

Supporting Information for "Propane/Propylene Diffusion in Zeolites: Framework Dynamics"

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Calculated and Experimental Lattice Parameters.

Table 1: Si-SAS and Si-CHA calculated and experimental lattice parameters.

| Potential | a [Å] | c [Å] | Si - O [Å] | Si - Si [Å] | \angle Si - O - Si | \angle O - Si - O |
|------------------------|---------|---------|---------------|---------------|----------------------|---------------------|
| SAS | | | | | | |
| BKS | 14.43 | 10.28 | 1.594 - 1.616 | 3.149 - 3.161 | 156.154 - 161.993 | 106.080 - 114.073 |
| | | | 1.608 | 3.152 | 157.454 | 109.396 |
| PMM06 | 13.564 | 9.668 | 1.497 - 1.501 | 2.956 - 2.982 | 160.169 - 167.940 | 103.197 - 119.055 |
| | | | 1.499 | 2.962 | 162.716 | 109.381 |
| Exp¹ | 14.1039 | 10.1875 | 1.595 | | 150.1 | |
| CHA | | | | | | |
| BKS | 13.85 | 14.82 | 1.599 - 1.615 | 3.121 - 3.158 | 153.650 - 155.701 | 106.908 - 114.458 |
| | | | 1.609 | 3.140 | 154.852 | 109.391 |
| PMM06 | 12.98 | 14.09 | 1.498 - 1.499 | 2.939 - 2.958 | 157.3742 - 162.089 | 102.383 - 117.969 |
| | | | 1.499 | 2.953 | 160.440 | 109.361 |
| Exp² | 13.53 | 14.75 | 1.603 | | 148.4/148.0 | 109.47 |

Calculated and Experimental Volume and Window Size Data: Si-CHA

Table 2: Thermal changes in Si-CHA 8 MR window geometry. Oxygen to oxygen effective distances in the 8 MR extracted from NVE MD trajectories at the specified temperatures using either the BKS or PMM FF. The values given are the effective distances obtained by subtracting twice the oxygen VDW radius ($2 \times 1.35 = 2.7$ Å, as suggested by the International Zeolite Association³). The calculated volume ($\langle V \rangle^{NPT}$) refers to the NPT ensemble average volume and corresponding standard deviation. The $\Delta V^{|Exp-Calc|}$ corresponds to the absolute value of the percent difference between the NPT ensemble average volume and the experimental volume at the given temperature reported by Woodcock et al.⁴

| Si-CHA | | | | |
|--------|-----------------|-----------------|---|-----------------------------|
| BKS | d_1 [Å] | d_2 [Å] | $\langle V \rangle^{NPT}$ [Å ³] | $\Delta V^{ Exp-Calc }$ [%] |
| 300 K | 3.83 ± 0.14 | 4.20 ± 0.17 | 2442 ± 2.4 | 4.6 |
| 400 K | 3.84 ± 0.16 | 4.18 ± 0.19 | 2439 ± 2.8 | 4.6 |
| 600 K | 3.82 ± 0.20 | 4.17 ± 0.23 | 2434 ± 3.6 | 4.8 |
| 800 K | 3.82 ± 0.23 | 4.16 ± 0.27 | 2428 ± 4.9 | 5.2 |
| PMM | d_1 [Å] | d_2 [Å] | $\langle V \rangle^{NPT}$ [Å ³] | $\Delta V^{ Exp-Calc }$ [%] |
| 300 K | 3.96 ± 0.14 | 4.12 ± 0.16 | 2470 ± 2.0 | 5.8 |
| 400 K | 3.95 ± 0.16 | 4.11 ± 0.19 | 2469 ± 2.6 | 5.9 |
| 600 K | 3.92 ± 0.19 | 4.12 ± 0.23 | 2467 ± 3.3 | 6.2 |
| 800 K | 3.92 ± 0.22 | 4.10 ± 0.26 | 2465 ± 4.3 | 6.8 |
| EXP | d_1 [Å] | d_2 [Å] | V^{Exp} [Å ³] | REF |
| 293 K | – | – | 2334 | 4 |
| 298 K | 3.70 | 4.17 | 2348 | 5 |
| 300 K | – | – | 2392 | 2 |

Calculated and Experimental Volume and Window Size Data: Si-SAS

Table 3: Thermal changes in Si-SAS 8 MR window geometry. Oxygen to oxygen distances in the 8 MR were extracted from MD trajectories at the specified temperatures and using both of the FFs. The values given are the effective distances obtained by subtracting twice the oxygen VDW radius ($2 \times 1.35 = 2.7$ Å, as suggested by the International Zeolite Association³). The calculated volume ($\langle V \rangle^{NPT}$) refers to the NPT ensemble average volume and corresponding standard deviation. The $\Delta V^{|Exp-Calc|}$ corresponds to the absolute value of the percent difference between the NPT ensemble average volume and the experimental volume at the given temperature reported by Wragg et al.¹

| Si-SAS | | | | |
|--------|-----------------|-----------------|--|-----------------------------|
| BKS | d_1 [Å] | d_2 [Å] | $\langle V \rangle^{Calc}$ [Å ³] | $\Delta V^{ Exp-Calc }$ [%] |
| 300 K | 4.24 ± 0.16 | 4.26 ± 0.16 | 2119 ± 2.7 | 4.6 |
| 600 K | 4.22 ± 0.22 | 4.28 ± 0.22 | 2109 ± 4.3 | N/A |
| 800 K | 4.21 ± 0.25 | 4.24 ± 0.25 | 2102 ± 5.0 | N/A |
| PMM | d_1 [Å] | d_2 [Å] | $\langle V \rangle^{Calc}$ [Å ³] | $\Delta V^{ Exp-Calc }$ [%] |
| 300 K | 4.24 ± 0.16 | 4.28 ± 0.15 | 2140 ± 2.3 | 5.6 |
| 600 K | 4.25 ± 0.20 | 4.26 ± 0.21 | 2135 ± 4.0 | N/A |
| 800 K | 4.20 ± 0.23 | 4.29 ± 0.24 | 2132 ± 4.9 | N/A |
| EXP | d_1 [Å] | d_2 [Å] | V^{Exp} [Å ³] | REF |
| 298 K | 4.2 | 4.2 | 2027 | 1 |

References

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