Inorganic Chemistry
including bioinorganic chemistry
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Table 1. Crystal data and structure refinement for **2**.

Identification code	arp
Empirical formula	C40 H96 Ga4 Na4 O18 P4
Formula weight	1359.89
Temperature	133(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 12.367(5) A alpha = 90 deg. b = 13.788(7) A beta = 102.339(14) deg. c = 19.498(8) A gamma = 90 deg.
Volume	3248(2) A^3
Z, Calculated density	2, 1.391 Mg/m^3
Absorption coefficient	1.823 mm^-1
F(000)	1416
Crystal size	0.20 x 0.20 x 0.10 mm
Theta range for data collection	2.24 to 26.41 deg.
Index ranges	-15<=h<=15, 0<=k<=17, 0<=l<=24
Reflections collected / unique	6639 / 6639 [R(int) = 0.0000]
Completeness to 2theta = 26.41	95.4%
Max. and min. transmission	0.8387 and 0.7119
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6639 / 261 / 379
Goodness-of-fit on F^2	1.227
Final R indices [I>2sigma(I)]	R1 = 0.0413, wR2 = 0.0765
R indices (all data)	R1 = 0.0521, wR2 = 0.0825
Largest diff. peak and hole	0.506 and -0.434 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ga(1)	7432(1)	7253(1)	-4710(1)	25(1)
Ga(2)	7321(1)	9174(1)	-6432(1)	24(1)
Na(1)	4054(1)	8227(1)	-4687(1)	29(1)
Na(2)	5170(1)	10359(1)	-4190(1)	26(1)
P(1)	7413(1)	9565(1)	-4812(1)	20(1)
P(2)	5564(1)	7693(1)	-6061(1)	25(1)
O(1)	5493(2)	8764(2)	-3800(1)	29(1)
O(2)	4737(2)	7961(2)	-5629(1)	29(1)
O(3)	5892(2)	8629(2)	-6413(1)	26(1)
O(4)	6605(2)	7176(2)	-5654(1)	31(1)
O(5)	6361(2)	10170(1)	-4971(1)	23(1)
O(6)	7198(2)	8592(1)	-4462(1)	24(1)
O(7)	7912(2)	9372(2)	-5450(1)	25(1)
C(1)	4926(3)	6868(2)	-6765(2)	32(1)
C(2)	5777(3)	6554(3)	-7188(2)	47(1)
C(3)	4504(4)	5971(3)	-6431(2)	49(1)
C(4)	3954(3)	7376(3)	-7252(2)	46(1)
C(5)	8465(2)	10215(2)	-4180(2)	25(1)
C(6)	8669(3)	11208(2)	-4486(2)	33(1)
C(7)	8072(3)	10360(3)	-3492(2)	33(1)
C(8)	9539(2)	9617(2)	-4035(2)	32(1)
C(9)	7010(3)	10482(3)	-6835(2)	38(1)
C(10)	8268(3)	8202(3)	-6748(2)	37(1)
C(15)	6628(3)	6500(2)	-4121(2)	41(1)
C(16)	8993(3)	7074(2)	-4742(2)	36(1)
O(11)	3144(2)	6936(2)	-4349(1)	50(1)
C(11)	2761(13)	6113(9)	-4750(6)	81(5)
C(12)	2125(17)	5535(12)	-4327(9)	69(5)
C(13)	2448(15)	5935(13)	-3605(8)	71(4)
C(14)	3343(9)	6625(7)	-3614(4)	62(2)
C(11')	2282(9)	6966(6)	-3928(6)	69(3)
C(12')	2089(16)	5955(11)	-3760(9)	82(5)
C(13')	2391(18)	5376(11)	-4330(12)	73(5)
C(14')	3243(12)	5983(7)	-4549(8)	79(4)
O(20)	6146(2)	8859(2)	-2385(1)	44(1)
C(20)	6152(4)	9837(3)	-2144(2)	57(1)
C(21)	5807(5)	9835(4)	-1467(3)	74(2)
C(22)	5288(6)	8859(5)	-1432(4)	52(2)
C(23)	5838(4)	8241(3)	-1880(2)	61(1)
C(22')	5800(2)	8799(10)	-1251(7)	105(12)

Table 3. Bond lengths [A] and angles [deg] for **2**.

Ga(1)-O(4)	1.908(2)
Ga(1)-O(6)	1.946(2)
Ga(1)-C(16)	1.962(3)
Ga(1)-C(15)	1.968(3)
Ga(2)-O(7)	1.917(2)
Ga(2)-O(3)	1.928(2)
Ga(2)-C(10)	1.964(3)
Ga(2)-C(9)	1.971(3)
Ga(2)-Na(2)#1	3.6011(16)
Na(1)-O(2)	2.210(3)
Na(1)-O(11)	2.276(3)
Na(1)-O(1)	2.322(3)
Na(1)-O(5)#1	2.334(3)
Na(1)-Na(2)#1	3.2285(19)
Na(1)-Na(2)	3.304(2)
Na(2)-O(1)	2.334(3)
Na(2)-O(5)#1	2.339(2)
Na(2)-O(5)	2.350(2)
Na(2)-O(2)#1	2.350(3)
Na(2)-O(3)#1	2.390(2)
Na(2)-P(2)#1	2.9103(18)
Na(2)-Na(1)#1	3.2285(19)
Na(2)-Na(2)#1	3.252(3)
Na(2)-P(1)#1	3.3684(17)
Na(2)-P(1)	3.4350(17)
Na(2)-Ga(2)#1	3.6012(16)
P(1)-O(5)	1.520(2)
P(1)-O(7)	1.526(2)
P(1)-O(6)	1.553(2)
P(1)-C(5)	1.824(3)
P(1)-Na(2)#1	3.3685(17)
P(2)-O(2)	1.504(2)
P(2)-O(4)	1.537(2)
P(2)-O(3)	1.555(2)
P(2)-C(1)	1.827(3)
P(2)-Na(2)#1	2.9103(19)
O(2)-Na(2)#1	2.350(3)
O(3)-Na(2)#1	2.390(2)
O(5)-Na(1)#1	2.334(3)
O(5)-Na(2)#1	2.339(2)
C(1)-C(4)	1.532(5)
C(1)-C(2)	1.532(5)
C(1)-C(3)	1.540(5)
C(5)-C(7)	1.536(4)
C(5)-C(8)	1.537(4)
C(5)-C(6)	1.537(4)
O(11)-C(14')	1.384(9)
O(11)-C(11)	1.402(10)
O(11)-C(14)	1.465(7)
O(11)-C(11')	1.478(7)
C(11)-C(12)	1.486(11)
C(12)-C(13)	1.484(13)
C(13)-C(14)	1.462(11)
C(11')-C(12')	1.463(12)
C(12')-C(13')	1.480(13)
C(13')-C(14')	1.479(12)
O(20)-C(23)	1.414(4)
O(20)-C(20)	1.428(4)
C(20)-C(21)	1.471(6)
C(21)-C(22')	1.490(14)
C(21)-C(22)	1.499(8)
C(22)-C(23)	1.485(8)
C(23)-C(22')	1.456(12)

