Supporting Information

Hiding Extra-Framework Cations in Zeolites L and Y by Internal Ion Exchange and its

Effect on CO₂ Adsorption

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S1. Synthesis and ion exchange of Potassium Zeolite L.

Solution A was prepared by dissolving aluminium isopropoxide (1.54 g, Sigma-Aldrich) in potassium hydroxide (1.28 g, Alfa Aesar) and water (2.51 g) at 373 K, until clear. After solution A was cooled to room temperature the water loss due to evaporation was corrected. Solution B was prepared by mixing Ludox HS-40 (5.52 g, Sigma-Aldrich) with water (4.82 g) until homogeneous, which took around 3 min. Solution A was then added to solution B and the mixture was stirred until thickening of the gel started. The gel was loaded into a 40 mL PTFE (Teflon) liner inside a stainless-steel autoclave and heated at 453 K for 48 h. After crystallisation the autoclave was cooled to room temperature and the product was filtered and washed five times with distilled water (650 mL), ensuring the pH of the final wash water was 7. The product was then dried at 333 K overnight.

1.0 g of zeolite K_{9.0}-L (K_{9.0}Al_{9.0}Si_{27.0}O₇₂) was repeatedly ion exchanged with 0.5 M lanthanum nitrate solution or 0.5 M calcium nitrate solution at 333 K for 2-4 h. Sample was then filtered and washed with deionised water, dried in a 343 K oven overnight and a cation content was measured using SEM-EDX. When the La³⁺(Ca²⁺)/Al³⁺ ratio remained constant, the sample was calcined at 1073 K in flowing oxygen gas for 10 h. Then the process of ion exchange and calcination was repeated to reach required unit cell compositions, for example for the fully-exchanged La-L, K_{9.0}-L was exchanged 100x and calcined 10x. Each time 0.05-0.1 g of sample

with required content of cations, before and after calcination, was kept for further analysis. The studied compositions were: $K_{5.7}La_{1.1}Al_{9.0}Si_{27.0}O_{72}$ ($K_{5.7}La_{1.1}-L$), $K_{2.7}La_{2.1}Al_{9.0}Si_{27.0}O_{72}$ ($K_{2.7}La_{2.1}-L$), $La_{3.0}Al_{9.0}Si_{27.0}O_{72}$ ($La_{3.0}-L$), $K_{6.2}Ca_{1.4}Al_{9.0}Si_{27.0}O_{72}$ ($K_{6.2}Ca_{1.4}-L$) and $Ca_{3.8}K_{1.4}Al_{9.0}Si_{27.0}O_{72}$ ($Ca_{3.8}K_{1.4}-L$).

For comparison, commercially-obtained $Na_{56.0}$ -Y ($Na_{56.0}Al_{56.0}Si_{136.0}O_{384}$), was also ion exchanged 10× with 0.5 M lanthanum nitrate solution at 333 K for 6 h and heated twice at 673 K to obtain $La_{18.7}$ -Y ($La_{18.7}Al_{56.0}Si_{136.0}O_{384}$).

S2. EDX Spectra of K-L, K,La-L and La-L samples.



S3. Crystallographic details of dehydrated samples.

| | | K₅ ₂La₁ ₁-L | K5 7La1 1-L | K ₂₇ La ₂₁ -L |
|-----------------------|---|---|---|---|
| | K _{9.0} -L | (before calcination) | (after calcination) | (before calcination) |
| Unit cell | K _{9.0} Al _{9.0} Si _{27.0} O ₇₂ | K _{5.7} La _{1.1} Al _{9.0} Si _{27.0} O ₇₂ | K _{5.7} La _{1.1} Al _{9.0} Si _{27.0} O ₇₂ | K _{2.7} La _{2.1} Al _{9.0} Si _{27.0} O ₇₂ |
| Temperature/K | 298 | 298 | 298 | 298 |
| Space group | P6/mmm | P6/mmm | P6/mmm | P6/mmm |
| X-ray source | Cu | Cu | Cu | Cu |
| Diffractometer | Stoe | Stoe | Stoe | Stoe |
| Wavelength (Å) | 1.54056 | 1.54056 | 1.54056 | 1.54056 |
| a/ Å | 18.43881(16) | 18.28369(21) | 18.39583(24) | 18.30167(23) |
| c/ Å | 7.48766(7) | 7.50227(10) | 7.42565(12) | 7.43186(13) |
| Volume/Å ³ | 2204.66(4) | 2171.96(5) | 2176.23(6) | 2155.81(6) |
| R _p | 0.0324 | 0.0374 | 0.0402 | 0.0388 |
| R _{wp} | 0.0441 | 0.0501 | 0.0530 | 0.0519 |
| X ² | 2.275 | 1.959 | 2.276 | 2.027 |
| | K _{2.7} La _{2.1} -L | | | |
| | (after calcination) | La _{3.0} -L | Na _{56.0} -Y | La _{18.7} -Y |
| Unit cell | K _{2.7} La _{2.1} Al _{9.0} Si _{27.0} O ₇₂ | La _{3.0} Al _{9.0} Si _{27.0} O ₇₂ | Na _{56.0} Al _{56.0} Si _{136.0} O ₃₈₄ | La _{18.7} Al _{56.0} Si _{136.0} O ₃₈₄ |
| Temperature/K | 298 | 298 | 298 | 298 |
| Space group | P6/mmm | P6/mmm | Fd3m | Fd3m |

| X-ray source | Cu | Cu | Cu | Cu |
|-----------------------|--------------|-------------|--------------|------------|
| Diffractometer | Stoe | Stoe | Stoe | Stoe |
| Wavelength (Å) | 1.54056 | 1.54056 | 1.54056 | 1.54056 |
| a/ Å | 18.38886(29) | 18.1425(6) | 24.78528(26) | 24.7938(4) |
| c/ Å | 7.37587(14) | 7.36463(21) | | |
| Volume/Å ³ | 2160.00(7) | 2099.32(12) | 15225.9(5) | 15241.5(8) |
| R _p | 0.0366 | 0.0328 | 0.0285 | 0.0407 |
| R _{wp} | 0.0485 | 0.0423 | 0.0395 | 0.0544 |
| X ² | 1.907 | 1.564 | 1.682 | 2.140 |

S4. Fractional atomic coordinates, occupancies and isotropic displacement parameters (in $Å^2$) for dehydrated samples.

