

Correction to "Mechanism of Si Island Formation in SAPO-34"

Torstein Fjermestad, Stian Svelle, and Ole Swang*

J. Phys. Chem. C 2015, 119 (4), 2086-2095. DOI: 10.1021/jp510845z

Te have become aware of an error in the microkinetic calculations in our recent publication (J. Phys. Chem. C 2015, 119, 2086-2095), causing the water vapor pressures to be unrealistically high. Correcting the error gives the results in Table 1 below, which should be substituted for Table 1 in the

Table 1. Temperature and Pressure Dependence of the Forward Rate, r+, and the Amount of Si(OH)₄, $n_{Si(OH)}$, at Equilibrium of the Desilication^a

temp. (K)	press. (atm)	forward rate at equilib. (s^{-1})	amount of Si(OH) ₄
298	0.02	2.63×10^{-13}	3.70×10^{-17}
623	0.02	6.65×10^{-17}	8.77×10^{-20}
623	0.42	1.06×10^{-11}	1.40×10^{-14}
623	1	2.91×10^{-10}	3.83×10^{-13}
623	1.6	1.62×10^{-9}	2.14×10^{-12}
623	2	3.56×10^{-9}	4.69×10^{-12}
623	3	1.46×10^{-8}	1.92×10^{-11}
623	4	3.87×10^{-8}	5.11×10^{-11}
623	5	8.15×10^{-8}	1.07×10^{-10}
623	6	1.48×10^{-7}	1.96×10^{-10}
723	0.02	1.43×10^{-17}	1.97×10^{-20}
723	0.42	2.61×10^{-12}	3.60×10^{-15}
723	1	8.42×10^{-11}	1.16×10^{-13}
723	1.6	5.38×10^{-10}	7.43×10^{-13}
723	2	1.27×10^{-9}	1.76×10^{-12}
723	3	6.10×10^{-9}	8.42×10^{-12}
723	4	1.83×10^{-8}	2.53×10^{-11}
723	5	4.26×10^{-8}	5.88×10^{-11}
723	6	8.43×10^{-8}	1.16×10^{-10}
823	0.02	1.83×10^{-19}	1.03×10^{-21}
823	0.42	3.42×10^{-14}	1.92×10^{-16}
823	1	1.14×10^{-12}	6.38×10^{-15}
823	1.6	7.51×10^{-12}	4.21×10^{-14}
823	2	1.81×10^{-11}	1.01×10^{-13}
823	3	9.10×10^{-11}	5.10×10^{-13}
823	4	2.86×10^{-10}	1.60×10^{-12}
823	5	6.93×10^{-10}	3.89×10^{-12}
823	6	1.43×10^{-9}	8.00×10^{-12}

 a r+ is given in units of s⁻¹, and $n_{Si(OH)_{4}}$ is given as a fraction of the total amount of Si species. r+ and $n_{Si(OH)_4}$ are good descriptors of the Si(OH)₄ mobility in the SAPO material. The mobility of the Si(OH)₄ species further affects the Si/P exchange process which again influences the Si island formation.

original article. The corrected data lead to a different conclusion: r+ and $n_{Si(OH)_4}$ decrease with increasing temperature for all water vapor pressures investigated. The overall, qualitative mechanistic picture remains the same, however.

Below, we indicate the changes to the manuscript.

The fourth and fifth paragraphs in the subsection "Influence of the Reaction Temperature" should read:

"From the information in Table 1, we draw the following conclusions about the pressure and temperature dependence of the desilication: For a given temperature in the range 623-873 K, r+ and $n_{Si(OH)}$, both increase with increasing water vapor pressure. At a given water vapor pressure, on the other hand, both r+ and $n_{Si(OH)_4}$ decrease with increasing temperature."

The third paragraph in the subsection "Suggestions on How To Inhibit Si Island Formation" should read:

"A second possible way to inhibit the initiation of the Si island formation is to control the water vapor pressure and the temperature. From the microkinetic results, we see that r+ and $n_{\mathrm{Si(OH)_4}}$ decrease with increasing temperature. On the other hand, the same quantities increase with an increased water vapor pressure. A high water vapor pressure and a low temperature will therefore promote the Si island formation. To inhibit the Si island formation, the water vapor pressure should thus be kept as low as possible and the temperature as high as possible. This may be attempted by deliberate process design."

The last sentence in the conclusion should read:

"Microkinetic modeling of the desilication suggests that the Si island formation can be inhibited by lowering the water vapor pressure and increasing the temperature."

Published: August 20, 2015