Supplementary Material (ESI) for PCCP

Supplementary Data

Rotation dynamics of 2-methyl butane and n-pentane in MCM-22 zeolite: A molecular dynamics simulation study

Shiping Huang[a], Vincent Finsy[a], Jeroen Persoons[a], Mark T.F. Telling[b], Gino V. Baron[a] and Joeri F.M. Denayer[a]

[a] Department of Chemical Engineering, Vrije Universiteit Brussel, Pleinlaan 2, B-1050 Brussel, Belgium, Tel: + 32 2 629 17 87, Fax: + 32 2 629 32 48

Joeri.denayer@vub.ac.be

[b] ISIS Facility, Rutherford Appleton Laboratory, Chilton, OXON, OX11 0QX, UK

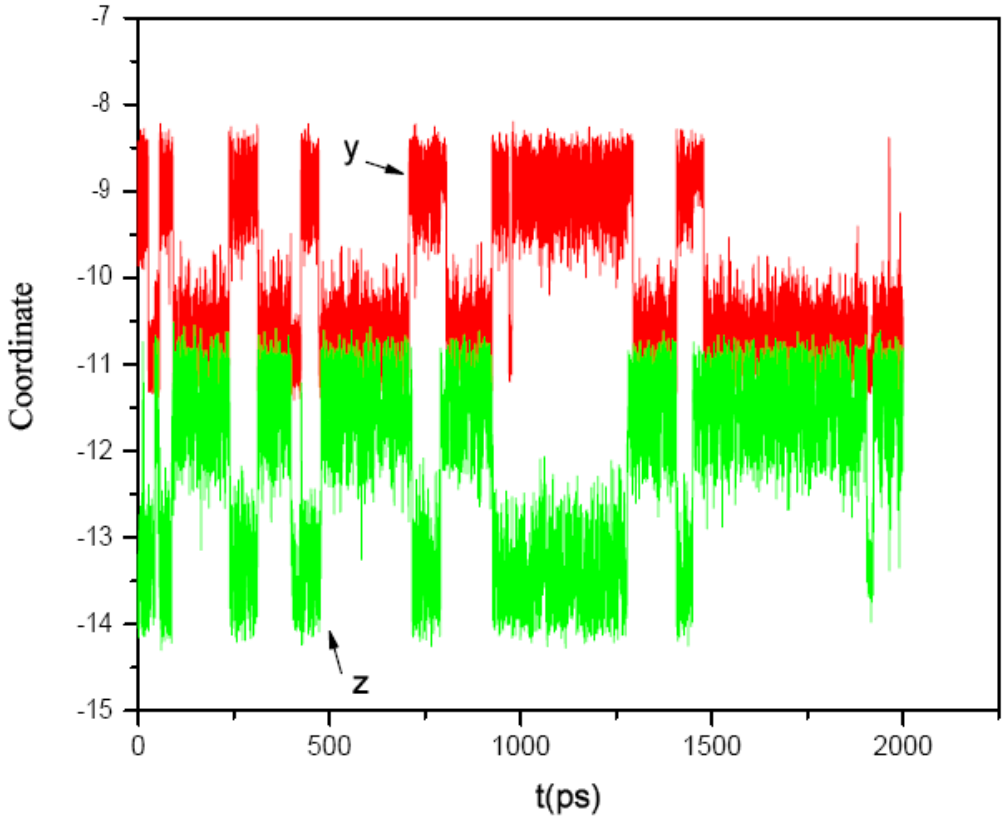
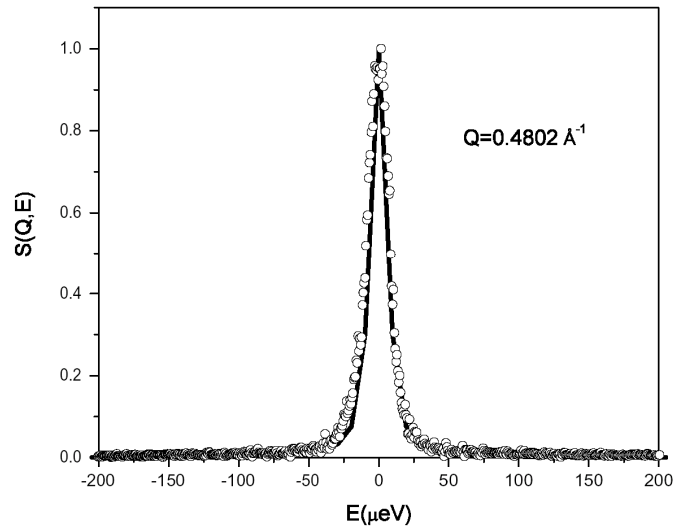
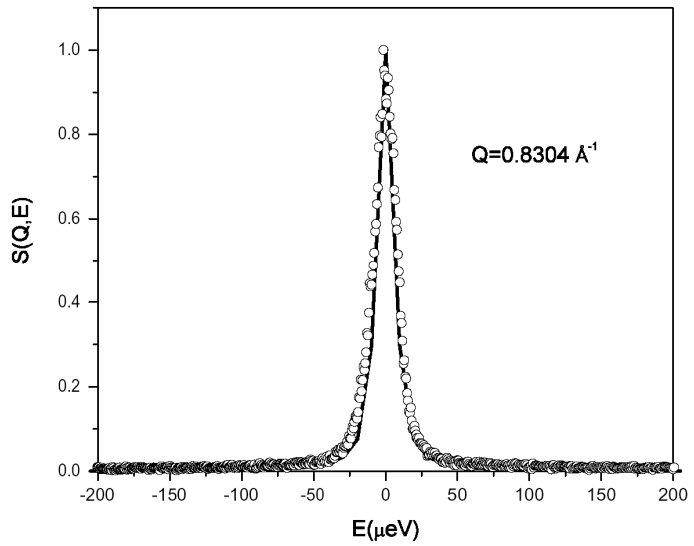


