Supporting Information

$PuCl_3\{CoCp[OP(OEt)_2]_3\}$: Transuranic Elements Entering the Field of Heterometallic Molecular Chemistry.

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Table S1. Crystallographic parameters for $PuCl_3\{CoCp[OP(OEt)_2]_3\}$.

Formula weight	883.64
Temperature/K	288(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a, b, c	10.7630(16), 15.914(2), 18.230(3)
α, β, γ	90, 95.148(5), 90
Volume/Å^3	3109.8(8)
Z	4
ρ_{calc}g/cm^3	1.887
μ/mm^{-1}	3.085
F(000)	1704.0
Crystal size/mm^3	0.116 × 0.066 × 0.036
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.236 to 50.78
Index ranges	$-12 \leq h \leq 12$, $-19 \leq k \leq 19$, $-21 \leq l \leq 21$
Reflections collected	93339
Independent reflections	5704 [R_{int} = 0.0643, R_{sigma} = 0.0241]
Data/restraints/parameters	5704/1376/534
Goodness-of-fit on F^2	1.084
Final R indexes [I>=2σ (I)]	R_1 = 0.0385, wR_2 = 0.0792
Final R indexes [all data]	R_1 = 0.0503, wR_2 = 0.0837
Largest diff. peak/hole / e Å^{-3}	1.01/-1.36

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Table S2: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for $PuCl_3\{CoCp[OP(OEt)_2]_3\}$. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Pu1	4826.6(2)	7218.7(2)	8029.1(2)	45.93(9)
Co1	5842.0(8)	5051.9(5)	6915.4(5)	49.5(2)
Cl1	2740(20)	7320(30)	8600(20)	89(5)
Cl1B	2654(8)	7534(16)	8440(13)	83(3)
Cl2	4900(30)	8599(16)	7300(20)	82(4)
Cl2B	4840(40)	8696(16)	7460(30)	78(5)
Cl3	6150(20)	7550(30)	9239(9)	84(5)
Cl3B	6050(20)	7760(20)	9209(6)	70(4)
P1	4350.4(16)	5890.2(11)	6509.5(10)	52.7(4)
P2	7098.6(16)	6088.6(11)	7180.3(10)	54.1(4)
P3	5265.0(19)	5043.9(11)	8019.9(10)	57.6(4)
O1	3957(4)	6571(3)	7035(2)	56.8(11)
O2	4977(4)	5885(3)	8375(3)	59.1(11)
O3	6551(4)	6875(3)	7504(3)	52.5(11)
O4	3166(7)	5454(6)	6121(6)	63(3)
C1	2117(16)	5212(13)	6555(8)	100(5)
C2	975(16)	5167(19)	6009(17)	152(10)
O4B	3132(19)	5301(16)	6480(20)	74(6)
C1B	1820(20)	5590(20)	6350(20)	76(8)
C2B	1170(30)	4900(30)	5880(30)	96(12)
O5	4744(5)	6355(3)	5792(3)	76.2(14)
C3	3934(9)	6999(6)	5447(5)	87(2)
C4	4679(13)	7662(8)	5176(8)	135(4)
O6	7480(20)	6369(13)	6394(7)	84(3)
C5	7640(30)	7050(13)	6020(13)	89(3)
C6	8130(30)	6950(20)	5345(13)	108(5)
O6B	7996(12)	6344(8)	6575(7)	75(2)
C5B	8102(19)	7082(10)	6260(10)	93(3)
C6B	8820(20)	7138(13)	5662(12)	118(5)
O7	8506(14)	5920(20)	7450(20)	74(3)
C7	9410(30)	6390(20)	7860(30)	81(4)
C8	10430(30)	5930(30)	8190(30)	91(6)
O7B	8152(8)	5759(5)	7788(5)	72(2)
C7B	9059(11)	6270(7)	8158(7)	84(3)

