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Probing packing interactions in pharmaceuticals and other small (bio) molecules using solid-state NMR spectroscopy combined with DFT calculations and X-ray diffraction

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Solid-state NMR (SSNMR) is a powerful atomic-level characterization technique able to study the local chemical environment of a nucleus in crystalline/amorphous solids. Towards a better understanding of how drug hydrates self-assemble in the solid-state and reorganizes to produce its anhydrous form, we present an experimental SSNMR, X-ray diffraction (XRD), and computational study of the supramolecular assemblies of two interconvertible crystalline forms of the antibiotic ciprofloxacin (CIP), emphasizing the effect of nonconventional hydrogen bonds and water on NMR chemical shifts. The effect of crystal packing on the ^{1}H and ^{13}C chemical shifts including interionic hydrogen bonds, π...π and CH...π contacts, is quantified through computer simulations. We show that such chemical shifts are sensitive detectors of hydration/dehydration in the highly insoluble CIP antibiotics.

Recently, SSNMR became an important gadget in the process of crystal structure solution in powders. This is a non-trivial task and using powder XRD methods alone may often lead to the wrong structure solution. In this talk, we also present a new hybrid approach for structure determination of crystalline solids based on the combination of SSNMR, XRD and an ensemble of computational-assisted structure solution tools including a genetic algorithm based on evolution-inspired operators repeatedly applied to populations of possible crystal structure solutions that evolve to eventually produce the best new offspring candidates. This methodology is successfully applied to challenging cases involving multiple component crystals composed by flexible molecules such as a trihydrate β-lactamic antibiotic and an azole-based co-crystal featuring an hydrogen bond network of α-helixes involving NH...N/CH...π intermolecular interactions.

Biography

Luis Mafra has completed his B.Sc. at Universidade Nova de Lisboa, Portugal (2003), Ph.D. from two European institutes (2006): University of Aveiro (Portugal) and University of Caen-Basse Normandie (France). Invited researcher at the Max-Planck-Institut für Polymerforschung, Mainz, Germany during 2011. He is the recipient of two NMR related awards-Celestino da Costa/Jean Perrin and António Xavier (instituted by Bruker) prizes. Since 2007, he is researcher at CICECO lab, Univ. of Aveiro, with 10 years experience in SSNMR spectroscopy and has published about 52 international publications listed at the SCI. He is member of the editorial board of the solid-state NMR journal (Elsevier).

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