

Supporting Information for

High-field multinuclear MAS NMR and synchrotron XANES reveal the influence of strontium salt chemistry on geopolymer nanostructure

Kyle T. O'Donoghue¹, Daniel A. Geddes¹, Tom J. Wilkinson¹, Martin C. Stennett¹, Byoungkwan Kim¹, Dinu Iuga², Martin Hayes³, Brant Walkley^{1*}

¹*School of Chemical, Materials and Biological Engineering, The University of Sheffield, Sheffield, UK*

²*Department of Physics, University of Warwick, Coventry, UK*

³*United Kingdom National Nuclear Laboratory, Warrington, UK*

Corresponding author: Email: b.walkley@sheffield.ac.uk

)					reaction (%)
KGP	3 Days	25	54	20	1	1.32	82.17
OH_5	3 Days	27	35	34	4	1.40	87.28
KGP	28 Days	28	44	26	2	1.34	88.00
OH_5	28 Days	31	32	30	7	1.39	87.44

* Estimated error due to spectral noise is $\pm 2\%$

2. Effect of addition of strontium carbonate to geopolymers

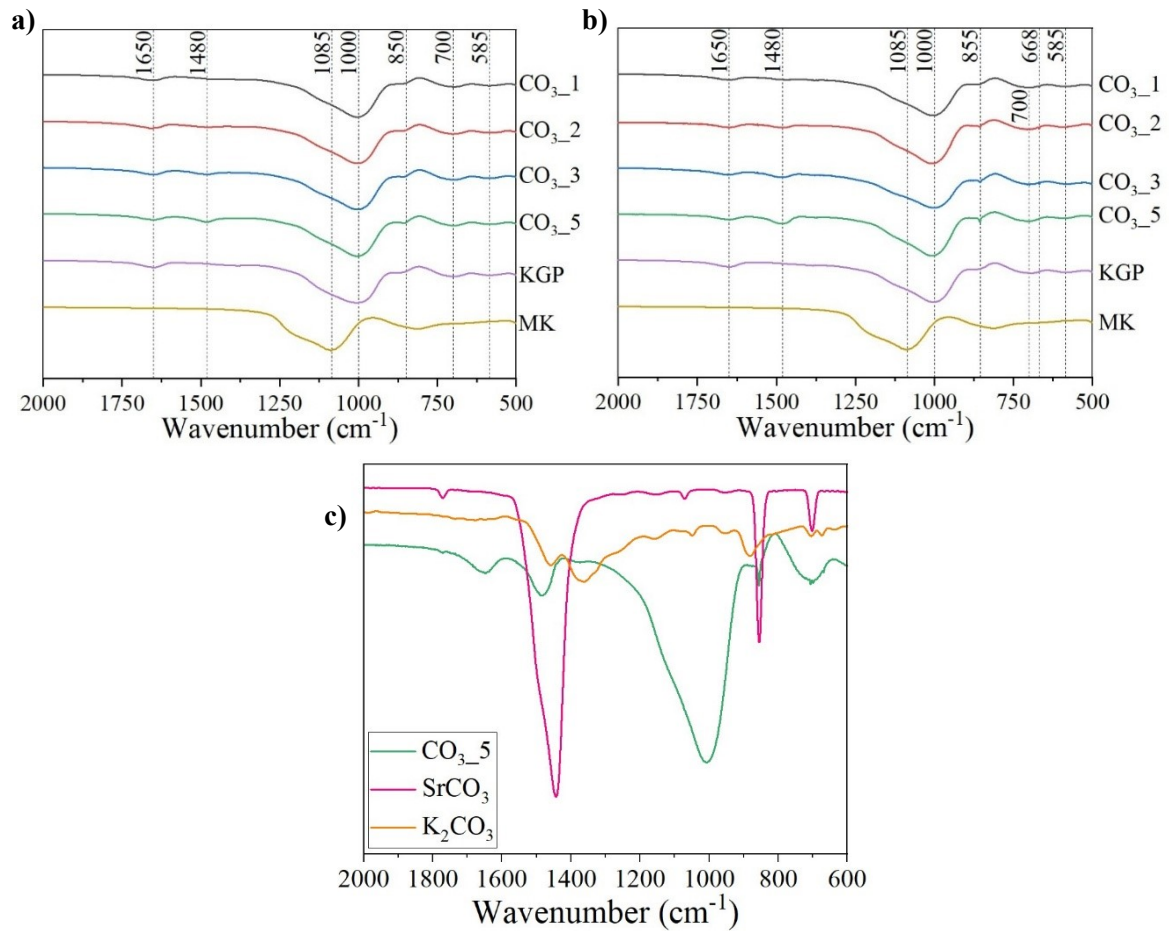


