

**Electronic Supplementary Information for:**

**Low-energy optical switching of SO<sub>2</sub> linkage**

**isomerisation in single crystals of a ruthenium-based coordination complex**

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### S1 – Single-crystal Raman Spectroscopy for 1

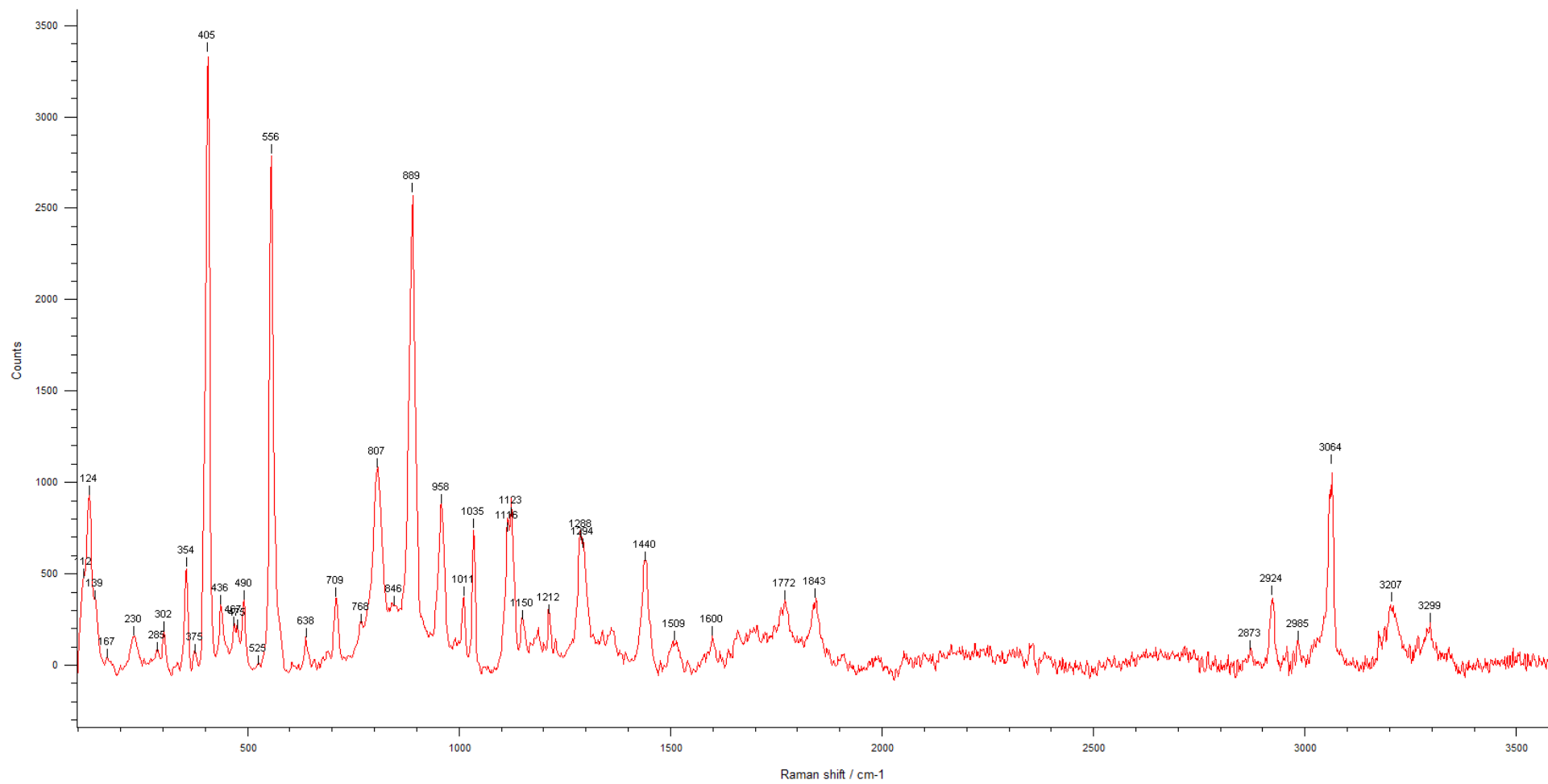
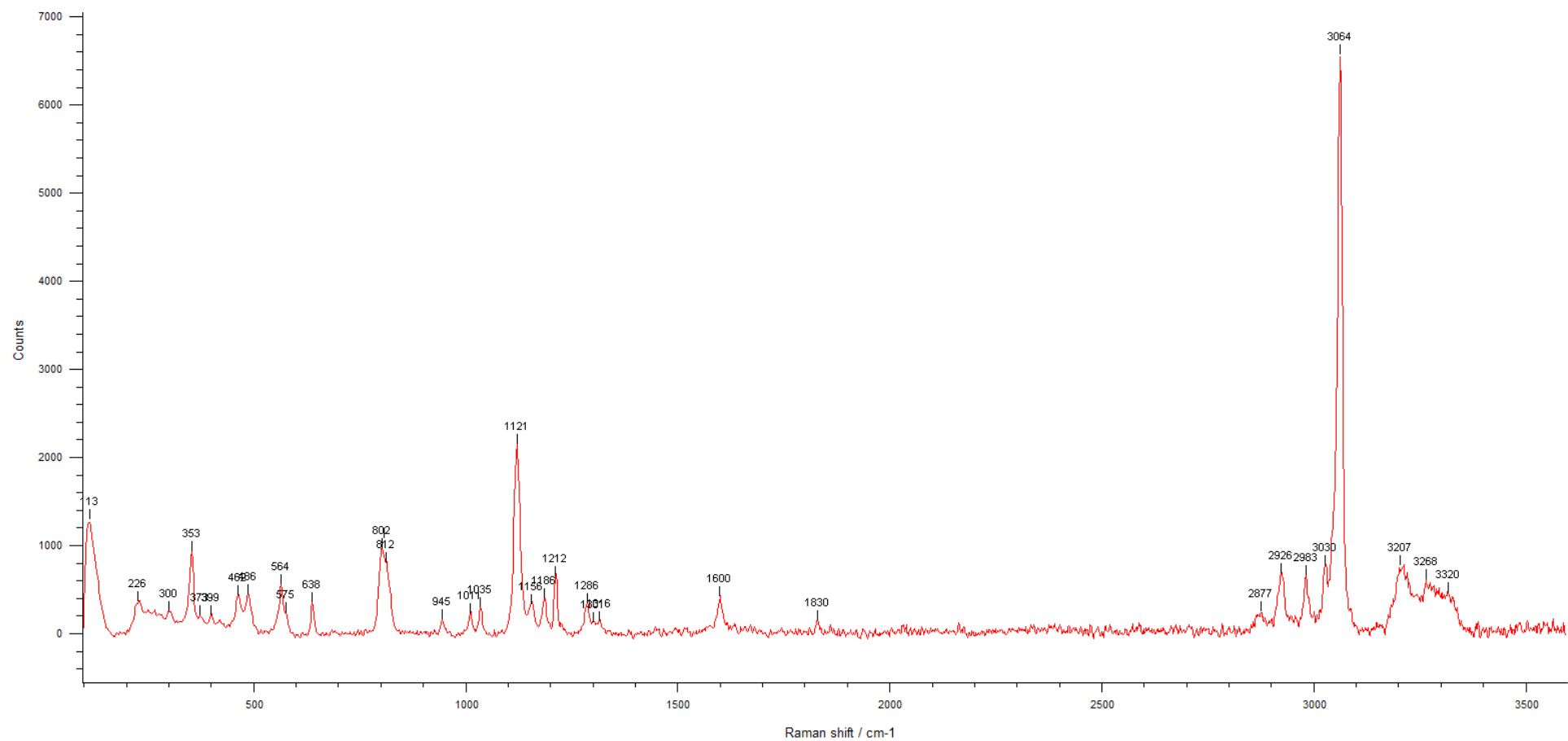
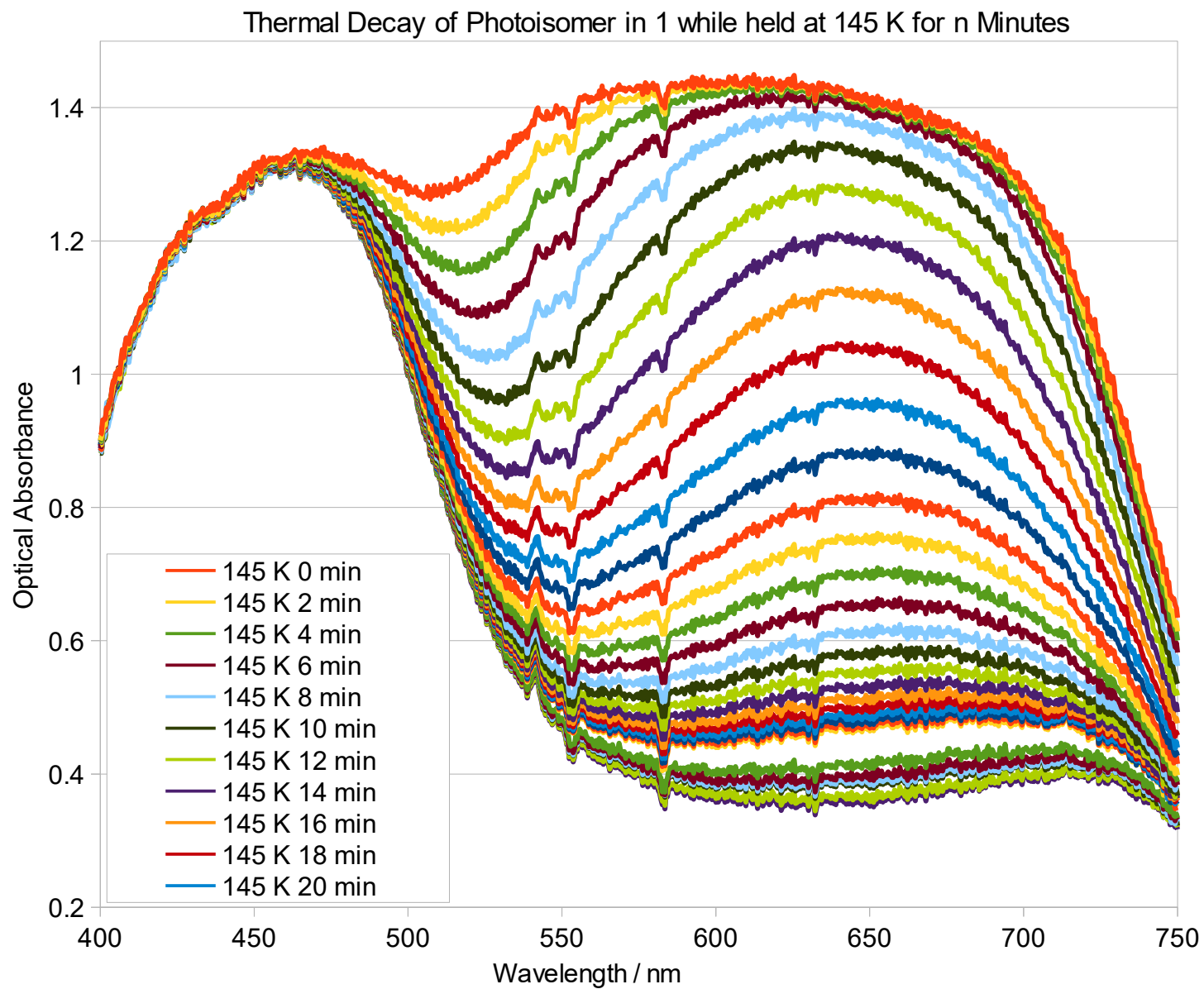


