Electronic Supplementary Material (ESI) for Catalysis Science & Technology.


# Understanding the Impact of One-Dimensional Pore Containing 10MR and 12MR and Aluminium Content on MTH Reaction Pathways: Direct Synthesis of Heteroatom Containing UZM-55

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Figure S1. SEM Photos at 10µm scale of Al-UZM-55- (A) 278, (B) 144, (C) 95 & (D) 63.

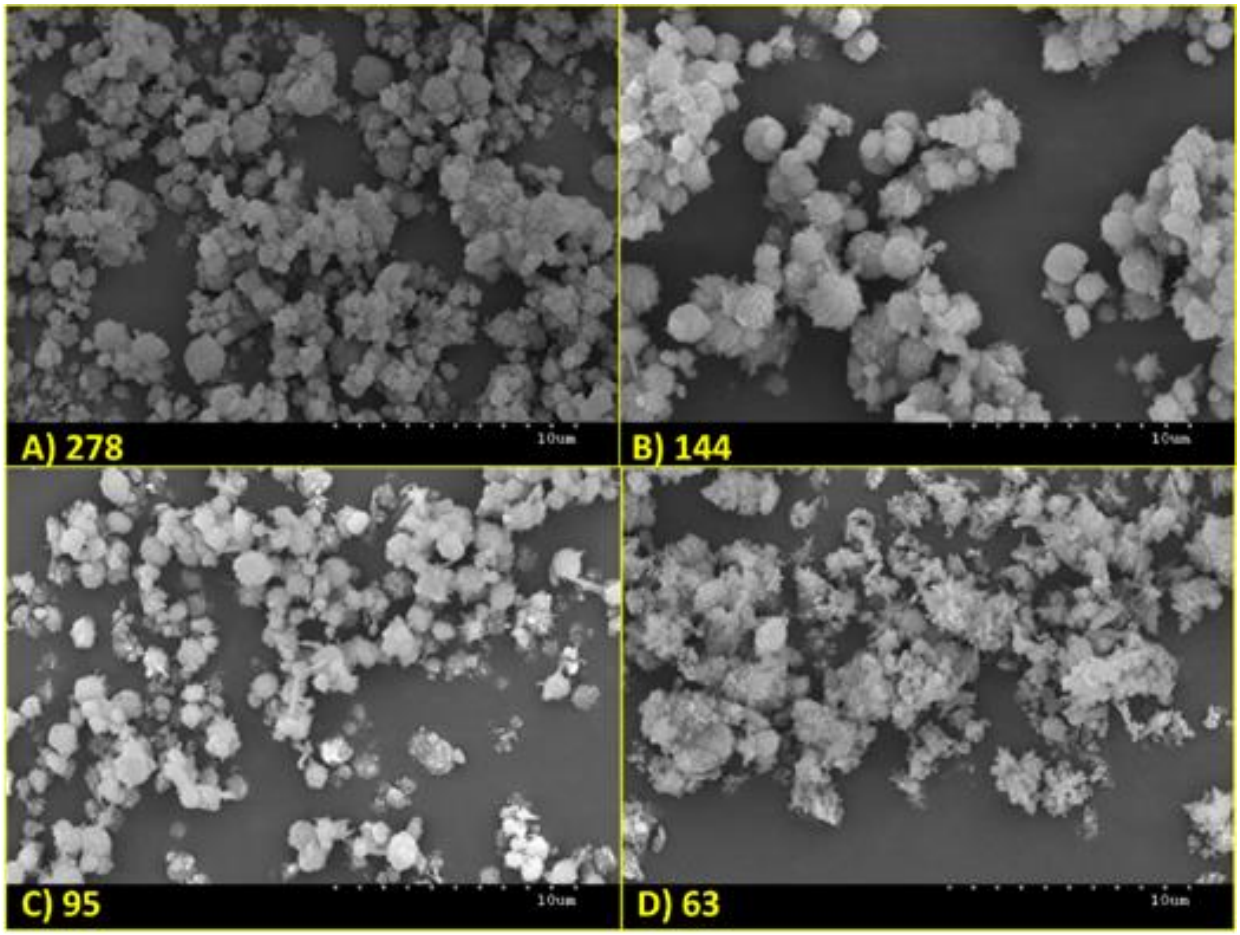
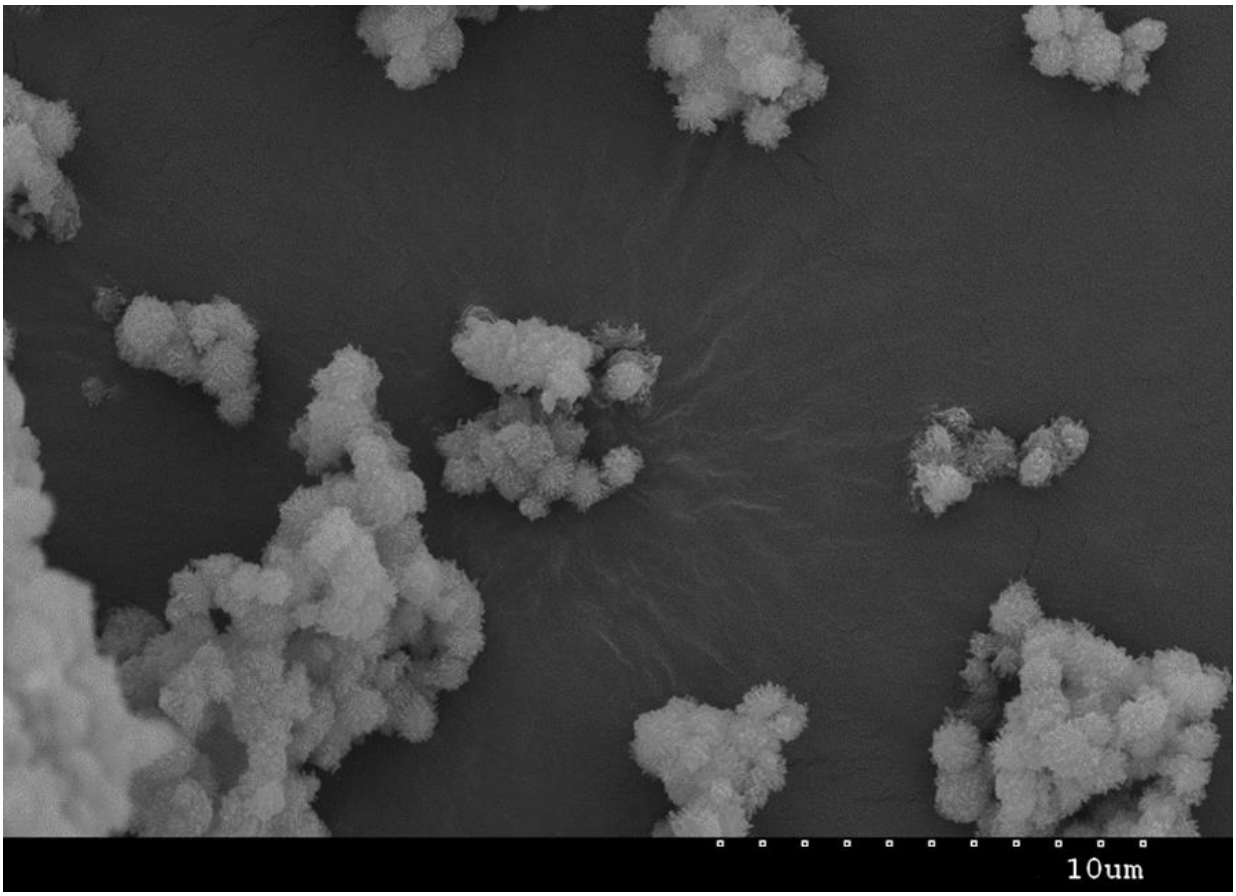


