

New insights on the vibrational dynamics of 2-methoxy-, 4-methoxy- and 4-ethoxy-benzaldehyde from INS spectra and periodic DFT calculations

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Supplementary Material

Figure S1. *INS spectra of 2-methoxybenzaldehyde (a), 4-methoxybenzaldehyde (b) and 4-ethoxybenzaldehyde (c) up to 4000 cm⁻¹.*

Figure S2. *Discrete (G09) and periodic (CASTEP) INS spectra of 2-methoxybenzaldehyde (a), 4-methoxybenzaldehyde (b) and 4-ethoxybenzaldehyde (c) up to 900 cm⁻¹, compared with the experimental spectrum.*

Figure S3. *Experimental and calculated INS spectra for 4-ethoxybenzaldehyde*

Figure S4. *Experimental and calculated Far-IR spectra for 4-ethoxybenzaldehyde*

Figure S1. (a) *2-methoxybenzaldehyde*

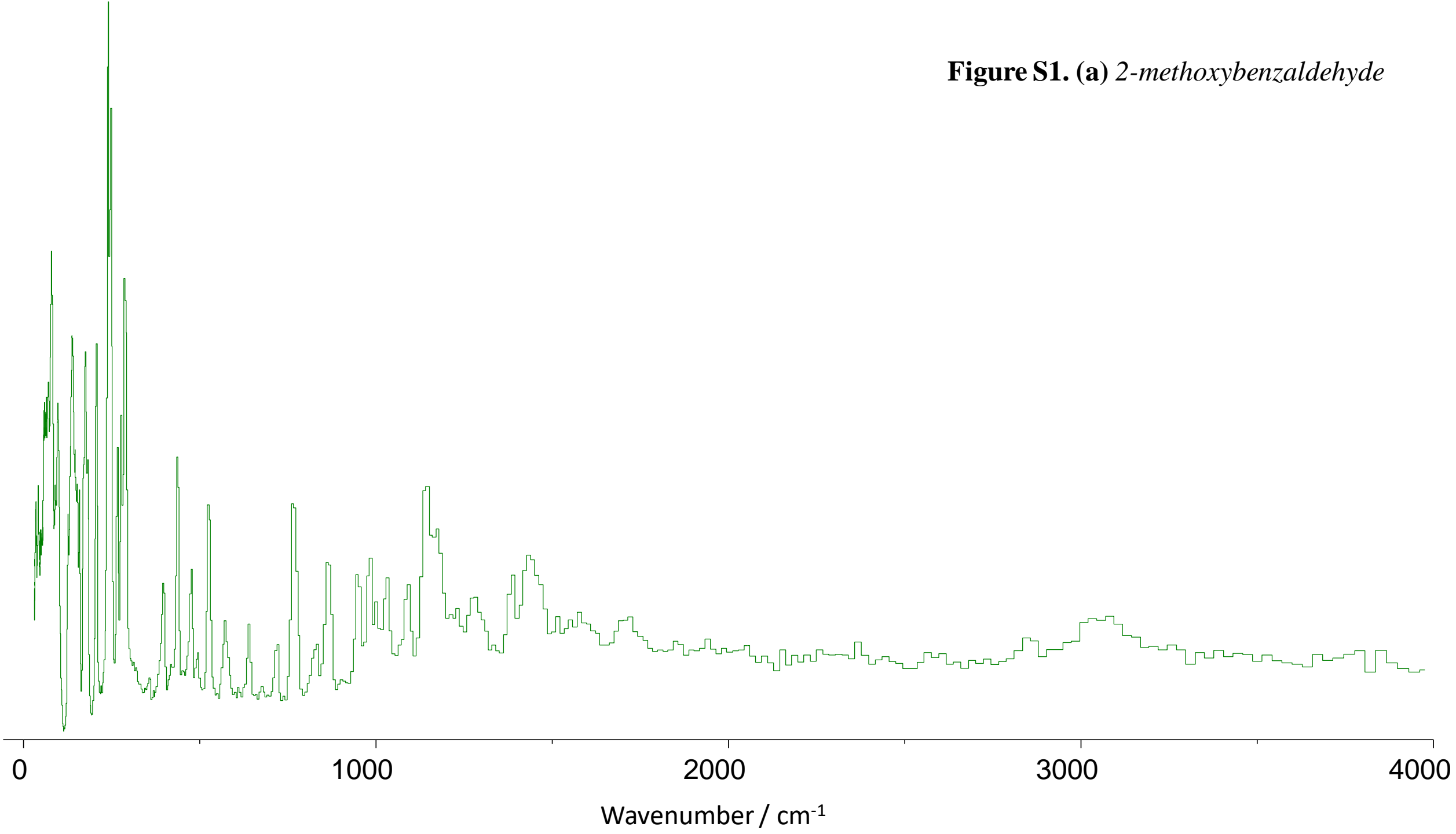