Figure S1 - Single-crystal Raman spectrum of 1 at 90 K

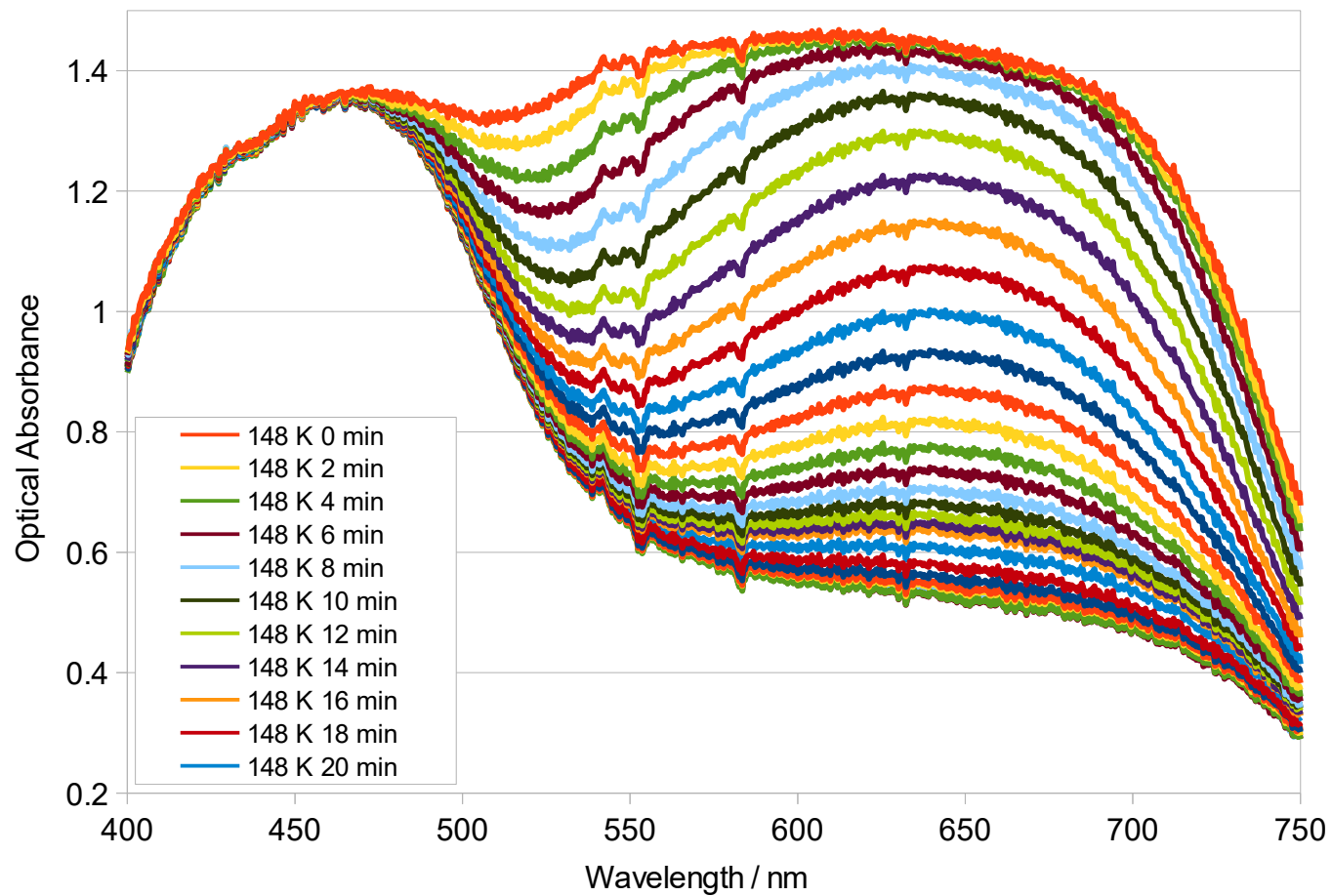


**Figure S2** - Single-crystal Raman spectrum of **1** at 300 K

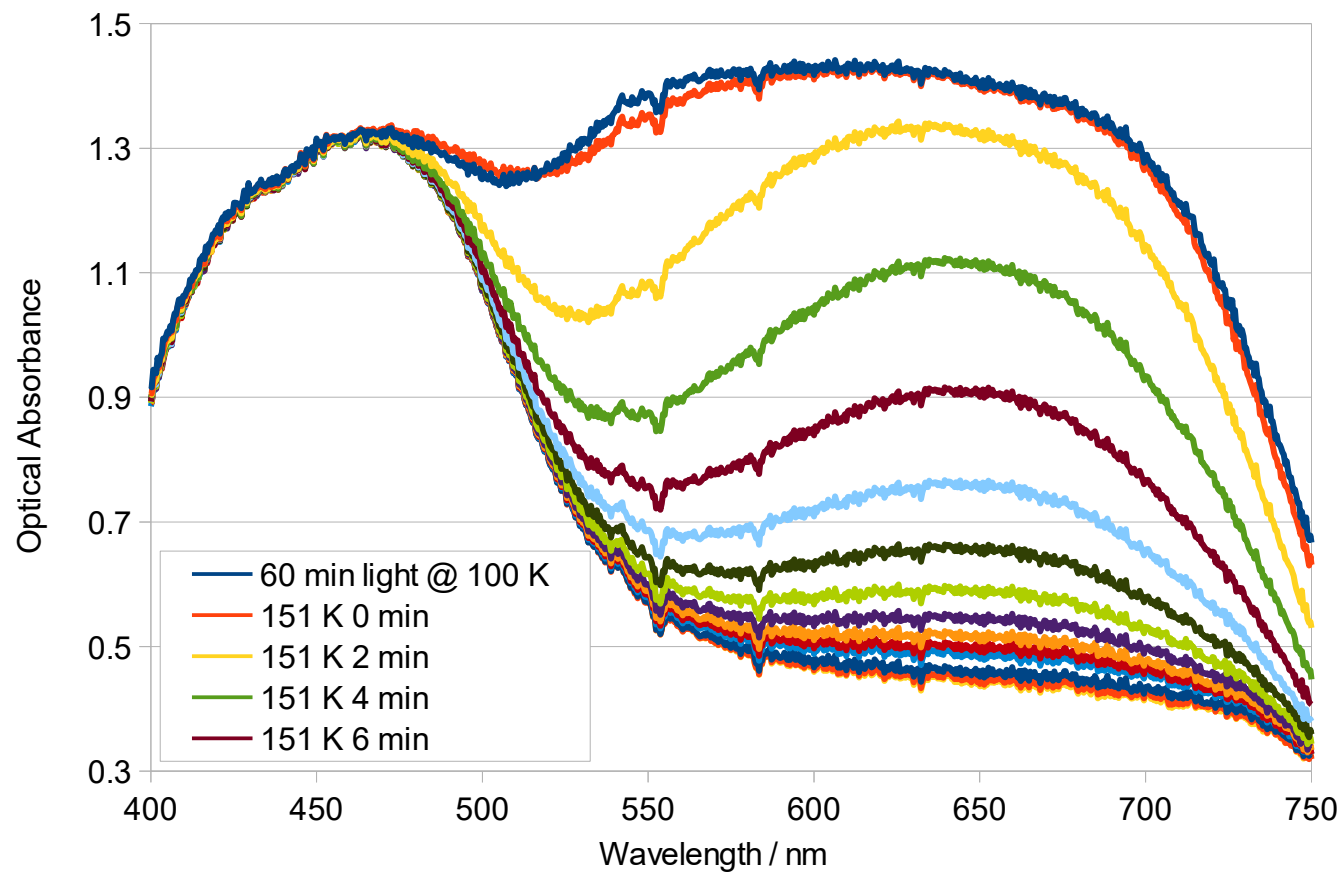
S2 - Single-crystal optical absorption spectra of 1 as a function of thermal decay at seven temperatures



