Computational models for dual Cu sites in Pseudoazurin from Achromobacter cycloclastes (AcPAz) [dataset]

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Description
Atomic positional coordinates (XYZ), computational log files (OUT), and binary (CHK) and formatted (FCHK) checkpoint files for electronic structure calculations are deposited. The levels of theory used in the simulations are denoted in the filenames. The full computational details can be obtained from the computational log files. The filenames are organised according to the peer reviewed publications.Fig.3 corresponds to the fully optimised inner sphere environment of the Type-1 Cu site i AcPAz for oxidised (panels A-C) and one-electron reduced (panels D-E) structures. Fig.5 contains the refined structures for the oxidised axial and rhombic Type-1 Cu environment as quantum chemical refinement of the inner sphere environments in the presence of a single Cu site. Fig.6 contains the refined structures for the reduced axial and rhombic Type-1 Cu environment as quantum chemical refinement of the inner sphere environments in the presence of a single Cu site. Additional electronic supporting information are also available upon request from the corresponding authors at szilagyi@montana.edu or takamitsu.kohzuma.qbs@vc.ibaraki.ac.jp.

Citations
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