Figure S1: Trajectory of one hydrogen atom of CH_3 in n-C5 molecule from MD simulation at a temperature of 200K.





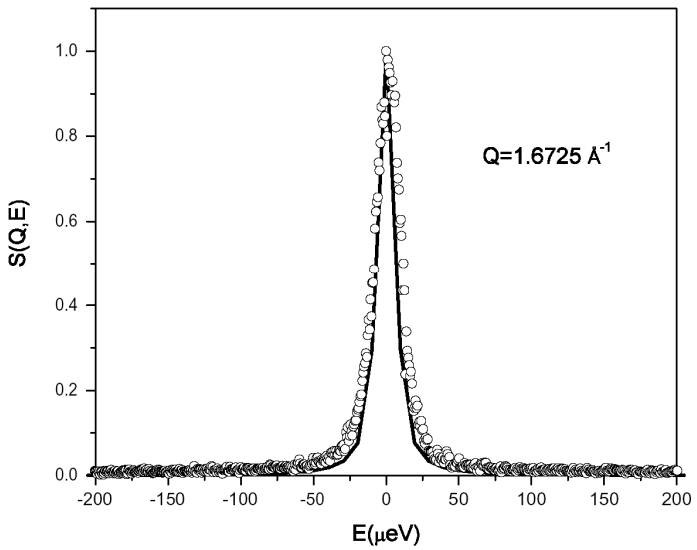


Figure S2: A comparison of the MD simulation results (red line) and the incoherent dynamic structure factor $S_{inc}(Q,t)$ in neutron scattering experiments (open dots) for 2-MeC4. The MD simulation is at a loading condition of 3.0 molec/UC, and the temperature is 200K. The spectra are normalized to their maximum values.

