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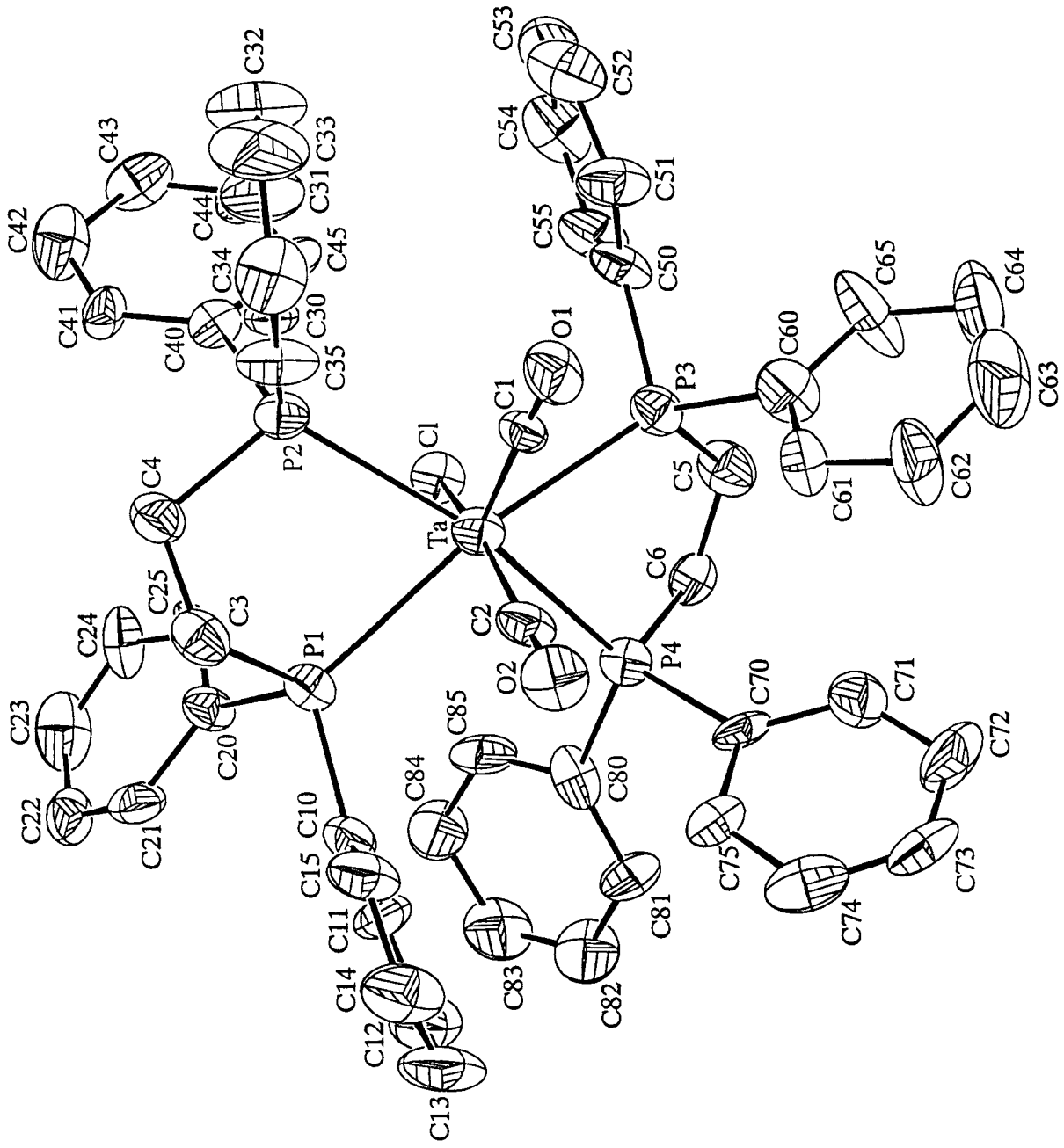

Figure S1. ORTEP diagram of **1** showing 30% probability displacement ellipsoids and the numbering scheme; hydrogen atoms are omitted for clarity.

