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**(DIS)AGREEMENT BETWEEN NMR RELAXOMETRY
AND DIELECTRIC SPECTROSCOPY RESULTS
FOR BIOMOLECULES**

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NMR relaxometry and dielectric spectroscopy are powerful methods used to study molecular dynamics in a broad range of time scales. The two methods have different physical backgrounds. Dielectric spectroscopy probes reorientation of electric dipole moments of molecules in response to the applied electric field, while NMR relaxometry is sensitive to fluctuations of magnetic dipole-dipole interactions on the atomistic level. In consequence, in other words, one can say that dielectric spectroscopy is a “macroscopic” method in this sense that only detects rotation of an effective electric dipole moment created by the whole molecule (or its large part), while using NMR relaxometry one can get access to local dynamics of single structural elements (like for example back bone fluctuations).

A thorough comparison of results obtained for proteins in solid state by means of both methods has lead to interesting observations that will be presented and discussed.

Taking into account the different physical background of the two methods, one should be able to provide a consistent interpretation of their results in terms of parameters which have a well-defined physical meaning. The strategy of data analysis applied by us is as follows. As far as NMR relaxometry is concerned, the ¹H spin-lattice relaxation dispersion profiles have been decomposed into ¹H-¹H and ¹H-¹⁴N relaxation contributions. The first contribution has been, then, further decomposed into relaxation terms associated with three motional processes referred as slow, intermediate and fast ones. It has been assumed that the corresponding spectral density functions are of a Lorentzian form. The extracted ¹H-¹H relaxation contributions have been transformed to a susceptibility representation to be compared with the shape of dielectric relaxation peaks in terms of their positions (taking into account the relationship between rank-one and rank-two rotational correlation times) and shapes.

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