Supplementary Material (ESI) for PCCP

Ab Initio Study of the Antiferromagnetic Coupling in the Wheel-Shaped $[Cu_{20}Cl(OH)_{24}(H_2O)_{12}(P_8W_{48}O_{184})]^{25-}$ Anion

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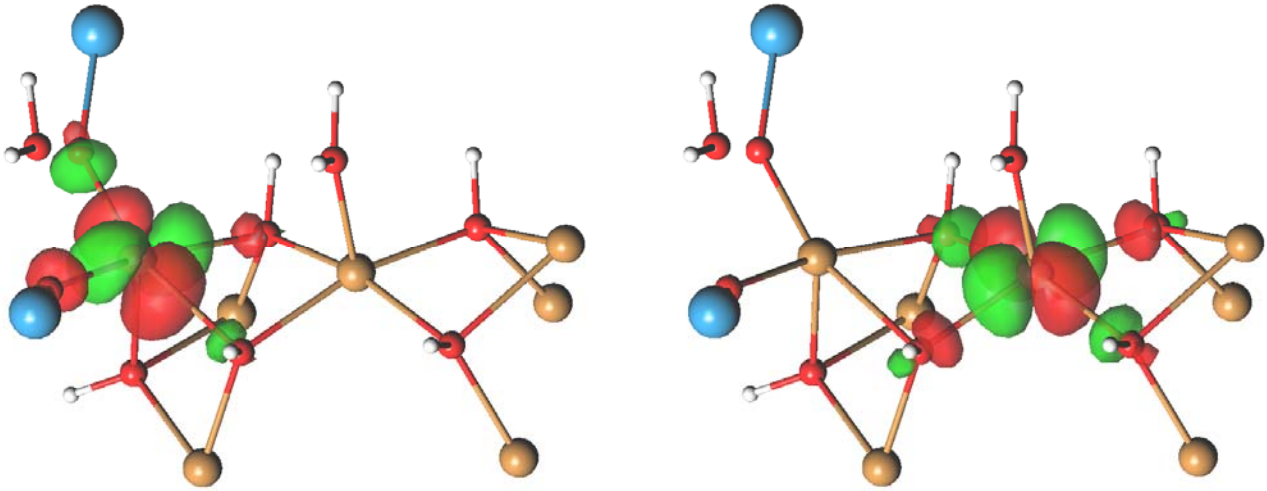
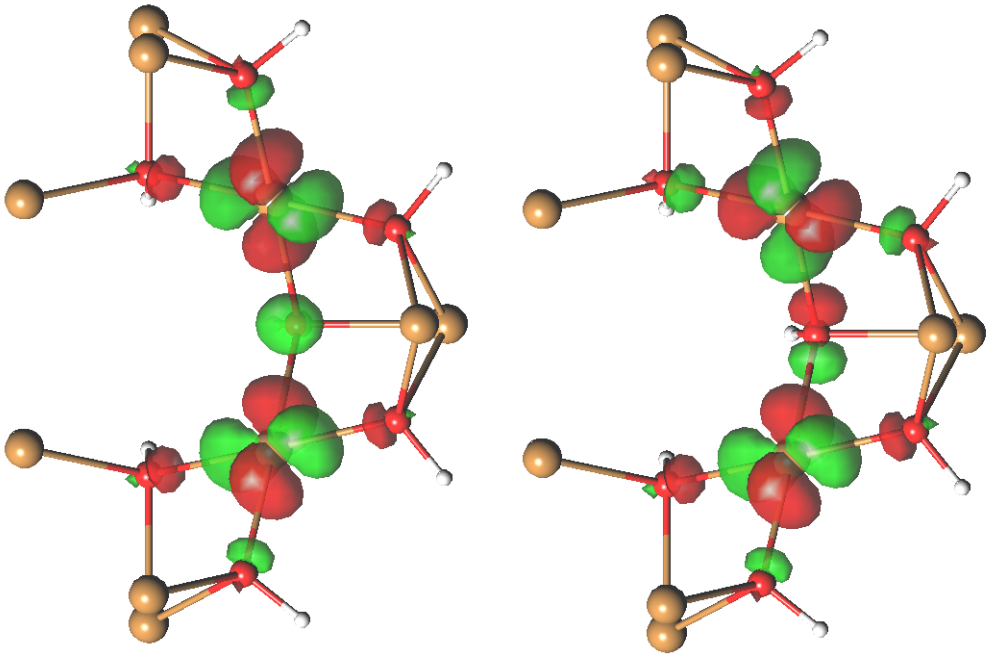
Electronic Supplementary Information

(a)



(b)



