

Supporting Information

A Combined, Modulation Enhanced X-ray Powder Diffraction
and Raman Spectroscopic Study of Structural Transitions in the
Spin Crossover Material $[\text{Fe}(\text{Htrz})_2(\text{trz})](\text{BF}_4)$

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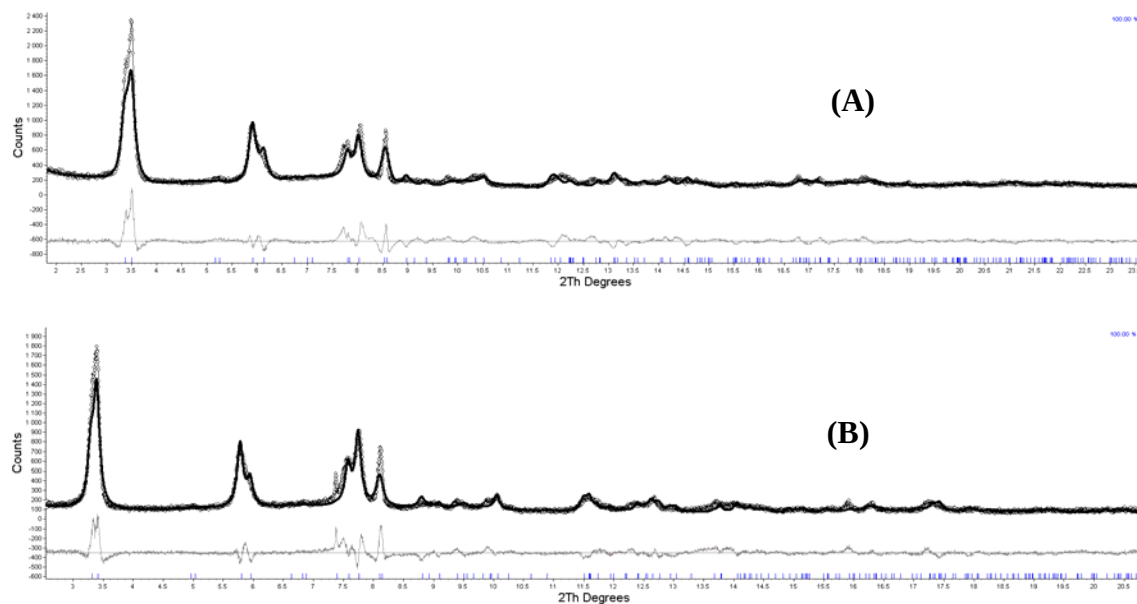


Figure S-1. High-resolution XRPD patterns of (A) low-spin and (B) high-spin structure of **1**. Gray line with circle and black line are experimental and calculated ones, respectively. The differences are shown below

