Electronic Supplementary Material (ESI) for RSC Advances.

Dynamics of an amorphous pharmacologically active compound - diazepam: A QENS study combined with molecular dynamics simulations

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SUPPLEMENTARY MATERIALS

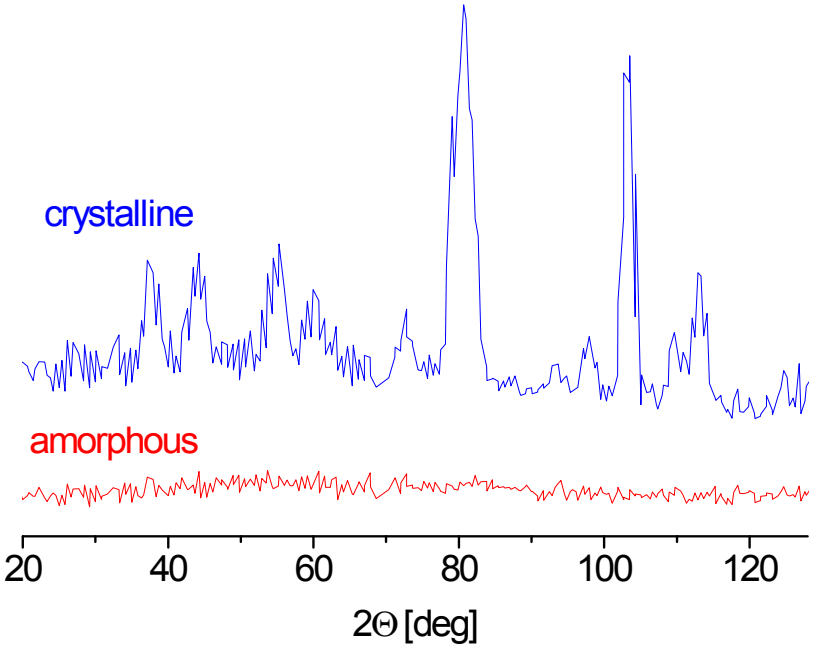
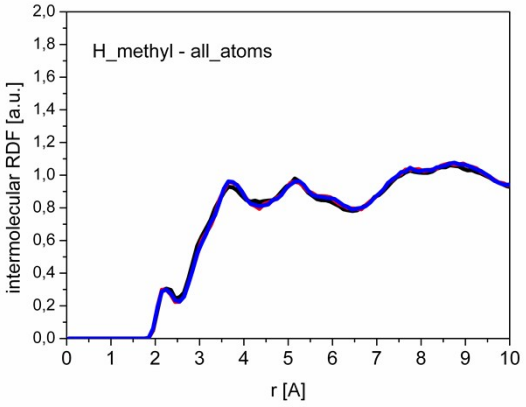
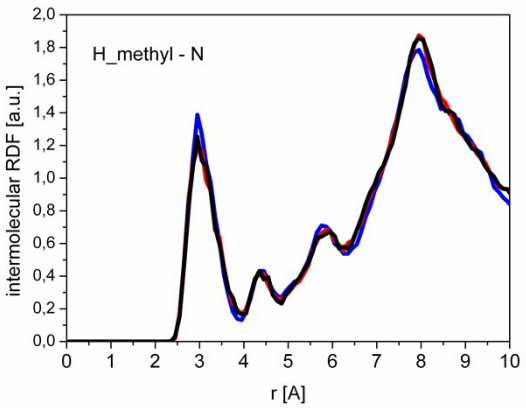
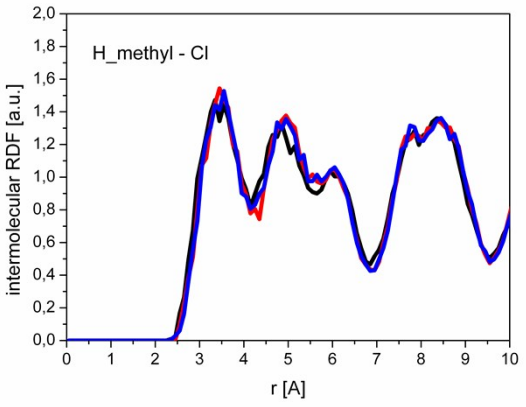


Fig. 1S. Neutron diffraction pattern for crystalline (top) and amorphous (bottom) samples at 300K.

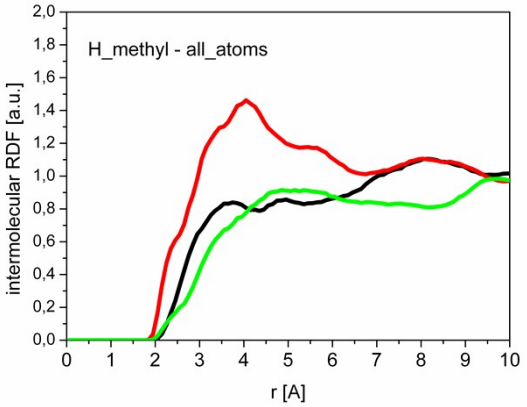
a)

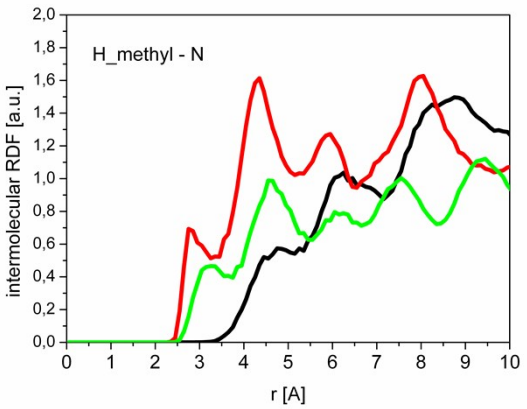

H_methyl - all_atoms
intermolecular RDF [a.u.]
r [A]

