Supporting Information

Modification of the Supramolecular Structure of [(thione)IY] (Y= Cl, Br) Systems by Cooperation of Strong Halogen Bonds and Hydrogen Bonds

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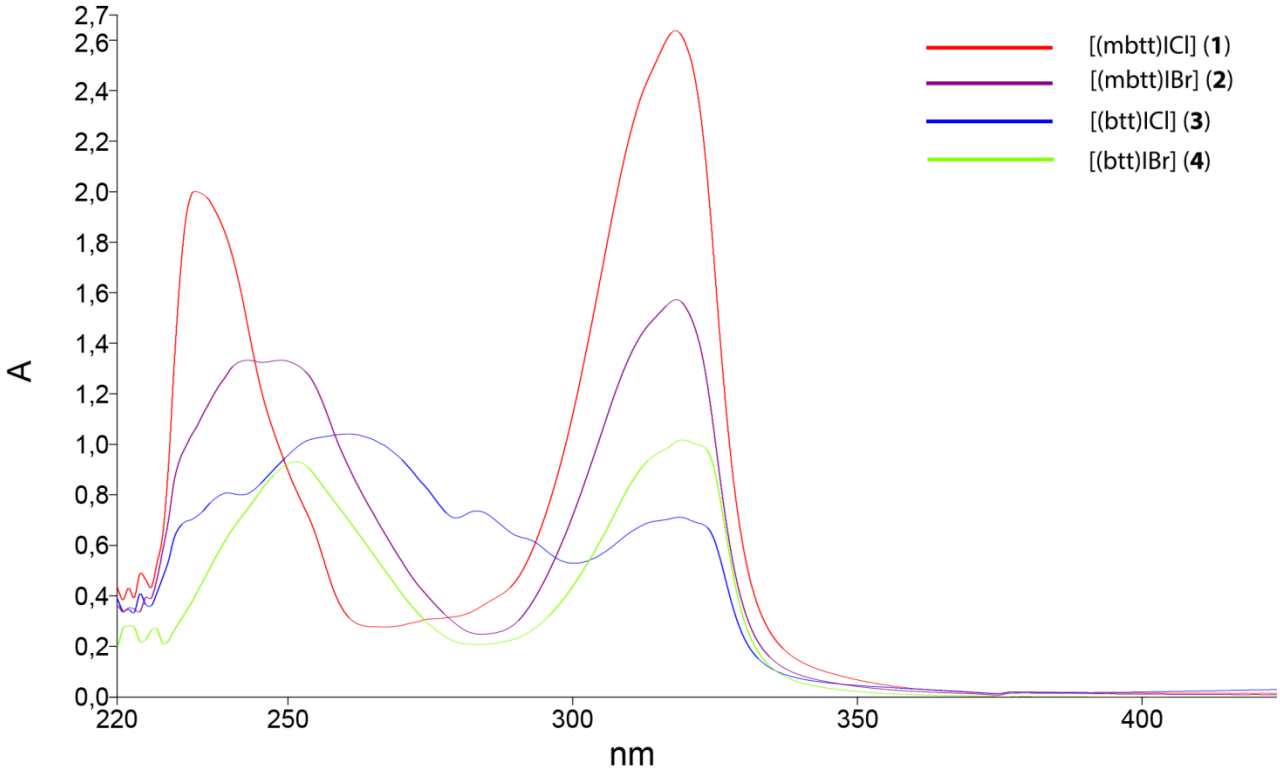

Figure S1. UV-Vis spectra of **1**-**4** in THF.

Table S1. Properties of the electron density at the C=S or I···Y bond critical points of the free mbtt and btt molecules and the dihalogens ICl, IBr, and I_2.

Compound	d (Å)	ρ (eÅ^{-3})	|V|/G	E_{int} (kJmol^{-1})	Ω(A, B)	q(S)	q(I)[b]	q(Y)[c]
mbtt	1.712	1.3487	2.28	-536	1.53	-0.061		
btt	1.709	1.3510	2.25	-544	1.56	-0.037		
ICl[a]	2.313	0.7209	1.83	-140	1.35		0.323	-0.323
IBr[a]	2.462	0.6316	1.93	-101	1.38		0.187	-0.187
I_2[a]	2.654	0.5323	1.98	-73	1.41		0.000	0.000

[a] computationally optimized structures; [b] the interacting iodine I(1) in the thione···I-Y adduct; [c] the non-interacting halogen Y.