

Supplementary Material for PCCP
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SUPPORTING INFORMATION

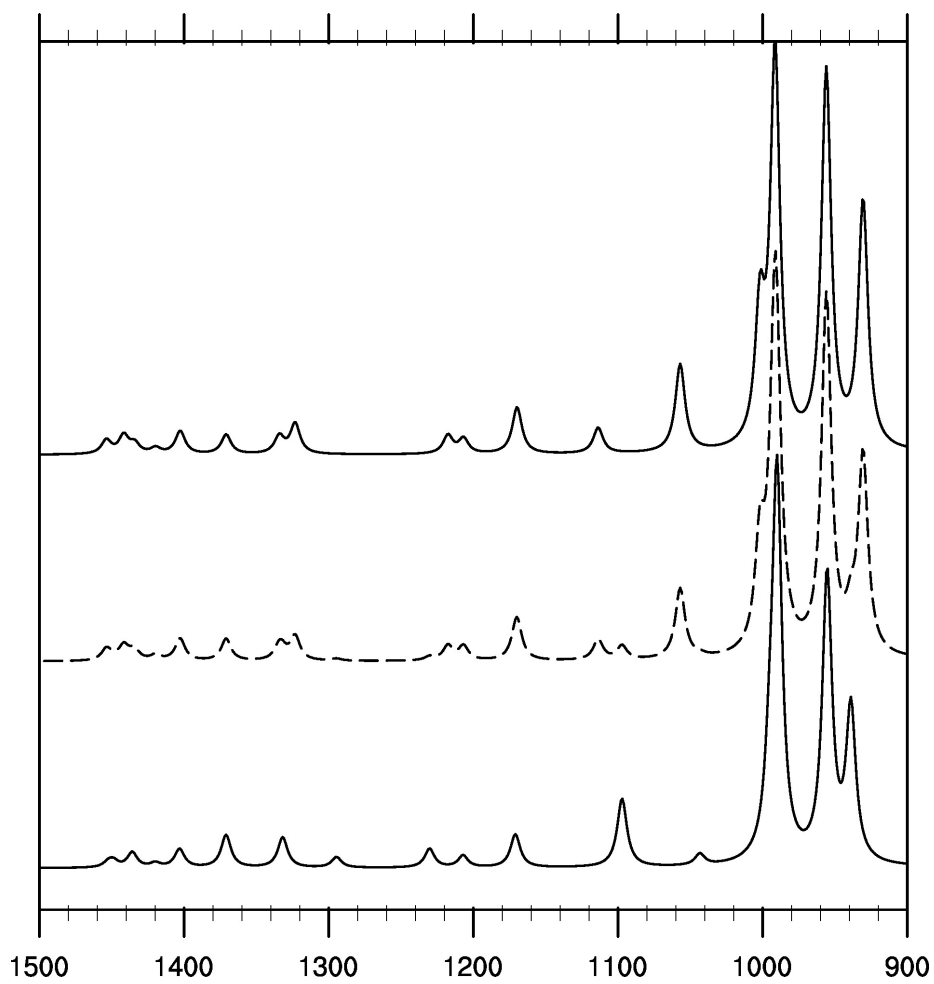


Figure S3-1: Simulated IR spectra (B3LYP; def2-TZVPP) for **3a-c1** (top), the Boltzmann-averaged **3a-c1/c2** (80%/20%; middle), **3a-c2** (bottom).

