



Oxamido-N-aminopropyl-N'-benzoic acid, H<sub>3</sub>obap (1)



N,N'-bis(3-aminopropyl) ethanediamide,  $H_2(apox)$  (2)



**Figure S2.** IR spectra of the Potassium-[(oxamido-*N*-aminopropyl-*N*'-benzoato)palladium(II)] trihydrate,  $KH[Pd(obap)]_2 \cdot 3H_2O$  (3) and *N*,*N*'-bis(3-aminopropyl)oxamide palladium(II), [Pd(apox)] (4) complexes

PotassiumHydrogen-[(oxamido-*N*-aminopropyl-*N*'-benzoato)palladium(II)]trihydrate, KH[Pd(obap)]<sub>2</sub>·3H<sub>2</sub>O (**3**)



*N*,*N*'-bis(3-aminopropyl)oxamide palladium(II), [Pd(apox)] (4)

**Figure S3.** <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of the oxamido-*N*-aminopropyl-*N*'-benzoic acid, H<sub>3</sub>obap (1) and *N*,*N*'-bis(3-aminopropyl) ethanediamide, H<sub>2</sub>(apox) (2) ligands





**Figure S4.** <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of the Potassium-[(oxamido-*N*-aminopropyl-*N*'-benzoato)palladium(II)] trihydrate,  $KH[Pd(obap)]_2 \cdot 3H_2O$  (3) and *N*,*N*'-bis(3-aminopropyl)oxamide palladium(II), [Pd(apox)] (4) complexes









PotassiumHydrogen-[(oxamido-*N*-aminopropyl-*N*'-benzoato)palladium(II)]trihydrate, KH[Pd(obap)]<sub>2</sub>·3H<sub>2</sub>O (**3**)



*N*,*N*'-bis(3-aminopropyl)oxamide palladium(II), [Pd(apox)] (4)

Figure S6. Distribution diagrams of the H<sub>3</sub>obap and H<sub>2</sub>apox ligands



Distribution diagram for H<sub>3</sub>obap. The concentration H<sub>3</sub>obap is 1.0 mmol dm<sup>-3</sup>.



Distribution diagram for  $H_2$  apox. The concentration  $H_2$  apox is 1.0 mmol dm<sup>-3</sup>.

Figure S7. Distribution diagrams of the Adenosine and Cytidine



Fig. 1c. Distribution diagram for HAdo. The concentration HAdo is 2.5 mmol dm<sup>-3</sup>.



Fig. 1d. Distribution diagram for HCyt. The concentration HCyt is 2.5 mmol dm<sup>-3</sup>.

Figure S8. Distribution diagram of the Pd-adenosine an Pd-cytidine complexes



Distribution diagram of Pd - Ado species at ligand-to-metal concentration ratio = 2:1 and total palladium concentration 1.0 mmol  $dm^{-3}$ 

Figure S9. Distribution diagram of the Pd-cytidine complex



Distribution diagram of Pd - Cyt species at ligand-to-metal concentration ratio = 2:1 and total palladium concentration 1.0 mmol dm<sup>-3</sup>



Figure S10. Distribution diagram of the Pd(II) - apox – Ado and Cyt system

Distribution diagram of Pd - apox - Ado species at Ado-to-apox-to-metal concentration ratio = 1:1:1 and total palladium concentration  $1.0 \text{ mmol dm}^{-3}$ 



Distribution diagram of Pd - apox - Cyt species at Cyt-to-apox-to-metal concentration ratio = 1:1:1 and total palladium concentration 1.0 mmol dm<sup>-3</sup>



**Figure S11**. Plots of log  $(F_0 - F)/F$  versus log [Q] of HSA-[Pd(obap)]<sup>-</sup> complex



Fig. S12. The DFT optimized conformers of the [Pd(apox)] complex

				NE	BOs	3	3-center hyt	orids
No	Hyperbond A:-B-:C	%A-B/%B-C	OCC.	BD <sup>1</sup> (A-B)	LP <sup>2</sup> (C)	h(A)	h(B)	h(C)
1	N 3:- C 1-: O 13	49.5/50.5	3.981	3	56	5	6	89
2	N 4:- C 2-: O 14	49.3/50.7	3.981	6	59	11	12	92
3	N 3:-Pd 15-: N 12	55.8/44.2	3.974	9	53	17	18	86
4	N 4:-Pd 15-: N 8	55.9/44.1	3.970	11	52	21	22	85

## Table S13 3-Center, 4-Electron A:-B-:C Hyperbonds (A-B :C <=> A: B-C) in case of [Pd(apox)] complex.

<sup>1</sup>BD means Bonding orbital <sup>2</sup>LP means Lone Pair

## Table S14. Crystallographic data and tables

A single crystal of complex **KPdOBAP** was selected and mounted on a glass fiber. Diffraction data were collected using a Oxford Diffraction Gemini S four-circle goniometer equipped with Sapphire CCD detector. The crystal to detector distance was 45.0 mm and graphite monochromated MoK $\alpha$  ( $\lambda = 0.71073$ Å) radiation was used for the experiments. The data were reduced using the program CrysAlisPRO [1]. A semiempirical absorption-correction based upon the intensities of equivalent reflections was applied, and the data were corrected for Lorentz, polarization, and background effects. The structure was solved by direct methods using Sir 97 program [2] and refined by full-matrix least-squares procedures on  $F^2$  using SHELXL-97 programs [3] as implemented in the WinGX program suite [4]. The non-H atoms were refined anisotropically. At the final stage of the refinement, H atoms were positioned geometrically and refined using a riding model with fixed isotropic displacement parameters (except those involved in disordered water molecules which could not be positioned from a difference Fourier map). Contributions from disordered solvent molecules were removed by the SOUEEZE routine (PLATON) [6] and the output from the SQUEEZE calculations is attached to CIF file. The refinement on the 5463 observed reflections reached at the discrepancy index R = 0.0763, with rather large e.s.d. on the structural parameters. A subsequent diference Fourier map showed regions of residual electron density (highest value = 4.6 e.Å<sup>-3</sup>), mainly confned in the cavities . This fact was interpreted as the presence of disordered solvent (water). We model this reather unpronounced peaks of the electron density as wather oxygen atoms (Ow, OwA, OwB) (Fig. bellow). The U(eq) value of an OW atom compared with the average U(eq) for to non-hydrogen atoms is high, but we did not performed any action since it was not of importance.

Crystallographic data and refinement parameters are listed in Table bellow. The figures representing molecular structure were made using ORTEP-3 [5] and PLATON [6] programs.

The perspective view of asymetric unit cell is shown in Fig. bellow. Selected bond lengths, bond angles and torsion angles are given in Tables bellow.