Zeolite L (LTL)

| K _{9.0} -L | x | У | z | Occup. | Multipl. | Uiso |
|---------------------------------------|-------------|-------------|-------------|------------|----------|-----------|
| Si1 | 0.09332(15) | 0.35680(16) | 0.5 | 0.75 | 12 | 0.0008(4) |
| Al1 | 0.09332(15) | 0.35680(16) | 0.5 | 0.25 | 12 | 0.0008(4) |
| Si2 | 0.16557(16) | 0.49789(14) | 0.21146(17) | 0.75 | 24 | 0.0008(4) |
| Al2 | 0.16557(16) | 0.49789(14) | 0.21146(17) | 0.25 | 24 | 0.0008(4) |
| 01 | 0.0 | 0.2735(4) | 0.5 | 1.0 | 6 | 0.0008(4) |
| 02 | 0.16534(20) | 0.3307(4) | 0.5 | 1.0 | 6 | 0.0008(4) |
| 03 | 0.26384(15) | 0.52767(29) | 0.2543(6) | 1.0 | 12 | 0.0008(4) |
| 04 | 0.10256(22) | 0.3243(4) | 1.0 | 1.0 | 24 | 0.0008(4) |
| O5 | 0.42487(15) | 0.84973(31) | 0.2713(6) | 1.0 | 12 | 0.0008(4) |
| O6 | 0.14649(28) | 0.47819(28) | 0.0 | 1.0 | 12 | 0.0008(4) |
| K1 (site I) | 0.3333 | 0.6667 | 0.5 | 1.023(5) | 2 | 0.025 |
| K2 (site II) | 0.0 | 0.5 | 0.5 | 1.005(4) | 3 | 0.025 |
| K3 (site III) | 0.0 | 0.31904(25) | 0.0 | 0.6410(29) | 6 | 0.025 |
| K _{5.7} La _{1.1} -L | | | | | | |
| (before calcination) | X | y | Z | Occup. | Multipl. | |
| Si1 | 0.09313(21) | 0.35716(22) | 0.5 | 0.75 | 12 | 0.0067(5) |
| All | 0.09313(21) | 0.35716(22) | 0.5 | 0.25 | 12 | 0.0067(5) |
| Si2 | 0.16412(22) | 0.49741(19) | 0.20972(26) | 0.75 | 24 | 0.0067(5) |
| Al2 | 0.16412(22) | 0.49741(19) | 0.20972(26) | 0.25 | 24 | 0.0067(5) |
| 01 | 0.0 | 0.2730(6) | 0.5 | 1.0 | 6 | 0.0067(5) |
| 02 | 0.16697(29) | 0.3339(6) | 0.5 | 1.0 | 6 | 0.0067(5) |
| 03 | 0.26372(21) | 0.5274(4) | 0.2556(9) | 1.0 | 12 | 0.0067(5) |
| 04 | 0.10009(28) | 0.41576(31) | 0.3245(5) | 1.0 | 24 | 0.0067(5) |
| O5 | 0.42676(21) | 0.8535(4) | 0.2696(9) | 1.0 | 12 | 0.0067(5) |
| O6 | 0.1434(4) | 0.4766(4) | 0.0 | 1.0 | 12 | 0.0067(5) |
| K1 (site I) | 0.3333 | 0.6667 | 0.5 | 1.026(7) | 2 | 0.025 |
| K2 (site II) | 0.0 | 0.5 | 0.5 | 0.734(7) | 3 | 0.025 |
| K3 (site III) | 0.0 | 0.321(7) | 0.0 | 0.245(4) | 6 | 0.05 |
| La2 (site II) | 0.0 | 0.5 | 0.5 | 0.26445 | 3 | 0.025 |
| La3 (site III) | 0.0 | 0.323(11) | 0.0 | 0.04623 | 6 | 0.025 |
| | | | | | | |
| K _{5.7} La _{1.1} -L | | | | | | |
| (after calcination) | x | У | z | Occup. | Multipl. | Uiso |
| Si1 | 0.09171(22) | 0.35388(25) | 0.5 | 0.75 | 12 | 0.0075(5) |
| Al1 | 0.09171(22) | 0.35388(25) | 0.5 | 0.25 | 12 | 0.0075(5) |
| Si2 | 0.16574(23) | 0.49792(20) | 0.21439(28) | 0.75 | 24 | 0.0075(5) |
| Al2 | 0.16574(23) | 0.49792(20) | 0.21439(28) | 0.25 | 24 | 0.0075(5) |
| 01 | 0.0 | 0.2710(6) | 0.5 | 1.0 | 6 | 0.0075(5) |
| 02 | 0.16609(30) | 0.3321(6) | 0.5 | 1.0 | 6 | 0.0075(5) |
| 03 | 0.26514(20) | 0.5301(4) | 0.2576(9) | 1.0 | 12 | 0.0075(5) |

