Supplementary material (ESI) for Journal of Materials Chemistry

Electronic Supplementary Information for

A Hybrid Cobalt Disulfonate with a Novel Inorganic Layer Architecture Exhibiting a Field-Induced Magnetic Transition

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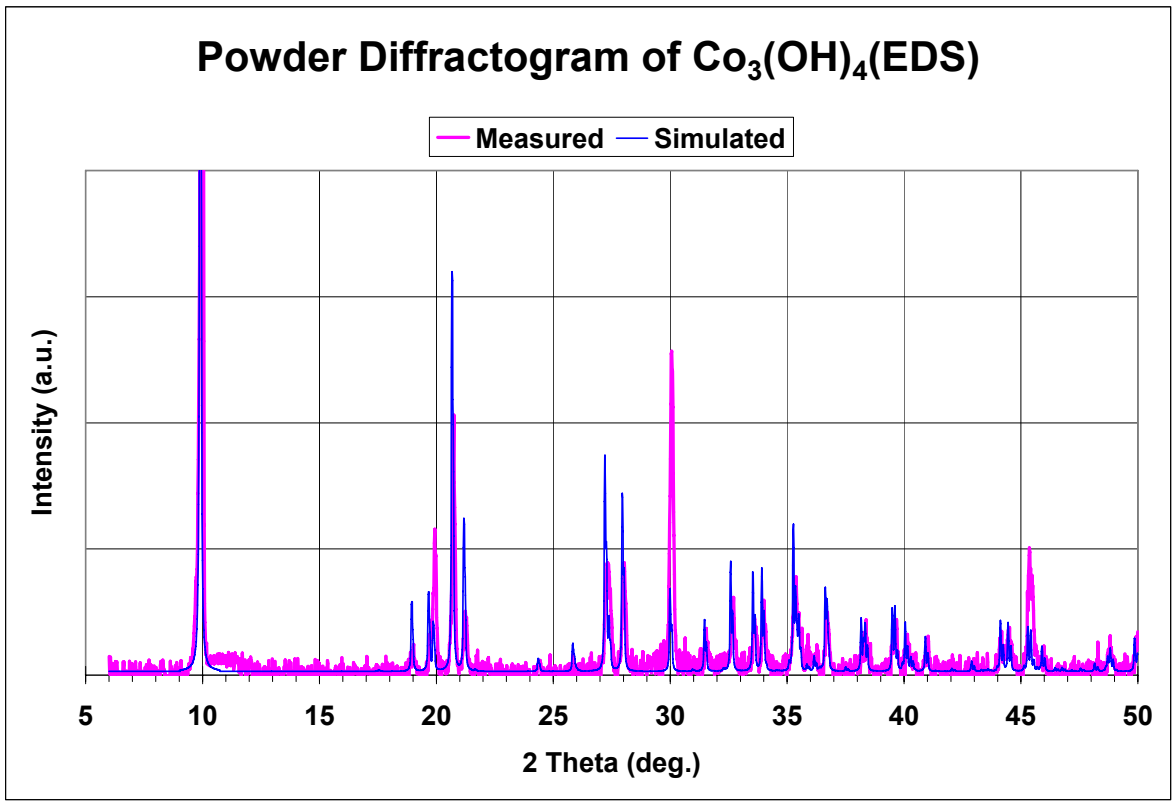
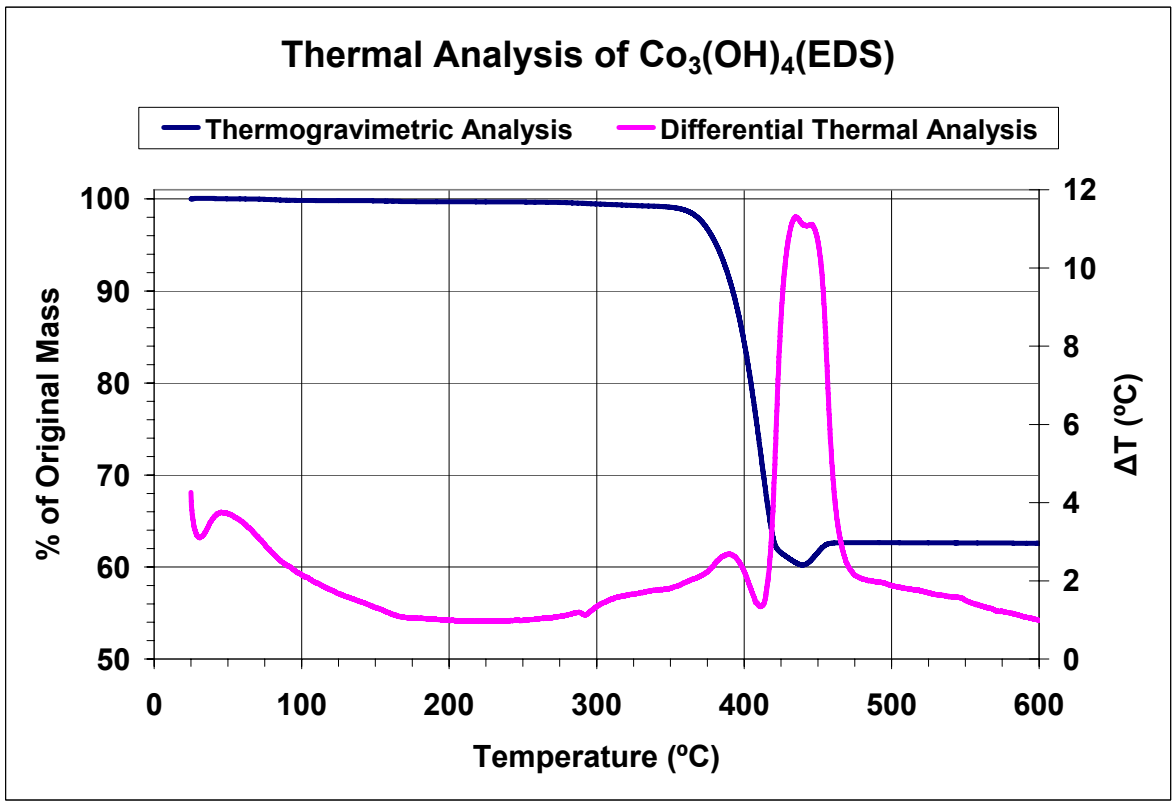
including tables of bond lengths and angles, anisotropic displacement parameters, hydrogen coordinates and hydrogen bond parameters; powder diffractogram and thermal analysis.





