Supplementary data

Structural Characterization and Comparison of Monovalent Cation-Exchanged Zeolite-W

Figure S1. Polyhedral representations of (a) Li-MER, (b) Na-MER, (c) Ag-MER, (d) K-MER, and (e) Rb-MER along the (001) direction. Grey sticks represent disordered Al/Si framework. Each colored beach ball represents an extra-framework cation. Equatorial, hatched, and striped red balls represent oxygens of WO(1)–WO(3), WO(4) and WO(5), respectively.
Figure S2. Comparison of channel opening area of d8r (black symbol) and pau (red symbol) along the (001) direction and sum of two areas.

Figure S3. Thermogravimetric analysis results of Li-, Na-, Ag-, and K-MER.
### Table S1. Cation-exchange conditions of MERs and chemical composition from Rietveld refinement and stoichiometric analysis.

| Material | Reagent | Conc. Used (M) | No. of Treatments | Treatment Duration (days) | %H₂O<sup>a</sup> | Rietveld | EDX<sup>b</sup> |
|----------|---------|---------------|-------------------|---------------------------|-------------------|-----------|---------------|
| Li-MER   | LiCl, (99%) | sat.          | 3                 | 1                         | 19.7              | Li₆₋₈Al₆₋₈Si₂₅₋₈O₆₋₈·26H₂O | Li₆₋₈Al₆₋₈Si₂₅₋₈O₆₋₈·26H₂O |
| Na-MER   | NaCl, (99%) | sat.          | 3                 | 1                         | 13.3              | Na₇₋₈Al₇₋₈Si₂₅₋₈O₆₋₈·20H₂O| Na₇₋₈Al₇₋₈Si₂₅₋₈O₆₋₈·17.8H₂O |
| Ag-MER   | AgCl, (99%) | sat.          | 3                 | 1                         | 11.9              | Ag₇₋₈Al₇₋₈Si₂₅₋₈O₆₋₈·22H₂O| Ag₇₋₈Al₇₋₈Si₂₅₋₈O₆₋₈·22.5H₂O |
| K-MER<sup>c</sup> |         |               |                   |                           | 11.8              |                        |               |
| Rb-MER<sup>d</sup> |         |               |                   |                           | 9.82              |                        | Rb₅₋₆Al₅₋₆Si₂₅₋₆O₆₋₆·14H₂O |

<sup>a</sup> The water contents in wt%. Weight loss is measured by thermogravimetric analysis (TGA) up to ca. 800 °C; <sup>b</sup> Confirmed from chemical and energy-dispersive X-ray spectroscopy (EDS) and TG analysis; <sup>c</sup> Hydrothermal synthesis following method from Itabashi et al., 2008; <sup>d</sup> Results from Itabashi et al., 2008.

### Table 2. Chemical composition calculated from energy-dispersive spectroscopy (EDS) method.

#### Li-MER

| Measurement | 1   | 2   | 3   |
|-------------|-----|-----|-----|
| Atomic percent (%) |     |     |     |
| Al          | 6.1(1) | 6.2(1) | 6.3(1) |
| Si          | 22.7(1) | 23.0(1) | 23.5(1) |
| K           | 0     | 0     | 0     |
| O           | 71.1(1) | 70.8(1) | 70.2(1) |

#### Na-MER

| Measurement | 1   | 2   | 3   |
|-------------|-----|-----|-----|
| Atomic percent (%) |     |     |     |
| Al          | 5.7(1) | 5.9(1) | 5.4(1) |
| Si          | 20.4(1) | 21.4(1) | 19.3(1) |
| Na          | 6.2(1) | 6.1(1) | 6.0(1) |
| O           | 67.5(1) | 66.4(1) | 69.2(1) |

#### Ag-MER

| Measurement | 1   | 2   | 3   |
|-------------|-----|-----|-----|
| Atomic percent (%) |     |     |     |
| Al          | 5.3(1) | 5.6(1) | 5.4(1) |
| Si          | 18.6(1) | 20.1(1) | 19.4(1) |
| Ag          | 6.0(1) | 6.7(1) | 6.5(1) |
| O           | 70.1(1) | 67.6(1) | 68.6(1) |

#### K-MER

| Measurement | 1   | 2   | 3   | 4   | 5   |
|-------------|-----|-----|-----|-----|-----|
| Atomic percent (%) |     |     |     |     |     |
| Al          | 6.48(5) | 6.17(5) | 6.25(5) | 6.22(5) | 6.26(5) |
| Si          | 25.25(5) | 25.49(5) | 24.61(5) | 25.01(5) | 25.34(5) |
| K           | 5.37(5) | 5.39(5) | 7.03(5) | 6.31(5) | 5.56(5) |
| O           | 62.9(5) | 62.94(5) | 62.11(5) | 62.48(5) | 62.84(5) |
Table 3. Refined cell parameters and atomic coordinates of M-MER at ambient conditions (M = Li\textsuperscript{+}, Na\textsuperscript{+}, Ag\textsuperscript{+}, K\textsuperscript{+} and Rb\textsuperscript{+}).