| 04 | 0.10200(34) | 0.41314(33) | 14(33) 0.3274(6) 1.0 | | 24 | 0.0075(5) |
|--|--|---|--|---|--|--|
| O5 | 0.42546(22) | 0.8509(4) | 0.2728(9) | 1.0 | 12 | 0.0075(5) |
| 06 | 0.1503(5) | 0.4804(4) | 0.0 1.0 | | 12 | 0.0075(5) |
| K1 (site I) | 0.3333 | 0.6667 | 0.5 | 0.676(4) | 2 | 0.025 |
| K2 (site II) | 0.0 | 0.5 | 0.5 | 0.537(6) | 3 | 0.025 |
| K3 (site III) | 0.0 | 0.3180(5) | 0.0 | 0.465(4) | 6 | 0.025 |
| La1 (site I) | 0.3333 | 0.6667 | 0.5 | 0.324(4) | 2 | 0.025 |
| La2 (site II) | 0.0 | 0.5 | 0.5 | 0.16017 | 3 | 0.025 |
| | | | | | | |
| K _{2.7} La _{2.1} -L | | | | | | |
| (before calcination) | X | y | Z | Occup. | Multipl. | Uiso |
| Si1 | 0.09174(25) | 0.35465(27) | 0.5 | 0.75 | 12 | 0.0084(6) |
| Al1 | 0.09174(25) | 0.35465(27) | 0.5 | 0.25 | 12 | 0.0084(6) |
| Si2 | 0.16507(27) | 0.49769(22) | 0.21394(30) | 0.75 | 24 | 0.0084(6) |
| AI2 | 0.16507(27) | 0.49769(22) | 0.21394(30) | 0.25 | 24 | 0.0084(6) |
| 01 | 0.0 | 0.2711(7) | 0.5 | 10 | 6 | 0.0084(6) |
| 01 | 0.0 | 0.22111(1) | 0.0 | 1.0 | 6 | 0.0001(0) |
| 02 | 0.10707(32) | 0.3340(0 | 0.0 | 1.0 | 0 | 0.0084(0) |
| 03 | 0.26373(23) | 0.5274(5) | 0.2571(10) | 1.0 | 12 | 0.0084(6) |
| 04 | 0.1025(4) | 0.4148(4) | 0.3274(7) | 1.0 | 24 | 0.0084(6) |
| O5 | 0.42594(25) | 0.8519(5) | 0.2733(10) | 1.0 | 12 | 0.0084(6) |
| O6 | 0.1486(5) | 0.4809(5) | 0.0 | 1.0 | 12 | 0.0084(6) |
| K1 (site I) | 0.3333 | 0.6667 | 0.5 | 0.584(5) | 2 | 0.025 |
| K3 (site III) | 0.0 | 0.3244(10) | 0.0 | 0.253(4) | 6 | 0.025 |
| | 0.0 | 0.3244(10) | 0.0 | 0.233(4) | 0 | 0.025 |
| La'i (site i) | 0.3333 | 0.6667 | 0.5 | 0.372(5) | 2 | 0.055 |
| La2 (site II) | 0.0 | 0.5 | 0.5 | 0.4514(23) | 3 | 0.055 |
| | | | | | | |
| | | | | | | |
| $K_{2.7}La_{2.1}-L$ | | | - | Occup | Multipl | Uiao |
| K _{2.7} La _{2.1} -L (after calcination) | x | y | z | Occup . | Multipl. | Uiso |
| K _{2.7} La _{2.1} -L (after calcination) Si1 Al1 | x 0.09174(26) 0.09174(26) | y 0.35219(30) 0.35219(30) | z 0.5 | Occup. 0.75 | Multipl. 12 12 | Uiso 0.0077(7) 0.0077(7) |
| K _{2.7} La _{2.1} -L (after calcination) Si1 Al1 Si2 | x 0.09174(26) 0.09174(26) 0.16494(27) | y 0.35219(30) 0.35219(30) 0.49770(23) | z 0.5 0.5 0.21643(34) | Occup. 0.75 0.25 0.75 | Multipl. 12 12 24 | Uiso 0.0077(7) 0.0077(7) 0.0077(7) |
| K _{2.7} La _{2.1} -L (after calcination) Si1 Al1 Si2 Al2 | x 0.09174(26) 0.09174(26) 0.16494(27) 0.16494(27) | y 0.35219(30) 0.35219(30) 0.49770(23) 0.49770(23) | z 0.5 0.5 0.21643(34) 0.21643(34) | Occup. 0.75 0.25 0.75 0.25 | Multipl. 12 12 24 24 | Uiso 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) |
| K _{2.7} La _{2.1} -L (after calcination) Si1 Al1 Si2 Al2 O1 | x 0.09174(26) 0.09174(26) 0.16494(27) 0.16494(27) 0.0 | y 0.35219(30) 0.35219(30) 0.49770(23) 0.49770(23) 0.2742(7) | z 0.5 0.5 0.21643(34) 0.21643(34) 0.5 | Occup. 0.75 0.25 0.75 0.25 1.0 | Multipl. 12 12 24 24 6 | Uiso 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) |
| K2.7La2.1-L (after calcination) Si1 Al1 Si2 Al2 O1 O2 | x 0.09174(26) 0.16494(27) 0.16494(27) 0.0 0.1652(4) | y 0.35219(30) 0.49770(23) 0.49770(23) 0.2742(7) 0.3303(7) | z 0.5 0.21643(34) 0.21643(34) 0.5 0.5 | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 | Multipl. 12 12 24 24 6 6 | Uiso 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) |
| K2.7La2.1-L (after calcination) Si1 Al1 Si2 Al2 O1 O2 O3 | x 0.09174(26) 0.09174(26) 0.16494(27) 0.16494(27) 0.0 0.1652(4) 0.26584(23) | y 0.35219(30) 0.49770(23) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) | z 0.5 0.21643(34) 0.21643(34) 0.5 0.5 0.5 0.2613(11) | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 | Multipl. 12 12 24 24 6 6 6 12 | Uiso 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) |
| K2.7La2.1-L (after calcination) Si1 Al1 Si2 Al2 O1 O2 O3 O4 | x 0.09174(26) 0.09174(26) 0.16494(27) 0.16494(27) 0.0 0.1652(4) 0.26584(23) 0.1045(4) | y 0.35219(30) 0.35219(30) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) 0.4134(4) | z 0.5 0.21643(34) 0.21643(34) 0.5 0.5 0.5 0.2613(11) 0.3293(8) | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 1.0 | Multipl. 12 12 24 24 6 6 12 24 24 | Uiso 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) |
| K2.7La2.1-L (after calcination) Si1 Al1 Si2 Al2 O1 O2 O3 O4 O5 | x 0.09174(26) 0.09174(26) 0.16494(27) 0.16494(27) 0.0 0.1652(4) 0.26584(23) 0.1045(4) 0.42489(27) | y 0.35219(30) 0.35219(30) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) 0.4134(4) 0.8497(5) | z 0.5 0.21643(34) 0.21643(34) 0.5 0.5 0.2613(11) 0.3293(8) 0.2781(12) | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 1.0 1.0 | Multipl. 12 12 24 24 6 6 12 24 12 24 12 | Uiso 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) |
| K2.7La2.1-L (after calcination) Si1 Al1 Si2 Al2 O1 O2 O3 O4 O5 O6 | x 0.09174(26) 0.09174(26) 0.16494(27) 0.16494(27) 0.0 0.1652(4) 0.26584(23) 0.1045(4) 0.42489(27) 0.1520(5) | y 0.35219(30) 0.35219(30) 0.49770(23) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) 0.4134(4) 0.8497(5) 0.4831(5) 0.4831(5) | z 0.5 0.21643(34) 0.21643(34) 0.5 0.5 0.2613(11) 0.3293(8) 0.2781(12) 0.0 | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 1.0 1.0 1.0 | Multipl. 12 12 24 24 6 6 12 24 12 12 12 24 | Uiso 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) |
