Supplementary Materials: Different Erionite Species Bind Iron into the Structure: A Potential Explanation for Fibrous Erionite Toxicity

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Table S1. Experimental details and miscellaneous data of the Rietveld refinements. Statistical parameters as defined in Young [76].

Experimental details	
Instrument	Bruker AXS D8 Advance
Radiation	CuKα
Detector	PSD VÅNTEC-1
Sample mount	Rotating capillary (60 r/min)
Incident beam optics	60 mm focusing multilayer (Göbel) X-ray mirror
Angular range (°2θ)	5-145
(sin /)max (Å^{-1})	0.619
Step size (°2θ)	0.022
Counting time (s)	10

Miscellaneous data	**Samples**	
	Pristine	Fe (II) loaded
Calcite (wt %)	1.55(9)	-
Quartz (wt %)	0.63(2)	0.556(18)
RBragg (%)	0.23	0.14
RP (%)	1.49	0.97
RWP (%)	2.04	1.40

Table S2. Comparison of cell parameters and volume, ε_0 microstrain, and principal ellipsoid radii of pristine and Fe (II) loaded samples. For comparison purposes data of woolly erionite-Na from Durkee, Oregon [61] are reported.

Sample	*a* (Å)	*c* (Å)	*c*/*a*	Volume (Å^3)	ε_0	r_a (nm)	r_c (nm)	r_c/r_a
Pristine	13.2560(4)	15.0473(5)	1.1351	2289.90(15)	0.193(5)	18.6(2)	51.1(18)	2.75
500 μM $FeCl_2$	13.2627(4)	15.0409(5)	1.1341	2291.24(16)	0.168(5)	15.19(18)	51.3(2)	3.38
Woolly erionite-Na	13.2357(5)	15.0652(6)	1.1382	2285.6(2)	0.200(7)	15.5(2)	79(5)	5.10

Table S3. Si, Al partition at T1 and T2 sites and calculation of the R ratio following Jones [72].

Sample	<T1-O>	<T2-O>	T1	T2	T	R
Pristine	1.6279	1.6465	$Si_{20.28}Al_{3.72}$	$Si_{8.70}Al_{3.30}$	$Si_{28.98}Al_{7.02}$	0.805
500 μM $FeCl_2$	1.6255	1.6493	$Si_{20.64}Al_{3.36}$	$Si_{8.49}Al_{3.51}$	$Si_{29.13}Al_{6.87}$	0.809