Supporting Information

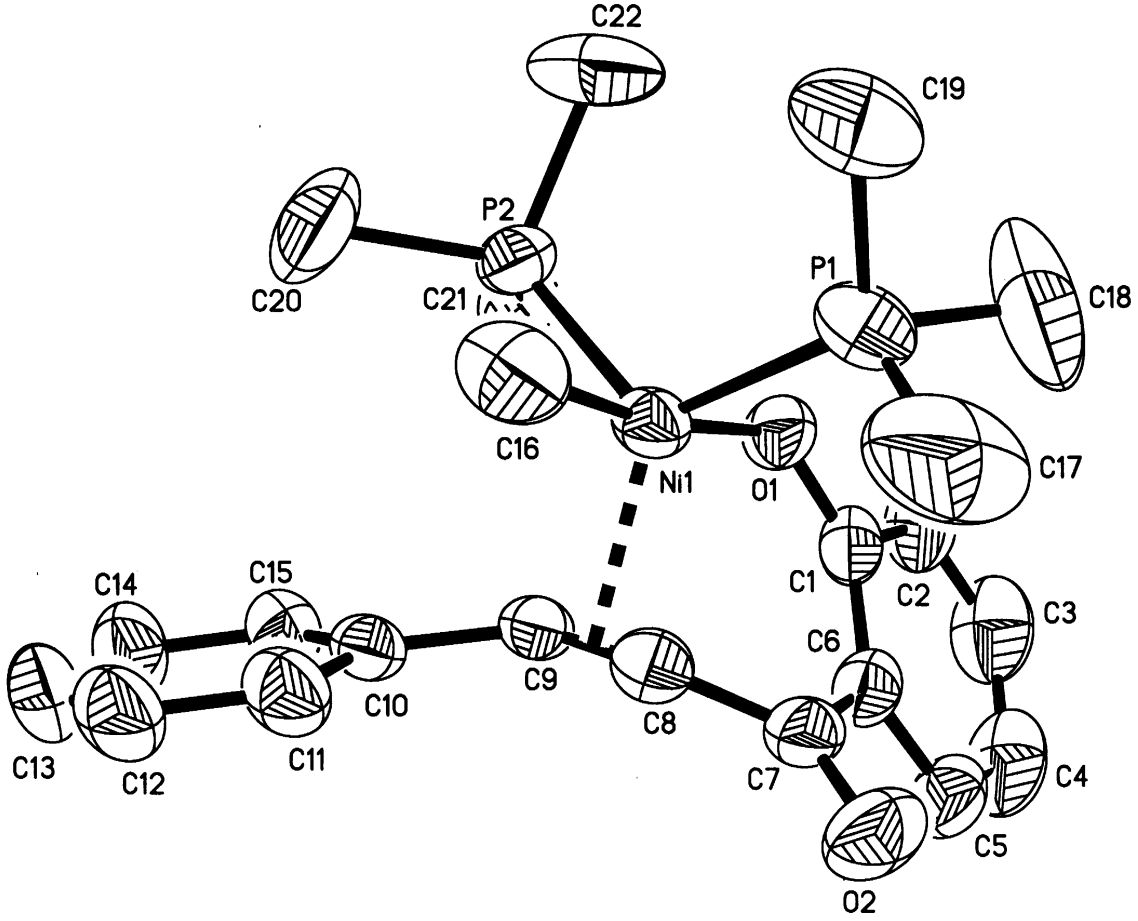

Table 1. Crystal data and structure refinement for k650.