| K2.7La2.1-L (after calcination) Si1 Al1 Si2 Al2 O1 O2 O3 O4 O5 O6 K1 (site I) | x 0.09174(26) 0.09174(26) 0.16494(27) 0.16494(27) 0.0 0.1652(4) 0.26584(23) 0.1045(4) 0.42489(27) 0.1520(5) 0.3333 0.0 | y 0.35219(30) 0.49770(23) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) 0.4134(4) 0.8497(5) 0.4831(5) 0.6667 | z 0.5 0.5 0.21643(34) 0.21643(34) 0.5 0.5 0.2613(11) 0.3293(8) 0.2781(12) 0.0 0.5 0.2 | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 1.0 1.0 0.365(5) | Multipl. 12 12 24 24 6 6 12 24 12 12 12 2 2 2 2 2 2 2 2 2 2 2 2 2 | Uiso 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0025 |
| $K_{2.7}La_{2.1}-L$ (after calcination) Si1 Al1 Si2 Al2 O1 O2 O3 O4 O5 O6 K1 (site I) K3 (site II) Lo4 (site I) | x 0.09174(26) 0.09174(26) 0.16494(27) 0.16494(27) 0.0 0.1652(4) 0.26584(23) 0.1045(4) 0.42489(27) 0.1520(5) 0.3333 0.0 0.2022 | y 0.35219(30) 0.49770(23) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) 0.4134(4) 0.8497(5) 0.4831(5) 0.6667 0.3186(9) 0.0007 | z 0.5 0.5 0.21643(34) 0.21643(34) 0.5 0.5 0.2613(11) 0.3293(8) 0.2781(12) 0.0 0.5 0.0 0.5 | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 1.0 0.365(5) 0.321(5) | Multipl. 12 12 24 24 6 6 12 24 12 12 12 2 6 6 2 2 2 2 2 2 2 2 2 2 2 2 2 | Uiso 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0025 0.034 0.055 |
| $K_{2.7}La_{2.1}-L$ (after calcination) Si1 Al1 Si2 Al2 O1 O2 O3 O4 O5 O6 K1 (site I) K3 (site II) La1 (site I) La2 (site II) | x 0.09174(26) 0.16494(27) 0.16494(27) 0.1652(4) 0.26584(23) 0.1045(4) 0.42489(27) 0.1520(5) 0.3333 0.0 0.3333 0.0 | y 0.35219(30) 0.49770(23) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) 0.4134(4) 0.8497(5) 0.4831(5) 0.6667 0.3186(9) 0.6667 | z 0.5 0.21643(34) 0.21643(34) 0.5 0.5 0.2613(11) 0.3293(8) 0.2781(12) 0.0 0.5 0.0 0.5 0.0 0.5 0.5 0.0 0.5 0.0 0.5 0.5 | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 1.0 0.365(5) 0.321(5) 0.635(5) | Multipl. 12 12 24 24 6 6 12 24 12 12 12 2 6 2 2 3 | Uiso 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0055 0.055 0.055 |
| $\begin{array}{c} \textbf{K}_{2.7}\textbf{L}\textbf{a}_{2.1}\textbf{-}\textbf{L} \\ \textbf{(after calcination)} \\ \hline \textbf{Si1} \\ \hline \textbf{A 1} \\ \hline \textbf{Si2} \\ \hline \textbf{A 2} \\ \hline \textbf{O1} \\ \hline \textbf{O2} \\ \hline \textbf{O3} \\ \hline \textbf{O4} \\ \hline \textbf{O5} \\ \hline \textbf{O6} \\ \hline \textbf{K1} (site I) \\ \hline \textbf{K3} (site II) \\ \hline \textbf{La1} (site I) \\ \hline \textbf{La2} (site II) \\ \hline \textbf{La2} (site II) \\ \hline \end{array}$ | x 0.09174(26) 0.16494(27) 0.16494(27) 0.0 0.1652(4) 0.26584(23) 0.1045(4) 0.42489(27) 0.1520(5) 0.3333 0.0 0.3333 0.0 | y 0.35219(30) 0.49770(23) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) 0.4134(4) 0.8497(5) 0.4831(5) 0.6667 0.3186(9) 0.6667 0.5 | z 0.5 0.21643(34) 0.21643(34) 0.5 0.5 0.2613(11) 0.3293(8) 0.2781(12) 0.0 0.5 0.0 0.5 0.0 0.5 0.5 | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 1.0 0.365(5) 0.321(5) 0.635(5) 0.2686(22) | Multipl. 12 12 24 24 6 6 12 24 12 12 2 6 2 3 3 | Uiso 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0055 0.055 |
| $\begin{array}{c} {\sf K}_{2.7}{\sf La}_{2.1}{\text{-}{\sf L}}\\ (after calcination)\\ \hline Si1\\ Al1\\ Si2\\ Al2\\ O1\\ O2\\ O3\\ O4\\ O5\\ O6\\ \hline K1 (site I)\\ \hline K3 (site I)\\ \hline La1 (site I)\\ \hline La2 (site II)\\ \hline \end{array}$ | x 0.09174(26) 0.16494(27) 0.16494(27) 0.0 0.1652(4) 0.26584(23) 0.1045(4) 0.42489(27) 0.1520(5) 0.3333 0.0 0.3333 0.0 | y 0.35219(30) 0.49770(23) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) 0.4134(4) 0.8497(5) 0.4831(5) 0.6667 0.3186(9) 0.6667 0.5 | z 0.5 0.21643(34) 0.21643(34) 0.5 0.5 0.2613(11) 0.3293(8) 0.2781(12) 0.0 0.5 0.0 0.5 0.0 0.5 0.5 | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 1.0 0.25 0.25 0.25 0.25 0.25 0.010 1.0 0.010 0.02685(5) 0.2686(22) | Multipl. 12 12 24 24 6 6 12 24 12 24 12 2 6 2 3 3 | Uiso 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0025 0.034 0.055 0.055 |
| $\begin{tabular}{ c c c c c } \hline K_{2.7} La_{2.1} - L & & & \\ \hline (after calcination) & & \\ \hline Si1 & & & \\ \hline Al1 & & & \\ Si2 & & & \\ Al2 & & & \\ O1 & & & \\ O2 & & & \\ O3 & & & \\ O4 & & & \\ O5 & & & \\ O4 & & & \\ O5 & & & \\ O5 & & & \\ O6 & & & \\ K1 & (site I) & & \\ K3 & (site II) & & \\ La1 & (site I) & & \\ La2 & (site II) & & \\ \hline La2 & (site II) & & \\ \hline La_{3.0} - L & & \\ \hline \end{tabular}$ | x 0.09174(26) 0.09174(26) 0.16494(27) 0.16494(27) 0.0 0.1652(4) 0.26584(23) 0.1045(4) 0.42489(27) 0.1520(5) 0.3333 0.0 0.3333 0.0 x | y 0.35219(30) 0.35219(30) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) 0.4134(4) 0.8497(5) 0.4831(5) 0.6667 0.3186(9) 0.6667 0.5 y | z 0.5 0.21643(34) 0.21643(34) 0.5 0.5 0.2613(11) 0.3293(8) 0.2781(12) 0.0 0.5 0.0 0.5 0.0 0.5 0.5 z | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 1.0 0.25 0.25 0.25 0.01 0.01 0.021 0.365(5) 0.2686(22) Occup. | Multipl. 12 12 24 24 6 6 12 24 12 24 12 24 12 2 6 2 3 Multipl. | Uiso 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.025 0.034 0.055 0.055 Uiso |