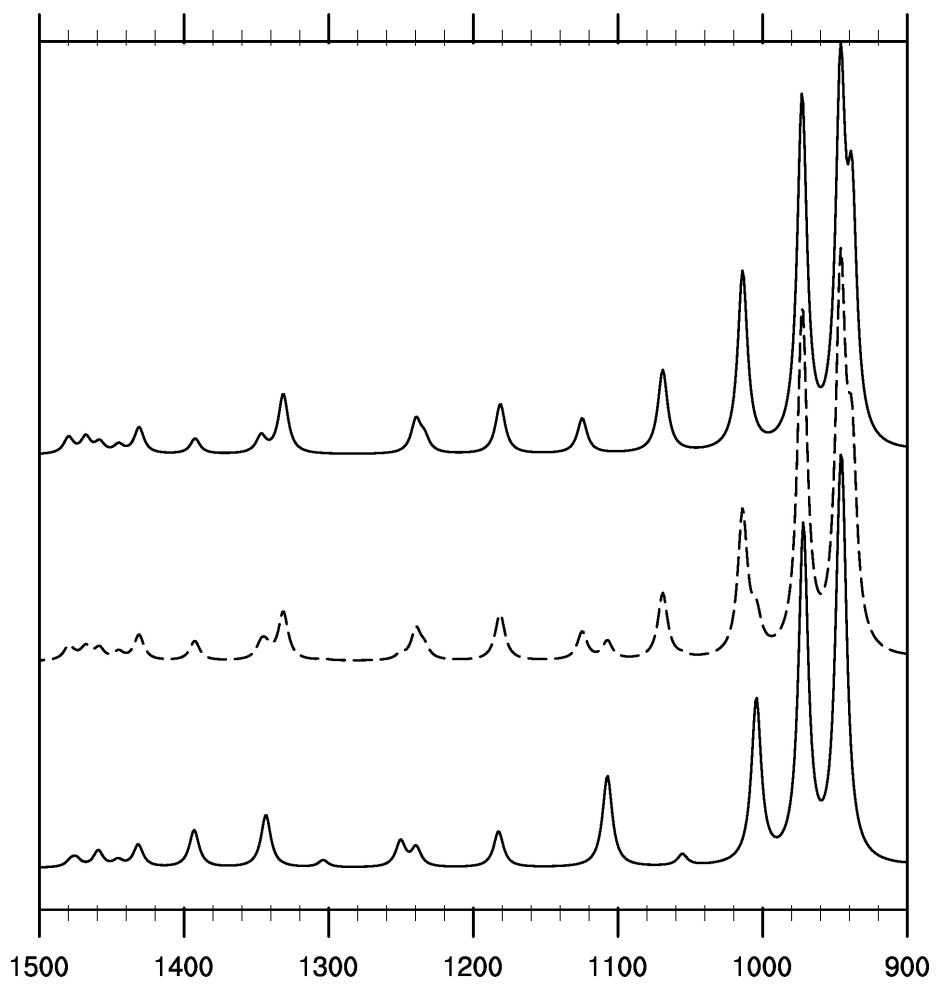


Figure S3-2: Simulated IR spectra (B3LYP; Stuttgart/6-31Gd) for **3a-c1** (top), the Boltzmann-averaged **3a-c1/c2** (80%/20%; middle), **3a-c2** (bottom).

