Supplementary material to:

M.S.A. Hamza, M.A. Elawady and H.M. Marques, *S. Afr. J. Chem.*, 2008, **61**, 68–73.

Table S1 Comparison of the logarithms of the equilibrium constants (in $dm^3\ mol^{-1}$) determined experimentally (K_{obs}) and estimated from molecular mechanics calculations (K_E).

	ΔE/kJ mol^{-1} [a]	% Equilibrium population	log K_E	log K_{obs}
Reactants				
ImH + (α-H_2O, β-CN^-)CbsPr	13.05	0.43		
ImH + (α-CN^-, β-H_2O)CbsPr	11.84	0.70		
Products				
H_2O + (α-ImH, β-CN^-)CbsPr	0	83.87		
H_2O + (α-CN^-, β-ImH)CbsPr	4.27	15.00	1.94	3.57(2)
Reactants				
Tz + (α-H_2O, β-CN^-)CbsPr	9.12	1.88		
Tz + (α-CN^-, β-H_2O)CbsPr	7.87	3.06		
Products				
H_2O + (α-Tz, β-CN^-)CbsPr	0	74.02		
H_2O + (α-CN^-, β-Tz)CbsPr	3.14	21.04	1.28	2.80(2)
Reactants				
Pz + (α-H_2O, β-CN^-)CbsPr	5.48	5.22		
Pz + (α-CN^-, β-H_2O)CbsPr	12.97	0.25		
Products				
H_2O + (α-Pz, β-CN^-)CbsPr	0	47.66		
H_2O + (α-CN^-, β-Pz)CbsPr	0.042	46.87	1.24	2.65(3)
Reactants				
ImH + (α-H_2O, β-Et)CbsPr	9.25	2.32		
ImH + (α-Et, β-H_2O)CbsPr	15.15	0.21		
Products				
H_2O + (α-ImH, β-Et)CbsPr	0	96.76		
H_2O + (α-Et, β-ImH)CbsPr	12.18	0.71	1.59	2.13(2)
Reactants				
Tz + (α-H_2O, β-Et)CbsPr	7.82	4.01		
Tz + (α-Et, β-H_2O)CbsPr	11.67	0.85		
Products				
H_2O + (α-Tz, β-Et)CbsPr	0	94.5		
H_2O + (α-Et, β-Tz)CbsPr	12.22	0.68	1.29	1.43(2)
Reactants				
Pz + (α-H_2O, β-Et)CbsPr	7.74	4.16		
Pz + (α-Et, β-H_2O)CbsPr	13.68	0.38		
Products				
H_2O + (α-Pz, β-Et)CbsPr	0	94.63		
H_2O + (α-Et, β-Pz)CbsPr	11.72	0.84	1.32	1.26(2)

[a] Relative strain energy, measured relative to the lowest energy species in each reaction.

