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On the use of XALOC BL for the characterisation of materials prepared under supercritical CO2 conditions

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During the last few years, the supercritical fluids and functional materials group (SFFM) at ICMAB, have been researching on the preparation of metalorganic materials using an unconventional technique based on supercritical CO2 technology (scCO2) as solvent.

In the field of coordination polymers and metal-organic-frameworks (MOFs), scCO2 is widely known for being used for the post-synthetic activation, or cleaning steps agent, however scCO2 can go further, as it can be used for the synthesis of these materials.

Thus, using this approach, we have widely proven that single molecules as well as 1D, 2D or 3D coordination polymers or MOFS can be prepared through the reaction of the right choice of building blocks.

On the other hand, scCO2 precipitation approach is generally governed by heterogeneous nucleation involving supersaturation of the reactants followed by nucleation and further crystal growth. However, in scCO2 nucleation generally dominates crystal growth, leading to the precipitation of very small crystals, which cannot be resolved by conventional diffractometers.

Under these lines, synchrotron radiation at ALBA though XALOC BL have been crucial for the determination of the structures of the materials precipitated in scCO2.

Herein, we report the scCO2 synthesis of single molecules, adducts and coordination polymers, based on the reaction between metals of the first transition row and nitrogen-based ligands. In all cases, the structure determination was carried out through single crystal diffraction using synchrotron radiation at ALBA.

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