

Table 7: One-shell simulations of Sr EXAFS Fourier peak I from the S₁, S₂, S₃, and S₀ states and the inactive Sr-PS II control.

Fit	Sample	Shell	$R, \text{Å}$	N (with $S_0^2 = 1.0$)	$\sigma^2 (\times 10^3), \text{Å}^2$	ΔE_0	$\Phi (\times 10^3)$	$\mathcal{E}^2 (\times 10^5)$
1	S ₁	Sr-O	2.56	8.3	8.4	-4	0.28	0.11
2	S ₂	Sr-O	2.56	7.0	7.3	-4	0.35	0.14
3	S ₃	Sr-O	2.55	7.8	8.9	-6	0.28	0.11
4	S ₀	Sr-O	2.53	7.6	7.5	-5	0.29	0.12
5	HYD	Sr-O	2.58	7.5	8.1	-3	0.33	0.13