O(4)-Ga(1)-O(6)	102.45(9)
O(4)-Ga(1)-C(16)	106.86(13)
O(6)-Ga(1)-C(16)	109.10(12)
O(4)-Ga(1)-C(15)	107.48(14)

O(6)-Ga(1)-C(15)	103.63(12)
C(16)-Ga(1)-C(15)	125.13(15)
O(7)-Ga(2)-O(3)	101.01(9)
O(7)-Ga(2)-C(10)	106.53(12)
O(3)-Ga(2)-C(10)	110.49(12)
O(7)-Ga(2)-C(9)	105.60(13)
O(3)-Ga(2)-C(9)	105.26(12)
C(10)-Ga(2)-C(9)	125.29(15)
O(7)-Ga(2)-Na(2)#1	79.00(7)
O(3)-Ga(2)-Na(2)#1	37.79(7)
C(10)-Ga(2)-Na(2)#1	146.91(11)
C(9)-Ga(2)-Na(2)#1	82.13(10)
O(2)-Na(1)-O(11)	114.30(10)
O(2)-Na(1)-O(1)	107.68(10)
O(11)-Na(1)-O(1)	112.41(11)
O(2)-Na(1)-O(5)#1	91.11(8)
O(11)-Na(1)-O(5)#1	136.93(11)
O(1)-Na(1)-O(5)#1	89.86(9)
O(2)-Na(1)-Na(2)#1	46.71(6)
O(11)-Na(1)-Na(2)#1	154.89(9)
O(1)-Na(1)-Na(2)#1	91.21(8)
O(5)#1-Na(1)-Na(2)#1	46.63(6)
O(2)-Na(1)-Na(2)	100.44(7)
O(11)-Na(1)-Na(2)	144.28(9)
O(1)-Na(1)-Na(2)	44.94(6)
O(5)#1-Na(1)-Na(2)	45.06(6)
Na(2)#1-Na(1)-Na(2)	59.69(5)
O(1)-Na(2)-O(5)#1	89.48(9)
O(1)-Na(2)-O(5)	91.12(9)
O(5)#1-Na(2)-O(5)	92.18(8)
O(1)-Na(2)-O(2)#1	165.39(10)
O(5)#1-Na(2)-O(2)#1	105.09(9)
O(5)-Na(2)-O(2)#1	87.36(8)
O(1)-Na(2)-O(3)#1	117.65(9)
O(5)#1-Na(2)-O(3)#1	94.47(8)
O(5)-Na(2)-O(3)#1	150.47(9)
O(2)#1-Na(2)-O(3)#1	63.13(8)
O(1)-Na(2)-P(2)#1	148.54(8)
O(5)#1-Na(2)-P(2)#1	99.81(7)
O(5)-Na(2)-P(2)#1	118.21(7)
O(2)#1-Na(2)-P(2)#1	30.96(6)
O(3)#1-Na(2)-P(2)#1	32.26(5)
O(1)-Na(2)-Na(1)#1	137.36(8)
O(5)#1-Na(2)-Na(1)#1	91.58(7)
O(5)-Na(2)-Na(1)#1	46.23(6)
O(2)#1-Na(2)-Na(1)#1	43.20(6)
O(3)#1-Na(2)-Na(1)#1	104.77(7)
P(2)#1-Na(2)-Na(1)#1	72.84(5)
O(1)-Na(2)-Na(2)#1	90.44(8)
O(5)#1-Na(2)-Na(2)#1	46.23(6)
O(5)-Na(2)-Na(2)#1	45.95(6)
O(2)#1-Na(2)-Na(2)#1	98.85(8)
O(3)#1-Na(2)-Na(2)#1	133.22(8)
P(2)#1-Na(2)-Na(2)#1	117.65(6)
Na(1)#1-Na(2)-Na(2)#1	61.31(5)
O(1)-Na(2)-Na(1)	44.66(7)
O(5)#1-Na(2)-Na(1)	44.96(6)
O(5)-Na(2)-Na(1)	89.52(6)
O(2)#1-Na(2)-Na(1)	149.75(8)
O(3)#1-Na(2)-Na(1)	115.15(7)
P(2)#1-Na(2)-Na(1)	138.16(5)
Na(1)#1-Na(2)-Na(1)	120.31(5)
Na(2)#1-Na(2)-Na(1)	59.00(4)
O(1)-Na(2)-P(1)#1	107.04(7)
O(5)#1-Na(2)-P(1)#1	22.97(5)
O(5)-Na(2)-P(1)#1	106.08(7)
O(2)#1-Na(2)-P(1)#1	87.31(6)
O(3)#1-Na(2)-P(1)#1	73.33(6)
P(2)#1-Na(2)-P(1)#1	77.13(3)
Na(1)#1-Na(2)-P(1)#1	88.38(4)
Na(2)#1-Na(2)-P(1)#1	62.49(4)
Na(1)-Na(2)-P(1)#1	64.73(4)
O(1)-Na(2)-P(1)	73.73(7)
O(5)#1-Na(2)-P(1)	104.36(7)

