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Quantification of Molecular and Nanostructural Topology RAMNATH RAMACHANDRAN, Univeristy of Cincinnati, GREGORY BEAUCAGE, University of Cincinnati — We have recently derived a method for the description of complex molecular and nanostructural topologies based on a statistical analysis. The method has been applied to a wide range of materials from long chain branched polyolefins, hyperbranched polymers, star polymers, H-branched polymers to cyclics, biopolymers, and branched nanostructured aggregates. This method, when applied to neutron scattering data from dilute polymer solutions, yields the mole fraction of a structure involved in long chain branching, the branching density, and the average branch length. Moreover, quantitative measures of the convolution or tortuosity of the structure and the connectivity of the molecules can be made, opening a new window for our understanding of complex molecular topologies. When applied to neutron scattering the approach is applied to the chain-scaling regime at low to moderate values of the scattering vector. At high scattering vector the Kuhn length is observed that has been shown to be directly related to short chain branching in polyolefins. By combining information of short and long chain branching a topological map of complex molecular structure becomes possible. The method is quite generally applicable. This understanding has recently been applied to model long-chain branched polyethylene.

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