

The H₂O Effect on Cu Speciation in Cu-CHA-Catalysts for NH₃-SCR Probed by NH₃ Titration

Roberta Villamaina ¹, Federica Gramigni ¹, Umberto Iacobone ¹, Shaojun Liu ¹, Isabella Nova ¹, Enrico Tronconi ^{1,*}, Maria Pia Ruggeri ², Jillian Collier ², Andrew P. E. York ² and David Thompsett ²

¹ Laboratory of Catalysis and Catalytic Processes, Dipartimento di Energia, Politecnico di Milano, via La Masa 34, 20156 Milano, Italy; roberta.villamaina@polimi.it (R.V.); federica.gramigni@polimi.it (F.G.);

umberto.iacobone@polimi.it (U.I.); shaojun.liu@polimi.it (S.L.); isabella.nova@polimi.it (I.N.)

² Johnson Matthey Technology Centre, Blounts Court Road, Sonning Common, Reading RG4 9NH, UK; MariaPia.Ruggeri@matthey.com (M.P.R.); jillian.collier@matthey.com (J.C.); andrew.york@matthey.com (A.P.E.Y.); david.thompsett@matthey.com (D.T.)

* Correspondence: enrico.tronconi@polimi.it

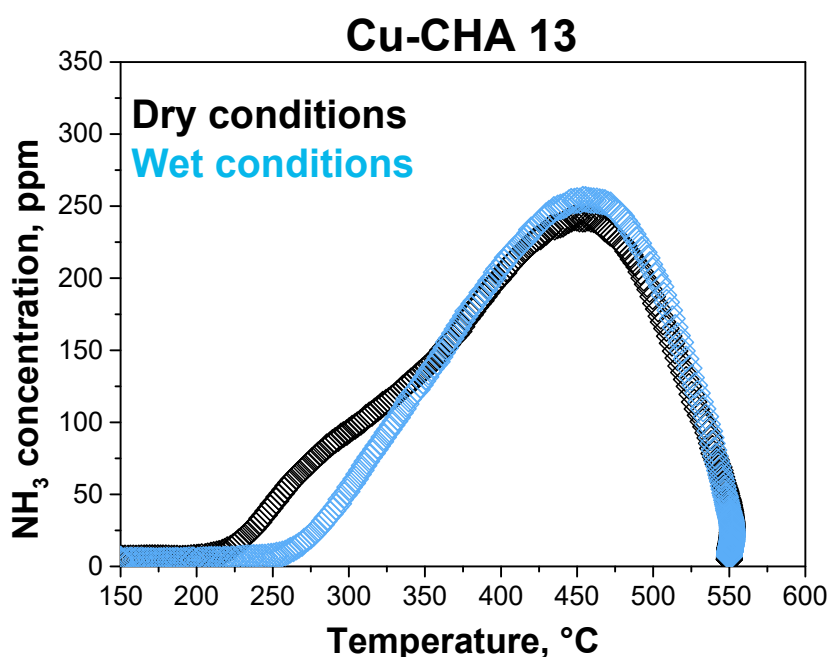


Figure S1. Comparison between dry and wet NH₃-TPD after adsorption at 150 °C on H-CHA catalysts with SAR=13. NH₃= 500 ppm, H₂O= 0-5% v/v; heating rate= 15 °C/min, He. GHSV= 266250 cm³/(g_{cat}*h) (STP).

Table S1 NH₃ adsorbed on different sites as estimated from NH₃-TPD deconvolution under dry conditions

SAMPLE	Cu loaded, μmol	NH ₃ Lewis, μmol	NH ₃ Bronsted, μmol	NH ₃ extra - framework, μmol	NH ₃ /Cu ^a	NH ₃ physisorbed, μmol	NH ₃ /Cu ^b	NH ₃ TPD, μmol
0.7% w/w Cu, SAR=25	1.8	2.79	8.02	1.1	1.55	3.60	3.60	12.00
1.7% w/w Cu, SAR=25	4.3	6.19	7.9	1.2	1.44	8.02	3.35	15.43
2.1% w/w Cu, SAR=25	5.2	6.86	7.07	1.1	1.32	10.10	3.26	15.10
1.7% w/w Cu, SAR=10	4.3	7.12	6.20	2.5	1.66	7.67	3.56	16.17
1.7% w/w Cu, SAR=13	4.3	7.03	8.30	2.0	1.63	8.00	3.55	16.90
1.7% w/w Cu, SAR=17	4.3	6.90	8.90	1.9	1.60	8.41	3.55	17.90
1.7% w/w Cu, SAR=22	4.3	6.06	8.00	1.7	1.41	9.18	3.54	15.90

Table S2 NH₃ adsorbed on different sites as estimated from NH₃-TPD deconvolution under wet conditions

SAMPLE	Cu loaded, μmol	NH ₃ Lewis, μmol	NH ₃ Bronsted, μmol	NH ₃ extra - framework, μmol	NH ₃ /Cu ^a	NH ₃ physisorbed, μmol	NH ₃ /Cu ^b	NH ₃ TPD, μmol
0.7% w/w Cu, SAR=25	1.8	2.32	8.38	/	1.28	3.50	3.23	10.50
1.7% w/w Cu, SAR=25	4.3	4.47	8.67	/	1.04	8.01	2.90	13.20
2.1% w/w Cu, SAR=25	5.2	5.27	8.07	/	1.00	8.07	2.93	13.40
1.7% w/w Cu, SAR=10	4.3	5.96	7.54	/	1.28	6.98	3.01	13.62
1.7% w/w Cu, SAR=13	4.3	4.58	9.50	/	1.07	8.00	2.93	14.08
1.7% w/w Cu, SAR=22	4.3	4.32	9.28	/	1.00	8.62	3.00	13.60

Table S3. Additional characterization measurements for the bare zeolites: BET surface area, pore volume, micropore area, micropore volume

SAMPLE	BET surface area (m²/g)	Pore volume [0.99ads] (cm³/g)	Micropore area (cm²/g)	Micropore volume (cm³/g)
SAR 25	722	0.26	718	0.25
SAR 13	644	0.23	637	0.22
SAR 22	763	0.29	729	0.25