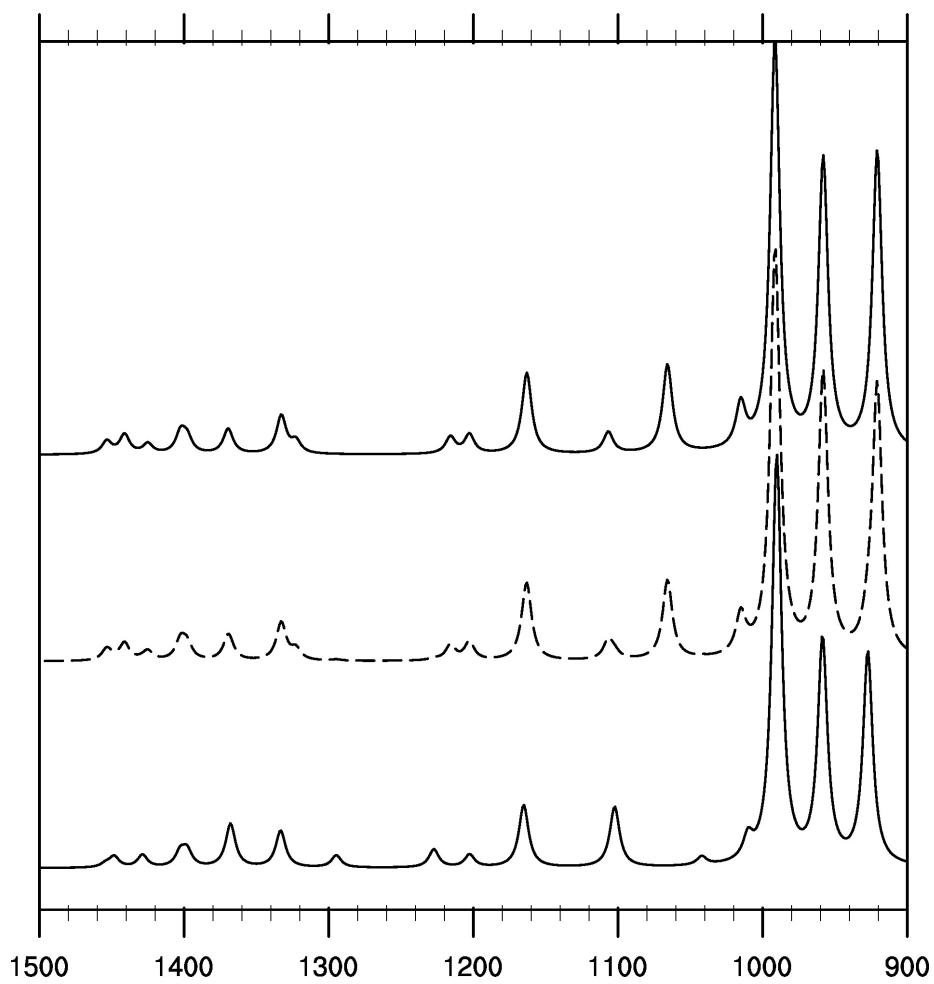


Figure S3-3: Simulated IR spectra (B3LYP; def2-TZVPP) for **3b-c1** (top), the Boltzmann-averaged **3b-c1/c2** (90%/10%; middle), **3b-c2** (bottom).

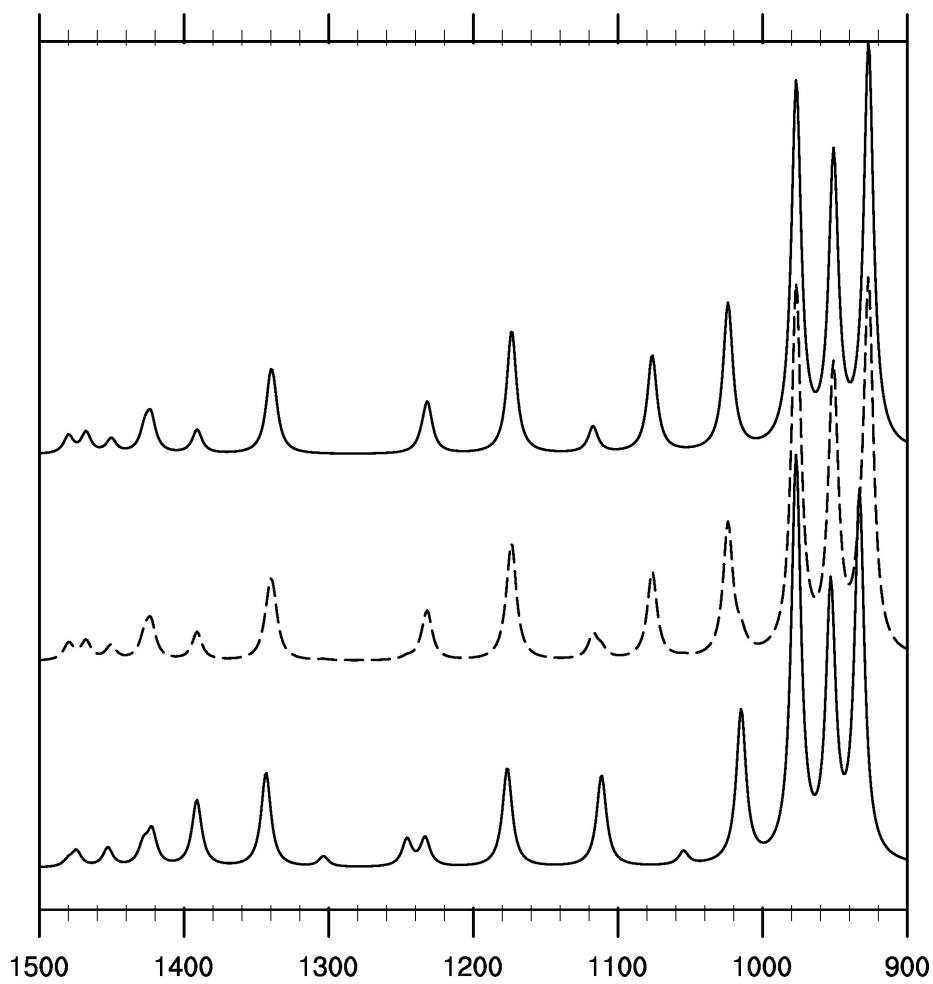


Figure S3-4: Simulated IR spectra (B3LYP; Stuttgart/6-31Gd) for **3b-c1** (top), the Boltzmann-averaged **3b-c1/c2** (90%/10%; middle), **3b-c2** (bottom).