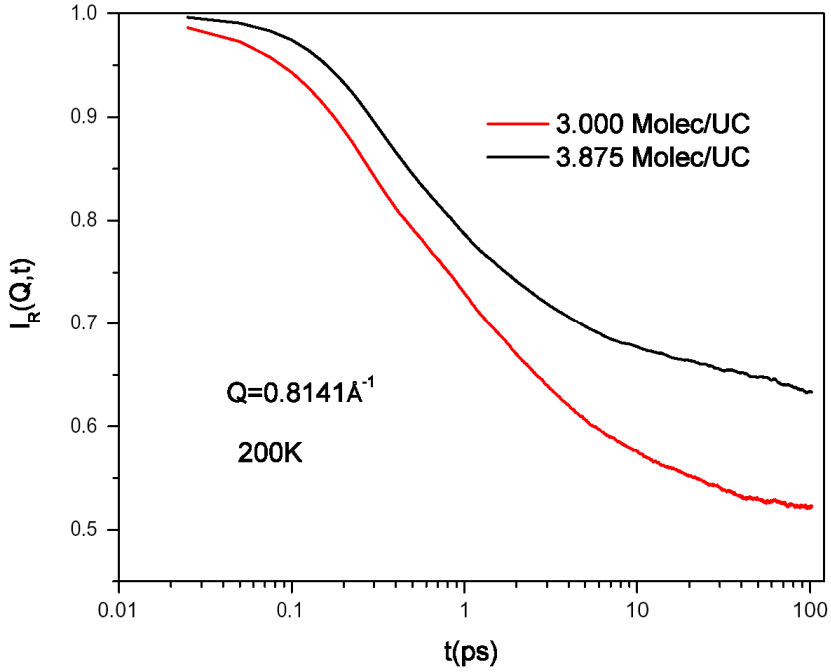


Figure S3: The rotational intermediate scattering functions for 2-MeC4 in zeolite MCM-22 as a function of temperature at Q=0.8141Å^{-1}.

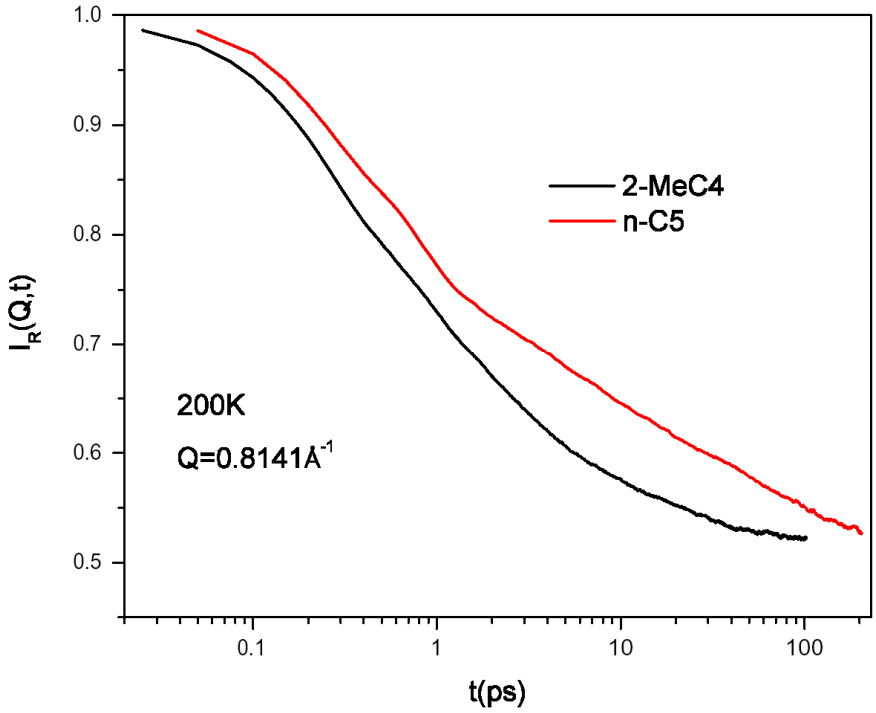


Figure S4: Comparison of the rotational intermediate scattering functions for 2-MeC4 and n-C5 at 200 K (Q=0. 0.8141Å^{-1}).

