Supplementary Material

Amino acids encapsulation in zeolite MOR: effect of spatial confinement

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Na-MOR characterization

Thermogravimetric analysis

Figure 1S shows the TG and DTG curves of Na-MOR. The total weight loss is 14.6% corresponding to 28 H_2O molecules p.u.c. The loss mainly occurs below 200° C (indicating that most of the water is weakly bonded), even if the weight loss continues up to about 500°C (temperature at which even the stronger bonded H_2O molecules are released).

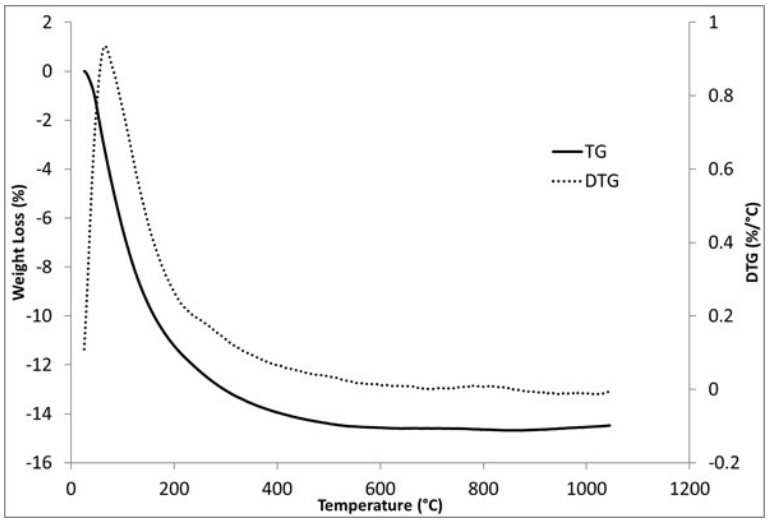

Figure 1S: TG and DTG curves of Na-MOR sample.

IR spectroscopy

The hydration state of Na-MOR is also studied by IR spectroscopy (Figure 2S). Besides the two signals at 1975 and 1860 cm^{-1}, corresponding to the combination modes of the lattice stretching vibration (νSi-O) - present in all the spectra - the main feature in the spectrum acquired in air (curve a) is the intense absorption around 1640 cm^{-1}, typically assigned to the water deformation mode (δH_2O), which is so intense to be out of scale. The outgas at room temperature (curve b) drastically

reduces the water contribution to the spectrum. Another common feature of the thermally untreated materials (curve a and b) is the presence of a weak adsorption located at 1466 cm^{-1} assigned to the antisymmetric deformation of satured aliphatic moieties ($\delta_{as}CH_3$ and δCH_2) that arises from small carbon species (e.g. hydrocarbons) typically adsorbed on these types of materials. When Na-MOR is treated at 200°C (curve c) the water deformation band dramatically drops, leaving - based on the integration of the water band - an estimated 5 % of water molecules of the material only outgassed at room temperature (corresponding to 1.4 H_2O molecules p.u.c.). Finally, the outgas at 500°C (curve d) completely removes all the water present in the sample - as confirmed by the comparison with the material outgassed after the exchange with D_2O (curve e) - leaving the underlying overtone mode of the Si-O bond located at 1650 cm^{-1}.

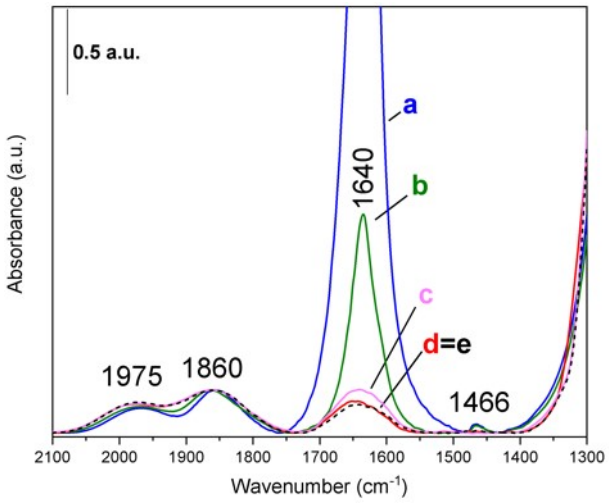

Figure 2S: Infrared profiles in the 2100 – 1300 cm^{-1} range of Na-MOR sample: a) in air, b) after outgas at rT, c) outgassed at 200°C, d) outgassed at 500°C and outgassed after the isotopic exchange with D_2O.

Structure refinement

Table 1S reports the sstructural refinement parameters, Table 2S atomic coordinates, occupancy factors and thermal parameters and Table S3 bond distances of Na-MOR sample, Figure 3S shows the refined XRPD pattern.

The starting model for the as-synthesized Na-MOR structure was taken from Simoncic & Armbruster (2004). In this paper the structure of mordenite is determined on single crystal in $Cmc2_1$ s.g. and described by two domains, shifted of *c*/2, related to framework defects and crystallographic faulting. In order to simplify the system, and to allow the refinement from powder data, only the predominant domain was used here. In this model, the position of the framework atom O8, placed on an inversion centre in the *Cmcm* s.g., is split into four closely spaced (about 0.5 Å) positions, with a site-occupancy factor of 0.25 each. For the refinement of Na-MOR+gly and Na-MOR+βala sample, to simplify the system, the framework oxygen O8 was set on a unique position, averaging the previously cited four and applying a higher $U_{iso,}$ respect to the other framework oxygen atoms.

