

Supplementary information

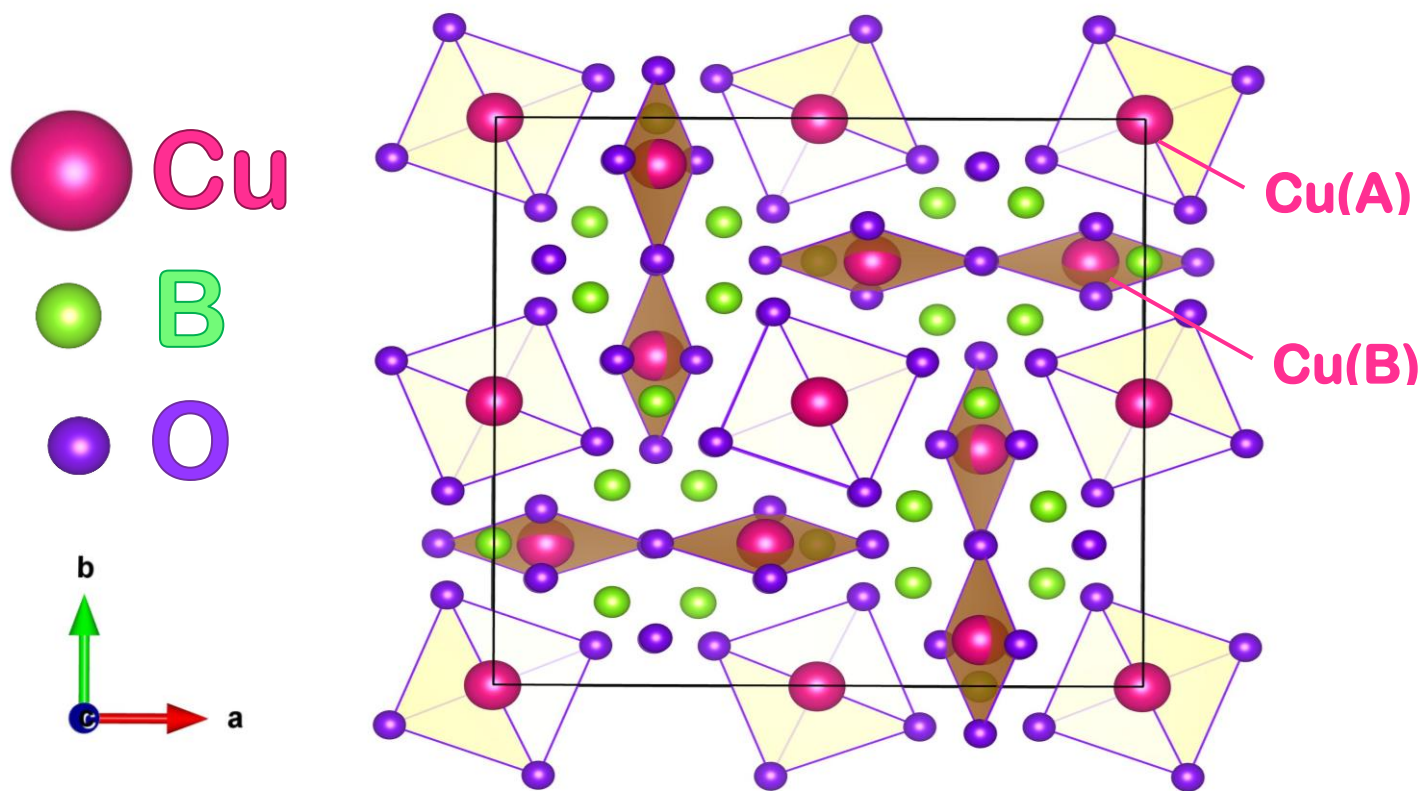
Anomalous boron isotope effects on electronic structure and lattice dynamics of CuB_2O_4

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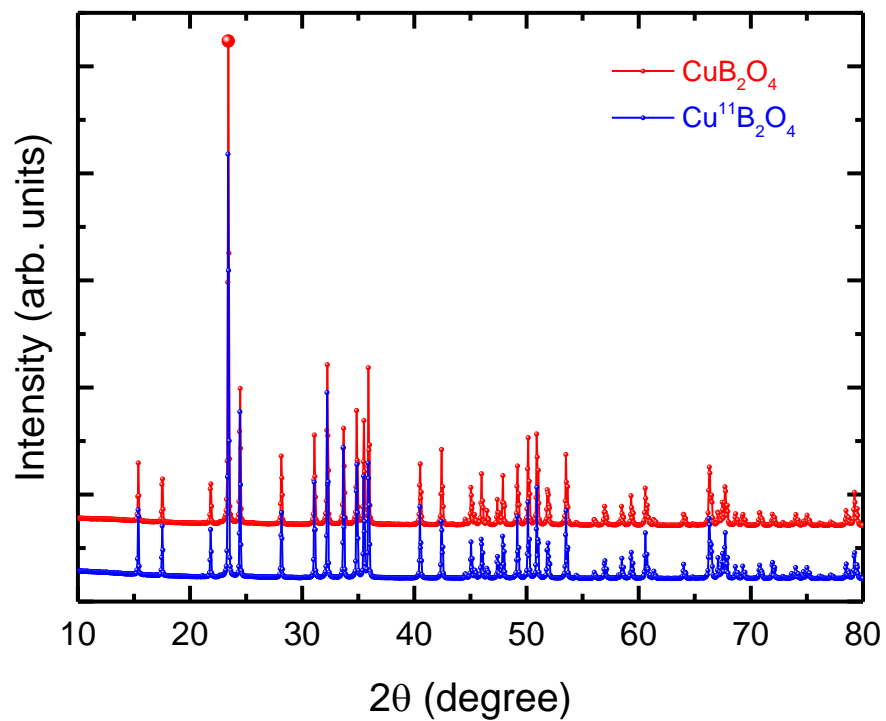
