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Monte Carlo Simulations on Phase Transitions and Conformational Properties of Catenated Double-ring Copolymers DACHUAN SUN, JUNHAN CHO, Dankook Univ — The thermodynamic and conformational properties of catenated double-ring A/B copolymer melts are investigated through lattice Monte Carlo simulations. The topological constraint on the catenated copolymers is shown to suppress demixing of A and B monomers. This action results in their order-to-disorder transition (ODT) at an increased segregation level and the lamellae below ODT with reduced order, when compared to diblock copolymers of linear or single-ring topology. The A and B rings are pulled closer by catenation in the copolymer, which leads to its smaller gyration radius, lamellar domain spacing, and distance between mass centers of the two rings than for the diblock copolymers. With increasing segregation tendencies, the gyration radii of the A rings of the catenated copolymers stretch along the direction normal to lamellae, while the A-block conformations of the single-ring copolymers change their shapes from ellipsoid to sphere.

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