

# Single-Crystal Structures, Optical Absorptions, and Electronic Distributions of Thorium Oxychalcogenides ThOQ (Q = S, Se, Te)

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## Supplementary Material

Table S1

Experimental Optical Bandgap Results for ThOQ (Q = S, Se, Te). All values in eV.

Measurement type	ThOS	ThOSe	ThOTe
Direct	2.27	1.91	1.46
	2.24	1.86	1.46
	2.24		
Average	2.25	1.89	1.46
Indirect	2.25	1.70	1.46
	2.21	1.60	1.46
	2.20		
Average	2.22	1.65	1.46

Figure S1. Absorbance vs. energy (eV) spectrum for ThOTe obtained with the visible detection scheme. The bandgap, 1.46 eV, is beyond the 3.2 – 1.5 eV range.

Figure S2. Absorption coefficients of ThOS and ThOTe obtained with the IR detection scheme. As expected from its 2.22 eV bandgap, the ThOS crystal has a flat and low absorption coefficient over the range 1.8 – 1.08 eV.