Figure S1. (b) *4-methoxybenzaldehyde*

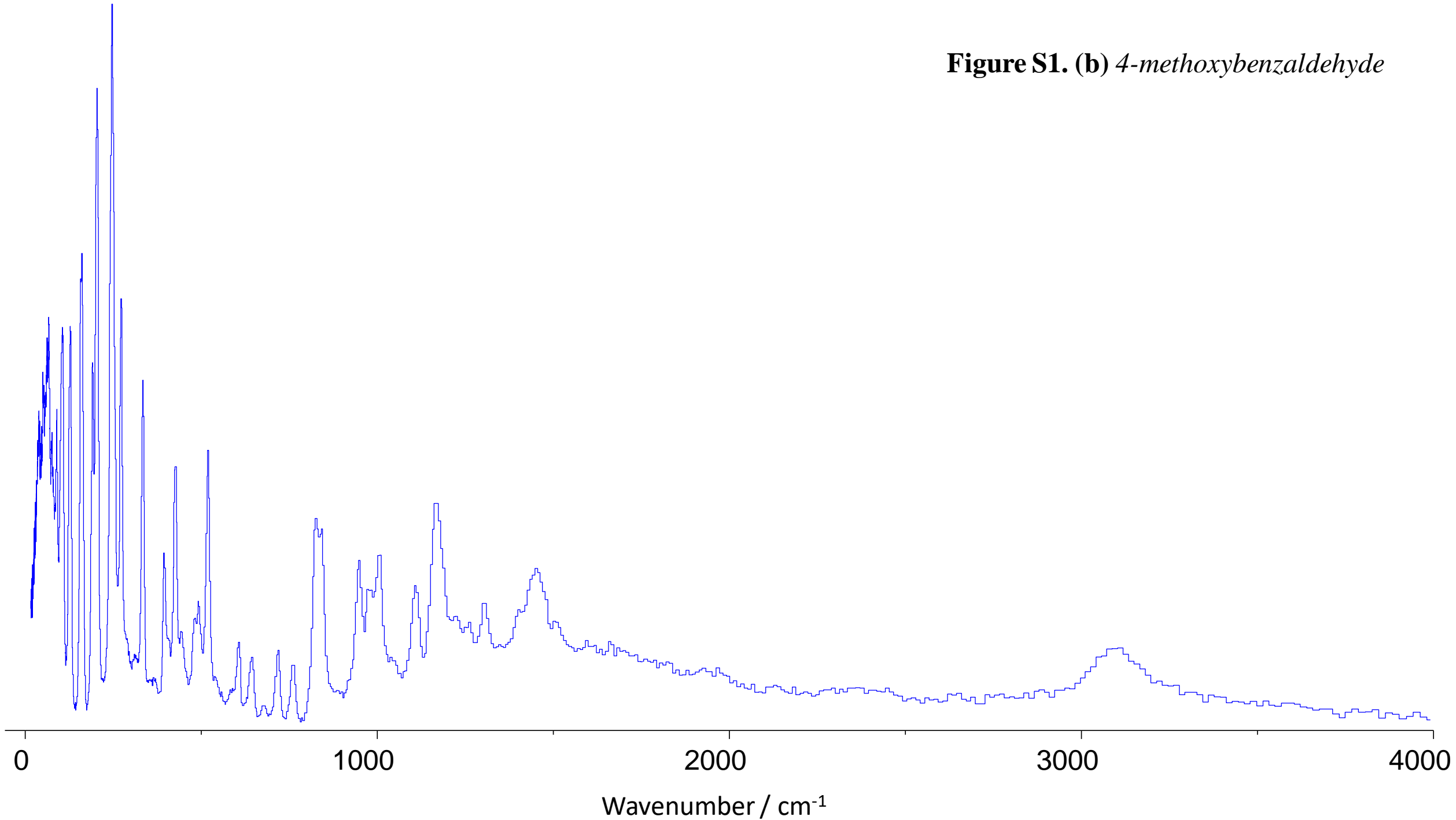


Figure S1. (c) *4-ethoxybenzaldehyde*

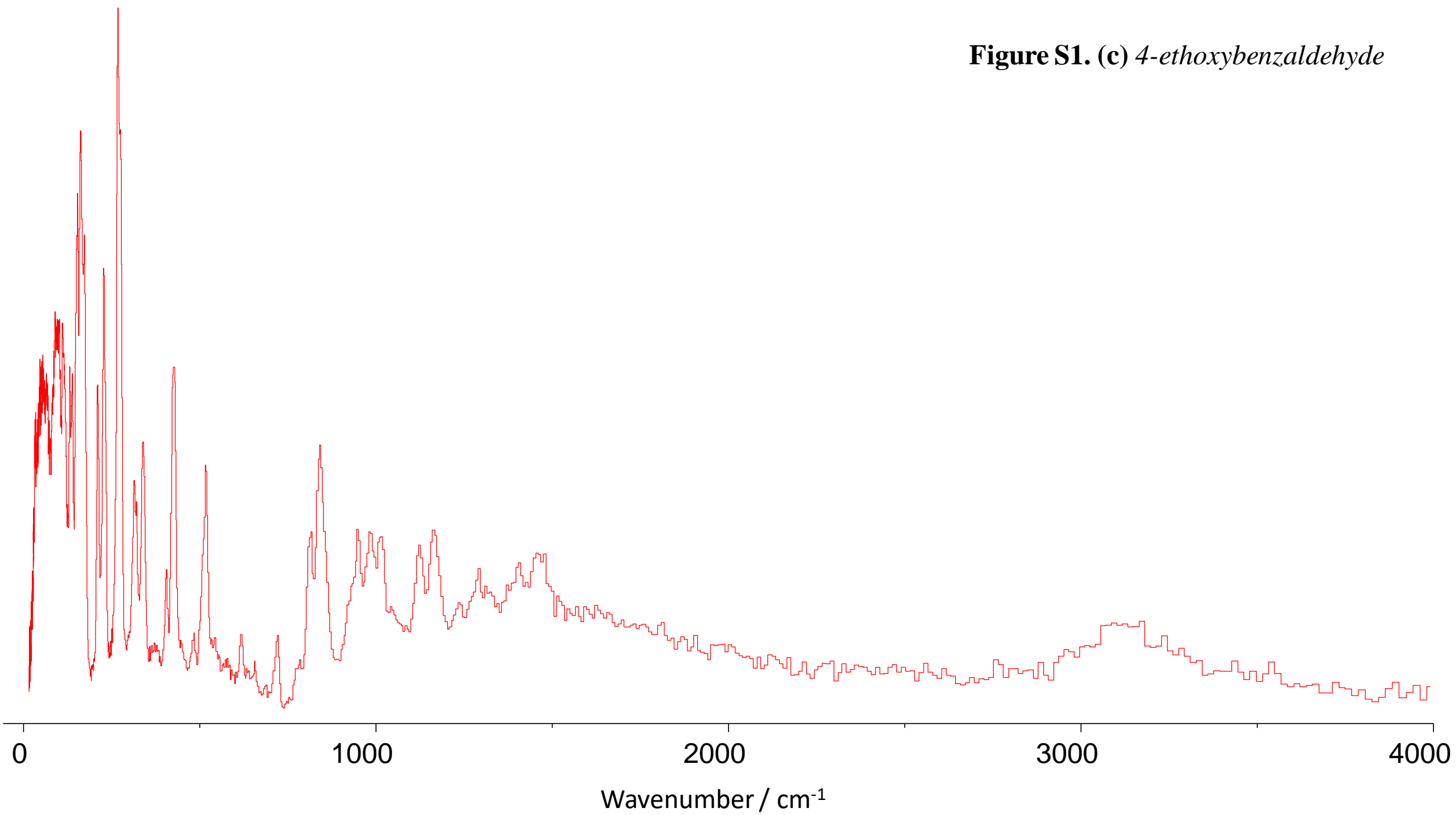


Figure S2. (a) *2-methoxybenzaldehyde*

