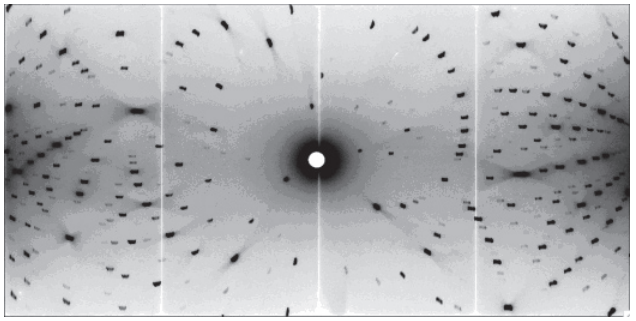
geometrical aspects of the manifestation of thermal diffuse scattering, and yield values of the sound velocities in good accord with values obtained by ultrasound attenuation measurements.



A typical long-exposure neutron Laue pattern for Al_2O_3

[1] G.J. McIntyre, M.-H. Lemée-Cailleau, C. Wilkinson *Physica B* **2006**, *385-386*, 1055-1058. [2] P.D.W. Boyd, A.J. Edwards, M.G. Gardiner, C.C. Ho, M.-H. Lemée-Cailleau, D.S. McGuinness, A. Riapanitra, J.W. Steed, D.N. Stringer, B.F. Yates *Angew. Chem.* **2010**, *49*, 6315-6318. [3] C.J. Carlile, B.T.M. Willis *Acta Cryst. A* **1989,** *45*, 708-715.

Keywords: neutron_Laue_diffraction, image-plate_detectors thermal_diffuse_scattering

MS.56.1

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Structural identification and antiproliferative activity of metallodrugs

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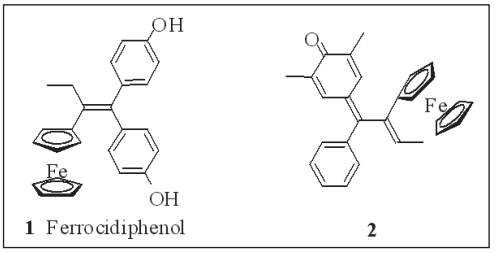
The first line drug used to combat hormone-dependent breast cancers is tamoxifen, the archetypal selective estrogen receptor modulator (SERM). Since tamoxifen is active only against tumours that are estrogen receptor positive (ER+), and frequently gives rise to resistance after prolonged use, the search for related but different agents has intensified considerably over the last few years.

We have designed novel therapeutic agents which are based on organometallic compounds that express high antiproliferative activity against breast cancer cells [1], [2]. We found that ferrocidiphenol **1** is characterized in vitro by a strong antiproliferative effect on both hormone-dependent (MCF-7) and hormone-independent (MDA-MB-231) breast cancer cells (IC_{50} values around 0.5 μM), whereas OH-Tam has an effect only on hormone-dependent cells.

Many complexes have been synthesized, allowing the study of the structure-activity relationship. Electrochemical experiments have suggested that the active metabolite of these compounds is a quinone methide. This hypothesis is now supported by isolation and X-ray structural determination of the quinone methide **2** [3].

The structural requirements for activity seem to be 1) the presence of a ferrocene group, 2) a conjugated linker, 3) aromatic para-substitution by a protic function and 4) an ethyl group residing on the same carbon as the ferrocene group. X-ray absorption spectroscopy has been used to obtain addition information on these compounds.



1 Ferrocidiphenol **2**

XANES spectra of ferrocidiphenol and its diphenyl analogue (2-ferrocenyl-1,1-diphenyl-but-1-ene) have been compared to XANES of ferrocene. Spectra indicate that the iron electronic properties are affected by the group that replaces a hydrogen of the unsubstituted Cp ring [4].

[1] S. Top, A. Vessières, G. Leclercq, J. Quivy, J. Tang, J. Vaissermann, M. Huché, G. Jaouen, *Chem. Eur. J.* **2003**, 9, 5223-5236. [2] A. Vessières, S. Top, P. Pigeon, E. Hillard, L. Boubeker, D. Spera, G. Jaouen *J. Med. Chem.* **2005**, *48*, 3937-3940. [3] D. Hamels, P. Dansette, E. A. Hillard, S. Top, A. Vessières, P. Herson, G. Jaouen, D. Mansuy *Angew. Chem. Ed. Int.* **2009**, *48*, 9124-9126 [4] I. Ascone, D. Hamels, P. Pigeon, M. Salome, Y Joly, T. Prange, A. Vessières, S. Top, G. Jaouen. Manuscript in preparation.

Keywords: organometallic, anticancer, XANES

MS.56.2

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XANES spectroscopy for determination of the 3D nanoscale atomic structure

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The status of modern theoretical analysis of the experimental x-ray absorption spectra to extract structural parameters will be presented. Novel method for extracting of 3D structural information on the basis of advanced quantitative analysis of X-ray absorption near edge structure (XANES) realized in "FitIt" software [1] is described. The approach is based on the fitting of experimental XANES data using multidimensional interpolation of spectra as a function of structural parameters and adva nced "ab-initio" XANES simulations. Small number of required ab-initio calculations is the main advantage of the approach, which allows one to use computationally time-expensive non-muffin-tin methods. The possibility to extract information on bond angles and bond-lengths is demonstrated and it opens new perspectives of quantitative XANES analysis as a 3D local structure probe. As XANES spectrum can be measured simultaneously, one can use XANES to study the local structure in time-dependent experiments within a time domain of 100 picoseconds and less.

Advanced theoretical analysis based either on self-consistent muffin-tin model or full potential (non-muffin-tin) theory, coupled with DFT geometry optimization have been applied to extract structural information from experimental XANES data. The status of modern research shows that XANES spectroscopy and its "ab initio" theoretical analysis can be a useful tool for the investigation of both local structure and electronic subsystem of many advanced materials without long range order. The present approach can provide a subatomic level (i.e., 0.01- 0.03 angstrom) of accuracy in the determination of the interatomic distances and several of degrees in the determination of the bonding angles at specific atomic site of nanostructured materials without long range order.