

Table S1. Crystal data and structure refinement for $[\text{Ru}_4(\text{CO})_{12}(\mu_4\text{-PNEt}_2)_2]$.

empirical formula	$\text{C}_{20}\text{H}_{20}\text{N}_2\text{O}_{12}\text{P}_2\text{Ru}_4$
formula weight	946.60
temperature (K)	173(2)
wavelength ($\text{\AA}$)	0.71070
crystal system	monoclinic
space group	$\text{P}2_{1/c}$
a , ($\text{\AA}$)	9.380(2)
b , ($\text{\AA}$)	16.917(3)
c , ($\text{\AA}$)	19.244(3)
α , ($^\circ$)	90.
β , ($^\circ$)	94.737(3)
γ , ($^\circ$)	90
V , $\text{\AA}^3$	3043.4(9)
Z ,	4
D_{calc} , g cm^{-3}	2.066
absorption coefficient mm^{-1}	2.110
$F(000)$	1824
crystal size, mm	0.2 x 0.3 x 0.3
θ range for data collection, ($^\circ$)	1.61 to 28.82
index ranges	$-12 \leq h \leq 11$, $-22 \leq k \leq 22$, $-25 \leq l \leq 26$
reflections collected / unique	30903 / 7892 [$R(\text{int}) = 0.0568$]
completeness to $2\theta = 28.82^\circ$	96.1%
refinement method	Full-matrix least-squares on F^2
data / restraints / parameters	7892 / 0 / 361
goodness-of-fit on F^2	1.033
final R indices [$I > 2\sigma(I)$]	$R1 = 0.0272$, $wR2 = 0.0616$
R indices (all data)	$R1 = 0.0387$, $wR2 = 0.0655$
largest diff. peak and hole	0.971 and $-0.811 \text{ e.\AA}^{-3}$

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ru}_4(\text{CO})_{12}(\mu_4\text{-PNEt}_2)_2]$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Ru(1)	3151(1)	7133(1)	2530(1)	27(1)
Ru(2)	463(1)	6302(1)	2366(1)	27(1)
Ru(3)	2107(1)	4900(1)	2696(1)	27(1)
Ru(4)	4381(1)	5693(1)	2063(1)	30(1)
P(1)	2884(1)	6039(1)	205(1)	26(1)
P(2)	2175(1)	6083(1)	1616(1)	28(1)
O(9)	6238(3)	7560(2)	2999(1)	54(1)
O(10)	2939(3)	8137(2)	1179(1)	63(1)
O(11)	1683(3)	8328(2)	3418(2)	63(1)
O(12)	-783(3)	6579(2)	3793(1)	63(1)
O(13)	-1764(2)	5112(1)	1800(1)	45(1)
O(14)	-1020(3)	7759(2)	1723(2)	66(1)
O(15)	-326(3)	4387(2)	3548(2)	57(1)
O(16)	4214(3)	3714(2)	3376(2)	63(1)
O(17)	1252(3)	3902(2)	1370(1)	0(1)
O(18)	6644(3)	5343(2)	3294(1)	63(1)
O(19)	4877(3)	4149(2)	1312(2)	64(1)
O(20)	6286(3)	6683(2)	1195(1)	59(1)
N(1)	3321(3)	6091(2)	4057(1)	37(1)
N(2)	1768(3)	6164(2)	764(1)	43(1)
C(1)	3892(4)	6808(2)	4414(2)	49(1)
C(2)	5460(5)	6752(3)	4664(2)	73(1)
C(3)	3133(4)	5412(2)	4525(2)	47(1)
C(4)	1803(5)	5458(3)	4907(2)	65(1)
C(5)	2823(4)	5994(3)	254(2)	54(1)
C(6)	2620(6)	5194(3)	-84(2)	81(2)
C(7)	339(4)	6353(3)	446(2)	55(1)
C(8)	196(5)	7180(3)	146(2)	74(1)
C(9)	5087(3)	7409(2)	2822(2)	37(1)
C(10)	3015(3)	7774(2)	1673(2)	38(1)
C(11)	2215(4)	7889(2)	3074(2)	40(1)
C(12)	-305(3)	6476(2)	3280(2)	38(1)
C(13)	-939(3)	5559(2)	2023(2)	32(1)

C(14)	-446(4)	7222(2)	1959(2)	41(1)
C(15)	588(4)	4577(2)	3231(2)	39(1)
C(16)	3433(4)	4156(2)	3105(2)	40(1)
C(17)	1532(3)	4263(2)	1857(2)	37(1)
C(18)	5833(3)	5483(2)	2842(2)	41(1)
C(20)	5579(3)	6319(2)	1519(2)	39(1)

Table S3. Bond lengths [Å] and angles [°] for [Ru₄(CO)₁₂(μ₄-PNEt₂)₂].

