

SUPPORTING INFORMATION

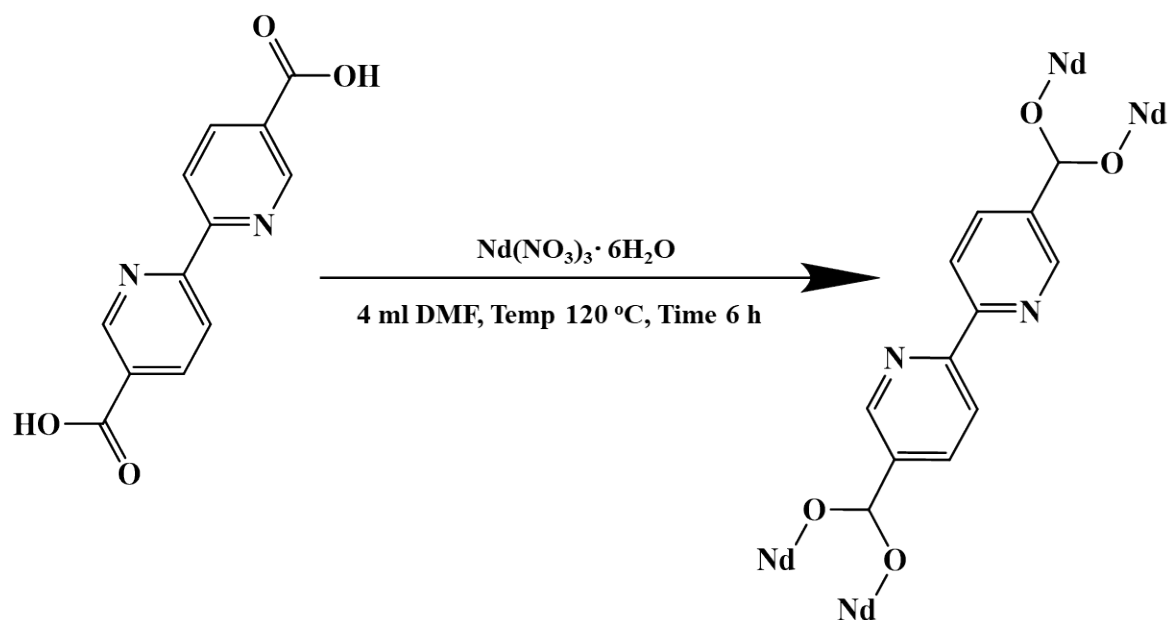
Synthesis and characterisation of neodymium based MOFs for application in carbon dioxide reduction to syngas

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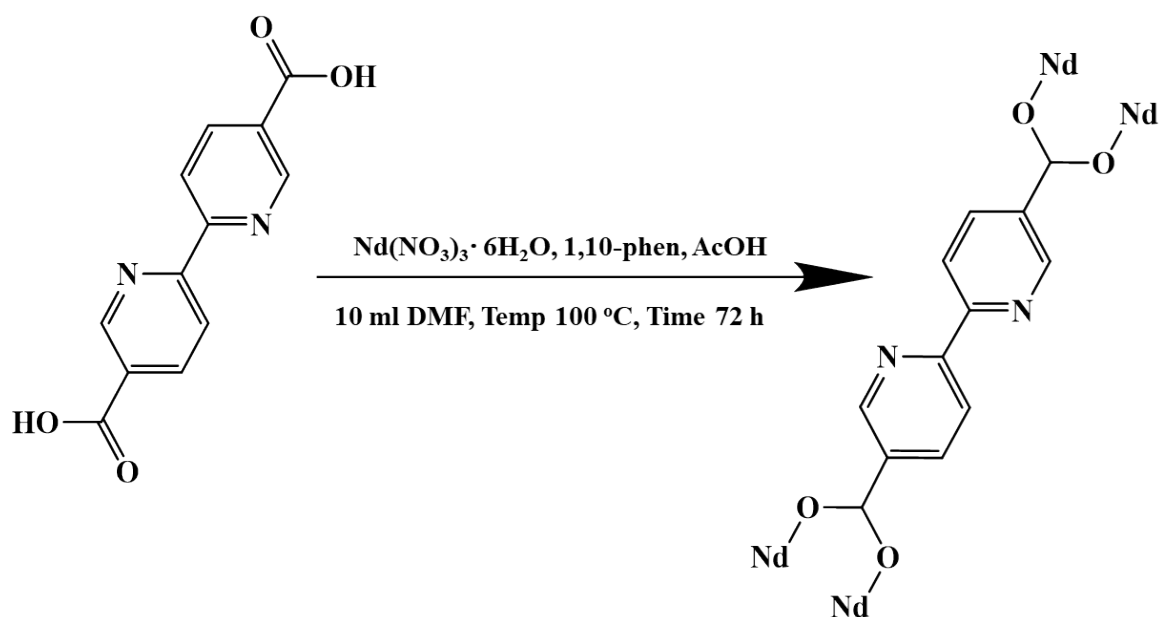
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Scheme 1: Synthetic scheme for JMS-10



