

Hybrid density functional approach to the isotropic and anisotropic hyperfine couplings with ^{14}N and ^1H nuclei in the blue copper proteins.

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We report UB1LYP hybrid density functional studies on the hyperfine parameters of wild-type azurin from *Pseudomonas aeruginosa* and M121Q mutant of azurin from *Alcaligenes denitrificans*. The large models of the copper site used in the calculations give quantitative insight into the spin density distribution and confirm highly delocalized character of the unpaired electron. Theoretically predicted isotropic and anisotropic hyperfine couplings are compared to the available EPR data and the assignment of the hyperfine splittings is verified.

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