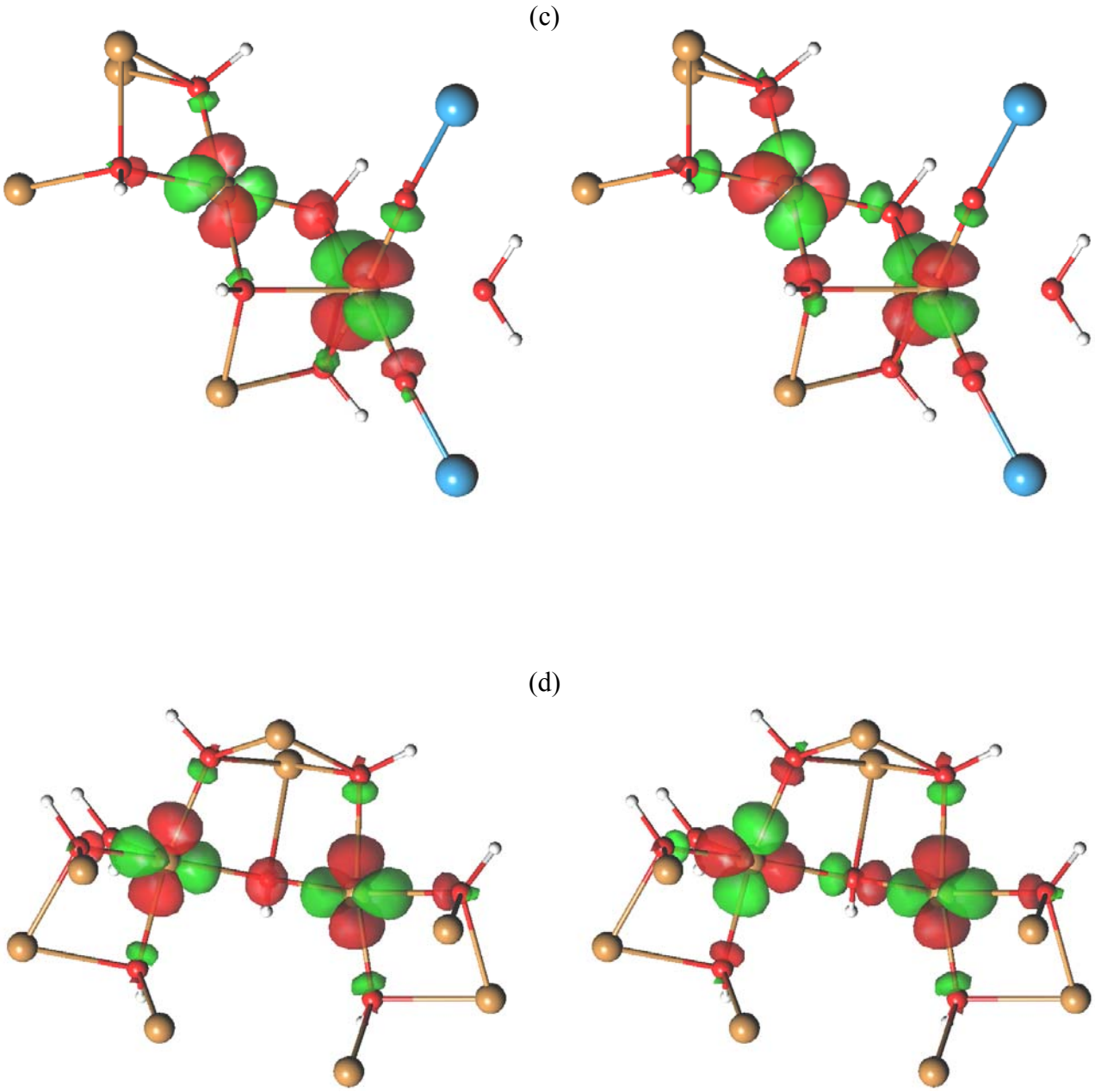


Fig. S1 Magnetic orbitals in the four Cu_{20} fragments: (a) yellow, (b) green, (c) red and (d) purple interactions. Small red spheres are oxygen, white spheres represent hydrogen, cyan spheres are tungsten total ion potentials and gold spheres are used to represent copper total ion potentials.