Table S1. Detailed Crystallographic Data for $TaCl(CO)_2(dppe)_2$.

(a) Crystal Parameters.

formula	$C_{68}\,H_{64}\,Cl\,O_2\,P_4\,Ta$
formula weight	1253.47 g mol^{-1}
crystal system	triclinic
space group	$P\bar{1}$ (No. 2)
a, Å	13.937(12)
b, Å	14.811(7)
c, Å	14.929(9)
α, deg	102.30(5)
β, deg	95.60(7)
γ, deg	98.41(5)
V, $Å^3$	2952(3)
Z	2
D_{calc}, g/cm^3	1.410
μ (Mo*K*α), mm^{-1}	2.06
crystal dimensions, mm	0.30 × 0.30 × 0.04
crystal colour	orange

(b) Data Collection.

diffractometer	Enraf-Nonius CAD-4
radiation	Mo$K\alpha$ (λ = 0.71069 Å)
monochromator	graphite
temperature, K	298(2)
data collected	$0 \le h \le 13$, $-14 \le k \le 14$, $-14 \le l \le 14$
θ scan range, deg	1.4-20.0
no. of reflns collected	5801
no. of independent reflns	5510 (R_{int} = 0.0525)
no. of ind obsd reflns [$I>2\sigma(I)$]	3629
absorption correction	DIFABS (transmission factors: 0.377-1.00)

(c) Structure Solution and Refinement.

solution method	Patterson and Fourier methods
refinement method	full-matrix least-squares on F^2 (for all ind data)
no. of variables	658
no. of restraints	90
data/variables ratio	8.4
function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0787P)^2 + 4.928P]$ where $P = (F_o^2 + 2F_c^2)/3$
R^a, $wR2^b$, ind obsd reflns	0.0560; 0.1275
R^a, $wR2^b$, all ind reflns	0.1275; 0.1560
goodness of fit indicator [c]	1.090 (all ind data)
max. shift/error, final cycle	0.032
max. resid electron dens, e/Å^3	0.954
min. resid electron dens, e/Å^3	-0.928

(*a*) $R = \Sigma \big| |F_o| - |F_c| \big| / \Sigma |F_o|$. (*b*) $wR2 = \{[\Sigma w(F_o^2 - F_c^2)^2] / [\Sigma w(F_o^2)^2]\}^{1/2}$.

(*c*) Goodness-of-fit on F^2, $S = \{[\Sigma w(F_o^2 - F_c^2)^2]/(N_{obs} - N_{var})\}^{1/2}$.

Table S2. Selected Bond Lengths [Å] and Angles [°] for $TaCl(CO)_2(dppe)_2$.

Ta-P1	2.632(4)	P2-C40	1.85(2)
Ta-P2	2.623(5)	P3-C5	1.85(2)
Ta-P3	2.573(4)	P3-C50	1.82(2)
Ta-P4	2.633(4)	P3-C60	1.84(2)
Ta-Cl	2.586(4)	P4-C6	1.836(14)
Ta-C1	2.029(14)	P4-C70	1.806(14)
Ta-C2	2.02(2)	P4-C80	1.874(14)
P1-C3	1.860(14)	C1-O1	1.153(14)
P1-C10	1.82(2)	C2-O2	1.15(2)
P1-C20	1.852(14)	C3-C4	1.49(2)
P2-C4	1.861(13)	C5-C6	1.48(2)
P2-C30	1.849(13)	C10-P1-C20	102.6(6)
P1-Ta-P2	74.25(13)	Ta-P2-C4	111.0(5)
P1-Ta-P3	166.42(11)	Ta-P2-C30	119.9(5)
P1-Ta-P4	95.60(13)	Ta-P2-C40	121.1(5)
P2-Ta-P3	116.40(13)	C4-P2-C30	99.3(6)
P2-Ta-P4	162.90(11)	C4-P2-C40	101.7(7)
P3-Ta-P4	71.94(13)	C30-P2-C40	100.5(6)
C1-Ta-C2	65.6(5)	Ta-P3-C5	113.2(5)
C1-Ta-Cl	130.8(4)	Ta-P3-C50	114.6(5)
C2-Ta-Cl	162.5(4)	Ta-P3-C60	120.9(6)
C1-Ta-P1	120.4(4)	C3-P1-C20	98.8(7)
C1-Ta-P2	73.8(4)	C5-P3-C50	104.1(7)
C1-Ta-P3	72.3(4)	C5-P3-C60	99.3(8)
C1-Ta-P4	123.3(4)	C50-P3-C60	102.3(7)
C2-Ta-P1	76.2(4)	Ta-P4-C6	109.2(5)
C2-Ta-P2	105.0(4)	Ta-P4-C70	116.7(5)
C2-Ta-P3	107.3(4)	Ta-P4-C80	120.8(6)
C2-Ta-P4	85.3(4)	C6-P4-C70	107.1(8)