Figure S3: FTIR data for the geopolymers cured for a) 3 and b) 28 days, as a function of the amount of SrCO₃ (wt. %) in the formulation, and unreacted metakaolin (MK), as well as c) FTIR data for the CO_{3_5} sample compared against that of reagents SrCO₃ and K₂CO₃.

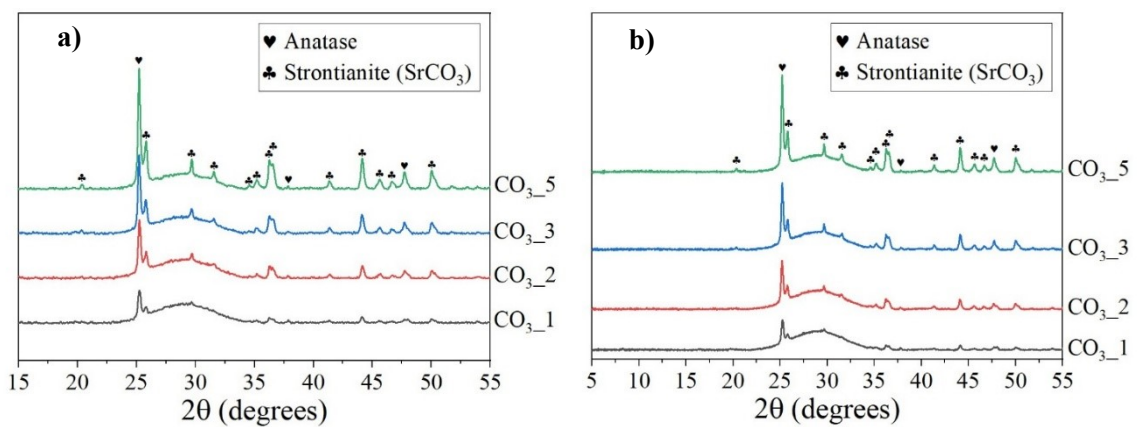


Figure S4: X-ray diffraction data for the geopolymers cured for a) 3 and b) 28 days, as a function of the amount of SrCO₃ (wt. %) in the formulation.

Table S2: Relative integral areas for Q⁴(mAl) sites and Si/Al ratios within K-A-S-H in each sample, as well as extent of reaction (mol. %), calculated from the deconvoluted ²⁹Si MAS NMR spectra

Sample	Time point	Relative Integral Area (%)				Si/Al	Extent of reaction (%)
		Q ⁴ (4Al)	Q ⁴ (3Al)	Q ⁴ (2Al)	Q ⁴ (1Al)		
KGP	3 Days	25	54	20	1	1.32	82.17
CO ₃ _5	3 Days	24	49	23	4	1.37	80.73
KGP	28 Days	28	44	26	2	1.34	88.00
CO ₃ _5	28 Days	24	48	27	1	1.36	83.01