O(5)-Na(2)-P(1)	21.59(5)
O(2)#1-Na(2)-P(1)	101.05(6)
O(3)#1-Na(2)-P(1)	158.36(7)
P(2)#1-Na(2)-P(1)	131.13(4)
Na(1)#1-Na(2)-P(1)	64.74(4)
Na(2)#1-Na(2)-P(1)	60.43(4)
Na(1)-Na(2)-P(1)	86.06(4)
P(1)#1-Na(2)-P(1)	122.91(4)
O(1)-Na(2)-Ga(2)#1	99.09(7)
O(5)#1-Na(2)-Ga(2)#1	70.62(6)
O(5)-Na(2)-Ga(2)#1	159.75(7)
O(2)#1-Na(2)-Ga(2)#1	86.98(6)
O(3)#1-Na(2)-Ga(2)#1	29.63(5)
P(2)#1-Na(2)-Ga(2)#1	57.21(3)
Na(1)#1-Na(2)-Ga(2)#1	121.34(4)
Na(2)#1-Na(2)-Ga(2)#1	116.06(5)
Na(1)-Na(2)-Ga(2)#1	85.65(4)
P(1)#1-Na(2)-Ga(2)#1	54.23(3)
P(1)-Na(2)-Ga(2)#1	171.54(4)
O(5)-P(1)-O(7)	113.95(12)
O(5)-P(1)-O(6)	110.18(11)
O(7)-P(1)-O(6)	110.10(12)
O(5)-P(1)-C(5)	108.96(13)
O(7)-P(1)-C(5)	106.39(13)
O(6)-P(1)-C(5)	106.96(13)
O(5)-P(1)-Na(2)#1	36.91(8)
O(7)-P(1)-Na(2)#1	91.86(9)
O(6)-P(1)-Na(2)#1	92.91(8)
C(5)-P(1)-Na(2)#1	145.76(10)
O(5)-P(1)-Na(2)	34.67(8)
O(7)-P(1)-Na(2)	147.27(9)
O(6)-P(1)-Na(2)	83.89(8)
C(5)-P(1)-Na(2)	96.82(10)
Na(2)#1-P(1)-Na(2)	57.09(4)
O(2)-P(2)-O(4)	114.78(13)
O(2)-P(2)-O(3)	108.39(12)
O(4)-P(2)-O(3)	110.13(12)
O(2)-P(2)-C(1)	109.74(14)
O(4)-P(2)-C(1)	106.23(14)
O(3)-P(2)-C(1)	107.31(14)
O(2)-P(2)-Na(2)#1	53.48(8)
O(4)-P(2)-Na(2)#1	126.75(9)
O(3)-P(2)-Na(2)#1	55.12(8)
C(1)-P(2)-Na(2)#1	126.93(12)
Na(1)-O(1)-Na(2)	90.40(9)
P(2)-O(2)-Na(1)	158.93(15)
P(2)-O(2)-Na(2)#1	95.56(11)
Na(1)-O(2)-Na(2)#1	90.09(8)
P(2)-O(3)-Ga(2)	131.20(13)
P(2)-O(3)-Na(2)#1	92.62(10)
Ga(2)-O(3)-Na(2)#1	112.58(10)
P(2)-O(4)-Ga(1)	133.62(13)
P(1)-O(5)-Na(1)#1	134.78(12)
P(1)-O(5)-Na(2)#1	120.12(11)
Na(1)#1-O(5)-Na(2)#1	89.99(8)
P(1)-O(5)-Na(2)	123.74(12)
Na(1)#1-O(5)-Na(2)	87.14(8)
Na(2)#1-O(5)-Na(2)	87.82(8)
P(1)-O(6)-Ga(1)	131.48(12)
P(1)-O(7)-Ga(2)	134.84(13)
C(4)-C(1)-C(2)	109.5(3)
C(4)-C(1)-C(3)	109.7(3)
C(2)-C(1)-C(3)	109.6(3)
C(4)-C(1)-P(2)	109.7(2)
C(2)-C(1)-P(2)	110.1(2)
C(3)-C(1)-P(2)	108.2(2)
C(7)-C(5)-C(8)	109.4(3)
C(7)-C(5)-C(6)	109.4(3)
C(8)-C(5)-C(6)	110.0(3)
C(7)-C(5)-P(1)	109.9(2)
C(8)-C(5)-P(1)	109.0(2)
C(6)-C(5)-P(1)	109.1(2)
C(14')-O(11)-C(11)	27.6(9)
C(14')-O(11)-C(14)	89.5(8)

C(11)-O(11)-C(14)	105.9(6)
C(14')-O(11)-C(11')	107.5(6)
C(11)-O(11)-C(11')	97.6(7)
C(14)-O(11)-C(11')	57.0(6)
C(14')-O(11)-Na(1)	125.6(6)
C(11)-O(11)-Na(1)	127.0(5)
C(14)-O(11)-Na(1)	121.5(3)
C(11')-O(11)-Na(1)	126.8(3)
O(11)-C(11)-C(12)	106.3(8)
C(13)-C(12)-C(11)	105.1(9)
C(14)-C(13)-C(12)	106.3(9)
C(13)-C(14)-O(11)	103.5(7)
C(12')-C(11')-O(11)	105.7(8)
C(11')-C(12')-C(13')	105.4(9)
C(14')-C(13')-C(12')	102.8(10)
O(11)-C(14')-C(13')	110.2(9)
C(23)-O(20)-C(20)	108.8(3)
O(20)-C(20)-C(21)	108.1(3)
C(20)-C(21)-C(22')	105.9(6)
C(20)-C(21)-C(22)	104.6(4)
C(22')-C(21)-C(22)	25.7(11)
C(23)-C(22)-C(21)	103.5(5)
O(20)-C(23)-C(22')	109.3(6)
O(20)-C(23)-C(22)	106.9(4)
C(22')-C(23)-C(22)	26.1(11)
C(23)-C(22')-C(21)	105.4(8)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+2,-z-1

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **2**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ga(1)	26(1)	20(1)	31(1)	1(1)	8(1)	1(1)
Ga(2)	23(1)	27(1)	24(1)	-1(1)	7(1)	0(1)
Na(1)	34(1)	23(1)	31(1)	0(1)	9(1)	-4(1)
Na(2)	24(1)	22(1)	32(1)	-1(1)	8(1)	0(1)
P(1)	19(1)	19(1)	23(1)	-1(1)	6(1)	-1(1)
P(2)	26(1)	20(1)	30(1)	-5(1)	7(1)	-2(1)
O(1)	26(1)	32(1)	31(1)	2(1)	11(1)	2(1)
O(2)	31(1)	23(1)	37(1)	-5(1)	13(1)	-4(1)
O(3)	25(1)	25(1)	30(1)	-3(1)	6(1)	-2(1)
O(4)	33(1)	24(1)	33(1)	-4(1)	4(1)	4(1)
O(5)	20(1)	20(1)	28(1)	-1(1)	6(1)	0(1)
O(6)	25(1)	20(1)	28(1)	1(1)	10(1)	-1(1)
O(7)	23(1)	28(1)	24(1)	-2(1)	7(1)	-2(1)
C(1)	35(2)	25(2)	37(2)	-9(1)	7(1)	-5(1)
C(2)	47(2)	52(2)	43(2)	-24(2)	13(2)	-4(2)
C(3)	62(3)	30(2)	55(2)	-10(2)	10(2)	-16(2)
C(4)	41(2)	38(2)	52(2)	-14(2)	-6(2)	-5(2)
C(5)	26(2)	26(2)	24(2)	0(1)	6(1)	-2(1)
C(6)	35(2)	26(2)	36(2)	-1(1)	2(1)	-9(1)
C(7)	37(2)	35(2)	27(2)	-6(1)	7(1)	-6(2)
C(8)	24(2)	37(2)	33(2)	1(1)	1(1)	-1(1)
C(9)	38(2)	39(2)	39(2)	10(2)	11(2)	-1(2)
C(10)	32(2)	45(2)	35(2)	-10(2)	10(1)	4(2)
C(15)	44(2)	29(2)	52(2)	8(2)	18(2)	0(2)
C(16)	31(2)	32(2)	46(2)	2(2)	10(2)	4(1)
O(11)	74(2)	33(1)	48(2)	2(1)	25(1)	-15(1)
C(11)	132(12)	67(8)	38(5)	-8(5)	8(6)	-52(8)
C(12)	84(9)	56(8)	60(7)	7(6)	-1(6)	-37(7)
C(13)	99(10)	65(7)	51(6)	9(5)	20(6)	-32(7)
C(14)	92(7)	56(5)	41(4)	-3(4)	21(4)	-27(5)
C(11')	102(7)	32(4)	93(7)	7(4)	69(6)	-3(4)
C(12')	106(11)	62(7)	95(11)	18(7)	60(9)	-13(7)
C(13')	101(11)	33(5)	82(9)	0(5)	18(8)	-19(6)
C(14')	95(9)	32(5)	132(12)	-4(6)	73(8)	7(5)
O(20)	62(2)	38(1)	33(1)	2(1)	12(1)	-2(1)
C(20)	79(3)	43(2)	50(2)	-4(2)	15(2)	-17(2)
C(21)	96(4)	64(3)	74(3)	-22(3)	42(3)	-17(3)
C(22)	55(4)	61(4)	42(4)	-6(3)	14(3)	-19(3)
C(23)	93(3)	44(2)	54(3)	10(2)	33(2)	-2(2)
C(22')	180(3)	101(19)	42(11)	-36(11)	49(16)	-100(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **2**.

