

{Co(HBpe)₂}V₄O₁₂: Pedal Motion Induced Order-Disorder P-1 → C-1 Transition and Disrupted C-1 → C2/m Displacive Transition due to Thermal Instability.

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SUPPORTING INFORMATION

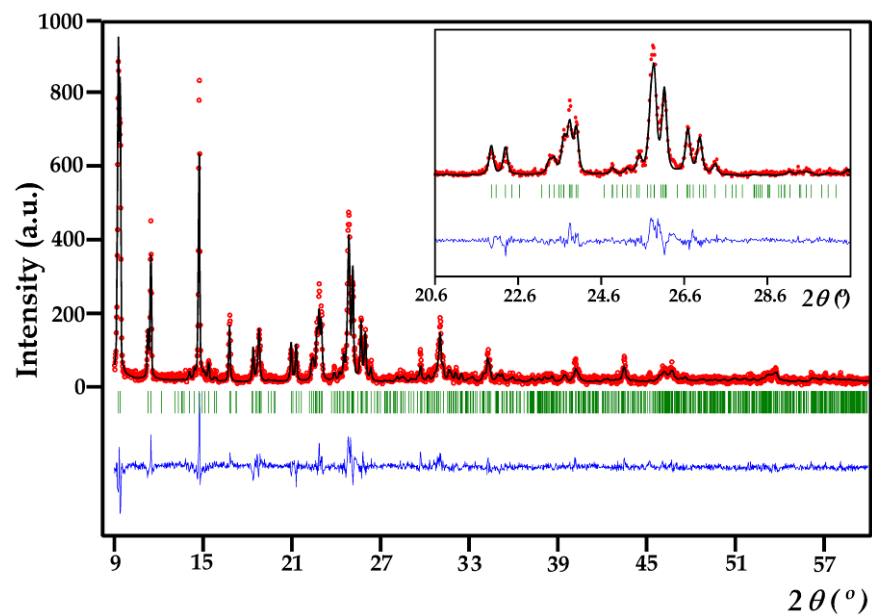


Figure S1. Rietveld refinement Red points: Experimental data; Black line: Calculated, Green bars: Reflection positions, Blue line: Experimental-Calculated.

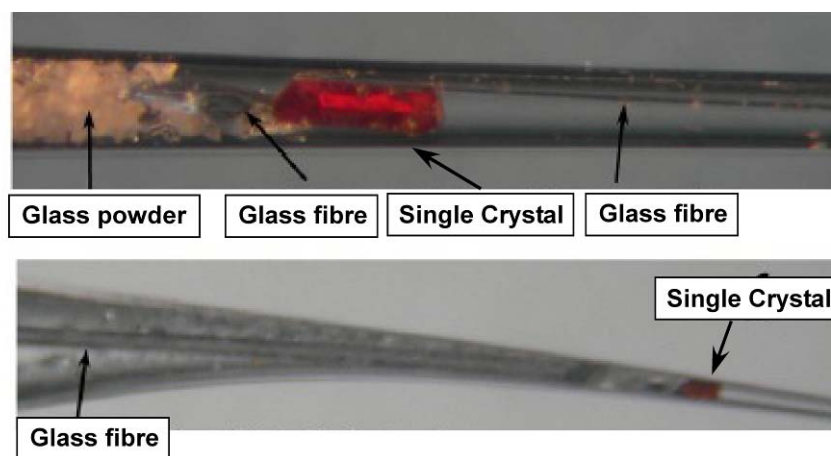


Figure S2. Device to measure the data single X-ray diffraction data at high temperatures.

