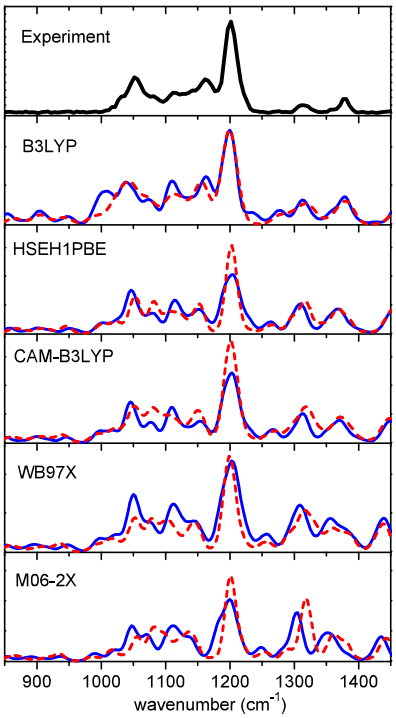

Supplementary Information. Fig. S1: Experimental IRMPD spectrum recorded for the nonactin–Na^+ complex compared to the IR spectra predicted for the $1\,C_2$ (blue, solid line) and $2\,S_4$ (red, dashed line) conformers, by computations with different density functionals (as indicated in each panel). The 6-311+G(d) basis set is employed in all cases. It can be noted that the B3LYP functional provides the best agreement with the shape of the IRMPD bands, in particular in the 950–1250 cm^{-1} range.