\text{Si-O-Si})$  at 1058.



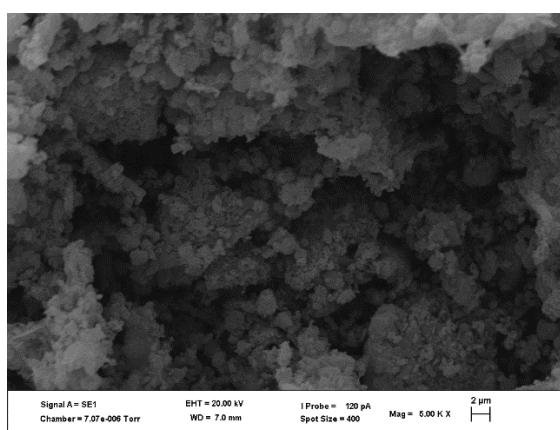
HL3



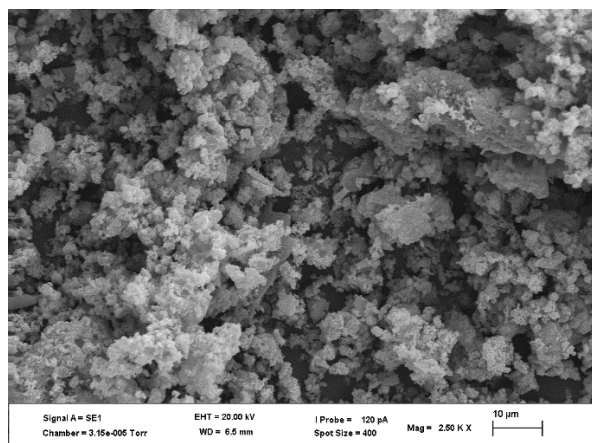
HL4



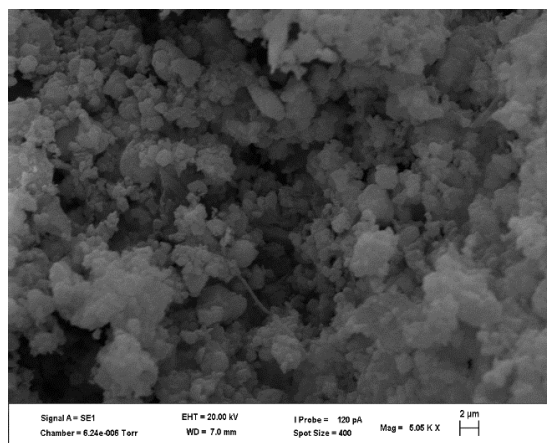
Complex 1



Complex 2

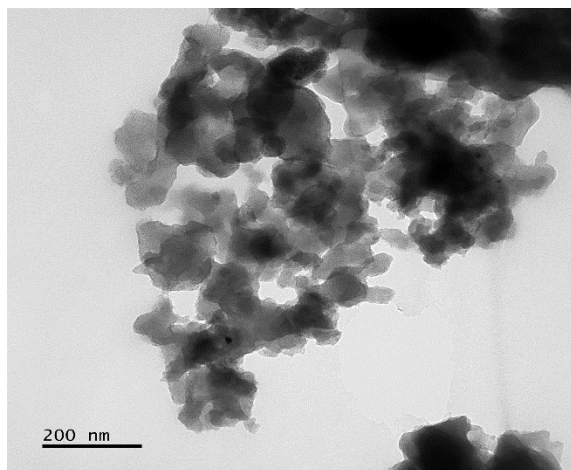


Complex 3

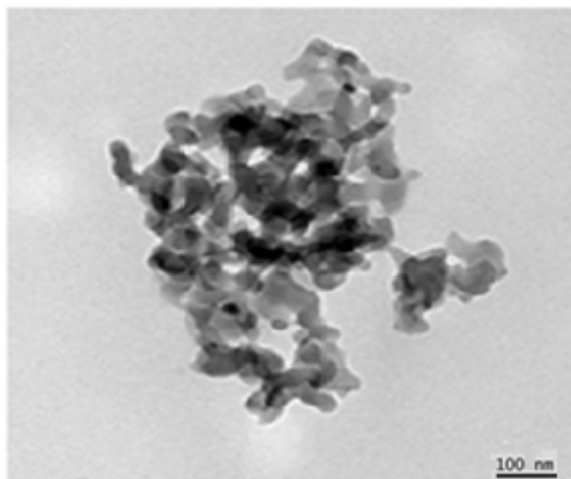


Complex 4

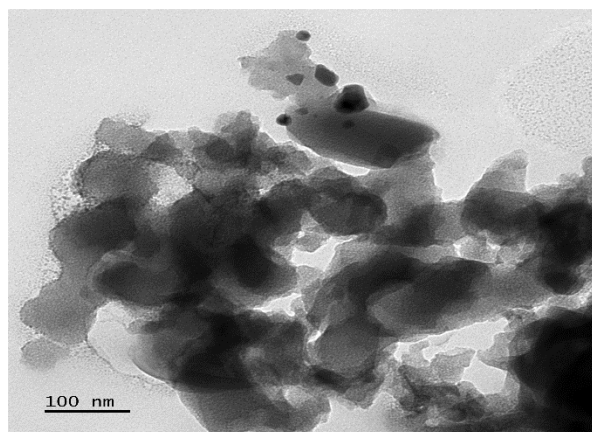
**Figure S7.** SEM images displaying the morphologies of the immobilized ligands and complexes 1-4.



