

Supporting Information

Synthesis and Characterization of Cobalt(II) Complexes with Tripodal Polypyridine Ligand Bearing Pivalamide Groups. Selective Formation of a Six-coordinate and a Seven-coordinate Cobalt(II) Complexes

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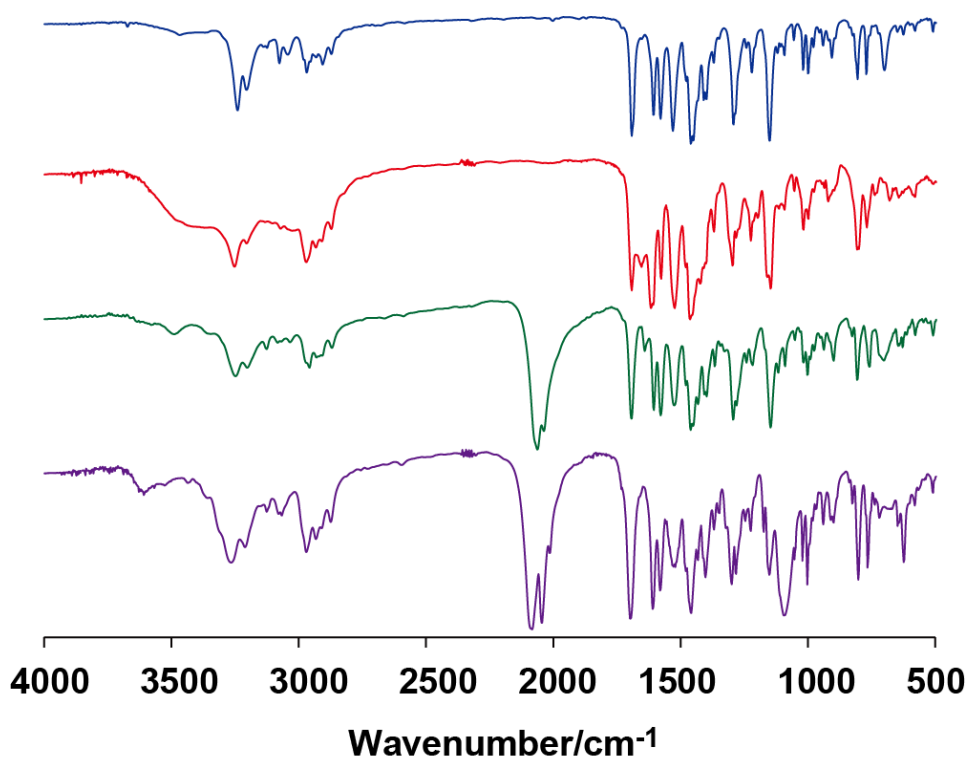


Fig. S1 IR spectra of 1^{Cl} (blue line), 1^{Br} (red line), 1^{azide} (green line), $3 \cdot (\text{ClO}_4^-)$ (purple line).

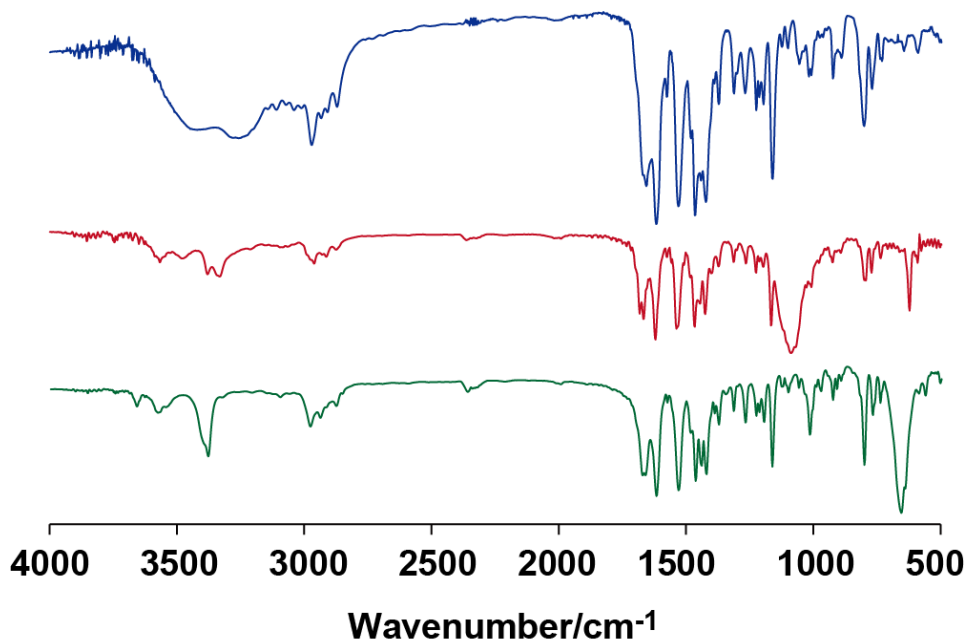


Fig. S2 IR spectra of $2^{\text{MeCN}} \cdot (\text{I})_2$ (blue line), $2^{\text{MeOH}} \cdot (\text{ClO}_4)_2$ (red line), $2^{\text{MeOH}} \cdot (\text{SbF}_6)_2$ (green line).

