Table 2. Arsenic K-edge extended x-ray absorption fine-structure (EXAFS) fit results*

	Atom	$N^{\dagger}$	R(Å)	σ^2(Å^2)
Sediment B	S	2	2.24	0.0029
($\chi^2 = 1.37$)	As	1	2.58	0.0031
	As	2.5	3.49	0.0043
	As	0.75	3.63	0.0114
	S	2.5	3.65	0.0064

Reference compounds:					Crystallographic values		
	Atom	$N^{\dagger}$	R(Å)	σ^2 (Å^2)	Atom	N	R(Å)
Realgar[‡]	S	2	2.24	0.0034	S	2	2.225-2.251
(AsS)	As	1	2.58	0.0048	As	1	2.565-2.579
($\chi^2 = 0.54$)					S	1	3.415-3.513
	As	2.5	3.47	0.0057	As	2.5	3.439-3.499
					As	0.5	3.562
	As	0.75	3.63	0.0118	As	0.75	3.624-3.627
					S	0.75	3.570-3.617
	S	2.5	3.67	0.0078	S	2.5	3.657-3.689
Orpiment[§]	S	3	2.28	0.0040	S	3	2.243-2.307
(As_2S_3)	As	1	3.19	0.0097	As	1	3.191
($\chi^2 = 0.24$)	S	1	3.22	0.0150	S	1	3.219, 3.291
	S	1	3.47	0.0168	S	1	3.475, 3.514
	As	1	3.52	0.0068	As	1	3.521
	As	1	3.57	0.0111	As	1	3.568
Arsenolite[¶]	O	3	1.80	0.0040	O	3	1.787
(As_2O_3)	As	3	3.24	0.0035	As	3	3.223
($\chi^2 = 0.57$)	As	6	3.88	0.017	As	6	3.946

*EXAFS fit results for arsenic spectra shown in Fig. 1*b*; N is the number of backscattering atoms at distance (R); σ^2, the Debye–Waller term, is the absorber-backscatterer mean-square relative displacement. R and σ^2 were varied in fits; N was fixed on crystallographic values. χ^2 is a reduced least-squares goodness-of-fit parameter [= (F-factor)/(# of points – # of variables)]. Based on empirical fits to reference

compounds, error in R is ±0.02 Å; error in σ^2 is ±25% (1). Crystallographic values for reference compounds from independent x-ray diffraction analyses were taken from the literature.

[†]Fixed parameter.

[‡]Realgar structure from ref. 2; average of four unique arsenic sites. Disordered sulfur shells at 3.415-3.513 Å and 3.570-3.617 Å cancel and do not contribute to EXAFS amplitudes.

[§]Orpiment crystal structure from ref. 2; average of two unique arsenic site.

[¶]Arsenolite crystal structure from ref. 3; additional oxygen shells at 3.049 Å and 3.450 Å scatter too weakly to contribute to EXAFS amplitudes.

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