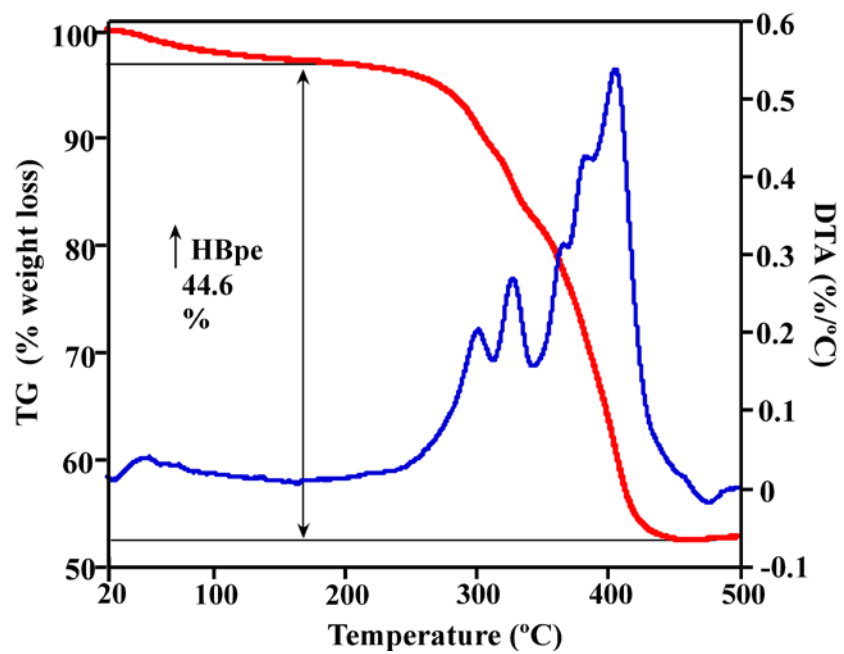


Figure S3. TGA and ATD Curves.

