Electronic Supplementary Information for Dalton Transactions

Synthesis and structural and magnetic characterization of a hexadecanuclear cobalt phosphonate compound

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Supporting materials

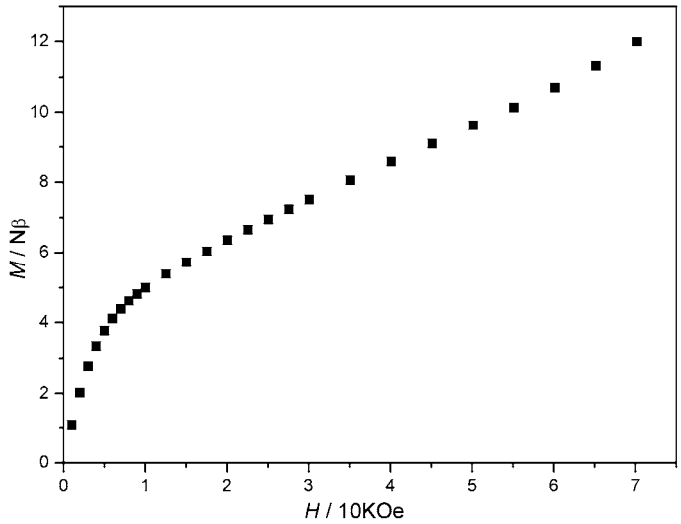

Figure S1 *M/Nβ* vs. *H* curve for **1**·10CH_2Cl_2·2H_2O

Table S1 Crystallographic and refinement details

Empirical formula	$C_{132}H_{122}Cl_{42}Co_{16}N_{22}O_{40}P_2$
FW	5150.24
Crystal system	Triclinic
Space group	P$\bar{1}$
a/Å	14.783(3)
b/Å	15.607(3)
c/Å	21.545(4)
α/^{o}	98.12(3)
β/^{o}	101.56(3)
γ/^{o}	93.29(3)
V	4802.4(17)
Z	1
ρ_{calcd}/ g cm^{-3}	1.781
F(000)	2564
Goodness-of-fit on F^2	1.056
R_1, wR_2 [I >2σ(I)]	0.0780, 0.1828
R_1, wR_2 (all data)	0.1257, 0.2091
$(\Delta\rho)_{max}$, $(\Delta\rho)_{min}$/e Å^{-3}	1.718, -1.281

Table S2 Selected bond lengths (Å) and angles (°)

Bond lengths/Å			
Co(1)-O(5)	2.055(5)	Co(5)-O(13)	1.991(6)
Co(1)-O(14)	2.056(5)	Co(5)-O(5)	2.051(5)
Co(1)-O(11)	2.062(6)	Co(5)-O(9)	2.146(6)
Co(1)-O(4)	2.098(6)	Co(5)-N(3)	2.204(6)
Co(1)-O(10)	2.096(5)	Co(5)-N(6)	2.215(6)
Co(1)-O(1)	2.167(5)	Co(5)-O(10)	2.277(5)
Co(2)-O(6)	2.001(5)	Co(6)-O(2)	2.042(5)
Co(2)-O(1)	2.011(5)	Co(6)-O(15)	2.092(5)
Co(2)-N(9)	2.064(6)	Co(6)-O(6)	2.114(5)
Co(2)-N(8)	2.108(6)	Co(6)-O(17)	2.120(3)
Co(2)-O(14)	2.262(5)	Co(6)-N(10)	2.169(6)
Co(3)-O(5)	1.994(5)	Co(6)-O(16)	2.194(5)
Co(3)-O(6)	2.032(5)	Co(7)-O(9)	2.015(5)
Co(3)-N(7)	2.066(6)	Co(7)-O(4)	2.027(6)
Co(3)-N(11)	2.095(6)	Co(7)-O(7)	2.055(5)
Co(4)-O(3)	2.021(5)	Co(7)-O(12)	2.074(5)
Co(4)-O(19)	2.059(3)	Co(7)-N(2)	2.089(7)
Co(4)-O(18)	2.127(3)	Co(8)-O(8)	1.944(7)
Co(4)-O(16A)	2.141(5)	Co(8)-O(4)	1.971(5)
Co(4)-O(7)	2.154(5)	Co(8)-N(5)	2.020(8)
Co(4)-O(12)	2.211(5)	Co(8)-N(4)	2.047(7)

Bond angles/°			
O(1)-Co(1)-O(4)	95.7(2)	O(13)-Co(5)-O(5)	87.6(2)
O(1)-Co(1)-O(5)	90.1(2)	O(13)-Co(5)-O(9)	159.8(2)
O(1)-Co(1)-O(10)	169.3(2)	O(13)-Co(5)-N(3)	101.4(3)
O(1)-Co(1)-O(11)	96.5(2)	O(13)-Co(5)-N(6)	108.8(2)
O(1)-Co(1)-O(14)	79.8(2)	O(13)-Co(5)-O(10)	92.7(2)
O(4)-Co(1)-O(5)	95.7(2)	O(5)-Co(5)-O(9)	108.2(2)
O(4)-Co(1)-O(10)	90.8(2)	O(5)-Co(5)-N(3)	163.2(2)
O(4)-Co(1)-O(11)	92.0(2)	O(5)-Co(5)-N(6)	90.0(2)
O(4)-Co(1)-O(14)	175.1(2)	O(5)-Co(5)-O(10)	76.7(2)
O(5)-Co(1)-O(10)	80.8(2)	O(9)-Co(5)-N(3)	60.2(2)
O(5)-Co(1)-O(11)	169.3(2)	O(9)-Co(5)-N(6)	84.3(2)
O(5)-Co(1)-O(14)	82.4(2)	O(9)-Co(5)-O(10)	79.3(2)
O(10)-Co(1)-O(11)	91.6(2)	N(3)-Co(5)-N(6)	100.3(2)
O(10)-Co(1)-O(14)	93.3(2)	N(3)-Co(5)-O(10)	88.6(2)
O(11)-Co(1)-O(14)	90.5(2)	N(6)-Co(5)-O(10)	154.4(2)
O(1)-Co(2)-O(6)	100.8(2)	O(2)-Co(6)-O(15)	90.4(2)
O(1)-Co(2)-N(9)	102.6(2)	O(2)-Co(6)-O(6)	103.6(2)
O(1)-Co(2)-N(8)	123.3(2)	O(2)-Co(6)-O(17)	90.4(2)