	x	y	z	U(eq)
H(2)	5970(3)	8640(3)	-3925(19)	31(11)
H(1)	5790(3)	8670(3)	-3270(2)	62(13)
H(2A)	5444	6072	-7540	70
H(2B)	6422	6270	-6871	70
H(2C)	6011	7120	-7424	70
H(3A)	3948	6171	-6169	74
H(3B)	5125	5658	-6111	74
H(3C)	4171	5513	-6800	74
H(4A)	4229	7930	-7479	69
H(4B)	3427	7604	-6977	69
H(4C)	3583	6918	-7611	69
H(6A)	8019	11622	-4507	49
H(6B)	8802	11122	-4961	49
H(6C)	9317	11514	-4187	49
H(7A)	7900	9729	-3310	50
H(7B)	7407	10768	-3579	50
H(7C)	8658	10677	-3146	50
H(8A)	10107	9958	-3692	48
H(8B)	9797	9531	-4472	48
H(8C)	9398	8981	-3847	48
H(9A)	6392	10769	-6665	57
H(9B)	6815	10436	-7349	57
H(9C)	7669	10890	-6694	57
H(10A)	8926	8519	-6848	55
H(10B)	7856	7885	-7175	55
H(10C)	8494	7715	-6379	55
H(15A)	5855	6714	-4210	61
H(15B)	6972	6602	-3625	61
H(15C)	6657	5810	-4235	61
H(16A)	9089	6443	-4954	54
H(16B)	9447	7096	-4264	54
H(16C)	9225	7591	-5024	54
H(11A)	3390	5731	-4845	97
H(11B)	2279	6304	-5203	97
H(12A)	1319	5607	-4512	83
H(12B)	2321	4839	-4332	83
H(13A)	1812	6265	-3473	85
H(13B)	2705	5410	-3263	85
H(14A)	4076	6309	-3470	74
H(14B)	3305	7181	-3299	74
H(11C)	2539	7348	-3494	82
H(11D)	1594	7263	-4201	82
H(12C)	1303	5852	-3744	98
H(12D)	2556	5774	-3299	98
H(13C)	2695	4736	-4156	87
H(13D)	1745	5278	-4721	87
H(14C)	3989	5736	-4330	95
H(14D)	3155	5948	-5065	95
H(20A)	5636	10235	-2490	68
H(20B)	6904	10115	-2086	68
H(21A)	5267	10359	-1451	89
H(21B)	6453	9922	-1073	89
H(21C)	5060	10121	-1519	89
H(21D)	6333	10214	-1114	89
H(22A)	5433	8614	-943	63
H(22B)	4479	8885	-1618	63
H(23A)	6500	7924	-1593	73
H(23B)	5324	7733	-2114	73
H(23C)	6381	7707	-1763	73
H(23D)	5102	7955	-2072	73
H(22C)	6457	8654	-874	126
H(22D)	5125	8647	-1080	126

Table 6. Crystal data and structure refinement for **3**.

Identification code	kgp
Empirical formula	C68 H154 Ga6 K6 O26 P6
Formula weight	2226.65
Temperature	133(2) K
Wavelength	0.71073 A
Crystal system, space group	hexagonal, P6(3)22
Unit cell dimensions	a = 17.812(3) A alpha = 90 deg. b = 17.812(3) A beta = 90 deg. c = 39.241(5) A gamma = 120 deg.
Volume	10782(3) A^3
Z, Calculated density	4, 1.372 Mg/m^3
Absorption coefficient	1.858 mm^-1
F(000)	4640
Crystal size	0.50 x 0.40 x 0.30 mm
Theta range for data collection	2.04 to 26.54 deg.
Index ranges	-18<=h<=0, 0<=k<=22, 0<=l<=49
Reflections collected / unique	7504 / 7504 [R(int) = 0.0000]
Completeness to 2theta = 26.54	99.8%
Max. and min. transmission	0.6056 and 0.4568
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7504 / 738 / 462
Goodness-of-fit on F^2	1.328
Final R indices [I>2sigma(I)]	R1 = 0.0564, wR2 = 0.1023
R indices (all data)	R1 = 0.0590, wR2 = 0.1033
Absolute structure parameter	0.031(15)
Largest diff. peak and hole	0.405 and -0.344 e.A^-3