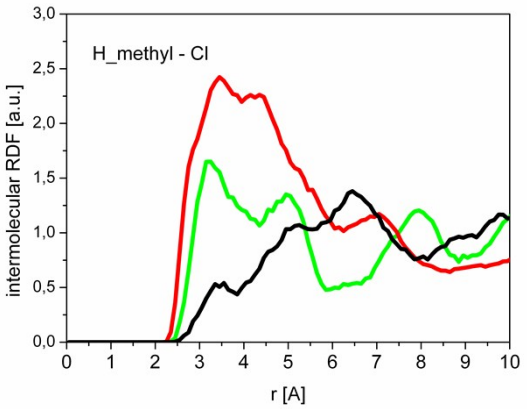

H_methyl - N
intermolecular RDF [a.u.]
r [A]


H_methyl - Cl
intermolecular RDF [a.u.]
r [A]

b)


H_methyl - all_atoms
intermolecular RDF [a.u.]
r [A]


H_methyl - N
intermolecular RDF [a.u.]
r [A]


H_methyl - Cl
intermolecular RDF [a.u.]
r [A]

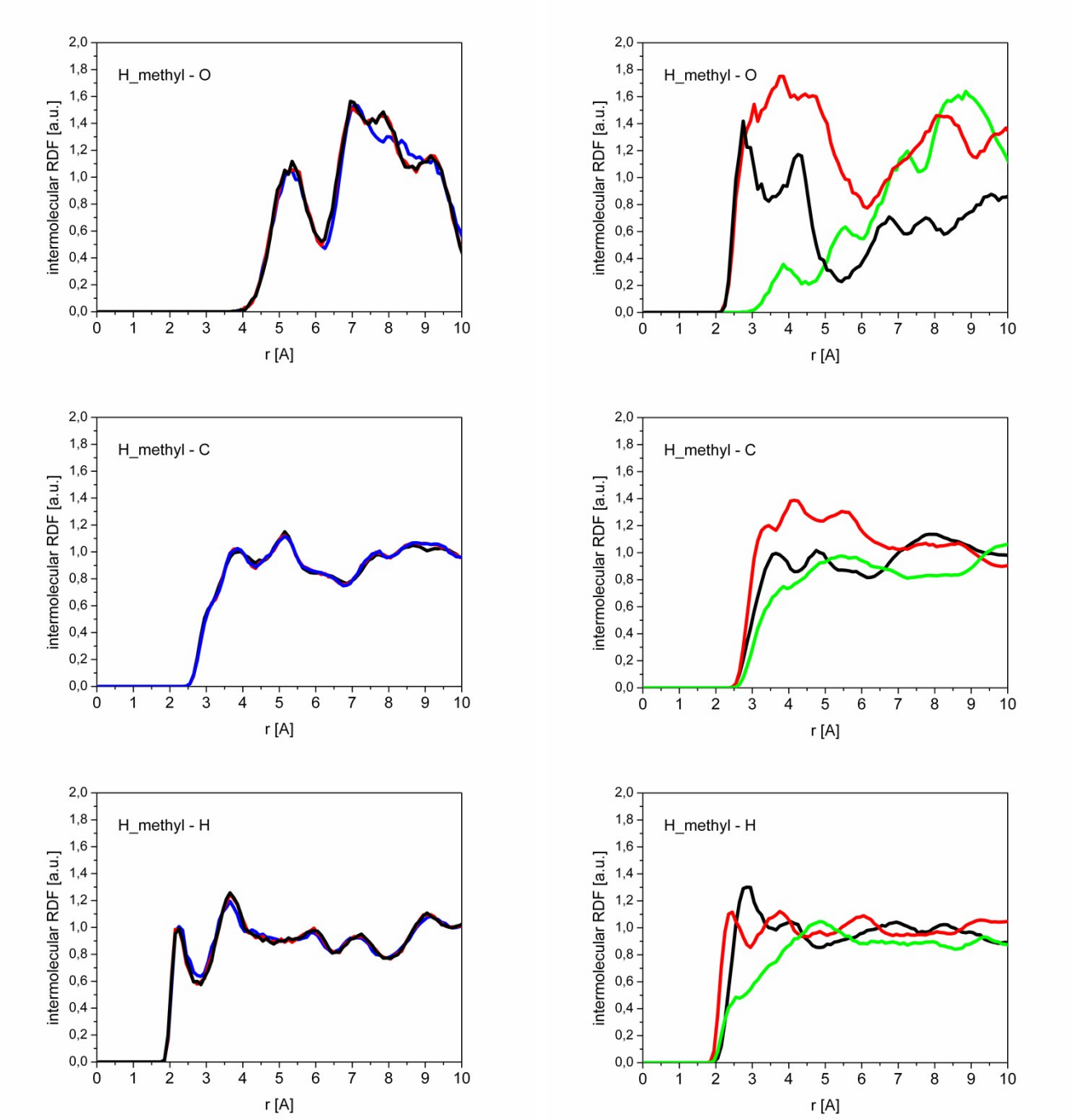


Fig. 2S. The separate contributions from different types of atoms to intermolecular H_iX RDF (eqn. 9) showing the distance distribution between methyl hydrogens and other atoms in a) crystalline and b) amorphous clusters for 3 selected molecules.