Table 2. Fitting results of the full k^3– weighted EXAFS spectra on Cu(I)DR1885

Cu(I)DR1885 $\Delta E = -10.3$ (eV)	**Ligand**	**r(Å)**	**$2\sigma^2 \cdot 10^3$(Å^2)**	**R-exafs**	**ε (fit index)**
Fit 1 (1 shell)	2S	2.299(3)	4(1)	0.446	0.49
Fit 2 (1 shell)	3S	2.301(2)	9(1)	0.403	0.41
Fit 3 (2 shells)	3S	2.300(2)	8(1)	0.334	0.29
	1N(no MS)	1.982(9)	4(1)		
Fit 4 (2 shells)*	3 S	2.303(2)	8(1)	0.305	0.27
	1N(His, MS)	1.999(4)	7(2)		

The values in parentheses are the estimated standard deviations from the diagonal elements of the covariance matrix (precisions). Accuracy of bond lengths can by estimated as ± 0.01 Å for the 1st shell atoms. MS, multiple scattering.

*Only the coordination distance of the N-imidazole from the histidine ligand is reported. The parameters of the remaining imidazole atoms which contribute to the multiple scattering calculations have been omitted for clarity since the aromatic ring has been treated as a rigid body during the fitting .