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ga(1)	-3389(1)	-1352(1)	-4867(1)	39(1)
K(1)	-1268(1)	-1268(1)	-5000	32(1)
P(1)	-2138(1)	-329(1)	-5475(1)	33(1)
O(1)	-2639(2)	-1139(2)	-5250(1)	34(1)
C(1)	-2516(4)	-681(4)	-5911(1)	46(1)
O(2)	-1179(2)	5(2)	-5450(1)	34(1)
C(2)	-1979(5)	101(5)	-6149(1)	65(2)
Ga(2)	-9396(1)	-2946(1)	-2638(1)	51(1)
K(2)	-8129(1)	-4064(1)	-2500	28(1)
P(2)	-8093(1)	-5607(1)	-2974(1)	38(1)
C(3)	-2398(4)	-1446(4)	-6009(1)	51(2)
K(3)	0	0	-5832(1)	37(1)
O(3)	-2416(2)	335(2)	-5395(1)	41(1)
K(4)	-6667	-3333	-3331(1)	40(1)
C(4)	-3464(4)	-934(5)	-5936(2)	69(2)
C(5)	-4432(3)	-1316(4)	-5003(2)	61(2)
O(11)	-8858(2)	-3135(2)	-2248(1)	39(1)
C(6)	-3385(5)	-2322(4)	-4625(2)	54(2)
O(12)	-7343(2)	-4701(2)	-2948(1)	32(1)
O(13)	-8437(2)	-2114(3)	-2890(1)	50(1)
C(11)	-8496(4)	-5824(4)	-3413(2)	58(2)
C(12)	-8860(5)	-5238(5)	-3505(2)	76(2)
C(13)	-7731(5)	-5656(5)	-3647(2)	71(2)
C(14)	-9209(5)	-6768(5)	-3446(2)	81(2)
C(15)	-10023(5)	-2352(5)	-2500(3)	92(3)
C(16)	-9896(5)	-4045(4)	-2892(2)	66(2)
K(5)	-3333	3333	-3734(1)	84(1)
O(20)	-3206(11)	4563(9)	-3300(3)	134(4)
C(21)	-2528(14)	5368(11)	-3351(5)	134(4)
C(22)	-2310(12)	5836(11)	-3045(4)	129(4)
C(23)	-3145(13)	5403(12)	-2848(4)	129(4)
C(24)	-3493(14)	4552(11)	-2947(4)	131(4)
O(20')	-3037(16)	4418(12)	-3226(5)	129(4)
C(21')	-2306(16)	5180(15)	-3296(9)	124(4)
C(22')	-2447(19)	5858(13)	-3212(7)	125(5)
C(23')	-3306(18)	5443(16)	-3025(7)	125(4)
C(24')	-3658(17)	4562(15)	-3057(8)	130(4)
O(30)	-4271(4)	1884(4)	-4118(1)	82(2)
C(31)	-4634(6)	988(5)	-4060(2)	90(2)
C(32)	-5424(9)	582(10)	-4241(4)	92(4)
C(33)	-5262(5)	1145(5)	-4551(2)	87(2)
C(34)	-4595(5)	1995(5)	-4430(2)	73(2)
C(32')	-5110(12)	507(8)	-4346(4)	92(4)
O(40)	60(2)	-20(5)	-6512(2)	98(6)
C(41)	-670(2)	-180(5)	-6713(5)	122(10)
C(42)	-340(3)	100(5)	-7040(6)	138(11)
C(43)	370(3)	-140(4)	-7060(5)	129(10)
C(44)	714(19)	50(4)	-6731(5)	102(9)
O(50)	-6610(6)	-3390(7)	-4034(2)	87(5)
C(51)	-6190(3)	-3750(3)	-4219(5)	101(7)
C(52)	-6020(2)	-3360(2)	-4540(5)	111(10)
C(53)	-6700(3)	-3110(4)	-4595(5)	124(12)
C(54)	-7070(3)	-3180(4)	-4271(6)	112(9)

Table 8. Bond lengths [A] and angles [deg] for **3**.

Ga(1)-O(3)#1	1.889(3)
Ga(1)-O(1)	1.919(3)
Ga(1)-C(5)	1.964(5)
Ga(1)-C(6)	1.975(6)
Ga(1)-K(1)	3.7422(12)
K(1)-O(1)	2.744(3)
K(1)-O(1)#2	2.744(3)
K(1)-O(2)#1	2.804(3)
K(1)-O(2)#3	2.805(3)
K(1)-O(2)#2	2.816(3)
K(1)-O(2)	2.816(3)
K(1)-P(1)	3.3556(13)
K(1)-P(1)#2	3.3556(13)
K(1)-Ga(1)#2	3.7422(12)
K(1)-K(1)#4	3.913(3)
K(1)-K(1)#3	3.913(3)
P(1)-O(2)	1.505(4)
P(1)-O(3)	1.526(4)
P(1)-O(1)	1.540(4)
P(1)-C(1)	1.833(5)
P(1)-K(3)	3.8182(16)
C(1)-C(4)	1.518(9)
C(1)-C(3)	1.528(8)
C(1)-C(2)	1.547(9)
O(2)-K(3)	2.584(4)
O(2)-K(1)#4	2.804(3)
Ga(2)-O(13)	1.887(4)
Ga(2)-O(11)	1.922(4)
Ga(2)-C(15)	1.961(6)
Ga(2)-C(16)	1.968(6)
Ga(2)-K(2)	3.7219(12)
K(2)-O(11)	2.747(3)
K(2)-O(11)#5	2.747(3)
K(2)-O(12)#6	2.795(3)
K(2)-O(12)#7	2.795(3)
K(2)-O(12)#5	2.814(3)
K(2)-O(12)	2.814(3)
K(2)-P(2)#5	3.3445(14)
K(2)-P(2)	3.3444(14)
K(2)-C(16)#5	3.519(7)
K(2)-Ga(2)#5	3.7218(11)
K(2)-K(2)#6	3.907(2)
P(2)-O(12)	1.497(3)
P(2)-O(13)#8	1.530(4)
P(2)-O(11)#5	1.542(4)
P(2)-C(11)	1.832(6)
P(2)-K(4)	3.8120(17)
K(3)-O(2)#4	2.584(3)
K(3)-O(2)#3	2.584(4)
K(3)-O(40)	2.670(8)
K(3)-O(40)#4	2.670(8)
K(3)-O(40)#3	2.670(8)
K(3)-P(1)#4	3.8182(16)
K(3)-P(1)#3	3.8183(16)
K(3)-K(1)#4	3.9704(18)
K(3)-K(1)#3	3.9704(18)
O(3)-Ga(1)#1	1.889(3)
K(4)-O(12)#6	2.592(3)
K(4)-O(12)#8	2.592(3)
K(4)-O(12)	2.592(3)
K(4)-O(50)	2.761(10)
K(4)-O(50)#6	2.761(10)
K(4)-O(50)#8	2.761(10)