3. Effect of addition of strontium nitrate to geopolymers

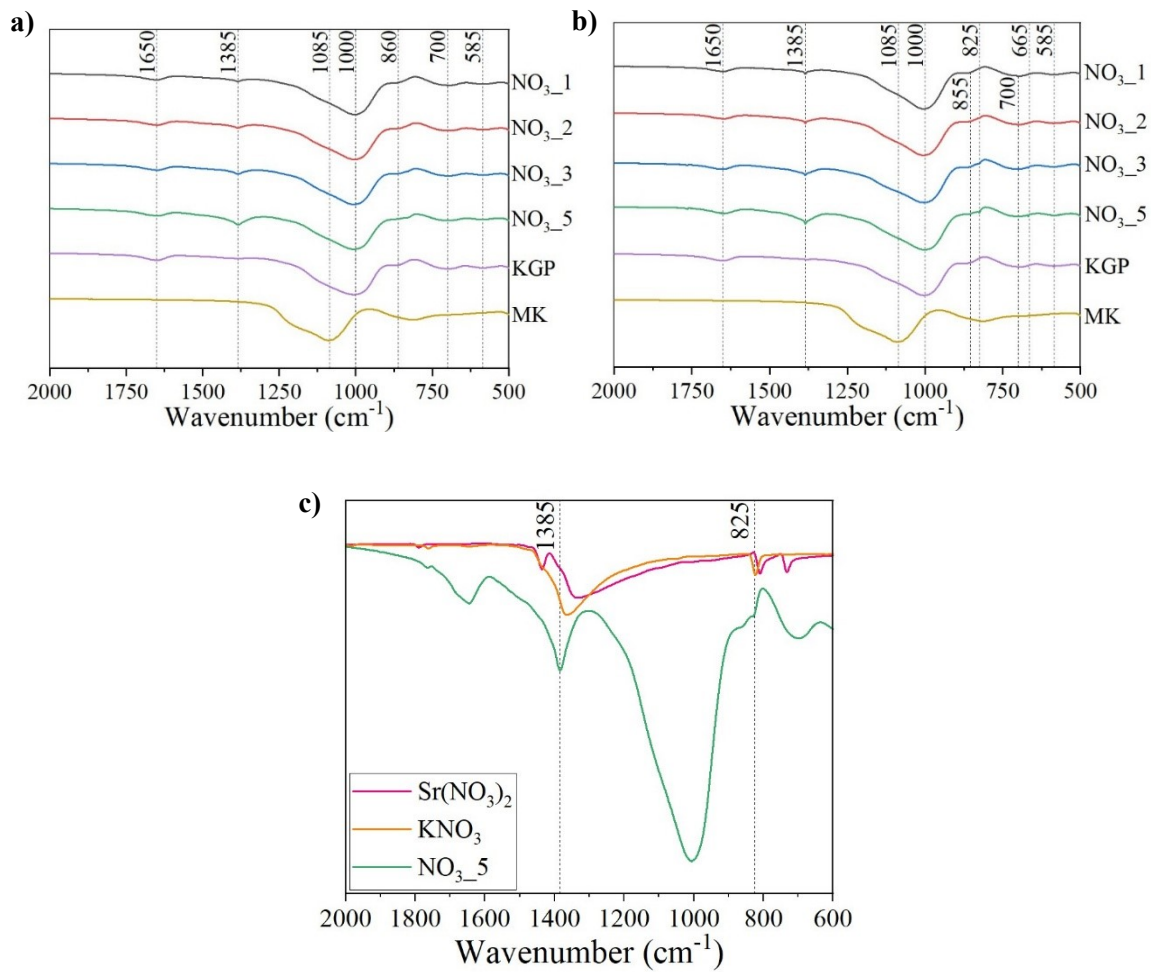


Figure S5: FTIR data for the geopolymers cured for a) 3 and b) 28 days, as a function of the amount of $\text{Sr}(\text{NO}_3)_2$ (wt. %) in the formulation, and unreacted metakaolin (MK). FTIR data for the reagents used to produce the geopolymer samples are shown in c).