	Х	У	Z	U(eq)
Pd(2)	2304(1)	4461(1)	401(1)	31(1)
Pd(1)	-2324(1)	10357(1)	-5539(1)	35(1)
K(1)	637(3)	11452(2)	-8201(2)	47(1)
O(2B)	2061(11)	7556(6)	-726(6)	56(2)
O(2A)	-3391(11)	9628(6)	-2819(5)	53(2)
O(1A)	-1021(11)	8068(6)	-3337(5)	51(2)
C(2A)	-2892(14)	9729(8)	-3655(7)	39(2)
N(3A)	-3091(14)	11870(8)	-6239(6)	49(2)
O(1B)	1481(11)	6666(6)	-1933(5)	51(2)
C(3A)	-667(14)	8084(8)	-5220(7)	38(2)
O(3A)	-1267(12)	10116(6)	-6740(5)	57(2)
O(3B)	2227(12)	3012(6)	452(5)	52(2)
N(3B)	2216(15)	3926(7)	1791(6)	48(2)
N(1B)	2294(10)	5015(6)	-929(5)	34(2)
C(8B)	2429(14)	3316(8)	-1178(7)	41(2)
N(1A)	-1499(11)	8897(6)	-4833(5)	36(2)
O(4B)	2262(16)	1698(7)	-50(6)	79(3)
N(2A)	-3327(11)	10538(7)	-4336(6)	40(2)
O(4A)	88(16)	9281(7)	-7709(6)	83(3)
C(1A)	-1630(12)	8780(8)	-3937(6)	34(2)
C(4A)	-351(16)	7042(8)	-4658(8)	48(3)
C(8A)	-142(15)	8248(8)	-6166(7)	43(3)
C(2B)	2133(13)	6568(8)	-487(7)	37(2)
C(7A)	670(20)	7391(10)	-6478(9)	63(4)
C(5A)	460(19)	6232(9)	-5014(9)	59(3)
N(2B)	2380(11)	5909(6)	295(5)	36(2)
C(7B)	2594(18)	2787(10)	-1821(9)	61(3)
C(9B)	2310(15)	2673(9)	-222(8)	47(3)
C(3B)	2449(12)	4389(8)	-1511(6)	35(2)
C(4B)	2737(17)	4840(10)	-2473(7)	55(3)
C(6B)	2848(19)	3206(11)	-2746(9)	67(4)

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

C(5B)	2930(19)	4252(12)	-3046(8)	67(4)
C(1B)	1941(13)	6074(7)	-1203(6)	35(2)
C(9A)	-467(17)	9276(9)	-6896(8)	50(3)
C(11A)	-4400(20)	12440(10)	-4868(9)	71(4)
C(12A)	-4551(15)	11461(8)	-4158(8)	47(3)
C(10A)	-4570(20)	12535(10)	-5789(9)	74(4)
C(6A)	1040(20)	6399(10)	-5941(9)	70(4)
C(12B)	2700(17)	6285(9)	1009(8)	52(3)
C(11B)	2960(40)	5486(13)	1860(9)	127(10)
C(10B)	2470(40)	4611(13)	2275(11)	122(9)
OW1	-4025(17)	8407(9)	-3545(7)	91(4)
OW2	4310(17)	6378(9)	-1564(7)	94(4)
OW	-153(18)	7610(7)	-2459(7)	105(5)

Pd(2)-N(2B)	1.957(8)
Pd(2)-O(3B)	1.981(7)
Pd(2)-N(1B)	1.983(8)
Pd(2)-N(3B)	2.061(9)
Pd(1)-N(2A)	1.962(9)
Pd(1)-N(1A)	1.984(8)
Pd(1)-O(3A)	1.995(8)
Pd(1)-N(3A)	2.028(9)
K(1)-OW#1	1.829(10)
K(1)-O(1B)#1	2.773(8)
K(1)-O(1A)#1	2.792(9)
K(1)-O(2B)#1	2.807(9)
K(1)-O(3B)#2	2.807(8)
K(1)-O(2A)#1	2.809(8)
K(1)-O(3A)	2.834(8)
K(1)-O(4B)#2	2.867(10)
K(1)-O(4A)	2.944(10)
K(1)-C(9A)	3.231(11)
K(1)-C(9B)#2	3.242(12)
K(1)-C(2B)#1	3.449(10)
O(2B)-C(2B)	1.277(12)
O(2B)-K(1)#1	2.807(9)
O(2A)-C(2A)	1.262(13)
O(2A)-K(1)#1	2.809(8)
O(1A)-C(1A)	1.205(11)
O(1A)-OW	1.551(10)
O(1A)-K(1)#1	2.792(9)
C(2A)-N(2A)	1.308(13)
C(2A)-C(1A)	1.570(14)
C(2A)-K(1)#1	3.474(10)
N(3A)-C(10A)	1.506(17)
N(3A)-H(3B)	0.90(2)
N(3A)-H(3A)	0.90(2)
O(1B)-C(1B)	1.243(11)

Bond lengths [Å] and angles [°] for KPdOBAP.

O(1B)-OW	1.730(11)
O(1B)-K(1)#1	2.773(8)
C(3A)-N(1A)	1.405(14)
C(3A)-C(4A)	1.416(14)
C(3A)-C(8A)	1.416(14)
O(3A)-C(9A)	1.251(14)
O(3B)-C(9B)	1.272(14)
O(3B)-K(1)#3	2.807(8)
N(3B)-C(10B)	1.454(18)
N(3B)-H(3C)	0.91(2)
N(3B)-H(3D)	0.91(2)
N(1B)-C(1B)	1.356(12)
N(1B)-C(3B)	1.414(13)
C(8B)-C(7B)	1.393(16)
C(8B)-C(3B)	1.400(14)
C(8B)-C(9B)	1.475(15)
N(1A)-C(1A)	1.349(12)
O(4B)-C(9B)	1.287(14)
O(4B)-K(1)#3	2.867(10)
N(2A)-C(12A)	1.469(14)
O(4A)-C(9A)	1.260(14)
C(1A)-K(1)#1	3.508(10)
C(4A)-C(5A)	1.370(17)
C(4A)-H(4A)	0.9300
C(8A)-C(7A)	1.386(17)
C(8A)-C(9A)	1.512(14)
C(2B)-N(2B)	1.293(12)
C(2B)-C(1B)	1.537(14)
C(2B)-K(1)#1	3.449(10)
C(7A)-C(6A)	1.353(17)
C(7A)-H(7A)	0.9300
C(5A)-C(6A)	1.393(18)
C(5A)-H(5A)	0.9300
N(2B)-C(12B)	1.465(14)
C(7B)-C(6B)	1.372(17)
C(7B)-H(7B)	0.9300