Atom	*x*	*y*	*z*	U(eq)
C8B	10019(12)	5826(9)	8573(9)	101(4)
O8	6038(12)	4480(7)	8608(5)	72(2)
C9	6585(19)	4808(11)	9283(8)	97(3)
C10	7350(20)	4343(14)	9711(11)	127(6)
O8B	6486(16)	4736(14)	8514(9)	86(3)
C9B	7050(20)	4973(16)	9208(11)	94(3)
C10B	8040(30)	4570(20)	9495(15)	110(6)
O9	3979(6)	4522(4)	7959(4)	74(2)
C11	3236(12)	4412(8)	8577(8)	94(3)
C12	3377(17)	3438(10)	8739(10)	132(5)
O9B	4650(20)	4260(11)	8385(13)	82(3)
C11B	3320(30)	4220(30)	8220(18)	89(3)
C12B	2870(30)	3860(30)	8960(20)	99(6)
C13	5390(14)	4302(10)	5989(8)	62(2)
C14	5357(13)	3830(8)	6638(10)	63(2)
C15	6575(15)	3852(9)	7018(7)	63(2)
C16	7330(10)	4336(9)	6603(9)	63(2)
C17	6606(17)	4632(8)	5965(7)	64(2)
C13B	5129(16)	4040(13)	6282(16)	62(2)
C14B	5720(20)	3743(12)	6951(14)	62(2)
C15B	7000(20)	3987(17)	6985(11)	63(3)
C16B	7173(18)	4446(16)	6354(15)	63(2)
C17B	6020(30)	4491(15)	5913(10)	63(2)

Table S3: Bond lengths (Å) and angles (°) for $PuCl_3\{CoCp[OP(OEt)_2]_3\}$.

Bond Lengths (Å)		Bond Angles (°)			
Pu1-Cl1	2.567(7)	Cl1-Pu1-Cl2	103.2(16)	O3-P2-Co1	117.23(18)
Pu1-Cl1B	2.569(4)	Cl1-Pu1-Cl3	94.2(11)	O3-P2-O6	104.9(8)
Pu1-Cl2	2.576(5)	Cl1B-Pu1-Cl2B	88.7(13)	O3-P2-O6B	109.9(5)
Pu1-Cl2B	2.573(7)	Cl3-Pu1-Cl2	103.3(14)	O3-P2-O7	114.5(11)
Pu1-Cl3	2.569(6)	Cl3B-Pu1-Cl1B	95.7(7)	O3-P2-O7B	106.0(4)
Pu1-Cl3B	2.569(5)	Cl3B-Pu1-Cl2B	90.6(15)	O6-P2-Co1	102.7(8)
Pu1-O1	2.218(4)	O1-Pu1-Cl1	92.4(8)	O6B-P2-Co1	116.7(5)
Pu1-O2	2.216(5)	O1-Pu1-Cl1B	90.0(4)	O6B-P2-O7B	97.4(7)
Pu1-O3	2.231(4)	O1-Pu1-Cl2	90.2(9)	O7-P2-Co1	120.2(12)
Co1-P1	2.166(2)	O1-Pu1-Cl2B	96.3(13)	O7-P2-O6	90.9(18)
Co1-P2	2.160(2)	O1-Pu1-Cl3	163.2(11)	O7B-P2-Co1	107.1(3)
Co1-P3	2.160(2)	O1-Pu1-Cl3B	171.1(9)	O2-P3-Co1	118.4(2)
Co1-C13	2.089(10)	O1-Pu1-O3	80.92(16)	O2-P3-O8	108.9(5)
Co1-C14	2.064(12)	O2-Pu1-Cl1	89.1(12)	O2-P3-O8B	102.5(8)
Co1-C15	2.069(13)	O2-Pu1-Cl1B	98.6(7)	O2-P3-O9	106.0(3)
Co1-C16	2.086(13)	O2-Pu1-Cl2	163.7(11)	O2-P3-O9B	113.8(9)
Co1-C17	2.093(12)	O2-Pu1-Cl2B	171.0(14)	O8-P3-Co1	117.3(5)
Co1-C13B	2.086(11)	O2-Pu1-Cl3	86.1(11)	O8-P3-O9	98.7(6)
Co1-C14B	2.088(19)	O2-Pu1-Cl3B	93.8(9)	O8B-P3-Co1	103.7(8)
Co1-C15B	2.10(2)	O2-Pu1-O1	78.59(17)	O9-P3-Co1	104.8(3)
Co1-C16B	2.07(2)	O2-Pu1-O3	81.10(16)	O9B-P3-Co1	124.1(10)
Co1-C17B	2.06(2)	O3-Pu1-Cl1	169.1(9)	O9B-P3-O8B	82.7(13)
P1-O1	1.531(5)	O3-Pu1-Cl1B	170.9(4)	P1-O1-Pu1	136.1(3)
P1-O4	1.564(8)	O3-Pu1-Cl2	85.5(10)	P3-O2-Pu1	136.8(3)
P1-O4B	1.61(2)	O3-Pu1-Cl2B	90.9(12)	P2-O3-Pu1	137.1(3)
P1-O5	1.593(6)	O3-Pu1-Cl3	90.0(7)	C1-O4-P1	120.1(9)
P2-O3	1.525(5)	O3-Pu1-Cl3B	93.4(6)	O4-C1-C2	105.9(14)
P2-O6	1.588(8)	P3-Co1-P2	91.30(8)	C1B-O4B-P1	126(2)
P2-O6B	1.584(7)	C13-Co1-P2	135.5(6)	O4B-C1B-C2B	104.2(16)
P2-O7	1.575(9)	C13-Co1-P3	133.2(6)	C3-O5-P1	119.3(5)
P2-O7B	1.601(6)	C13-Co1-C17	39.6(4)	C4-C3-O5	109.6(9)
P3-O2	1.531(5)	C14-Co1-P2	156.0(4)	C5-O6-P2	139.9(16)
P3-O8	1.577(7)	C14-Co1-P3	97.8(4)	O6-C5-C6	116.3(15)
P3-O8B	1.602(8)	C14-Co1-C13	39.5(5)	C5B-O6B-P2	128.0(10)
P3-O9	1.609(6)	C14-Co1-C15	40.4(4)	O6B-C5B-C6B	118.3(13)
P3-O9B	1.584(9)	C14-Co1-C16	66.5(5)	C7-O7-P2	133(2)
O4-C1	1.486(13)	C14-Co1-C17	66.8(5)	O7-C7-C8	115.1(18)
C1-C2	1.51(2)	C15-Co1-P2	117.3(5)	C7B-O7B-P2	124.3(7)
O4B-C1B	1.487(15)	C15-Co1-P3	92.8(4)	O7B-C7B-C8B	114.4(9)

