Contribution ID: **57** Type: **Poster**

Dynamics of pharmacologically active compounds - felodipine and lacidipine: QENS and NMR study combined with molecular dynamics and density functional theory simulations

Friday, 2 September 2016 17:50 (1h 25m)

Molecular dynamics of felodipine and lacidipine (derivatives of 1,4-dihydropyridines, calcium channel blockers) were explored by solid-state nuclear magnetic resonance (NMR) and quasi-elastic (QENS) neutron scattering experiments. The experimental results were further combined with DFT and molecular dynamics (MD) simulations, providing a quantitative description of the intramolecular motions.
Both NMR spin-lattice relaxation and QENS measurements - performed on spectrometers with different resolution (backscattering - IN16, time-of-flight - IN5 and IN6) revealed the existence of dynamically inequivalent methyl groups. The activation parameters for their reorientation were determined. The temperature dependence of the correlation times ⊠c established both from NMR and QENS experiments are in very good agreement. Our analysis, supported by the MD and DFT calculations, relates the different dynamics observed for each methyl group with the calculated potential barriers in the crystal structure [1].

1. A. Pajzderska, K. Drużbicki, A. Kiwilsza, M. A. Gonzalez, J. Jenczyk, J. Mielcarek, J. Wąsicki On the Molecular Dynamics in Long-Acting Calcium Channel Blocker Lacidipine: Solid-State NMR, Neutron Scattering and Periodic DFT Study, 2016 RSC Advances, in press

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Session Classification: Poster Session