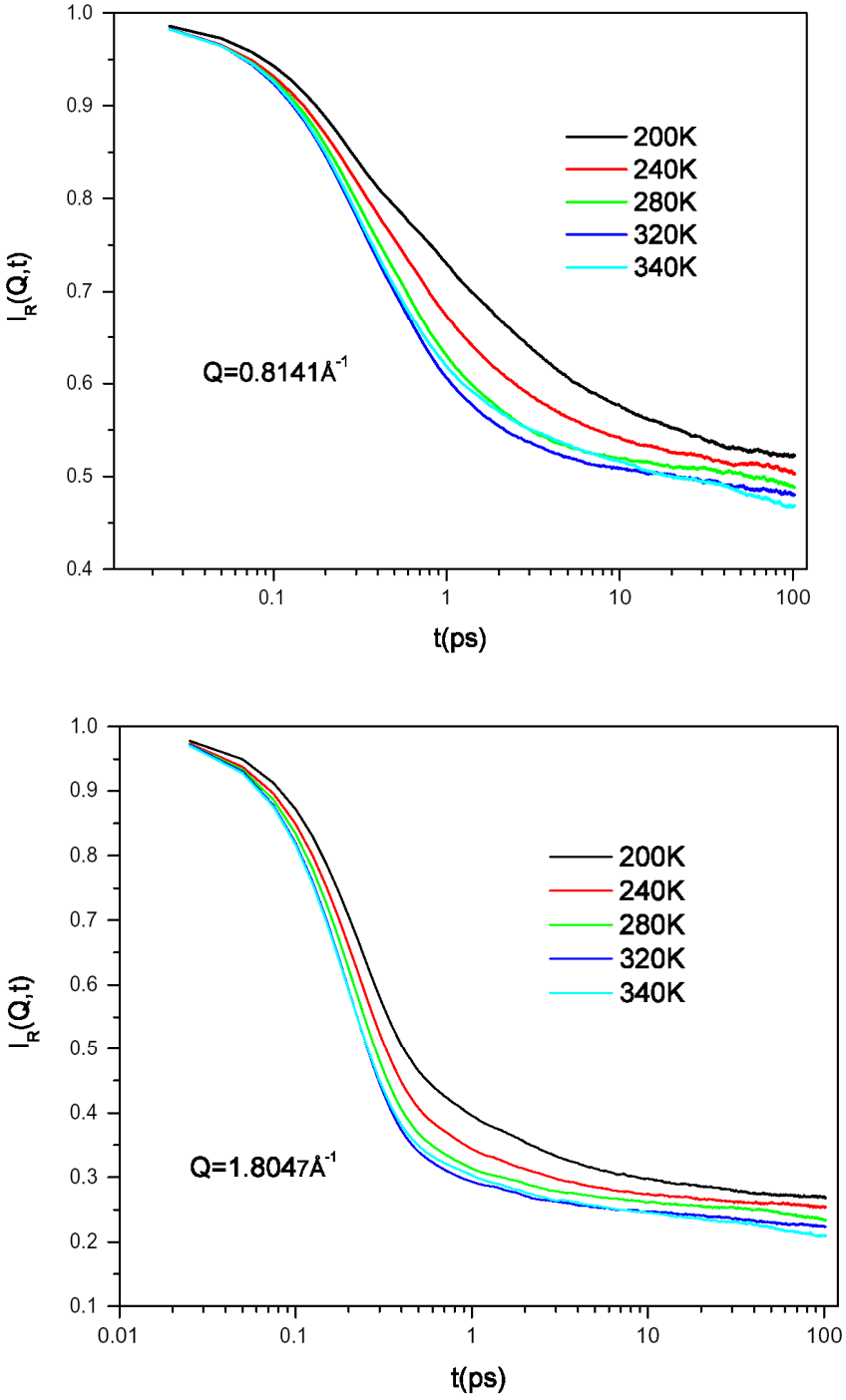
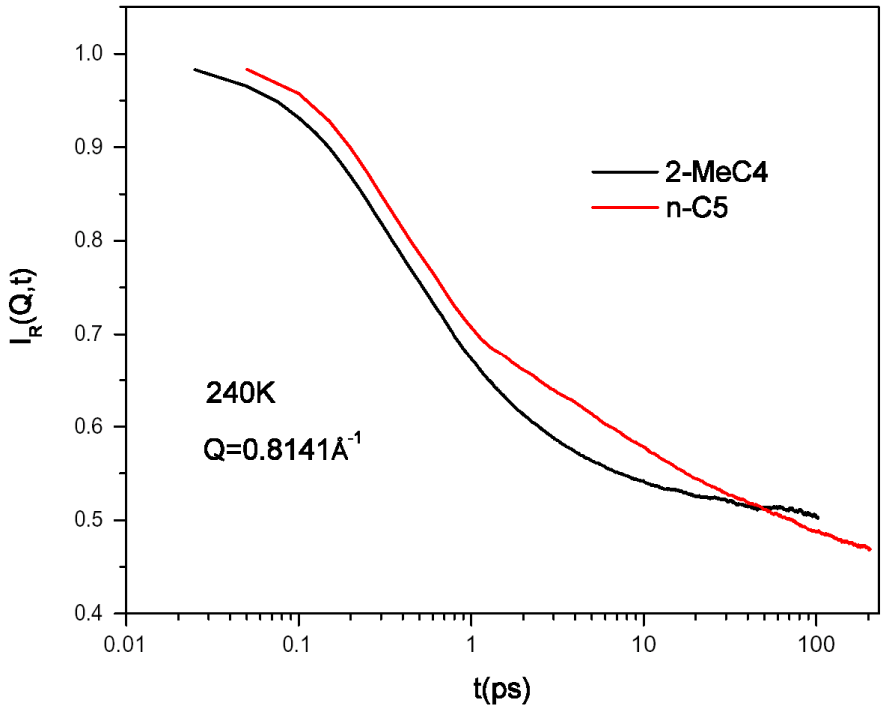
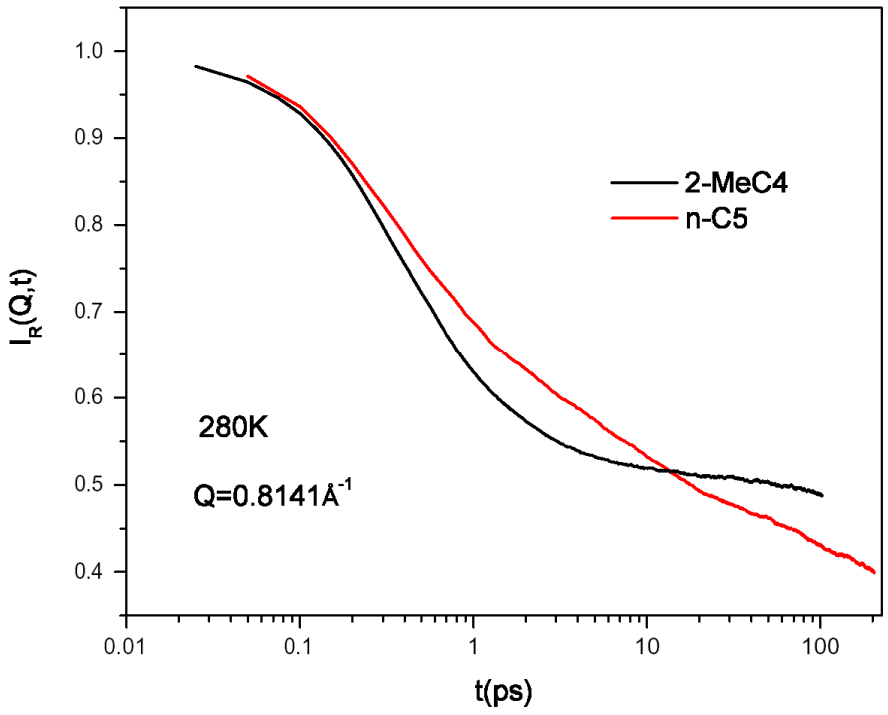