C1B-C2B	1.52(2)	C15-Co1-C13	66.7(5)	C9-O8-P3	122.3(10)
O5-C3	1.452(9)	C15-Co1-C16	39.1(4)	C10-C9-O8	120.0(14)
C3-C4	1.439(14)	C15-Co1-C17	66.7(5)	C9B-O8B-P3	133.7(15)
O6-C5	1.300(13)	C16-Co1-P2	89.9(3)	C10B-C9B-O8B	120.0(16)
C5-C6	1.392(16)	C16-Co1-P3	122.9(4)	C11-O9-P3	122.7(7)
O6B-C5B	1.316(12)	C16-Co1-C13	66.2(4)	O9-C11-C12	102.3(11)
C5B-C6B	1.392(15)	C16-Co1-C17	39.7(4)	C11B-O9B-P3	113(2)
O7-C7	1.392(14)	C17-Co1-P2	98.3(5)	O9B-C11B-C12B	102.2(16)
C7-C8	1.407(16)	C17-Co1-P3	159.5(3)	C14-C13-Co1	69.3(7)
O7B-C7B	1.397(11)	C13B-Co1-P2	154.8(9)	C14-C13-C17	108.5(10)
C7B-C8B	1.415(13)	C13B-Co1-P3	112.9(10)	C17-C13-Co1	70.4(6)
O8-C9	1.414(13)	C13B-Co1-C15B	39.4(5)	C13-C14-Co1	71.2(7)
C9-C10	1.308(15)	C14B-Co1-P2	66.3(6)	C13-C14-C15	107.8(11)
O8B-C9B	1.403(13)	C14B-Co1-P3	142.6(8)	C15-C14-Co1	70.0(7)
C9B-C10B	1.312(16)	C14B-Co1-C13B	86.6(6)	C14-C15-Co1	69.6(7)
O9-C11	1.450(13)	C14B-Co1-C15B	39.8(5)	C16-C15-Co1	71.1(7)
C11-C12	1.582(17)	C15B-Co1-P2	104.2(7)	C16-C15-C14	107.8(10)
O9B-C11B	1.446(16)	C15B-Co1-P3	99.1(6)	C15-C16-Co1	69.7(7)
C11B-C12B	1.584(19)	C16B-Co1-P2	91.1(6)	C15-C16-C17	108.9(10)
C13-C14	1.404(16)	C16B-Co1-P3	136.7(8)	C17-C16-Co1	70.4(7)
C13-C17	1.415(16)	C16B-Co1-C13B	66.7(6)	C13-C17-Co1	70.1(6)
C14-C15	1.426(15)	C16B-Co1-C14B	66.4(7)	C13-C17-C16	107.0(10)
C15-C16	1.392(14)	C16B-Co1-C15B	38.9(5)	C16-C17-Co1	69.9(7)
C16-C17	1.420(14)	C17B-Co1-P2	115.1(9)	C14B-C13B-Co1	70.4(9)
C13B-C14B	1.406(17)	C17B-Co1-P3	151.9(8)	C14B-C13B-C17B	108.0(12)
C13B-C17B	1.414(17)	C17B-Co1-C13B	39.9(5)	C17B-C13B-Co1	68.9(11)
C14B-C15B	1.427(16)	C17B-Co1-C14B	66.8(7)	C13B-C14B-Co1	70.2(9)
C15B-C16B	1.389(15)	C17B-Co1-C15B	66.5(7)	C13B-C14B-C15B	107.8(12)
C16B-C17B	1.419(16)	C17B-Co1-C16B	40.2(5)	C15B-C14B-Co1	70.6(11)
		O1-P1-Co1	117.40(19)	C14B-C15B-Co1	69.6(11)
		O1-P1-04	109.7(4)	C16B-C15B-Co1	69.4(12)
		O1-P1-O4B	99.4(11)	C16B-C15B-C14B	107.9(12)
		O1-P1-O5	107.2(3)	C15B-C16B-Co1	71.7(13)
		O4-P1-Co1	115.5(4)	C15B-C16B-C17B	108.7(12)
		O4-P1-O5	95.7(5)	C17B-C16B-Co1	69.3(12)
		O4B-P1-Co1	103.3(8)	C13B-C17B-Co1	71.2(10)
		O5-P1-Co1	108.8(2)	C13B-C17B-C16B	107.5(12)
		O5-P1-O4B	121.2(13)	C16B-C17B-Co1	70.5(12)