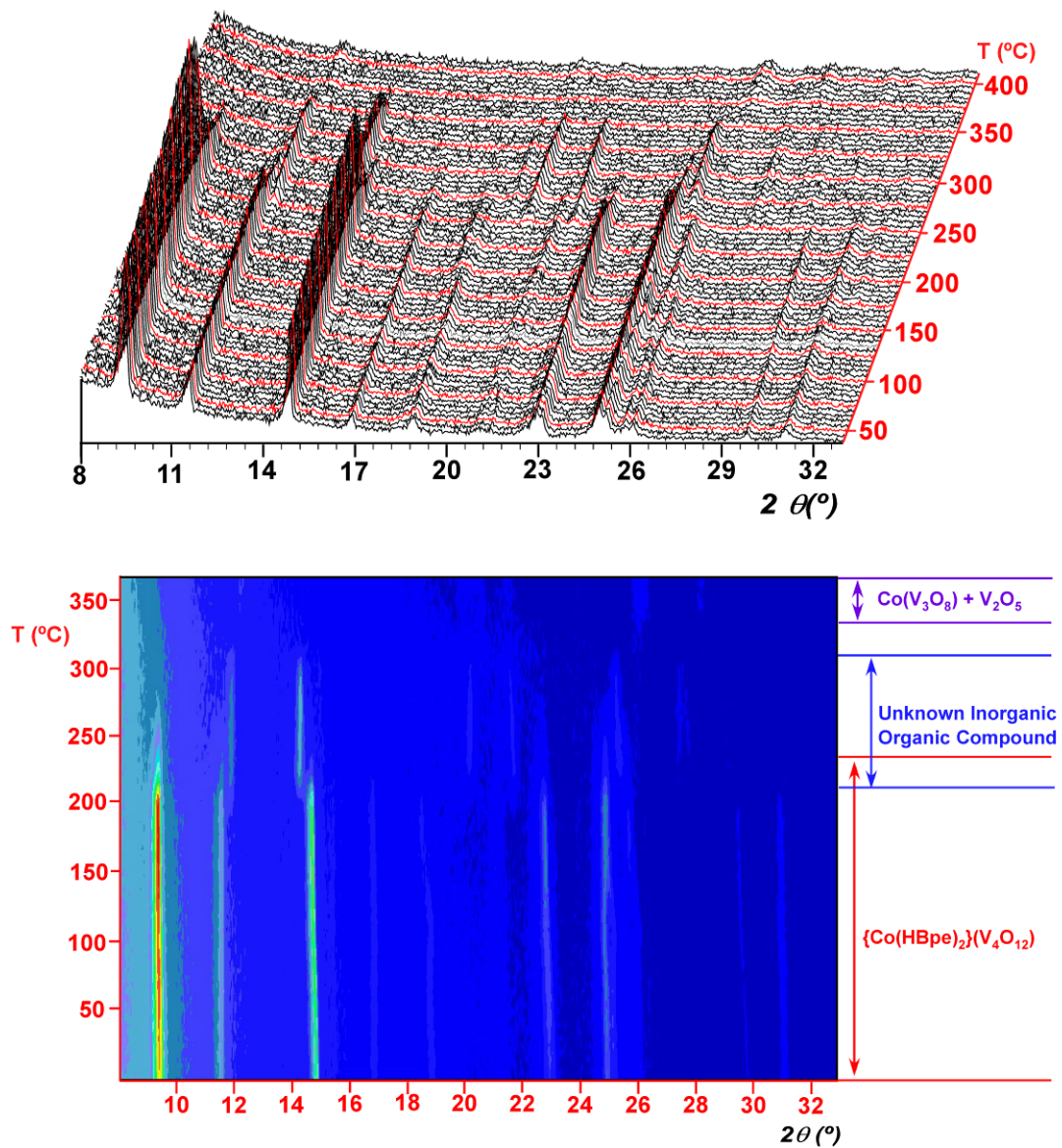


Figure S4. Thermodiffractometry experiment.