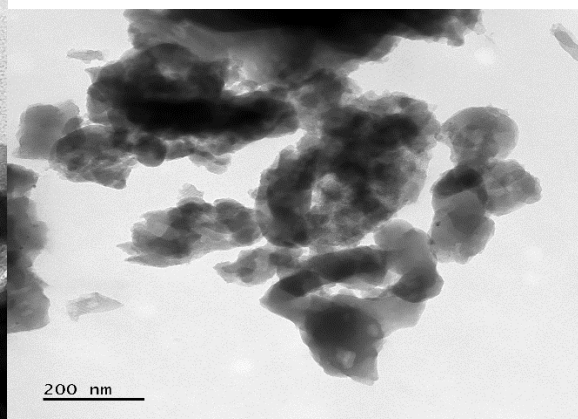
HL3



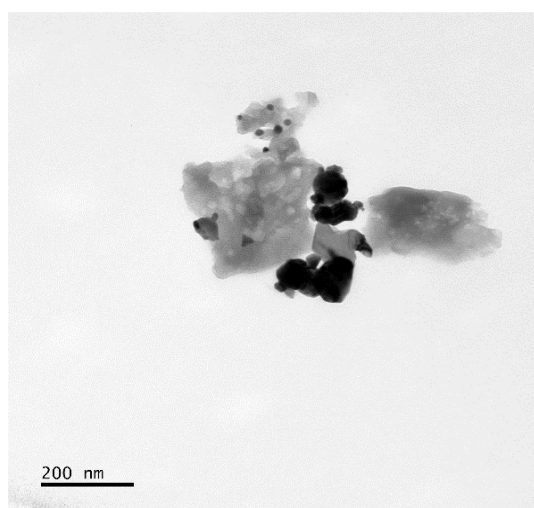
HL4



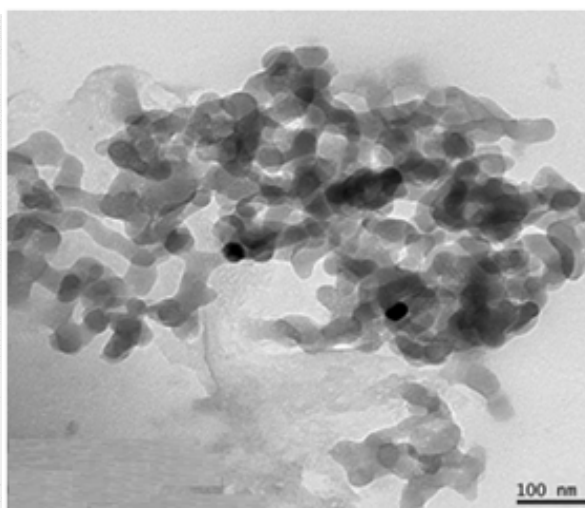
Complex 1



Complex 2

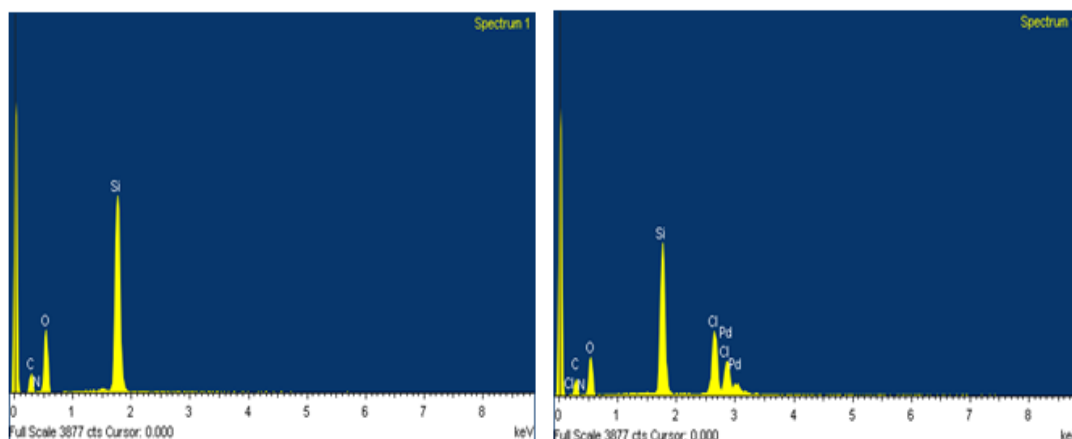