¹Department of Physics, National Taiwan Normal University, Taipei 11677, Taiwan

²Department of Physics, Tamkang University, Tamsui, New Taipei City 25137, Taiwan

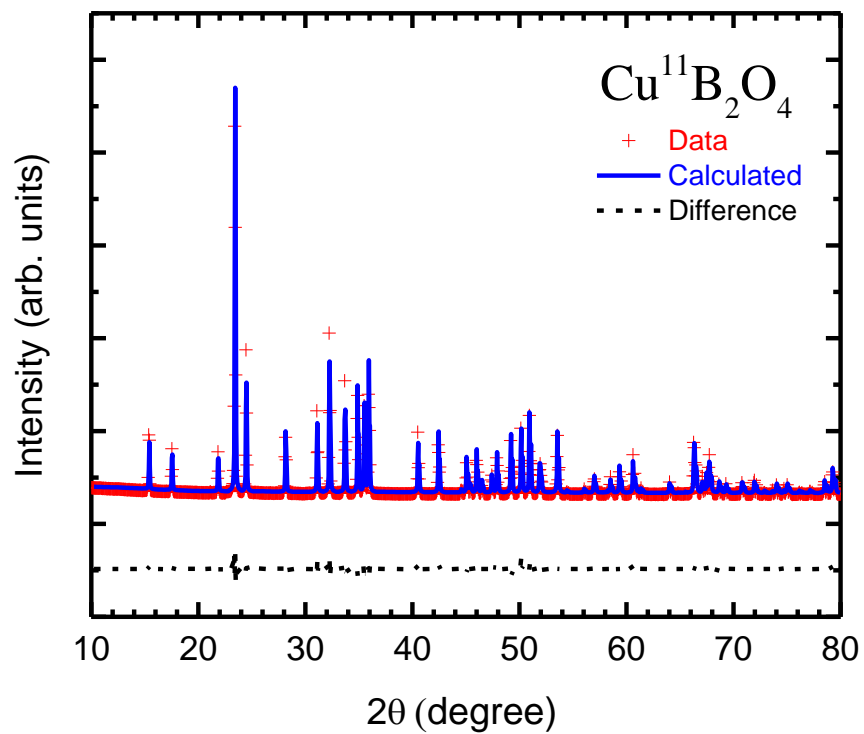
*Corresponding author: hliu@ntnu.edu.tw



Supplementary Fig. 1. The crystal structure of CuB_2O_4 .