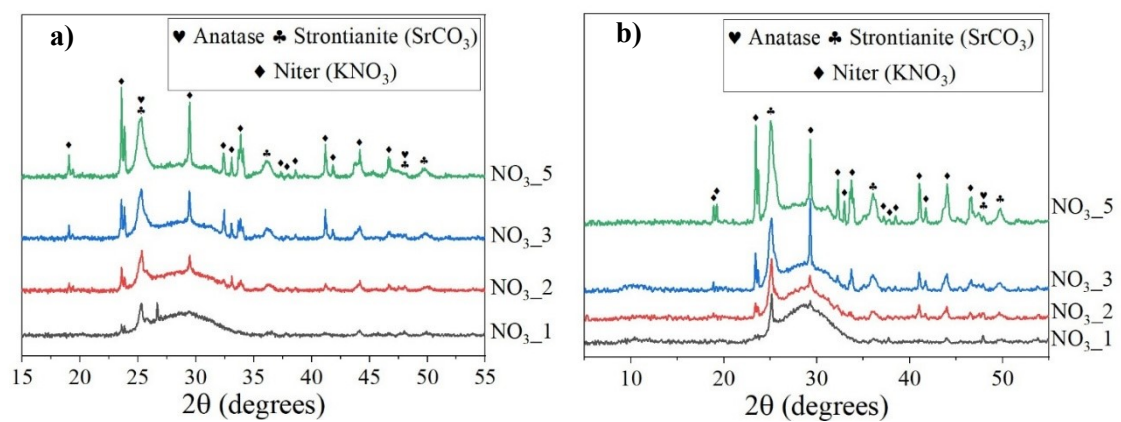


Figure S6: X-ray diffraction data for the geopolymers cured for a) 3 and b) 28 days, as a function of the amount of $\text{Sr}(\text{NO}_3)_2$ (wt. %) in the formulation.

Table S3: Relative integral areas for Q⁴(mAl) sites and Si/Al ratios within K-A-S-H in each sample, as well as extent of reaction (mol. %), calculated from the deconvoluted ²⁹Si MAS NMR spectra

Sample	Time point	Relative Integral Area (%)				Si/Al	Extent of reaction (%)
		Q ⁴ (4Al)	Q ⁴ (3Al)	Q ⁴ (2Al)	Q ⁴ (1Al)		
KGP	3 Days	25	54	20	1	1.32	82.17
NO ₃ _5	3 Days	30	38	30	2	1.35	73.32
KGP	28 Days	28	44	26	2	1.34	88.00
NO ₃ _5	28 Days	39	40	20	1	1.26	77.73