Complex 3

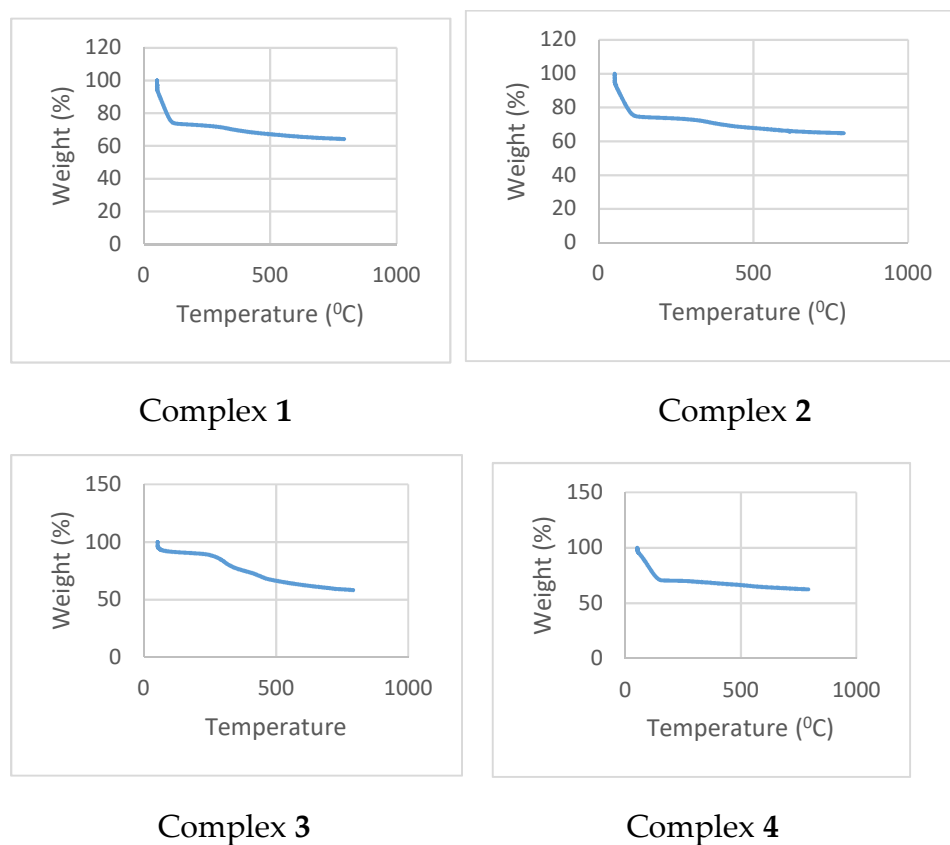


Complex 4

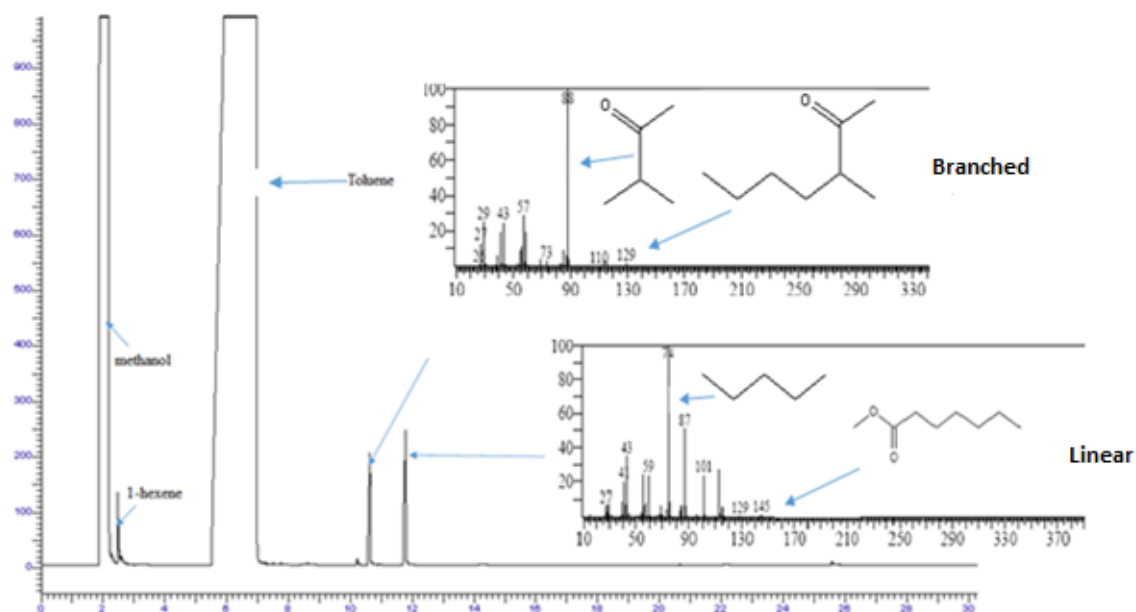
**Figure S8.** TEM images displaying the morphologies of the Immobilized ligands and their respective complexes.



