Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The Crystal Structure, Thermal Expansion and Far-IR Spectrum of Propanal (CH_3CH_2CHO) Determined using Powder X-ray Diffraction, Neutron Scattering, Periodic DFT and Synchrotron Techniques.

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Supplementary Information

Table S1: Table of lattice parameters presented in figure 4 of the main manuscript.

Temp (K)	a (Å)	b (Å)	c (Å)	β (°)	V (Å)
100.9	8.9837	4.2219	9.4758	97.473	356.32
102.9	8.9846	4.2219	9.4751	97.462	356.35
105.0	8.9851	4.2246	9.4747	97.468	356.42
107.0	8.9856	4.2276	9.4768	97.459	356.7
109.0	8.9867	4.2288	9.4763	97.464	356.95
111.1	8.9876	4.2318	9.4798	97.46	357.25
113.1	8.9902	4.2335	9.4782	97.467	357.54
115.1	8.9936	4.2361	9.481	97.431	357.94
117.2	8.9945	4.2382	9.4815	97.427	358.22
119.2	8.995	4.2414	9.484	97.42	358.52
121.2	8.9988	4.2434	9.4829	97.417	358.9
123.3	9.0009	4.2458	9.4844	97.387	359.23
125.3	9.0032	4.249	9.4862	97.376	359.61
127.3	9.0036	4.2499	9.4856	97.38	359.87
129.4	9.007	4.2533	9.4882	97.362	360.2
131.4	9.007	4.2558	9.49	97.36	360.54
133.4	9.0098	4.2585	9.4914	97.346	360.93
135.5	9.0116	4.2609	9.4924	97.352	361.26
137.5	9.0122	4.2633	9.4941	97.343	361.56
139.6	9.0124	4.2656	9.4927	97.342	361.72
141.6	9.0159	4.2681	9.4947	97.32	362.15
143.6	9.0175	4.2711	9.4976	97.302	362.54
145.6	9.0169	4.274	9.4957	97.331	362.69
147.7	9.0216	4.2788	9.4984	97.289	363.25
149.7	9.0216	4.281	9.4962	97.3	363.58
151.7	9.0262	4.2845	9.497	97.263	364
153.8	9.0264	4.2872	9.4968	97.264	364.31
155.8	9.0269	4.2901	9.4972	97.27	364.55
157.8	9.0281	4.2937	9.4995	97.269	364.94
159.9	9.0312	4.2957	9.4966	97.259	365.26
161.9	9.0334	4.2984	9.4971	97.269	365.54
163.9	9.0318	4.3003	9.4995	97.271	365.79