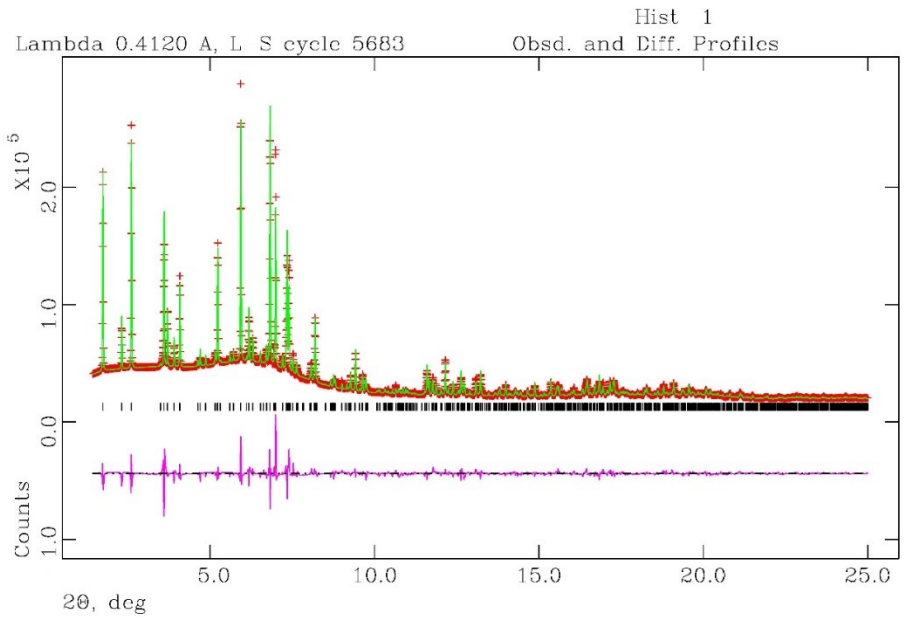

Figure 3S: Observed (red cross marks) and calculated (green line) diffraction patterns and final difference curve (purple line) from Rietveld refinements for Na-MOR.

On the basis of the distances and occupancy factors of the refined extraframework sites (Figure 4S, two Na cation sites are located in the unit cell: i) Na1, placed in the middle of 8MR channel and coordinated to six framework oxygen and two H_2O oxygen atoms, and ii) Na3, located in the 8MR window between the 12MR channel and the side pocket, slightly shifted from the (100) mirror plane (Figure 4S) and coordinated to two framework oxygen and three H_2O oxygen atoms. On the basis of the refined occupancy factors, the total amount of Na is 4.9 atoms p.u.c., slightly higher than that determined by the chemical analysis (4 atoms p.u.c.).

H_2O molecules are located in seven crystallographic independent sites: W1 in the 8MR channel, coordinated to Na1; W6 inside the side pocket coordinated to Na3; and five H_2O molecules (W2, W3, W4, W7 and W10) in the 12MR channel forming a hydrogen bonded cluster, with interatomic distances ranging between 2.50 and 3.16 Å (Table 3S). W1, W3 and W4 weakly interact also with framework oxygen atoms. The resulting total amount of H_2O is 26.6 molecules p.u.c., in good agreement with the TG results (28 molecules p.u.c.). However, it cannot be excluded that W4 site (located in the 12MR channel) is alternatively occupied by Na atom, being this position always present also in the nominally anhydrous hybrid samples (see below).

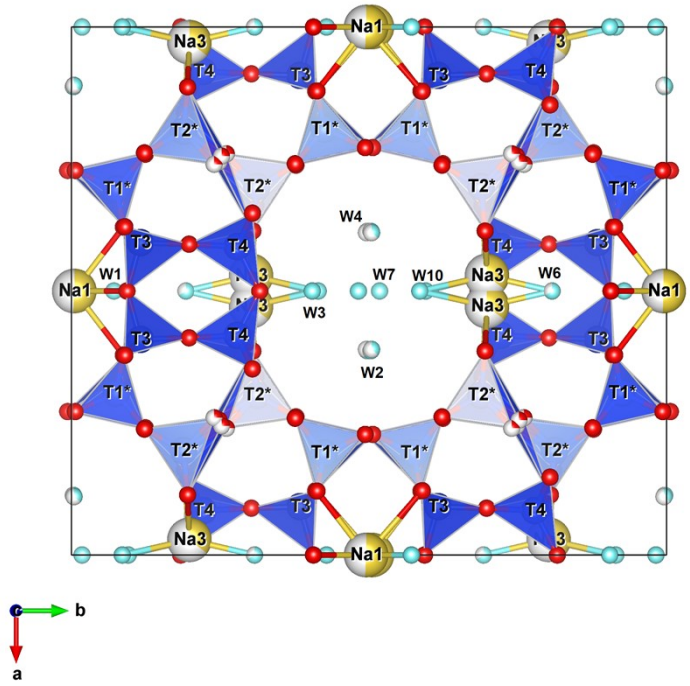

Figure 4S: View along [001] of the as synthesized Na-MOR structure.