C(9B)-K(1)#3	3.242(12)
C(3B)-C(4B)	1.429(14)
C(4B)-C(5B)	1.356(18)
C(4B)-H(4B)	0.9300
C(6B)-C(5B)	1.374(19)
C(6B)-H(6B)	0.9300
C(5B)-H(5B)	0.9300
C(1B)-K(1)#1	3.472(10)
C(11A)-C(10A)	1.44(2)
C(11A)-C(12A)	1.457(16)
C(11A)-H(11A)	0.9700
C(11A)-H(11B)	0.9700
C(12A)-H(12A)	0.9700
C(12A)-H(12B)	0.9700
C(10A)-H(10A)	0.9700
C(10A)-H(10B)	0.9700
C(6A)-H(6A)	0.9300
C(12B)-C(11B)	1.451(18)
C(12B)-H(12C)	0.9700
C(12B)-H(12D)	0.9700
C(11B)-C(10B)	1.28(2)
C(11B)-H(11C)	0.9700
C(11B)-H(11D)	0.9700
C(10B)-H(10C)	0.9700
C(10B)-H(10D)	0.9700
OW-K(1)#1	1.829(10)
N(2B)-Pd(2)-O(3B)	177.6(3)
N(2B)-Pd(2)-N(1B)	83.1(3)
O(3B)-Pd(2)-N(1B)	94.5(3)
N(2B)-Pd(2)-N(3B)	95.8(4)
O(3B)-Pd(2)-N(3B)	86.6(3)
N(1B)-Pd(2)-N(3B)	177.6(4)
N(2A)-Pd(1)-N(1A)	83.5(3)
N(2A)-Pd(1)-O(3A)	177.8(3)
N(1A)-Pd(1)-O(3A)	94.3(3)

N(2A)-Pd(1)-N(3A)	95.6(4)
N(1A)-Pd(1)-N(3A)	177.5(4)
O(3A)-Pd(1)-N(3A)	86.6(4)
OW#1-K(1)-O(1B)#1	37.6(3)
OW#1-K(1)-O(1A)#1	31.2(3)
O(1B)#1-K(1)-O(1A)#1	68.3(2)
OW#1-K(1)-O(2B)#1	95.8(3)
O(1B)#1-K(1)-O(2B)#1	58.4(2)
O(1A)#1-K(1)-O(2B)#1	125.4(3)
OW#1-K(1)-O(3B)#2	83.8(4)
O(1B)#1-K(1)-O(3B)#2	74.3(2)
O(1A)#1-K(1)-O(3B)#2	99.3(2)
O(2B)#1-K(1)-O(3B)#2	78.5(2)
OW#1-K(1)-O(2A)#1	87.5(3)
O(1B)#1-K(1)-O(2A)#1	124.8(3)
O(1A)#1-K(1)-O(2A)#1	57.9(2)
O(2B)#1-K(1)-O(2A)#1	176.7(3)
O(3B)#2-K(1)-O(2A)#1	101.9(3)
OW#1-K(1)-O(3A)	88.6(4)
O(1B)#1-K(1)-O(3A)	97.6(2)
O(1A)#1-K(1)-O(3A)	75.6(2)
O(2B)#1-K(1)-O(3A)	99.0(3)
O(3B)#2-K(1)-O(3A)	171.7(3)
O(2A)#1-K(1)-O(3A)	81.0(2)
OW#1-K(1)-O(4B)#2	128.9(4)
O(1B)#1-K(1)-O(4B)#2	108.7(2)
O(1A)#1-K(1)-O(4B)#2	139.5(3)
O(2B)#1-K(1)-O(4B)#2	73.6(3)
O(3B)#2-K(1)-O(4B)#2	45.2(2)
O(2A)#1-K(1)-O(4B)#2	104.3(3)
O(3A)-K(1)-O(4B)#2	141.9(3)
OW#1-K(1)-O(4A)	131.6(4)
O(1B)#1-K(1)-O(4A)	135.0(3)
O(1A)#1-K(1)-O(4A)	110.2(2)
O(2B)#1-K(1)-O(4A)	99.3(3)
O(3B)#2-K(1)-O(4A)	144.3(3)

O(2A)#1-K(1)-O(4A)	78.4(3)
O(3A)-K(1)-O(4A)	43.8(3)
O(4B)#2-K(1)-O(4A)	99.5(3)
OW#1-K(1)-C(9A)	108.7(4)
O(1B)#1-K(1)-C(9A)	119.9(3)
O(1A)#1-K(1)-C(9A)	88.9(3)
O(2B)#1-K(1)-C(9A)	106.4(3)
O(3B)#2-K(1)-C(9A)	165.7(3)
O(2A)#1-K(1)-C(9A)	72.4(3)
O(3A)-K(1)-C(9A)	22.6(3)
O(4B)#2-K(1)-C(9A)	122.4(3)
O(4A)-K(1)-C(9A)	23.0(3)
OW#1-K(1)-C(9B)#2	105.7(4)
O(1B)#1-K(1)-C(9B)#2	88.4(3)
O(1A)#1-K(1)-C(9B)#2	121.7(3)
O(2B)#1-K(1)-C(9B)#2	70.2(3)
O(3B)#2-K(1)-C(9B)#2	22.9(3)
O(2A)#1-K(1)-C(9B)#2	108.9(3)
O(3A)-K(1)-C(9B)#2	162.6(3)
O(4B)#2-K(1)-C(9B)#2	23.3(3)
O(4A)-K(1)-C(9B)#2	122.7(3)
C(9A)-K(1)-C(9B)#2	145.6(3)
OW#1-K(1)-C(2B)#1	80.5(3)
O(1B)#1-K(1)-C(2B)#1	43.5(2)
O(1A)#1-K(1)-C(2B)#1	111.7(2)
O(2B)#1-K(1)-C(2B)#1	20.4(2)
O(3B)#2-K(1)-C(2B)#1	63.5(2)
O(2A)#1-K(1)-C(2B)#1	161.9(3)
O(3A)-K(1)-C(2B)#1	112.0(3)
O(4B)#2-K(1)-C(2B)#1	73.7(3)
O(4A)-K(1)-C(2B)#1	119.7(3)
C(9A)-K(1)-C(2B)#1	124.3(3)
C(9B)#2-K(1)-C(2B)#1	62.2(3)
C(2B)-O(2B)-K(1)#1	109.5(7)
C(2A)-O(2A)-K(1)#1	111.4(7)
C(1A)-O(1A)-OW	153.1(9)