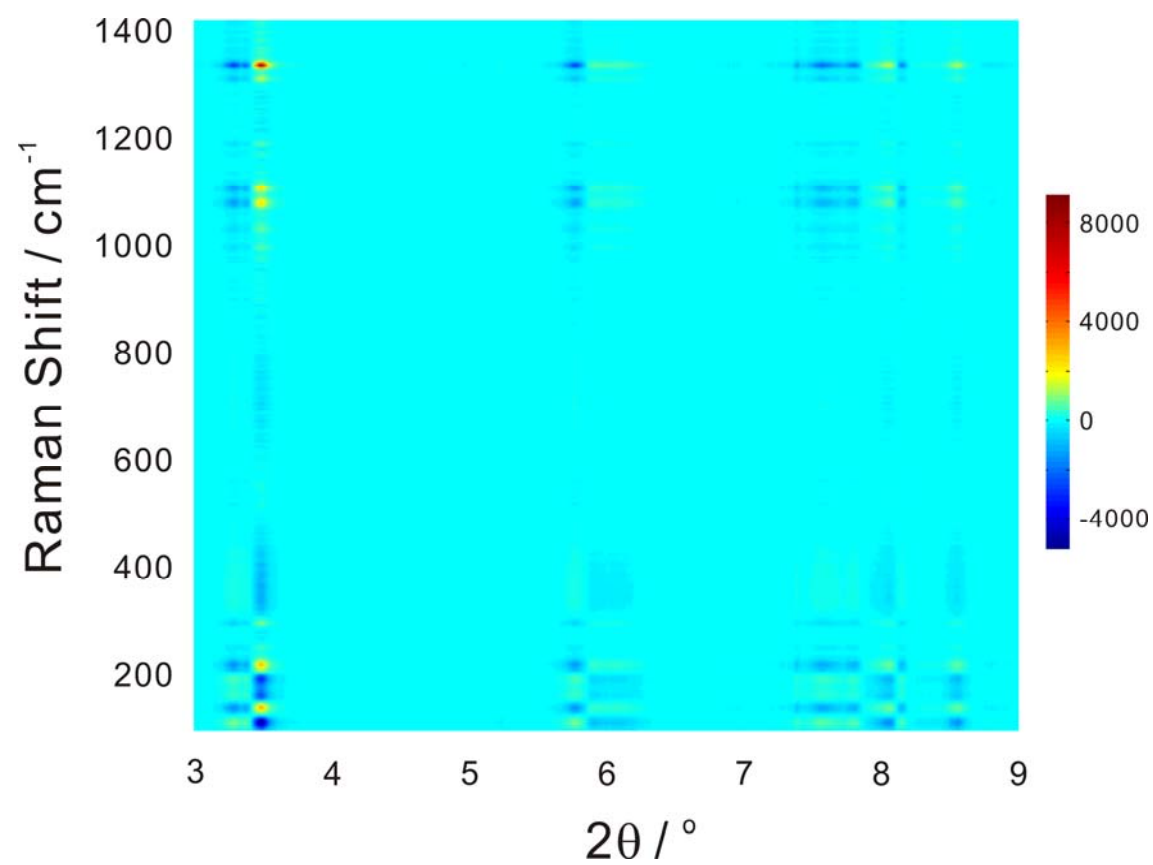


Figure S-2. 2D XRPD-Raman covariance plot.