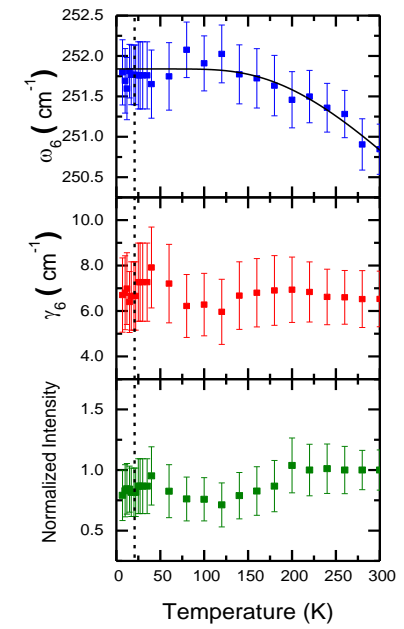
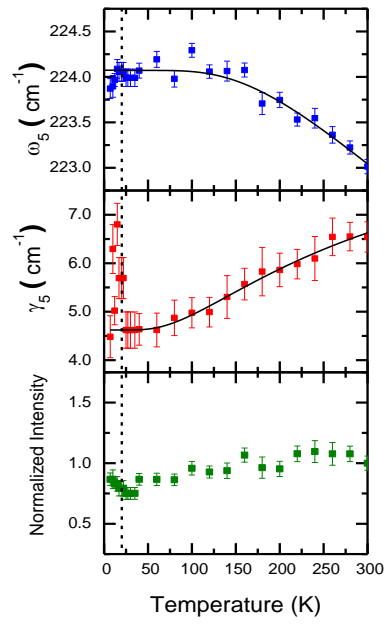
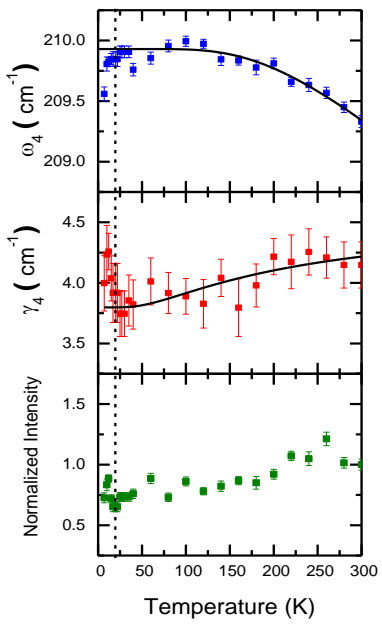
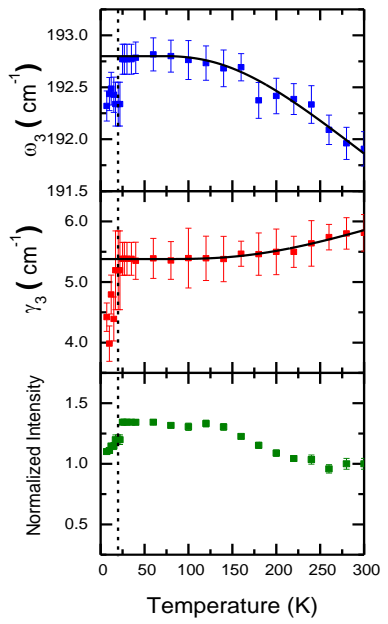
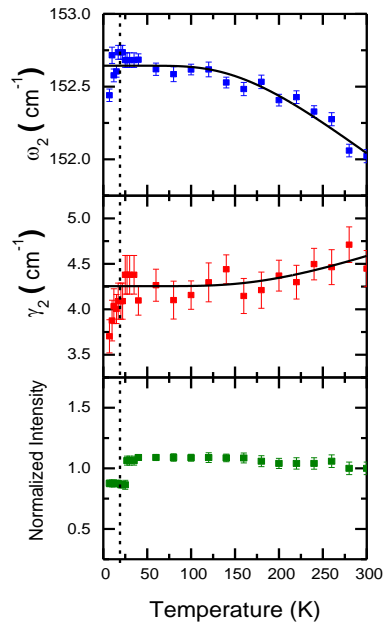
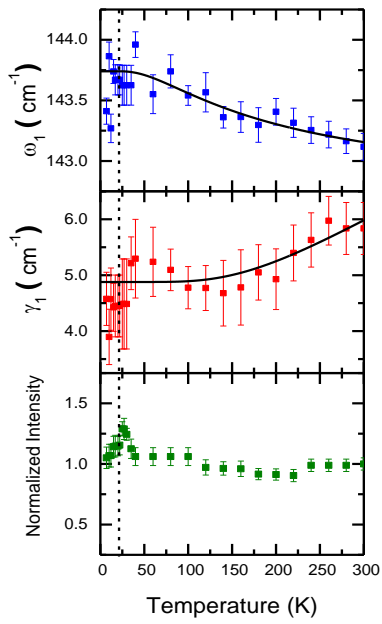
Supplementary Fig. 2. X-ray powder diffraction patterns for CuB_2O_4 and $\text{Cu}^{11}\text{B}_2\text{O}_4$ show high similarity.

