Novel example of a chain structure formed by 1,4-dioxane and cobalt(II) links. Chain [Co-3(mu-OOCCF3)(4)(mu-H2O)(2)(OOCCF3)(2)(H2O)(2)(C4H8O2)]center dot 2C(4)H(8)O(2)

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A Novel Example of a Chain Structure Formed by 1,4-Dioxane and Cobalt(II) Links. Chain $Co_3(\mu\text{-}OOC\text{-}CF_3)_4(\mu\text{-}H_2O)_2(OOC\text{-}CF_3)_2(H_2O)_2(C_4H_8O_2).2(C_4H_8O_2)$.

Víctor Calvo-Pérez, Sergei Ostrovsky, Andrés Vega, Juraj Pelikan, Evgenia Spodine, Wolfgang Haase

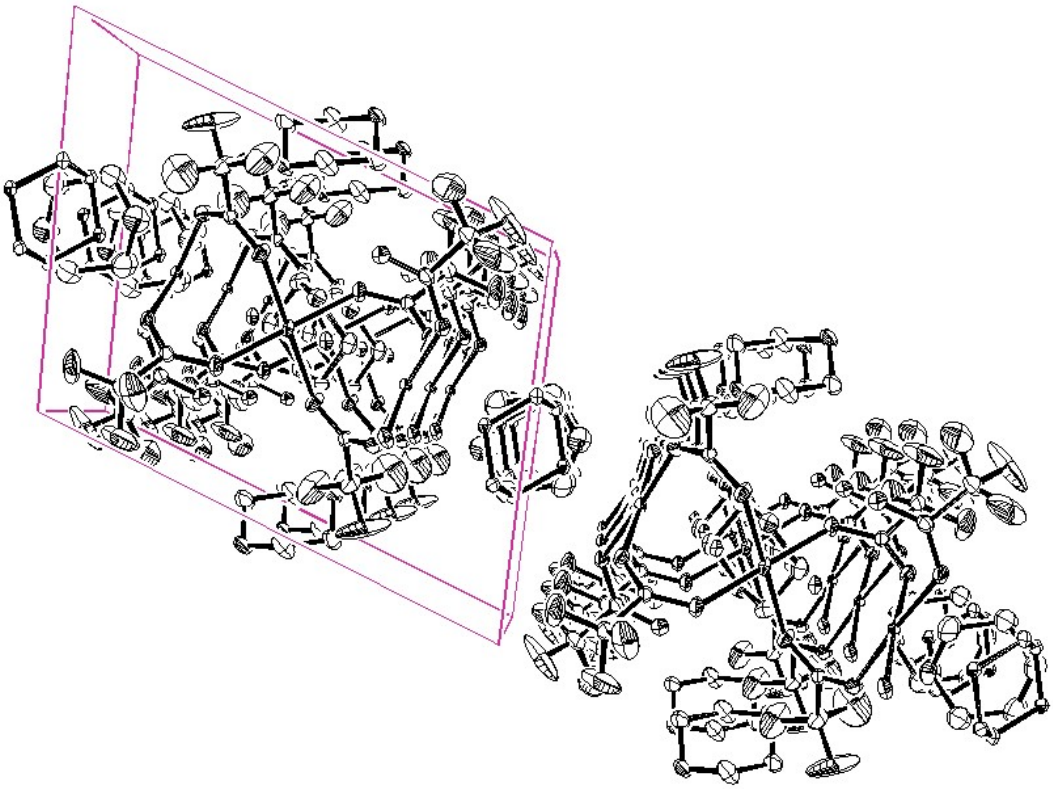

Figure S1

Illustration of the 1D chain of trimers along the longitudinal axis surrounded by a 1,4-dioxane scaffold. The hydrogen atoms are not shown for clarity.