Ru(1)-C(11)	1.912(3)
Ru(1)-C(9)	1.914(3)
Ru(1)-C(10)	1.969(3)
Ru(1)-P(1)	2.2852(8)
Ru(1)-P(2)	2.6117(8)
Ru(1)-Ru(4)	2.8711(5)
Ru(1)-Ru(2)	2.8808(5)
Ru(1)-Ru(3)	3.9217(7)
Ru(2)-C(13)	1.897(3)
Ru(2)-C(14)	1.911(3)
Ru(2)-C(12)	1.978(3)
Ru(2)-P(2)	2.2755(8)
Ru(2)-P(1)	2.7118(8)
Ru(2)-Ru(3)	2.8712(5)
Ru(2)-Ru(4)	3.9062(7)
Ru(3)-C(16)	1.895(3)
Ru(3)-C(15)	1.906(3)
Ru(3)-C(17)	1.978(3)
Ru(3)-P(1)	2.2557(8)
Ru(3)-Ru(4)	2.8749(5)
Ru(3)-P(2)	2.8890(8)
Ru(4)-C(19)	1.907(3)
Ru(4)-C(20)	1.917(3)
Ru(4)-C(18)	1.973(3)
Ru(4)-P(2)	2.2715(8)
Ru(4)-P(1)	2.7668(8)
P(1)-N(1)	1.660(2)
P(2)-N(2)	1.659(3)
O(9)-C(9)	1.135(4)
O(10)-C(10)	1.129(4)
O(11)-C(11)	1.137(4)
O(12)-C(12)	1.130(4)
O(13)-C(13)	1.140(4)
O(14)-C(14)	1.132(4)
O(15)-C(15)	1.139(4)
O(16)-C(16)	1.141(4)
O(17)-C(17)	1.131(4)

O(18)-C(18)	1.133(4)
O(19)-C(19)	1.132(4)
O(20)-C(20)	1.130(4)
N(1)-C(1)	1.471(4)
N(1)-C(3)	1.479(4)
N(2)-C(7)	1.461(5)
N(2)-C(5)	1.478(5)
C(1)-C(2)	1.513(6)
C(3)-C(4)	1.502(5)
C(5)-C(6)	1.506(6)
C(7)-C(8)	1.516(6)

C(11)-Ru(1)-C(9)	98.26(14)
C(11)-Ru(1)-C(10)	95.10(15)
C(9)-Ru(1)-C(10)	96.01(13)
C(11)-Ru(1)-P(1)	98.87(10)
C(9)-Ru(1)-P(1)	100.19(10)
C(10)-Ru(1)-P(1)	156.80(9)
C(11)-Ru(1)-P(2)	132.28(10)
C(9)-Ru(1)-P(2)	129.39(10)
C(10)-Ru(1)-P(2)	79.40(10)
P(1)-Ru(1)-P(2)	77.48(3)
C(11)-Ru(1)-Ru(4)	162.54(10)
C(9)-Ru(1)-Ru(4)	84.41(10)
C(10)-Ru(1)-Ru(4)	101.81(10)
P(1)-Ru(1)-Ru(4)	63.72(2)
P(2)-Ru(1)-Ru(4)	48.668(19)
C(11)-Ru(1)-Ru(2)	87.12(10)
C(9)-Ru(1)-Ru(2)	162.16(10)
C(10)-Ru(1)-Ru(2)	100.47(9)
P(1)-Ru(1)-Ru(2)	62.07(2)
P(2)-Ru(1)-Ru(2)	48.647(17)
Ru(4)-Ru(1)-Ru(2)	85.548(14)
C(11)-Ru(1)-Ru(3)	118.12(10)
C(9)-Ru(1)-Ru(3)	116.65(10)
C(10)-Ru(1)-Ru(3)	126.84(9)
P(1)-Ru(1)-Ru(3)	30.055(19)
P(2)-Ru(1)-Ru(3)	47.443(18)
Ru(4)-Ru(1)-Ru(3)	47.000(11)

