Electronic Supplementary Material (ESI) for Faraday Discussions.

Experimental and Theoretical Investigations on the Anti-Perovskite Nitrides Co_3CuN, Ni_3CuN and Co_3MoN for Ammonia Synthesis

Faraday Discussions

Angela Daisley[1]*, Michael Higham[2], C. Richard A. Catlow[2,3] and Justin S. J. Hargreaves[1]

[1] *University of Glasgow, UK*

[2] *University College London, UK*

[3] *Cardiff University, UK*

Supplementary Information

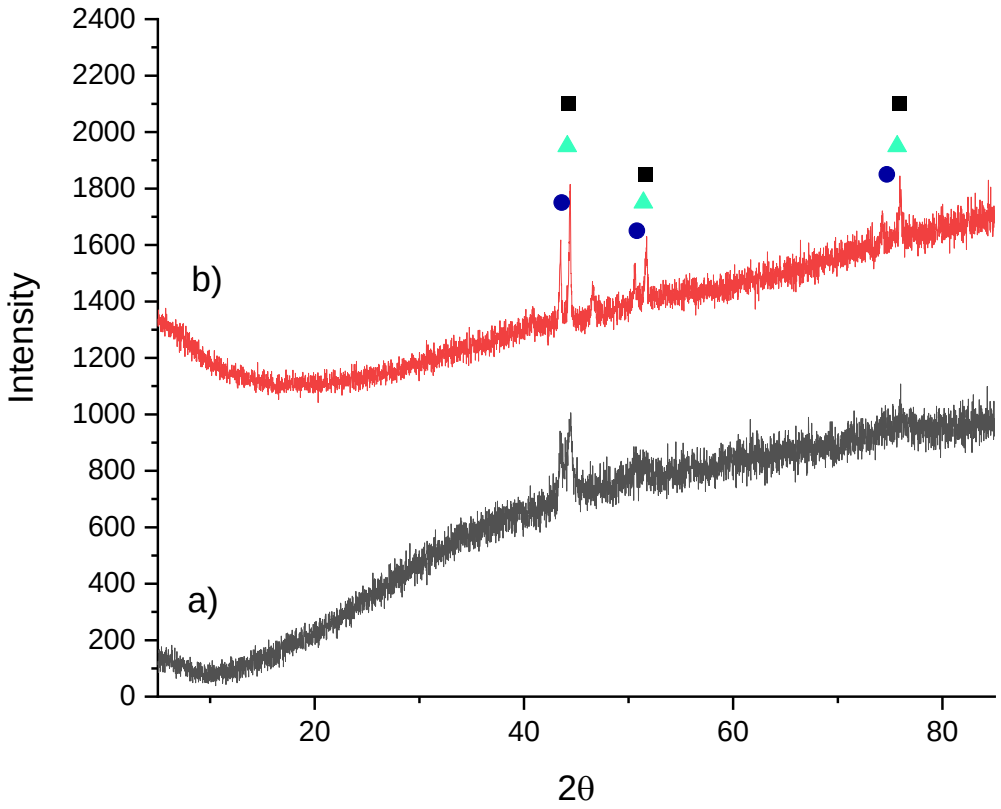

Figure 1: XRD patterns of Co_3Cu: a) prepared with 3:1 H_2/N_2 at 500°C and b) prepared with 3:1 H_2/N_2 at 700°C. (■) Co_3Cu, (Δ) Co and (●) Cu

[1] Corresponding author: A. Daisley (angela.daisley@glasgow.ac.uk)