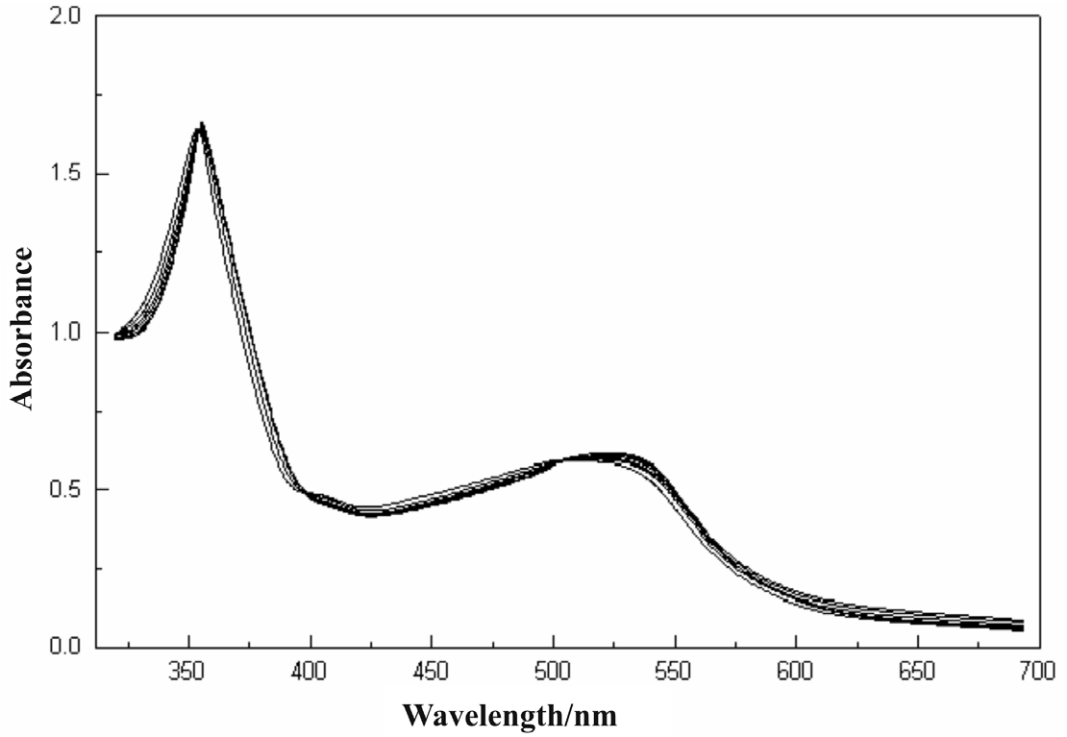

Figure S1 Spectral changes accompanying the reaction of 1,2,4-triazole with ACCbs-Pr in aqueous solution at 25 °C. λ_{max} of the product, (Tz)(CN)Cbs-Pr occurs at 360, 516 and 548 nm. Well-defined isobestic points occur at 355.5, 395 and 511 nm.

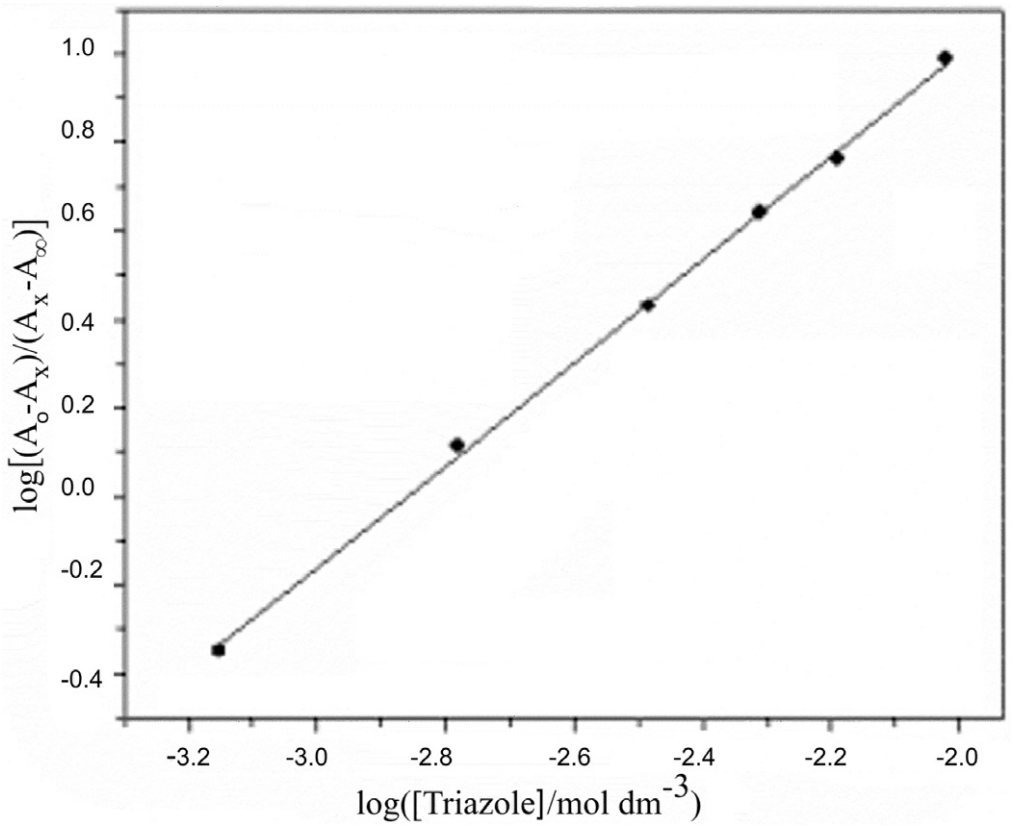

Figure S2 A log-log plot of ACCbs-Pr (in aqueous solution, pH = 9.0, I = 0.1 mol dm^{-3}, 25 °C) with Tz. The slope $n = 1.04 \pm 0.03$ shows that a single Tz ligand is complexed, i.e. H_2O, but not CN^-, is displaced from Co(III).