Figure S2. SEM Photos at 10µm scale of B-UZM-55 Material.



**Analysis of OSDA content (CHN / TGA)**

Table S1. CHN Analysis of the as-synthesized UZM-55 materials

| Si/Al ratio | C(%) | H(%) | N(%) | Expected SDA C/N | C/N Ratio | OSDA / UC |
|---|---|---|---|---|---|---|
| >4000 | 7.67 | 1.58 | 0.98 | 9.00 | 9.12 | 1.02 |
| 278 | 7.46 | 1.68 | 0.97 | | 9.01 | 1.01 |
| 144 | 7.87 | 1.71 | 0.96 | | 9.55 | 1.00 |
| 95 | 7.83 | 1.42 | 0.99 | | 9.26 | 1.03 |
| 63 | 8.21 | 1.75 | 1.03 | | 9.30 | 1.07 |
| 124 (B) | 7.85 | 1.69 | 0.98 | | 9.34 | 1.02 |

Thermogravimetric analysis was utilized to understand SDA decomposition as a function of aluminum content, with results obtained (Figure S3) consistent with that previously published. For each sample, 1-2% water loss is observed around 100-120ºC. With increasing temperature, relatively consistent mass loss up to ~800°C is observed, at which point all organic material has been removed from the UZM-55 materials. Total mass loss of ~12-13% is consistent with the CHN results and corresponds to 1 OSDA/UC.

