Table 2. Orbitals used in the parameterization of the unpaired electron spin density

Center	Type	Z_{eff}	ρ*, %
Cu	$3d_{x^2-y^2}$	6.0	46
Cys-89 S^{γ}	$3p_{xy}$	4.3	42
His-39 N^{δ}	$2p^{\dagger}$	3.2	5
His-92 N^{δ}	$2p^{\dagger}$	3.2	5
Met-97 S^{δ}	$3p_z$	4.3	1.4
Cys-89 H^{β_1}	1s	1.0	0.5
Cys-89 H^{β_2}	1s	1.0	0.4

The hydrogen-like Slater-type orbitals used in the structure calculation of the metal site of *A.v.* plastocyanin. The molecular coordinate system is defined by the copper ion at the origin, the Met-97 S^{δ} along the z-axis, and Cys-89 S^{γ} with an azimuth angle of $\pi/4$.

* Average values of atomic spin densities obtained from XAS, ENDOR, and NMR (see text).

† The orientation of the 2p orbitals at the His-39 N^{δ} and His-92 N^{δ} ligands were defined so that the symmetry axis of the 2p orbital points toward the copper ion.