Table S4: Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for $PuCl_3\{CoCp[OP(OEt)_2]_3\}$. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pu1	44.75(14)	43.44(13)	49.19(14)	-9.68(11)	1.96(9)	-1.41(11)
Co1	53.0(5)	43.3(5)	50.6(5)	-7.2(4)	-4.6(4)	8.6(4)
Cl1	71(6)	92(11)	107(10)	-4(8)	32(6)	-7(5)
Cl1B	61(3)	86(7)	104(6)	-11(4)	23(3)	10(3)
Cl2	101(5)	53(4)	90(8)	8(5)	-3(5)	3(4)
Cl2B	86(6)	44(4)	100(11)	-1(6)	-7(8)	8(4)
Cl3	101(6)	75(10)	72(5)	-19(4)	-24(4)	-7(6)
Cl3B	80(5)	69(8)	60(3)	-9(3)	-6(3)	-19(4)
P1	52.6(10)	51.1(9)	51.5(10)	-11.6(8)	-11.1(8)	9.2(8)
P2	46.8(9)	53.5(10)	62.4(11)	-4.6(8)	7.5(8)	1.9(8)
P3	70.2(12)	45.8(9)	56.6(11)	3.9(8)	4.1(9)	-1.9(8)
O1	58(3)	59(3)	52(3)	-13(2)	-7(2)	9(2)
O2	74(3)	52(2)	53(3)	-4(2)	10(2)	-5(2)
O3	43(2)	43(2)	73(3)	-6(2)	13(2)	-2.8(18)
O4	59(4)	72(5)	53(5)	-13(4)	-14(3)	4(3)
C1	90(7)	110(9)	100(8)	18(7)	-3(5)	-22(7)
C2	80(9)	190(20)	182(17)	15(15)	-30(10)	-30(12)
O4B	58(7)	73(8)	87(11)	-14(8)	-10(7)	-1(6)
C1B	62(8)	79(11)	84(12)	-5(9)	-7(8)	1(7)
C2B	71(16)	105(18)	105(19)	-11(14)	-24(14)	-16(13)
O5	89(3)	78(3)	62(3)	3(2)	7(2)	28(2)
C3	94(4)	86(4)	80(4)	6(3)	1(3)	25(3)
C4	144(8)	111(7)	148(8)	24(6)	6(7)	4(6)
O6	83(6)	88(5)	84(5)	0(4)	25(5)	-15(5)
C5	85(6)	98(5)	86(5)	14(5)	16(5)	-3(5)
C6	111(11)	126(10)	88(8)	12(8)	22(8)	0(9)
O6B	62(5)	83(4)	84(4)	0(4)	20(4)	-4(4)
C5B	93(6)	99(5)	88(5)	13(4)	18(5)	-5(5)
C6B	123(10)	132(9)	105(9)	24(8)	35(7)	-8(8)
O7	59(4)	78(5)	86(5)	-7(5)	4(4)	1(4)
C7	70(5)	82(6)	90(6)	-4(5)	-3(5)	-4(5)
C8	77(9)	93(10)	99(11)	-6(10)	-7(9)	-2(9)
O7B	55(3)	71(4)	87(4)	-7(3)	-13(3)	2(3)
C7B	74(4)	85(5)	91(5)	-4(4)	-8(4)	-7(4)
C8B	80(7)	103(7)	115(8)	-17(7)	-22(6)	-1(6)
O8	79(4)	73(4)	65(4)	19(3)	4(4)	-6(4)
C9	95(6)	104(6)	88(5)	11(4)	-13(5)	-2(5)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C10	132(10)	128(10)	113(9)	17(8)	-32(8)	8(8)
O8B	96(5)	91(6)	71(5)	15(5)	-2(5)	11(5)
C9B	93(6)	98(6)	87(5)	15(5)	-9(5)	-9(5)
C10B	104(9)	116(10)	105(10)	22(9)	-11(8)	2(8)
O9	81(4)	67(4)	76(4)	2(3)	9(3)	-25(3)
C11	93(5)	100(5)	91(5)	0(4)	14(4)	-24(4)
C12	134(9)	129(7)	135(9)	37(7)	13(8)	-30(7)
O9B	88(5)	76(5)	82(5)	7(5)	10(4)	-15(4)
C11B	91(5)	87(6)	89(6)	0(5)	10(5)	-18(5)
C12B	102(10)	95(11)	102(10)	5(9)	21(9)	-18(10)
C13	71(4)	55(4)	61(4)	-16(3)	2(4)	7(3)
C14	72(4)	50(3)	66(4)	-13(3)	-1(4)	5(3)
C15	69(4)	50(4)	70(4)	-8(3)	-1(4)	11(4)
C16	70(4)	55(4)	65(4)	-10(4)	4(3)	15(3)
C17	71(4)	58(4)	62(4)	-12(3)	4(4)	9(4)
C13B	69(4)	52(4)	64(4)	-13(4)	0(4)	5(4)
C14B	69(5)	51(4)	66(4)	-9(4)	2(4)	8(4)
C15B	67(4)	53(4)	69(4)	-8(4)	3(4)	12(4)
C16B	68(4)	57(4)	65(4)	-10(4)	4(4)	11(4)
C17B	69(4)	56(4)	62(4)	-13(4)	3(4)	7(4)