Table 1S. Structural refinement parameters of Na-MOR, Na-MOR+gly, Na-MOR+βala, Na-MOR+gly_P_{amb}R

refinement	Na-MOR	Na-MOR+gly	Na-MOR+βala	Na-MOR+gly_P_{amb}R
wRp	0.0443	0.0164	0.0163	0.001
Rp	0.027	0.0108	0.0123	0.0006
RF²	0.152	0.097	0.0472	0.17
***a* (Å)**	18.0801(5)	18.075(1)	18.0617(7)	18.075(2)
***b* (Å)**	20.3795(4)	20.350(1)	20.3611(6)	20.337(2)
***c* (Å)**	7.4886(2)	7.4912(4)	7.4855(2)	7.4877(6)
***V* (Å³)**	2759.3(1)	2755.5(3)	2752.8(2)	2752.4(6)
n. observation	4332	2167	5976	1963
n. variables	148	146	132	151

Table 2S. Site fractional coordinates, occupancy factors (frac.) and equivalent/isotropic displacement parameters (U_{iso}, $Å^2$) of Na-MOR sample.

atoms	x	y	z	frac	Uiso
T1	0.304(1)	0.0685(9)	0.026(3)	1	0.018(1)
T1a	-0.307(1)	-0.0753(9)	-0.063(3)	1	0.018(1)
T2	0.3080(7)	0.3083(6)	0.045(3)	1	0.018(1)
T2a	-0.3027(8)	-0.3116(5)	-0.049(3)	1	0.018(1)
T3	0.0916(6)	0.3841(5)	0.242(4)	1	0.018(1)
T4	0.0841(6)	0.2213(5)	0.212(3)	1	0.018(1)
O1	0.122(2)	0.410(2)	0.434(4)	1	0.028(2)
O1a	-0.121(2)	-0.413(2)	-0.449(4)	1	0.028(2)
O2	0.147(1)	0.196(2)	0.361(3)	1	0.028(2)
O2a	-0.114(1)	-0.195(2)	-0.486(4)	1	0.028(2)
O3	-0.241(2)	-0.124(1)	-0.987(5)	1	0.028(2)
O3a	0.238(2)	0.123(1)	0.025(5)	1	0.028(2)
O4	0.089(1)	0.3024(6)	0.260(5)	1	0.028(2)
O5	0.162(1)	0.190(2)	0.750(3)	1	0.028(2)
O6	0.163(1)	0.417(1)	0.729(3)	1	0.028(2)
O7	0.272(1)	-0.006(1)	0.010(5)	1	0.028(2)
O8a	0.2401	0.2602	0.532	0.25	0.028(2)
O8b	-0.2401	-0.2602	-0.532	0.25	0.028(2)
O8c	0.2446	0.2521	0.48	0.25	0.028(2)
O8d	-0.2446	-0.2521	-0.48	0.25	0.028(2)
O9	0	0.407(1)	0.227(8)	1	0.028(2)
O10	0	0.184(1)	0.198(6)	1	0.028(2)
Na1	0	-0.495(3)	0.492(8)	0.51(1)	0.04(1)
Na3	0.028(2)	0.198(1)	0.680(6)	0.353(7)	0.05(2)
W1	0	0.429(2)	0.719(5)	1	0.109(9)
W2	0.113(2)	-0.003(3)	0.296(5)	0.64(3)	0.109(9)
W3	0	0.095(1)	0.491(4)	1	0.109(9)
W4	0.111(3)	0.004(6)	-0.083(7)	0.36(3)	0.109(9)
W6	0.5	0.192(1)	0.22(2)	0.66(2)	0.109(9)
W7	0.5	0.482(1)	0.615(5)	1	0.109(9)
W10	0.5	0.4146(8)	0.323(4)	1	0.109(9)

Table 3S. Selected interatomic distances (Å) of Na-MOR sample.

Atom1	Atom2	distance		Atom1	Atom2	distance	
T1	O1	1.57(1)		W1	O1	3.09(3)	x2
	O3a	1.62(1)			O6	2.95(2)	x2
	O6	1.66(1)			Na1	2.3(2)	
	O7	1.64(1)			Na1	2.46(2)	
T1a	O1a	1.57(1)			W6	2.47(5)	
	O3	1.65(1)		W2	W4	2.85(6)	
	O6	1.66(1)			W7	3.16(5)	
	O7	1.64(1)			W7	2.49(2)	
T2	O2	1.59(1)			W10	2.65(5)	
	O3	1.66(1)		W3	O10	2.84(4)	
	O5	1.63(1)			Na3	2.58(3)	x2
	O8a	1.647(7)			W4	2.90(9)	x2
	O8b	1.672(7)			W7	2.49(2)	
	O8c	1.629(7)			W10	2.50(1)	
	O8d	1.631(7)		W4	O7	3.00(2)	
T2a	O2a	1.59(1)			W3	2.90(9)	
	O3a	1.63(1)			W2	2.85(6)	
	O5	1.64(1)			W7	3.05(7)	
	O8a	1.657(7)			W7	2.51(2)	
	O8b	1.659(7)			W10	2.69(9)	
	O8c	1.618(7)		W6	Na3	2.31(2)	x2
	O8d	1.638(7)			W1	2.47(5)	
T3	O1	1.63(1)		W7	W3	2.49(2)	
	O1a	1.63(1)			W2	3.16(5)	x2
	O4	1.67(1)			W2	2.49(2)	x2
	O9	1.72(1)			W4	3.05(7)	x2
T4	O2	1.68(1)			W4	2.51(2)	x2
	O2a	1.67(1)			W10	2.59(2)	
	O4	1.69(1)			W10	2.61(2)	
	O10	1.70(1)		W10	Na3	2.59(3)	x2
Na1	O1	2.96(4)	x2		W3	2.50(1)	
	O1a	2.80(4)	x2		W2	2.65(5)	x2
	O9	2.82(5)			W4	2.69(9)	x2
	O9	2.52(5)			W7	2.59(2)	
	W1	2.30(2)			W7	2.61(2)	
	W1	2.46(2)					
Na3	O2a	2.94(3)					
	O5	2.47(2)					
	W3	2.58(3)					
	W6	2.31(2)					
	W10	2.59(3)					

Table 4S. Site fractional coordinates, occupancy factors (frac.) and equivalent/isotropic displacement parameters (U_{iso}, $Å^2$) of Na-MOR+gly sample, XRPD collected in capillary.

