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Synchrotron-based Mössbauer spectroscopy of photo- and catalytically- active Iridium complexes

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Iridium complexes have highly interesting photochemical, photophysical and catalytic properties. They are used for example in organic light-emitting diodes (OLEDs), organic solar cells and automotive exhaust catalysts.[1,2,3] Iridium complexes have also been used to initiate "water oxidation reactions".[4,5] They also hold promise as photosensitisers and photocatalysts for directed photodynamic cancer therapy (PDT).[3,6] Recently nuclear forward scattering (NFS) on 193Ir at 73 keV has been established at beamline P01, PETRA III, DESY, Hamburg.[7] This technique can be regarded as Mössbauer spectroscopy in the time domain. We have applied 193Ir-NFS to yield information about the electronic properties of selected catalytically active Iridium complexes via the determination of Mössbauer parameters like the quadrupole splitting (ΔEQ) (Figure 1). We have also performed Density Functional Theory (DFT) calculations to calculate the Mössbauer parameters of the complexes under investigation.

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