C(1A)-O(1A)-K(1)#1	117.0(7)
OW-O(1A)-K(1)#1	37.7(4)
O(2A)-C(2A)-N(2A)	127.6(10)
O(2A)-C(2A)-C(1A)	117.9(8)
N(2A)-C(2A)-C(1A)	114.5(9)
O(2A)-C(2A)-K(1)#1	48.8(5)
N(2A)-C(2A)-K(1)#1	150.4(7)
C(1A)-C(2A)-K(1)#1	78.2(5)
C(10A)-N(3A)-Pd(1)	118.4(7)
C(10A)-N(3A)-H(3B)	101(10)
Pd(1)-N(3A)-H(3B)	105(10)
C(10A)-N(3A)-H(3A)	102(7)
Pd(1)-N(3A)-H(3A)	111(7)
H(3B)-N(3A)-H(3A)	120(10)
C(1B)-O(1B)-OW	146.4(9)
C(1B)-O(1B)-K(1)#1	114.2(7)
OW-O(1B)-K(1)#1	40.1(4)
N(1A)-C(3A)-C(4A)	119.9(9)
N(1A)-C(3A)-C(8A)	123.0(9)
C(4A)-C(3A)-C(8A)	117.1(10)
C(9A)-O(3A)-Pd(1)	127.8(7)
C(9A)-O(3A)-K(1)	96.8(7)
Pd(1)-O(3A)-K(1)	126.4(4)
C(9B)-O(3B)-Pd(2)	126.3(7)
C(9B)-O(3B)-K(1)#3	98.1(7)
Pd(2)-O(3B)-K(1)#3	131.3(4)
C(10B)-N(3B)-Pd(2)	119.4(8)
C(10B)-N(3B)-H(3C)	104(5)
Pd(2)-N(3B)-H(3C)	109(6)
C(10B)-N(3B)-H(3D)	102(8)
Pd(2)-N(3B)-H(3D)	94(8)
H(3C)-N(3B)-H(3D)	130(10)
C(1B)-N(1B)-C(3B)	123.6(8)
C(1B)-N(1B)-Pd(2)	111.7(6)
C(3B)-N(1B)-Pd(2)	124.4(6)
C(7B)-C(8B)-C(3B)	116.6(10)

C(7B)-C(8B)-C(9B)	116.1(10)
C(3B)-C(8B)-C(9B)	127.3(10)
C(1A)-N(1A)-C(3A)	122.2(8)
C(1A)-N(1A)-Pd(1)	113.0(7)
C(3A)-N(1A)-Pd(1)	124.4(6)
C(9B)-O(4B)-K(1)#3	95.0(7)
C(2A)-N(2A)-C(12A)	119.5(9)
C(2A)-N(2A)-Pd(1)	114.8(7)
C(12A)-N(2A)-Pd(1)	125.7(7)
C(9A)-O(4A)-K(1)	91.4(7)
O(1A)-C(1A)-N(1A)	131.2(10)
O(1A)-C(1A)-C(2A)	116.8(9)
N(1A)-C(1A)-C(2A)	111.8(8)
O(1A)-C(1A)-K(1)#1	45.2(6)
N(1A)-C(1A)-K(1)#1	162.8(6)
C(2A)-C(1A)-K(1)#1	75.8(5)
C(5A)-C(4A)-C(3A)	121.3(11)
C(5A)-C(4A)-H(4A)	119.4
C(3A)-C(4A)-H(4A)	119.4
C(7A)-C(8A)-C(3A)	118.4(10)
C(7A)-C(8A)-C(9A)	115.3(11)
C(3A)-C(8A)-C(9A)	126.2(11)
O(2B)-C(2B)-N(2B)	127.8(10)
O(2B)-C(2B)-C(1B)	117.7(9)
N(2B)-C(2B)-C(1B)	114.5(9)
O(2B)-C(2B)-K(1)#1	50.1(5)
N(2B)-C(2B)-K(1)#1	148.6(7)
C(1B)-C(2B)-K(1)#1	78.0(5)
C(6A)-C(7A)-C(8A)	124.8(13)
C(6A)-C(7A)-H(7A)	117.6
C(8A)-C(7A)-H(7A)	117.6
C(4A)-C(5A)-C(6A)	121.6(11)
C(4A)-C(5A)-H(5A)	119.2
C(6A)-C(5A)-H(5A)	119.2
C(2B)-N(2B)-C(12B)	119.0(9)
C(2B)-N(2B)-Pd(2)	115.1(7)

C(12B)-N(2B)-Pd(2)	125.9(7)
C(6B)-C(7B)-C(8B)	126.4(12)
C(6B)-C(7B)-H(7B)	116.8
C(8B)-C(7B)-H(7B)	116.8
O(3B)-C(9B)-O(4B)	117.1(10)
O(3B)-C(9B)-C(8B)	124.9(10)
O(4B)-C(9B)-C(8B)	118.0(10)
O(3B)-C(9B)-K(1)#3	59.0(6)
O(4B)-C(9B)-K(1)#3	61.8(6)
C(8B)-C(9B)-K(1)#3	160.4(8)
C(8B)-C(3B)-N(1B)	122.1(9)
C(8B)-C(3B)-C(4B)	117.9(10)
N(1B)-C(3B)-C(4B)	119.9(9)
C(5B)-C(4B)-C(3B)	121.0(12)
C(5B)-C(4B)-H(4B)	119.5
C(3B)-C(4B)-H(4B)	119.5
C(7B)-C(6B)-C(5B)	115.2(12)
C(7B)-C(6B)-H(6B)	122.4
C(5B)-C(6B)-H(6B)	122.4
C(4B)-C(5B)-C(6B)	122.8(12)
C(4B)-C(5B)-H(5B)	118.6
C(6B)-C(5B)-H(5B)	118.6
O(1B)-C(1B)-N(1B)	128.6(10)
O(1B)-C(1B)-C(2B)	118.1(9)
N(1B)-C(1B)-C(2B)	113.3(8)
O(1B)-C(1B)-K(1)#1	46.7(5)
N(1B)-C(1B)-K(1)#1	156.8(7)
C(2B)-C(1B)-K(1)#1	76.3(5)
O(3A)-C(9A)-O(4A)	118.2(10)
O(3A)-C(9A)-C(8A)	123.9(11)
O(4A)-C(9A)-C(8A)	117.9(11)
O(3A)-C(9A)-K(1)	60.6(6)
O(4A)-C(9A)-K(1)	65.6(6)
C(8A)-C(9A)-K(1)	152.4(8)
C(10A)-C(11A)-C(12A)	120.3(13)
C(10A)-C(11A)-H(11A)	107.3