atoms	x	y	z	frac	Uiso
T1	0.3015(7)	0.0732(7)	0.082(3)	1	0.017(1)
T1a	-0.3093(7)	-0.0734(6)	0.002(3)	1	0.017(1)
T2	0.3054(7)	0.3135(7)	0.110(4)	1	0.017(1)
T2a	-0.3031(7)	0.3054(7)	0.008(3)	1	0.017(1)
T3	0.0859(5)	0.3843(4)	0.295(4)	1	0.017(1)
T4	0.0886(4)	0.2250(5)	0.278(4)	1	0.017(1)
O1	0.122(1)	0.408(1)	0.484(4)	1	0.025
O1a	-0.115(1)	-0.422(1)	-0.383(4)	1	0.025
O2	0.139(1)	0.201(1)	0.446(4)	1	0.025
O2a	-0.123(1)	-0.179(1)	-0.380(4)	1	0.025
O3	0.236(1)	0.128(1)	0.073(4)	1	0.025
O3a	-0.247(1)	-0.123(1)	-0.921(4)	1	0.025
O4	0.099(1)	0.3050(4)	-0.281(7)	1	0.025
O5	0.1625(7)	0.198(1)	0.809(3)	1	0.025
O6	0.1735(7)	0.4214(5)	0.790(3)	1	0.025
O7	0.2772(6)	-0.004(8)	0.073(3)	1	0.025
O8	0.257(1)	0.243(1)	0.580(4)	1	0.04
O9	0	0.410(1)	0.29(1)	1	0.025
O10	0	0.207(2)	0.296(6)	1	0.025
Na1	0	-0.493(5)	0.518(13)	0.43(1)	0.03(2)
Na3	0	0.232(1)	0.762(6)	0.78(1)	0.05(2)
W1	0.5	0.918(2)	0.75(1)	0.83(2)	0.11(3)
W4	0.357(1)	0.514(4)	-0.033(8)	0.43(2)	0.05(3)
C1	0	-0.082(2)	0.16(1)	0.32(1)	0.08
O1g	0.5	0.391(6)	0.013(14)	0.32(1)	0.08
O2g	0	0.112(6)	-0.194(14)	0.32(1)	0.08
C2	0	-0.007(3)	0.20(2)	0.32(1)	0.08
Ng	0.5	0.435(4)	0.68(2)	0.32(1)	0.08

Table 5S. Selected interatomic distances of Na-MOR+gly sample, XRPD collected in capillary.

atom1	atom2	distance	
T1	O1	1.618(5)	
	O3	1.619(5)	
	O6	1.626(5)	
	O7	1.624(5)	
T1a	O1a	1.622(5)	
	O3a	1.620(5)	
	O6	1.620(5)	
	O7	1.626(5)	
T2	O2	1.615(5)	
	O3a	1.619(5)	
	O5	1.617(5)	
	O8	1.621(5)	
T2a	O2a	1.618(5)	
	O3	1.613(5)	
	O5	1.614(5)	
	O8	1.615(5)	
T3	O1	1.624(5)	
	O1a	1.627(5)	
	O4	1.635(5)	
	O9	1.638(5)	
T4	O2	1.628(5)	
	O2a	1.628(5)	
	O4	1.639(5)	
	O10	1.647(5)	
Na1	O1	2.99(4)	x2
	O1a	2.64(4)	x2
	O9	2.65(5)	
	W1	2.51(9)	x2
Na3	O5	3.04(3)	x2
	C1	3.15(2)	
	O1g	3.12(3)	
	O2g	2.46(2)	

atom1	atom2	distance	
W1	O1	2.98(3)	x2
	O6	3.15(1)	x2
	Na1	2.51(9)	x2
W4	O3	2.98(3)	
	O7	2.58(1)	
	C2	3.12(11)	
	Ng	3.2(1)	
C1	Na3	3.15(2)	
	O1g	1.25(1)	
	O2g	1.25(1)	
	C2	1.522(8)	
O1g	O10	2.57(4)	
	Na3	3.12(3)	
	C1	1.25(1)	
	N	2.67(14)	
O2g	Na3	2.46(2)	
	C1	1.25(1)	
	Ng	2.9(1)	
C2	W4	3.1(1)	x2
	C1	1.52(1)	
	N	1.482(8)	
Ng	O10	3.03(4)	
	W4	3.2(1)	x2
	O2g	2.9(1)	
	C2	1.482(8)	

Table 6S. Site fractional coordinates, occupancy factors (frac.) and equivalent/isotropic displacement parameters (U_{iso}, $Å^2$) of Na-MOR+βala sample, XRPD collected in capillary.

