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Antiplasticization of polymer melts diluted by low molar mass species EVGENY STUKALIN, Department of Chemistry, The University of North Carolina at Chapel Hill, NC 27599, JACK DOUGLAS, Polymers Division, National Institute of Standards and Technology, Gaithersburg, MD 20899, KARL FREED, The James Franck Institute, The University of Chicago, Chicago, IL 60637 — An analysis is made of glass formation in polymers diluted by molecular additives by combining the Adam-Gibbs model and computations of the configurational entropy using the lattice cluster theory. Plasticization and antiplasticization of polymer melts is shown to depend on the molecular properties of the additive. Antiplasticization is accompanied by a toughening of the glass mixture and occurs when the diluent is a small species having strongly attractive interactions with the polymer chains. Plasticization leads the softening of the host polymer and emerges for small additives with weakly attractive interactions. Shifts in T_g and changes in compressibility and density of polymer melts with a diluent are evaluated to characterize the efficiency of (anti-)plasticizers. The general reduction in the T_g and fragility of polymers by molecular additives is rationalized by analyzing the influence of the diluent's properties (cohesive energy, chain length, and stiffness) on glass formation. We also study the vitrification of mixtures at fixed temperature due to increasing polymer concentration. The zero mobility concentration is found to scale linearly with the inverse degree of polymerization.

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