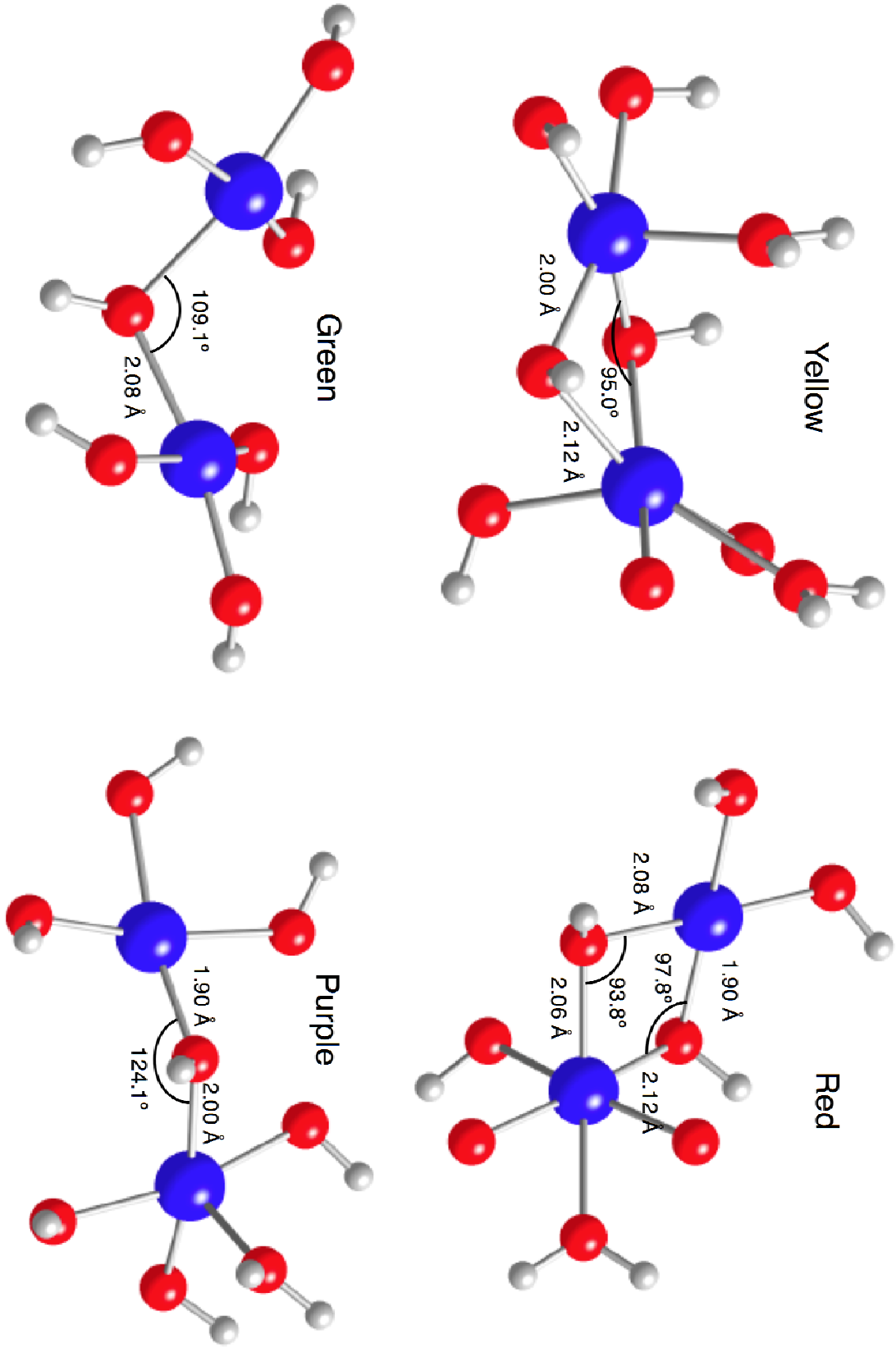


Fig S2: Geometrical details of the four clusters used to calculate the magnetic coupling parameters of the different interaction paths in the Cu_{20} unit. Red is oxygen, blue is copper, grey is hydrogen, only atoms from the first cluster region are shown.