atoms	x	y	z	frac	Uiso	mult
T1	0.3078(5)	0.0727(5)	0.102(1)	1	0.016(1)	8
T1a	-0.3012(4)	-0.0709(6)	0.020(1)	1	0.016(1)	8
T2	0.3035(4)	0.3089(5)	0.109(2)	1	0.016(1)	8
T2a	-0.3065(4)	-0.3117(5)	0.012(1)	1	0.016(1)	8
T3	0.0868(2)	0.3847(2)	0.309(2)	1	0.016(1)	8
T4	0.0884(2)	0.2256(2)	0.288(2)	1	0.016(1)	8
O1	0.1134(6)	0.4123(7)	0.505(2)	1	0.025	8
O1a	-0.1243(6)	-0.4215(6)	-0.362(2)	1	0.025	8
O2	0.1351(5)	0.1933(8)	0.454(2)	1	0.025	8
O2a	-0.1129(5)	-0.1907(7)	-0.398(2)	1	0.025	8
O3	0.2401(7)	0.1229(7)	0.062(2)	1	0.025	8
O3a	-0.2356(7)	-0.1201(6)	-0.917(2)	1	0.025	8
O4	0.0979(4)	0.3054(2)	0.298(3)	1	0.025	8
O5	0.1642(4)	0.2006(7)	0.810(2)	1	0.025	8
O6	0.1721(5)	0.4206(5)	0.813(2)	1	0.025	8
O7	0.2686(4)	0.0005(6)	0.084(3)	1	0.025	8
O8	0.253(1)	0.253(1)	0.585(3)	1	0.025	8
O9	0	0.4067(4)	0.278(3)	1	0.025	4
O10	0	0.2026(6)	0.297(3)	1	0.025	4
Na1	0	-0.494(3)	0.565(9)	0.309(7)	0.025	4
Na3	0	0.2449(5)	0.750(2)	0.790(7)	0.08	4
W1	0.5	0.9276(9)	0.770(4)	0.87(1)	0.07(3)	4
W2	0.625(1)	0.490(2)	0.373(4)	0.54(1)	0.08	8
W4	0.375(2)	0.506(3)	0.014(5)	0.46(1)	0.08	8
C1g	0.5	0.4161(6)	0.202(2)	0.554(2)	0.04(2)	4
O2g	0	0.0208(7)	-0.275(3)	0.554(2)	0.12(2)	4
C3g	0	-0.059(2)	-0.126(2)	0.554(2)	0.13(2)	4
O1g	0	0.374(1)	0.334(3)	0.554(2)	0.02(3)	4
Ng	0	0.066(2)	0.173(3)	0.554(2)	0.08(2)	4
C2g	0.5	0.390(1)	0.016(3)	0.554(2)	0.06(2)	4

Table 7S. Selected interatomic distances of Na-MOR+βala sample, XRPD collected in capillary.

atom1	atom2	distance	
T1	O1	1.628(3)	
	O3	1.622(3)	
	O6	1.624(3)	
	O7	1.638(3)	
T1a	O1a	1.616(3)	
	O3a	1.623(3)	
	O6	1.629(3)	
	O7	1.639(3)	
T2	O2	1.610(3)	
	O3a	1.621(3)	
	O5	1.619(3)	
	O8	1.629(3)	
T2a	O2a	1.605(3)	
	O3	1.621(3)	
	O5	1.624(3)	
	O8	1.633(3)	
T3	O1	1.642(3)	
	O1a	1.636(3)	
	O4	1.628(3)	
	O9	1.647(3)	
T4	O2	1.636(3)	
	O2a	1.627(3)	
	O4	1.636(3)	
	O10	1.666(3)	
Na1	O1	2.83(4)	x2
	O1p	2.73(4)	x2
	O9	2.96(6)	
	O9	2.36(6)	
	W1	2.21(8)	
	W1	2.59(8)	
Na3	O5	3.13(4)	x2
	O1g	2.51(1)	

atom1	atom2	distance	
W1	O1	2.87(2)	x2
	O6	3.13(1)	x2
	Na1	2.21(8)	
	Na1	2.59(8)	
W2	O7	3.04(1)	
	W4	2.71(5)	
	C1g	3.00(3)	
	O2g	2.52(3)	
	C3g	2.65(3)	
	Ng	3.12(3)	
W4	O7	2.641(8)	
	O2g	2.82(3)	
	C3g	2.82(5)	
	W2	2.71(5)	
	Ng	2.84(4)	
C1g	O2g	1.30(1)	
	O1g	1.30(1)	
	W2	3.00(3)	x2
	C2g	1.49(2)	
C3g	O10	2.99(1)	
	W4	2.82(5)	x2
	W2	2.65(3)	x2
	Ng	1.51(1)	
	C2g	1.50(1)	
O1g	O2p	3.15(1)	x2
	Na3	2.51(2)	
	C1g	1.30(1)	
O2g	W4	2.82(2)	x2
	C1g	1.30(1)	
	W2	2.52(3)	
Ng	O10	2.92(1)	
	W4	2.84(4)	x2
	C3g	1.51(1)	
	W2	3.12(3)	x2

Table 8S. Site fractional coordinates, occupancy factors (frac.) and equivalent/isotropic displacement parameters (U_{iso}, $Å^2$) of Na-MOR+gly_P_{amb}R sample, XRPD collected in DAC at ambient pressure after pressure release.