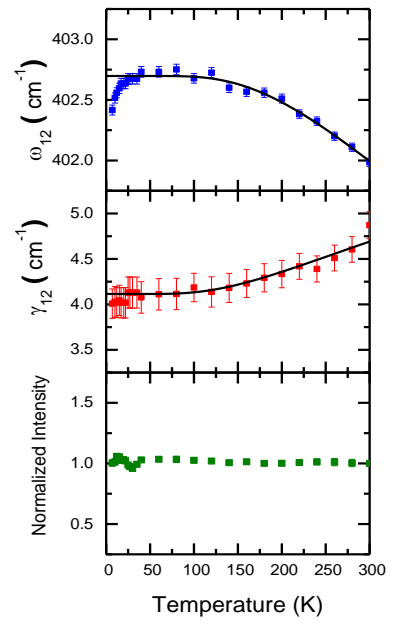
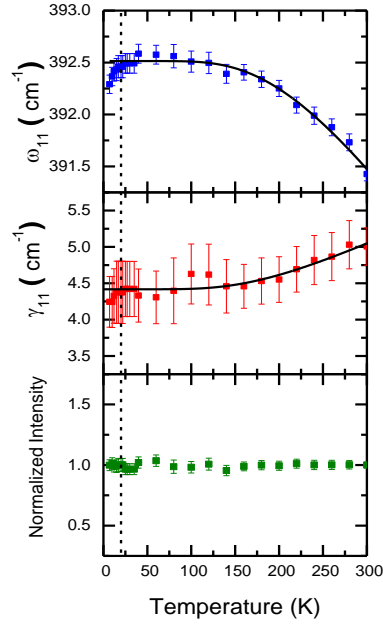
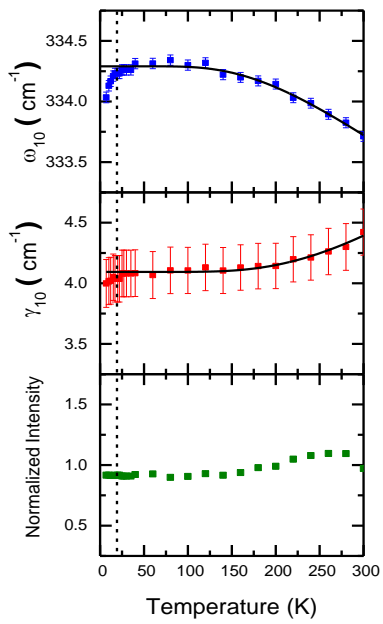
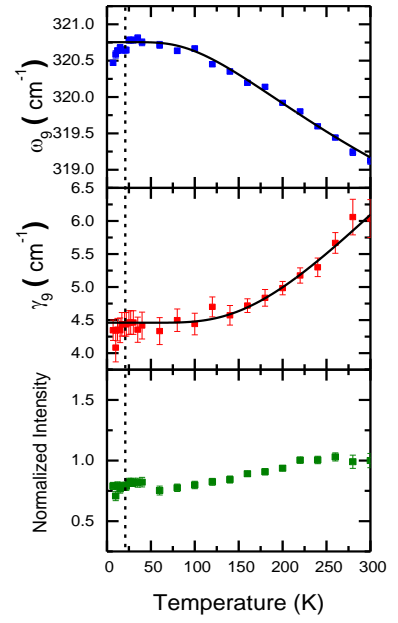
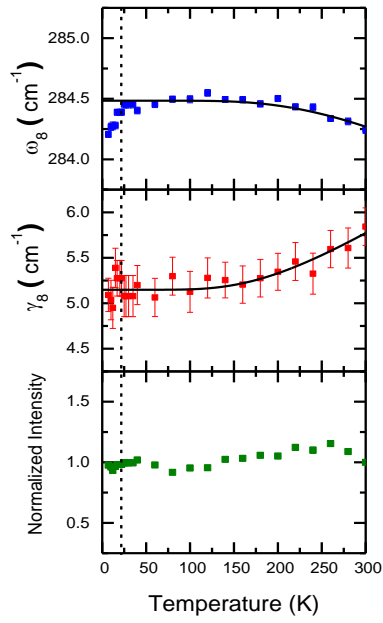
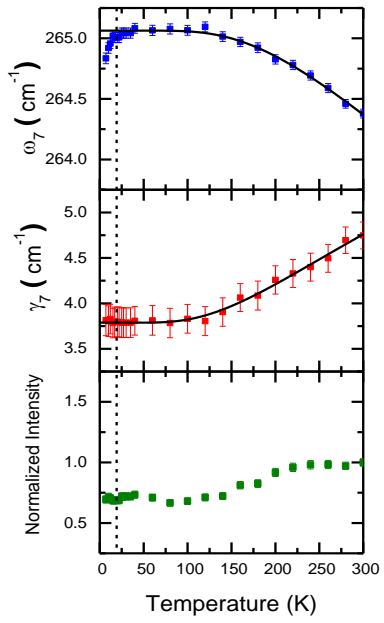


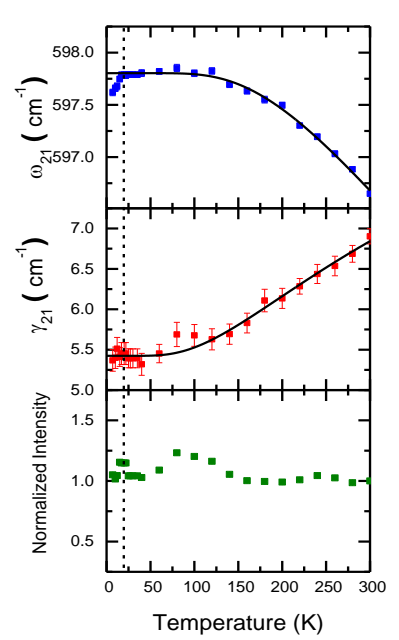
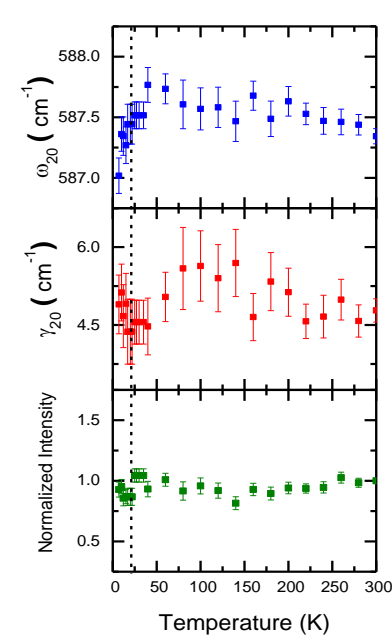