C(12A)-C(11A)-H(11A)	107.3
C(10A)-C(11A)-H(11B)	107.3
C(12A)-C(11A)-H(11B)	107.3
H(11A)-C(11A)-H(11B)	106.9
C(11A)-C(12A)-N(2A)	115.1(10)
C(11A)-C(12A)-H(12A)	108.5
N(2A)-C(12A)-H(12A)	108.5
C(11A)-C(12A)-H(12B)	108.5
N(2A)-C(12A)-H(12B)	108.5
H(12A)-C(12A)-H(12B)	107.5
C(11A)-C(10A)-N(3A)	113.8(11)
C(11A)-C(10A)-H(10A)	108.8
N(3A)-C(10A)-H(10A)	108.8
C(11A)-C(10A)-H(10B)	108.8
N(3A)-C(10A)-H(10B)	108.8
H(10A)-C(10A)-H(10B)	107.7
C(7A)-C(6A)-C(5A)	116.7(13)
C(7A)-C(6A)-H(6A)	121.6
C(5A)-C(6A)-H(6A)	121.6
C(11B)-C(12B)-N(2B)	114.8(10)
C(11B)-C(12B)-H(12C)	108.6
N(2B)-C(12B)-H(12C)	108.6
C(11B)-C(12B)-H(12D)	108.6
N(2B)-C(12B)-H(12D)	108.6
H(12C)-C(12B)-H(12D)	107.5
C(10B)-C(11B)-C(12B)	135.7(16)
C(10B)-C(11B)-H(11C)	103.3
C(12B)-C(11B)-H(11C)	103.3
C(10B)-C(11B)-H(11D)	103.3
C(12B)-C(11B)-H(11D)	103.3
H(11C)-C(11B)-H(11D)	105.2
C(11B)-C(10B)-N(3B)	122.1(14)
С(11В)-С(10В)-Н(10С)	106.8
N(3B)-C(10B)-H(10C)	106.8
C(11B)-C(10B)-H(10D)	106.8
N(3B)-C(10B)-H(10D)	106.8

H(10C)-C(10B)-H(10D)	106.7
O(1A)-OW-O(1B)	144.6(8)
O(1A)-OW-K(1)#1	111.2(6)
O(1B)-OW-K(1)#1	102.3(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z-1 #2 x,y+1,z-1 #3 x,y-1,z+1

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Pd(2)	37(1)	30(1)	24(1)	0(1)	-8(1)	-9(1)
Pd(1)	37(1)	32(1)	29(1)	4(1)	-5(1)	-8(1)
K(1)	63(2)	35(1)	32(1)	3(1)	-6(1)	-7(1)
O(2B)	67(5)	33(4)	59(5)	3(4)	-14(4)	-13(4)
O(2A)	56(5)	53(5)	40(4)	-10(4)	-1(4)	-1(4)
O(1A)	62(5)	34(4)	48(5)	3(3)	-23(4)	3(4)
C(2A)	38(6)	33(5)	37(6)	-1(4)	-4(4)	-4(4)
N(3A)	58(6)	44(5)	29(5)	3(4)	-2(4)	-2(5)
O(1B)	64(5)	42(4)	30(4)	3(3)	-6(4)	0(4)
C(3A)	41(6)	36(5)	32(5)	4(4)	-8(4)	-17(5)
O(3A)	75(6)	44(5)	43(5)	-7(4)	-3(4)	-6(4)
O(3B)	77(6)	36(4)	42(4)	-3(3)	-16(4)	-14(4)
N(3B)	69(7)	37(5)	35(5)	1(4)	-22(5)	-8(5)
N(1B)	33(4)	37(4)	25(4)	-4(3)	2(3)	-7(4)
C(8B)	36(6)	37(6)	42(6)	-6(5)	-6(5)	-1(4)
N(1A)	35(4)	38(5)	30(4)	-5(4)	-1(3)	-8(4)
O(4B)	138(10)	35(5)	59(6)	-14(4)	0(6)	-16(5)
N(2A)	38(5)	41(5)	34(5)	-1(4)	-11(4)	-5(4)
O(4A)	146(10)	58(6)	35(5)	-9(4)	-4(5)	-12(6)
C(1A)	29(5)	36(5)	25(5)	6(4)	0(4)	-9(4)
C(4A)	60(7)	35(6)	44(6)	1(5)	-11(5)	-13(5)
C(8A)	58(7)	36(6)	34(6)	0(4)	-10(5)	-18(5)
C(2B)	31(5)	43(6)	30(5)	-7(4)	4(4)	-6(4)
C(7A)	95(11)	46(7)	51(7)	-18(6)	-10(7)	-15(7)
C(5A)	84(9)	30(6)	60(8)	-5(5)	-17(7)	-7(6)
N(2B)	34(4)	34(4)	34(5)	1(4)	-7(4)	-10(4)
C(7B)	70(9)	51(7)	60(8)	-26(6)	1(7)	-4(6)
C(9B)	45(6)	45(7)	43(6)	-11(5)	-3(5)	3(5)
C(3B)	26(5)	45(6)	28(5)	-4(4)	3(4)	-10(4)
C(4B)	73(8)	51(7)	29(6)	0(5)	-13(6)	-1(6)
C(6B)	90(10)	56(8)	44(7)	-17(6)	-8(7)	8(7)

Anisotropic displacement parameters (Å<sup>2</sup>x 10<sup>3</sup>) for KPdOBAP. The anisotropic displacement factor exponent takes the form:  $-2\pi^2$ [ h<sup>2</sup>a<sup>\*2</sup>U<sup>11</sup> + ... + 2 h k a<sup>\*</sup> b<sup>\*</sup> U<sup>12</sup> ]

C(5B)	71(9)	83(10)	33(6)	-12(6)	-4(6)	2(7)
C(1B)	35(5)	31(5)	28(5)	2(4)	-3(4)	-4(4)
C(9A)	65(8)	38(6)	38(6)	5(5)	-13(6)	-11(6)
C(11A)	85(10)	50(8)	62(9)	-18(7)	13(7)	4(7)
C(12A)	45(6)	43(6)	46(6)	-8(5)	-4(5)	-1(5)
C(10A)	75(9)	50(8)	59(9)	14(6)	-3(7)	16(7)
C(6A)	109(12)	45(7)	57(8)	-19(6)	-20(8)	-3(7)
C(12B)	57(7)	51(7)	50(7)	-16(6)	-12(6)	-6(6)
C(11B)	300(30)	81(12)	37(8)	-2(7)	-42(12)	-102(16)
C(10B)	260(30)	68(11)	55(10)	5(8)	-70(14)	-62(14)
OW1	128(10)	100(8)	50(6)	-3(5)	-16(6)	-55(7)
OW2	125(10)	102(8)	53(6)	13(6)	-18(6)	-63(8)
OW	203(14)	49(6)	69(7)	-15(5)	-104(9)	37(7)