Scheme 2: Synthetic scheme for JMS-11

Table S1: Crystallographic and refinement parameters of JMS-10 and JMS-11

	JMS-10	JMS-11
Empirical formula	$\text{C}_{36}\text{H}_{18}\text{Nd}_2\text{N}_6\text{O}_{14}$	$\text{C}_{47.25}\text{H}_{44.25}\text{Nd}_2\text{N}_{9.75}\text{O}_{16.75}$
Formula weight (g mol^{-1})	1067.08	1305.15
Crystal system	Monoclinic	Monoclinic
T/K	173	143
Space group	$P2_1/c$	$P2_1/c$
a/Å	26.3857(12)	27.4090(3)
b/Å	14.0955(7)	11.1853(2)
c/Å	16.9025(8)	16.97965(19)
$\alpha/^\circ$	90	90
$\beta/^\circ$	98.528 (2)	98.5206(12)
$\gamma/^\circ$	90	90

Volume/Å ³	6216.878 (5)	5148.13 (13)
Z	4	4
Calculated density (g/cm ³)	1.136	1.684
F(000)	2080	2600
μ, mm ⁻¹	1.701	15.91
Crystal size/mm ³	0.090 x 0.120 x 0.120	0.196 x 0.084 x 0.029
Radiation	0.71073	1.54184
2θ max	60.90°	75.7°
Goodness of fit S	1.15	1.03
Final R indexes [I>=2σ (I)]	0.0737 (15969)	0.0541(8615)
Final wR ₂ indexes [all data]	0.1648 (19050)	0.1417(10133)
Highest peak	5.14	3.46
Deepest hole	-2.84	-1.93

