

# Supporting Information for "Vibronic relaxation pathways in molecular spin qubit

## $\text{Na}_9[\text{Ho}(\text{W}_5\text{O}_{18})_2]\cdot 35\text{H}_2\text{O}$ under pressure"

Janice L. Musfeldt,<sup>\*,†,‡</sup> Zhenxian Liu,<sup>¶</sup> Diego López-Alcalá,<sup>§</sup> Yan Duan,<sup>§</sup>

Alejandro Gaita-Ariño,<sup>§</sup> José J. Baldoví,<sup>§</sup> and Eugenio Coronado<sup>§</sup>

<sup>†</sup>*Department of Chemistry, University of Tennessee, Knoxville, Tennessee 37996, USA*

<sup>‡</sup>*Department of Physics, University of Tennessee, Knoxville, Tennessee 37996, USA*

<sup>¶</sup>*Department of Physics, University of Illinois Chicago, IL 60607-7059, USA*

<sup>§</sup>*Instituto de Ciencia Molecular, Universitat de Valencia, Paterna 46980, Spain*

E-mail: musfeldt@utk.edu

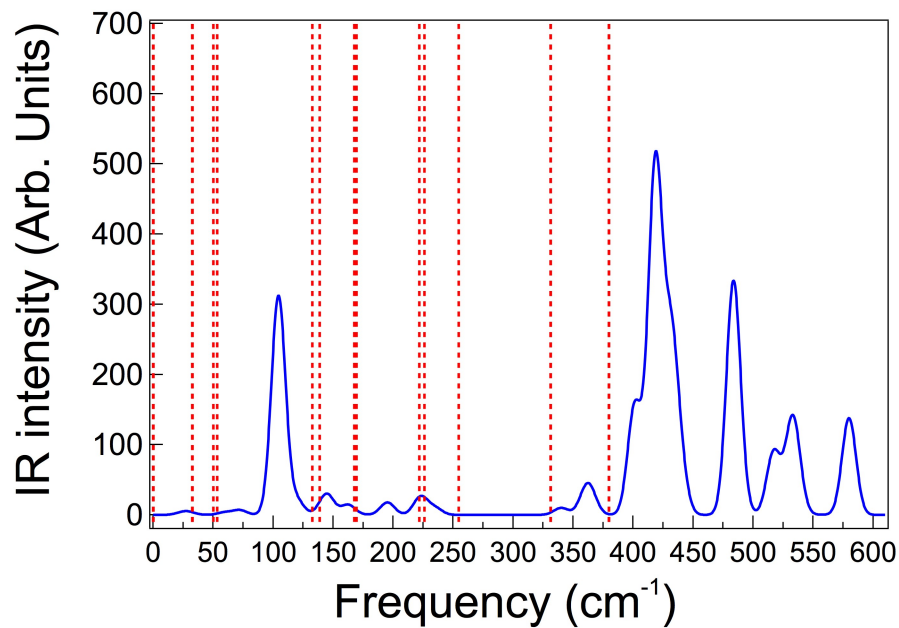


Figure S1: Calculated infrared spectrum (blue solid line) and spin energy levels (vertical red dashed lines) of  $\text{Ho}(\text{W}_5\text{O}_{18})_2]^{9-}$  without any applied strain.