Three regimes are typically visible in the first derivative of the mass loss curve. The first is centred at about 370°C with a second around 500°C and a third at 620°C. Most weight loss occurs prior to 600°C. From this, we determined that 600°C would be the preferred calcination temperature for future studies of the UZM-55 materials.

Figure S3. Representative TGA analysis of the as-synthesized Al-UZM-55 products at 0.3 OH/Si ratio. TGA results shown as the weight loss (green, left axis), and the first derivative thereof (blue, right axis). Shown here is the Al-UZM-55-95 product measured by heating at 10°C per minute in air to 900°C.

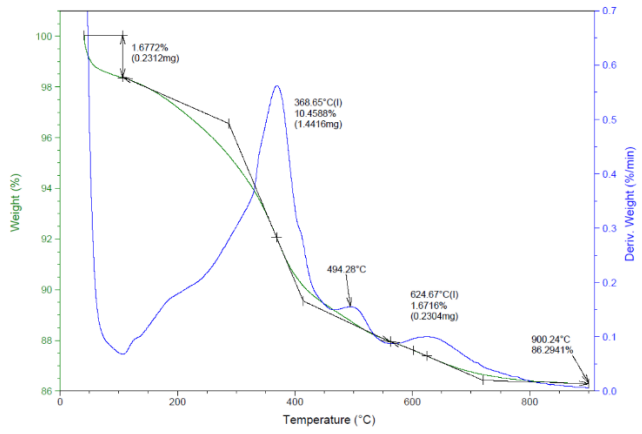


Figure S4. $^{27}$Al NMR Spectra of UZM-55 materials before and after calcination at 600°C (blue: as-synthesized, red: calcined at 600° for 4 hours). Samples are Al-UZM-55- A) 278, B) 144, C) 95, and D) 63.