Figure S5: The rotational intermediate scattering functions for 2-MeC4 in zeolite MCM-22 as a function of temperature at Q=0.8141Å^{-1} and 1.8047 Å^{-1}.





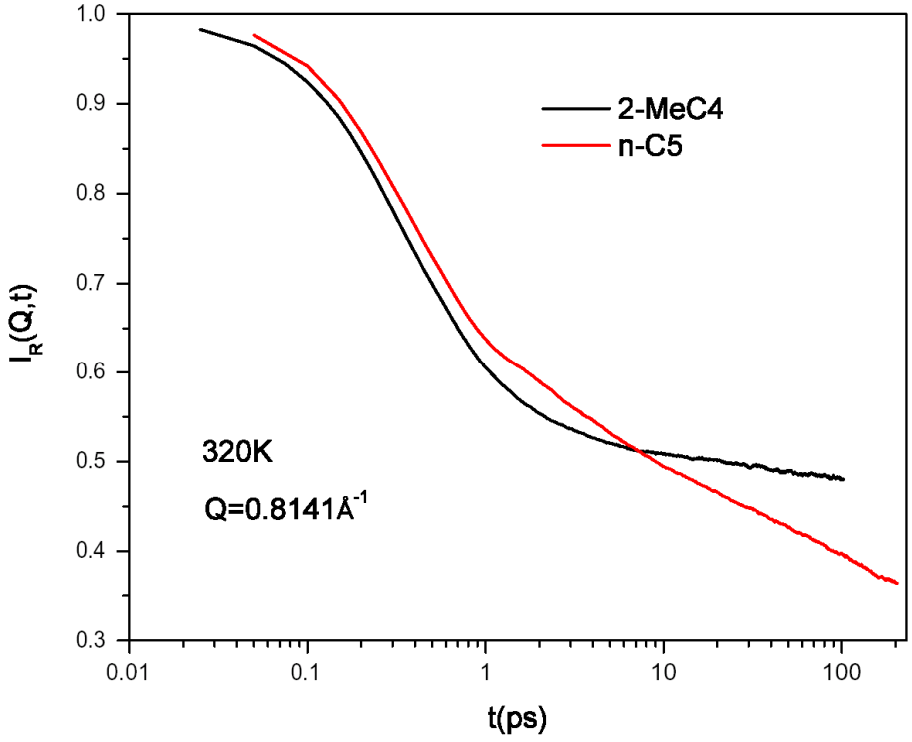


Figure S6: Comparison of the rotational intermediate scattering functions for 2-MeC4 and n-C5 at different temperatures (Q=0.8141Å^{-1}).

