Magnetic Spin Relaxation in dimethylpyridines investigated by Nuclear Magnetic Resonance

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Magnetic Spin Relaxation is a versatile tool for studying molecular motions under conditions of local interactions both in ordered as well as non-ordered molecular environments. In the case of molecular chemically symmetric systems, as in this example of 2,6-dimethylpyridine, two methyl groups in symmetric positions to the main planar C_2 axial rotation axis are magnetically inequivalent what is a consequence of the central symmetric nitrogen atom (N) similar to the circular ring. Although chemically equivalent both methyl groups through the carbons connecting hydrogen atoms are magnetically non-equivalent. Consequently, this allows to study both groups directly without taking into account fast spin magnetic diffusion processes through the net between them and rest of the spin system.

In the present study, the magnetic spin-lattice relaxation T_1 was the main physical parameter to test that anisotropic methyl group rotation is the dominant source of magnetic spin ordering after external experimental magnetic disturbance, and therefore was utilized to find what type of the local dynamics for both CH_3 appears and if methyl groups rotations are independent phenomena in the common spin system ring and also how the remaining proton spin groups behave in the ring. Therefore, it was used the standard spin saturation pulse sequence as a one of the best options, after which macroscopic magnetization M has a zero value and is deprived of direction. Over time local spin-spin processes leading to building the magnetic order which can be tested by additional magnetic pulse allowing to establish the estimated spin-lattice relaxation time T_1, finally as a function of reciprocal scale temperature. With the use of the spin relaxation theory proposed by Bloembergen-Purcell-Pound (BPP theory), it was possible to distinguish the anisotropic axial rotation for two chemically non-equivalent groups as independent, and the magnetic screening effect (Chemical Shift Anisotropy) can be revealed only by the subjective Fourier analysis temporarily dependent induction signals as a response on earlier pulse excitation. Moreover, for rest three CH groups both magnetic screening and spin relaxation behaviour allow stating that the main factor of their differentiation comes in the ring nitrogen atom, which is the heaviest atom in the structure an stabilizes it. These observations can be spread from 3.2 up to 3.7 on the β scale (reciprocal temperature scale).

In conclusion, the use of magnetic spin relaxation to study the symmetric 2,6-dimethylpyridine system made it possible to identify spin relaxation processes, propose dynamical models leading to the averaging of macroscopic net magnetization consistent with the experimental data, estimate the values of physical parameters describing these processes, and confirm the lack of magnetic symmetry in the atomic structure over the entire investigated temperature range.