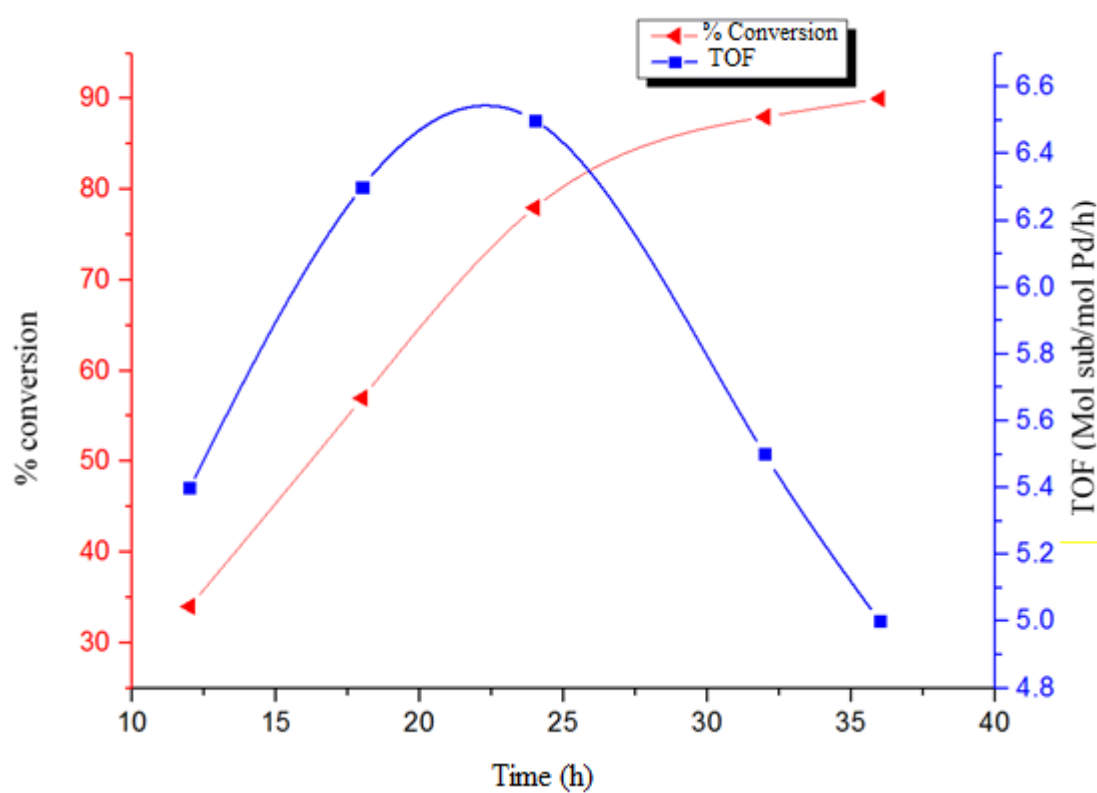
**Figure S9.** The Energy Dispersive X-ray Spectroscopy (EDX) spectrum of ligand **L4** and complex **4** showing the presence of a Pd signal in **4**.