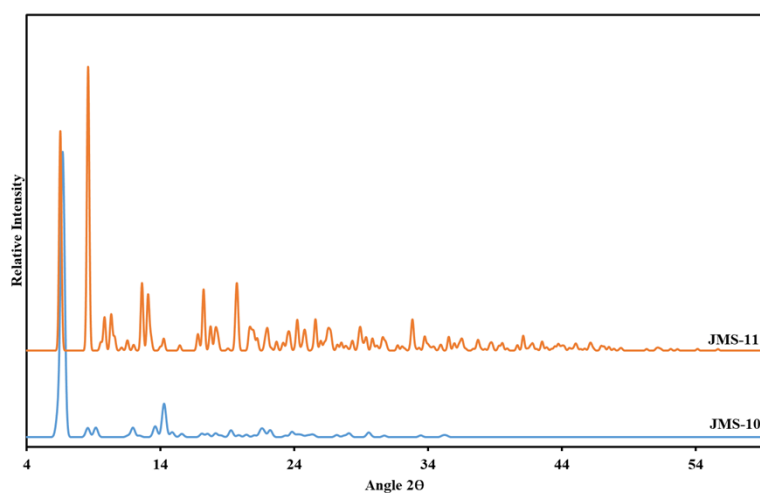


Figure S1: A comparison of the simulated patterns of JMS-10 and JMS-11

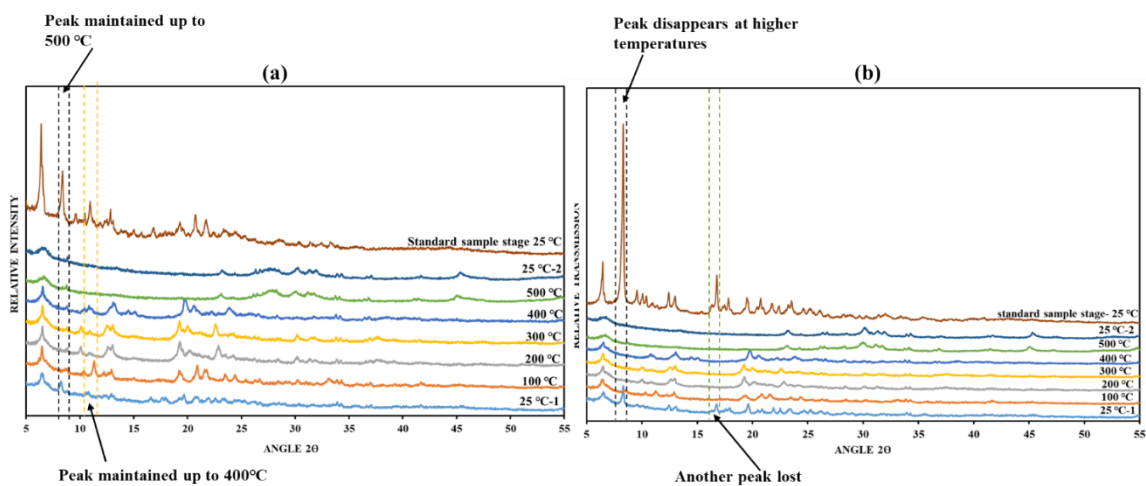


Figure S2: Variable temperature PXRD for (a) JMS-10 and (b) JMS-11, comparing the plots of the samples ran in the VT chamber with a sample ran at the standard sample stage.

