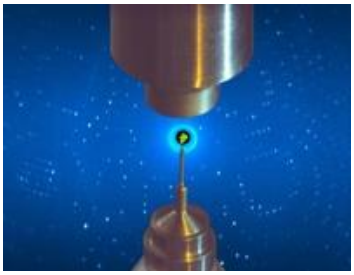

Contribution ID: **79** Type: **invited talk**

Neutrons reveal (some of) the secrets of heme peroxidases

Tuesday, 8 June 2021 16:40 (30 minutes)

We have used the ability of neutron crystallography to locate hydrogen atoms in our studies to investigate the mechanisms of the heme peroxidases cytochrome c peroxidase and ascorbate peroxidase. In order to do this we have cryo-trapped the labile intermediates known as Compound I and Compound II in crystals. A key question about these intermediates has been the protonation states of the ferryl oxygen atom. This should be indirectly resolvable from the Fe-O bond length, and this could be determined by X-ray crystallography. However, photoreduction makes this challenging, as these highly oxidised Fe(IV) intermediates are particularly sensitive to the direct and indirect reducing consequences of X-rays. In solving the structures by neutron crystallography we revealed that assumptions about the charge state of the active site histidine need to be revised. These results will be presented in the context of complimentary enabling spectroscopic and XFEL investigations. The protonation states of the residues in the pathway of proton-coupled electron transport in ascorbate peroxidase was also examined, showing that the arginine side chain can exist in the neutral form within the enzyme.

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Session Classification: Protein structure, function and dynamics

Track Classification: Protein structure, function and dynamics