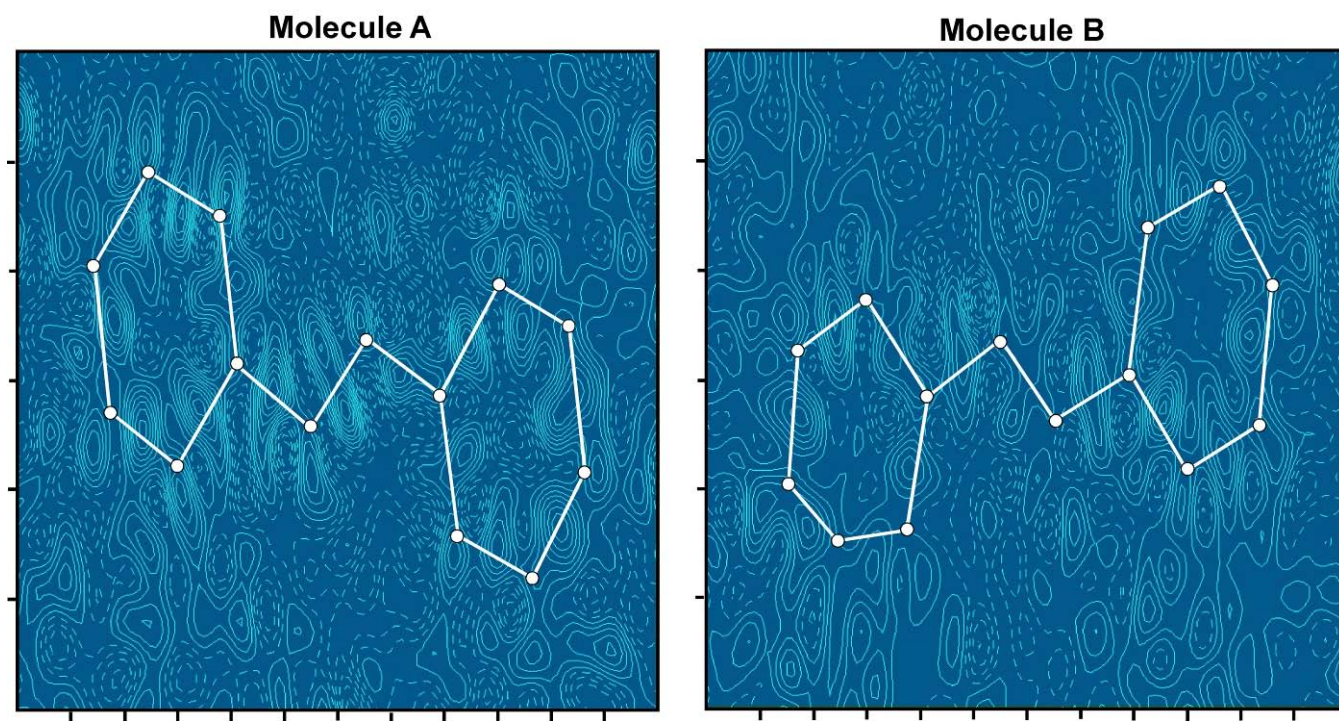


Figure S5. Difference electron density maps of the two crystallographically independent HBpe molecules at 100K. Minimum electron density: $-0.60 \text{ e}\text{\AA}^{-3}$. Maximum electron density: $0.60 \text{ e}\text{\AA}^{-3}$.

