Electronic Supplementary Material (ESI) for Soft Matter.

Supporting Information

Effect of Polar Group Content on the Glass Transition Temperature of ROMP Copolymers

Yi-Lin Li,[a] Xiang-Meng Jia,[a,†] Xu-Ze Zhang,[a] Zhong-Yuan Lu[a] and Hu-Jun Qian[a]*

a. State Key Laboratory of Supramolecular Structure and Materials, Institute of Theoretical Chemistry, College of Chemistry, Jilin University, Changchun 130021, China.

† Current address: South China Advanced Institute for Soft Matter Science and Technology, School of Emergent Soft Matter, South China University of Technology, Guangzhou 510640, China.

*Corresponding author. E-mail: hjqian@jlu.edu.cn

Taking the COC2 system as an example, the fitting process using datapoints from different temperature window are shown in the following figure. It can be seen that when we use more data points from lower temperatures, the VFT fitting will lead to a lower T_g value. However, such variation in extrapolated T_g value slowly converges during this process. In particular, when the τ_α increases from 10^3 ps 10^4 ps, the T_g value decreases from 323 K from 321 K, the difference is in the order of < 1%. Therefore, we stop the further decrease of the simulation temperature for the purpose of computational efficiency.

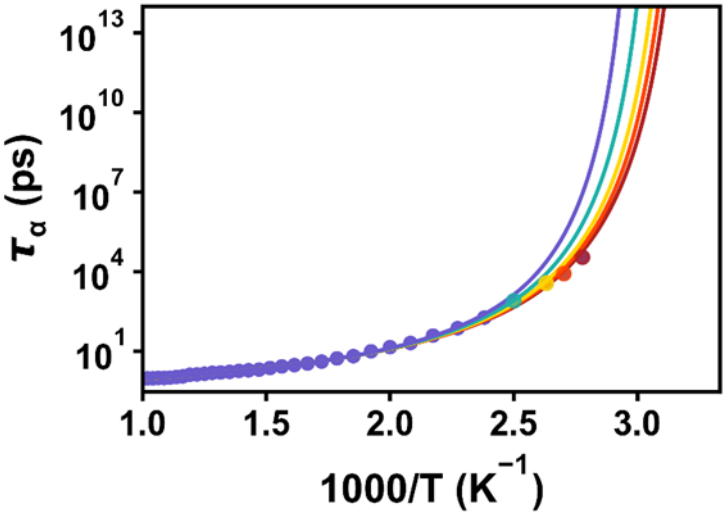

Figure S1. Temperature dependence of segmental relaxation time for COC2 polymers with different windows, lines represent the least-squares fitting with VFT equation.