Using Free Rotating Groups in RDC analysis of Small Molecules

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Residual Dipolar Couplings (RDCs) are more and more becoming a complementary tool to NOEs and scalar couplings for the stereochemical analysis of small organic compounds.[1] However, their application can be hampered by the lack of enough independent vectors to span the 3D space and reliably determine the alignment tensor. It would be therefore convenient to use all available vectors as possible. The C-H vectors from rotatable methyl [2] and phenyl groups can provide additional vectors which can be of invaluable help for determination of stereochemistry in cyclic molecules, where the number of independent vectors can be very low.

To facilitate the use of these groups we have implemented, inside the RDC analysis MSpin code developed in our group, automatic recognition of methyl and phenyl groups from molecular geometry. Averaged matrixes are built in a completely transparent form for the user and alignment tensor and back-computed averaged RDCs are provided. As a test case we have analyzed, the conformation of phenylmenthol, where the alignment tensor can be determined only by using all available RDCs. These were recorded in PELG/CHCl3 by using a combination of 1D 13C and 2D F1 and F2 coupled HSQC experiments.

[1] Thiele, C. M. Concepts in Magnetic Resonance Part A **2007**, *30A*, 65-80.
[2] Haberz, P.; Farjon, J.; Griesinger, C. *Angew. Chem. Int. Ed*. **2005**, *44*, 427-429.

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