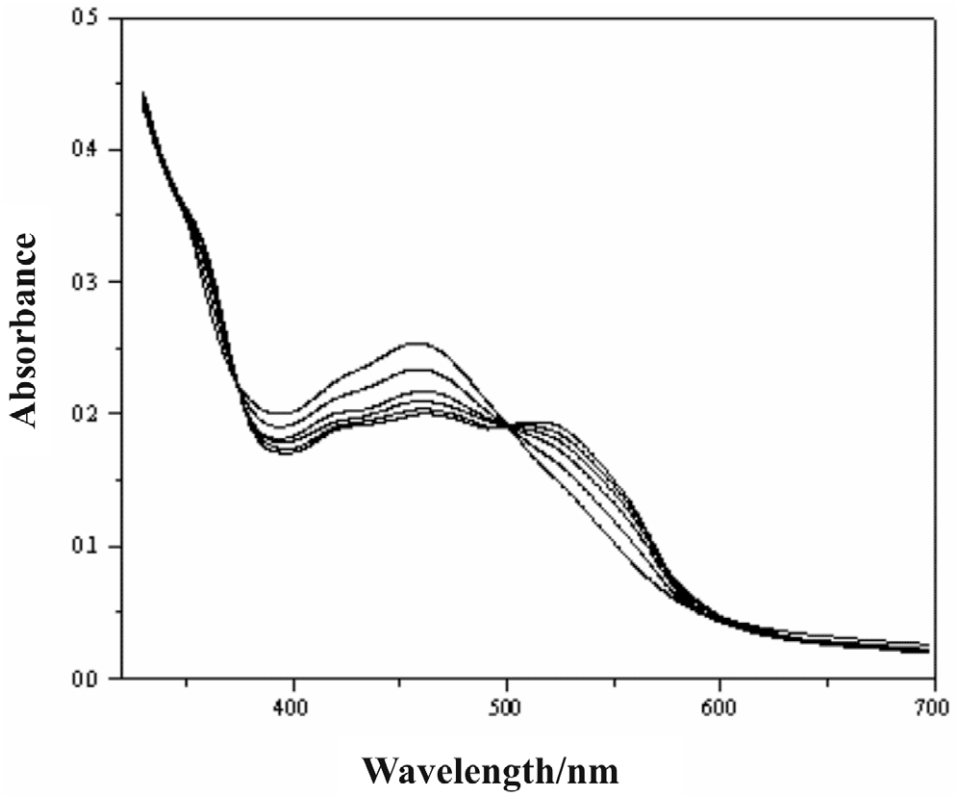

Figure S3 Spectral changes accompanying the spectrophotometric titration of SCBs-Pr in ethyl acetate with ImH at 25 °C.