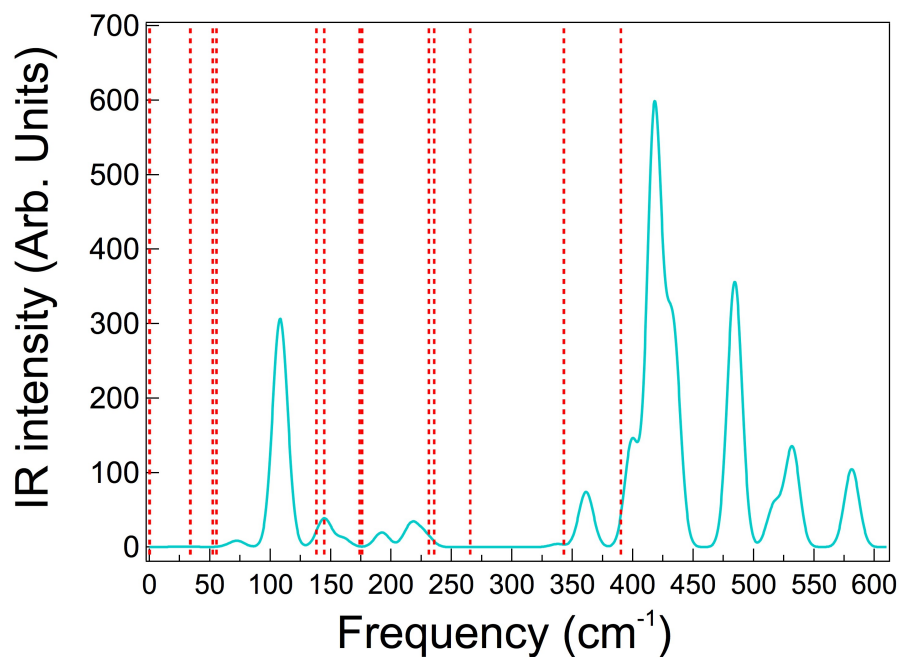


Figure S2: Calculated infrared spectrum (clear blue solid line) and spin energy levels (vertical red dashed lines) of  $\text{Ho}(\text{W}_5\text{O}_{18})_2]^{9-}$  under 0.5% compressive strain.

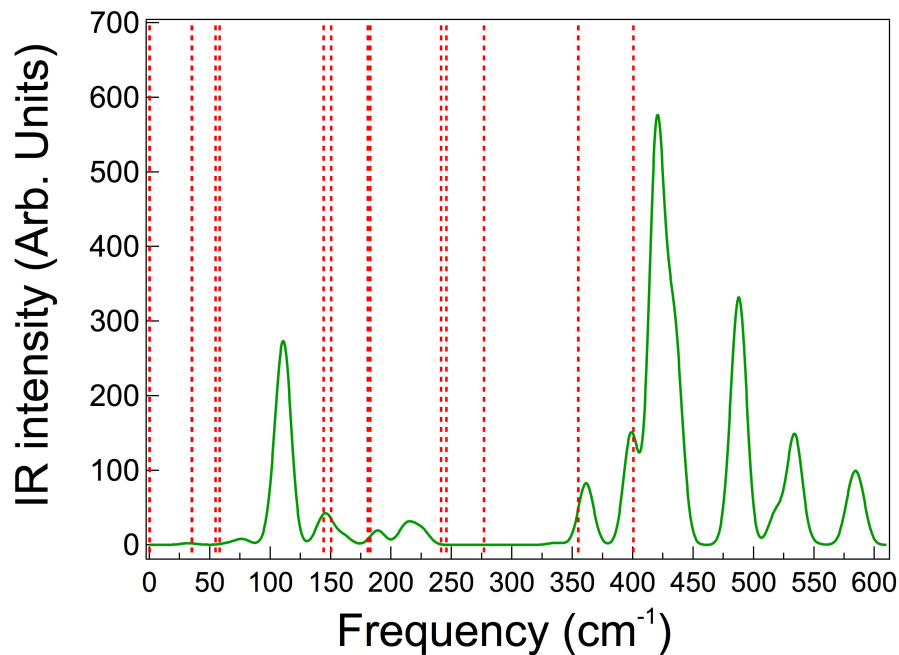


Figure S3: Calculated infrared spectrum (green solid line) and spin energy levels (vertical red dashed lines) of Ho(W<sub>5</sub>O<sub>18</sub>)<sub>2</sub>]<sup>9-</sup> under 1% compressive strain.

