

**Table 6: Simulations of the entire Mn EXAFS from the S<sub>1</sub>, S<sub>2</sub>, S<sub>3</sub>, and S<sub>0</sub> states.**

Fit	Sample	Shell	$R, \text{\AA}$	$N$ (with $S_0^2 = 0.85$ )	$\sigma^2(\times 10^3), \text{\AA}^2$	$\Delta E_0$	$\Phi(\times 10^3)$	$\epsilon^2(\times 10^5)$
1	S <sub>1</sub>	Mn-O	1.84	1.6	0.8	-20	0.60	0.31
		Mn-Mn	2.70	0.9				
		Mn-Mn	3.19	0.3				
		Mn-Sr	3.52	0.5				
2	S <sub>2</sub>	Mn-O	1.84	2.1	1.5	-20	0.55	0.27
		Mn-Mn	2.72	1.0				
		Mn-Mn	3.15	0.2				
		Mn-Sr	3.48	0.6				
3	S <sub>3</sub>	Mn-O	1.87	2.2	2.0*	-13	1.07	0.54
		Mn-Mn	2.73	1.1	1.0*			
		Mn-Mn	2.87	0.5	1.0*			
4	S <sub>0</sub>	Mn-O	1.85	2.0	2.3	-20	0.63	0.32
		Mn-Mn	2.71	1.0				
		Mn-Mn	3.12	0.3				
		Mn-Sr	3.52	0.7				

\* parameter was fixed.