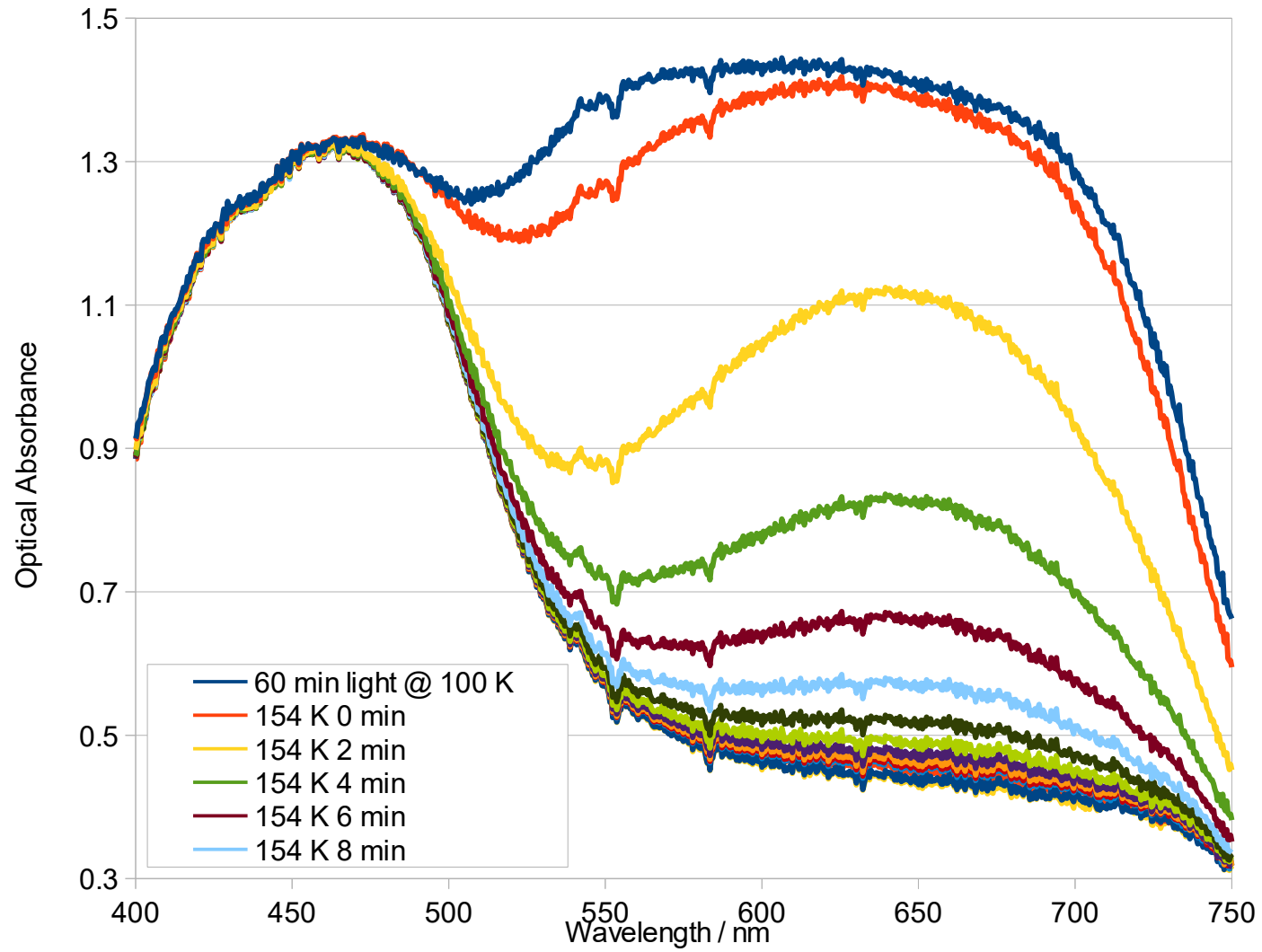
Thermal Decay of 1 while held at 148 K for n Minutes



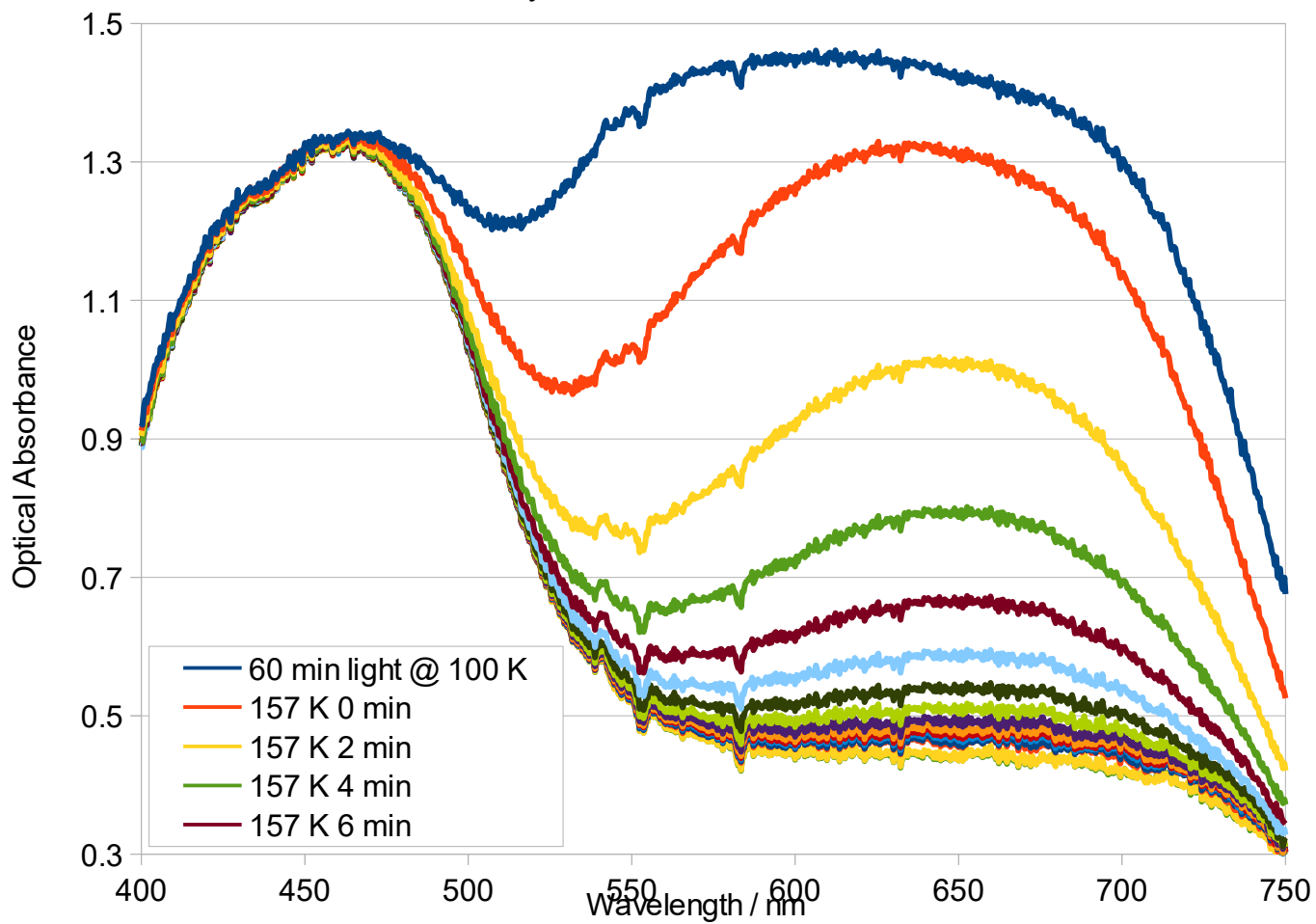
Thermal Decay of 1 while held at 151 K for n Minutes



