

## **Does that "green" plasticiser make my PVC flexible enough for you?**

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What gives plastic objects their flexibility and reduces their brittleness is the concentration of plasticiser. For example, a chemical solvent of the phthalate family called DOP is often used. The trouble is there are concerns that phthalates present health risks. So there is a demand for more alternatives. Now, scientists from China have examined the effect of using DEHHP, a new eco-friendly plasticiser, used in combination with PVC. For a plasticiser to work, there has to be adequate hydrogen bonding with the plastic.. By combining experiments and simulations, the team revealed why the polymer-solvent hydrogen bonding interaction's strength decreases with dilution at a molecular level - which is a phenomenon also observed in the DOP-PVC combination. These findings have been published in EPJ Plus by Yang Liu from Nanjing University and colleagues.

The team studied the polymer-<u>solvent</u> interactions at various temperatures and concentrations. Specifically, they looked at the effects of DEHHP concentration in relation to hydrogen bonding interactions, as a means to evaluate its ability to make plastics flexible. This eco-friendly plasticiser is an ideal model because it has only one kind of hydrogen bonding interaction - between polymer and solvent - and is free of other potentially interfering hydrogen bonding interactions.

They found in stretching experiments that when the temperature increases or the PVC concentration decreases, the interactions between polymer and solvent were weaker in the PVC-DEHHP mix than in the PVC-DOP combination.



Then, they used what they refer to as low-field hydrogen Nuclear Magnetic Resonance (NMR). This shows that the number of polymersolvent complexes decreased as temperature increased. Furthermore, they looked into simulations of the molecular dynamics to study the role of polymer-solvent hydrogen bonding interactions. They demonstrated that when the temperature was high or the PVC <u>concentration</u> was low, faster molecular motions resulted. This also led to the disassociation of the <u>hydrogen bonds</u> in the hydrogen bonding system.

**More information:** "Hydrogenation induced deviation of temperature and concentration dependences of polymer-solvent interactions in poly(vinyl chloride) and a new eco-friendly plasticizer," *European Physical Journal* Plus 130: 116, DOI 1140/epjp/i2015-15116-3

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