Ru(2)-Ru(1)-Ru(3)	46.914(7)
C(13)-Ru(2)-C(14)	97.13(13)
C(13)-Ru(2)-C(12)	96.58(13)
C(14)-Ru(2)-C(12)	93.39(15)
C(13)-Ru(2)-P(2)	100.23(9)
C(14)-Ru(2)-P(2)	100.83(11)
C(12)-Ru(2)-P(2)	156.37(9)
C(13)-Ru(2)-P(1)	128.38(9)
C(14)-Ru(2)-P(1)	134.46(10)
C(12)-Ru(2)-P(1)	80.99(9)
P(2)-Ru(2)-P(1)	75.57(3)
C(13)-Ru(2)-Ru(3)	82.78(9)
C(14)-Ru(2)-Ru(3)	167.63(11)
C(12)-Ru(2)-Ru(3)	98.92(10)
P(2)-Ru(2)-Ru(3)	67.14(2)
P(1)-Ru(2)-Ru(3)	47.553(17)
C(13)-Ru(2)-Ru(1)	159.50(9)
C(14)-Ru(2)-Ru(1)	90.25(10)
C(12)-Ru(2)-Ru(1)	102.07(9)
P(2)-Ru(2)-Ru(1)	59.49(2)
P(1)-Ru(2)-Ru(1)	48.118(18)
Ru(3)-Ru(2)-Ru(1)	85.967(15)
C(13)-Ru(2)-Ru(4)	114.06(9)
C(14)-Ru(2)-Ru(4)	123.18(11)
C(12)-Ru(2)-Ru(4)	126.06(9)
P(2)-Ru(2)-Ru(4)	30.759(19)
P(1)-Ru(2)-Ru(4)	45.090(18)
Ru(3)-Ru(2)-Ru(4)	47.212(7)
Ru(1)-Ru(2)-Ru(4)	47.121(11)
C(16)-Ru(3)-C(15)	94.56(14)
C(16)-Ru(3)-C(17)	95.90(14)
C(15)-Ru(3)-C(17)	96.81(13)
C(16)-Ru(3)-P(1)	102.11(10)
C(15)-Ru(3)-P(1)	103.89(10)
C(17)-Ru(3)-P(1)	151.19(10)
C(16)-Ru(3)-Ru(2)	164.33(10)
C(15)-Ru(3)-Ru(2)	86.83(10)
C(17)-Ru(3)-Ru(2)	99.43(10)
P(1)-Ru(3)-Ru(2)	62.52(2)

C(16)-Ru(3)-Ru(4)	90.10(10)
C(15)-Ru(3)-Ru(4)	167.69(10)
C(17)-Ru(3)-Ru(4)	94.03(9)
P(1)-Ru(3)-Ru(4)	63.94(2)
Ru(2)-Ru(3)-Ru(4)	85.655(14)
C(16)-Ru(3)-P(2)	134.93(10)
C(15)-Ru(3)-P(2)	130.47(10)
C(17)-Ru(3)-P(2)	79.11(10)
P(1)-Ru(3)-P(2)	72.23(3)
Ru(2)-Ru(3)-P(2)	46.536(17)
Ru(4)-Ru(3)-P(2)	46.418(16)
C(16)-Ru(3)-Ru(1)	120.93(10)
C(15)-Ru(3)-Ru(1)	121.54(10)
C(17)-Ru(3)-Ru(1)	120.75(9)
P(1)-Ru(3)-Ru(1)	30.490(19)
Ru(2)-Ru(3)-Ru(1)	47.119(11)
Ru(4)-Ru(3)-Ru(1)	46.919(7)
P(2)-Ru(3)-Ru(1)	41.751(16)
C(19)-Ru(4)-C(20)	95.89(14)
C(19)-Ru(4)-C(18)	94.63(15)
C(20)-Ru(4)-C(18)	96.63(14)
C(19)-Ru(4)-P(2)	103.86(11)
C(20)-Ru(4)-P(2)	100.98(10)
C(18)-Ru(4)-P(2)	152.85(10)
C(19)-Ru(4)-P(1)	131.42(10)
C(20)-Ru(4)-P(1)	132.53(10)
C(18)-Ru(4)-P(1)	78.36(9)
P(2)-Ru(4)-P(1)	74.50(3)
C(19)-Ru(4)-Ru(1)	163.54(11)
C(20)-Ru(4)-Ru(1)	88.39(10)
C(18)-Ru(4)-Ru(1)	100.66(10)
P(2)-Ru(4)-Ru(1)	59.69(2)
P(1)-Ru(4)-Ru(1)	47.780(16)
C(19)-Ru(4)-Ru(3)	86.64(10)
C(20)-Ru(4)-Ru(3)	168.07(10)
C(18)-Ru(4)-Ru(3)	94.78(10)
P(2)-Ru(4)-Ru(3)	67.12(2)
P(1)-Ru(4)-Ru(3)	47.086(17)
Ru(1)-Ru(4)-Ru(3)	86.081(14)

