Electronic Supplementary Material (ESI) for CrystEngComm.

σ-hole halogen bonding interactions in a mixed valence cobalt(III/II) complex and anti-electrostatic hydrogen bonding interaction in a cobalt(III) complex: A theoretical insight

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Table S1: Selected bond lengths (Å) of complexes **1** and **2.**

	1	**2**
Co(1)–O(1)	1.9024(18)	1.8946(16)
Co(1)–O(1AC)	1.8973(19)	–
Co(1)–O(2)	1.9199(18)	–
Co(1)–N(1)	1.9240(2)	1.9252(19)
Co(1)–N(2)	1.9230(2)	1.9601(19)
Co(1)–N(3)	1.8990(2)	–
Co(2)–O(1)	2.1381(18)	–
Co(2)–O(2)	2.1177(18)	–
Co(2)–O(3)	2.1461(18)	1.9166(15)
Co(2)–O(2AC)	2.0356(19)	–

Co(2)–O(4)	2.0674(17)	–
Co(2)–O(3AC)	2.0524(19)	–
Co(3)–O(4AC)	1.9063(19)	–
Co(3)–O(3)	1.9263(17)	–
Co(3)–O(4)	1.9033(18)	–
Co(3)–N(4)	1.9340(2)	–
Co(3)–N(5)	1.9270(2)	–
Co(3)–N(6)	1.8970(2)	–
Co(1)–N(1)[a]	–	1.9252(19)
Co(1)–O(1)[a]	–	1.8946(16)
Co(1)–N(2)[a]	–	1.9601(19)
Co(2)–N(5)	–	1.9244(19)
Co(2)–O(3)[b]	–	1.9166(15)
Co(2)–N(5)[b]	–	1.9244(19)
Co(2)–N(6)	–	1.9610(2)
Co(2)–N(6)[b]	–	1.9610(2)
Co(3)–N(9)	–	1.9234(18)
Co(3)–N(10)	–	1.9740(19)
Co(3)–N(11)	–	1.9590(2)
Co(3)–N(14)	–	1.9630(2)
Co(3)–N(17)	–	1.9763(19)
Co(3)–O(5)	–	1.9008(16)

Symmetry transformation: [a] = 1–X,1–Y, –Z and [b] = 1–X,2–Y,1–Z.

Table S2: Selected bond angles (°) of complexes **1** and **2.**

	1	**2**
O(1)–Co(1)–O(1AC)	94.15(8)	
O(1)–Co(1)–O(2)	81.12(8)	
O(1)–Co(1)–N(1)	92.97(9)	90.37(8)
O(1)–Co(1)–N(2)	172.48(9)	87.79(8)
O(1)–Co(1)–N(3)	90.28(9)	
O(1AC)–Co(1)–O(2)	92.98(8)	
O(1AC)–Co(1)–N(1)	85.15(9)	
O(1AC)–Co(1)–N(2)	86.81(9)	
O(1AC)–Co(1)–N(3)	174.31(9)	
O(2)–Co(1)–N(1)	173.67(9)	
O(2)–Co(1)–N(2)	91.39(9)	
O(2)–Co(1)–N(3)	91.24(9)	
N(1)–Co(1)–N(2)	94.54(10)	88.67(8)
N(1)–Co(1)–N(3)	91.06(10)	
N(2)–Co(1)–N(3)	89.27(10)	
O(1)–Co(2)–O(2)	71.46(7)	
O(1)–Co(2)–O(3)	105.10(7)	