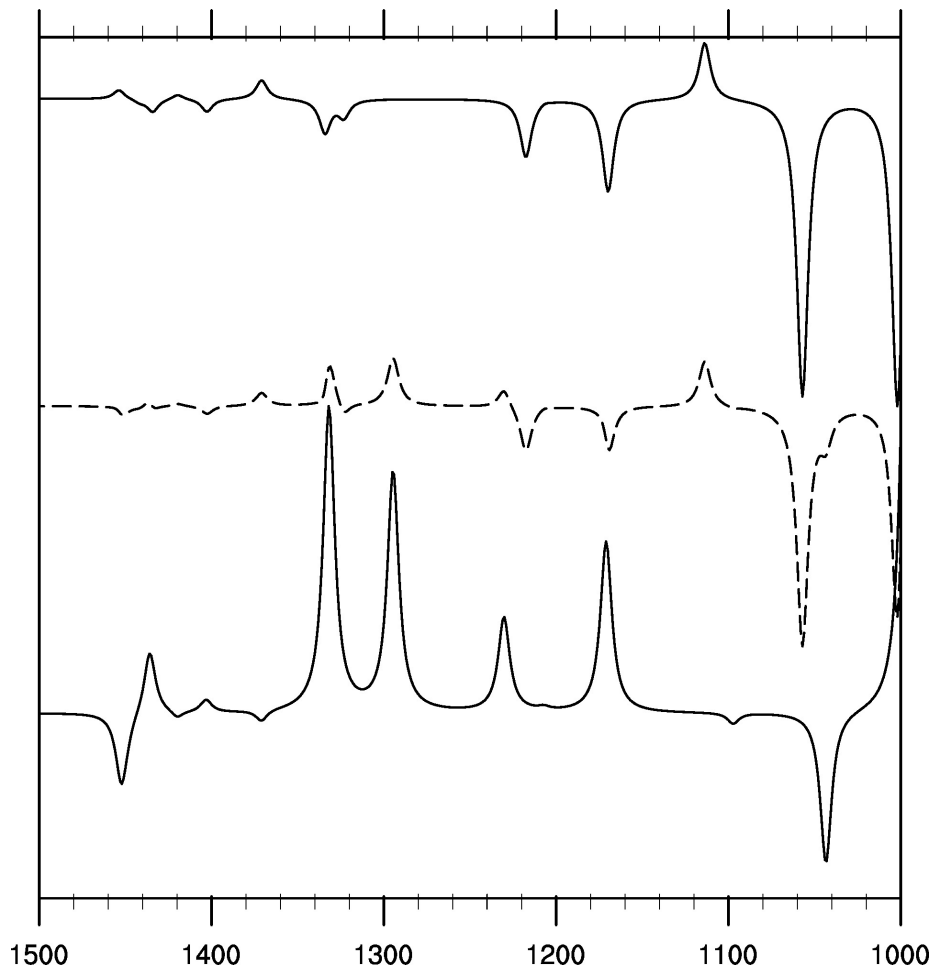


Figure S3-5: Simulated VCD spectra (B3LYP; def2-TZVPP) for **3a-c1** (top), the Boltzmann-averaged **3a-c1/c2** (80%/20%; middle), **3a-c2** (bottom).