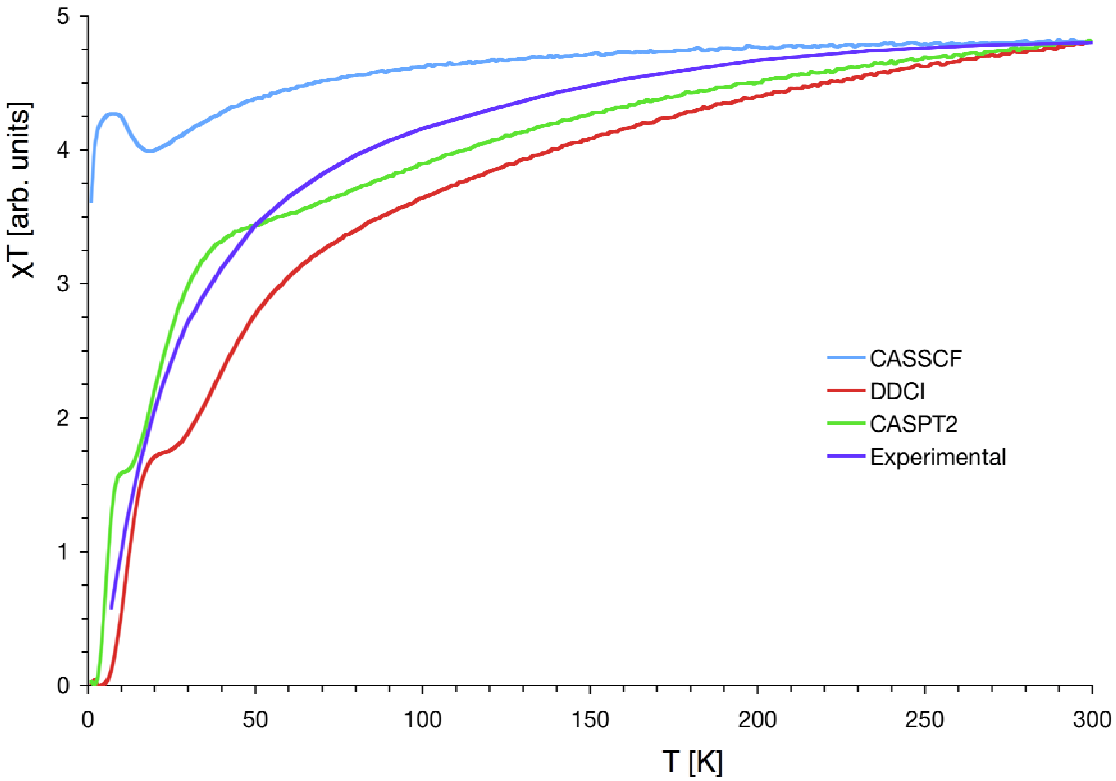


Fig. S3 χT curve of the Cu_{20} unit obtained from Monte Carlo simulations of the Ising model. The results of three different sets of magnetic interaction parameters (CASSCF, CASPT2 and DDCI) are compared to experimental data (taken from ref. 16)

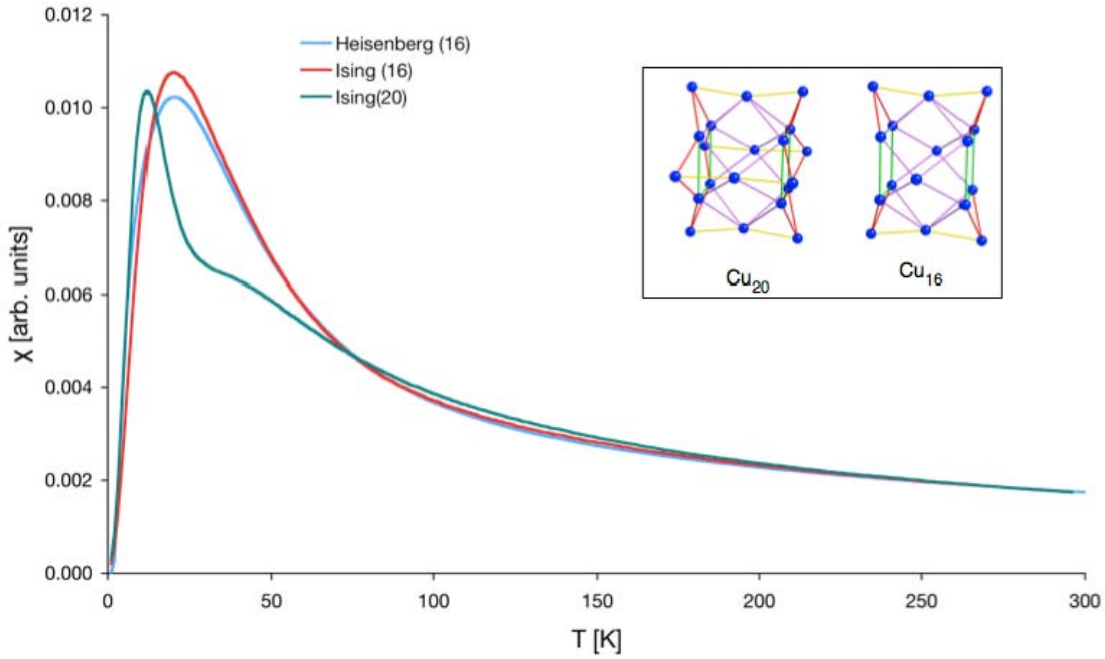


Fig. S4 Magnetic susceptibility curve obtained by diagonalization the exact Heisenberg Hamiltonian of a model containing 16 Cu^{2+} centres (light blue); by Monte Carlo simulation of the same 16-centres model applying the Ising Hamiltonian (red); and by Monte Carlo simulation of the complete Cu_{20} unit (green). The 16-centres model is constructed by removing 4 Cu^{2+} centres on the edge of the complete Cu_{20} cluster (see inset).