

# Supporting Information

## Experimental and Theoretical Investigations of the Ligand Structure of Water-Soluble CdTe Nanocrystals

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**Table S1** Structural information from elemental analysis for TGA-capped CdTe sample A2 upon purification.

| Applied precipitation steps | Cd : Te : S     | NC concentration |
|-----------------------------|-----------------|------------------|
| 0                           | 1 : 0.02 : 1.54 | 0.01 mM          |
| 1                           | 1 : 0.07 : 1.15 | 0.02 mM          |
| 2                           | 1 : 0.11 : 0.96 | 0.02 mM          |