Cl-Ta-P1	96.04(12)	C6-P4-C80	99.0(6)
Cl-Ta-P2	87.44(13)	C70-P4-C80	101.9(7)
Cl-Ta-P3	76.84(12)	Ta-C1-O1	176.0(12)
Cl-Ta-P4	79.87(14)	Ta-C2-O2	176.7(11)
Ta-P1-C3	105.4(5)	P1-C3-C4	107.7(10)
Ta-P1-C10	118.1(5)	P2-C4-C3	112.4(10)
Ta-P1-C20	124.5(5)	P3-C5-C6	115.4(10)
C3-P1-C10	104.1(7)	P4-C6-C5	113.9(10)
P1-C3-C4-P2	-52.5(11)	P3-C5-C6-P4	-17.1(16)
C3-C4-P2-Ta	22.2(10)	C5-C6-P4-Ta	40.3(13)
C4-P2-Ta-P1	9.7(5)	C6-P4-Ta-P3	-34.6(5)
P2-Ta-P1-C3	-32.9(5)	P4-Ta-P3-C5	27.2(6)
Ta-P1-C3-C4	59.1(10)	Ta-P3-C5-C6	-14.3(14)

Table S3. Anisotropic Displacement Parameters ($Å^2$) for $TaCl(CO)_2(dppe)_2$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ta	0.0546(5)	0.0576(4)	0.0537(4)	0.0149(3)	0.0094(3)	0.0094(3)
P1	0.061(3)	0.053(2)	0.060(2)	0.021(2)	0.011(2)	0.008(2)
P2	0.054(3)	0.058(2)	0.060(2)	0.013(2)	0.014(2)	0.010(2)
P3	0.068(3)	0.058(3)	0.062(2)	0.018(2)	0.009(2)	0.007(2)
P4	0.057(3)	0.058(3)	0.068(2)	0.017(2)	0.010(2)	0.014(2)
Cl	0.069(3)	0.066(2)	0.061(2)	0.013(2)	0.007(2)	0.013(2)
C1	0.053(10)	0.095(12)	0.041(8)	0.022(8)	-0.008(8)	0.010(9)
O1	0.093(8)	0.098(8)	0.049(6)	0.025(5)	0.015(6)	0.027(7)
C2	0.079(11)	0.027(8)	0.068(9)	0.011(7)	0.028(9)	-0.004(8)
O2	0.100(9)	0.057(7)	0.086(7)	0.001(6)	0.002(7)	0.009(7)
C3	0.082(13)	0.061(10)	0.079(10)	0.023(8)	0.020(9)	0.016(10)
C4	0.064(11)	0.063(10)	0.064(9)	0.027(7)	0.015(8)	0.008(9)
C5	0.091(13)	0.061(11)	0.098(12)	0.028(9)	0.025(11)	0.023(10)
C6	0.055(10)	0.076(11)	0.083(10)	0.028(8)	0.008(9)	0.025(9)
C10	0.070(12)	0.051(10)	0.061(9)	0.025(8)	0.000(8)	0.001(8)
C11	0.036(10)	0.084(12)	0.087(11)	0.023(9)	-0.010(9)	0.002(10)
C12	0.09(2)	0.12(2)	0.093(14)	0.030(13)	0.011(12)	-0.003(13)
C13	0.10(2)	0.14(2)	0.096(14)	0.044(14)	-0.014(13)	-0.05(2)
C14	0.12(2)	0.10(2)	0.078(12)	0.006(11)	0.003(13)	-0.03(2)
C15	0.091(14)	0.071(12)	0.071(10)	0.014(9)	0.012(10)	-0.024(11)
C20	0.055(10)	0.064(11)	0.066(9)	0.033(9)	0.016(8)	0.006(8)
C21	0.043(10)	0.075(11)	0.080(12)	0.022(9)	0.013(8)	0.001(8)
C22	0.067(12)	0.12(2)	0.071(12)	0.058(11)	0.018(10)	0.034(12)
C23	0.15(2)	0.13(2)	0.041(10)	0.031(13)	0.020(12)	0.06(2)
C24	0.14(2)	0.10(2)	0.059(12)	0.029(10)	-0.018(11)	0.046(13)
C25	0.15(2)	0.049(11)	0.064(11)	0.030(8)	0.008(11)	0.006(11)
C30	0.035(9)	0.061(10)	0.075(10)	0.021(9)	0.014(8)	0.006(8)
C31	0.080(13)	0.112(14)	0.083(11)	0.010(10)	0.034(11)	-0.004(12)