K(4)-P(2)#6	3.8119(17)
K(4)-P(2)#8	3.8119(17)
K(4)-K(2)#6	3.9658(17)
K(4)-K(2)#8	3.9658(18)
O(11)-P(2)#5	1.542(4)
O(12)-K(2)#8	2.795(3)
O(13)-P(2)#6	1.530(4)
C(11)-C(14)	1.523(9)
C(11)-C(12)	1.523(10)
C(11)-C(13)	1.544(9)
K(5)-O(20')#9	2.639(13)
K(5)-O(20')	2.639(13)
K(5)-O(20')#10	2.639(13)
K(5)-O(20)#9	2.694(10)
K(5)-O(20)#10	2.694(9)
K(5)-O(20)	2.694(10)
K(5)-O(30)	2.723(5)
K(5)-O(30)#10	2.723(5)
K(5)-O(30)#9	2.723(5)
K(5)-C(21')#9	3.33(3)
K(5)-C(21')#10	3.33(3)
K(5)-C(21')	3.33(3)
O(20)-C(21)	1.350(12)
O(20)-C(24)	1.472(13)
C(21)-C(22)	1.401(14)
C(22)-C(23)	1.503(14)
C(23)-C(24)	1.376(13)
O(20')-C(21')	1.359(13)
O(20')-C(24')	1.420(14)
C(21')-C(22')	1.391(15)
C(22')-C(23')	1.514(15)
C(23')-C(24')	1.373(14)
O(30)-C(34)	1.408(7)
O(30)-C(31)	1.409(8)
C(31)-C(32')	1.410(12)
C(31)-C(32)	1.411(12)
C(32)-C(33)	1.509(13)
C(33)-C(34)	1.460(9)
C(33)-C(32')	1.523(13)
O(40)-C(44)	1.411(13)
O(40)-C(41)	1.413(14)
C(41)-C(42)	1.393(16)
C(42)-C(43)	1.535(17)
C(43)-C(44)	1.392(15)
O(50)-C(54)	1.411(14)
O(50)-C(51)	1.412(14)
C(51)-C(52)	1.394(14)
C(52)-C(53)	1.515(17)
C(53)-C(54)	1.407(14)

O(3)#1-Ga(1)-O(1)	102.20(14)
O(3)#1-Ga(1)-C(5)	104.1(2)
O(1)-Ga(1)-C(5)	110.9(2)
O(3)#1-Ga(1)-C(6)	108.3(2)
O(1)-Ga(1)-C(6)	104.0(2)
C(5)-Ga(1)-C(6)	125.2(3)
O(3)#1-Ga(1)-K(1)	85.78(11)
O(1)-Ga(1)-K(1)	45.00(10)
C(5)-Ga(1)-K(1)	155.9(2)
C(6)-Ga(1)-K(1)	69.9(2)
O(1)-K(1)-O(1)#2	132.49(15)
O(1)-K(1)-O(2)#1	81.39(9)
O(1)#2-K(1)-O(2)#1	119.61(9)
O(1)-K(1)-O(2)#3	119.62(9)
O(1)#2-K(1)-O(2)#3	81.39(9)
O(2)#1-K(1)-O(2)#3	129.37(15)
O(1)-K(1)-O(2)#2	160.78(9)

O(1)#2-K(1)-O(2)#2	53.34(10)
O(2)#1-K(1)-O(2)#2	80.89(14)
O(2)#3-K(1)-O(2)#2	77.86(11)
O(1)-K(1)-O(2)	53.34(10)
O(1)#2-K(1)-O(2)	160.78(9)
O(2)#1-K(1)-O(2)	77.87(11)
O(2)#3-K(1)-O(2)	80.89(14)
O(2)#2-K(1)-O(2)	128.94(15)
O(1)-K(1)-P(1)	26.93(7)
O(1)#2-K(1)-P(1)	155.00(9)
O(2)#1-K(1)-P(1)	78.62(7)
O(2)#3-K(1)-P(1)	100.47(7)
O(2)#2-K(1)-P(1)	151.62(9)
O(2)-K(1)-P(1)	26.42(7)
O(1)-K(1)-P(1)#2	155.00(9)
O(1)#2-K(1)-P(1)#2	26.92(7)
O(2)#1-K(1)-P(1)#2	100.47(7)
O(2)#3-K(1)-P(1)#2	78.62(7)
O(2)#2-K(1)-P(1)#2	26.42(7)
O(2)-K(1)-P(1)#2	151.63(9)
P(1)-K(1)-P(1)#2	177.91(7)
O(1)-K(1)-Ga(1)	29.63(7)
O(1)#2-K(1)-Ga(1)	116.53(8)
O(2)#1-K(1)-Ga(1)	65.89(7)
O(2)#3-K(1)-Ga(1)	148.99(7)
O(2)#2-K(1)-Ga(1)	133.10(7)
O(2)-K(1)-Ga(1)	76.63(7)
P(1)-K(1)-Ga(1)	52.33(3)
P(1)#2-K(1)-Ga(1)	129.06(4)
O(1)-K(1)-Ga(1)#2	116.53(8)
O(1)#2-K(1)-Ga(1)#2	29.63(7)
O(2)#1-K(1)-Ga(1)#2	148.98(7)
O(2)#3-K(1)-Ga(1)#2	65.89(7)
O(2)#2-K(1)-Ga(1)#2	76.63(7)
O(2)-K(1)-Ga(1)#2	133.10(7)
P(1)-K(1)-Ga(1)#2	129.07(4)
P(1)#2-K(1)-Ga(1)#2	52.33(3)
Ga(1)-K(1)-Ga(1)#2	116.73(4)
O(1)-K(1)-K(1)#4	85.84(8)
O(1)#2-K(1)-K(1)#4	140.38(8)
O(2)#1-K(1)-K(1)#4	46.00(7)
O(2)#3-K(1)-K(1)#4	87.36(8)
O(2)#2-K(1)-K(1)#4	87.20(8)
O(2)-K(1)-K(1)#4	45.76(7)
P(1)-K(1)-K(1)#4	64.44(3)
P(1)#2-K(1)-K(1)#4	113.57(3)
Ga(1)-K(1)-K(1)#4	91.97(2)
Ga(1)#2-K(1)-K(1)#4	150.95(2)
O(1)-K(1)-K(1)#3	140.38(8)
O(1)#2-K(1)-K(1)#3	85.84(7)
O(2)#1-K(1)-K(1)#3	87.36(8)
O(2)#3-K(1)-K(1)#3	46.00(7)
O(2)#2-K(1)-K(1)#3	45.76(7)
O(2)-K(1)-K(1)#3	87.20(8)
P(1)-K(1)-K(1)#3	113.57(3)
P(1)#2-K(1)-K(1)#3	64.44(3)
Ga(1)-K(1)-K(1)#3	150.95(2)
Ga(1)#2-K(1)-K(1)#3	91.97(2)
K(1)#4-K(1)-K(1)#3	60.0
O(2)-P(1)-O(3)	115.0(2)
O(2)-P(1)-O(1)	110.18(19)
O(3)-P(1)-O(1)	110.4(2)
O(2)-P(1)-C(1)	110.2(2)
O(3)-P(1)-C(1)	104.5(2)
O(1)-P(1)-C(1)	106.0(2)
O(2)-P(1)-K(1)	56.36(13)
O(3)-P(1)-K(1)	133.04(14)