**Figure S10.** A TGA graphical plot showing the decomposition phases of complexes **1–4**.

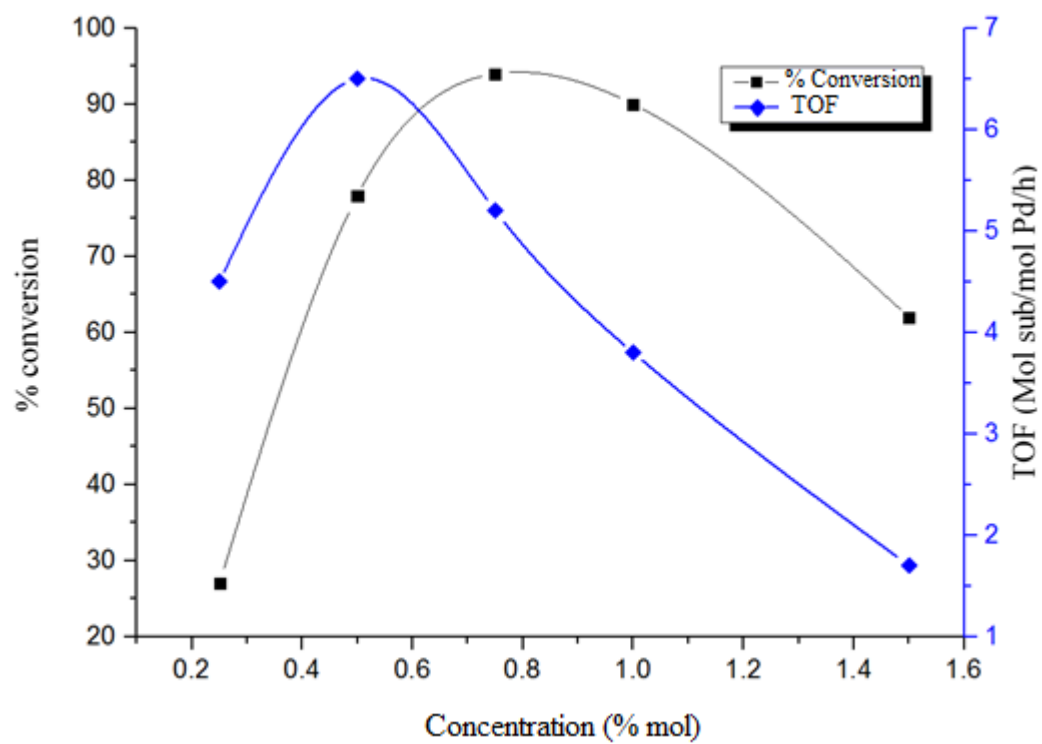


**Figure S11.** The GC and GC-MS spectra of methoxycarbonylation products identified as branched (methyl 2-methylhexanoate) and linear (methyl heptanoate) esters.

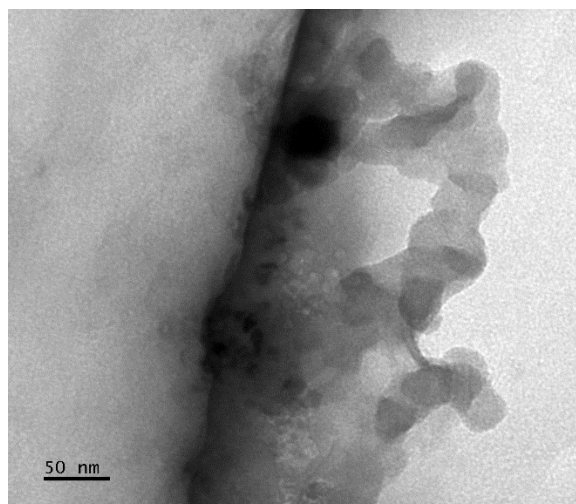


**Figure S12.** A graphical plot showing the variations of TOF and the % conversion with the reaction time for complex 2.