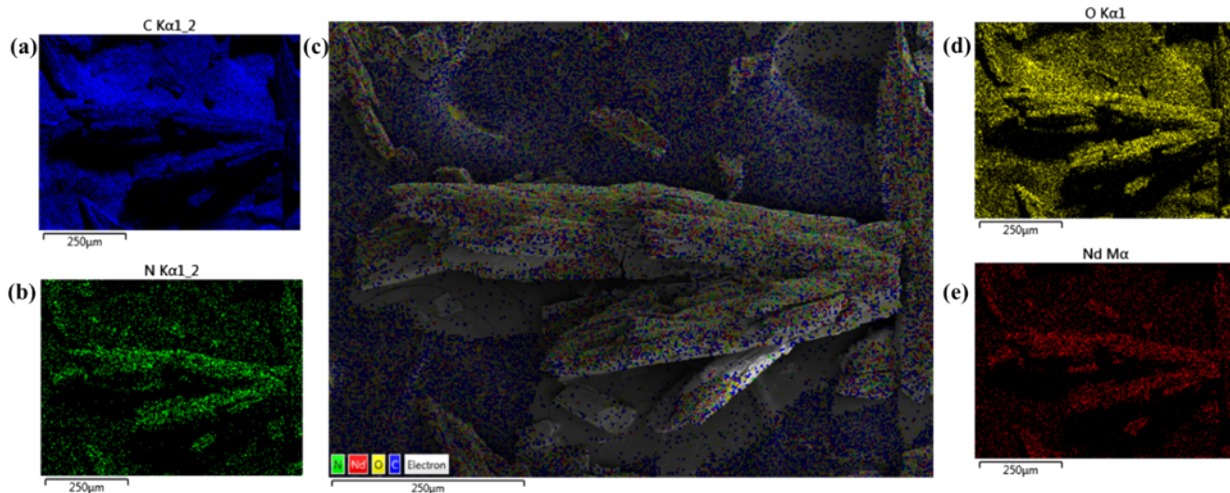


Figure S3: Elementary mapping of JMS-10 crystal as obtained from SEM-EDX

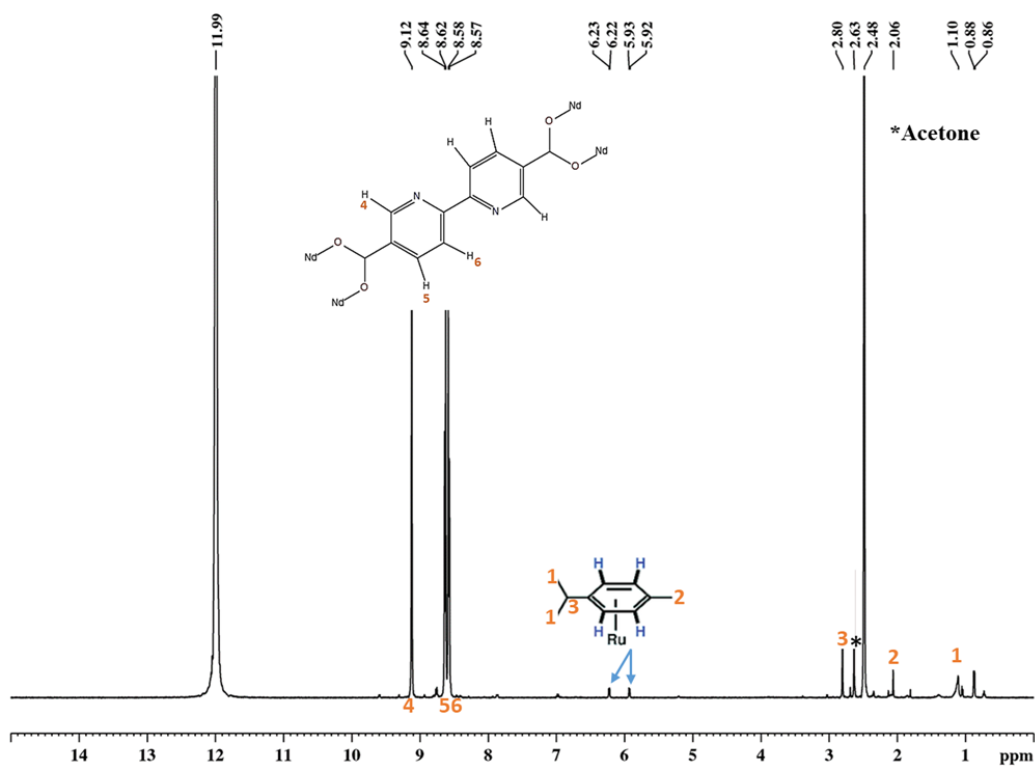


Figure S5: Proton NMR for Ru(II)@JMS-10