Identification code	k650	
Empirical formula	C22 H32 Ni O2 P2	
Formula weight	449.13	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.6720(10) Å	α= 68.880(10)°.
	b = 11.2510(10) Å	β= 74.540(10)°.
	c = 13.458(2) Å	γ = 74.890(10)°.
Volume	1160.6(2) $Å^3$	
Z	2	
Density(calculated)	1.285 Mg/m^3	
F(000)	476	
Crystall size	0.18×0.58×0.30 mm	
θ range for data collection	2.14 to 27.50°	
Limiting indices	$-1 \leq h \leq 11$, $-13 \leq k \leq 13$, $-17 \leq l \leq 17$	
Reflections collected	6299	
Independent corrections	5252(R_{int} = 0.0137)	
Absorption correction	Psi-scans	
Max. And min. Transmission	0.942 and 0.795	
Refinment method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5252 / 0 /245	
Goodness-of fir on F^2	1.008	
Final R indices [I>2σ(I)]	R1 = 0.0430, wR2 = 0.0947	
R indices (all data)	R1 = 0.0694, wR2 = 0.1068	
Extinction coefficient	0.0000(9)	
Largest diff. Peak and hole	0.398 and –0.377 e $Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for k650. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni(1)	2318(1)	2730(1)	2719(1)	46(1)
P(1)	-84(1)	3087(1)	3817(1)	71(1)
P(2)	2297(1)	2749(1)	1047(1)	59(1)
O(1)	2176(2)	4586(2)	2072(2)	51(1)
O(2)	3809(3)	3441(2)	4938(2)	74(1)
C(1)	2808(3)	5345(2)	2330(2)	46(1)
C(2)	2607(4)	6671(3)	1709(3)	63(1)
C(3)	3222(5)	7535(3)	1925(3)	80(1)
C(4)	4048(5)	7146(4)	2760(4)	83(1)
C(5)	4225(4)	5885(3)	3402(3)	64(1)
C(6)	3612(3)	4955(3)	3212(2)	47(1)
C(7)	3798(3)	3629(3)	3979(2)	49(1)
C(8)	4046(3)	2497(3)	3616(2)	46(1)
C(9)	4877(3)	2457(2)	2586(2)	41(1)
C(10)	5963(3)	1316(2)	2323(2)	44(1)
C(11)	6149(4)	75(3)	3067(3)	58(1)
C(12)	7221(4)	-947(3)	2774(3)	71(1)
C(13)	8150(4)	-752(3)	1755(3)	75(1)
C(14)	7995(4)	465(3)	1007(3)	71(1)
C(15)	6914(3)	1489(3)	1293(2)	54(1)
C(16)	2137(4)	880(3)	3294(3)	79(1)
C(17)	12(6)	2513(7)	5240(4)	156(3)
C(18)	-978(6)	4770(5)	3595(5)	153(3)
C(19)	-1750(5)	2388(6)	3854(5)	130(2)
C(20)	3143(6)	1293(4)	646(4)	112(2)
C(21)	3323(4)	3952(3)	-40(3)	72(1)
C(22)	241(5)	3185(5)	773(4)	105(2)

Table 3. Bond lengths [Å] and angles [°] for k650.

Ni(1)-O(1)	1.9359(18)
Ni(1)-C(16)	1.975(3)
Ni(1)-C(8)	2.075(3)
Ni(1)-C(9)	2.127(2)
Ni(1)-P(1)	2.2443(10)
Ni(1)-P(2)	2.2477(10)
P(1)-C(18)	1.795(5)
P(1)-C(19)	1.798(4)
P(1)-C(17)	1.804(5)
P(2)-C(21)	1.808(4)
P(2)-C(20)	1.820(4)
P(2)-C(22)	1.822(4)
O(1)-C(1)	1.308(3)
O(2)-C(7)	1.234(3)
C(1)-C(6)	1.412(4)
C(1)-C(2)	1.413(4)
C(2)-C(3)	1.368(5)
C(3)-C(4)	1.370(5)
C(4)-C(5)	1.363(5)
C(5)-C(6)	1.414(4)
C(6)-C(7)	1.473(4)
C(7)-C(8)	1.468(4)
C(8)-C(9)	1.393(4)
C(9)-C(10)	1.476(3)
C(10)-C(15)	1.386(4)
C(10)-C(11)	1.393(4)
C(11)-C(12)	1.384(4)
C(12)-C(13)	1.365(5)
C(13)-C(14)	1.374(5)
C(14)-C(15)	1.385(4)
O(1)-Ni(1)-C(16)	170.77(12)
O(1)-Ni(1)-C(8)	95.05(9)
C(16)-Ni(1)-C(8)	93.89(13)

O(1)-Ni(1)-C(9)	91.22(9)
C(16)-Ni(1)-C(9)	97.19(12)
C(8)-Ni(1)-C(9)	38.69(10)
O(1)-Ni(1)-P(1)	88.88(6)
C(16)-Ni(1)-P(1)	86.65(12)
C(8)-Ni(1)-P(1)	104.76(8)
C(9)-Ni(1)-P(1)	143.29(7)
O(1)-Ni(1)-P(2)	85.11(6)
C(16)-Ni(1)-P(2)	89.87(12)
C(8)-Ni(1)-P(2)	137.23(8)
C(9)-Ni(1)-P(2)	98.57(7)
P(1)-Ni(1)-P(2)	117.99(4)
C(18)-P(1)-C(19)	102.8(3)
C(18)-P(1)-C(17)	102.8(3)
C(19)-P(1)-C(17)	100.3(3)
C(18)-P(1)-Ni(1)	114.18(17)
C(19)-P(1)-Ni(1)	120.24(17)
C(17)-P(1)-Ni(1)	114.21(16)
C(21)-P(2)-C(20)	102.5(2)
C(21)-P(2)-C(22)	102.77(18)
C(20)-P(2)-C(22)	103.1(2)
C(21)-P(2)-Ni(1)	114.21(11)
C(20)-P(2)-Ni(1)	120.32(15)
C(22)-P(2)-Ni(1)	111.93(16)
C(1)-O(1)-Ni(1)	127.49(17)
O(1)-C(1)-C(6)	125.0(2)
O(1)-C(1)-C(2)	117.5(3)
C(6)-C(1)-C(2)	117.4(3)
C(3)-C(2)-C(1)	121.4(3)
C(2)-C(3)-C(4)	121.1(3)
C(5)-C(4)-C(3)	119.5(3)
C(4)-C(5)-C(6)	121.5(3)
C(1)-C(6)-C(5)	119.0(3)
C(1)-C(6)-C(7)	123.4(2)
C(5)-C(6)-C(7)	117.6(3)
O(2)-C(7)-C(8)	118.3(3)

