

Supplementary Information

Electronic Supplementary Information 1

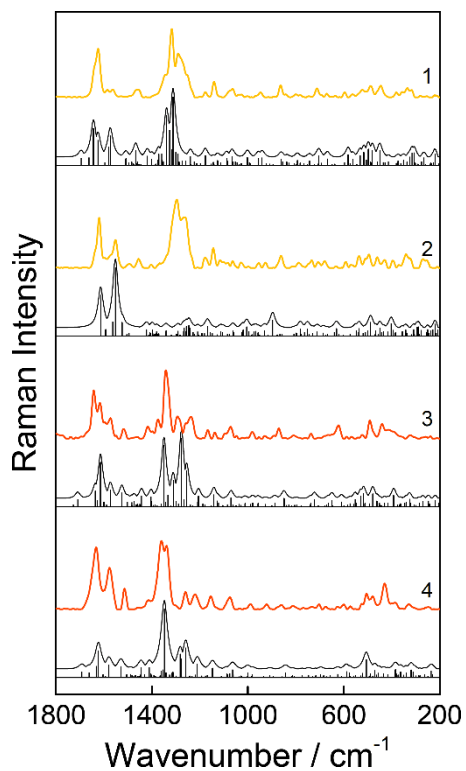


Figure S1. Alignment of the experimental FT-Raman spectra of TC (1), ETC (2), ATC (3), and EATC (4) with the calculated scattering activities (calculation method: B3LYP/cc-pVTZ) and their Lorentzian peak profile (FWHM = 27 cm⁻¹). Here, the scaling factors and the resulting MAE values for the investigated wavenumber region (1800–200 cm⁻¹) are 0.98 and 1.23 (1), 0.93 and 1.92 (2), 0.98 and 2.47 (3), and 0.98 and 2.50 (4).