Thermal Decay of 1 while held at 154 K for n Minutes

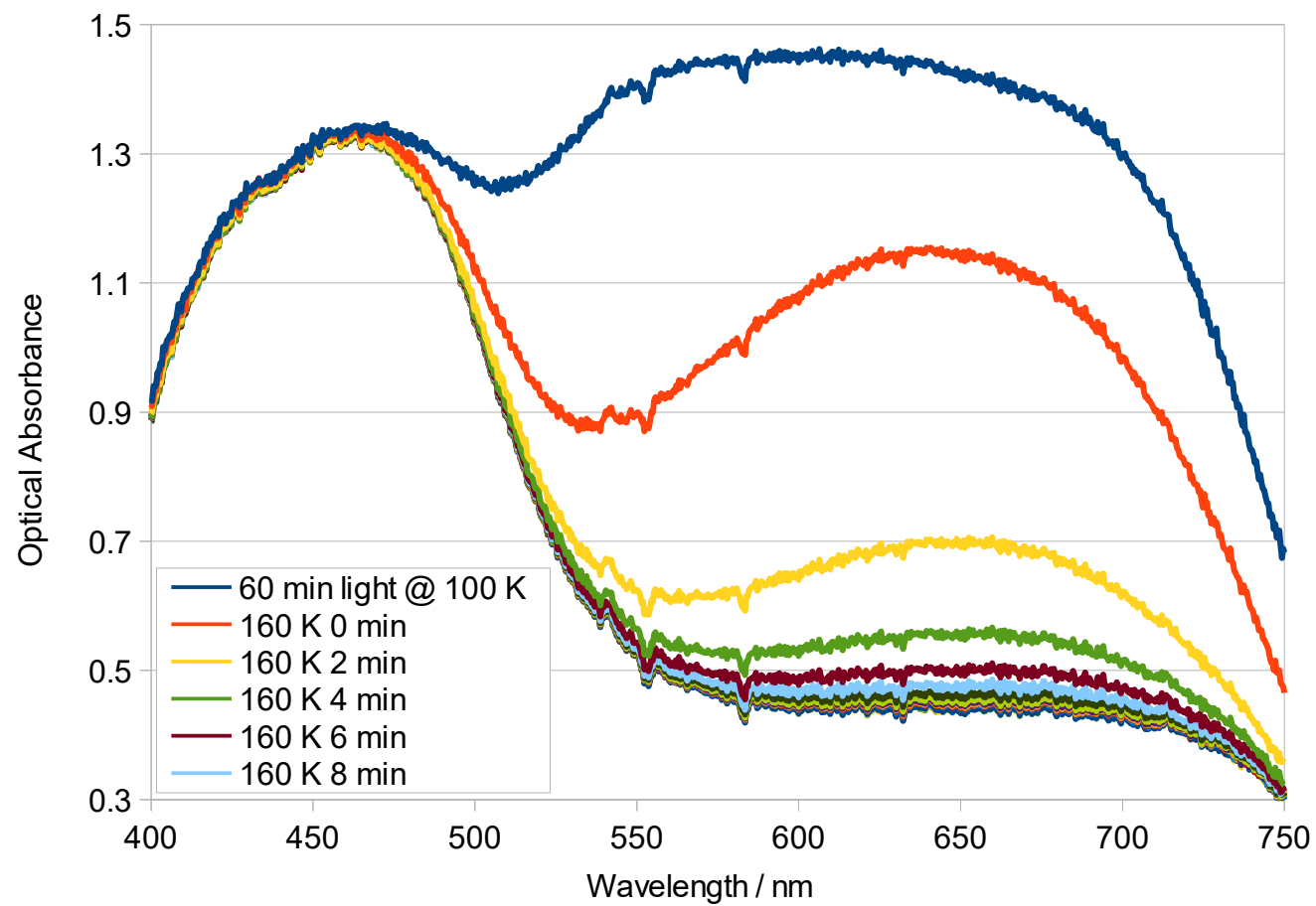


Thermal Decay of 1 while held at 157 K for n Minutes