C(19)-Ru(4)-Ru(2)	118.47(10)
C(20)-Ru(4)-Ru(2)	122.51(10)
C(18)-Ru(4)-Ru(2)	122.21(9)
P(2)-Ru(4)-Ru(2)	30.82(2)
P(1)-Ru(4)-Ru(2)	43.960(16)
Ru(1)-Ru(4)-Ru(2)	47.331(7)
Ru(3)-Ru(4)-Ru(2)	47.134(10)
N(1)-P(1)-Ru(3)	121.27(10)
N(1)-P(1)-Ru(1)	119.24(10)
Ru(3)-P(1)-Ru(1)	119.45(3)
N(1)-P(1)-Ru(2)	134.91(10)
Ru(3)-P(1)-Ru(2)	69.93(2)
Ru(1)-P(1)-Ru(2)	69.81(2)
N(1)-P(1)-Ru(4)	134.11(10)
Ru(3)-P(1)-Ru(4)	68.97(2)
Ru(1)-P(1)-Ru(4)	68.50(2)
Ru(2)-P(1)-Ru(4)	90.95(2)
N(2)-P(2)-Ru(4)	121.73(11)
N(2)-P(2)-Ru(2)	119.77(11)
Ru(4)-P(2)-Ru(2)	118.42(3)
N(2)-P(2)-Ru(1)	130.46(11)
Ru(4)-P(2)-Ru(1)	71.64(2)
Ru(2)-P(2)-Ru(1)	71.86(2)
N(2)-P(2)-Ru(3)	138.72(11)
Ru(4)-P(2)-Ru(3)	66.46(2)
Ru(2)-P(2)-Ru(3)	66.32(2)
Ru(1)-P(2)-Ru(3)	90.81(3)
C(1)-N(1)-C(3)	114.4(3)
C(1)-N(1)-P(1)	123.7(2)
C(3)-N(1)-P(1)	121.8(2)
C(7)-N(2)-C(5)	114.0(3)
C(7)-N(2)-P(2)	124.0(2)
C(5)-N(2)-P(2)	121.9(2)
N(1)-C(1)-C(2)	113.8(3)
N(1)-C(3)-C(4)	113.8(3)
N(2)-C(5)-C(6)	113.2(3)
N(2)-C(7)-C(8)	114.3(3)
O(9)-C(9)-Ru(1)	178.8(3)
O(10)-C(10)-Ru(1)	179.5(3)

O(11)-C(11)-Ru(1)	177.6(3)
O(12)-C(12)-Ru(2)	178.0(3)
O(13)-C(13)-Ru(2)	178.0(3)
O(14)-C(14)-Ru(2)	178.1(3)
O(15)-C(15)-Ru(3)	179.6(3)
O(16)-C(16)-Ru(3)	177.3(3)
O(17)-C(17)-Ru(3)	177.5(3)
O(18)-C(18)-Ru(4)	178.0(3)
O(19)-C(19)-Ru(4)	178.9(3)
O(20)-C(20)-Ru(4)	179.5(3)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ru}_4(\text{CO})_{12}(\mu_4\text{-PNEt}_2)_2]$.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2[h^2a^{*2}U11+2hka^*b^*U12]$$