| K2.7La2.1-L (after calcination) Si1 Al1 Si2 Al2 O1 O2 O3 O4 O5 O6 K1 (site I) La1 (site I) La2 (site II) La2 (site II) Si1 | x 0.09174(26) 0.09174(26) 0.16494(27) 0.16494(27) 0.0 0.1652(4) 0.26584(23) 0.1045(4) 0.42489(27) 0.1520(5) 0.3333 0.0 0.3333 0.0 x 0.0 x 0.0887(4) | y 0.35219(30) 0.49770(23) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) 0.4134(4) 0.8497(5) 0.4831(5) 0.6667 0.3186(9) 0.6667 0.5 y 0.3512(4) | z 0.5 0.21643(34) 0.21643(34) 0.5 0.5 0.2613(11) 0.3293(8) 0.2781(12) 0.0 0.5 0.0 0.5 0.5 z 0.5 | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 1.0 0.25 0.75 0.25 0.01 0.01 0.025 0.01 1.0 0.365(5) 0.321(5) 0.635(5) 0.2686(22) Occup. 0.75 | Multipl. 12 12 24 24 6 6 12 24 12 24 12 24 12 2 6 2 3 Multipl. 12 | Uiso 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0055 0.034 0.055 0.055 Uiso 0.0030(8) |
| K2.7La2.1-L (after calcination) Si1 Al1 Si2 Al2 O1 O2 O3 O4 O5 O6 K1 (site I) La1 (site I) La2 (site II) La2 (site II) La1 (site I) Al2 (site II) Al1 | x 0.09174(26) 0.09174(26) 0.16494(27) 0.16494(27) 0.0 0.1652(4) 0.26584(23) 0.1045(4) 0.42489(27) 0.1520(5) 0.3333 0.0 0.3333 0.0 x 0.0887(4) 0.0887(4) | y 0.35219(30) 0.35219(30) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) 0.4134(4) 0.8497(5) 0.4831(5) 0.6667 0.3186(9) 0.6667 0.5 | z 0.5 0.21643(34) 0.21643(34) 0.5 0.5 0.2613(11) 0.3293(8) 0.2781(12) 0.0 0.5 0.0 0.5 0.5 0.5 0.5 0.5 | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 1.0 0.365(5) 0.321(5) 0.635(5) 0.2686(22) Occup. 0.75 0.25 | Multipl. 12 12 24 24 6 6 12 24 12 24 12 24 12 22 6 2 3 Multipl. 12 12 12 12 12 12 12 12 12 12 | Uiso 0.0077(7) 0.0075(7) 0.0077(7) 0.0075(7) 0.0075(7) 0.0075(7) 0.0034 0.0055 0.034 0.0055 0.030(8) 0.0030(8) 0.0030(8) |
| K2.7La2.1-L (after calcination) Si1 Al1 Si2 Al2 O1 O2 O3 O4 O5 O6 K1 (site I) La1 (site I) La2 (site II) La2 (site II) Si1 Al1 Si2 | x 0.09174(26) 0.09174(26) 0.16494(27) 0.16494(27) 0.0 0.1652(4) 0.26584(23) 0.1045(4) 0.42489(27) 0.1520(5) 0.3333 0.0 0.3333 0.0 x 0.0887(4) 0.0887(4) 0.1671(4) | y 0.35219(30) 0.35219(30) 0.49770(23) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) 0.4134(4) 0.8497(5) 0.4831(5) 0.6667 0.3186(9) 0.6667 0.5 y 0.3512(4) 0.4989(4) | z 0.5 0.21643(34) 0.21643(34) 0.5 0.5 0.2613(11) 0.3293(8) 0.2781(12) 0.0 0.5 0.0 0.5 0.5 0.5 0.5 0.5 | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 1.0 0.365(5) 0.321(5) 0.635(5) 0.2686(22) Occup. 0.75 0.25 0.75 | Multipl. 12 12 24 24 6 12 24 12 24 6 12 24 12 24 12 13 14 <td>Uiso 0.0077(7) 0.0075 0.0034 0.055 0.035 0.030(8) 0.0030(8) 0.0030(8) 0.0030(8)</td> | Uiso 0.0077(7) 0.0075 0.0034 0.055 0.035 0.030(8) 0.0030(8) 0.0030(8) 0.0030(8) |
| K2.7La2.1-L (after calcination) Si1 Al1 Si2 Al2 O1 O2 O3 O4 O5 O6 K1 (site I) K3 (site II) La1 (site I) La2 (site II) La2 (site II) Si1 Al1 Si2 Al2 | x 0.09174(26) 0.16494(27) 0.16494(27) 0.0 0.1652(4) 0.26584(23) 0.1045(4) 0.42489(27) 0.1520(5) 0.3333 0.0 0.3333 0.0 x 0.0887(4) 0.0887(4) 0.1671(4) 0.1671(4) | y 0.35219(30) 0.35219(30) 0.49770(23) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) 0.4134(4) 0.8497(5) 0.4831(5) 0.6667 0.3186(9) 0.6667 0.55 y 0.3512(4) 0.4989(4) | z 0.5 0.21643(34) 0.21643(34) 0.5 0.5 0.2613(11) 0.3293(8) 0.2781(12) 0.0 0.5 0.0 0.5 0.5 0.5 z 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 1.0 1.0 0.365(5) 0.321(5) 0.635(5) 0.2686(22) Occup. 0.75 0.25 0.75 | Multipl. 12 12 24 24 6 6 12 24 12 12 2 6 2 3 Multipl. 12 12 24 24 24 24 24 | Uiso 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0055 0.034 0.055 Uiso Uiso 0.0030(8) 0.0030(8) 0.0030(8) |
| K2.7La2.1-L (after calcination) Si1 Al1 Si2 Al2 O1 O2 O3 O4 O5 O6 K1 (site I) K3 (site II) La1 (site I) La2 (site II) La1 (site I) L3.0-L Si1 Al1 Si2 Al2 O1 | x 0.09174(26) 0.16494(27) 0.16494(27) 0.1652(4) 0.26584(23) 0.1045(4) 0.42489(27) 0.1520(5) 0.3333 0.0 0.3333 0.0 x 0.0887(4) 0.0887(4) 0.1671(4) 0.1671(4) 0.0 | y 0.35219(30) 0.35219(30) 0.49770(23) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) 0.4134(4) 0.8497(5) 0.4831(5) 0.6667 0.3186(9) 0.6667 0.5 y 0.3512(4) 0.4989(4) 0.4989(4) 0.2631(12) | z 0.5 0.21643(34) 0.21643(34) 0.5 0.5 0.2613(11) 0.3293(8) 0.2781(12) 0.0 0.5 0.0 0.5 0.5 z 0.5 0.5 0.2156(5) 0.5 0.5 | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 1.0 1.0 0.365(5) 0.321(5) 0.635(5) 0.2686(22) Occup. 0.75 0.25 0.75 0.25 1.0 | Multipl. 12 12 24 6 6 12 24 6 12 24 12 24 12 24 12 24 12 12 3 Multipl. 12 12 24 24 24 24 6 6 | Uiso 0.0077(7) 0.0030(8) 0.003 |
| K2.7La2.1-L (after calcination) Si1 Al1 Si2 Al2 O1 O2 O3 O4 O5 O6 K1 (site I) K3 (site II) La1 (site I) La2 (site II) La2 (site II) Al1 Si1 Al1 Si2 Al2 O1 | x 0.09174(26) 0.16494(27) 0.16494(27) 0.16494(27) 0.0 0.1652(4) 0.26584(23) 0.1045(4) 0.42489(27) 0.1520(5) 0.3333 0.0 0.3333 0.0 x 0.0887(4) 0.0887(4) 0.1671(4) 0.1671(4) 0.0 0.1637(5) | y 0.35219(30) 0.35219(30) 0.49770(23) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) 0.4134(4) 0.8497(5) 0.4831(5) 0.6667 0.3186(9) 0.6667 0.5 y 0.3512(4) 0.4989(4) 0.4989(4) 0.2631(12) 0.3275(10) | z 0.5 0.21643(34) 0.21643(34) 0.5 0.5 0.2613(11) 0.3293(8) 0.2781(12) 0.0 0.5 0.0 0.5 0.5 0.5 0.5 0.2156(5) 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 1.0 1.0 0.365(5) 0.321(5) 0.635(5) 0.2686(22) Occup. 0.75 0.25 1.0 1.10 | Multipl. 12 12 24 24 6 6 12 24 12 24 12 22 6 2 3 Multipl. 12 12 2 4 2 4 6 6 2 3 4 2 4 6 6 6 2 3 3 4 5 6 6 6 6 7 7 7 7 7 7 7 7 7 7 7 7 7 | Uiso 0.0077(7) 0.0030(8) 0.003 |