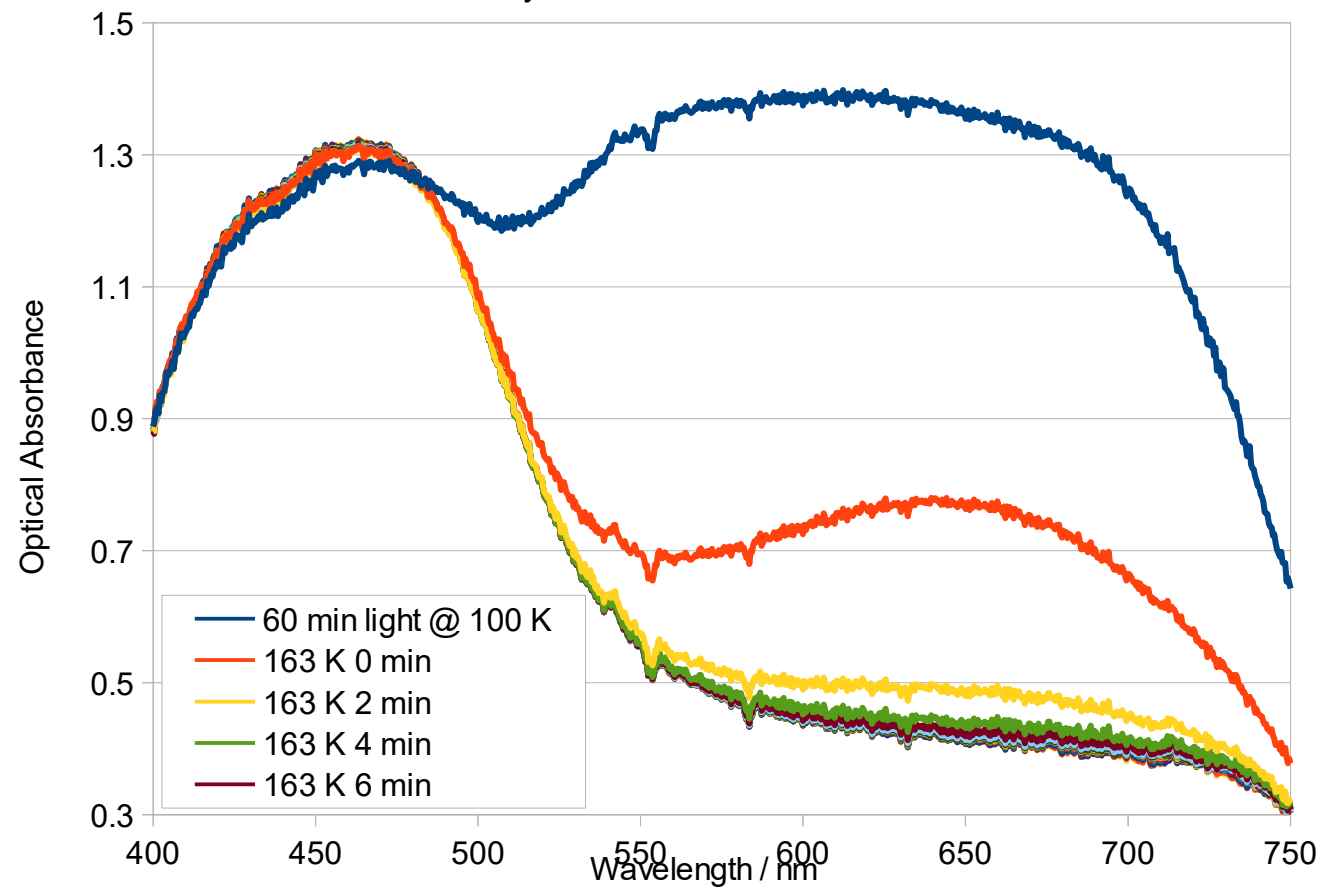




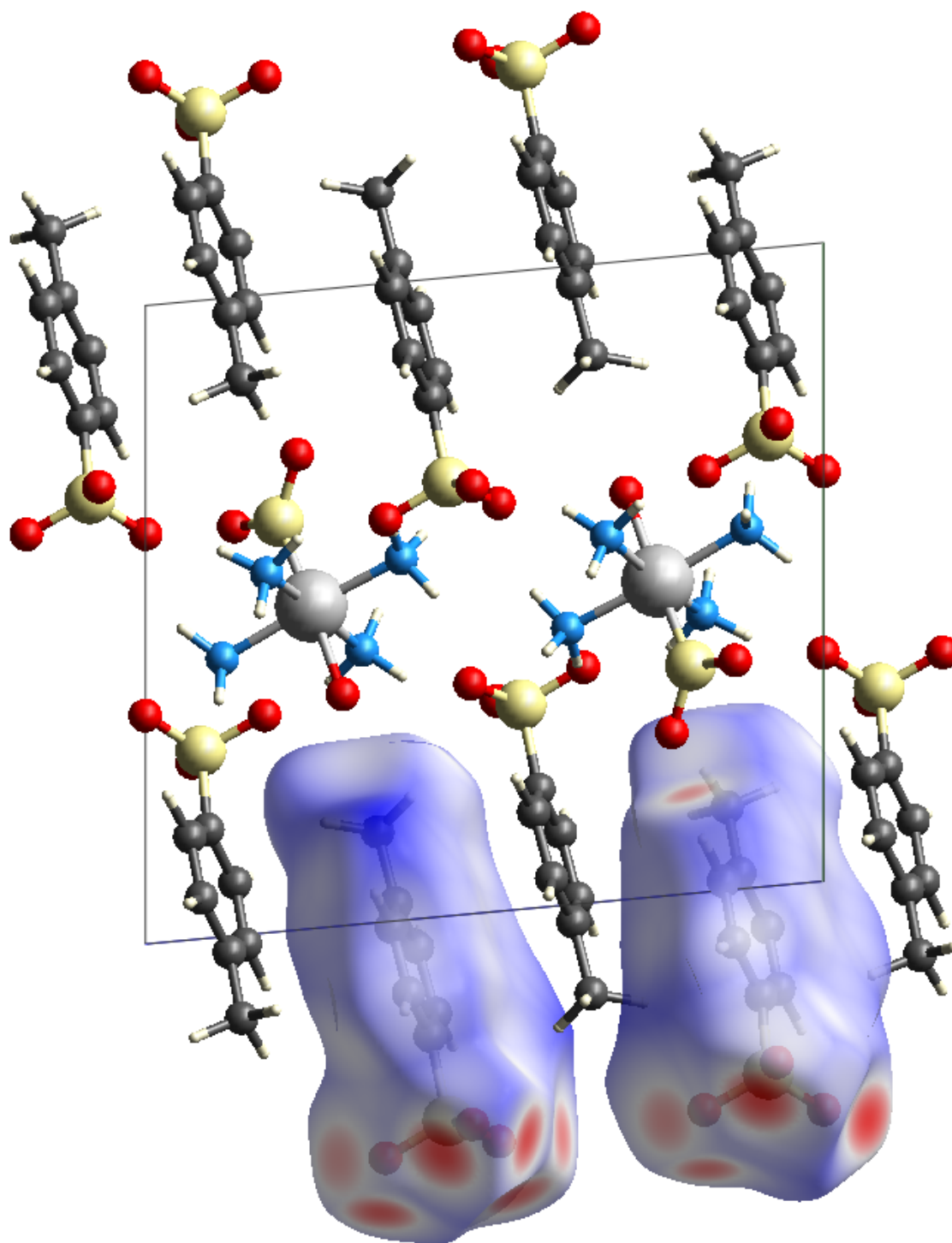
Thermal Decay of 1 while held at 160 K for n Minutes



