FLORENCE MEETS fiRelax – IMPLEMENTATION OF PARAMAGNETIC RELAXATION MODELS INTO A NOVEL WEB-BASED FITTING PLATFORM

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Fitting Nuclear Magnetic Relaxation Dispersion (NMRD) profiles with suitable relaxation functions provides insights into the molecular dynamics and interactions of a system, by revealing structural, dynamic and electronic parameters. In paramagnetic molecules and nanoparticles, the total water proton relaxation rate often comprises multiple contributions, arising from the inner-, second- or outer-sphere protons, as well as effects from fast internal mobility. Furthermore, in the presence of static Zero-Field-Splitting (ZFS), the Florence [1] and modified Florence models [2] offer a more accurate description of the field dependence of the relaxation rates. However, software solutions integrating a robust fitting algorithm and an easily accessible library of paramagnetic relaxation models are still lacking.

We present a novel fitting platform with a Graphical User-Interface (GUI) called fiRelax, which is available online as a web application at https://firelax.cerm.unifi.it. The software is composed of a front end web application, which allows the user to analyze experimental profiles and simulate theoretical relaxation curves. It has a dynamic interface, enabling interaction and results updates without requiring page reloads by the user. The application's core is running in Java, providing stability and longevity. Users can use fiRelax without in-depth knowledge of programming tools or the theory of paramagnetic systems. On the back end side, calculations and minimization procedures are done using One-Fit-Engine [3] (OFE). OFE has been developed as an open-source algorithm running in Raku and C, and is the fitting core also used by other fitting programs. For paramagnetic systems, the Florence model has been implemented by adapting the modified Fortran code into OFE's C environment. This integration allows a faster fitting process compared to the original Fortran minimalization algorithm.

The platform has been tested with various datasets, including contributions from multiple relaxation processes for inner-, outer-sphere and fast internal mobility. Multiple datasets can be fit simultaneously by (1) performing fits with shared parameters or (2) using Arrhenius equations to calculate temperature dependences.

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References
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[2] J. Chem. Phys., 1999, 111, 5795.
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