O(1)–Co(2)–O(2AC)	86.27(7)	
O(1)–Co(2)–O(4)	105.88(7)	
O(1)–Co(2)–O(3AC)	164.34(7)	
O(2)–Co(2)–O(3)	108.04(7)	
O(2)–Co(2)–O(2AC)	89.35(7)	
O(2)–Co(2)–O(4)	177.34(7)	
O(2)–Co(2)–O(3AC)	93.57(7)	
O(3)–Co(2)–O(2AC)	161.42(7)	
O(3)–Co(2)–O(4)	72.47(7)	
O(3)–Co(2)–O(3AC)	83.54(7)	
O(2AC)–Co(2)–O(4)	90.46(7)	
O(2AC)–Co(2)–O(3AC)	89.04(7)	
O(4)–Co(2)–O(3AC)	89.08(7)	
O(4AC)–Co(3)–O(3)	92.79(8)	
O(4AC)–Co(3)–O(4)	92.84(8)	
O(4AC)–Co(3)–N(4)	87.29(9)	
O(4AC)–Co(3)–N(5)	86.16(8)	
O(4AC)–Co(3)–N(6)	175.07(9)	
O(3)–Co(3)–O(4)	81.16(7)	
O(3)–Co(3)–N(4)	93.10(8)	
O(3)–Co(3)–N(5)	171.67(8)	
O(3)–Co(3)–N(6)	91.09(8)	
O(4)–Co(3)–N(4)	174.25(8)	

O(4)–Co(3)–N(5)	90.63(8)	
O(4)–Co(3)–N(6)	90.76(9)	
N(4)–Co(3)–N(5)	95.11(9)	
N(4)–Co(3)–N(6)	89.48(9)	
N(5)–Co(3)–N(6)	90.43(9)	
O(1)–Co(1)–O(1)[a]	–	180.00
O(1)–Co(1)–N(1)[a]	–	89.63(8)
O(1)–Co(1)–N(2)[a]	–	92.21(8)
O(1)[a]–Co(1)–N(1)	–	89.63(8)
N(1)–Co(1)–N(1)[a]	–	180.00
N(1)–Co(1)–N(2)[a]	–	91.33(8)
O(1)[a]–Co(1)–N(2)	–	92.21(8)
N(1)[a]–Co(1)–N(2)	–	91.33(8)
N(2)–Co(1)–N(2)[a]	–	180.00
O(1)[a]–Co(1)–N(1)[a]	–	90.37(8)
O(1)[a]–Co(1)–N(2)[a]	–	87.79(8)
N(1)[a]–Co(1)–N(2)[a]	–	88.67(8)
O(3)–Co(2)–O(3)[b]	–	180.00
O(3)–Co(2)–N(5)[b]	–	90.96(7)
O(3)–Co(2)–N(6)[b]	–	91.94(7)
N(5)–Co(2)–N(6)	–	88.50(8)
O(3)[b]–Co(2)–N(5)	–	90.96(7)
N(5)–Co(2)–N(5)[b]	–	180.00

N(5)–Co(2)–N(6)[b]	–	91.50(8)
O(3)[b]–Co(2)–N(6)	–	91.94(7)
N(5)[b]–Co(2)–N(6)	–	91.50(8)
N(6)–Co(2)–N(6)[b]	–	180.00
O(3)[b]–Co(2)–N(5)[b]	–	89.04(7)
O(3)[b]–Co(2)–N(6)[b]	–	88.06(7)
N(5)[b]–Co(2)–N(6)[b]	–	88.50(8)
O(3)–Co(2)–N(6)	–	88.06(7)
O(3)–Co(2)–N(5)	–	89.04(7)
O(5)–Co(3)–N(17)	–	90.44(7)
O(5)–Co(3)–N(14)	–	91.09(7)
N(9)–Co(3)–N(14)	–	176.94(8)
N(9)–Co(3)–N(17)	–	91.24(8)
N(10)–Co(3)–N(11)	–	87.91(8)
N(10)–Co(3)–N(14)	–	83.66(8)
N(10)–Co(3)–N(17)	–	87.58(8)
N(11)–Co(3)–N(14)	–	88.57(8)
N(11)–Co(3)–N(17)	–	175.44(8)
N(14)–Co(3)–N(17)	–	90.26(8)
O(5)–Co(3)–N(10)	–	174.38(8)
O(5)–Co(3)–N(11)	–	93.99(8)
O(5)–Co(3)–N(9)	–	91.57(7)
N(9)–Co(3)–N(11)	–	89.74(8)

N(9)–Co(3)–N(10)	–	93.73(8)

Symmetry transformation: [a] = 1–X,1–Y, –Z and [b] = 1–X,2–Y,1–Z.