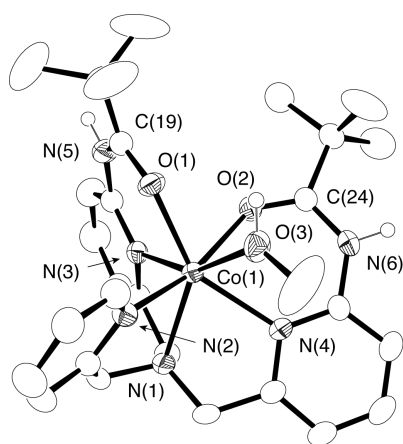


Fig S3. ORTEP diagram of the molecular structure of $2^{\text{MeOH}} \cdot (\text{SbF}_6^-)_2$ with 50% thermal ellipsoid probability. The hydrogen atoms and SbF_6^- anion have been omitted for clarity.

Table S1 Crystallographic and structure refinement data for compounds $2^{\text{MeOH}} \cdot (\text{SbF}_6^-)_2$

Chemical formula	$\text{C}_{29}\text{H}_{40}\text{CoF}_{12}\text{N}_6\text{O}_3\text{Sb}_2$	$\beta / ^\circ$	121.1594(12)	Independent reflections	8822
Formula weight	1051.09	$V / \text{\AA}^3$	7730.5(18)	$R(\text{int})$	0.0338
Crystal system	Monoclinic	Z	8	$RI(I > 2\sigma(I))^a$	0.0370
Space group	$C2/c$ (#15)	$D_c / \text{g cm}^{-3}$	1.806	RI (all)	0.0465
$a / \text{\AA}$	28.793(4)	$\mu(\text{Mo-K}\alpha) / \text{cm}^{-1}$	19.065	$wR2$ (all)	0.0898
$b / \text{\AA}$	13.5107(17)	$F(000)$	4136	GOF	1.056
$c / \text{\AA}$	23.222(4)	Reflections collected	30145	CCDC number	851269

$$^a R_1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}, wR_2 = \left\{ \frac{\sum [w(F_o^2 - F_c^2)^2]}{\sum [w(F_o^2)]} \right\}^{1/2}.$$

Table S2 Selected bond lengths [\AA] and angles [$^\circ$] of $2^{\text{MeOH}} \cdot (\text{SbF}_6^-)_2$

Co(1)–N(1)	2.206(3)	N(1)–Co(1)–N(2)	74.09(11)	N(3)–Co(1)–N(4)	115.00(10)
Co(1)–N(2)	2.200(4)	N(1)–Co(1)–N(3)	74.60(10)	N(3)–Co(1)–O(1)	82.26(9)
Co(1)–N(3)	2.174(3)	N(1)–Co(1)–N(4)	72.19(10)	N(3)–Co(1)–O(2)	78.36(11)
Co(1)–N(4)	2.269(3)	N(1)–Co(1)–O(1)	139.86(10)	N(3)–Co(1)–O(3)	154.68(10)
Co(1)–O(1)	2.132(2)	N(1)–Co(1)–O(2)	123.94(11)	N(4)–Co(1)–O(1)	147.95(9)
Co(1)–O(2)	2.148(4)	N(1)–Co(1)–O(3)	130.72(11)	N(4)–Co(1)–O(2)	76.53(11)
Co(1)–O(3)	2.243(2)	N(2)–Co(1)–N(3)	105.83(11)	N(4)–Co(1)–O(3)	78.27(8)
O(1)–C(19)	1.234(5)	N(2)–Co(1)–N(4)	116.04(12)	O(1)–Co(1)–O(2)	81.35(10)
O(2)–C(24)	1.219(4)	N(2)–Co(1)–O(1)	81.50(11)	O(1)–Co(1)–O(3)	76.78(8)
N(5)–C(19)	1.353(5)	N(2)–Co(1)–O(2)	161.60(8)	O(2)–Co(1)–O(3)	84.53(11)
N(6)–C(24)	1.354(4)	N(2)–Co(1)–O(3)	85.11(11)		