Table 3. Iron K-edge EXAFS fit results*

	Nonsulfide component†					Sulfide component‡				
	Atom	*N*	*R* (Å)	σ^2 (Å^2)	ΔE_0 (eV)	Atom	*N*	*R* (Å)	σ^2 (Å^2)	ΔE_0 (eV)
Sed. A $\chi^2 = 0.44$	O	1.8§	2.01§	0.0050	-1.0§	S	1.0§	2.25	0.0012	-5.8§
	Fe	0.5§	3.08§	0.0050		S	1.0¶	3.44	0.0066	
	Si	0.6§	3.26	0.0065		Fe	2.0¶	3.82	0.0066	
Sed. B $\chi^2 = 0.35$	O	2.1§	2.00§	0.0060	-1.1§	S	0.7§	2.25	0.0012	-6.9§
	Fe	0.7§	3.08§	0.0050		S	0.7¶	3.44	0.0066	
	Si	0.6§	3.26	0.0065		Fe	1.3¶	3.82	0.0100	
Pyrite: Illite 50:50 $\chi^2 = 0.68$	O	3.5§	2.01§	0.0072	-0.3§	S	0.9§	2.25	0.0012	-3.8§
	Al	1.7§	3.02§	0.0088		S	0.9¶	3.44	0.0032	
	Fe	0.6§	3.02§	0.0059		Fe	1.8¶	3.82	0.0027	
	Si	2.3§	3.26	0.0045						

*EXAFS fit results for iron spectra shown in Fig. 1*c*; variables are as in Table 2.

†For sediment samples, the nonsulfide component represents a composite of Fe-bearing phyllosilicate and oxide minerals. Values for σ^2 were fixed for all shells based on empirical fits to reference compounds of similar composition and structure; *R* and *N* were varied, except for the Fe-Si shell, which will covary with Fe shells if floated independently. This shell was fixed on a typical crystallographic distance for Fe-Si in phyllosilicates (see ref. 1).

‡Sulfide component: Interatomic distances (*R*) were fixed on crystallographic values from pyrite and σ^2 was fixed on values determined from fits to several reference sulfide compounds; *N* for each shell was floated as a linked variable in proportions based on the known coordination in pyrite (see ref. 1).

§Parameter varied in least-squares fit.

¶Parameter linked to the above variable in a constant ratio.

1. O'Day, P. A., Rivera, N., Root, R. & Carroll, S. A. (2004) *Am. Mineral.* **89,** 572–585.