Table S5: Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for $PuCl_3\{CoCp[OP(OEt)_2]_3\}$.

Atom	*x*	*y*	*z*	U(eq)
H1A	2001.93	5627.52	6931.86	120
H1B	2277.09	4671.03	6789.63	120
H2A	811.86	4592.32	5873.12	229
H2B	1118.89	5486.72	5577.42	229
H2C	270.5	5394.85	6228.32	229
H1BA	1772.5	6122.95	6082	91
H1BB	1443.89	5661.95	6806.76	91
H2BA	1784.83	4560.74	5671.24	143
H2BB	620.29	5142.87	5498.41	143
H2BC	699.59	4553.59	6190.16	143
H3A	3404.55	6757.03	5042.54	105
H3B	3403.4	7223.81	5802.24	105
H4A	5275.45	7851.47	5563.86	202
H4B	4148.07	8122.08	5009.93	202
H4C	5109	7456.52	4773.33	202
H5A	8183.98	7421.39	6321.13	107
H5B	6835.48	7330.77	5933.14	107
H6A	8942.57	6700.18	5422.85	162
H6B	8183.57	7482.03	5109.72	162
H6C	7592.32	6582.25	5037.46	162
H5B1	8448.79	7469.96	6634.06	111
H5B2	7268.48	7277.85	6099.33	111
H6B1	9668.82	7253.71	5835.3	178
H6B2	8502.25	7583.2	5341.95	178
H6B3	8774	6616.35	5396.62	178
H7A	9009.35	6677.42	8250.47	98
H7B	9714.11	6817.83	7546.31	98
H8A	10707.51	6175.61	8655.53	136
H8B	11094.88	5946.36	7871.33	136
H8C	10182.47	5359.53	8258	136
H7BA	8655.04	6640.63	8485.97	101
H7BB	9430.39	6618.24	7799.61	101
H8BA	10292.8	5367.06	8286.48	151
H8BB	9709.99	5612.67	9014.62	151
H8BC	10707.75	6197.83	8700.93	151
H9A	7034.6	5313.23	9170.04	116
H9B	5910.81	4980.22	9568.44	116