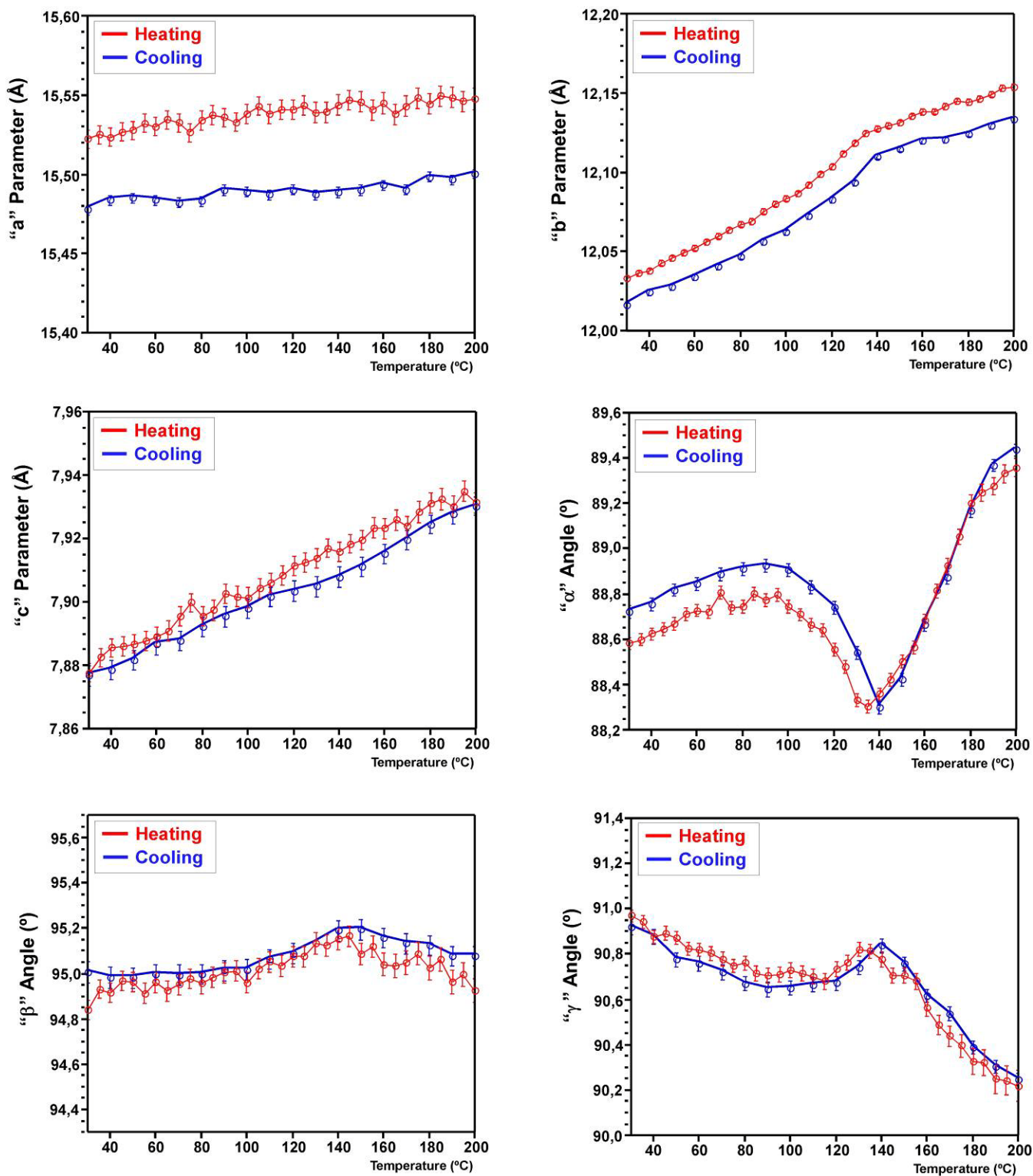


Figure S6. Comparison between the thermal evolution of the cell parameters on cooling (blue lines and points) and heating (red lines and points).

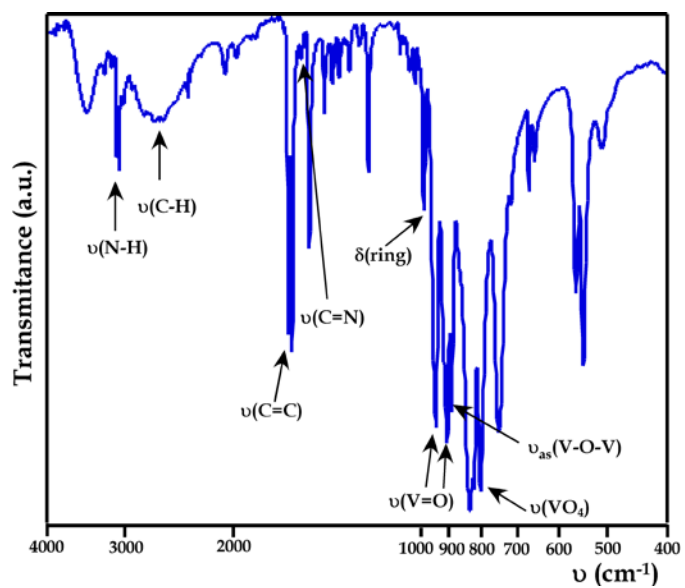


Figure S7. IR spectrum.

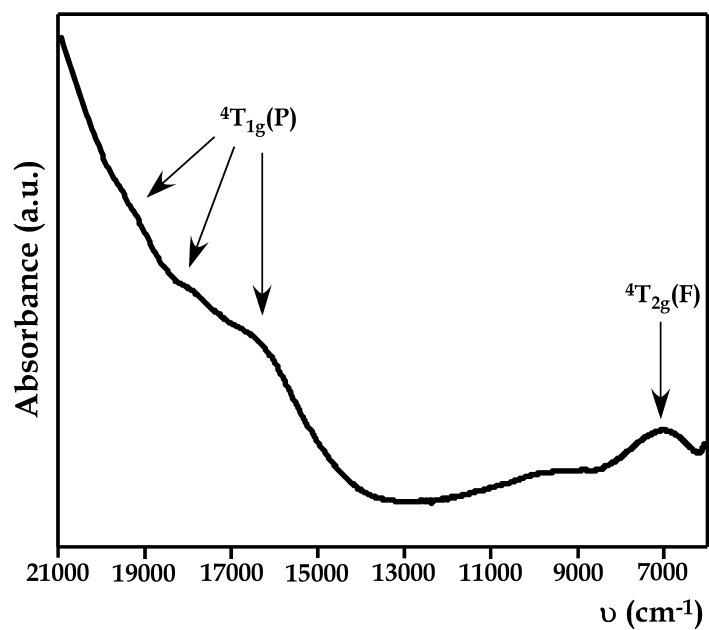


Figure S8. UV-spectrum.