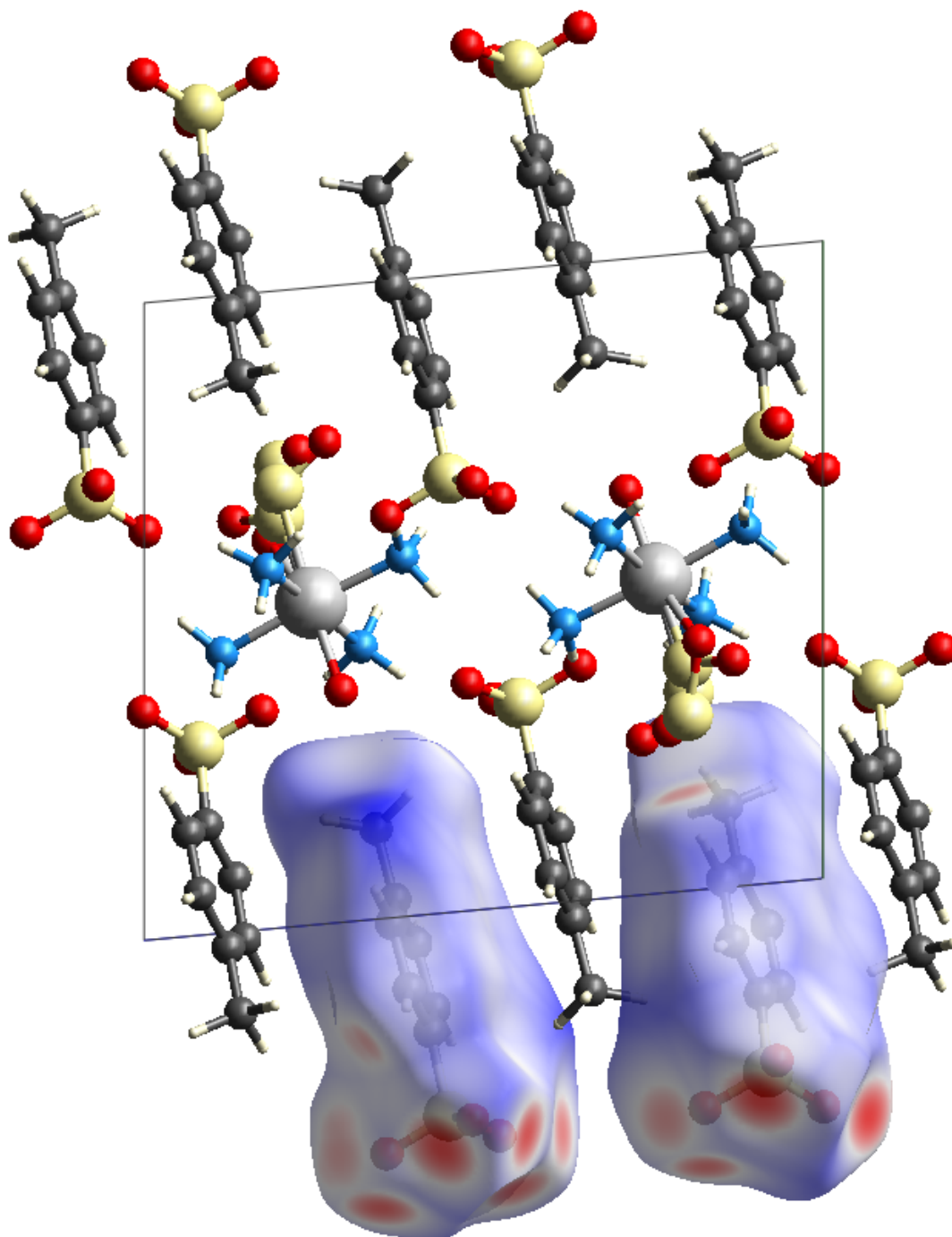
Thermal Decay at 1 while held at 163 K for n Minutes



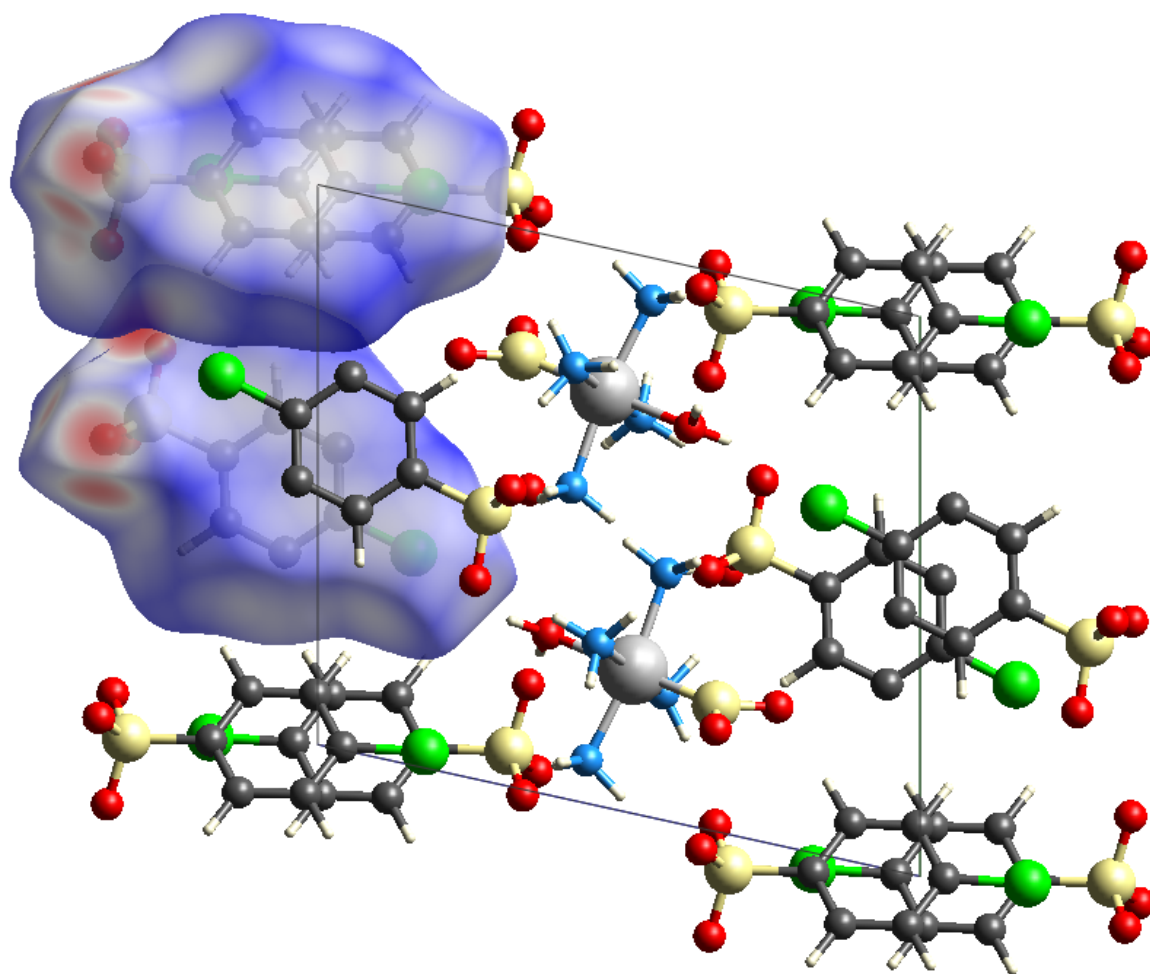
S3 - Hirshfeld surfaces of the anions in the dark and light-induced crystal structures of **1** and *trans*-[Ru(SO<sub>2</sub>)(NH<sub>3</sub>)<sub>4</sub>(H<sub>2</sub>O)]chlorobenzenesulfonate<sub>2</sub>