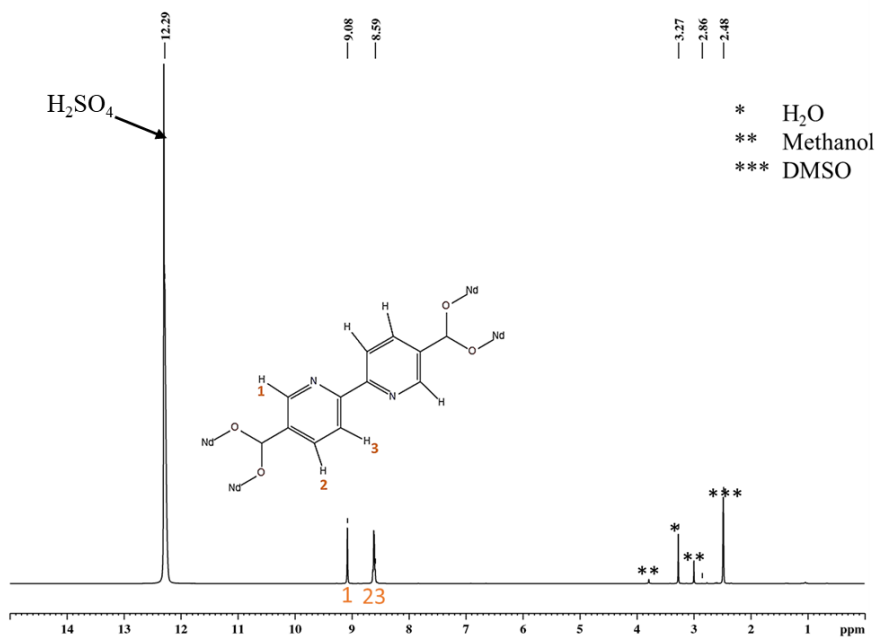


Figure S6: Proton NMR for JMS-10

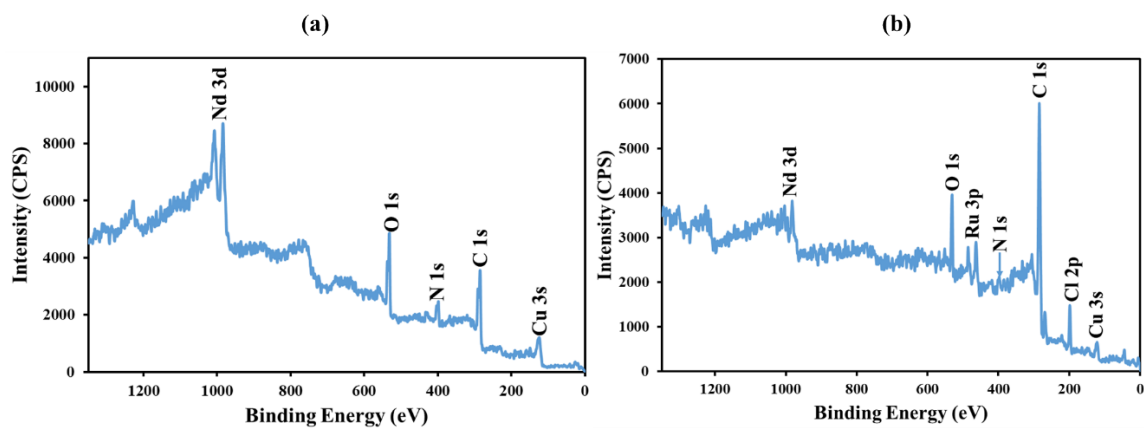


Figure S7: XPS of (a) JMS-10 and (b) Ru(II)@JMS-10

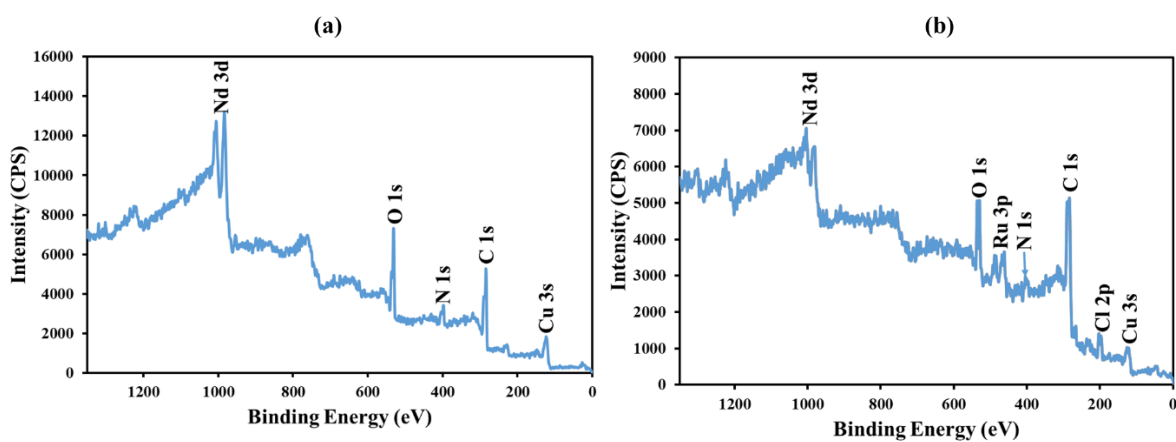