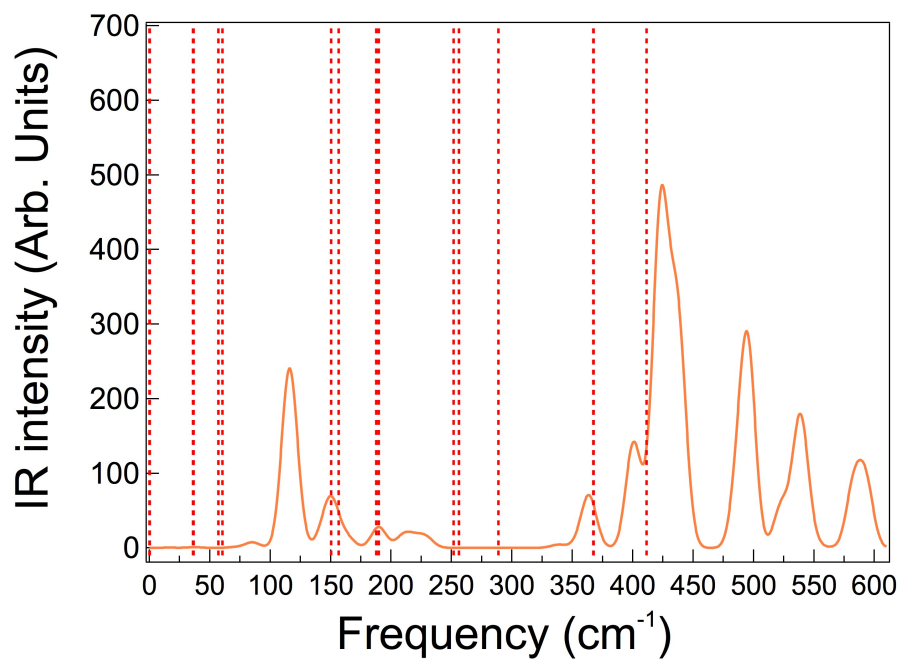


Figure S4: Calculated infrared spectrum (orange solid line) and spin energy levels (vertical red dashed lines) of Ho(W<sub>5</sub>O<sub>18</sub>)<sub>2</sub>]<sup>9-</sup> under 1.5% compressive strain.

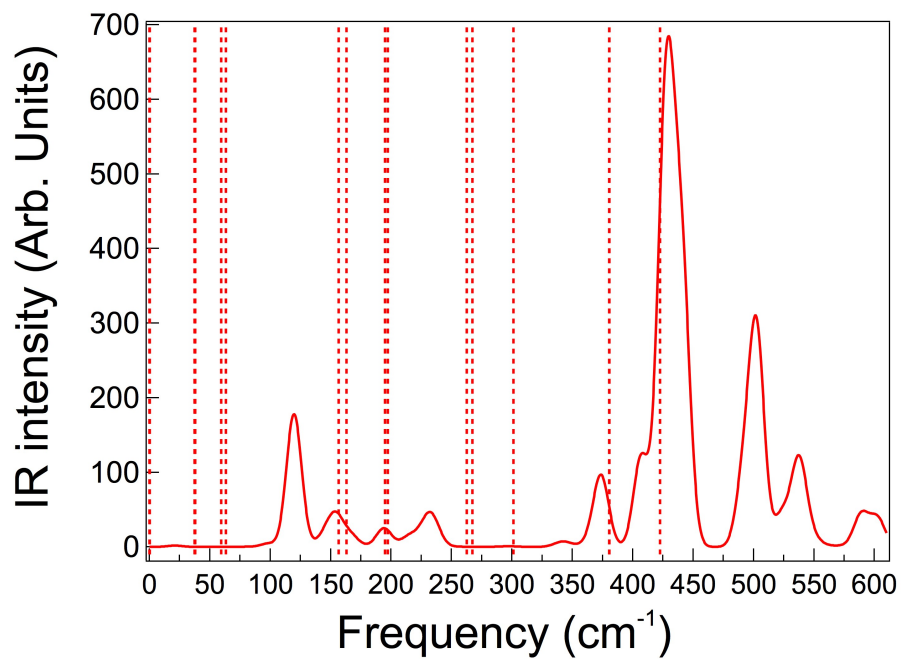


Figure S5: Calculated infrared spectrum (red solid line) and spin energy levels (vertical red dashed lines) of  $\text{Ho}(\text{W}_5\text{O}_{18})_2]^{9-}$  under 2% compressive strain.