TABLE S1. Atomic Coordinates (Å x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **1**

atom	x	y	z	U(eq)
Co1	5000	10000	5000	33(1)
Co2	5056(1)	8702(1)	7557(1)	30(1)
O1	3547(4)	10566(4)	5652(3)	50(1)
C1	3053(5)	10253(5)	6388(4)	35(1)
O2	3293(3)	9435(3)	7034(3)	45(1)
C2	1990(7)	11010(7)	6547(5)	62(2)
F1	1405(7)	11507(8)	5745(5)	167(3)
F2	1109(8)	10411(8)	6953(8)	217(5)
F3	2660(10)	12080(8)	7257(7)	207(4)
O3	6671(4)	11324(3)	6243(2)	46(1)
C3	6967(5)	11374(5)	7256(4)	37(1)
O4	6442(4)	10603(3)	7804(3)	47(1)
C4	8196(6)	12606(7)	7933(4)	65(2)
F4	8092(6)	13734(4)	7546(4)	128(2)
F5	9410(5)	12504(7)	7876(6)	165(3)
F6	8276(6)	12811(5)	8939(3)	138(2)
O5	6823(3)	7972(4)	8181(3)	45(1)
C5	7772(5)	7995(5)	7749(4)	42(1)
O6	7753(4)	8169(4)	6816(3)	60(1)
C6	9140(7)	7753(8)	8487(6)	69(2)
F7	8923(5)	6808(8)	9046(7)	194(4)
F8	9925(7)	8748(7)	9136(7)	216(4)
F9	9956(7)	7420(10)	8004(6)	196(4)
O7	5046(3)	9034(3)	9193(2)	42(1)
C7	3781(5)	8938(5)	9505(4)	44(1)
C8	6301(5)	9701(5)	10104(4)	46(1)
O8	3709(4)	6817(3)	7409(3)	46(1)
O9	5187(3)	8355(3)	5924(2)	33(1)
C10	5600(10)	4890(10)	9186(7)	113(3)
O10	4288(6)	5247(6)	8981(4)	112(2)
O11	6002(4)	4232(3)	5148(3)	53(1)
C11	3532(8)	4660(10)	9663(7)	101(3)
C12	5260(7)	4364(6)	5923(5)	57(1)
C13	6168(6)	5424(5)	4631(5)	56(1)
O12	1179(4)	5738(4)	5862(3)	62(1)
C14	81(7)	4726(8)	6026(5)	86(2)
C15	629(7)	6326(7)	4926(6)	82(2)

U(eq) is defined as 1/3 the trace of the Uij tensor.

TABLE S2. Bond lengths (Å) and angles (degrees) for **1**

Co1-O1a	2.067(3)	Co1-O1	2.067(3)
Co1-O3a	2.076(3)	Co1-O3	2.076(3)
Co1-O9	2.143(3)	Co1-O9a	2.143(3)
Co2-O8	2.044(3)	Co2-O2	2.053(3)
Co2-O4	2.055(3)	Co2-O5	2.072(3)
Co2-O7	2.120(3)	Co2-O9	2.160(3)
O1-C1	1.224(5)	C1-O2	1.238(5)
C1-C2	1.518(7)	C2-F2	1.227(7)
C2-F1	1.241(7)	C2-F3	1.284(9)
O3-C3	1.249(5)	C3-O4	1.225(5)
C3-C4	1.542(7)	C4-F6	1.277(7)
C4-F5	1.282(8)	C4-F4	1.304(7)
O5-C5	1.241(6)	C5-O6	1.225(6)
C5-C6	1.522(7)	C6-F8	1.218(8)
C6-F7	1.262(8)	C6-F9	1.263(8)
O7-C7	1.435(5)	O7-C8	1.439(5)
C7-C8a	1.478(7)	C8-C7a	1.478(7)
C10-O10	1.42(1)	C10-C11a	1.47(1)
O10-C11	1.403(8)	O11-C13	1.429(6)
O11-C12	1.432(6)	C11-C10a	1.47(1)
C12-C13a	1.491(8)	C13-C12a	1.491(8)
O12-C14	1.406(7)	O12-C15	1.415(7)
C14-C15a	1.46(1)	C15-C14a	1.46(1)

