Local ordering of simple organic liquids in the nanometre range

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X-ray scattering experiments with simple organic liquids (aldehydes, alcohols and acids) have revealed that these substances, in addition to the usual short-range ordering, also exhibit longer-range correlations that extend into the nanometre range. To gain insight into the structure of such liquids, we performed configurational bias Monte Carlo (CBMC) simulations utilizing the TraPPE-UA force field which had already been proven to reproduce—at least qualitatively—the main structural properties of such systems. A favourable comparison of the theoretical scattering curves to the experimental SAXS/WAXS data enabled us to study the structure of the simulated systems in various ways: via pair distribution functions, via partial scattering factors and by analysis of molecule clustering. As expected, the strength of the long-range correlations depends greatly on the functional group: alcohols and acids are strongly correlated, whereas aldehydes, not being capable of forming hydrogen bonds, exhibit only weak long-range ordering.

X-ray scattering curves of pure organic acids