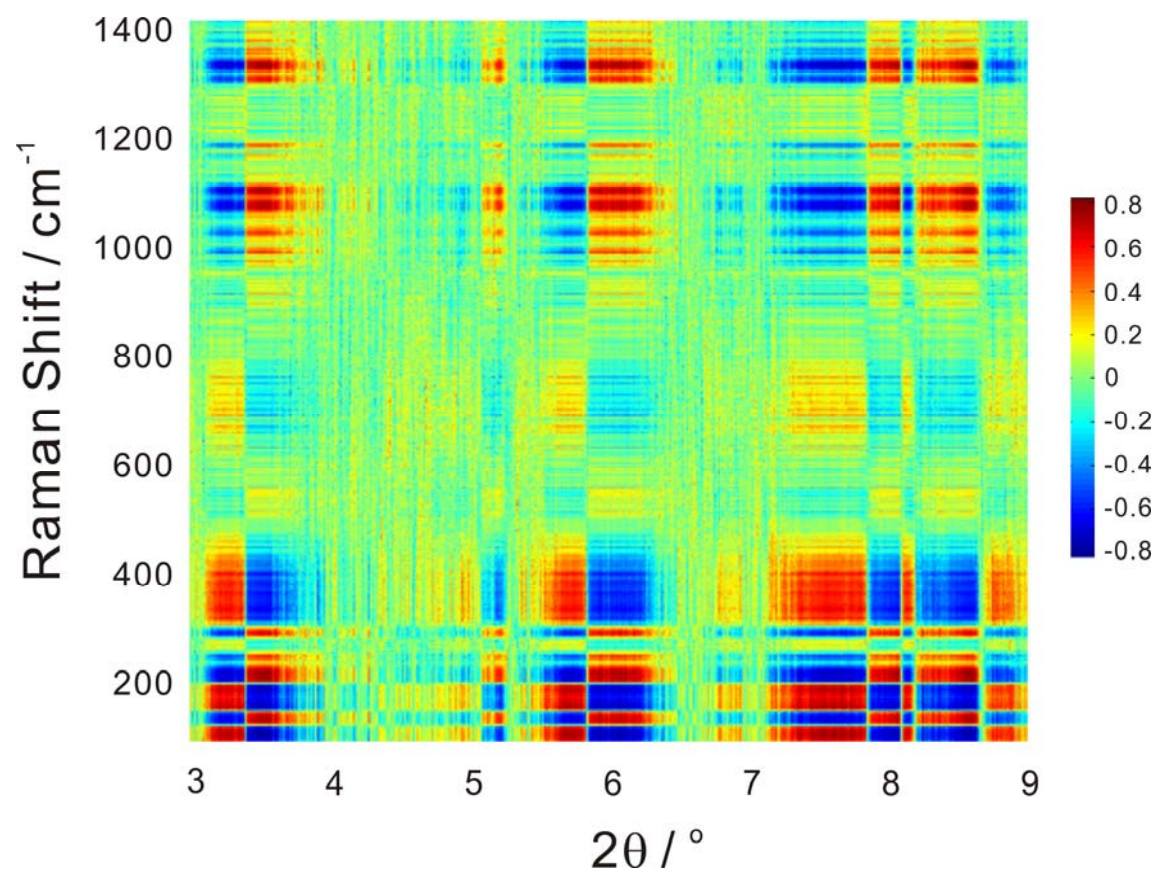


Figure S-3. 2D XRPD-Raman correlation plots.

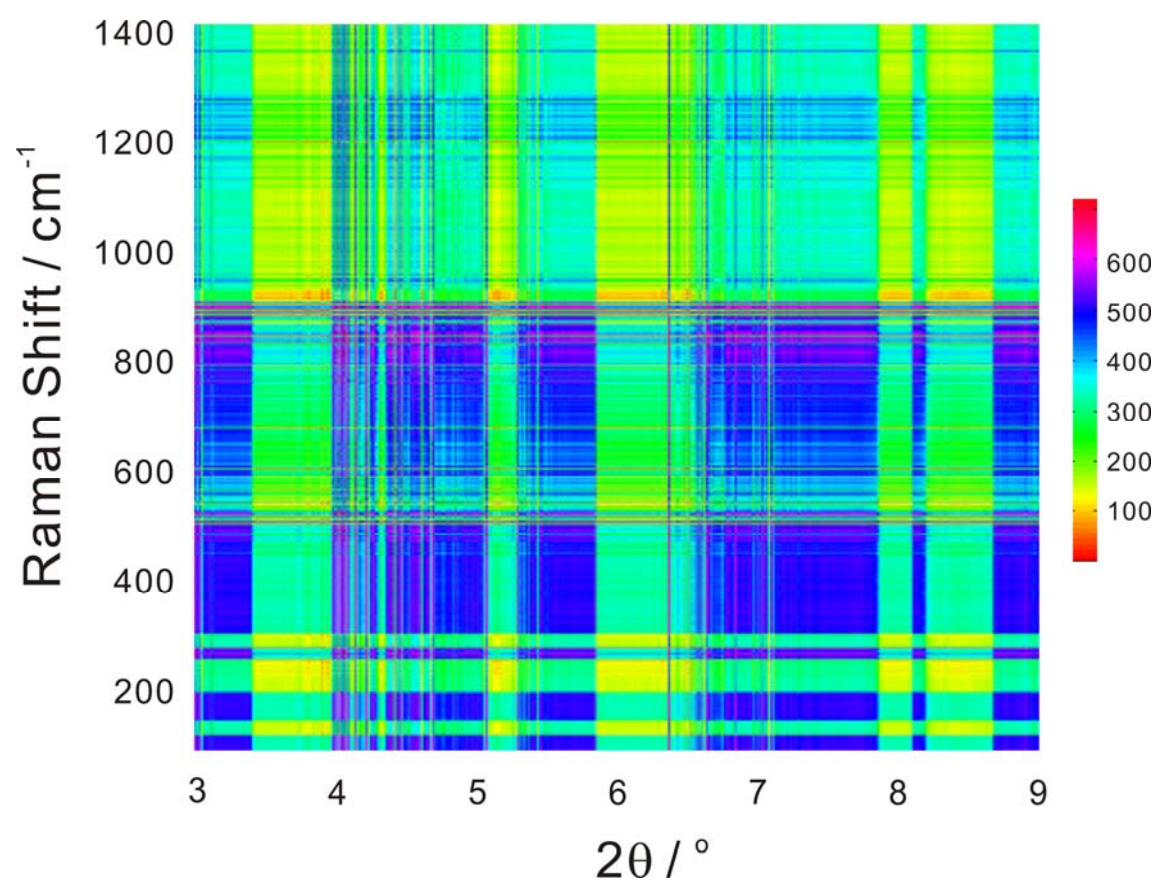


Figure S-4. 2D XRPD-Raman sum of in-phase angle plot.