atoms	x	y	z	frac	Uiso	mult
T1	0.2962(1)	0.0666(1)	0.0701(4)	1	0.007(4)	8
T1a	-0.3129(1)	-0.0782(1)	-0.0262(3)	1	0.007(4)	8
T2	0.2980(1)	0.3107(1)	0.0697(3)	1	0.007(4)	8
T2a	-0.3053(1)	-0.3083(1)	-0.0326(3)	1	0.007(4)	8
T3	0.0849(1)	0.3854(1)	0.3130(3)	1	0.007(4)	8
T4	0.0869(1)	0.2268(1)	0.2680(3)	1	0.007(4)	8
O1	0.1311(8)	0.394(1)	0.4984(9)	1	0.015(6)	8
O1a	-0.1344(5)	-0.4150(4)	-0.3505(8)	1	0.015(6)	8
O2	0.1379(4)	0.1896(4)	0.4166(8)	1	0.015(6)	8
O2a	-0.1174(3)	-0.1992(11)	-0.4230(12)	1	0.015(6)	8
O3	0.2357(5)	0.1244(4)	1.0313(17)	1	0.015(6)	8
O3a	-0.2364(2)	-0.1185(3)	-0.9904(16)	1	0.015(6)	8
O4	0.0961(15)	0.3056(3)	0.305(7)	1	0.015(6)	8
O5	0.1634(3)	0.1815(6)	0.7652(3)	1	0.015(6)	8
O6	0.1651(3)	0.4198(6)	0.7630(3)	1	0.015(6)	8
O7	0.2727(3)	-0.0083(1)	0.0173(7)	1	0.015(6)	8
O8	0.2453(7)	0.2485(5)	0.4669(9)	1	0.015(6)	8
O9	0	0.4100(7)	0.345(4)	1	0.015(6)	4
O10	0	0.2049(13)	0.277(21)	1	0.015(6)	4
Na1	0	-0.499(7)	0.51(4)	0.41(2)	0.04(4)	4
Na3	0	0.220(2)	0.728(12)	0.88(3)	0.10(4)	4
W4	0.3302(2)	0.5265(2)	-0.2243(4)	0.44(2)	0.08	8
C1	0	-0.083(4)	0.210(34)	0.30(1)	0.1	4
O1g	0.5	0.395(8)	0.05(4)	0.30(1)	0.1	4
O2g	0	0.120(8)	-0.15(4)	0.30(1)	0.1	4
C2	0	-0.008(4)	0.212(29)	0.30(1)	0.1	4
N	0.5	0.473(9)	0.887(33)	0.30(1)	0.1	4
W1	0.5	0.898(2)	0.866(10)	0.84(4)	0.10(5)	4

Table 9S. Selected interatomic distances of Na-MOR+gly_P_{amb}R samples, XRPD collected in DAC at ambient pressure after the pressure treatment.

T1	O1	1.630(1)	
	O3	1.630(1)	
	O6	1.629(1)	
	O7	1.630(1)	
T1a	O1a	1.630(1)	
	O3a	1.630(1)	
	O6	1.628(1)	
	O7	1.630(1)	
T2	O2	1.630(1)	
	O3a	1.630(1)	
	O5	1.629(1)	
	O8	1.629(1)	
T2a	O2a	1.628(1)	
	O3	1.630(1)	
	O5	1.629(1)	
	O8	1.629(1)	
T3	O1	1.630(1)	
	O1a	1.632(1)	
	O4	1.635(1)	
	O9	1.634(1)	
T4	O2	1.631(1)	
	O2a	1.632(1)	
	O4	1.635(1)	
	O10	1.634(1)	
Na1	O1a	3.15(1)	x2
	O9	2.22(8)	
	O9	2.90(29)	
	W1	2.30(1)	

Na3	O5	3.07(1)	
	C1	2.79(5)	
	O1g	2.69(6)	
	O2g	2.20(5)	
W1	O6	3.113(8)	x2
	Na1	2.300(1)	
W4	O3	3.01(1)	
	O3p	2.70(1)	
	O5	3.16(1)	
	O7	2.690(4)	
	O7	2.709(4)	
C1	Na3	2.79(5)	
	O1g	1.265(1)	
	O2g	1.267(1)	
	C2	1.516(1)	
	N	2.67(2)	
O1g	O10	2.90(2)	
	Na4	2.69(6)	
	C1	1.265(1)	
	N	2.00(21)	
O2g	O2a	3.17(2)	
	Na3	2.20(5)	
	C1	1.267(1)	
	N	3.02(2)	
C2	C1	1.516(1)	
	N	1.50(1)	
N	O1g	2.00(21)	
	O2g	3.02(2)	
	C2	1.50(1)	

Table 10S. Unit cell parameters and volume of Na-MOR+gly measured under compression and decompression in DAC. The cell parameters normalized to those collected in capillary at ambient conditions are also reported. REV indicates data collected during pressure release.

10S:

P (Gpa)	*a*	*b*	*c*	*V*	*a/a0*	*b/b0*	*c/c0*	*V/V0*
0	18.080(1)	20.348(1)	7.4908(4)	2755.9(4)	1,0003	0,9999	0,9999	1,0001
0,44	17.999(5)	20.156(4)	7.445(1)	2701(1)	0,9958	0,9905	0,9938	0,9802
1,02	17.781(2)	19.830(2)	7.337(1)	2587(1)	0,9837	0,9744	0,9794	0,9388
1,57	17.539(8)	19.564(6)	7.255(2)	2489(2)	0,9703	0,9614	0,9685	0,9033
2,06	17.43(1)	19.33(1)	7.222(4)	2432(3)	0,9643	0,9499	0,9641	0,8826
1,68	17.44(1)	19.42(1)	7.223(5)	2447(4)	0,9649	0,9543	0,9642	0,8880
1,1	17.661(4)	19.718(3)	7.298(1)	2541(1)	0,9771	0,9689	0,9742	0,9222
0	18.075(2)	20.337(2)	7.4877(6)	2752.4(6)	1,0000	0,9994	0,9995	0,9989

Figures

Figure 5S: Observed (red cross marks) and calculated (green line) diffraction patterns and final difference curve (purple line) from Rietveld refinements for Na-MOR+gly in capillary.

