A Monte Carlo Study of Dilute Solution Properties of Semiflexible Ring Polymers

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A Monte Carlo (MC) study is made of dilute solution properties, the mean-square radius of gyration $\langle S^2 \rangle$ ($R_g = \langle S^2 \rangle^{1/2}$),[1,2] particle scattering function $P(k)$ with k the magnitude of the scattering vector,[1,3] intrinsic viscosity $[\eta]$,[4] and second virial coefficient A_2,[1,2,5] of semiflexible ring polymers by the use of the discrete version of the Kratky–Porod wormlike[6] ring model proposed by Frank-Kamenetskii *et al.*[7] The behavior of those properties is examined as a function of the reduced contour length λL, where λ^{-1} and L are the stiffness parameter (equal to twice of the persistence length) and contour length, respectively, of the wormlike ring and then effects of chain stiffness on the dilute solution properties are clarified. Further, the MC results for the wormlike rings without the intramolecular topological constraints are compared with the results for the wormlike rings of the trivial knot[1–4] and for those of the trefoil knot,[8] and then, effects of the intramolecular topological are also examined.

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