Replacing Polyvinyl Chloride with Novel Thermoplastics Derived from Natural Gas

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The primary research objective of this proposal is to synthesize novel polyoxymethylene copolymers—derived from natural gas feedstocks—having thermomechanical properties suitable for replacing the common thermoplastic polyvinyl chloride (PVC). Polyoxymethylene (POM) is already a commercial material with many excellent properties, but complex copolymers based on POM are rare and poorly understood. The organic feedstock for POM is methanol, which currently is derived from natural gas, a fossil fuel with a projected availability longer than that of petroleum.

Our previous investigations of alkyl-branched polyoxymethylenes revealed that considerably more branches are required to plasticize polyoxymethylene than polyethylene. About 2.6 times more branches are required to effect a comparable melting point depression in POM versus PE. The present computational model studies help to explain the diminished response of POM to chain disruptions.

- The numerous local dipoles of POM lock adjacent helical chains together.
- Within a chain, the observed helical conformation has two reinforcing effects: intramolecular 1,5 H···O interactions and anomeric stabilization.
- The penalty for disrupting these (simultaneously) is calculated to be 2.2 to 3.2 kcal/mol, depending on the computational method.
- The strong inter- and intramolecular forces suggest that significantly plasticized polyoxymethylene copolymers will require rather high comonomer compositions.

Thus, we continue our pursuit of more effective and economical approaches to polyoxymethylene plasticization via synthesis of novel POM copolymers.