The hydrogenases catalyse the reversible interconversion of protons to hydrogen. Recently, the X-ray crystal structures of all-iron hydrogenase from Clostridium pasteurianum and Desulfovibrio desulfuricans were reported. The active site, the H-centre, in each is comprised of a 6-Fe cluster, with 2 [4FeS] clusters forming an electron transfer pathway from the site to the surface of the protein. In the active site, a [4FeS] cluster is linked through a cysteinyl sulfur to a novel [2FeS] unit, the sub-site, which is ligated by CO and CN-. Model chemistry can provide an understanding of the spectroscopic properties of H-centre redox and mechanistic insights into how the enzyme works. There has been considerable debate as to whether the epr active redox state of the sub-site comprises a Fe(II)-Fe(II) or Fe(II)-Fe(I) pair. The Fe(II)-Fe(I) state is unprecedented in biology and recent structural and spectroscopic data for synthetic sub-site assemblies, including, the first class of artificial [2FeS] complexes and two biologically active organogermanium compounds, we have synthesized a number of compounds. The crystal structures of three of these have been determined and will be presented in the poster. Crystal data: (I): CuH2GeO2, FW = 509.15, monoclinic, P2_1/c, a = 9.1051(5), b = 16.3832(6), c = 18.1040(7) A, beta = 113.857(1)°, V = 2788.33(13) A^3, Z = 4, Dx = 1.213 Mg/m^3, T = 170 K, F(000) = 1064, R = 0.054, GoF = 1.03, for 6347 reflections collected on a KappaCCD diffractometer, and using full-matrix least-squares calculations on F^2 with the aid of SHELXL97, Crystal data (II): CuH2GeO2, FW = 471.04, monoclinic, P2_1/c, a = 9.7250(1), b = 17.9074(3), c = 13.54008(2) A, beta = 113.857(1)°, V = 2597.5(2) A^3, Z = 4, Dx = 1.320 Mg/m^3, T = 170 K, F(000) = 1064, R = 0.043, GoF = 1.01, for 5870 reflections collected on a KappaCCD diffractometer, and using full-matrix least-squares calculations on F^2 with the aid of SHELXL97. Crystal data (III): CuH2GeO2, FW = 471.04, monoclinic, P2_1/c, a = 9.7250(1), b = 17.9074(3), c = 13.54008(2) A, beta = 113.857(1)°, V = 2597.5(2) A^3, Z = 4, Dx = 1.320 Mg/m^3, T = 170 K, F(000) = 1064, R = 0.043, GoF = 1.01, for 5870 reflections collected on a KappaCCD diffractometer, and using full-matrix least-squares calculations on F^2 with the aid of SHELXL97. Crystal data (IV): CuH2GeO2, FW = 471.04, monoclinic, P2_1/c, a = 9.7250(1), b = 17.9074(3), c = 13.54008(2) A, beta = 113.857(1)°, V = 2597.5(2) A^3, Z = 4, Dx = 1.320 Mg/m^3, T = 170 K, F(000) = 1064, R = 0.043, GoF = 1.01, for 5870 reflections collected on a KappaCCD diffractometer, and using full-matrix least-squares calculations on F^2 with the aid of SHELXL97. Crystal data (V): CuH2GeO2, FW = 471.04, monoclinic, P2_1/c, a = 9.7250(1), b = 17.9074(3), c = 13.54008(2) A, beta = 113.857(1)°, V = 2597.5(2) A^3, Z = 4, Dx = 1.320 Mg/m^3, T = 170 K, F(000) = 1064, R = 0.043, GoF = 1.01, for 5870 reflections collected on a KappaCCD diffractometer, and using full-matrix least-squares calculations on F^2 with the aid of SHELXL97. Crystal data (VI): CuH2GeO2, FW = 471.04, monoclinic, P2_1/c, a = 9.7250(1), b = 17.9074(3), c = 13.54008(2) A, beta = 113.857(1)°, V = 2597.5(2) A^3, Z = 4, Dx = 1.320 Mg/m^3, T = 170 K, F(000) = 1064, R = 0.043, GoF = 1.01, for 5870 reflections collected on a KappaCCD diffractometer, and using full-matrix least-squares calculations on F^2 with the aid of SHELXL97. Crystal data (VII): CuH2GeO2, FW = 471.04, monoclinic, P2_1/c, a = 9.7250(1), b = 17.9074(3), c = 13.54008(2) A, beta = 113.857(1)°, V = 2597.5(2) A^3, Z = 4, Dx = 1.320 Mg/m^3, T = 170 K, F(000) = 1064, R = 0.043, GoF = 1.01, for 5870 reflections collected on a KappaCCD diffractometer, and using full-matrix least-squares calculations on F^2 with the aid of SHELXL97. Crystal data (VIII): CuH2GeO2, FW = 471.04, monoclinic, P2_1/c, a = 9.7250(1), b = 17.9074(3), c = 13.54008(2) A, beta = 113.857(1)°, V = 2597.5(2) A^3, Z = 4, Dx = 1.320 Mg/m^3, T = 170 K, F(000) = 1064, R = 0.043, GoF = 1.01, for 5870 reflections collected on a KappaCCD diffractometer, and using full-matrix least-squares calculations on F^2 with the aid of SHELXL97.

References

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