Atom	*x*	*y*	*z*	U(eq)
H10A	6872.86	3999.12	10017.24	190
H10B	7897.61	4698.98	10015.43	190
H10C	7825.01	3991.16	9415.01	190
H9B1	7268.57	5562.18	9178.42	113
H9B2	6418.4	4930.64	9554.17	113
H10D	7821.6	4003.3	9601.82	164
H10E	8358.99	4847.16	9941.76	164
H10F	8667.52	4573.35	9152.21	164
H11A	2371.11	4563.25	8446.8	113
H11B	3561.01	4742.88	8998.05	113
H12A	2568.53	3178.61	8691.66	199
H12B	3759.22	3355.51	9229.55	199
H12C	3889.14	3189.07	8392.3	199
H11C	3086.61	3852.34	7808.04	107
H11D	2969.99	4777.84	8110.34	107
H12D	2564.54	3300.63	8881.52	148
H12E	2210.13	4210.71	9117.52	148
H12F	3554.39	3861.13	9335.6	148
H13	4686.07	4392.21	5618.13	75
H14	4636.1	3522.87	6792.62	76
H15	6838.2	3562.92	7481.04	76
H16	8215.51	4456.38	6732	76
H17	6900.64	4983.6	5575.13	76
H13B	4252.26	3953.33	6104.69	74
H14B	5331.19	3412.23	7321.57	75
H15B	7643.63	3858.48	7384.59	76
H16B	7963.32	4690.18	6228.91	76
H17B	5874.59	4759.49	5429.46	75

Figure S1 (p 11). The solution-state UV-Vis spectra of $Na\{CoCp[OP(OEt)_2]_3\}$ in MeCN.

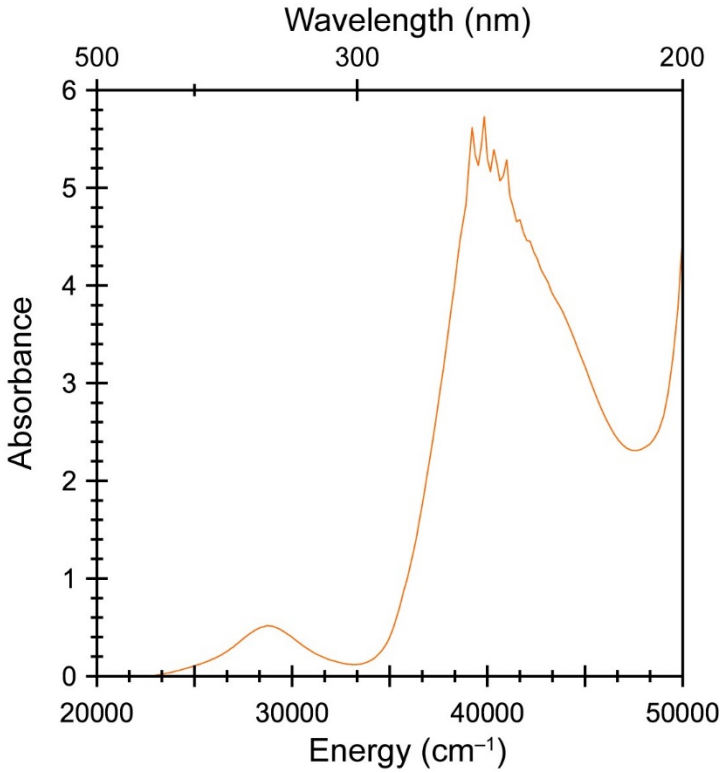

Figure S2 (p 12). The solution-state ^{1}H NMR spectrum of $Na\{CoCp[OP(OEt)_2]_3\}$ in $CDCl_3$.