	Х	У	Z	U(eq)
H(4A)	-701	6904	-4034	58
H(7A)	974	7506	-7102	75
H(5A)	628	5555	-4628	71
H(7B)	2524	2081	-1601	73
H(4B)	2793	5546	-2710	66
H(6B)	2957	2810	-3142	80
H(5B)	3127	4571	-3667	81
H(11A)	-5289	12982	-4679	86
H(11B)	-3260	12602	-4881	86
H(12A)	-5749	11340	-4070	57
H(12B)	-4353	11536	-3595	57
H(10A)	-4617	13261	-6144	89
H(10B)	-5680	12343	-5788	89
H(6A)	1650	5856	-6180	84
H(12C)	3737	6612	789	63
H(12D)	1704	6819	1124	63
H(11C)	4238	5307	1824	153
H(11D)	2577	5872	2307	153
H(10C)	1353	4760	2655	147
H(10D)	3316	4207	2681	147
H(3C)	3090(80)	3360(40)	1930(60)	20(20)
H(3B)	-2200(200)	12190(170)	-6290(160)	180(110)
H(3D)	1030(40)	3970(100)	1900(80)	60(40)
H(3A)	-3510(140)	11910(80)	-6750(40)	40(30)
H(1)	-6300(130)	9430(80)	-2610(70)	40(30)

Hydrogen coordinates (  $x \ 10^4$ ) and isotropic displacement parameters (Å<sup>2</sup>x 10<sup>3</sup>) for KPdOBAP.

Torsion angles [°] for KPdOBAP.

K(1)#1-O(2A)-C(2A)-N(2A)	-141.6(10)
K(1)#1-O(2A)-C(2A)-C(1A)	39.7(11)
N(2A)-Pd(1)-N(3A)-C(10A)	-20.4(11)
N(1A)-Pd(1)-N(3A)-C(10A)	-89(9)
O(3A)-Pd(1)-N(3A)-C(10A)	159.7(11)
N(2A)-Pd(1)-O(3A)-C(9A)	4(10)
N(1A)-Pd(1)-O(3A)-C(9A)	3.0(11)
N(3A)-Pd(1)-O(3A)-C(9A)	-179.3(11)
N(2A)-Pd(1)-O(3A)-K(1)	-136(9)
N(1A)-Pd(1)-O(3A)-K(1)	-136.3(5)
N(3A)-Pd(1)-O(3A)-K(1)	41.3(5)
OW#1-K(1)-O(3A)-C(9A)	-153.1(8)
O(1B)#1-K(1)-O(3A)-C(9A)	170.4(7)
O(1A)#1-K(1)-O(3A)-C(9A)	-124.4(7)
O(2B)#1-K(1)-O(3A)-C(9A)	111.3(7)
O(3B)#2-K(1)-O(3A)-C(9A)	-176.9(16)
O(2A)#1-K(1)-O(3A)-C(9A)	-65.4(7)
O(4B)#2-K(1)-O(3A)-C(9A)	36.4(9)
O(4A)-K(1)-O(3A)-C(9A)	17.2(7)
C(9B)#2-K(1)-O(3A)-C(9A)	61.1(13)
C(2B)#1-K(1)-O(3A)-C(9A)	127.7(7)
OW#1-K(1)-O(3A)-Pd(1)	-4.3(6)
O(1B)#1-K(1)-O(3A)-Pd(1)	-40.9(5)
O(1A)#1-K(1)-O(3A)-Pd(1)	24.3(4)
O(2B)#1-K(1)-O(3A)-Pd(1)	-100.0(5)
O(3B)#2-K(1)-O(3A)-Pd(1)	-28(2)
O(2A)#1-K(1)-O(3A)-Pd(1)	83.3(5)
O(4B)#2-K(1)-O(3A)-Pd(1)	-174.9(5)
O(4A)-K(1)-O(3A)-Pd(1)	165.9(7)
C(9A)-K(1)-O(3A)-Pd(1)	148.8(10)
C(9B)#2-K(1)-O(3A)-Pd(1)	-150.2(8)
C(2B)#1-K(1)-O(3A)-Pd(1)	-83.5(5)
N(2B)-Pd(2)-O(3B)-C(9B)	5(9)
N(1B)-Pd(2)-O(3B)-C(9B)	5.1(10)

N(3B)-Pd(2)-O(3B)-C(9B)	-177.0(10)
N(2B)-Pd(2)-O(3B)-K(1)#3	-146(8)
N(1B)-Pd(2)-O(3B)-K(1)#3	-146.6(5)
N(3B)-Pd(2)-O(3B)-K(1)#3	31.3(5)
N(2B)-Pd(2)-N(3B)-C(10B)	-8.1(15)
O(3B)-Pd(2)-N(3B)-C(10B)	172.0(15)
N(1B)-Pd(2)-N(3B)-C(10B)	-70(9)
N(2B)-Pd(2)-N(1B)-C(1B)	-13.9(7)
O(3B)-Pd(2)-N(1B)-C(1B)	166.1(7)
N(3B)-Pd(2)-N(1B)-C(1B)	49(9)
N(2B)-Pd(2)-N(1B)-C(3B)	172.3(8)
O(3B)-Pd(2)-N(1B)-C(3B)	-7.7(8)
N(3B)-Pd(2)-N(1B)-C(3B)	-125(9)
C(4A)-C(3A)-N(1A)-C(1A)	16.7(14)
C(8A)-C(3A)-N(1A)-C(1A)	-164.5(9)
C(4A)-C(3A)-N(1A)-Pd(1)	-171.2(7)
C(8A)-C(3A)-N(1A)-Pd(1)	7.6(13)
N(2A)-Pd(1)-N(1A)-C(1A)	-13.7(7)
O(3A)-Pd(1)-N(1A)-C(1A)	166.3(7)
N(3A)-Pd(1)-N(1A)-C(1A)	55(9)
N(2A)-Pd(1)-N(1A)-C(3A)	173.6(8)
O(3A)-Pd(1)-N(1A)-C(3A)	-6.5(8)
N(3A)-Pd(1)-N(1A)-C(3A)	-117(8)
O(2A)-C(2A)-N(2A)-C(12A)	-0.7(17)
C(1A)-C(2A)-N(2A)-C(12A)	177.9(9)
K(1)#1-C(2A)-N(2A)-C(12A)	-71.7(17)
O(2A)-C(2A)-N(2A)-Pd(1)	-177.9(9)
C(1A)-C(2A)-N(2A)-Pd(1)	0.8(11)
K(1)#1-C(2A)-N(2A)-Pd(1)	111.1(14)
N(1A)-Pd(1)-N(2A)-C(2A)	6.6(7)
O(3A)-Pd(1)-N(2A)-C(2A)	6(9)
N(3A)-Pd(1)-N(2A)-C(2A)	-171.1(8)
N(1A)-Pd(1)-N(2A)-C(12A)	-170.3(9)
O(3A)-Pd(1)-N(2A)-C(12A)	-171(9)
N(3A)-Pd(1)-N(2A)-C(12A)	12.0(9)
OW#1-K(1)-O(4A)-C(9A)	-3.9(11)