C32	0.08(2)	0.12(2)	0.108(14)	-0.016(13)	0.037(13)	-0.020(13)
C33	0.10(2)	0.16(2)	0.13(2)	0.04(2)	0.08(2)	0.04(2)
C34	0.11(2)	0.103(14)	0.053(9)	-0.001(9)	0.005(11)	0.032(13)
C35	0.072(12)	0.081(12)	0.067(9)	0.010(9)	0.025(9)	-0.005(10)
C40	0.060(11)	0.052(11)	0.052(9)	0.007(7)	0.004(8)	0.015(9)
C41	0.056(10)	0.056(10)	0.072(10)	0.016(9)	-0.030(9)	0.004(9)
C42	0.12(2)	0.13(2)	0.060(11)	0.019(12)	0.000(11)	0.06(2)
C43	0.074(14)	0.07(2)	0.097(14)	-0.009(11)	-0.003(11)	0.009(11)
C44	0.070(14)	0.11(2)	0.089(13)	0.002(13)	0.006(11)	0.013(13)
C45	0.040(10)	0.093(14)	0.069(10)	-0.007(10)	-0.014(8)	0.002(10)
C50	0.090(13)	0.051(10)	0.064(9)	0.018(8)	0.011(10)	-0.012(9)
C51	0.075(13)	0.072(12)	0.108(13)	0.012(10)	0.010(12)	-0.010(11)
C52	0.12(2)	0.09(2)	0.14(2)	0.024(14)	0.05(2)	0.000(14)
C53	0.10(2)	0.09(2)	0.099(14)	0.040(13)	-0.017(14)	-0.022(13)
C54	0.17(2)	0.044(11)	0.068(11)	0.002(9)	-0.006(14)	-0.020(14)
C55	0.12(2)	0.043(10)	0.074(11)	0.005(9)	0.013(10)	-0.029(11)
C60	0.105(14)	0.059(11)	0.065(10)	0.010(10)	0.002(10)	-0.004(10)
C61	0.082(13)	0.089(14)	0.081(12)	0.040(10)	0.000(10)	0.020(11)
C62	0.15(2)	0.13(2)	0.056(12)	0.031(11)	-0.020(12)	0.03(2)
C63	0.20(3)	0.20(3)	0.08(2)	0.09(2)	-0.01(2)	0.03(2)
C64	0.25(4)	0.14(2)	0.14(2)	0.09(2)	-0.06(2)	-0.01(2)
C65	0.23(3)	0.082(14)	0.071(13)	0.042(11)	-0.01(2)	-0.03(2)
C70	0.035(9)	0.081(12)	0.052(9)	0.013(9)	-0.013(7)	-0.013(9)
C71	0.071(13)	0.098(14)	0.098(14)	0.027(13)	0.012(12)	0.014(11)
C72	0.08(2)	0.16(2)	0.083(13)	0.013(13)	-0.032(12)	-0.01(2)
C73	0.045(12)	0.12(2)	0.10(2)	0.004(14)	-0.022(10)	-0.001(13)
C74	0.048(13)	0.10(2)	0.12(2)	-0.01(2)	0.025(13)	0.011(12)
C75	0.045(10)	0.075(13)	0.091(12)	0.007(10)	0.000(10)	0.001(10)
C80	0.09(2)	0.064(10)	0.057(10)	0.014(8)	0.023(10)	0.033(10)
C81	0.036(11)	0.12(2)	0.110(14)	0.038(11)	0.017(10)	0.022(10)

