

Structure and Dynamics of Co-ordination Compounds by Neutron Scattering

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The importance of transition metal hydrido-complexes, both classical and non-classical (i.e. compounds containing the M-H or M-H₂ moieties) in catalytic reactions, in particular hydrogenations, is well known, and much work has been carried out in recent years to obtain a detailed understanding of the nature and reactivity of the M-H and M-H₂ moieties.

Single crystal neutron diffraction, at low temperature, has been instrumental in establishing the correct co-ordination geometry in non-classical hydrides. It has been established that the H-H separation can cover a wide range of distances, from ~ 0.8 Å (strong H-H bond) to ~ 1.4 Å (weak H-H bond), corresponding to various degree of the H-H activation, thus neatly spanning the oxidative addition pathway and giving support to the mechanistic studies.

However, it is worth noting that a complete description of the reactivity in hydrido-compounds can only be achieved by combining the diffraction results with the knowledge of their dynamics that can be obtained from neutron incoherent inelastic scattering (INS) experiments.

I will discuss some recent structural results on transition metal poly-hydrides and show how, by combining neutron diffraction, INS and DFT calculations, the H₂ dynamics can be explained.

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