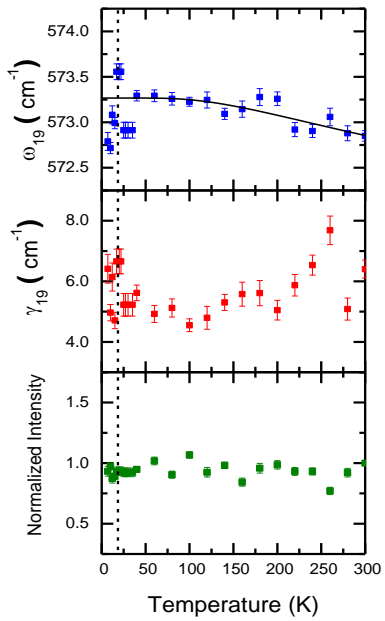
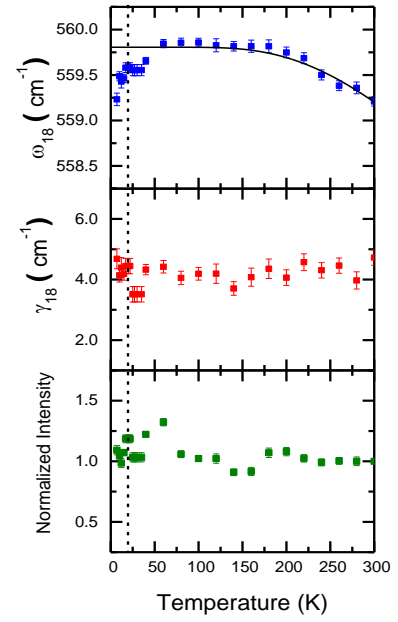
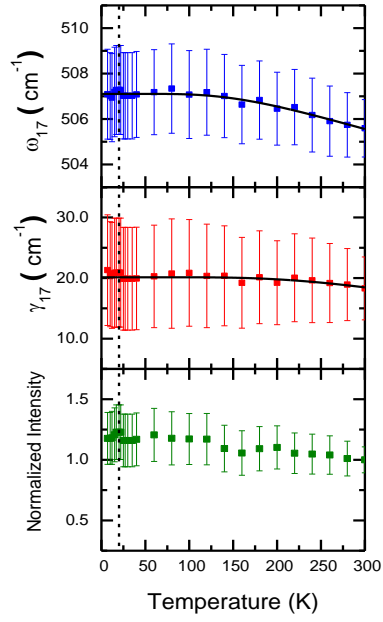
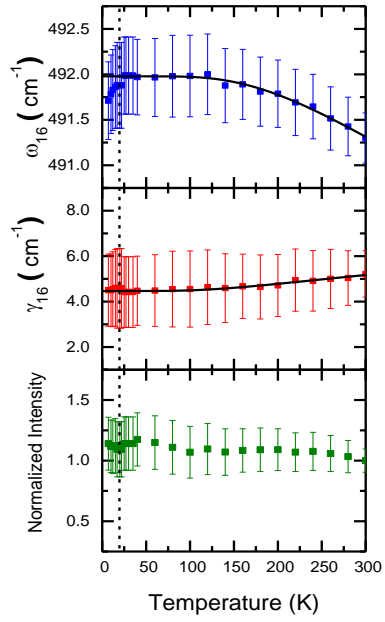
Supplementary Fig. 3. Observed, calculated, and difference of X-ray powder diffraction patterns for $\text{Cu}^{11}\text{B}_2\text{O}_4$.

