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Molecular and Electronic Structure of an Unusual Cobalt NNO pincer ligand complex

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1. Table for CShm calculation.
2. Selected bond length and bond angle table
3. Magnetic measurement for complex **2.**

Table S1. Table for CShm calculation.

Geometry	Pentagon	Vacant octahedron	Trigonal bipyramid	Spherical square pyramid	Johnson trigonal bipyramid
Point group	D5h	C4v	D3h	C4v	D3h
Deviation from the indicated geometry	32.209	3.242	5.173	**1.714**	7.805

Table S2-S3. Table for the selected bond length and bond angle for complex **2.**

Atom	Atom	Length/ Å
Co(11)-N(112)		1.8364(11)
Co(11)-O(111)		1.9411(10)
Co(11)-N(111)		1.9486(12)
Co(11)-P(161)		2.1993(4)
Co(11)-P(151)		2.2338(4)
Co(2)-C(14)		1.9380(14)
Co(2)-C(13)		2.1159(14)
Co(2)-C(15)		2.1357(14)
Co(2)-P(71)		2.1654(4)
Co(2)-P(81)		2.1676(4)
Co(2)-P(91)		2.1847(4)
Co(1)-N(12)		1.8397(11)
Co(1)-N(11)		1.9469(12)
Co(1)-O(11)		1.9501(10)
Co(1)-P(61)		2.2079(4)
Co(1)-P(51)		2.2387(4)
Co(12)-C(114)		1.9366(14)
Co(12)-C(113)		2.1087(14)
Co(12)-C(115)		2.1367(14)
Co(12)-P(171)		2.1642(4)
Co(12)-P(181)		2.1672(4)
Co(12)-P(191)		2.1839(4)

Atom Atom Atom	Angle/˚
N(112)-Co(11)-O(111)	80.64(5)
N(112)-Co(11)-N(111)	81.34(5)
O(111)-Co(11)-N(111)	149.73(5)
N(112)-Co(11)-P(161)	160.33(4)
O(111)-Co(11)-P(161)	85.55(3)
N(111)-Co(11)-P(161)	104.67(3)
N(112)-Co(11)-P(151)	92.29(4)
O(111)-Co(11)-P(151)	95.40(3)
N(111)-Co(11)-P(151)	109.45(4)
P(161)-Co(11)-P(151)	102.946(16)
C(14)-Co(2)-C(13)	41.46(6)
C(14)-Co(2)-C(15)	40.98(5)
C(13)-Co(2)-C(15)	68.34(5)
C(14)-Co(2)-P(71)	111.80(4)
C(13)-Co(2)-P(71)	151.81(4)
C(15)-Co(2)-P(71)	84.52(4)
C(14)-Co(2)-P(81)	101.04(4)
C(13)-Co(2)-P(81)	96.71(4)
C(15)-Co(2)-P(81)	136.88(4)
P(71)-Co(2)-P(81)	98.187(16)
C(14)-Co(2)-P(91)	134.87(4)
C(13)-Co(2)-P(91)	98.65(4)
C(15)-Co(2)-P(91)	117.20(4)
P(71)-Co(2)-P(91)	100.531(17)
P(81)-Co(2)-P(91)	104.660(17)
N(12)-Co(1)-N(11)	81.02(5)
N(12)-Co(1)-O(11)	80.61(5)
N(11)-Co(1)-O(11)	150.28(5)

N(12)-Co(1)-P(61)	160.91(4)
N(11)-Co(1)-P(61)	104.74(4)
O(11)-Co(1)-P(61)	86.27(3)
N(12)-Co(1)-P(51)	92.44(4)
N(11)-Co(1)-P(51)	108.65(4)
O(11)-Co(1)-P(51)	95.29(3)
P(61)-Co(1)-P(51)	102.586(16)
C(114)-Co(12)-C(113)	41.48(6)
C(114)-Co(12)-C(115)	40.93(5)
C(113)-Co(12)-C(115)	68.42(5)
C(114)-Co(12)-P(171)	112.37(4)
C(113)-Co(12)-P(171)	152.34(4)
C(115)-Co(12)-P(171)	84.87(4)
C(114)-Co(12)-P(181)	100.81(4)
C(113)-Co(12)-P(181)	96.90(4)
C(115)-Co(12)-P(181)	136.31(4)
P(171)-Co(12)-P(181)	97.722(16)
C(114)-Co(12)-P(191)	134.04(4)
C(113)-Co(12)-P(191)	97.45(4)
C(115)-Co(12)-P(191)	117.58(4)
P(171)-Co(12)-P(191)	101.348(16)
P(181)-Co(12)-P(191)	104.712(16)