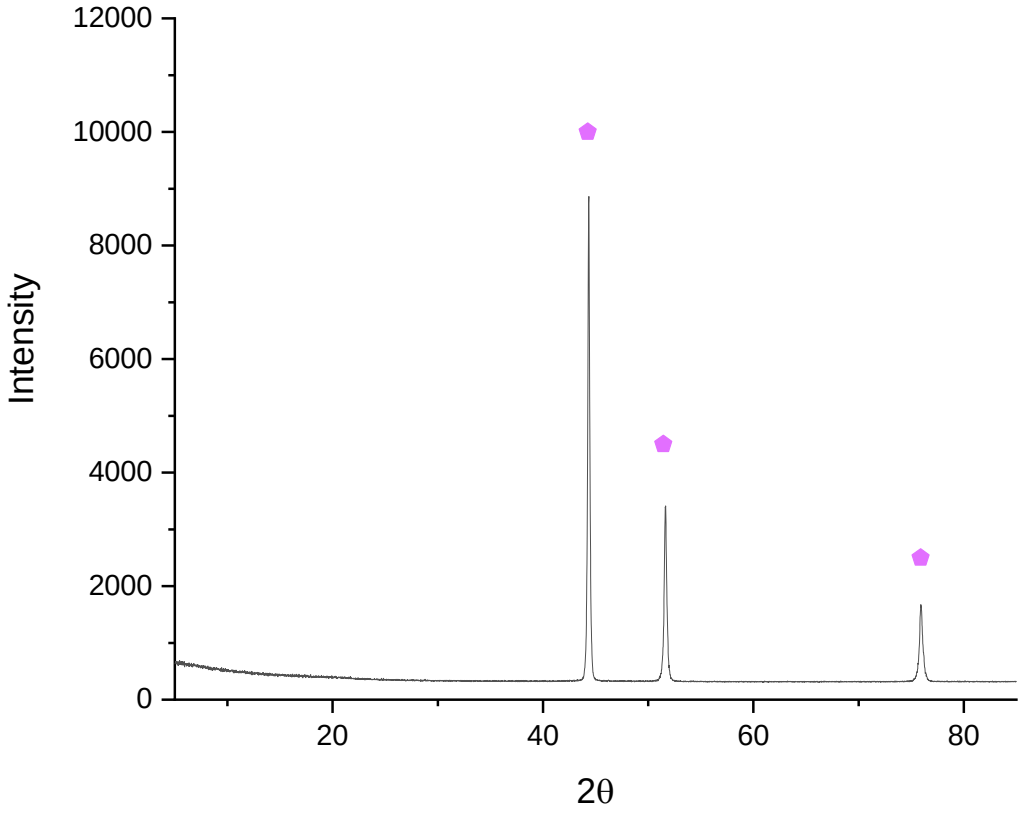

Figure 2: XRD pattern of Ni_3Cu prepared with 3:1 H_2/N_2 at 500°C. (⌂) Ni_3Cu

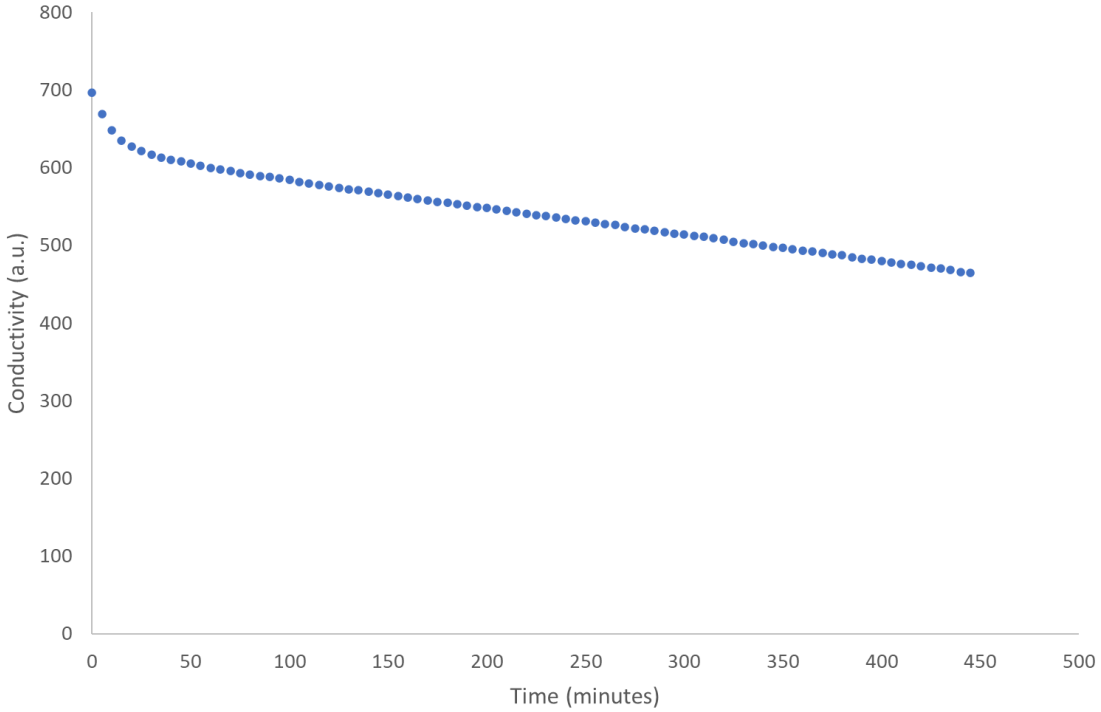

Figure 3: Ammonia production reaction profile of 'Co_3MoN' reacted with 60 mL/min of 3:1 H_2/N_2 for 7 hours 25 minutes at 400^oC

Material	Nitrogen content (wt.%)
‘Co_3MoN’	4.03
‘Co_3MoN’ post N_2/H_2 400°C	0.98

Table 1: Nitrogen analysis pre- and post-reaction for ‘Co_3MoN’ reacted with 60 mL/min of 3:1 H_2/N_2 for 7 hours 25 minutes at 400°C