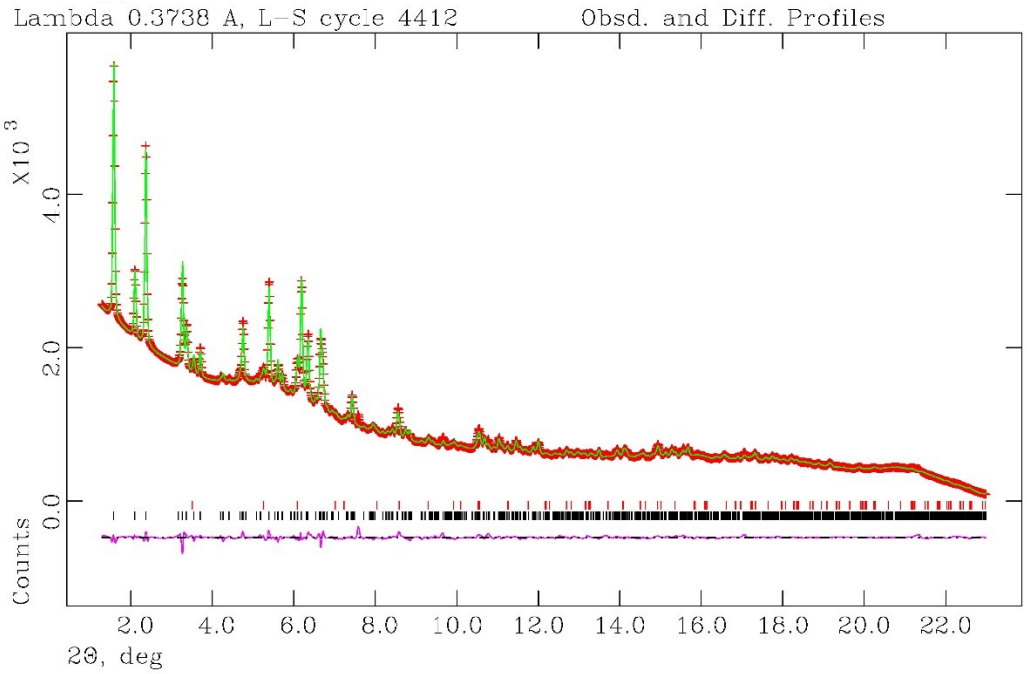

Figure 6S: Observed (red cross marks) and calculated (green line) diffraction patterns and final difference curve (purple line) from Rietveld refinements for Na-MOR+βala.

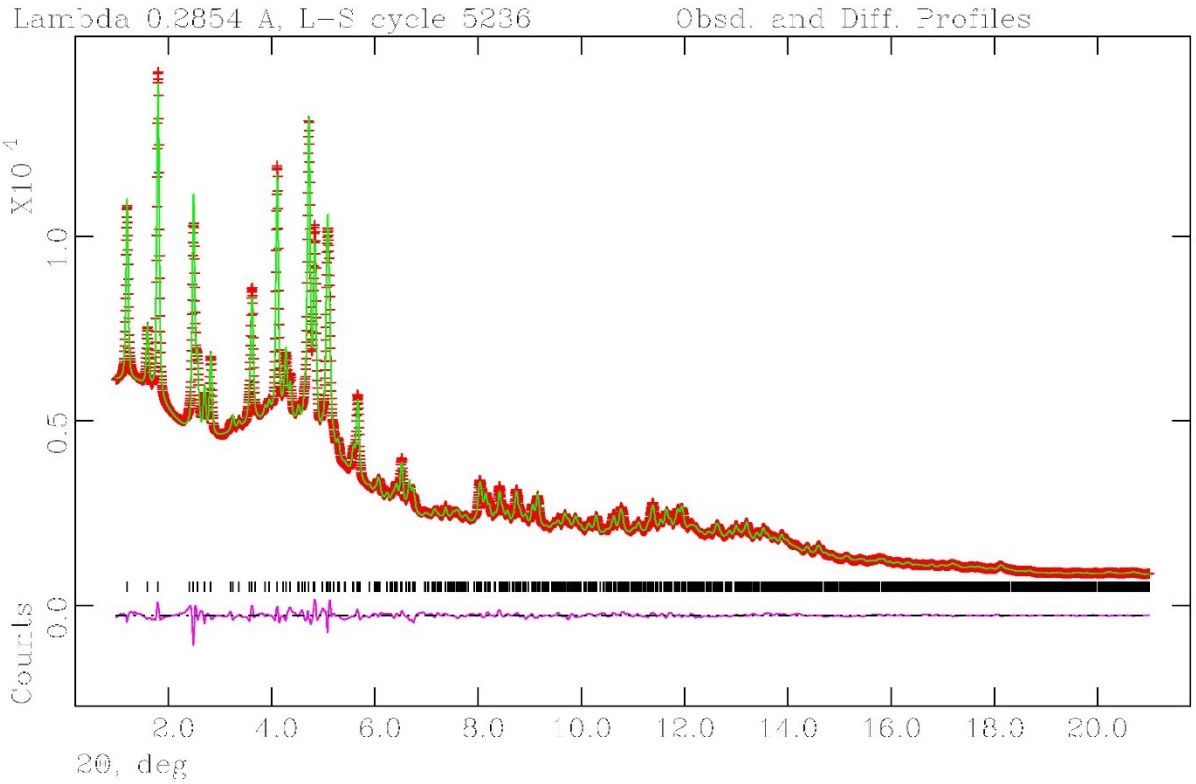

Figure 7S: Observed (red cross marks) and calculated (green line) diffraction patterns and final difference curve (purple line) from Rietveld refinements for Na-MOR+gly_P_{amb}R in DAC in selected 2theta range.