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Crystallographic Data for $Co_3(OH)_4(EDS)$:

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$):

	x	y	z	U_{eq}
Co(1)	0	0	0	11(1)
Co(2)	-801(1)	-4787(1)	1402(1)	12(1)
S(1)	-3208(1)	-12(1)	1538(1)	13(1)
C(1)	-4973(3)	502(6)	700(3)	16(1)
O(1)	-2902(2)	-2734(4)	1514(2)	20(1)
O(2)	-2120(2)	1445(4)	791(2)	17(1)
O(3)	-3333(2)	935(4)	2874(2)	21(1)
O(4)	-571(2)	1543(4)	-1821(2)	14(1)
O(5)	-916(2)	-3375(3)	-513(2)	14(1)

(U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor)

Bond lengths [Å] and angles [°]:

Co(1)-O(5)	2.0171(18)	S(1)-C(1)	1.771(3)
Co(1)-O(5)#1	2.0171(18)	C(1)-C(1)#5	1.512(5)
Co(1)-O(4)#1	2.0532(17)	C(1)-H(1)	0.98(3)
Co(1)-O(4)	2.0532(17)	C(1)-H(2)	0.99(3)
Co(1)-O(2)	2.2349(18)	O(2)-Co(2)#6	2.3774(19)
Co(1)-O(2)#1	2.2349(18)	O(4)-Co(2)#7	2.0250(17)
Co(2)-O(4)#2	2.0250(17)	O(4)-Co(2)#1	2.1362(19)
Co(2)-O(5)#3	2.0667(18)	O(4)-H(3)	0.83(4)
Co(2)-O(5)	2.0736(19)	O(5)-Co(2)#3	2.0667(18)
Co(2)-O(4)#1	2.1362(19)	O(5)-H(4)	0.80(4)
Co(2)-O(1)	2.1787(19)	----------	----------
Co(2)-O(2)#4	2.3774(19)	O(5)-Co(1)-O(5)#1	180.00(11)
S(1)-O(3)	1.4526(19)	O(5)-Co(1)-O(4)#1	87.53(7)
S(1)-O(1)	1.464(2)	O(5)#1-Co(1)-O(4)#1	92.47(7)
S(1)-O(2)	1.4822(19)	O(5)-Co(1)-O(4)	92.47(7)