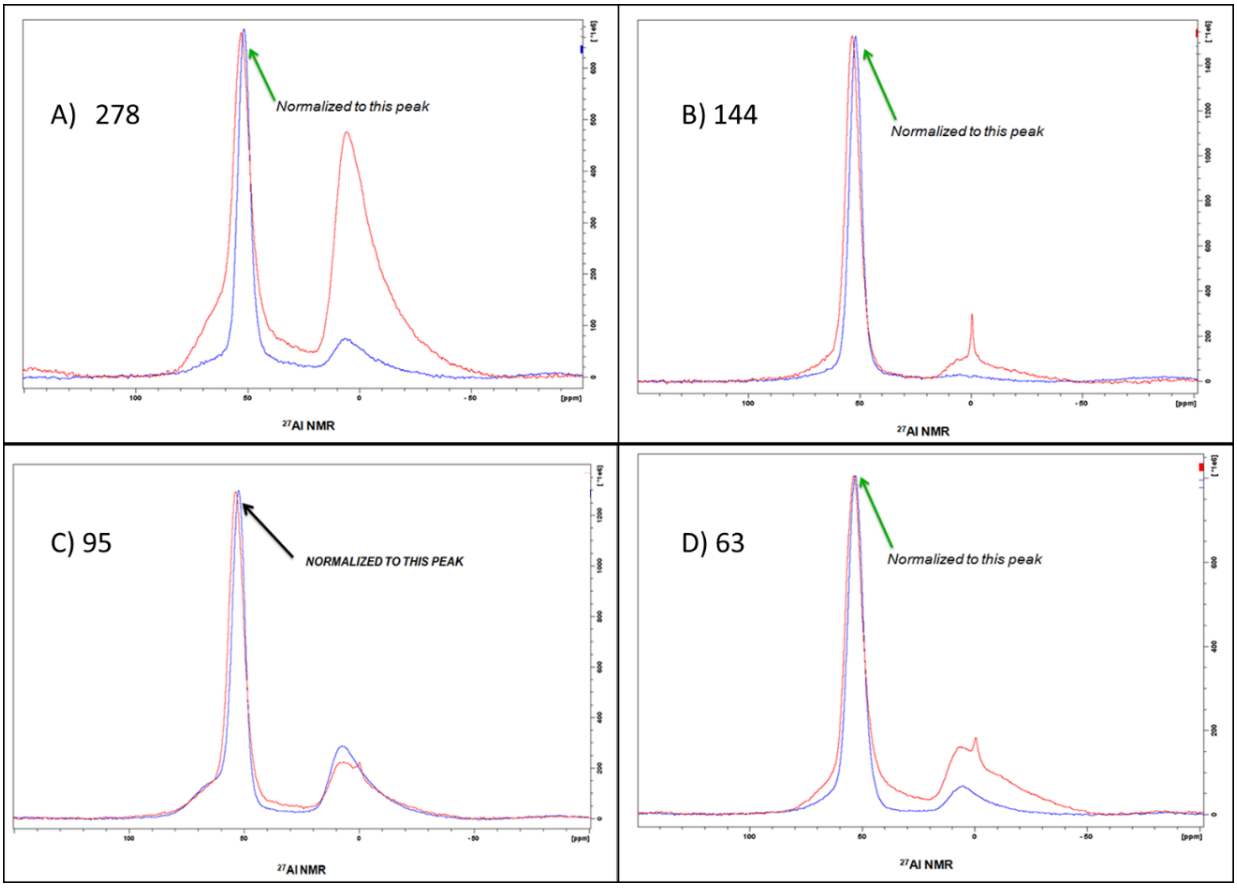


Figure S5. FTIR spectra of Al-UZM-55 materials in the hydroxyl region. Samples were ground and pressed into self-supporting pellets (~8 mg/cm$^2$) and heated at 10ºC/min to 350$^{o}$C in synthetic air and held for 2 h before cooling to room temperature for data acquisition.

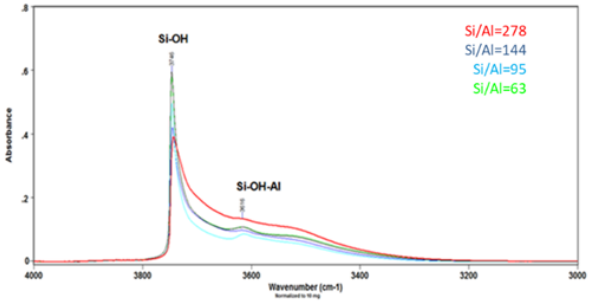



Figure S6. FTIR spectra during pyridine adsorption experiments. Initial spectra were acquired at room temperature after preactivation in He at 500ºC for 2 hours. The samples were cooled and equilibrated in pyridine/He at 150ºC for an hour. Stepwise desorption of pyridine was then performed at 150 (red), 300 (blue) or 450ºC (green). After 1h hold at desorption temperature, the sample was cooled to room temperature and a spectrum recorded. We believe low frequency Lewis shoulders at 150ºC are due to pyridine weakly coordinating with, but not protonating, silanol groups as no additional cations are present. Integrated values are given in Table 4.