O1-Co1a-O1	180.000(1)	O1-Co1a-O3a	89.8(1)
O1-Co1-O3a	90.2(2)	O1-Co1a-O3	90.2(2)
O1-Co1-O3	89.8(2)	O3-Co1a-O3	180.000(1)
O1-Co1a-O9	85.4(1)	O1-Co1-O9	94.6(1)
O3-Co1a-O9	89.6(1)	O3-Co1-O9	90.4(1)
O1-Co1a-O9a	94.6(1)	O1-Co1-O9a	85.4(1)
O3-Co1a-O9a	90.4(1)	O3-Co1-O9a	89.6(1)
O9-Co1-O9a	180.000(1)	O8-Co2-O2	88.7(1)
O8-Co2-O4	176.6(1)	O2-Co2-O4	92.3(1)
O8-Co2-O5	90.8(1)	O2-Co2-O5	176.4(1)
O4-Co2-O5	87.9(1)	O8-Co2-O7	87.5(1)
O2-Co2-O7	90.0(1)	O4-Co2-O7	89.2(1)
O5-Co2-O7	86.4(1)	O8-Co2-O9	93.4(1)
O2-Co2-O9	93.0(1)	O4-Co2-O9	89.7(1)
O5-Co2-O9	90.6(1)	O7-Co2-O9	176.8(1)
C1-O1-Co1	135.9(3)	O1-C1-O2	130.6(4)
O1-C1-C2	114.7(4)	O2-C1-C2	114.7(4)
C1-O2-Co2	129.8(3)	F2-C2-F1	110.9(7)
F2-C2-F3	102.2(7)	F1-C2-F3	101.3(7)
F2-C2-C1	115.4(5)	F1-C2-C1	115.8(5)
F3-C2-C1	109.3(6)	C3-O3-Co1	129.4(3)
O4-C3-O3	130.6(4)	O4-C3-C4	114.6(4)
O3-C3-C4	114.8(4)	C3-O4-Co2	137.9(3)
F6-C4-F5	108.9(6)	F6-C4-F4	106.6(6)
F5-C4-F4	103.0(6)	F6-C4-C3	113.8(4)
F5-C4-C3	111.6(6)	F4-C4-C3	112.3(5)
C5-O5-Co2	124.3(3)	O6-C5-O5	129.1(5)
O6-C5-C6	116.1(5)	O5-C5-C6	114.8(5)
F8-C6-F7	106.3(8)	F8-C6-F9	102.9(8)
F7-C6-F9	103.2(8)	F8-C6-C5	113.9(6)
F7-C6-C5	113.7(6)	F9-C6-C5	115.7(6)
C7-O7-C8	110.1(3)	C7-O7-Co2	124.6(3)
C8-O7-Co2	123.7(3)	O7-C7-C8a	110.9(4)
O7-C8-C7a	110.3(4)	Co1-O9-Co2	115.1(1)
O10-C10-C11a	110.2(8)	C11-O10-C10	110.4(6)

C13-O11-C12	109.7(4)	O10-C11-C10a	110.0(7)
O11-C12-C13a	110.4(4)	O11-C13-C12a	110.1(4)
C14-O12-C15	110.3(5)	O12-C14-C15a	112.1(6)
O12-C15-C14a	110.0(6)		

Estimated standard deviations are given in the parenthesis.
Symmetry operators ::
1: x, y, z 2: -x, -y, -z

TABLE S3. Anisotropic displacement parameters ($Å^2$ x 10^3) for **1**.