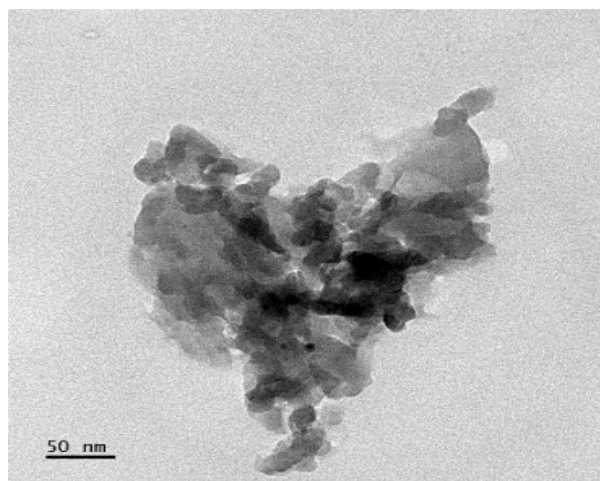




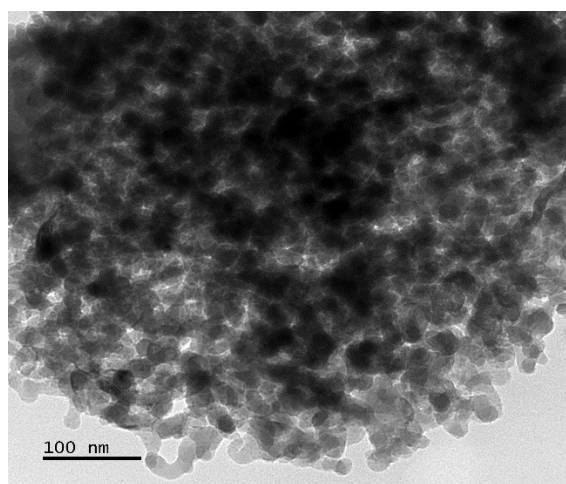
**Figure S13.** A graphical plot showing the variations of TOF and the % conversion with the catalyst concentration for complex 2.



