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Hg-coordination studies of several different types of small organic compounds by ^{199m}Hg -TDPAC

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Time differential perturbed angular correlation (TD-PAC) of γ -rays spectroscopy belongs to the family of spectroscopic techniques which allow for measurements of hyperfine interactions, and is a useful tool in the study of biomolecules [1,2], for example for the elucidation of how the function of a metalloprotein is related to the structure and dynamics of the metal ion binding site. In order to obtain empirical data correlating structure nuclear quadrupole parameters for Hg(II) containing compounds with biologically relevant ligands, we conducted ^{199m}Hg PAC experiments on a series of model compounds in 2007 and 2008 at ISOLDE-CERN. The aims of these experiments were to 1) use the empirical data in the interpretation of ^{199m}Hg PAC experiments on proteins, and 2) provide reference data for density functional and *ab initio* calculations of electric field gradients in Hg(II) complexes [3].

[1]L. Hemmingsen et al., *Hyperfine Interact.*, 197, 255-267, (2010)

[2]L. Hemmingsen et al., *Chem. Rev.*, 104, 4027-4061, (2004)

[3]V. Arcisauskaitė et al., *Phys. Chem. Chem. Phys.*, 14, 16070-9, (2012)

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