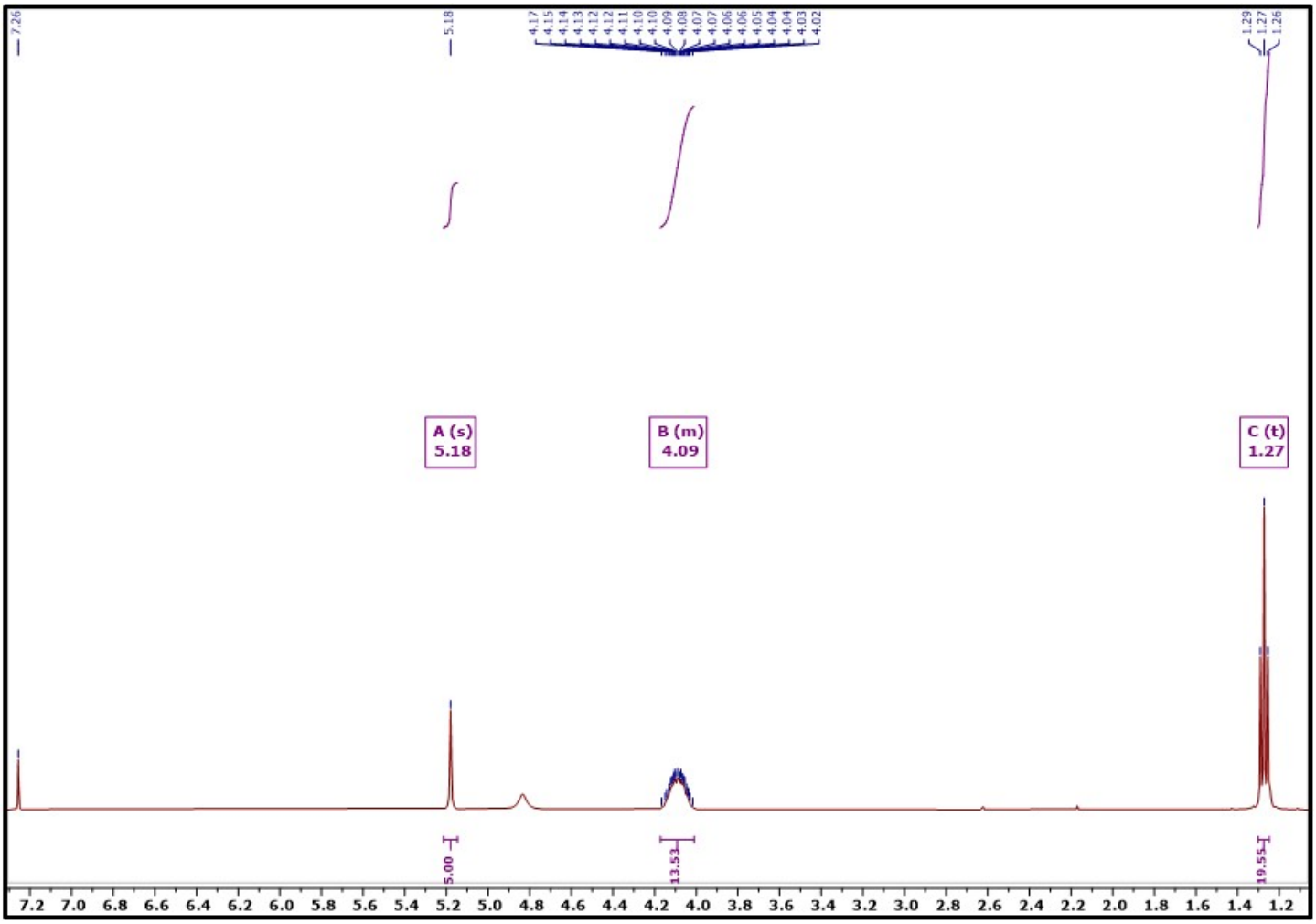

Figure S3 (p 13). The solution-state ^{1}H NMR spectrum of $PuCl_3\{CoCp[OP(OEt)_2]_3\}$ in $CDCl_3$. The inset is a zoomed in view of the doublet of quintets at 3.03 ppm that correspond to the methylene protons of the $CoCp[OP(OEt)_2]_3^-$ ligand.