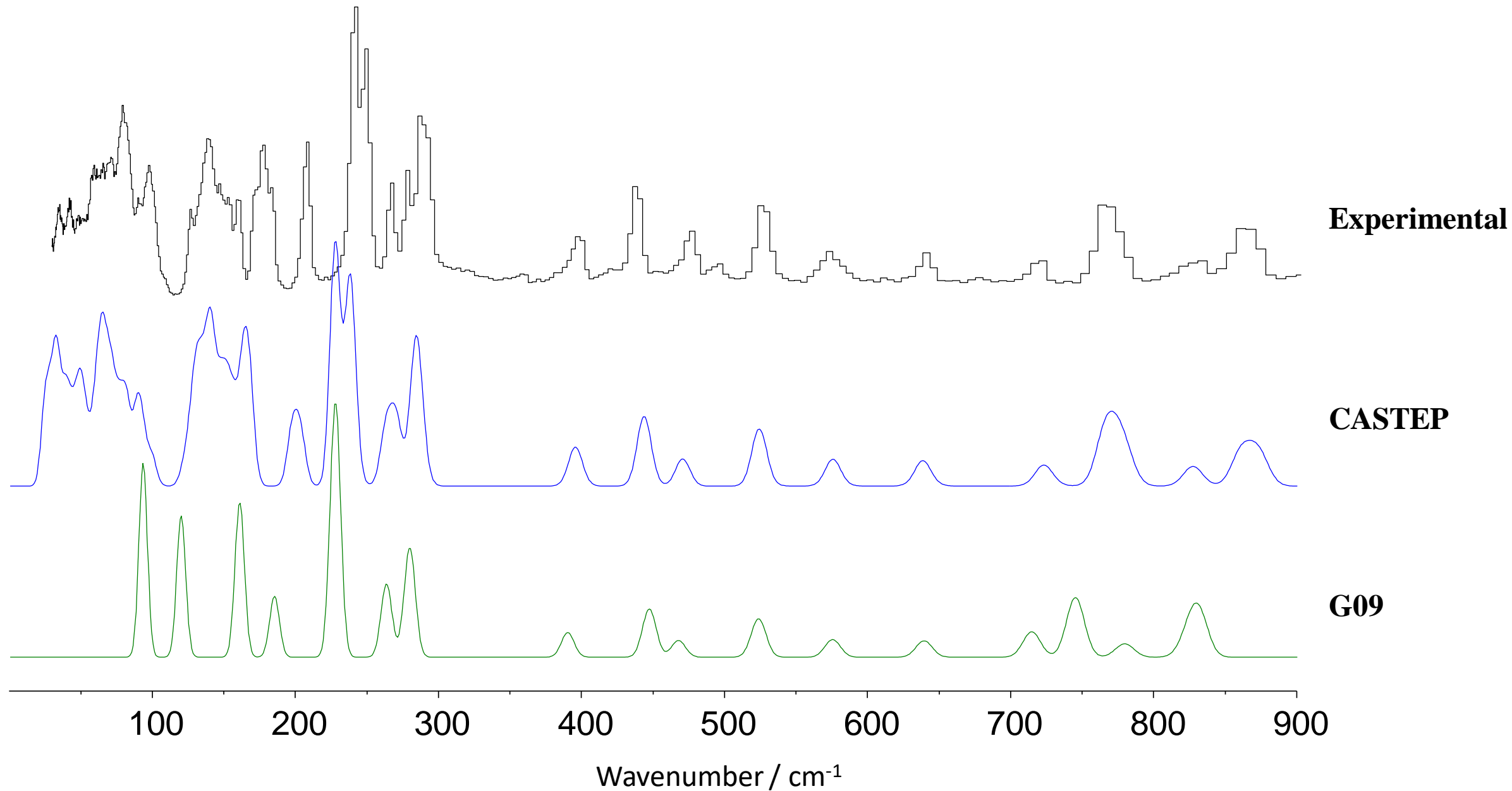


Figure S2. (b) *4-methoxybenzaldehyde*

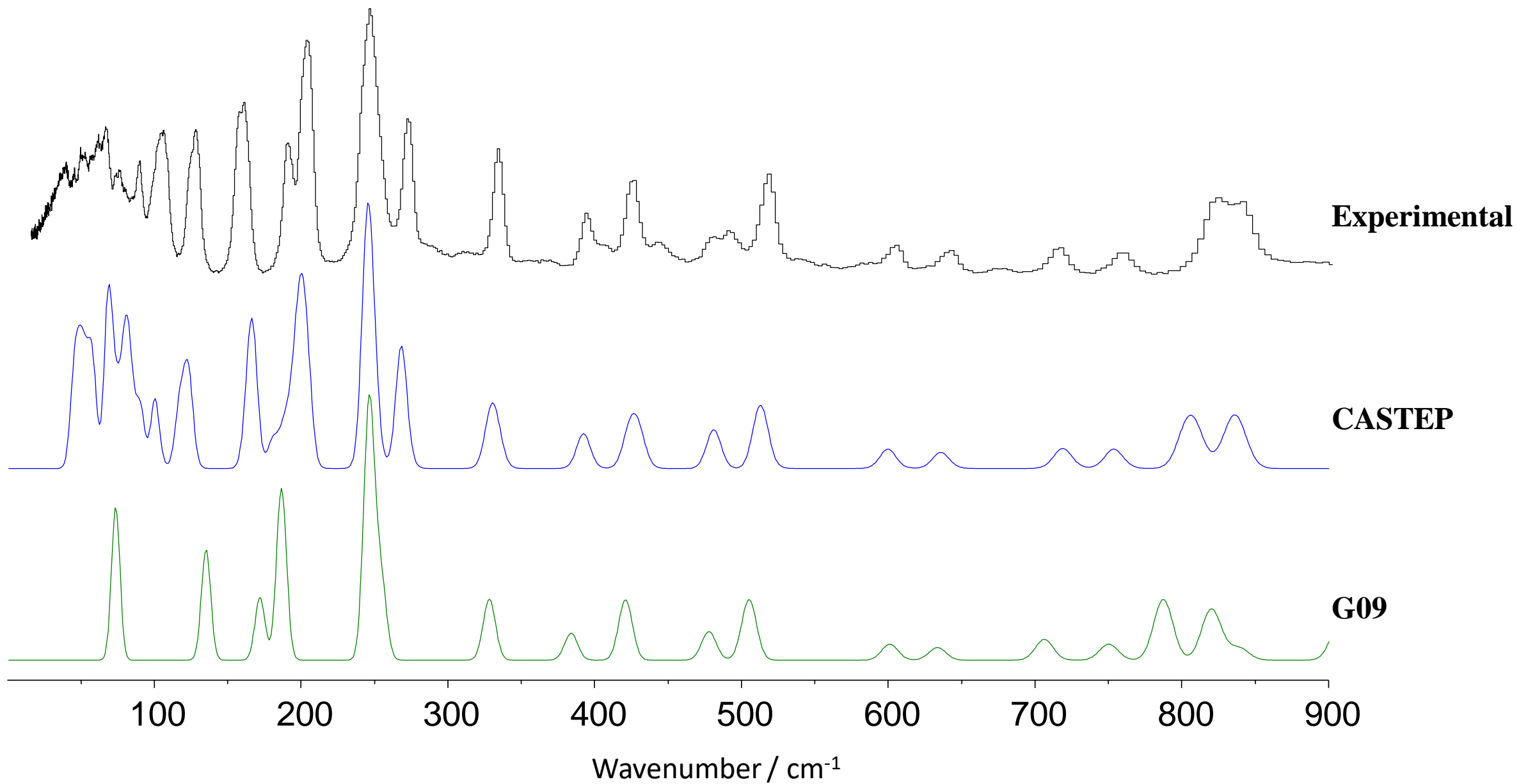


Figure S2. (c) *4-ethoxybenzaldehyde*

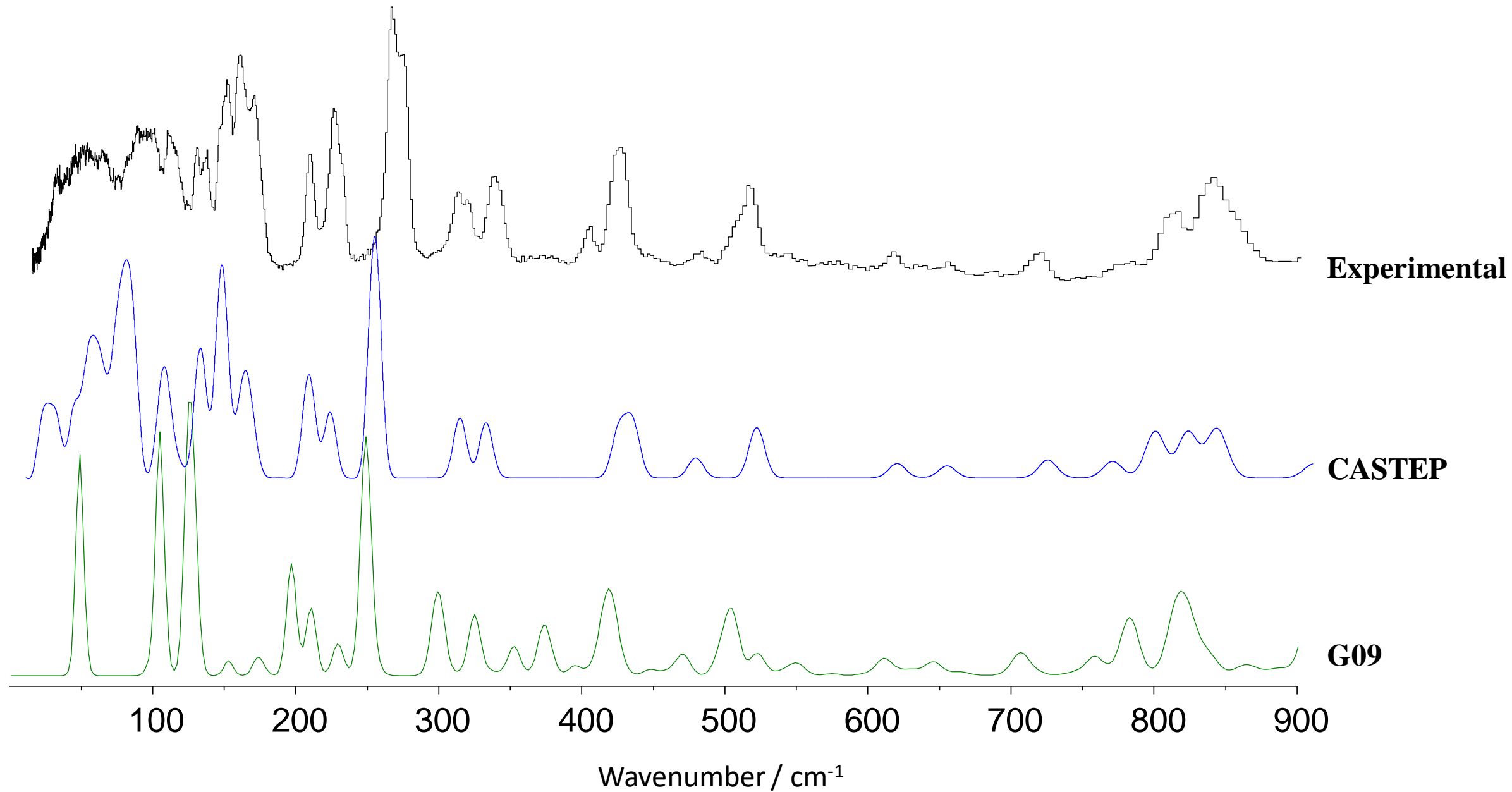