O(1B)#1-K(1)-O(4A)-C(9A)	-56.2(9)
O(1A)#1-K(1)-O(4A)-C(9A)	22.9(9)
O(2B)#1-K(1)-O(4A)-C(9A)	-110.3(8)
O(3B)#2-K(1)-O(4A)-C(9A)	166.5(7)
O(2A)#1-K(1)-O(4A)-C(9A)	72.1(8)
O(3A)-K(1)-O(4A)-C(9A)	-16.9(7)
O(4B)#2-K(1)-O(4A)-C(9A)	174.9(8)
C(9B)#2-K(1)-O(4A)-C(9A)	177.3(7)
C(2B)#1-K(1)-O(4A)-C(9A)	-108.5(8)
OW-O(1A)-C(1A)-N(1A)	140.7(19)
K(1)#1-O(1A)-C(1A)-N(1A)	156.9(9)
OW-O(1A)-C(1A)-C(2A)	-43(2)
K(1)#1-O(1A)-C(1A)-C(2A)	-27.1(11)
OW-O(1A)-C(1A)-K(1)#1	-16.2(18)
C(3A)-N(1A)-C(1A)-O(1A)	6.1(17)
Pd(1)-N(1A)-C(1A)-O(1A)	-166.9(9)
C(3A)-N(1A)-C(1A)-C(2A)	-170.1(8)
Pd(1)-N(1A)-C(1A)-C(2A)	17.0(10)
C(3A)-N(1A)-C(1A)-K(1)#1	76(3)
Pd(1)-N(1A)-C(1A)-K(1)#1	-97(2)
O(2A)-C(2A)-C(1A)-O(1A)	-10.0(14)
N(2A)-C(2A)-C(1A)-O(1A)	171.2(9)
K(1)#1-C(2A)-C(1A)-O(1A)	19.5(8)
O(2A)-C(2A)-C(1A)-N(1A)	166.8(9)
N(2A)-C(2A)-C(1A)-N(1A)	-12.0(12)
K(1)#1-C(2A)-C(1A)-N(1A)	-163.8(7)
O(2A)-C(2A)-C(1A)-K(1)#1	-29.4(8)
N(2A)-C(2A)-C(1A)-K(1)#1	151.8(9)
N(1A)-C(3A)-C(4A)-C(5A)	-179.9(11)
C(8A)-C(3A)-C(4A)-C(5A)	1.3(16)
N(1A)-C(3A)-C(8A)-C(7A)	-179.9(11)
C(4A)-C(3A)-C(8A)-C(7A)	-1.1(16)
N(1A)-C(3A)-C(8A)-C(9A)	-3.6(17)
C(4A)-C(3A)-C(8A)-C(9A)	175.2(10)
K(1)#1-O(2B)-C(2B)-N(2B)	-139.4(9)
K(1)#1-O(2B)-C(2B)-C(1B)	41.8(10)

C(3A)-C(8A)-C(7A)-C(6A)	-2(2)
C(9A)-C(8A)-C(7A)-C(6A)	-178.4(13)
C(3A)-C(4A)-C(5A)-C(6A)	1(2)
O(2B)-C(2B)-N(2B)-C(12B)	-3.0(16)
C(1B)-C(2B)-N(2B)-C(12B)	175.9(9)
K(1)#1-C(2B)-N(2B)-C(12B)	-76.3(16)
O(2B)-C(2B)-N(2B)-Pd(2)	177.6(9)
C(1B)-C(2B)-N(2B)-Pd(2)	-3.6(11)
K(1)#1-C(2B)-N(2B)-Pd(2)	104.3(13)
O(3B)-Pd(2)-N(2B)-C(2B)	9(9)
N(1B)-Pd(2)-N(2B)-C(2B)	9.5(7)
N(3B)-Pd(2)-N(2B)-C(2B)	-168.3(8)
O(3B)-Pd(2)-N(2B)-C(12B)	-170(8)
N(1B)-Pd(2)-N(2B)-C(12B)	-169.9(9)
N(3B)-Pd(2)-N(2B)-C(12B)	12.3(9)
C(3B)-C(8B)-C(7B)-C(6B)	3(2)
C(9B)-C(8B)-C(7B)-C(6B)	-175.1(13)
Pd(2)-O(3B)-C(9B)-O(4B)	179.1(9)
K(1)#3-O(3B)-C(9B)-O(4B)	-22.0(12)
Pd(2)-O(3B)-C(9B)-C(8B)	-1.9(16)
K(1)#3-O(3B)-C(9B)-C(8B)	157.0(10)
Pd(2)-O(3B)-C(9B)-K(1)#3	-158.9(9)
K(1)#3-O(4B)-C(9B)-O(3B)	21.4(11)
K(1)#3-O(4B)-C(9B)-C(8B)	-157.7(9)
C(7B)-C(8B)-C(9B)-O(3B)	177.0(12)
C(3B)-C(8B)-C(9B)-O(3B)	-0.9(18)
C(7B)-C(8B)-C(9B)-O(4B)	-4.0(16)
C(3B)-C(8B)-C(9B)-O(4B)	178.2(11)
C(7B)-C(8B)-C(9B)-K(1)#3	-88(2)
C(3B)-C(8B)-C(9B)-K(1)#3	94(2)
C(7B)-C(8B)-C(3B)-N(1B)	-180.0(10)
C(9B)-C(8B)-C(3B)-N(1B)	-2.1(16)
C(7B)-C(8B)-C(3B)-C(4B)	-3.5(15)
C(9B)-C(8B)-C(3B)-C(4B)	174.3(10)
C(1B)-N(1B)-C(3B)-C(8B)	-165.8(9)
Pd(2)-N(1B)-C(3B)-C(8B)	7.3(13)