| Chemical composition | Li-MER | Na-MER | Ag-MER | K-MER | Rb-MER<sup>a</sup> |
|----------------------|--------|--------|--------|--------|-------------------|
| Space group          | 14/mmm | 14/mmm | 14/mmm | 14/mmm | 14/mmm            |
| a<sub>sR<sup>s</sup>(%), X<sup>2</sup> | 1.91, 8.80 | 1.83, 0.36 | 2.50, 0.67 | 2.08, 3.01 |                  |
| Cell parameters      |       |        |        |        |                  |
| V (Å<sup>3</sup>)    | 1995.25(14) | 2005.81(25) | 2005.56(28) | 2005.46(15) | 1996.76(7)        |
| Li<sub>1.0</sub>Si<sub>0.5</sub>O<sub>4</sub>H<sub>2</sub>O | 0.11125(19) | 0.11030(7) | 0.116571(2) | 0.11051(10) | 0.11046(14) |
| Na<sub>1.0</sub>Si<sub>0.5</sub>O<sub>4</sub>H<sub>2</sub>O | 0.11621(18) | 0.15681(18) | 0.15767(13) | 0.15966(15) | 0.115637(14)   |
| Ag<sub>1.0</sub>Si<sub>0.5</sub>O<sub>4</sub>H<sub>2</sub>O | 0.16212(18) | 0.15681(18) | 0.15767(13) | 0.15966(15) | 0.115637(14)   |
| K<sub>2.0</sub>SiO<sub>4</sub>H<sub>2</sub>O | 0.12054(8) | 0.20902(6) | 0.25875(4) | 0.1200(5) | 0.1243(3)        |
| Rb<sub>2.0</sub>SiO<sub>4</sub>H<sub>2</sub>O | 0.16212(18) | 0.15681(18) | 0.15767(13) | 0.15966(15) | 0.115637(14)   |

<sup>a</sup>Values are given in parentheses.
| Occupancies | Materials |
|-------------|-----------|
| Esd’s        | Esd’s     |


\[ \text{Esd’s} = \frac{1}{n} \sum_{i=1}^{n} \sigma_i \]

Table 4. Selected interatomic distances (Å) and angles (°) for M-MER at ambient conditions (M = Li⁺, Na⁺, Ag⁺, K⁺, and Rb⁺).  

| Li-MER | Na-MER | Ag-MER | K-MER | Rb-MER* |
|--------|--------|--------|-------|---------|
| Si–O(1) | 1.6395(12) | 1.64813(29) | 1.6481(4) | 1.6502(7) | 1.330 |
| Si–O(2) | 1.6349(13) | 1.64815(28) | 1.6479(4) | 1.6480(7) | 1.946 |
| Si–O(3) | 1.6368(13) | 1.64813(28) | 1.6479(4) | 1.6479(8) | 1.823 |
| Si–O(4) | 1.6402(13) | 1.64806(27) | 1.6482(4) | 1.6458(7) | 1.916 |
| Mean⁴ | 1.6378(1) | 1.64811(1) | 1.6480(1) | 1.6479(1) | 1.753(1) |
| Si–O(1)–Si | 159.4(6) | 145.1(4) | 139.02(25) | 148.8(4) | 119.456 |
| Si–O(2)–Si | 149.0(6) | 142.35(23) | 177.68(21) | 144.25(31) | 124.978 |
| Si–O(3)–Si | 124.5(5) | 121.39(34) | 119.38(15) | 119.85(32) | 109.975 |
| Si–O(4)–Si | 152.1(6) | 177.36(27) | 145.83(18) | 172.1(5) | 153.949 |

Channel opening area of pau unit along (010) direction  

\[ \text{M(1)–O(1)} = 3(1) \quad 3.059(13) \quad 3.295(6) \quad 3.166(7) \quad 2.850 \]

\[ \text{M(1)–O(2)} = 3.062(6) \quad 3.205 \]

\[ \text{M(1)–WO(3)} = 2.7(18) \quad 2.733(11) \quad 2.815(6) \]

\[ \text{M(1)–WO(4)} = 2.364(17) \quad 2.59 \]

\[ \text{M(1)–WO(5)} = \]

\[ \text{M(2)–O(3)} = 3.114(8) \quad 2.967(8) \quad 3.1482(23) \quad 2.901(5) \quad 3.130 \]

\[ \text{M(2)–WO(1)} = 2.39(5) \quad 2.478(16) \quad 2.668(7) \quad 2.607(4) \quad 2.380 \]

\[ \text{M(2)–WO(2)} = 2.58(5) \quad 2.535(16) \quad 2.352(7) \quad 2.371(4) \quad 2.585 \]

\[ \text{WO(1)–WO(4)} = 2.729(30) \quad 2.837(16) \quad 2.741 \]

\[ \text{WO(1)–WO(5)} = 2.3995(18) \]

\[ \text{WO(3)–O(4)} = 3.0902(31) \quad 3.088 \]

\[ \text{WO(4)–O(1)} = 2.613(4) \]

\[ \text{WO(4)–O(3)} = 2.926(6) \]

\[ \text{WO(4)–WO(4)} = 2.633 \]

\[ \text{WO(4)–WO(5)} = 2.382(6) \quad 2.520(17) \quad 2.3976(18) \]

Bond Valence sum  

\[ \text{M(1)} = 0.102 \quad 0.426 \quad 0.251 \quad 1.48 \quad 0.642 \]

\[ \text{M(2)} = 0.179 \quad 0.515 \quad 0.511 \quad 1.429 \quad 1.736 \]

\[ a \text{ Esd’s are in parentheses, and WO denotes oxygen site of water molecules; } b \text{ Model from Itabashi et al., 2008; } c \text{ Interatomic distance was restrained by Al/Si ratio from EDS result; } d \text{ Standard deviations computed using } \sigma = 1/n[\sum_{i=1}^{n} \sigma_i^2]^{1/2}. \]