C82	0.09(2)	0.16(2)	0.093(14)	0.043(13)	0.046(14)	0.050(13)
C83	0.09(2)	0.15(2)	0.082(14)	0.035(12)	0.042(13)	0.024(13)
C84	0.10(2)	0.12(2)	0.080(12)	0.027(11)	0.030(12)	0.027(13)
C85	0.054(10)	0.092(12)	0.084(12)	0.017(9)	0.032(10)	0.011(9)
C101	0.25(2)	0.17(3)	0.26(2)	-0.02(2)	0.11(3)	-0.06(2)
C102	0.25(2)	0.17(2)	0.25(2)	0.01(2)	0.04(3)	-0.05(3)
C103	0.25(2)	0.19(3)	0.21(3)	-0.01(2)	0.01(3)	-0.09(2)
C104	0.29(3)	0.21(3)	0.19(2)	0.00(2)	0.01(3)	-0.03(3)
C105	0.30(3)	0.18(2)	0.21(2)	-0.04(2)	0.04(3)	-0.03(3)
C106	0.28(3)	0.16(2)	0.28(3)	0.01(2)	0.04(3)	-0.01(3)
C107	0.25(2)	0.30(4)	0.24(3)	-0.01(3)	0.08(3)	-0.03(4)

Table S4. Hydrogen Fractional Coordinates and Isotropic Displacement Parameters ($Å^2$) for $TaCl(CO)_2(dppe)_2$.

	x	y	z	U(eq)
H3A	0.3628(11)	-0.0633(10)	0.3803(10)	0.087
H3B	0.3664(11)	-0.0402(10)	0.2823(10)	0.087
H4A	0.5220(11)	0.0049(9)	0.3616(9)	0.074
H4B	0.4832(11)	0.0622(9)	0.4474(9)	0.074
H5A	0.2912(12)	0.4797(10)	0.2995(11)	0.096
H5B	0.2207(12)	0.4436(10)	0.2064(11)	0.096
H6A	0.1148(10)	0.4037(10)	0.2895(10)	0.082
H6B	0.1941(10)	0.4104(10)	0.3737(10)	0.082
H11	0.0919(12)	0.0648(12)	0.4331(11)	0.085
H12	-0.057(2)	-0.019(2)	0.3849(13)	0.121
H13	-0.088(2)	-0.144(2)	0.2584(14)	0.140
H14	0.049(2)	-0.1931(13)	0.1911(12)	0.130
H15	0.2004(13)	-0.1010(11)	0.2336(10)	0.098
H21	0.2256(10)	-0.0366(10)	0.5128(11)	0.079
H22	0.2385(12)	-0.0057(14)	0.6689(12)	0.094
H23	0.340(2)	0.126(2)	0.7552(11)	0.122
H24	0.414(2)	0.2346(13)	0.6843(11)	0.118
H25	0.3778(14)	0.2157(11)	0.5264(10)	0.104
H31	0.6804(13)	0.2203(13)	0.2832(11)	0.113
H32	0.7797(14)	0.171(2)	0.1761(13)	0.134
H33	0.729(2)	0.030(2)	0.071(2)	0.150
H34	0.579(2)	-0.0543(13)	0.0673(10)	0.109
H35	0.4809(11)	-0.0094(11)	0.1814(10)	0.090
H41	0.6305(11)	0.1406(11)	0.4882(11)	0.078
H42	0.751(2)	0.245(2)	0.5930(11)	0.119
H43	0.7746(14)	0.4043(14)	0.5889(13)	0.105
H44	0.6790(14)	0.4490(14)	0.4794(13)	0.111