| K2.7La2.1-L (after calcination) Si1 Al1 Si2 Al2 O1 O2 O3 O4 O5 O6 K1 (site I) La1 (site I) La2 (site II) La2 (site II) La3.0-L Si1 Al1 Si2 Al2 O1 O2 O3 | x 0.09174(26) 0.16494(27) 0.16494(27) 0.16494(27) 0.0 0.1652(4) 0.26584(23) 0.1045(4) 0.42489(27) 0.1520(5) 0.3333 0.0 0.3333 0.0 0.3333 0.0 0.3333 0.0 0.3333 0.0 0.3333 0.0 0.1671(4) 0.1671(4) 0.1671(4) 0.1637(5) 0.2634(4) | y 0.35219(30) 0.35219(30) 0.49770(23) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) 0.4134(4) 0.8497(5) 0.4831(5) 0.6667 0.3186(9) 0.6667 0.5 y 0.3512(4) 0.4989(4) 0.4989(4) 0.2631(12) 0.3275(10) 0.5267(8) | z 0.5 0.21643(34) 0.21643(34) 0.5 0.5 0.2613(11) 0.3293(8) 0.2781(12) 0.0 0.5 0.0 0.5 0.5 0.5 0.5 0.5 | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 1.0 0.365(5) 0.365(5) 0.2686(22) Occup. 0.75 0.25 1.0 1.0 1.0 1.0 1.0 0.365(5) 0.2686(22) 0.75 0.25 1.0 1.0 1.0 1.0 | Multipl. 12 12 24 24 6 6 12 24 12 24 12 24 12 2 6 2 3 Multipl. 12 24 6 2 3 Multipl. 12 24 6 6 12 2 4 6 6 12 2 4 12 2 2 6 2 2 3 12 2 4 12 2 4 12 2 4 12 2 4 12 2 4 12 2 4 12 2 4 12 2 4 12 2 4 12 2 4 12 2 12 2 4 12 2 12 1 | Uiso 0.0077(7) 0.0030(8) 0.003 |
| K2.7La2.1-L (after calcination) Si1 Al1 Si2 Al2 O1 O2 O3 O4 O5 O6 K1 (site I) La1 (site I) La2 (site II) La2 (site II) La3.0-L Si1 Al1 Si2 Al2 O1 O2 O3 O4 | x 0.09174(26) 0.16494(27) 0.16494(27) 0.16494(27) 0.0 0.1652(4) 0.26584(23) 0.1045(4) 0.42489(27) 0.1520(5) 0.3333 0.0 0.3333 0.0 0.3333 0.0 0.3333 0.0 0.3333 0.0 0.3333 0.0 0.1657(4) 0.1671(4) 0.1671(4) 0.1637(5) 0.2634(4) 0.1008(5) | y 0.35219(30) 0.35219(30) 0.49770(23) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) 0.4134(4) 0.8497(5) 0.4831(5) 0.6667 0.3186(9) 0.6667 0.5 y 0.3512(4) 0.4989(4) 0.2631(12) 0.3275(10) 0.5267(8) 0.4095(5) | z 0.5 0.21643(34) 0.21643(34) 0.5 0.5 0.2613(11) 0.3293(8) 0.2781(12) 0.0 0.5 0.0 0.5 0.5 z 0.5 0.5 0.5 0.2156(5) 0.5 0.5 0.5 0.5 0.5 0.5 0.2709(16 0.3330(10) | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 1.0 1.0 1.0 0.365(5) 0.321(5) 0.635(5) 0.2686(22) Occup. 0.75 0.25 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 | Multipl. 12 12 24 6 6 12 24 6 12 24 12 24 12 24 12 12 2 6 2 6 2 6 12 12 24 6 6 12 24 24 24 24 24 24 24 24 24 24 24 24 | Uiso 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0037(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) |
| K2.7La2.1-L (after calcination) Si1 Al1 Si2 Al2 O1 O2 O3 O4 O5 O6 K1 (site I) K3 (site II) La1 (site I) La2 (site II) La3.0-L Si1 Al1 Si2 Al2 O1 O2 O3 O4 O5 O6 K1 (site I) La2 (site II) La2 (site II) O1 O2 O3 O4 O5 O4 O5 | x 0.09174(26) 0.16494(27) 0.16494(27) 0.1652(4) 0.26584(23) 0.1045(4) 0.42489(27) 0.1520(5) 0.3333 0.0 0.3333 0.0 0.3333 0.0 x 0.0887(4) 0.1671(4) 0.1671(4) 0.1671(4) 0.1637(5) 0.2634(4) 0.1008(5) 0.4334(5) | y 0.35219(30) 0.35219(30) 0.49770(23) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) 0.4134(4) 0.8497(5) 0.4831(5) 0.6667 0.3186(9) 0.6667 0.3512(4) 0.3512(4) 0.4989(4) 0.4989(4) 0.2631(12) 0.3275(10) 0.5267(8) 0.4095(5) 0.8667(9) | z 0.5 0.21643(34) 0.21643(34) 0.21643(34) 0.5 0.5 0.2613(11) 0.3293(8) 0.2781(12) 0.0 0.5 0.0 0.5 0.5 0.5 0.5 0.5 | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 1.0 1.0 1.0 0.365(5) 0.321(5) 0.635(5) 0.2686(22) Occup. 0.75 0.25 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 | Multipl. 12 12 24 6 6 12 24 6 12 24 12 24 12 24 12 2 6 2 3 Multipl. 12 24 6 6 6 12 24 24 12 24 24 24 24 24 12 24 12 24 12 24 12 24 12 24 12 24 12 24 12 24 12 24 12 | Uiso 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0055 0.034 0.055 0.055 0.055 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) 0.0030(8) |
| K2.7La2.1-L (after calcination) Si1 Al1 Si2 Al2 O1 O2 O3 O4 O5 O6 K1 (site I) K3 (site II) La1 (site I) La2 (site II) La3.0-L Si1 Al1 Si2 Al2 O1 O2 O3 O4 O5 O6 K1 (site I) La2 (site II) La2 (site II) O1 O2 O3 O4 O5 O6 O3 O4 O5 O6 | x 0.09174(26) 0.16494(27) 0.16494(27) 0.16494(27) 0.0 0.1652(4) 0.26584(23) 0.1045(4) 0.42489(27) 0.1520(5) 0.3333 0.0 0.3333 0.0 0.3333 0.0 0.3333 0.0 0.3333 0.0 0.1671(4) 0.1671(4) 0.1671(4) 0.1671(4) 0.1671(4) 0.1671(4) 0.1637(5) 0.2634(4) 0.1008(5) 0.4334(5) 0.1500(8) 0.1500(8) | y 0.35219(30) 0.35219(30) 0.49770(23) 0.49770(23) 0.2742(7) 0.3303(7) 0.5316(5) 0.4134(4) 0.8497(5) 0.4831(5) 0.6667 0.3186(9) 0.6667 0.5 y 0.3512(4) 0.4989(4) 0.4989(4) 0.2631(12) 0.3275(10) 0.5267(8) 0.4095(5) 0.4853(8) | z 0.5 0.21643(34) 0.21643(34) 0.21643(34) 0.5 0.5 0.2613(11) 0.3293(8) 0.2781(12) 0.0 0.5 0.5 0.5 0.5 0.5 0.5 0.2156(5) 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 | Occup. 0.75 0.25 0.75 0.25 1.0 1.0 1.0 1.0 1.0 1.0 0.365(5) 0.321(5) 0.635(5) 0.258 0.75 0.25 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 | Multipl. 12 12 24 24 6 12 24 6 12 24 12 24 12 24 12 24 12 2 6 2 6 12 24 24 6 6 12 24 24 12 24 24 12 24 12 24 12 24 12 24 12 12 12 12 12 12 12 12 12 12 12 12 12 12 | Uiso 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0077(7) 0.0030(8) 0.003 |

