

Supplementary Materials of Supramolecular Structure, Hirshfeld Surface Analysis, Morphological Study and DFT Calculations of Triphenyltetrazolium Cobalt Thiocyanate Complex

by

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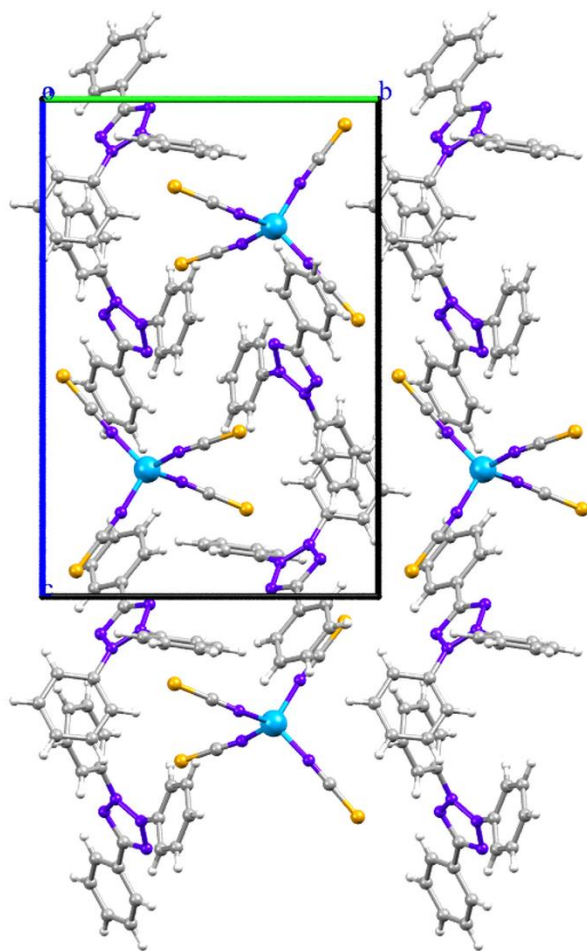


Figure S1. The crystal packing of (1) along *a* axis.

Table S1: Calculated UV-Vis spectrum, oscillator strength and the major contribution calculated using B3LYP functional.

λ_{cal} (nm)	Excitation energy (eV)	Oscillator strength	Major contributions
501.82	2.4707	0.0184	H-2Alpha -->L +12Alpha (0.70465)
431.81	2.8713	0.0120	H-3beta -->L +14beta (0.26804) H-1 beta-->L+14beta (0.31129) H beta -->L+14 beta (0.33366) H beta -->L+15 beta (0.39659)