O(1)-Co(2)-O(14)	78.5(2)	O(2)-Co(6)-N(10)	158.1(2)
O(6)-Co(2)-N(9)	106.3(2)	O(2)-Co(6)-O(16)	96.4(2)
O(6)-Co(2)-N(8)	109.1(2)	O(15)-Co(6)-O(6)	87.3(2)
O(6)-Co(2)-O(14)	80.9(2)	O(15)-Co(6)-O(17)	173.9(2)
N(9)-Co(2)-N(8)	113.1(2)	O(15)-Co(6)-N(10)	92.8(2)
N(9)-Co(2)-O(14)	172.2(2)	O(15)-Co(6)-O(16)	97.5(2)
N(8)-Co(2)-O(14)	60.9(2)	O(6)-Co(6)-O(17)	86.6(2)
O(5)-Co(3)-O(6)	109.4(2)	O(6)-Co(6)-N(10)	98.2(2)
O(5)-Co(3)-N(7)	115.5(2)	O(6)-Co(6)-O(16)	159.4(2)
O(5)-Co(3)-N(11)	103.5(2)	O(17)-Co(6)-N(10)	88.6(2)
O(6)-Co(3)-N(7)	116.1(2)	O(17)-Co(6)-O(16)	88.4(2)
O(6)-Co(3)-N(11)	102.9(2)	N(10)-Co(6)-O(16)	61.7(2)
N(7)-Co(3)-N(11)	107.9(2)	O(9)-Co(7)-O(4)	93.3(2)
O(3)-Co(4)-O(19)	100.0(2)	O(9)-Co(7)-O(7)	171.2(2)
O(3)-Co(4)-O(18)	162.7(2)	O(9)-Co(7)-O(12)	90.0(2)
O(3)-Co(4)-O(16A)	93.8(2)	O(9)-Co(7)-N(2)	92.2(3)
O(3)-Co(4)-O(7)	84.0(2)	O(4)-Co(7)-O(7)	90.8(2)
O(3)-Co(4)-O(12)	89.8(2)	O(4)-Co(7)-O(12)	99.9(2)
O(19)-Co(4)-O(18)	96.5(2)	O(4)-Co(7)-N(2)	112.4(3)
O(19)-Co(4)-O(16A)	83.6(2)	O(7)-Co(7)-O(12)	81.6(2)
O(19)-Co(4)-O(7)	164.7(2)	O(7)-Co(7)-N(2)	93.4(3)
O(19)-Co(4)-O(12)	88.9(2)	O(12)-Co(7)-N(2)	147.4(3)
O(18)-Co(4)-O(16A)	83.1(2)	O(8)-Co(8)-O(4)	103.0(3)
O(18)-Co(4)-O(7)	81.3(2)	O(8)-Co(8)-N(5)	113.9(3)
O(18)-Co(4)-O(12)	95.5(2)	O(8)-Co(8)-N(4)	108.4(3)
O(16A)-Co(4)-O(7)	111.0(2)	O(4)-Co(8)-N(5)	105.3(3)
O(16A)-Co(4)-O(12)	172.1(2)	O(4)-Co(8)-N(4)	111.5(3)
O(7)-Co(4)-O(12)	76.4(2)	N(5)-Co(8)-N(4)	114.2(3)
Co(1)-O(1)-Co(2)	103.1(2)	Co(2)-O(6)-Co(3)	111.8(2)
Co(1)-O(14)-Co(2)	98.4(2)	Co(2)-O(6)-Co(6)	104.3(2)
Co(1)-O(4)-Co(8)	97.2(2)	Co(6)-O(6)-Co(3)	111.7(2)
Co(1)-O(4)-Co(7)	129.6(3)	Co(7)-O(7)-Co(4)	100.7(2)
Co(7)-O(4)-Co(8)	108.0(2)	Co(7)-O(9)-Co(5)	115.0(2)
Co(3)-O(5)-Co(5)	110.4(2)	Co(1)-O(10)-Co(5)	94.8(2)
Co(3)-O(5)-Co(1)	110.6(2)	Co(7)-O(12)-Co(4)	98.3(2)
Co(5)-O(5)-Co(1)	103.3(2)	Co(4A)-O(16)-Co(6)	129.4(3)
Symmetry code: (A) –x, -y+1, -z			

Table S3 BVS calculations for Co and O atoms

Atom	BVS	atom	BVS
Co1	1.997	Co7	1.948
Co2	1.936	Co8	1.918
Co3	1.726	O4	1.171
Co4	1.859	O5	1.158
Co5	1.925	O6	1.116
Co6	1.926		