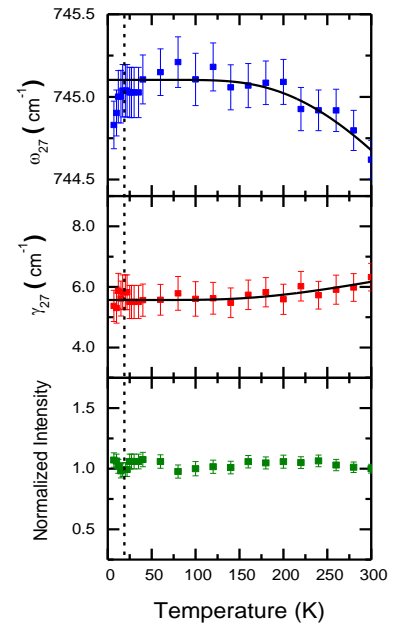
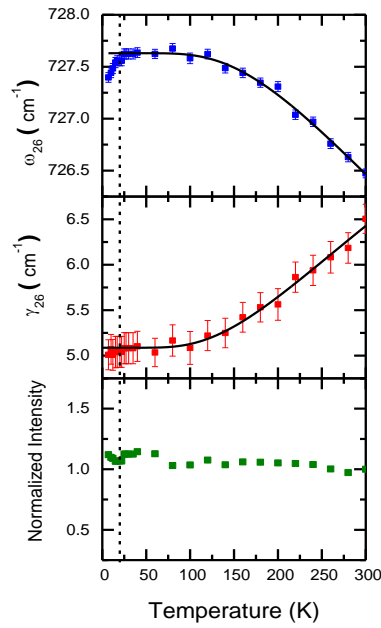
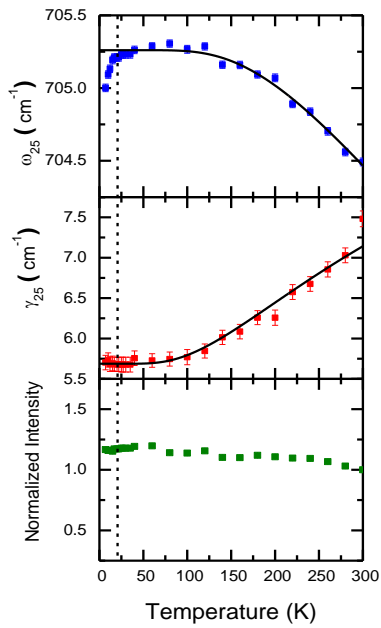
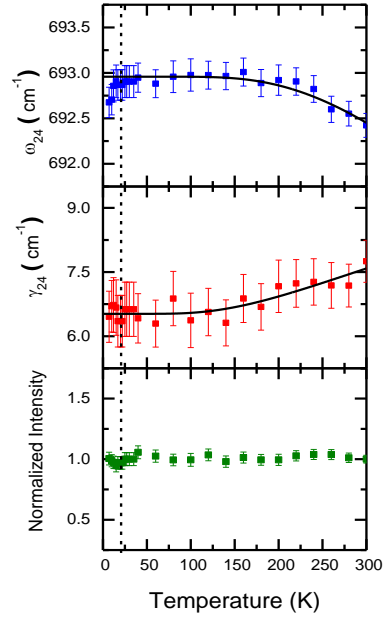
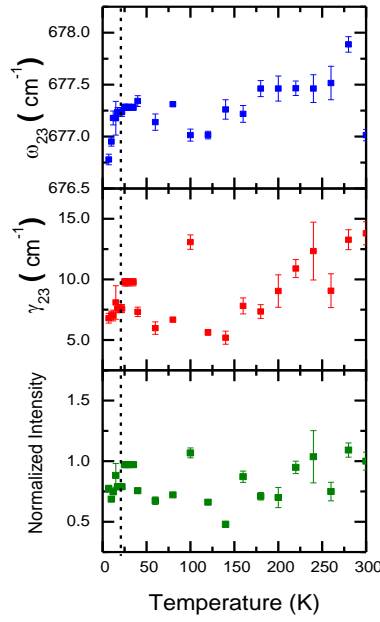
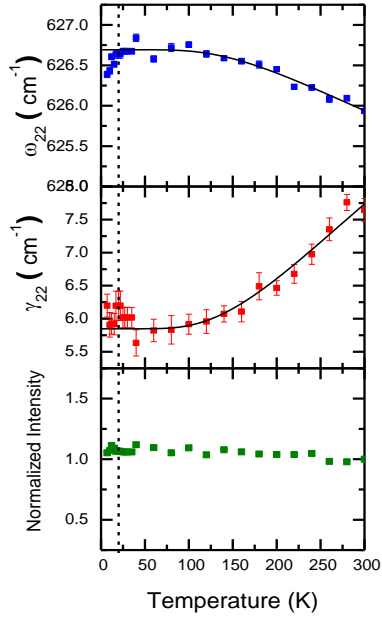
Supplementary Table 1. Crystallographic data for Cu¹¹B₂O₄.