O(5)#1-Co(1)-O(4)	87.53(7)	O(3)-S(1)-O(2)	112.65(12)
O(4)#1-Co(1)-O(4)	180.00(11)	O(1)-S(1)-O(2)	111.89(11)
O(5)-Co(1)-O(2)	93.06(7)	O(3)-S(1)-C(1)	106.19(12)
O(5)#1-Co(1)-O(2)	86.94(7)	O(1)-S(1)-C(1)	107.76(13)
O(4)#1-Co(1)-O(2)	89.23(7)	O(2)-S(1)-C(1)	105.63(12)
O(4)-Co(1)-O(2)	90.77(7)	C(1)#5-C(1)-S(1)	112.0(2)
O(5)-Co(1)-O(2)#1	86.94(7)	C(1)#5-C(1)-H(1)	110.6(19)
O(5)#1-Co(1)-O(2)#1	93.06(7)	S(1)-C(1)-H(1)	103(2)
O(4)#1-Co(1)-O(2)#1	90.77(7)	C(1)#5-C(1)-H(2)	118(2)
O(4)-Co(1)-O(2)#1	89.23(7)	S(1)-C(1)-H(2)	97(2)
O(2)-Co(1)-O(2)#1	180.00(9)	H(1)-C(1)-H(2)	115(3)
O(4)#2-Co(2)-O(5)#3	97.60(7)	S(1)-O(1)-Co(2)	130.69(11)
O(4)#2-Co(2)-O(5)	173.06(7)	S(1)-O(2)-Co(1)	126.95(11)
O(5)#3-Co(2)-O(5)	76.12(8)	S(1)-O(2)-Co(2)#6	129.23(11)
O(4)#2-Co(2)-O(4)#1	99.38(4)	Co(1)-O(2)-Co(2)#6	87.73(6)
O(5)#3-Co(2)-O(4)#1	91.75(7)	Co(2)#7-O(4)-Co(1)	128.59(10)
O(5)-Co(2)-O(4)#1	83.93(7)	Co(2)#7-O(4)-Co(2)#1	124.87(9)
O(4)#2-Co(2)-O(1)	103.00(7)	Co(1)-O(4)-Co(2)#1	91.68(7)
O(5)#3-Co(2)-O(1)	157.17(8)	Co(2)#7-O(4)-H(3)	103(2)
O(5)-Co(2)-O(1)	82.72(7)	Co(1)-O(4)-H(3)	104(2)
O(4)#1-Co(2)-O(1)	94.48(7)	Co(2)#1-O(4)-H(3)	100(3)
O(4)#2-Co(2)-O(2)#4	82.61(7)	Co(1)-O(5)-Co(2)#3	103.08(8)
O(5)#3-Co(2)-O(2)#4	82.15(7)	Co(1)-O(5)-Co(2)	94.58(8)
O(5)-Co(2)-O(2)#4	93.48(7)	Co(2)#3-O(5)-Co(2)	103.88(8)
O(4)#1-Co(2)-O(2)#4	173.80(7)	Co(1)-O(5)-H(4)	119(3)
O(1)-Co(2)-O(2)#4	90.76(7)	Co(2)#3-O(5)-H(4)	115(2)
O(3)-S(1)-O(1)	112.21(12)	Co(2)-O(5)-H(4)	118(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 x,-y-1/2,z+1/2 #3 -x,-y-1,-z #4 x,y-1,z #5 -x-1,-y,-z #6 x,y+1,z #7 x,-y-1/2,z-1/2

Anisotropic displacement parameters ($Å^2 \times 10^3$):

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co(1)	13(1)	11(1)	10(1)	0(1)	-1(1)	0(1)
Co(2)	13(1)	13(1)	10(1)	1(1)	0(1)	1(1)
S(1)	9(1)	16(1)	12(1)	0(1)	-1(1)	1(1)
C(1)	10(1)	22(1)	16(1)	-2(1)	-2(1)	1(1)
O(1)	17(1)	15(1)	27(1)	3(1)	2(1)	2(1)
O(2)	15(1)	18(1)	19(1)	1(1)	2(1)	-1(1)
O(3)	17(1)	29(1)	15(1)	-4(1)	1(1)	0(1)
O(4)	14(1)	15(1)	13(1)	-1(1)	-2(1)	3(1)
O(5)	13(1)	16(1)	14(1)	-1(1)	-2(1)	1(1)

(The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$)

Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$):

	x	y	z	U_{eq}
H(1)	-5060(40)	2350(60)	700(30)	31(7)
H(2)	-5580(40)	-370(60)	1340(30)	31(7)
H(3)	-1410(40)	2160(70)	-1740(30)	30(7)
H(4)	-1710(40)	-3410(70)	-920(30)	30(7)

Hydrogen bond parameters:

D-H...A	d (D-H)	d (H...A)	d (D...A)	< (DHA)
O(4)-H(3)...O(3)#1	0.83(4)	2.01(4)	2.809(3)	161(3)
O(5)-H(4)...O(3)#2	0.80(4)	2.27(4)	2.961(3)	144(4)

Symmetry transformations used to generate equivalent atoms: #1 x,-y+1/2,z-1/2 #2 x,-y-1/2,z-1/2