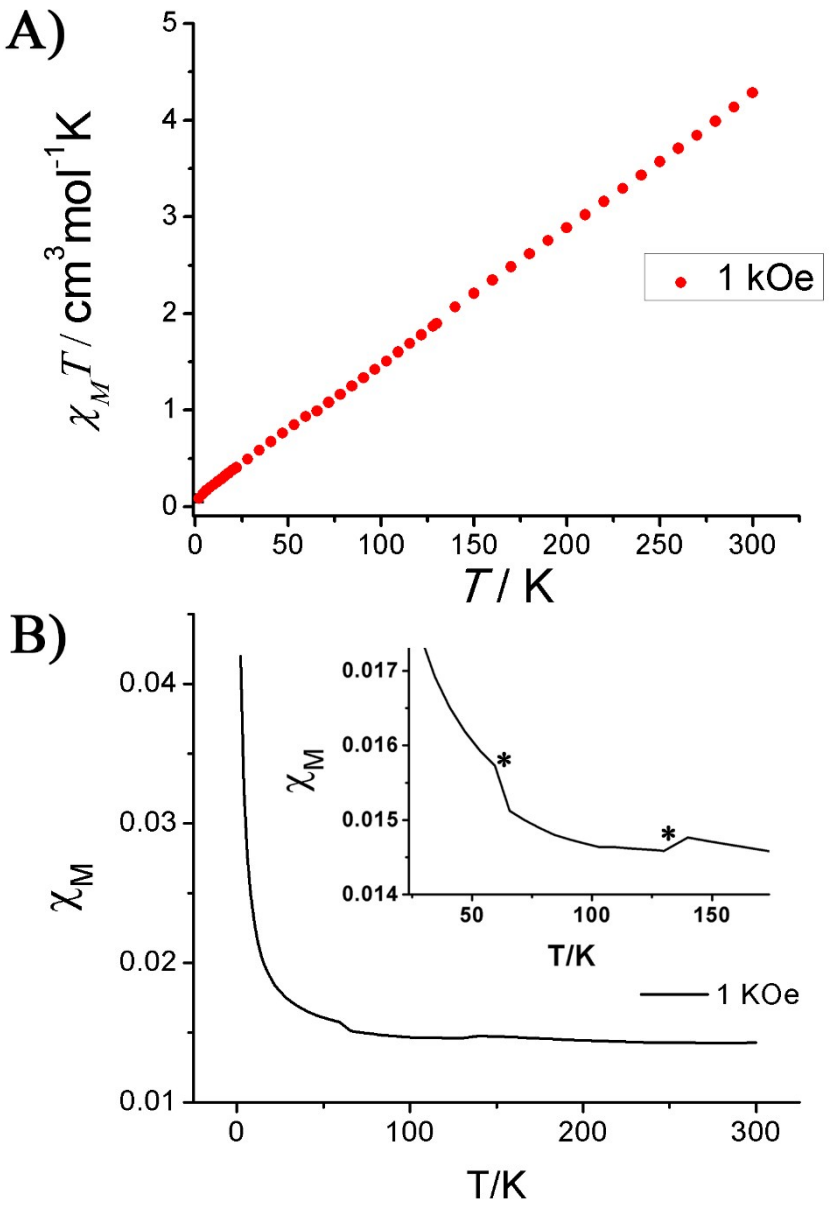

Figure S1. Temperature dependent magnetic susceptibility performed on polycrystalline sample of 2 in the presence of an external magnetic field of 1 kOe A) molar magnetic susceptibility temperature product as a function of temperature B) molar magnetic susceptibility as a function of temperature. Inset: Zoomed in region of χ_M = f(T) plot where the maxima appears at two different temperature (*) are indicated.