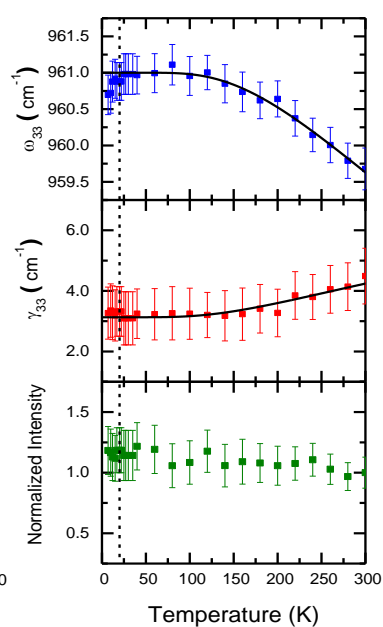
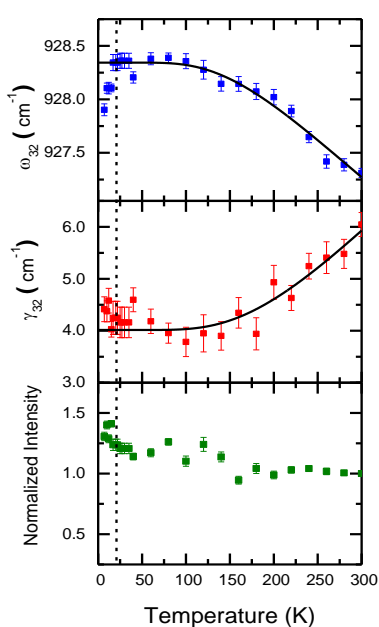
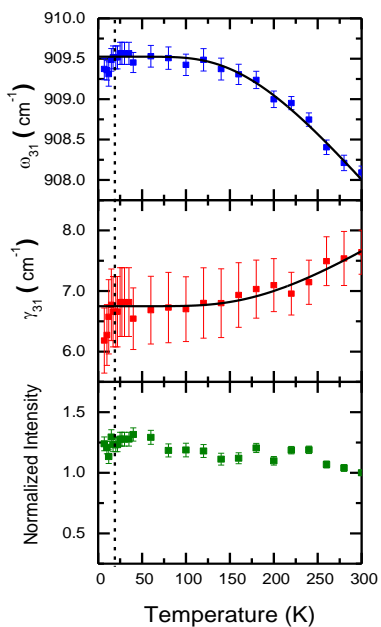
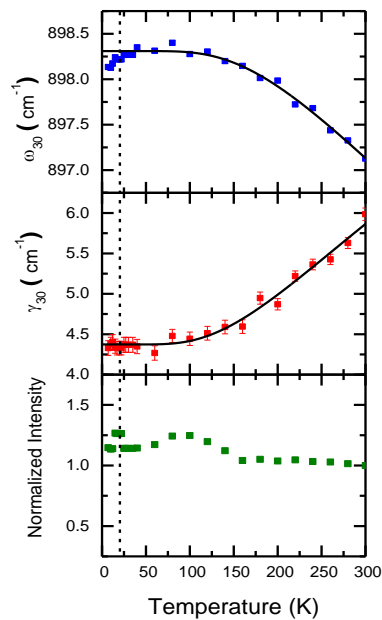
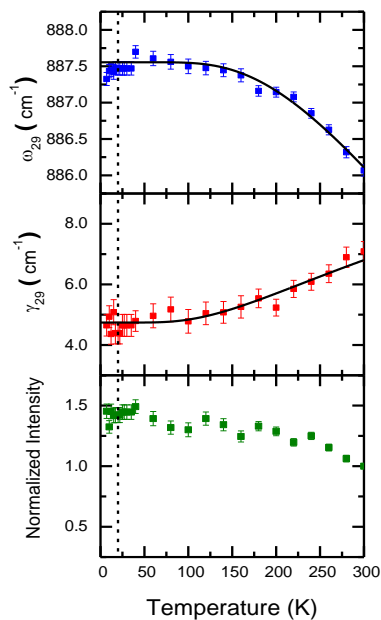
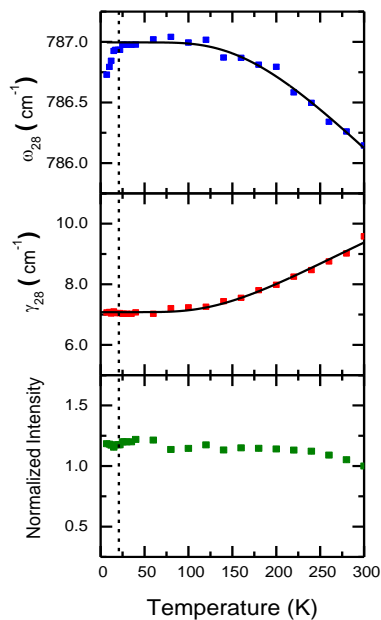
Parameters				
Lattice parameters				
a	11.4935 Å			
b	11.4935 Å			
c	5.6239 Å			
volume	742.919 Å ³			
Atomic position				
Label	Wyckoff position	x	y	z
O1	16e	0.16285	0.06764	0.49052
O2	8d	0.25074	0.25000	0.62500
O3	8d	0.25000	0.08335	0.87500
O4	16e	0.07236	0.18819	0.80329
B1	16e	0.18587	0.15422	0.69674
B2	8d	0.00933	0.25000	0.6250