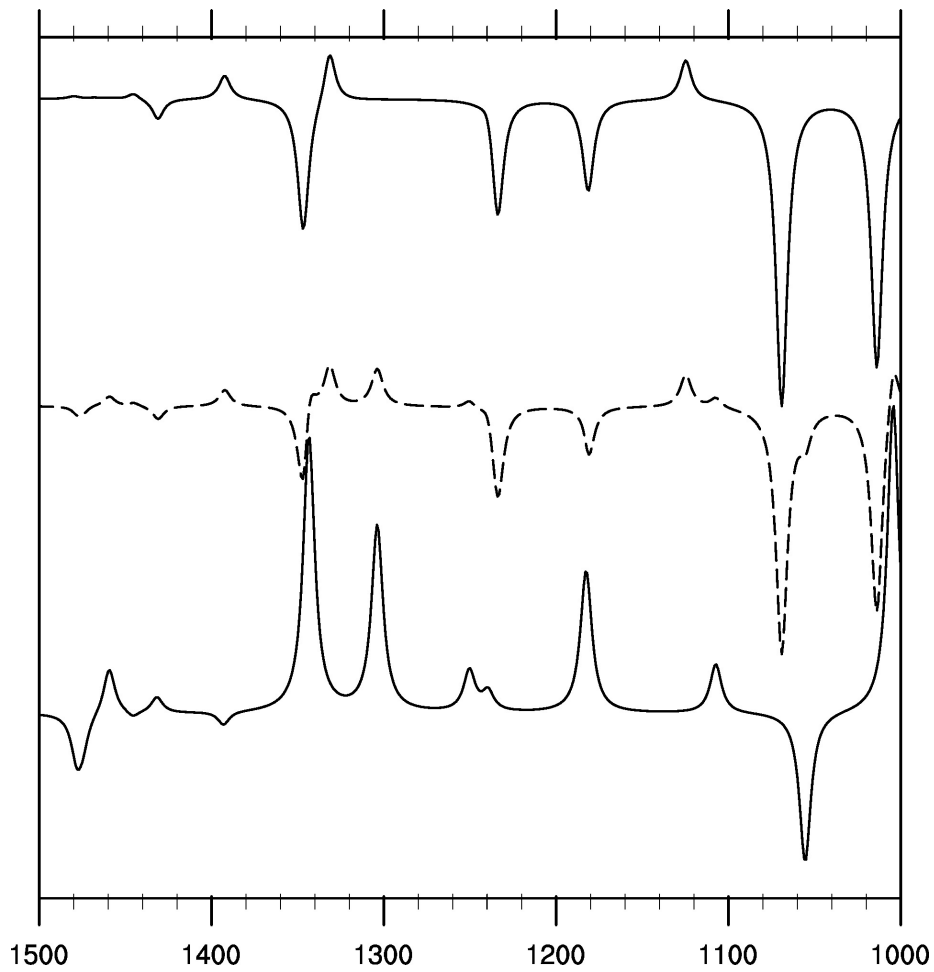


Figure S3-6: Simulated VCD spectra (B3LYP; Stuttgart/6-31Gd) for **3a-c1** (top), the Boltzmann-averaged **3a-c1/c2** (80%/20%; middle), **3a-c2** (bottom).