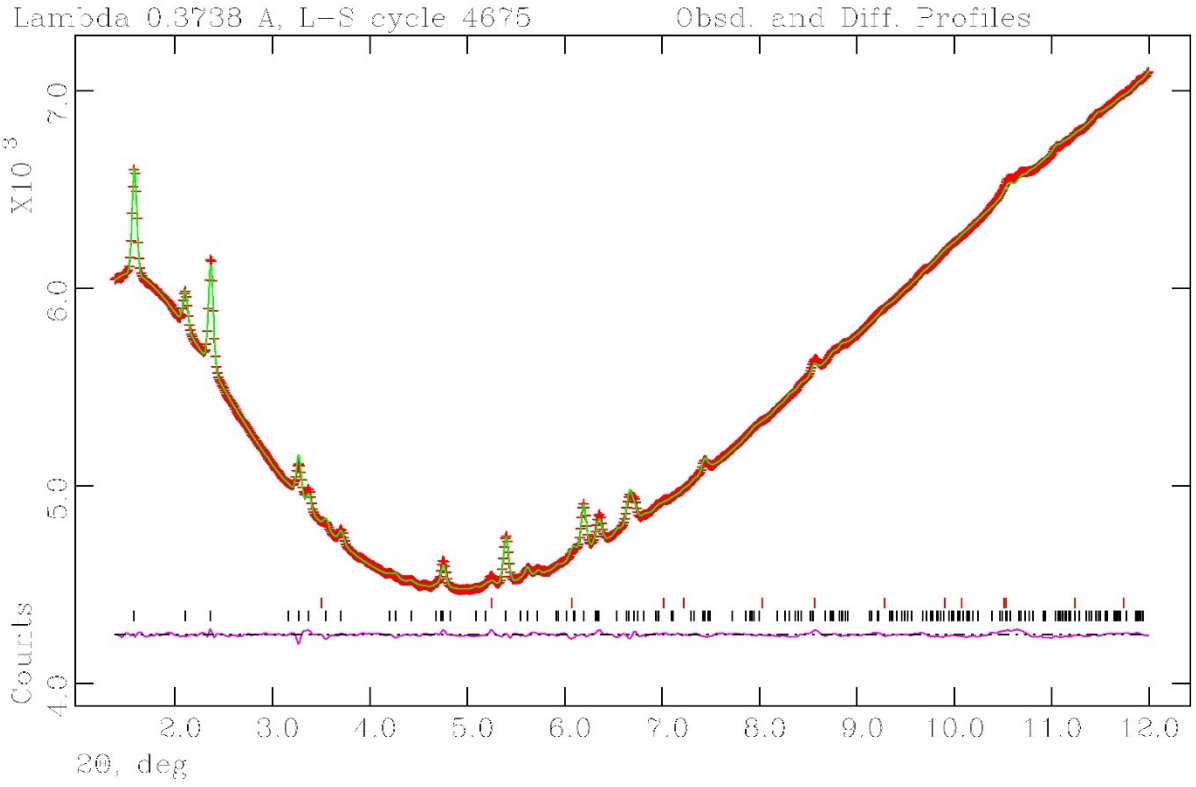

Figure 8S: Diffraction patterns collected on sample Na-MOR+gly at increasing pressures.

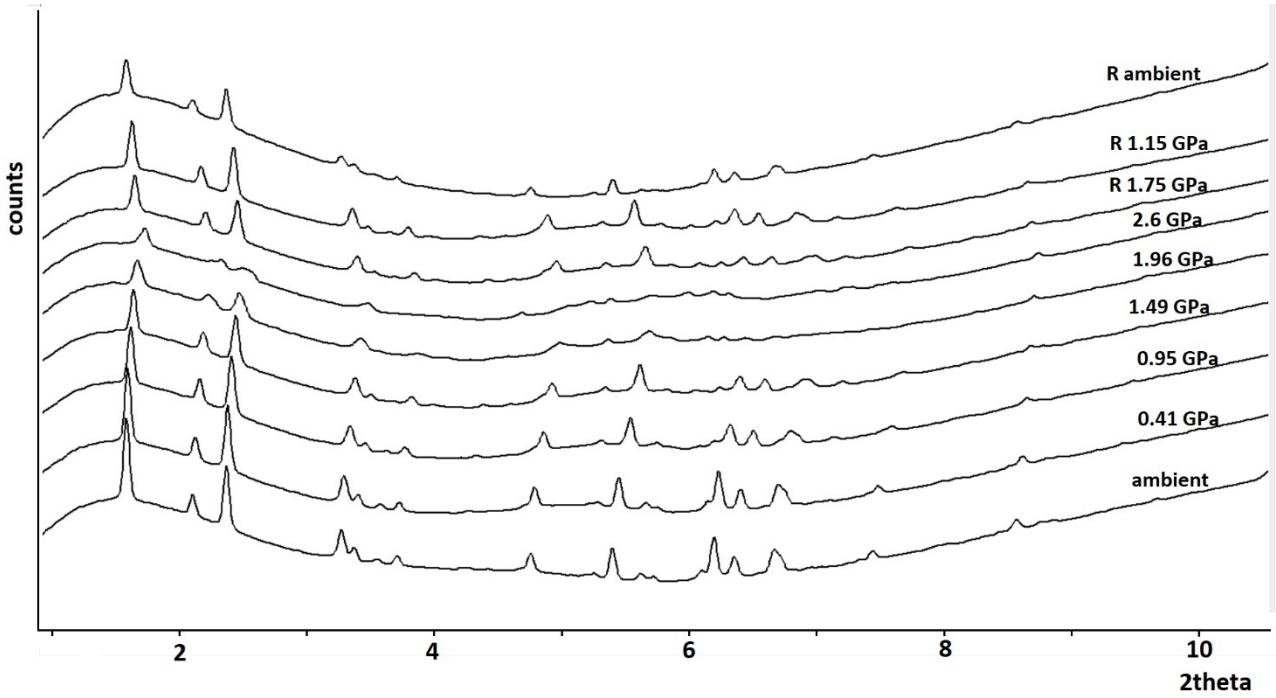

Figure 9S: Unit cell parameters as a function of pressure for Na-MOR+gly.