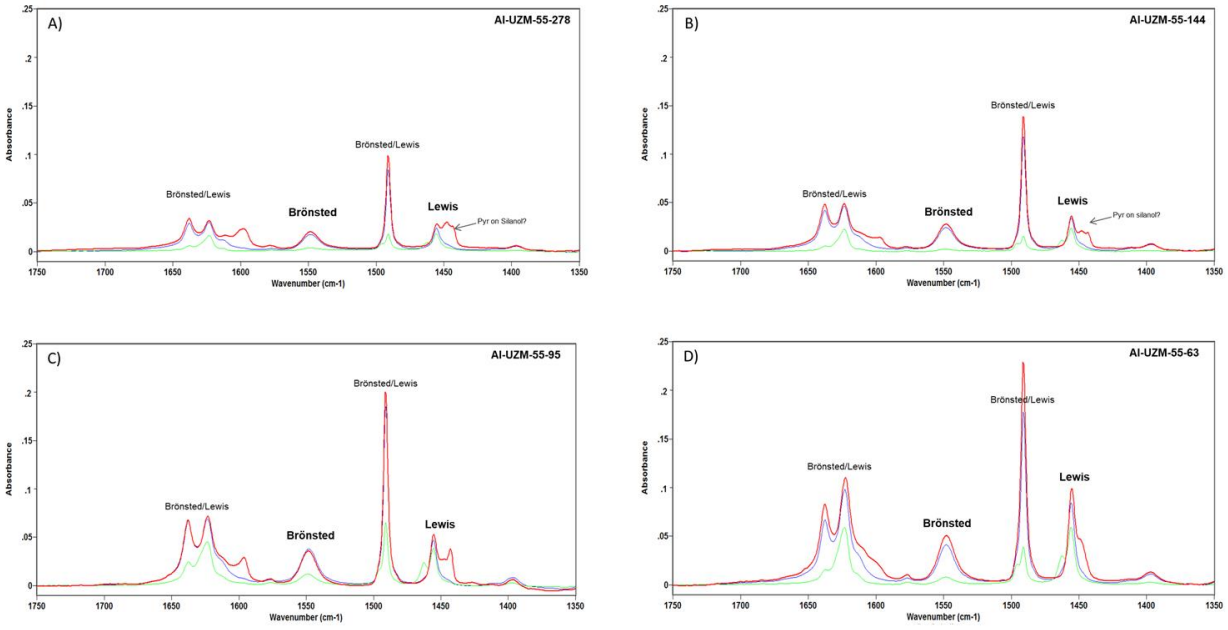


Figure S7. Characterization of reference MFI-76 obtained from Zeolyst at 150 $SiO_2/Al_2O_3$. ICP analysis showed a Si/Al ratio of 76. $^{27}Al$ NMR analysis shows 13% EFAL, 87% TFAL. Crystallite size by SEM is approximately 200-400nm.

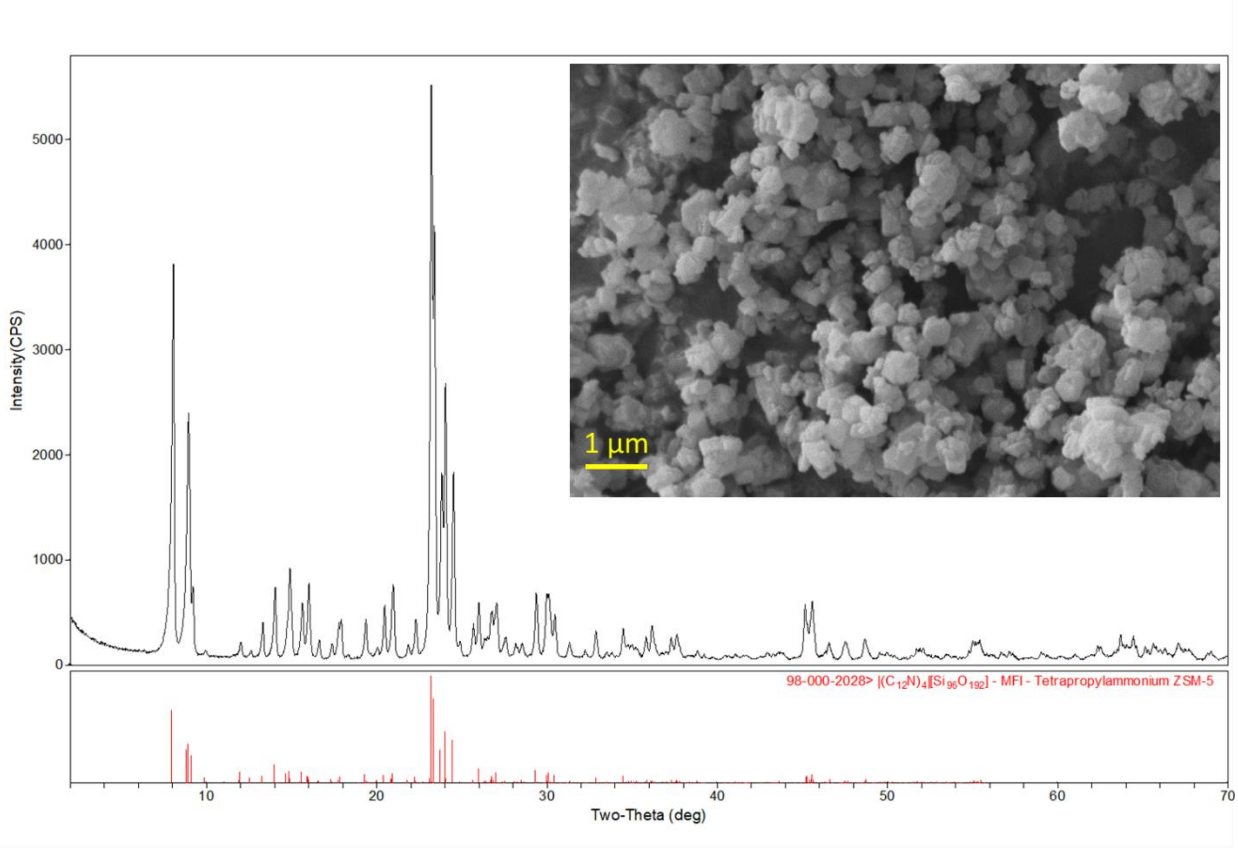


Figure S8. Full selectivity profiles for each of the catalysts tested. Reference catalyst MFI-76 is shown at the top, with Al-UZM-55-XX materials below.