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Example

Stability of cocrystals by Molecular Dynamics simulations

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A cocrystal is a system with at least two components that can be solids or liquids at room conditions. Molecules in a cocrystal interact by hydrogen bonds producing a new crystal which has different properties than the original compounds.
In the present work it was studied by molecular dynamics simulations the formic acid/pyridine and the isonicotinamide/formamide cocrystals at 173 K and 150 K, respectively. The OPLS/AA force field is used with two set of parameters for the liquids: a) the original set obtained by matching the simulations results to experimental density and heat of vaporization at room conditions and b) new values that reproduce the dielectric constant, surface tension and density at different temperatures. The parameters of pyridine and formamide have been published previously (Salas FJ et al.(2015) J. Chem. Theory Comput. 11(2):683). The liquid formic acid is parameterized in this work using the same procedure. The new parameters improved the predictions of the original values. The isonicotinamide parameters are obtained from those of pyridine and formamide assuming they are transferable. The structure and stability of cocrystals are determined through the calculation of distances and angles of atoms that form hydrogen bonds in different molecules. The simulation results were compared with experimental measurements of X-ray diffraction and a good agreement is found.