Figure S8: XPS of (a) JMS-11 and (b) Ru(II)@JMS-11

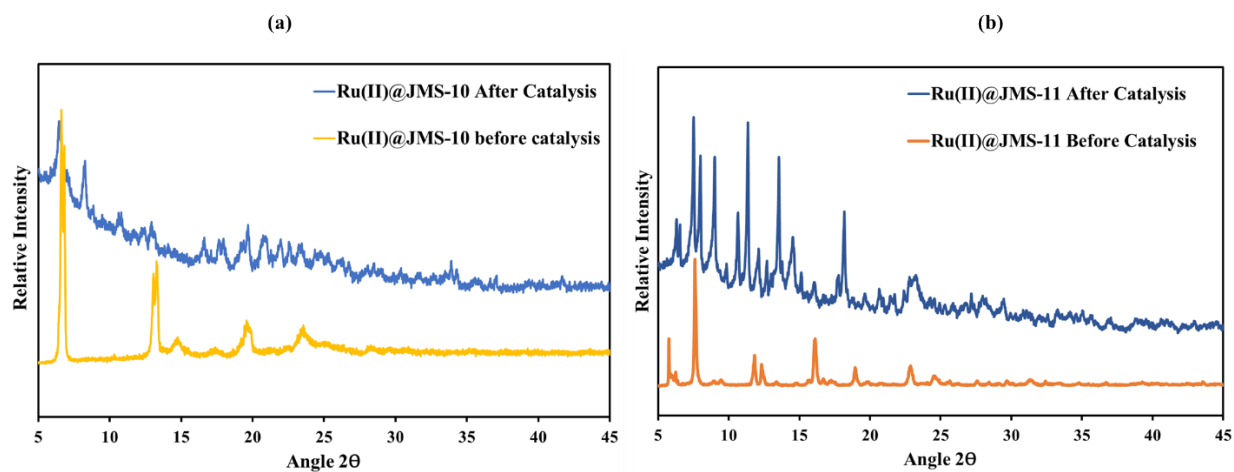


Figure S9: PXRD plots for the and Ru functionalised JMS-10 and JMS-11 before and after catalysis