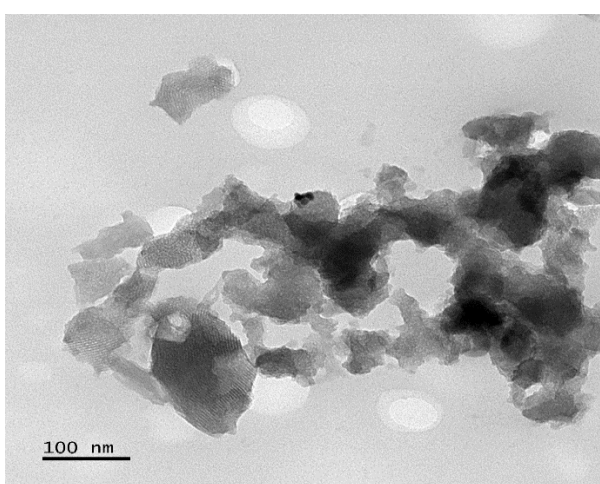
Complex 1



Complex 2

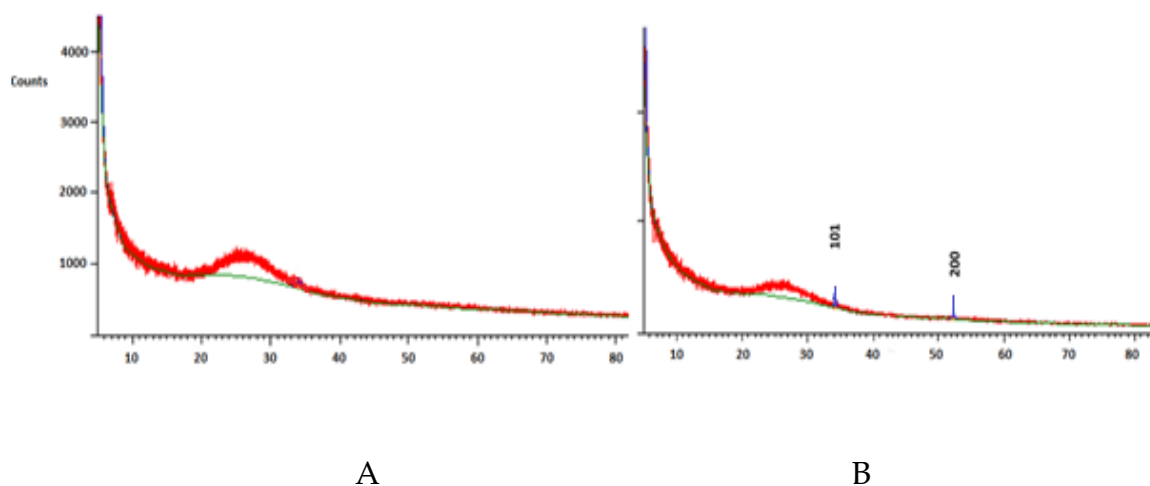


Complex 3



Complex 4

**Figure S14.** TEM images showing changes in the morphologies of the immobilized catalyst after four cycles of catalysis experiments.



**Figure S15.** XRD patterns for the native MCM-41 (**A**) and complex 2 (**B**).

**Table S1.** The EDX data for the fresh immobilized complexes showing elemental compositions.

| Element       | Complex 1 |        | Complex 2 |        | Complex 3 |        | Complex 4 |        |
|---------------|-----------|--------|-----------|--------|-----------|--------|-----------|--------|
|               | Weight    | Atomic | Weight    | Atomic | Weight    | Atomic | Weight    | Atomic |
|               | (%)       | (%)    | (%)       | (%)    | (%)       | (%)    | (%)       | (%)    |
| <b>C</b>      | 5.52      | 8.71   | 10.62     | 14.56  | 15.61     | 26.59  | 10.84     | 18.86  |
| <b>N</b>      | 10.34     | 15.64  | 10.30     | 15.54  | 5.97      | 8.72   | 6.89      | 10.18  |
| <b>O</b>      | 48.40     | 54.00  | 45.97     | 50.22  | 32.67     | 41.75  | 36.45     | 47.14  |
| <b>Si</b>     | 34.26     | 20.38  | 31.26     | 19.38  | 17.98     | 13.09  | 19.03     | 14.02  |
| <b>Cl</b>     | -         | -      | -         | -      | 11.73     | 6.77   | 12.30     | 7.28   |
| <b>Pd</b>     | 1.47      | 1.26   | 1.85      | 1.32   | 16.04     | 3.08   | 14.48     | 2.82   |
| <b>Totals</b> | 100.00    |        | 100.00    |        | 100.00    |        | 100.00    |        |

**Table S2.** The residual masses of the complexes after heating to 800 °C.

| Complex  | Original mass (g) | Residual weight (%) | Activity (%) |
|----------|-------------------|---------------------|--------------|
| <b>1</b> | 5.03              | 64                  | 76           |
| <b>2</b> | 5.47              | 65                  | 78           |
| <b>3</b> | 5.65              | 66                  | 59           |
| <b>4</b> | 10.61             | 62                  | 61           |

**Table S3.** The EDX data for the recycled immobilized complexes showing elemental compositions.

| Element       | Complex 1 |        | Complex 2 |        | Complex 3 |        | Complex 4 |        |
|---------------|-----------|--------|-----------|--------|-----------|--------|-----------|--------|
|               | Weight    | Atomic | Weight    | Atomic | Weight    | Atomic | Weight    | Atomic |
|               | (%)       | (%)    | (%)       | (%)    | (%)       | (%)    | (%)       | (%)    |
| <b>C</b>      | 6.56      | 10.31  | 10.58     | 13.46  | 16.05     | 26.88  | 11.15     | 18.90  |
| <b>N</b>      | 11.58     | 16.62  | 11.35     | 15.33  | 6.54      | 7.79   | 7.23      | 10.37  |
| <b>O</b>      | 49.12     | 52.31  | 45.52     | 51.06  | 32.12     | 42.05  | 37.09     | 47.30  |
| <b>Si</b>     | 35.44     | 19.66  | 31.20     | 18.94  | 18.98     | 13.09  | 19.35     | 14.15  |
| <b>Cl</b>     | -         | -      | -         | -      | 11.55     | 7.61   | 13.42     | 7.32   |
| <b>Pd</b>     | 1.30      | 1.10   | 1.35      | 1.21   | 14.76     | 2.58   | 11.76     | 1.96   |
| <b>Totals</b> | 100.00    |        | 100.00    |        | 100.00    |        | 100.00    |        |