C(1B)-N(1B)-C(3B)-C(4B)	17.9(14)
Pd(2)-N(1B)-C(3B)-C(4B)	-169.1(8)
C(8B)-C(3B)-C(4B)-C(5B)	2.0(17)
N(1B)-C(3B)-C(4B)-C(5B)	178.5(11)
C(8B)-C(7B)-C(6B)-C(5B)	0(2)
C(3B)-C(4B)-C(5B)-C(6B)	1(2)
C(7B)-C(6B)-C(5B)-C(4B)	-1(2)
OW-O(1B)-C(1B)-N(1B)	116.7(15)
K(1)#1-O(1B)-C(1B)-N(1B)	149.8(9)
OW-O(1B)-C(1B)-C(2B)	-62.5(18)
K(1)#1-O(1B)-C(1B)-C(2B)	-29.4(11)
OW-O(1B)-C(1B)-K(1)#1	-33.1(12)
C(3B)-N(1B)-C(1B)-O(1B)	10.1(16)
Pd(2)-N(1B)-C(1B)-O(1B)	-163.8(9)
C(3B)-N(1B)-C(1B)-C(2B)	-170.8(8)
Pd(2)-N(1B)-C(1B)-C(2B)	15.4(10)
C(3B)-N(1B)-C(1B)-K(1)#1	78.7(19)
Pd(2)-N(1B)-C(1B)-K(1)#1	-95.1(16)
O(2B)-C(2B)-C(1B)-O(1B)	-9.9(14)
N(2B)-C(2B)-C(1B)-O(1B)	171.1(9)
K(1)#1-C(2B)-C(1B)-O(1B)	21.6(8)
O(2B)-C(2B)-C(1B)-N(1B)	170.8(9)
N(2B)-C(2B)-C(1B)-N(1B)	-8.2(12)
K(1)#1-C(2B)-C(1B)-N(1B)	-157.7(8)
O(2B)-C(2B)-C(1B)-K(1)#1	-31.5(8)
N(2B)-C(2B)-C(1B)-K(1)#1	149.5(8)
Pd(1)-O(3A)-C(9A)-O(4A)	179.1(9)
K(1)-O(3A)-C(9A)-O(4A)	-32.8(13)
Pd(1)-O(3A)-C(9A)-C(8A)	-0.2(18)
K(1)-O(3A)-C(9A)-C(8A)	147.9(10)
Pd(1)-O(3A)-C(9A)-K(1)	-148.1(10)
K(1)-O(4A)-C(9A)-O(3A)	31.2(12)
K(1)-O(4A)-C(9A)-C(8A)	-149.4(9)
C(7A)-C(8A)-C(9A)-O(3A)	176.0(12)
C(3A)-C(8A)-C(9A)-O(3A)	-0.4(19)
C(7A)-C(8A)-C(9A)-O(4A)	-3.4(17)

C(3A)-C(8A)-C(9A)-O(4A)	-179.8(11)
C(7A)-C(8A)-C(9A)-K(1)	-93.6(19)
C(3A)-C(8A)-C(9A)-K(1)	90(2)
OW#1-K(1)-C(9A)-O(3A)	28.5(8)
O(1B)#1-K(1)-C(9A)-O(3A)	-11.0(8)
O(1A)#1-K(1)-C(9A)-O(3A)	53.0(7)
O(2B)#1-K(1)-C(9A)-O(3A)	-73.6(7)
O(3B)#2-K(1)-C(9A)-O(3A)	178.2(9)
O(2A)#1-K(1)-C(9A)-O(3A)	109.6(7)
O(4B)#2-K(1)-C(9A)-O(3A)	-154.3(7)
O(4A)-K(1)-C(9A)-O(3A)	-148.4(13)
C(9B)#2-K(1)-C(9A)-O(3A)	-152.4(7)
C(2B)#1-K(1)-C(9A)-O(3A)	-62.6(8)
OW#1-K(1)-C(9A)-O(4A)	176.9(9)
O(1B)#1-K(1)-C(9A)-O(4A)	137.4(8)
O(1A)#1-K(1)-C(9A)-O(4A)	-158.6(8)
O(2B)#1-K(1)-C(9A)-O(4A)	74.8(9)
O(3B)#2-K(1)-C(9A)-O(4A)	-33.4(16)
O(2A)#1-K(1)-C(9A)-O(4A)	-102.0(8)
O(3A)-K(1)-C(9A)-O(4A)	148.4(13)
O(4B)#2-K(1)-C(9A)-O(4A)	-5.9(9)
C(9B)#2-K(1)-C(9A)-O(4A)	-4.0(11)
C(2B)#1-K(1)-C(9A)-O(4A)	85.8(9)
OW#1-K(1)-C(9A)-C(8A)	-79.1(19)
O(1B)#1-K(1)-C(9A)-C(8A)	-118.7(18)
O(1A)#1-K(1)-C(9A)-C(8A)	-54.6(18)
O(2B)#1-K(1)-C(9A)-C(8A)	178.7(18)
O(3B)#2-K(1)-C(9A)-C(8A)	71(2)
O(2A)#1-K(1)-C(9A)-C(8A)	1.9(18)
O(3A)-K(1)-C(9A)-C(8A)	-108(2)
O(4B)#2-K(1)-C(9A)-C(8A)	98.0(18)
O(4A)-K(1)-C(9A)-C(8A)	104(2)
C(9B)#2-K(1)-C(9A)-C(8A)	99.9(18)
C(2B)#1-K(1)-C(9A)-C(8A)	-170.3(17)
C(10A)-C(11A)-C(12A)-N(2A)	55.9(18)
C(2A)-N(2A)-C(12A)-C(11A)	155.5(12)

Pd(1)-N(2A)-C(12A)-C(11A)	-27.7(15)
C(12A)-C(11A)-C(10A)-N(3A)	-67.1(19)
Pd(1)-N(3A)-C(10A)-C(11A)	46.3(17)
C(8A)-C(7A)-C(6A)-C(5A)	4(2)
C(4A)-C(5A)-C(6A)-C(7A)	-4(2)
C(2B)-N(2B)-C(12B)-C(11B)	-180.0(14)
Pd(2)-N(2B)-C(12B)-C(11B)	-0.6(18)
N(2B)-C(12B)-C(11B)-C(10B)	-28(4)
C(12B)-C(11B)-C(10B)-N(3B)	33(5)
Pd(2)-N(3B)-C(10B)-C(11B)	-9(3)
C(1A)-O(1A)-OW-O(1B)	-135.8(18)
K(1)#1-O(1A)-OW-O(1B)	-160(2)
C(1A)-O(1A)-OW-K(1)#1	24(3)
C(1B)-O(1B)-OW-O(1A)	-148.6(16)
K(1)#1-O(1B)-OW-O(1A)	161(2)
C(1B)-O(1B)-OW-K(1)#1	50.6(18)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z-1 #2 x,y+1,z-1 #3 x,y-1,z+1



Molecular structure of the complex with the non H atom numbering scheme with thermal ellipsoids at 30% probability level.



Drawing showing the crystal packing of KPdOBAP complex. Hydrogen atoms are omitted for clarity.

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