H45	0.5621(11)	0.3435(13)	0.3761(10)	0.088
H51	0.5062(14)	0.3454(12)	0.1263(12)	0.107
H52	0.672(2)	0.4158(14)	0.167(2)	0.137
H53	0.711(2)	0.550(2)	0.278(2)	0.122
H54	0.603(2)	0.5918(11)	0.3798(12)	0.122
H55	0.4422(14)	0.5115(11)	0.3478(10)	0.102
H61	0.2417(12)	0.1935(12)	0.0593(11)	0.097
H62	0.180(2)	0.186(2)	-0.0942(12)	0.131
H63	0.223(2)	0.306(2)	-0.159(2)	0.183
H64	0.306(2)	0.447(2)	-0.071(2)	0.212
H65	0.363(2)	0.4566(14)	0.0809(13)	0.158
H71	0.0711(13)	0.3296(13)	0.1408(13)	0.106
H72	-0.044(2)	0.271(2)	0.0103(13)	0.139
H73	-0.1077(13)	0.114(2)	-0.0270(14)	0.115
H74	-0.0705(13)	0.018(2)	0.067(2)	0.118
H75	0.0460(12)	0.0790(12)	0.1974(12)	0.088
H81	-0.0521(12)	0.2047(12)	0.3044(12)	0.101
H82	-0.1390(14)	0.1893(14)	0.4266(14)	0.125
H83	-0.064(2)	0.2168(14)	0.5708(14)	0.124
H84	0.112(2)	0.2511(13)	0.6008(12)	0.120
H85	0.1963(11)	0.2760(11)	0.4781(11)	0.091
H102	0.381(3)	0.630(2)	0.210(2)	0.285
H103	0.524(2)	0.659(2)	0.144(3)	0.288
H104	0.530(2)	0.751(2)	0.037(2)	0.295
H105	0.395(3)	0.815(2)	-0.005(2)	0.298
H106	0.252(2)	0.785(2)	0.060(2)	0.299
H10A	0.166(2)	0.705(2)	0.148(2)	0.421
H10B	0.224(2)	0.687(2)	0.237(2)	0.421
H10C	0.197(2)	0.607(2)	0.146(2)	0.421
H10D	0.226(2)	0.628(2)	0.206(2)	0.421

H10E	0.168(2)	0.646(2)	0.117(2)	0.421
H10F	0.194(2)	0.726(2)	0.208(2)	0.421
H212	0.148(5)	0.623(4)	0.723(4)	0.215
H213	0.176(6)	0.624(5)	0.879(4)	0.256
H214	0.097(7)	0.502(6)	0.934(3)	0.336
H215	-0.009(7)	0.379(5)	0.833(5)	0.325
H216	-0.037(6)	0.378(4)	0.678(5)	0.293
H21A	-0.002(5)	0.438(4)	0.551(3)	0.352
H21B	0.108(5)	0.487(4)	0.562(3)	0.352
H21C	0.024(5)	0.548(4)	0.568(3)	0.352
H21D	0.088(5)	0.544(4)	0.570(3)	0.352
H21E	-0.021(5)	0.495(4)	0.558(3)	0.352
H21F	0.063(5)	0.435(4)	0.553(3)	0.352
H222	0.178(8)	0.623(7)	0.828(6)	0.187
H223	0.131(9)	0.559(8)	0.949(4)	0.181
H224	0.009(8)	0.428(7)	0.920(4)	0.174
H225	-0.065(7)	0.361(5)	0.770(6)	0.167
H226	-0.019(6)	0.425(6)	0.649(3)	0.078
H22A	0.075(8)	0.538(7)	0.592(6)	0.325
H22B	0.181(8)	0.574(7)	0.645(6)	0.325
H22C	0.101(8)	0.637(7)	0.660(6)	0.325
H22D	0.163(8)	0.628(7)	0.673(6)	0.325
H22E	0.057(8)	0.592(7)	0.619(6)	0.325
H22F	0.138(8)	0.529(7)	0.604(6)	0.325
H232	-0.008(8)	0.405(5)	0.780(6)	0.169
H233	-0.021(8)	0.403(6)	0.623(5)	0.154
H234	0.066(7)	0.525(6)	0.573(3)	0.124
H235	0.165(6)	0.648(5)	0.679(5)	0.103
H236	0.178(7)	0.650(6)	0.836(5)	0.143
H23A	0.139(10)	0.583(8)	0.961(4)	0.481