| La2 (site II) | 0.0 | 0.5 | 0.5 | 0.3323(31) | 3 | 0.025 |
|----------------|-----|------------|-----|------------|---|-------|
| La3 (site III) | 0.0 | 0.3471(26) | 0.0 | 0.0432(20) | 6 | 0.025 |

Zeolite Y (FAU)

| Na _{56.0} -Y | X | У | z | Occup. | Multipl. | Uiso |
|-----------------------|-------------|-------------|-------------|------------|----------|------------|
| Si1 | 0.12496(12) | 0.94508(11) | 0.03571(12) | 0.71 | 192 | 0.0060(4) |
| Al1 | 0.12496(12) | 0.94508(11) | 0.03571(12) | 0.29 | 192 | 0.0060(4) |
| 01 | 0.17637(20) | 0.17637(20) | 0.96588(35) | 1.0 | 96 | 0.0060(4) |
| 02 | 0.17846(22) | 0.17846(22) | 0.31876(28) | 1.0 | 96 | 0.0060(4) |
| O3 | 0.25289(22) | 0.25289(22) | 0.14493(28) | 1.0 | 96 | 0.0060(4) |
| 04 | 0.10637(19) | 0.89363(19) | 0.0 | 1.0 | 96 | 0.0060(4) |
| Na2 | 0.05539(32) | 0.05539(32) | 0.05539(32) | 0.555(11) | 32 | 0.045 |
| Na3 | 0.23386(20) | 0.23386(20) | 0.23386(20) | 0.950(11) | 32 | 0.045 |
| Na4 | 0.0 | 0.0 | 0.0 | 0.472(13) | 16 | 0.045 |
| | | | | | | |
| La _{18.7} -Y | x | У | z | Occup. | Multipl. | Uiso |
| Si1 | 0.12647(19) | 0.94602(17) | 0.03748(21) | 0.71 | 192 | 0.0277(13) |
| Al1 | 0.12647(19) | 0.94602(17) | 0.03748(21) | 0.29 | 192 | 0.0277(13) |
| 01 | 0.17765(31) | 0.17765(31) | 0.9724(4) | 1.0 | 96 | 0.0277(13) |
| 02 | 0.17886(35) | 0.17886(35) | 0.3210(5) | 1.0 | 96 | 0.0277(13) |
| O3 | 0.24893(30) | 0.24893(30) | 0.1393(4) | 1.0 | 96 | 0.0277(13) |
| 04 | 0.11011(34) | 0.88990(34) | 0.0 | 1.0 | 96 | 0.0277(13) |
| La2 | 0.06831(10) | 0.06831(10) | 0.06831(10) | 0.6044(27) | 32 | 0.005 |