atom	U11	U22	U33	U23	U13	U12
Co1	46(1)	35(1)	19(1)	6(1)	9(1)	14(1)
Co2	34(1)	32(1)	21(1)	3(1)	6(1)	7(1)
O1	63(2)	67(2)	39(2)	23(2)	26(2)	37(2)
C1	36(2)	39(2)	30(2)	6(2)	8(2)	11(2)
O2	43(2)	57(2)	46(2)	25(2)	19(2)	24(2)
C2	74(4)	79(4)	60(4)	31(3)	36(3)	50(4)
F1	207(6)	282(8)	129(4)	114(5)	86(4)	216(6)
F2	205(7)	234(8)	410(10)	227(8)	259(8)	179(6)
F3	204(7)	192(7)	220(8)	-96(6)	37(6)	119(6)
O3	54(2)	48(2)	28(2)	6(1)	7(2)	3(2)
C3	37(2)	38(2)	31(2)	8(2)	7(2)	5(2)
O4	54(2)	43(2)	33(2)	4(1)	14(2)	-5(2)
C4	52(4)	80(4)	40(3)	20(3)	7(3)	-16(3)
F4	154(5)	54(2)	112(4)	14(2)	-11(3)	-27(3)
F5	49(3)	157(5)	242(8)	-47(5)	22(4)	-8(3)
F6	156(5)	131(4)	50(2)	-19(2)	18(3)	-78(4)
O5	44(2)	64(2)	33(2)	13(2)	11(2)	23(2)
C5	35(3)	44(3)	38(3)	0(2)	5(2)	7(2)
O6	45(2)	89(3)	47(2)	11(2)	17(2)	19(2)
C6	46(3)	89(5)	67(4)	11(4)	3(3)	25(3)
F7	73(3)	261(8)	253(8)	188(7)	14(4)	59(4)
F8	125(5)	152(6)	242(8)	-80(6)	-125(5)	57(4)
F9	118(4)	370(10)	147(5)	56(7)	33(4)	168(7)
O7	34(2)	59(2)	25(2)	-8(1)	9(1)	1(2)
C7	33(2)	58(3)	29(2)	-7(2)	10(2)	-8(2)
C8	37(3)	69(3)	26(2)	-3(2)	7(2)	10(2)
O8	47(2)	39(2)	35(2)	9(2)	-4(2)	1(2)
O9	41(2)	32(2)	23(2)	4(1)	5(1)	11(2)
C10	122(7)	144(8)	94(6)	63(6)	46(6)	51(6)
O10	106(4)	152(5)	92(4)	87(4)	29(3)	43(4)
O11	57(2)	43(2)	62(2)	0(2)	20(2)	19(2)
C11	80(5)	117(7)	103(6)	60(5)	21(5)	17(5)
C12	76(4)	48(3)	48(3)	3(2)	18(3)	19(3)
C13	62(4)	40(3)	70(4)	-4(3)	33(3)	12(3)
O12	38(2)	69(3)	57(2)	11(2)	-3(2)	-3(2)
C14	54(4)	117(6)	60(4)	32(4)	6(3)	-17(4)
C15	63(4)	63(4)	92(5)	33(4)	-8(4)	-1(3)

The anisotropic displacement factor exponent takes the form

$2\pi^2 [h^2a^2U(11) +...+ 2hka^*b^*U(12)]$

TABLE S4. Hydrogen Coordinates (Å 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **1**.

atom	x	y	z	U(eq)
H7A	3792	8376	10081	53
H7B	2940	8508	8882	53
H8A	7148	9789	9880	55
H8B	6376	9157	10694	55
H10A	6118	5312	8719	135
H10B	5406	3912	9015	135
H11A	3292	3680	9503	121
H11B	2646	4929	9526	121
H12A	5822	5128	6491	69
H12B	5137	3549	6265	69
H13A	6656	5327	4097	67
H13B	6748	6208	5175	67
H14A	-620	5140	6183	103
H14B	482	4313	6656	103
H15A	1403	6983	4794	98
H15B	-49	6797	5050	98
H2W	4720(50)	7600(30)	5520(30)	50(20)
H1W	6080(10)	8420(60)	6090(50)	60(20)
H3W	3880(50)	6330(40)	7910(30)	50(20)
H4W	2860(30)	6530(70)	6960(40)	90(20)