Cu1	4b	0.00000	0.00000	0.50000
Cu2	8b	0.08168	0.25000	0.12500
Bond Length				
B1 – O1	1.5509 Å			
B1 – O2	1.3894 Å			
B1 – O3	1.4872 Å			
B1 – O4	1.4878 Å			
⟨B1 – O⟩	1.4788 Å			
B2 – O1	1.4859 Å			
B2 – O4	1.4265 Å			
⟨B2 – O⟩	1.4562 Å			
Cu1 – O1	2.0274 Å			
⟨Cu1 – O⟩	2.0274 Å			
Cu2 – O2	1.9261 Å			
Cu2 – O3	1.8968 Å			
Cu2 – O4	1.9267 Å			
⟨Cu2 – O⟩	1.9291 Å			
R_B	4.36 %			
R_{wp}	9.4 %			

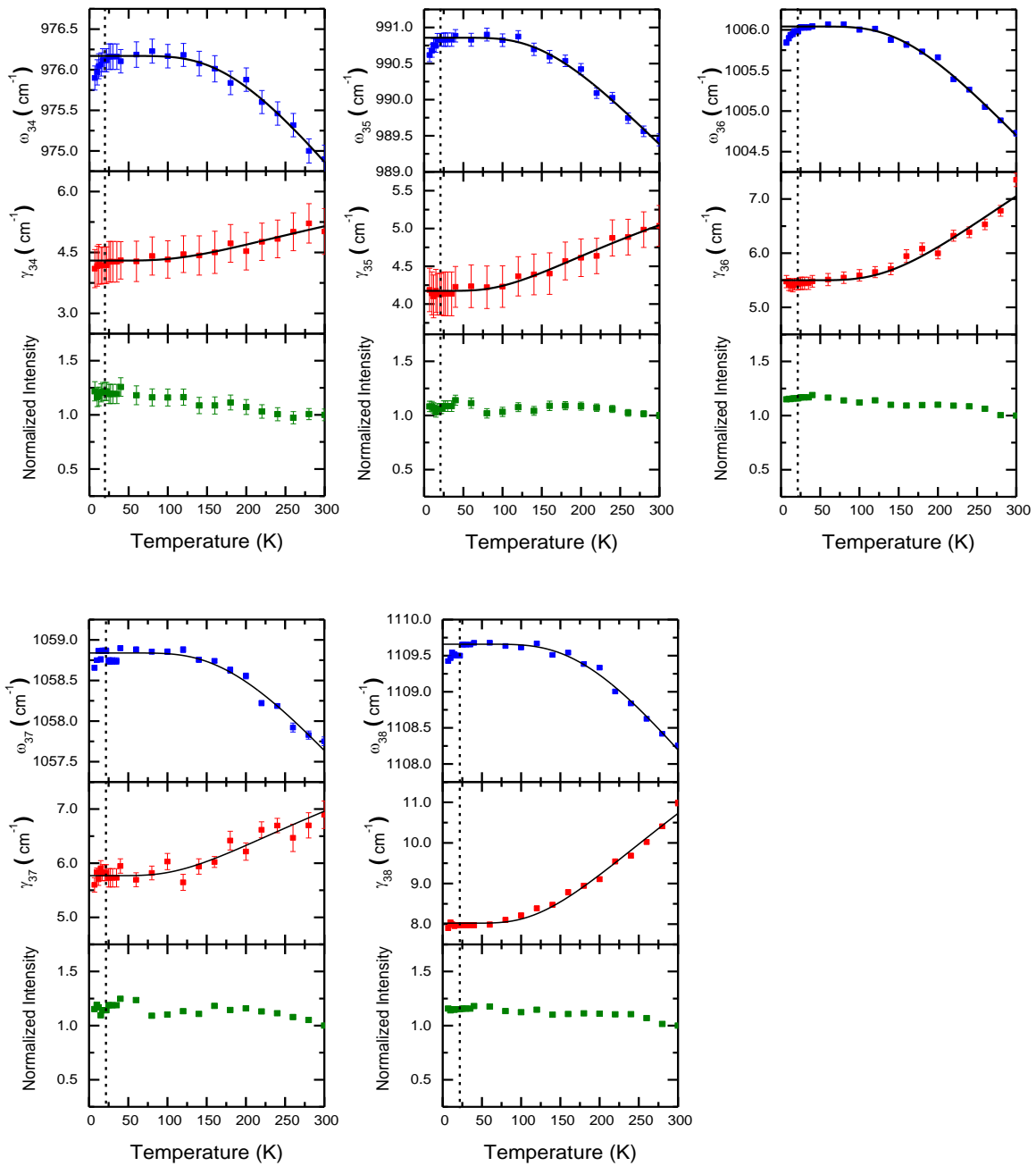












Supplementary Fig. 4. Temperature dependence of phonon peak energy, damping, and normalized intensity of $\text{Cu}^{11}\text{B}_2\text{O}_4$.