Figure S3. *Experimental and calculated INS spectra for 4-ethoxybenzaldehyde*

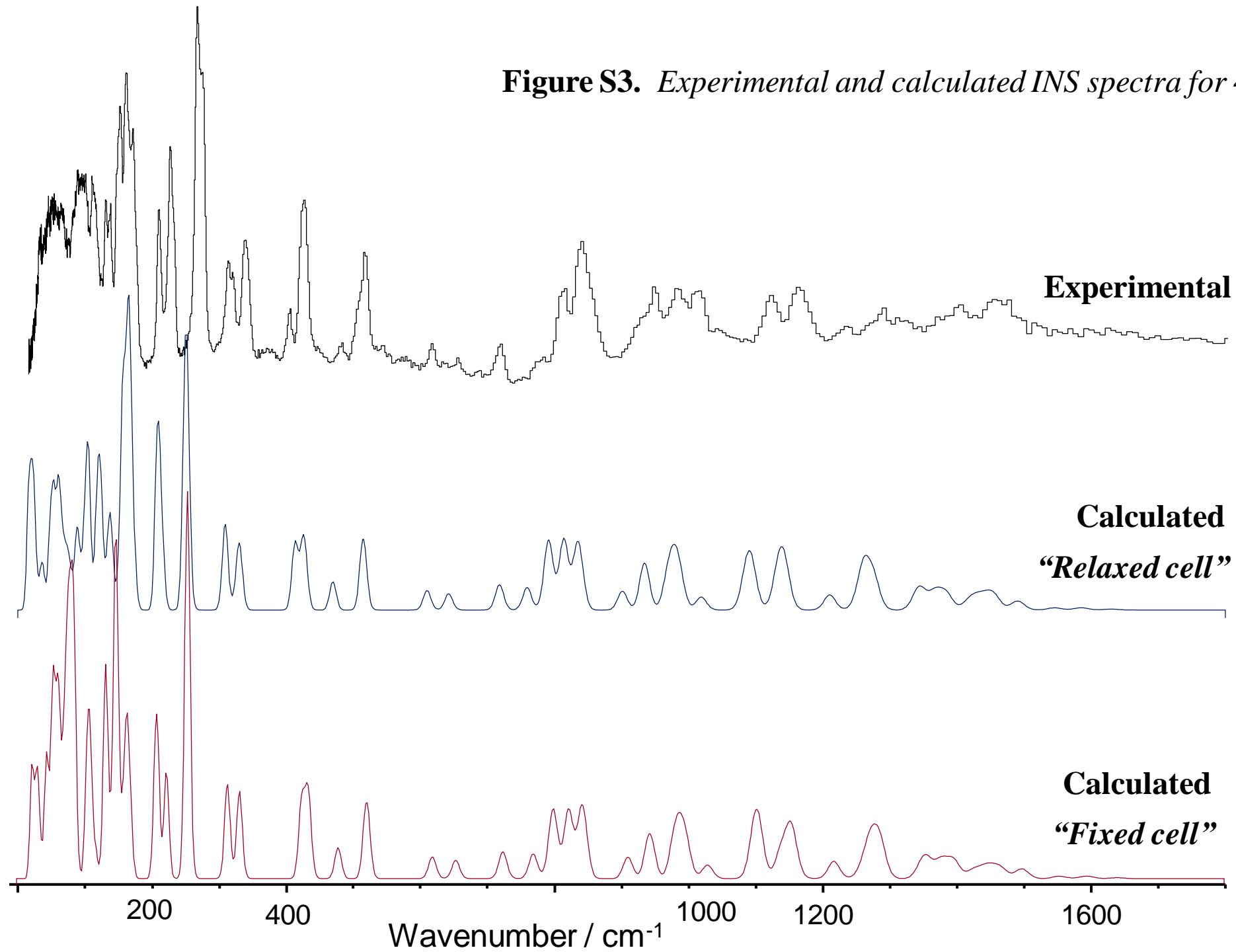


Figure S4. *Experimental and calculated Far-IR spectra for 4-ethoxybenzaldehyde*