	U11	U22	U33	U23	U13	U12
Ru(1)	25(1)	25(1)	31(1)	1(1)	1(1)	-3(1)
Ru(2)	21(1)	25(1)	35(1)	0(1)	2(1)	1(1)
Ru(3)	25(1)	24(1)	34(1)	1(1)	7(1)	1(1)
Ru(4)	24(1)	30(1)	35(1)	0(1)	8(1)	0(1)
P(1)	26(1)	26(1)	27(1)	1(1)	4(1)	1(1)
P(2)	26(1)	32(1)	28(1)	0(1)	2(1)	-5(1)
O(9)	35(1)	58(2)	67(2)	0(1)	-8(1)	-13(1)
O(10)	66(2)	64(2)	54(2)	26(1)	-12(1)	-19(1)
O(11)	65(2)	46(2)	79(2)	-17(1)	14(2)	12(1)
O(12)	54(2)	88(2)	50(2)	-21(2)	16(1)	2(2)
O(13)	33(1)	43(1)	60(2)	-11(1)	2(1)	-8(1)
O(14)	60(2)	34(1)	103(2)	11(1)	-10(2)	7(1)
O(15)	58(2)	50(2)	68(2)	6(1)	32(1)	-6(1)
O(16)	62(2)	55(2)	70(2)	4(1)	-5(2)	31(1)
O(17)	62(2)	63(2)	56(2)	-22(1)	9(1)	-15(1)
O(18)	43(2)	89(2)	57(2)	4(2)	-5(1)	13(2)
O(19)	75(2)	40(2)	80(2)	-16(1)	32(2)	1(1)
O(20)	50(2)	67(2)	63(2)	12(1)	19(1)	-18(1)
N(1)	44(2)	40(2)	26(1)	2(1)	2(1)	2(1)
N(2)	41(2)	58(2)	27(1)	4(1)	-2(1)	-17(1)
C(1)	64(2)	48(2)	33(2)	-8(1)	1(2)	1(2)
C(2)	78(3)	77(3)	59(3)	-2(2)	-19(2)	-11(3)
C(3)	60(2)	50(2)	30(2)	11(1)	1(2)	2(2)
C(4)	84(3)	68(3)	45(2)	-2(2)	22(2)	-16(2)
C(5)	56(2)	78(3)	0(2)	-3(2)	10(2)	-24(2)
C(6)	91(4)	102(4)	52(2)	-27(2)	27(2)	-34(3)
C(7)	44(2)	81(3)	37(2)	9(2)	-13(2)	-21(2)
C(8)	63(3)	93(4)	62(3)	35(2)	-13(2)	-14(2)
C(9)	36(2)	36(2)	38(2)	-1(1)	1(1)	-5(1)
C(10)	37(2)	38(2)	39(2)	7(1)	-3(1)	-10(1)
C(11)	37(2)	32(2)	51(2)	0(1)	3(2)	2(1)
C(12)	27(2)	41(2)	47(2)	-8(1)	2(1)	-2(1)
C(13)	26(2)	31(2)	41(2)	0(1)	9(1)	4(1)

C(14)	35(2)	28(2)	58(2)	3(1)	-1(2)	0(1)
C(15)	41(2)	32(2)	46(2)	1(1)	13(1)	1(1)
C(16)	42(2)	32(2)	47(2)	-4(1)	10(2)	6(1)
C(17)	34(2)	33(2)	45(2)	-1(1)	11(1)	-5(1)
C(18)	28(2)	47(2)	50(2)	2(2)	11(1)	5(1)
C(19)	39(2)	38(2)	50(2)	2(2)	16(2)	2(1)
C(20)	31(2)	40(2)	45(2)	-2(1)	5(1)	-2(1)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ru}_4(\text{CO})_{12}(\mu_4\text{-PNEt}_2)_2]$.

	x	y	z	U(eq)
H(1A)	3336	6914	4819	58
H(1B)	3752	7262	4091	58
H(2A)	5612	6300	4979	87
H(2B)	5758	7239	4911	87
H(2C)	6027	6682	4262	87
H(3A)	3974	5380	4870	56
H(3B)	3104	4920	4245	56
H(4A)	1810	5950	5176	78
H(4B)	1771	5006	5223	78
H(4C)	960	5449	4570	78
H(5A)	3798	6023	493	65
H(5B)	2749	6405	-113	65
H(6A)	2753	4781	273	97
H(6B)	3321	5124	-429	97
H(6C)	1651	5157	-315	97
H(7A)	-355	6290	803	66
H(7B)	83	5967	70	66
H(8A)	353	7568	522	89
H(8B)	-765	7249	-87	89
H(8C)	909	7258	-193	89