O(2)-C(7)-C(6)	120.5(3)
C(8)-C(7)-C(6)	121.2(2)
C(9)-C(8)-C(7)	123.2(2)
C(9)-C(8)-Ni(1)	72.69(15)
C(7)-C(8)-Ni(1)	110.77(18)
C(8)-C(9)-C(10)	125.9(2)
C(8)-C(9)-Ni(1)	68.63(14)
C(10)-C(9)-Ni(1)	120.57(17)
C(15)-C(10)-C(11)	117.5(3)
C(15)-C(10)-C(9)	118.6(2)
C(11)-C(10)-C(9)	123.9(3)
C(12)-C(11)-C(10)	120.8(3)
C(13)-C(12)-C(11)	120.6(3)
C(12)-C(13)-C(14)	119.7(3)
C(13)-C(14)-C(15)	119.9(3)
C(14)-C(15)-C(10)	121.4(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for k650. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	39(1)	40(1)	61(1)	-14(1)	-14(1)	-9(1)
P(1)	39(1)	90(1)	86(1)	-33(1)	-4(1)	-18(1)
P(2)	62(1)	51(1)	81(1)	-30(1)	-35(1)	-2(1)
O(1)	58(1)	39(1)	60(1)	-18(1)	-22(1)	-2(1)
O(2)	86(2)	96(2)	49(1)	-28(1)	-16(1)	-21(1)
C(1)	43(1)	43(1)	51(2)	-22(1)	1(1)	-9(1)
C(2)	74(2)	43(2)	66(2)	-19(1)	-4(2)	-10(2)
C(3)	93(3)	49(2)	91(3)	-23(2)	2(2)	-23(2)
C(4)	81(3)	70(2)	112(3)	-50(2)	12(2)	-39(2)
C(5)	55(2)	78(2)	75(2)	-45(2)	-1(2)	-23(2)
C(6)	44(1)	54(2)	51(2)	-26(1)	0(1)	-15(1)
C(7)	37(1)	67(2)	50(2)	-25(1)	-8(1)	-11(1)
C(8)	41(1)	48(1)	48(2)	-12(1)	-9(1)	-11(1)
C(9)	37(1)	41(1)	47(1)	-12(1)	-15(1)	-6(1)
C(10)	38(1)	41(1)	55(2)	-14(1)	-16(1)	-6(1)
C(11)	58(2)	46(2)	64(2)	-9(1)	-21(2)	-2(1)
C(12)	70(2)	44(2)	94(3)	-12(2)	-35(2)	2(2)
C(13)	65(2)	55(2)	106(3)	-37(2)	-26(2)	13(2)
C(14)	61(2)	70(2)	76(2)	-36(2)	-4(2)	4(2)
C(15)	51(2)	47(2)	59(2)	-15(1)	-12(1)	-3(1)
C(16)	68(2)	49(2)	114(3)	-8(2)	-24(2)	-21(2)
C(17)	76(3)	296(9)	89(3)	-63(4)	10(3)	-43(4)
C(18)	90(3)	111(4)	228(7)	-86(4)	48(4)	-2(3)
C(19)	51(2)	174(5)	192(5)	-92(4)	1(3)	-40(3)
C(20)	161(5)	76(3)	134(4)	-66(3)	-65(3)	4(3)
C(21)	73(2)	84(2)	63(2)	-31(2)	-18(2)	-5(2)
C(22)	84(3)	124(4)	121(4)	-18(3)	-63(3)	-29(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for k650.

	x	y	z	U(eq)
H(2)	2045	6962	1141	75
H(3)	3077	8400	1499	96
H(4)	4484	7738	2887	99
H(5)	4763	5630	3979	76
H(8)	3628	1772	4097	55
H(9)	4735	3218	2011	49
H(11)	5546	-69	3770	70
H(12)	7310	-1774	3275	85
H(13)	8884	-1439	1567	90
H(14)	8616	601	309	85
H(15)	6824	2310	783	64
H(16A)	1358	740	2976	118
H(16B)	1787	638	4068	118
H(16C)	3178	363	3116	118
H(17A)	874	2820	5343	235
H(17B)	216	1583	5489	235
H(17C)	-1004	2832	5645	235
H(18A)	-175	5239	3559	230
H(18B)	-1869	4857	4182	230
H(18C)	-1370	5112	2925	230
H(19A)	-1394	1474	3972	195
H(19B)	-2120	2787	3177	195
H(19C)	-2625	2530	4434	195
H(20A)	2671	580	1176	168
H(20B)	4301	1098	598	168
H(20C)	2903	1431	-48	168
H(21A)	2959	4773	92	108
H(21B)	3076	4027	-717	108
H(21C)	4476	3695	-73	108
H(22A)	-415	2594	1313	157

H(22B)	277	3138	68	157
H(22C)	-223	4051	793	157