O(1)-P(1)-K(1)	53.83(13)
C(1)-P(1)-K(1)	122.06(19)
O(2)-P(1)-K(3)	27.80(13)
O(3)-P(1)-K(3)	129.87(16)
O(1)-P(1)-K(3)	114.87(14)
C(1)-P(1)-K(3)	82.9(2)
K(1)-P(1)-K(3)	66.85(4)
P(1)-O(1)-Ga(1)	130.9(2)
P(1)-O(1)-K(1)	99.25(17)
Ga(1)-O(1)-K(1)	105.36(13)
C(4)-C(1)-C(3)	110.4(5)
C(4)-C(1)-C(2)	109.0(5)
C(3)-C(1)-C(2)	110.7(5)
C(4)-C(1)-P(1)	108.9(4)
C(3)-C(1)-P(1)	110.4(4)
C(2)-C(1)-P(1)	107.5(4)
P(1)-O(2)-K(3)	136.43(19)
P(1)-O(2)-K(1)#4	127.23(18)
K(3)-O(2)-K(1)#4	94.83(11)
P(1)-O(2)-K(1)	97.23(16)
K(3)-O(2)-K(1)	94.56(11)
K(1)#4-O(2)-K(1)	88.23(10)
O(13)-Ga(2)-O(11)	102.65(15)
O(13)-Ga(2)-C(15)	104.9(3)
O(11)-Ga(2)-C(15)	110.1(3)
O(13)-Ga(2)-C(16)	107.3(3)
O(11)-Ga(2)-C(16)	104.2(2)
C(15)-Ga(2)-C(16)	125.5(3)
O(13)-Ga(2)-K(2)	86.73(11)
O(11)-Ga(2)-K(2)	45.66(10)
C(15)-Ga(2)-K(2)	155.6(3)
C(16)-Ga(2)-K(2)	68.6(2)
O(11)-K(2)-O(11)#5	131.70(14)
O(11)-K(2)-O(12)#6	81.58(10)
O(11)#5-K(2)-O(12)#6	119.62(11)
O(11)-K(2)-O(12)#7	119.63(11)
O(11)#5-K(2)-O(12)#7	81.58(10)
O(12)#6-K(2)-O(12)#7	129.68(14)
O(11)-K(2)-O(12)#5	53.51(10)
O(11)#5-K(2)-O(12)#5	161.31(10)
O(12)#6-K(2)-O(12)#5	77.56(11)
O(12)#7-K(2)-O(12)#5	81.32(14)
O(11)-K(2)-O(12)	161.31(10)
O(11)#5-K(2)-O(12)	53.50(10)
O(12)#6-K(2)-O(12)	81.32(14)
O(12)#7-K(2)-O(12)	77.56(11)
O(12)#5-K(2)-O(12)	128.97(14)
O(11)-K(2)-P(2)#5	27.12(8)
O(11)#5-K(2)-P(2)#5	154.63(9)
O(12)#6-K(2)-P(2)#5	78.54(7)
O(12)#7-K(2)-P(2)#5	100.64(8)
O(12)#5-K(2)-P(2)#5	26.39(7)
O(12)-K(2)-P(2)#5	151.84(8)
O(11)-K(2)-P(2)	154.62(9)
O(11)#5-K(2)-P(2)	27.12(8)
O(12)#6-K(2)-P(2)	100.64(8)
O(12)#7-K(2)-P(2)	78.54(7)
O(12)#5-K(2)-P(2)	151.84(8)
O(12)-K(2)-P(2)	26.39(7)
P(2)#5-K(2)-P(2)	178.11(7)
O(11)-K(2)-C(16)#5	84.81(13)
O(11)#5-K(2)-C(16)#5	57.08(14)
O(12)#6-K(2)-C(16)#5	154.38(14)
O(12)#7-K(2)-C(16)#5	75.94(13)
O(12)#5-K(2)-C(16)#5	111.05(14)
O(12)-K(2)-C(16)#5	107.96(12)
P(2)#5-K(2)-C(16)#5	98.62(12)

P(2)-K(2)-C(16)#5	82.86(12)
O(11)-K(2)-Ga(2)	30.02(8)
O(11)#5-K(2)-Ga(2)	115.85(8)
O(12)#6-K(2)-Ga(2)	65.54(7)
O(12)#7-K(2)-Ga(2)	149.40(7)
O(12)#5-K(2)-Ga(2)	76.74(7)
O(12)-K(2)-Ga(2)	133.00(7)
P(2)#5-K(2)-Ga(2)	52.61(3)
P(2)-K(2)-Ga(2)	128.64(4)
C(16)#5-K(2)-Ga(2)	92.29(11)
O(11)-K(2)-Ga(2)#5	115.85(8)
O(11)#5-K(2)-Ga(2)#5	30.02(8)
O(12)#6-K(2)-Ga(2)#5	149.40(7)
O(12)#7-K(2)-Ga(2)#5	65.53(7)
O(12)#5-K(2)-Ga(2)#5	133.00(7)
O(12)-K(2)-Ga(2)#5	76.74(7)
P(2)#5-K(2)-Ga(2)#5	128.64(4)
P(2)-K(2)-Ga(2)#5	52.61(3)
C(16)#5-K(2)-Ga(2)#5	31.37(11)
Ga(2)-K(2)-Ga(2)#5	116.62(4)
O(11)-K(2)-K(2)#6	86.27(7)
O(11)#5-K(2)-K(2)#6	140.68(8)
O(12)#6-K(2)-K(2)#6	46.06(7)
O(12)#7-K(2)-K(2)#6	87.56(7)
O(12)#5-K(2)-K(2)#6	45.66(7)
O(12)-K(2)-K(2)#6	87.30(7)
P(2)#5-K(2)-K(2)#6	64.55(3)
P(2)-K(2)-K(2)#6	113.65(3)
C(16)#5-K(2)-K(2)#6	154.10(13)
Ga(2)-K(2)-K(2)#6	92.05(2)
Ga(2)#5-K(2)-K(2)#6	150.94(2)
O(12)-P(2)-O(13)#8	115.2(2)
O(12)-P(2)-O(11)#5	110.96(19)
O(13)#8-P(2)-O(11)#5	109.4(2)
O(12)-P(2)-C(11)	109.7(3)
O(13)#8-P(2)-C(11)	105.0(3)
O(11)#5-P(2)-C(11)	106.1(3)
O(12)-P(2)-K(2)	56.65(13)
O(13)#8-P(2)-K(2)	132.57(17)
O(11)#5-P(2)-K(2)	54.32(12)
C(11)-P(2)-K(2)	122.0(2)
O(12)-P(2)-K(4)	28.28(14)
O(13)#8-P(2)-K(4)	130.82(16)
O(11)#5-P(2)-K(4)	115.15(14)
C(11)-P(2)-K(4)	82.0(2)
K(2)-P(2)-K(4)	66.94(4)
O(2)-K(3)-O(2)#4	89.72(11)
O(2)-K(3)-O(2)#3	89.72(11)
O(2)#4-K(3)-O(2)#3	89.72(11)
O(2)-K(3)-O(40)	128.0(5)
O(2)#4-K(3)-O(40)	124.8(13)
O(2)#3-K(3)-O(40)	123.5(14)
O(2)-K(3)-O(40)#4	123.5(14)
O(2)#4-K(3)-O(40)#4	128.0(5)
O(2)#3-K(3)-O(40)#4	124.8(13)
O(40)-K(3)-O(40)#4	4.6(12)
O(2)-K(3)-O(40)#3	124.8(13)
O(2)#4-K(3)-O(40)#3	123.6(14)
O(2)#3-K(3)-O(40)#3	128.0(5)
O(40)-K(3)-O(40)#3	4.6(12)
O(40)#4-K(3)-O(40)#3	4.6(12)
O(2)-K(3)-P(1)#4	93.75(8)
O(2)#4-K(3)-P(1)#4	15.76(7)
O(2)#3-K(3)-P(1)#4	104.96(9)
O(40)-K(3)-P(1)#4	111.2(14)
O(40)#4-K(3)-P(1)#4	113.9(5)
O(40)#3-K(3)-P(1)#4	109.4(13)