4. Effect of addition of strontium sulfate to geopolymers

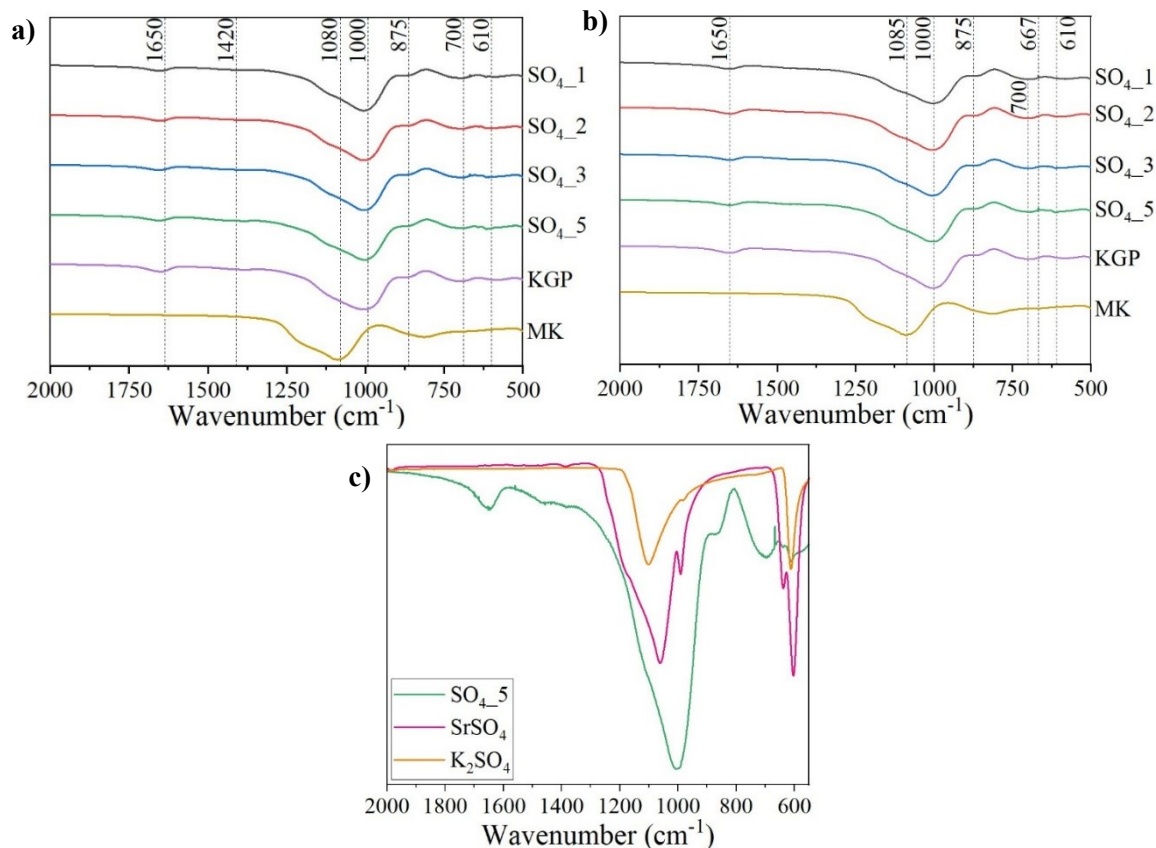


Figure S7: FTIR data for the geopolymers cured for 3 and 28 days, as a function of the amount of SrSO_4 (wt. %) in the formulation, the control geopolymer sample, unreacted metakaolin (MK), and SrSO_4 and K_2SO_4 reagents.

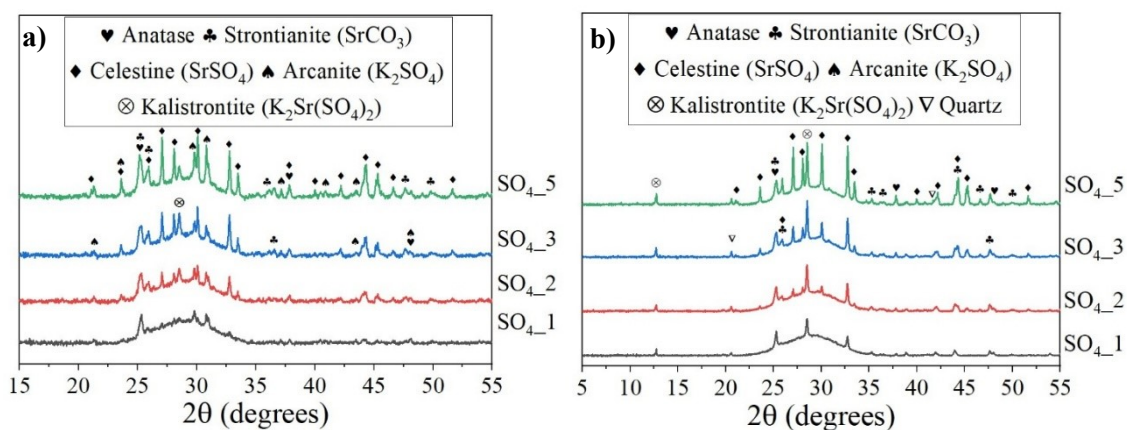


Figure S8: X-ray diffraction data for the geopolymers cured for a) 3 and b) 28 days, as a function of the amount of SrSO_4 (wt. %) in the formulation.

Table S4: Relative integral areas for Q⁴(mAl) sites and Si/Al ratios within K-A-S-H in each sample, as well as extent of reaction (mol. %), calculated from the deconvoluted ²⁹Si MAS NMR spectra

Sample	Time point	Relative Integral Area (%)				Si/Al	Extent of reaction (%)
		Q ⁴ (4Al)	Q ⁴ (3Al)	Q ⁴ (2Al)	Q ⁴ (1Al)		
KGP	3 Days	25	54	20	1	1.32	82.17
SO ₄ _5	3 Days	25	33	37	5	1.37	84.40
KGP	28 Days	28	44	26	2	1.34	88.00
SO ₄ _5	28 Days	31	34	28	7	1.36	86.61