Electronic Supplementary Information

Solid state NMR characterization of zeolite Beta based drug formulations containing Ag and sulfadiazine

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Figure S1. Experimental (blue) and deconvoluted (red) ²⁷Al MAS NMR spectrum of HB. The individual contributions are shown in dashed lines.



Figure S2. ¹³C CP MAS spectra of samples SD/HB, SD/AgB and AgSD/HB. For comparison, the ¹³C CPMAS NMR spectra of the pure SD and AgSD compounds are displayed.



Scheme S1. Mechanism of reinsertion of EFAI into the zeolite framework in the presence of Ag^+ (A, B) and SD (C). In this case further AI(OH) groups can be generated upon hydration, which might explain the residual low intensity broad signal at around 0 ppm in the spectra in Figure 1 of the paper.



Figure S3. ¹H MAS (30 kHz) NMR spectra of HB, AgB, SD/HB, SD/AgB and AgSD/HB, measured after heating the samples at 100 °C for one night.



Figure S4. (a) Single pulse ²⁹Si spectra of samples HB and AgB; Experimental (blue) and deconvoluted (red) ²⁹Al MAS NMR spectra of AgB (b) and HB (c), used to quantify the ratio of [Si(1OH) + Si(1AI)] to Si(OAI) species.



Figure S5. ¹H-²⁹Si CP HETCOR NMR correlation spectrum of AgSD/HB.



Figure S6. T₂ relaxation data (squares) and the best fit (red line) with mono- (SD and AgSD) and two-exponential functions (SD/HB, SD/AgB and AgSD/HB).