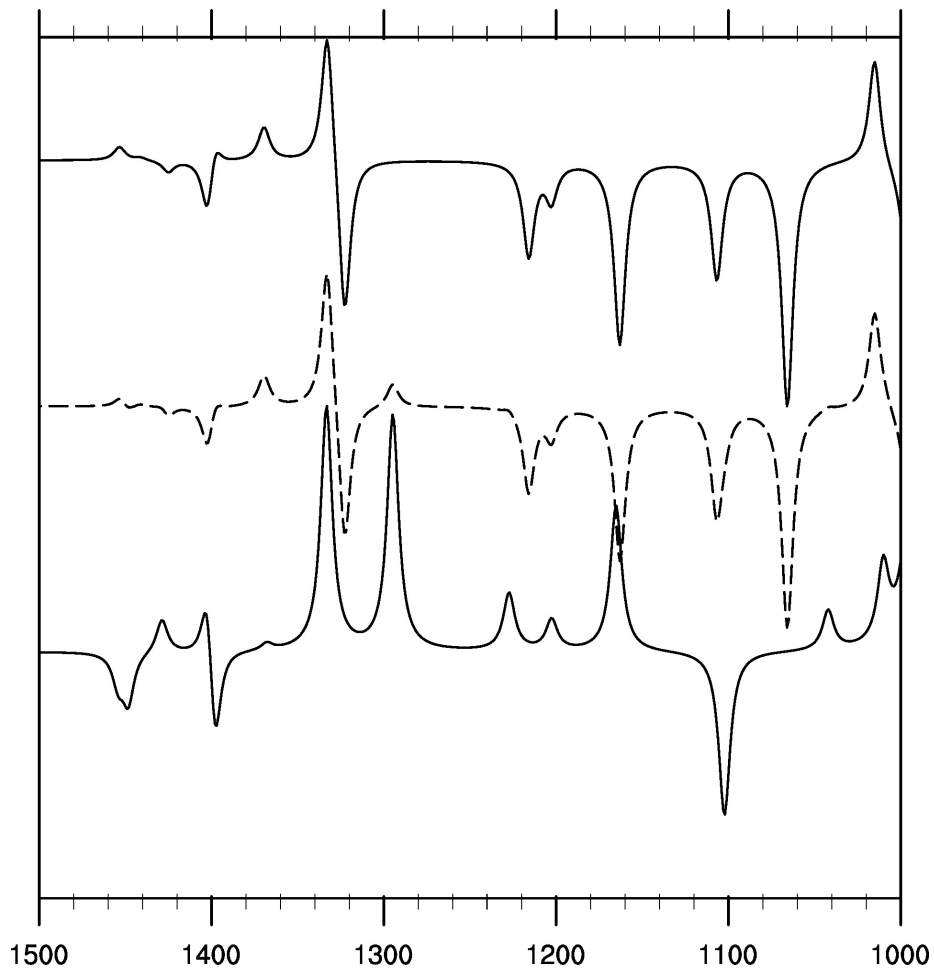


Figure S3-7: Simulated VCD spectra (B3LYP; def2-TZVPP) for **3b-c1** (top), the Boltzmann-averaged **3b-c1/c2** (90%/10%; middle), **3b-c2** (bottom).

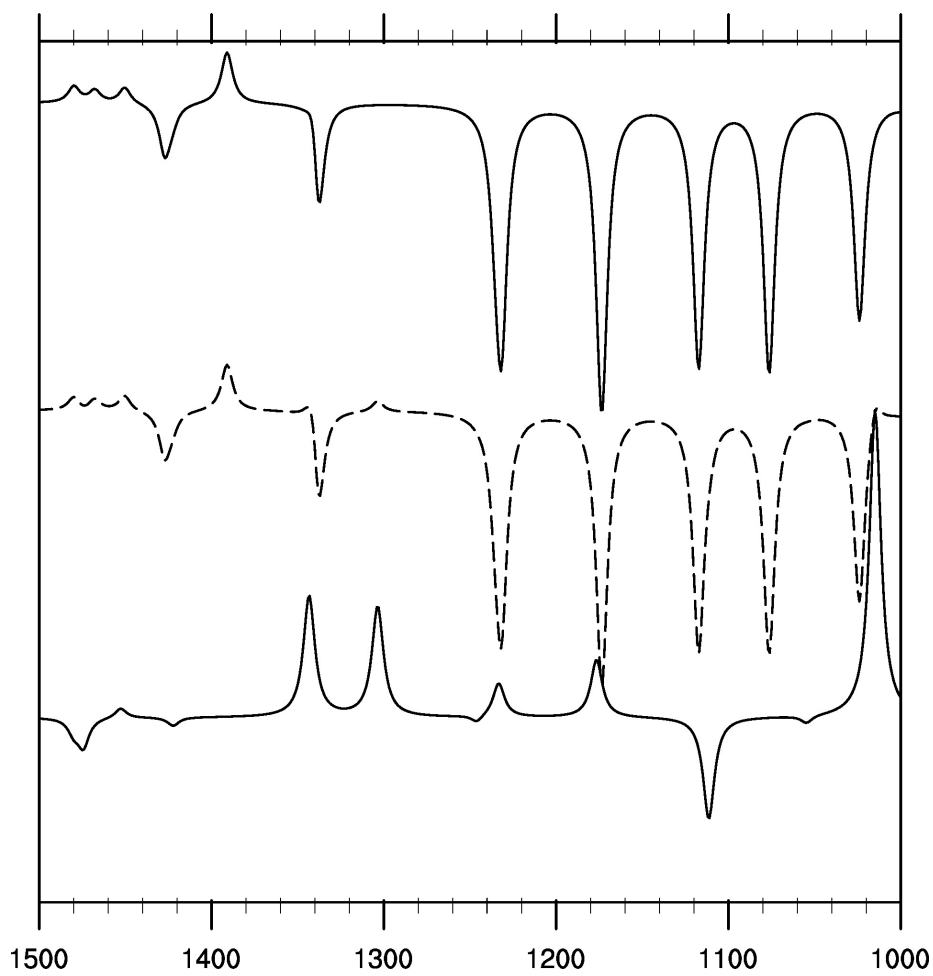


Figure S3-8: Simulated VCD spectra (B3LYP; Stuttgart/6-31Gd) for **3b-c1** (top), the Boltzmann-averaged **3b-c1/c2** (90%/10%; middle), **3b-c2** (bottom).