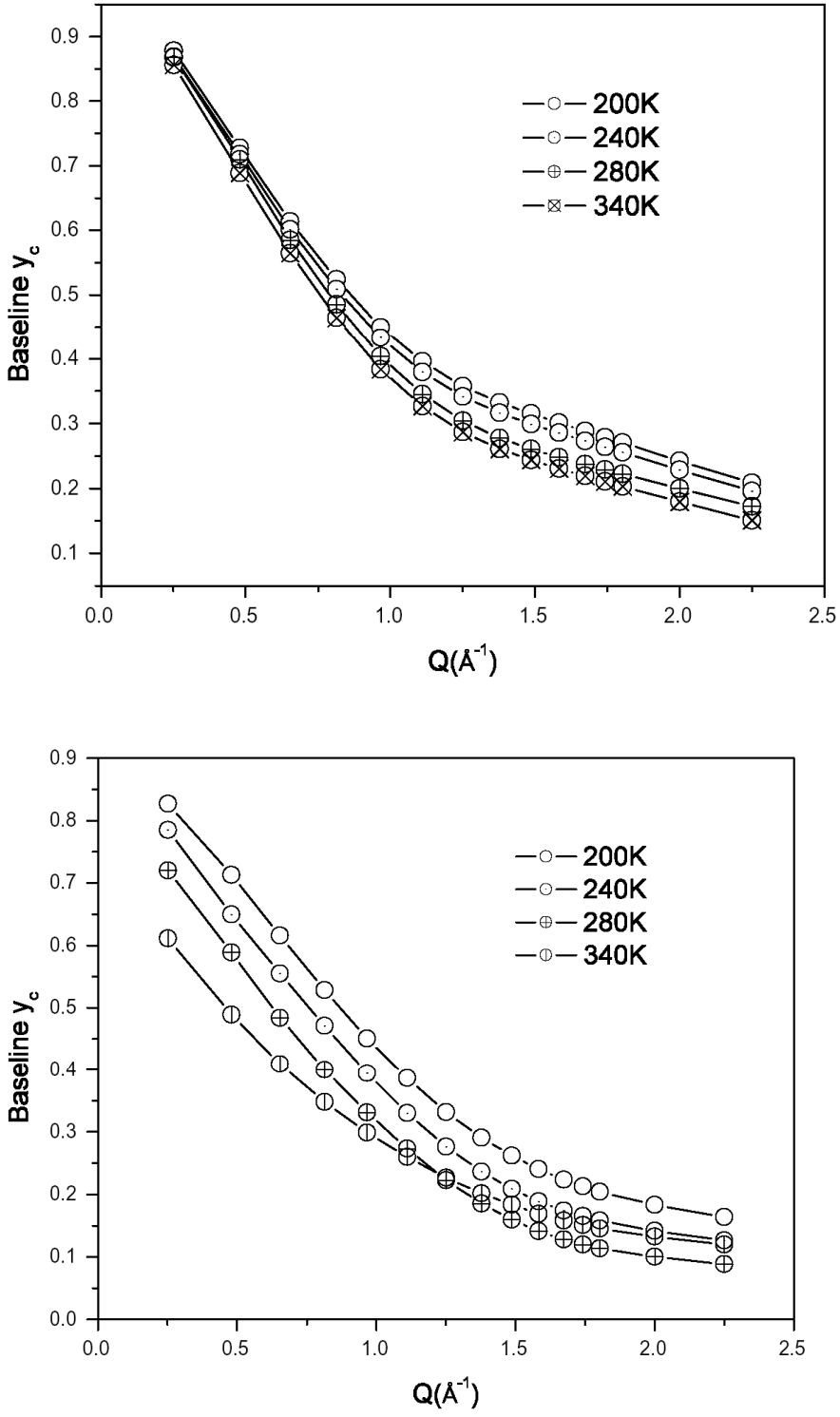


Figure S7: The rotation baselines y_c from MD simulations as a function of Q.

(a) 2-MeC4 (b) n-C5.