H23B	0.121(10)	0.473(8)	0.936(4)	0.481
H23C	0.032(10)	0.527(8)	0.947(4)	0.481
H23D	0.056(10)	0.472(8)	0.935(4)	0.481
H23E	0.074(10)	0.582(8)	0.960(4)	0.481
H23F	0.163(10)	0.529(8)	0.949(4)	0.481

The equivalent isotropic displacement parameter, U_{eq}, is calculated as

$U_{eq} = (1/3) \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \mathbf{a}_j$.

Table S5. Fractional Coordinates and Isotropic Displacement Parameters ($Å^2$) for the toluene solvate molecules in the crystal of $TaCl(CO)_2(dppe)_2$.

	x	y	z	U(eq)
C101	0.303(2)	0.7048(14)	0.141(2)	0.243(11)
C102	0.384(2)	0.6669(12)	0.1665(13)	0.238(10)
C103	0.469(2)	0.684(2)	0.127(2)	0.240(11)
C104	0.473(2)	0.740(2)	0.063(2)	0.246(12)
C105	0.392(2)	0.7776(13)	0.0377(12)	0.249(11)
C106	0.307(2)	0.7601(14)	0.077(2)	0.249(10)
C107	0.216(2)	0.674(2)	0.170(2)	0.281(14)
C211[a]	0.052(3)	0.501(3)	0.685(3)	0.19(2)
C212[a]	0.116(4)	0.574(3)	0.745(3)	0.18(2)
C213[a]	0.133(5)	0.575(4)	0.839(3)	0.21(3)
C214[a]	0.086(5)	0.502(5)	0.872(3)	0.28(3)
C215[a]	0.022(5)	0.428(4)	0.811(4)	0.27(3)
C216[a]	0.005(4)	0.428(3)	0.718(4)	0.24(3)
C217[a]	0.045(5)	0.493(4)	0.582(3)	0.23(3)
C221[b]	0.084(5)	0.530(4)	0.726(4)	0.11(2)
C222[b]	0.129(6)	0.571(5)	0.816(5)	0.16(3)
C223[b]	0.101(7)	0.532(6)	0.889(3)	0.15(3)
C224[b]	0.028(6)	0.453(5)	0.872(4)	0.14(3)
C225[b]	-0.017(5)	0.413(4)	0.782(4)	0.14(3)
C226[b]	0.011(4)	0.452(4)	0.709(3)	0.06(2)
C227[b]	0.113(8)	0.574(7)	0.649(6)	0.22(5)
C231[c]	0.086(5)	0.528(5)	0.823(3)	0.13(3)
C232[c]	0.027(6)	0.454(4)	0.760(4)	0.14(3)
C233[c]	0.019(6)	0.452(4)	0.666(4)	0.13(3)
C234[c]	0.071(5)	0.525(5)	0.636(3)	0.10(2)

C235[c]	0.131(5)	0.599(4)	0.700(4)	0.09(2)
C236[c]	0.138(5)	0.600(4)	0.793(4)	0.12(3)
C237[c]	0.096(10)	0.528(8)	0.926(4)	0.32(8)

(*a*) Atoms of the disordered solvent toluene molecule with site occupation factors of 0.52, (*b*) 0.25 and (*c*) 0.23, respectively.

The equivalent isotropic displacement parameter, U_{eq}, is calculated as

$U_{eq} = (1/3) \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$.