S5. XRD patterns of K,La-L samples heated at different temperatures.



S6. TGA graphs of K-, K,La- and La-L samples.



S7. Colour change from white (K-L) to light pink for La_{3.0}-L.





S8. Plots to derive Henry law constants at 298 K for (a) $K_{9.0}$ -L, (b) $K_{5.7}La_{1.1}$ -L, (c) $K_{2.7}La_{2.1}$ -L, (d) $La_{3.0}$ -L, (e) $Na_{56.0}$ -Y and (f) $La_{18.7}$ -Y.

S9. Fitted CO₂ adsorption isotherms for K-L (a,c and e) and La-L (b,d and f) at different temperatures: (a) and (b) 278 K, (c) and (d) 288 K, and (e) and (f) 298 K. The isotherms were fitted by virial equations using Desmos software. Clausius-Clapeyron equations for K-L (g) and La-L (h) at uptakes 0.75 (\blacksquare), 1.0 (\bullet), 1.25 (\blacktriangle) and 1.5 mmol g⁻¹ (\triangledown) used for the calculation of the isosteric heats of adsorption.



S10. XRD pattern of Ca_{4.0}K_{1.2}-L sample.



S11. Unit cell parameters vs. number of exchanging cations in (a) K,La-L and (b) K,Ca-L samples.



S12. CO₂ isotherms at 298 K on Ca,K-L samples.



S13. Rietveld plots of PXRD profiles ($\lambda = 1.54056$ Å, T = 298 K) of dehydrated (a) Na_{56.0}-Y and (b) La_{18.7}-Y (Observed – black, calculated – red, difference – blue, phase – pink and background – green).