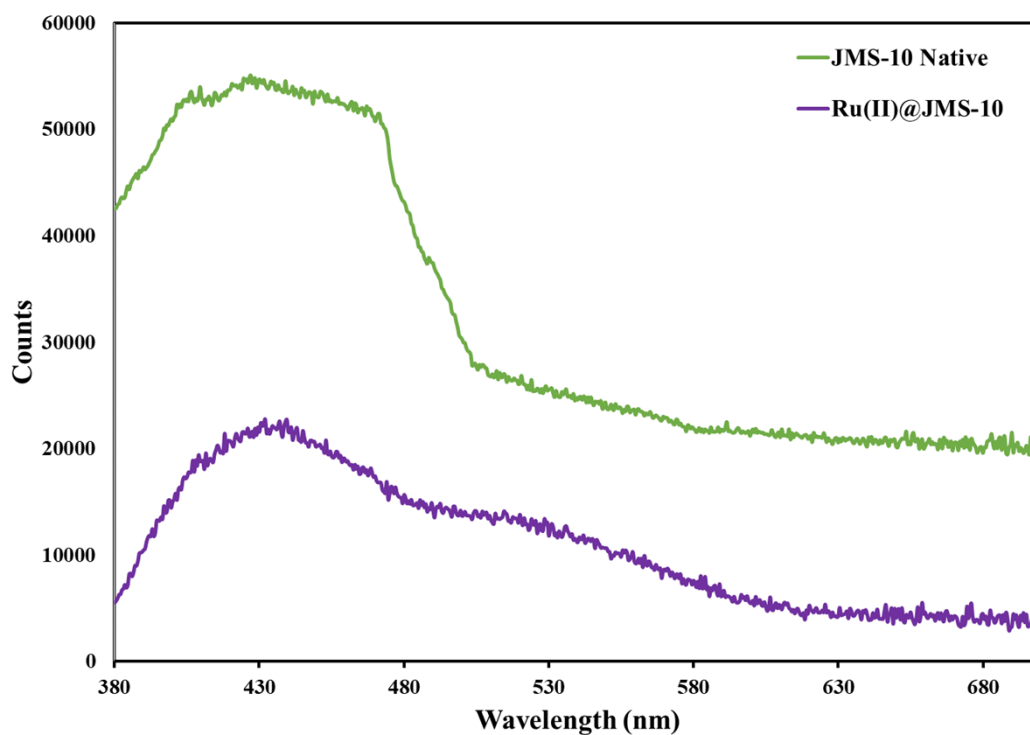


Figure S10: Photoluminescence results for JMS-10 and its functionalised form.

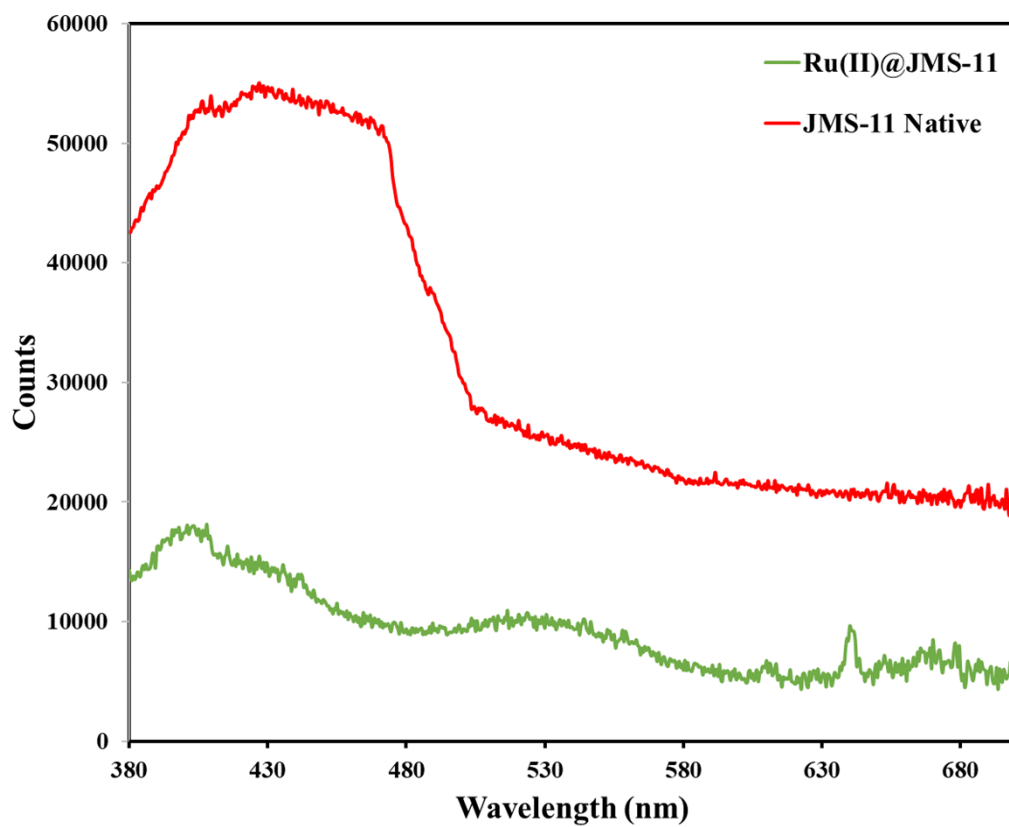


Figure S11: Photoluminescence of JMS-11 and its functionalised form.