

Monte Carlo Simulation of Water Adsorption in Hydrophobic MFI Zeolites with Hydrophilic Sites

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The numerical values of the parameters for the water–silicalite van der Waals interactions were erroneously reported in Table 4 of the original article. The correct values are given in Table 4 below. The results reported in the original article had been obtained using the correct parameter set and are still valid.

Table 4. Water–Silicalite van der Waals Interaction Parameters

A (kJ/mol·Å ¹²)	562 781
B (kJ/mol·Å ⁶)	2360
C (kJ/mol)	192.7
r_0 (Å)	0.9405
α (kJ/mol)	31 338
ρ_0 (Å)	0.3136
β (kJ/mol·Å ⁶)	2886
D (kJ/mol)	1.996×10^7
R_0 (Å)	0.2000

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