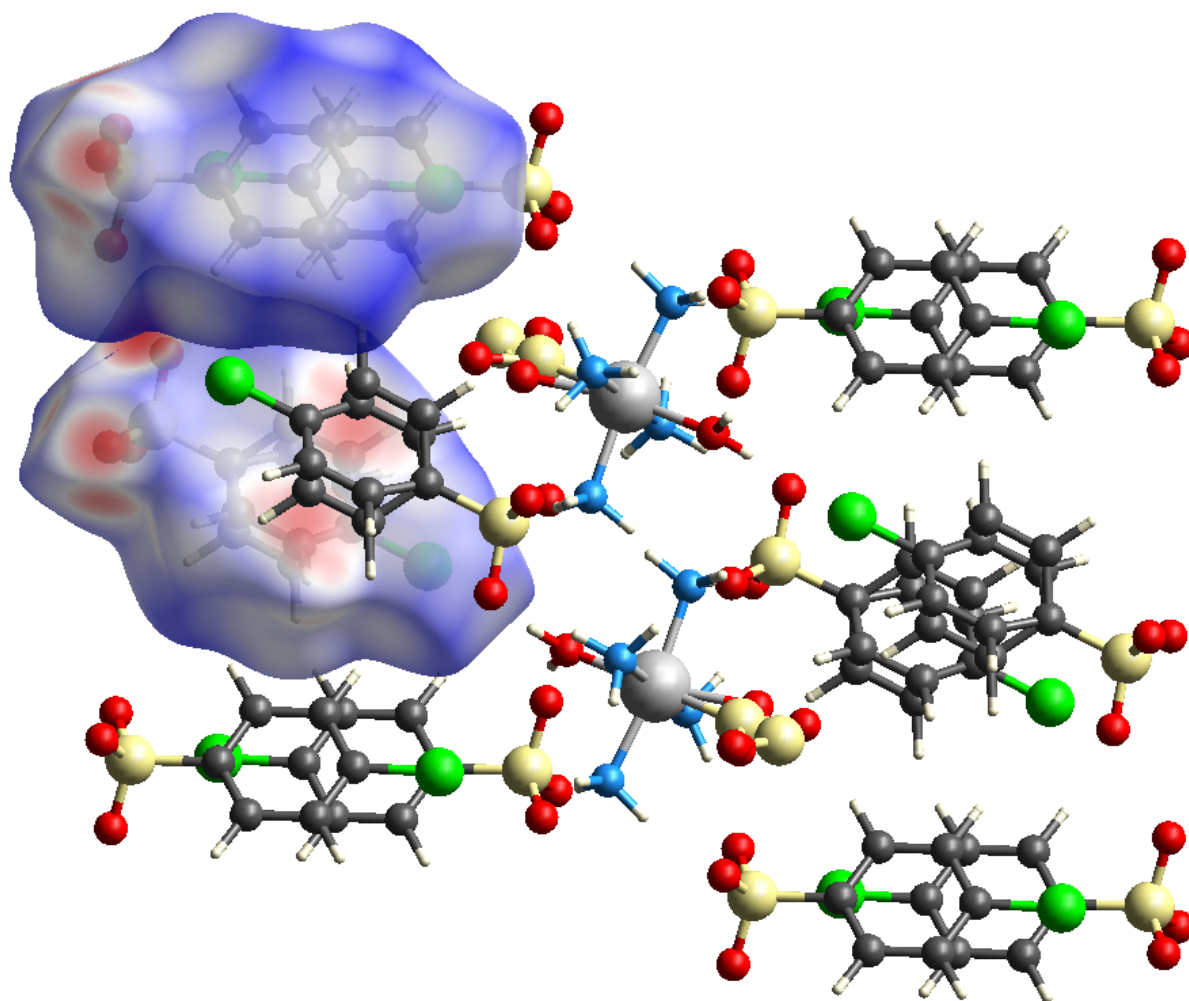
**Figure S10** Hirshfeld surfaces of anions in the dark-state crystal structure of **1**, viewed looking down the crystallographic *a* axis. The image was generated via CrystalExplorer.[1]



**Figure S11** Hirshfeld surfaces of anions in the light-induced crystal structure of **1**, viewed looking down the crystallographic *a* axis. The image was generated via CrystalExplorer.[1]



**Figure S12** Hirshfeld surfaces of anions in the dark-state crystal structure of *trans*-[Ru(SO<sub>2</sub>)(NH<sub>3</sub>)<sub>4</sub>(H<sub>2</sub>O)]chlorobenzenesulfonate<sub>2</sub>, viewed looking down the crystallographic *a* axis. The image was generated via CrystalExplorer.[1]



**Figure S13** Hirshfeld surfaces of anions in the light-induced crystal structure of *trans*-[Ru(SO<sub>2</sub>)(NH<sub>3</sub>)<sub>4</sub>(H<sub>2</sub>O)]chlorobenzenesulfonate<sub>2</sub>, viewed looking down the crystallographic *a* axis. The image was generated via CrystalExplorer.[1]

## S4 – References

[1] Turner, M. J.; McKinnon, J. J.; Wolff, S. K.; Grimwood, D. J.; Spackman, P. R.; Jayatilaka, D.; Spackman, M. A. CrystalExplorer17 (2017). University of Western Australia.  
<https://hirshfeldsurface.net>.