Supplementary Information

Structural, spectroscopic and redox properties of a mononuclear Co^{II} thiolate complex – the reactivity toward S-alkylation: an experimental and theoretical study

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Table S1. Summary of X-ray crystallographic data for **1**.

	1
Empirical formula	$C_{38}H_{30}CoN_2S_2$
Formula weight	637.69
Colour, habit	Black, long plate
Crystal size, mm	0.21x0.14x0.04
Crystal system	Triclinic
Space group	*P -1*
a, Å	9.0830(4)
b, Å	12.7159(7)
c, Å	13.1932(7)
α deg.	87.832(4)
β, deg.	76.838(4)
γ, deg.	85.366(4)
V, Å^3	1478.62(13)
Z	2
T, K	150(2)
ρ (calc), Mg/m^3	1.432
μ, mm^{-1}	0.753
θ range, deg.	3.41 to 26.37
No.of rflcn/obsv	9338 / 5934
GooF	0.632
*R*1	0.0375
*wR*2	0.0346

Table S2. Comparison between experimental data and predicted TD-DFT transitions (energies and intensities) for complexes **1*** and **1^{Me}***.

	Calc.		Exp.	
	λ (nm)	*f*	λ (nm)	ε (M^{-1}cm^{-1})
1*				
βHOMO-2 → βLUMO	742	0.038	750	1300
βHOMO-3 → βLUMO	543	0.073	530	1100
βHOMO-6 → βLUMO	457	0.072	460	1900
βHOMO-7 → βLUMO	438	0.071	420	2600
1^{Me} *				
βHOMO → βLUMO	566	0.005	530	350
βHOMO → βLUMO+1	489	0.028	450	1050