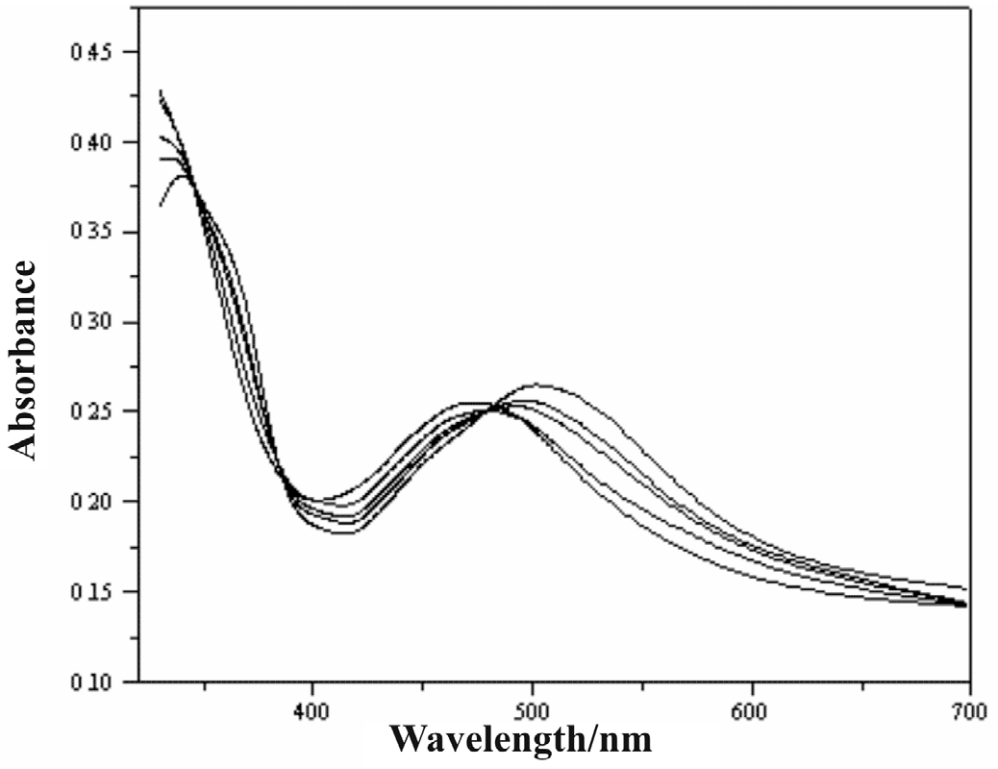

Figure S4 Spectrophotometric titration of MeCbs-Pr in H_2O with Pz at 25 °C.

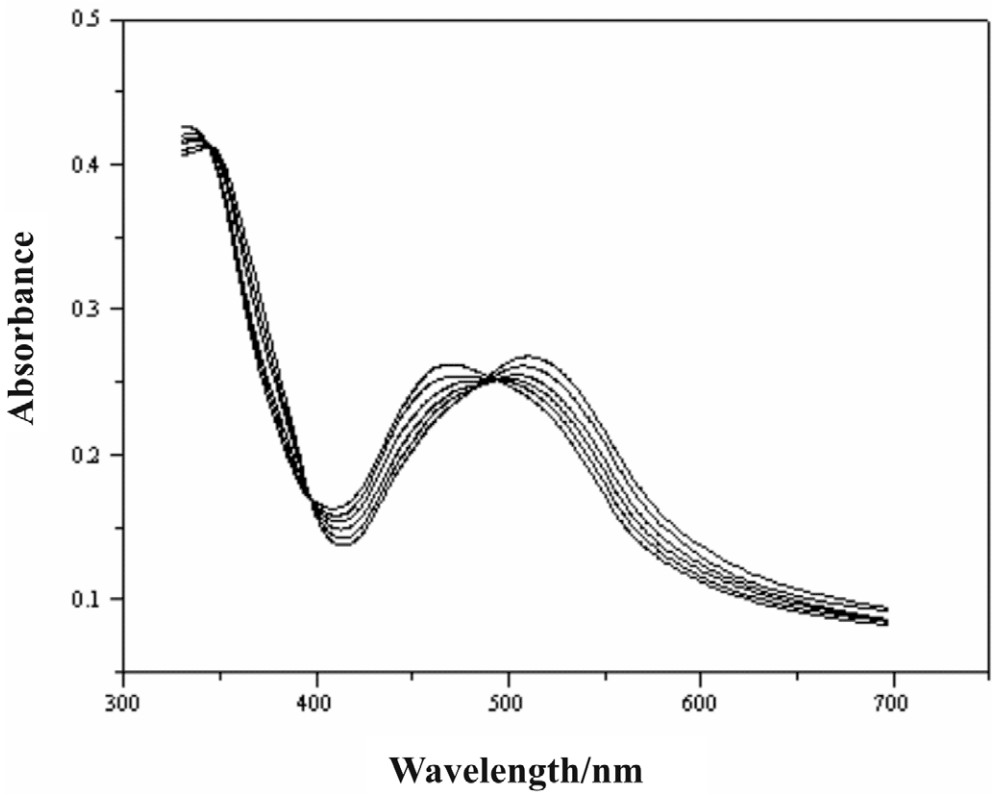

Figure S5 Spectrophotometric titration of EtCbs-Pr in H_2O with ImH at 25 °C.