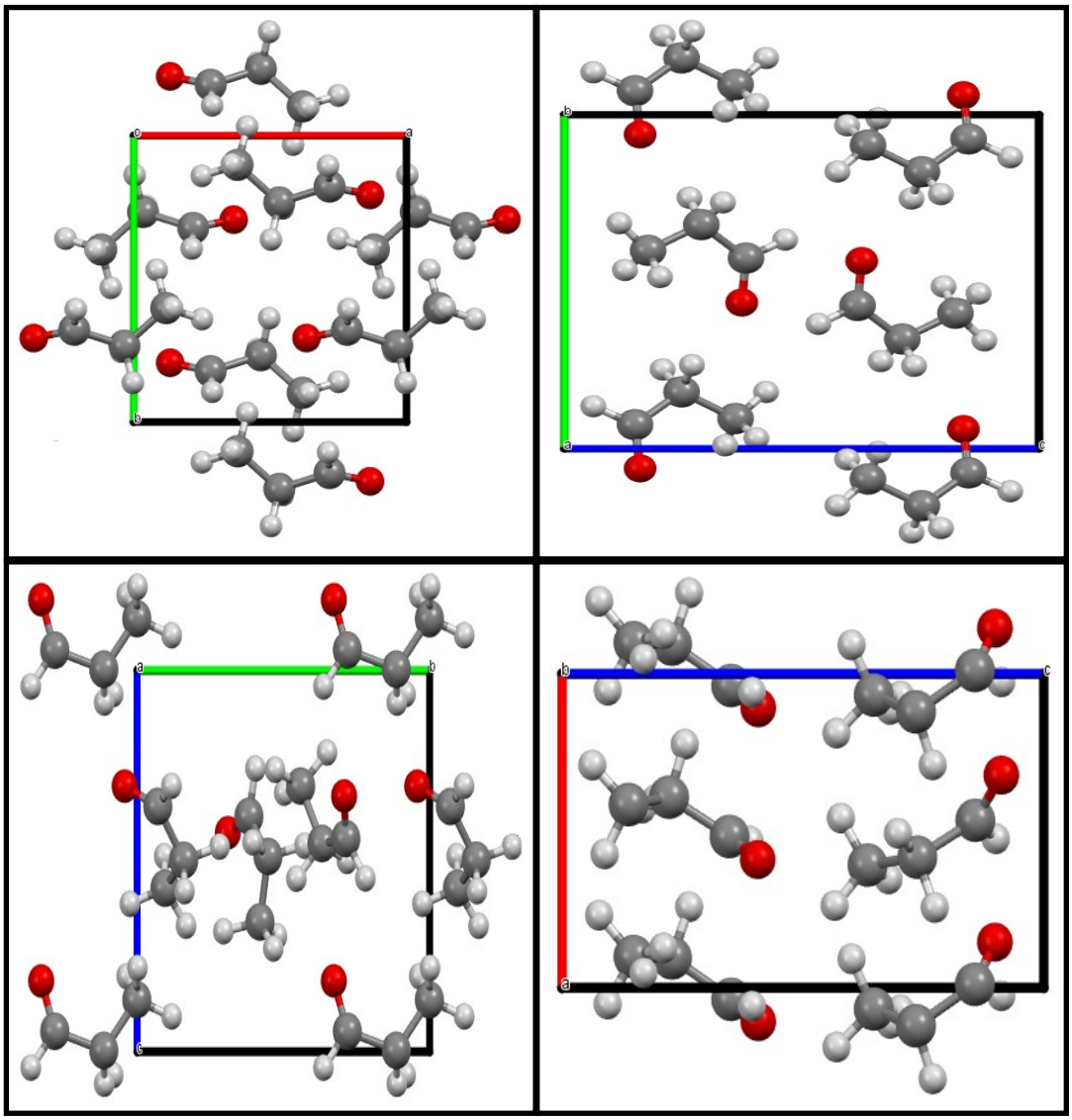

Figure S1: Predicted propanal unit cells generated from C17 calculations. Optimised geometries from modified (a) propionitrile, (b) propanoic acid, (c) N-methyl formamide, and (d) acetone literature structures reduced to *P*1 symmetry.

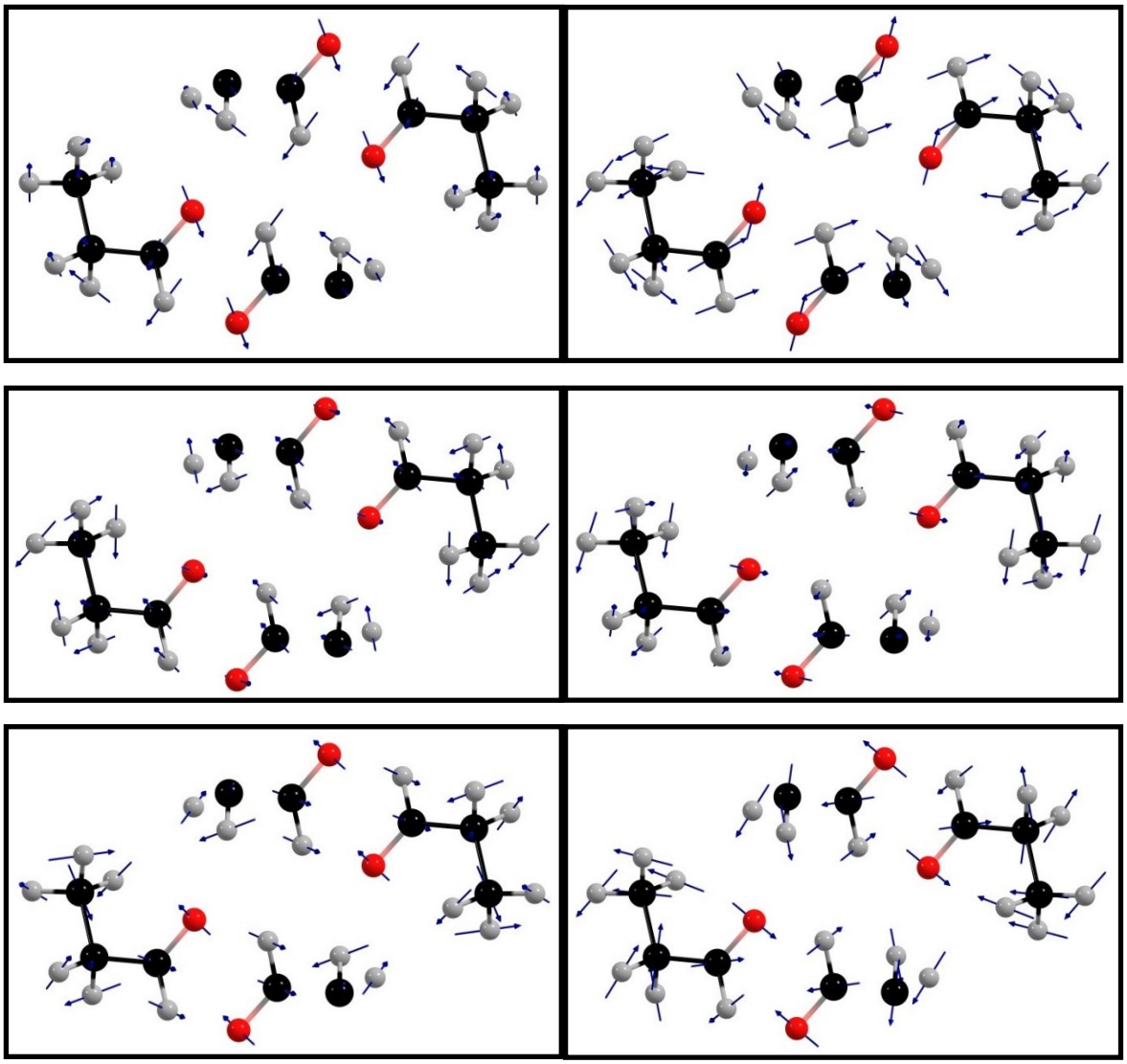

Figure S2: Atomic displacement vectors for low frequency vibration modes (a) 66 cm^{-1}, (b) 86 cm^{-1}, (c) 103 cm^{-1}, (d) 121 cm^{-1}, (e) 183 cm^{-1}, and (f) 264 cm^{-1} as calculated by C17 harmonic frequency calculations.