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Application of PAC spectroscopy to metalloproteins

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Time differential Perturbed Angular Correlation (PAC) of γ-rays spectroscopy may be applied to study the coordination geometry and dynamics at metal ion binding sites of proteins [1-2]. Selected examples relating to recent ^{199m}Hg and ^{111}Ag PAC experiments will be presented, such as 1) Ag(I) binding to human serum albumin - the major transport protein in blood; 2) A potential ^{111}Ag reference sample (Ag-benzoate(s)); 3) Modelling the effect of recoil energy on local structure upon the β-decay of ^{111}Ag [4]; 4) Hg(II) binding to an arsenic(III) biosensor - As(III) is one of the most important ubiquitous toxic elements in the environment.

References

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[2] S. Chakraborty, S. Pallada, J.T. Pedersen, A. Jancso, J.G. Correia, and L. Hemmingsen Nanosecond dynamics at protein metal sites: An application of perturbed angular correlation (PAC) of γ-rays spectroscopy Acc. Chem. Res., 2017, 50, 2225-2232
[4] R. Fromsejer, K.V. Mikkelsen, *L. Hemmingsen*
Dynamics of nuclear recoil: QM-BOMD simulations of model systems following β-decay
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