O(2)-K(3)-P(1)	15.76(7)
O(2)#4-K(3)-P(1)	104.96(9)
O(2)#3-K(3)-P(1)	93.74(8)
O(40)-K(3)-P(1)	113.9(5)
O(40)#4-K(3)-P(1)	109.4(13)
O(40)#3-K(3)-P(1)	111.2(14)
P(1)#4-K(3)-P(1)	107.33(3)
O(2)-K(3)-P(1)#3	104.96(9)
O(2)#4-K(3)-P(1)#3	93.74(8)
O(2)#3-K(3)-P(1)#3	15.76(7)
O(40)-K(3)-P(1)#3	109.4(13)
O(40)#4-K(3)-P(1)#3	111.2(14)
O(40)#3-K(3)-P(1)#3	113.9(5)
P(1)#4-K(3)-P(1)#3	107.33(3)
P(1)-K(3)-P(1)#3	107.33(3)
O(2)-K(3)-K(1)#4	44.74(8)
O(2)#4-K(3)-K(1)#4	44.99(8)
O(2)#3-K(3)-K(1)#4	89.22(9)
O(40)-K(3)-K(1)#4	147.2(14)
O(40)#4-K(3)-K(1)#4	145.9(14)
O(40)#3-K(3)-K(1)#4	142.8(5)
P(1)#4-K(3)-K(1)#4	51.00(3)
P(1)-K(3)-K(1)#4	60.12(3)
P(1)#3-K(3)-K(1)#4	102.82(5)
O(2)-K(3)-K(1)	44.99(8)
O(2)#4-K(3)-K(1)	89.21(9)
O(2)#3-K(3)-K(1)	44.74(8)
O(40)-K(3)-K(1)	145.9(14)
O(40)#4-K(3)-K(1)	142.8(5)
O(40)#3-K(3)-K(1)	147.2(14)
P(1)#4-K(3)-K(1)	102.82(5)
P(1)-K(3)-K(1)	50.99(3)
P(1)#3-K(3)-K(1)	60.12(3)
K(1)#4-K(3)-K(1)	59.04(4)
O(2)-K(3)-K(1)#3	89.22(9)
O(2)#4-K(3)-K(1)#3	44.73(8)
O(2)#3-K(3)-K(1)#3	44.99(8)
O(40)-K(3)-K(1)#3	142.8(5)
O(40)#4-K(3)-K(1)#3	147.2(14)
O(40)#3-K(3)-K(1)#3	145.9(14)
P(1)#4-K(3)-K(1)#3	60.12(3)
P(1)-K(3)-K(1)#3	102.82(5)
P(1)#3-K(3)-K(1)#3	51.00(3)
K(1)#4-K(3)-K(1)#3	59.04(4)
K(1)-K(3)-K(1)#3	59.04(4)
P(1)-O(3)-Ga(1)#1	139.1(2)
O(12)#6-K(4)-O(12)#8	89.67(11)
O(12)#6-K(4)-O(12)	89.66(11)
O(12)#8-K(4)-O(12)	89.66(11)
O(12)#6-K(4)-O(50)	129.0(6)
O(12)#8-K(4)-O(50)	123.7(18)
O(12)-K(4)-O(50)	124(2)
O(12)#6-K(4)-O(50)#6	124(2)
O(12)#8-K(4)-O(50)#6	129.0(6)
O(12)-K(4)-O(50)#6	123.7(18)
O(50)-K(4)-O(50)#6	6.0(10)
O(12)#6-K(4)-O(50)#8	123.7(18)
O(12)#8-K(4)-O(50)#8	124(2)
O(12)-K(4)-O(50)#8	129.0(6)
O(50)-K(4)-O(50)#8	6.0(10)
O(50)#6-K(4)-O(50)#8	6.0(11)
O(12)#6-K(4)-P(2)#6	15.88(7)
O(12)#8-K(4)-P(2)#6	93.49(8)
O(12)-K(4)-P(2)#6	105.08(8)
O(50)-K(4)-P(2)#6	115.0(8)
O(50)#6-K(4)-P(2)#6	110(2)
O(50)#8-K(4)-P(2)#6	109.4(16)

O(12)#6-K(4)-P(2)#8	105.08(8)
O(12)#8-K(4)-P(2)#8	15.88(7)
O(12)-K(4)-P(2)#8	93.49(8)
O(50)-K(4)-P(2)#8	109.4(16)
O(50)#6-K(4)-P(2)#8	115.0(8)
O(50)#8-K(4)-P(2)#8	110(2)
P(2)#6-K(4)-P(2)#8	107.28(4)
O(12)#6-K(4)-P(2)	93.48(8)
O(12)#8-K(4)-P(2)	105.08(8)
O(12)-K(4)-P(2)	15.88(7)
O(50)-K(4)-P(2)	110(2)
O(50)#6-K(4)-P(2)	109.4(16)
O(50)#8-K(4)-P(2)	115.0(8)
P(2)#6-K(4)-P(2)	107.28(4)
P(2)#8-K(4)-P(2)	107.28(4)
O(12)#6-K(4)-K(2)#6	45.05(7)
O(12)#8-K(4)-K(2)#6	44.62(7)
O(12)-K(4)-K(2)#6	89.16(9)
O(50)-K(4)-K(2)#6	147(2)
O(50)#6-K(4)-K(2)#6	147.0(19)
O(50)#8-K(4)-K(2)#6	141.9(6)
P(2)#6-K(4)-K(2)#6	50.89(3)
P(2)#8-K(4)-K(2)#6	60.17(3)
P(2)-K(4)-K(2)#6	102.75(5)
O(12)#6-K(4)-K(2)	44.62(7)
O(12)#8-K(4)-K(2)	89.16(9)
O(12)-K(4)-K(2)	45.05(8)
O(50)-K(4)-K(2)	147.0(19)
O(50)#6-K(4)-K(2)	141.9(6)
O(50)#8-K(4)-K(2)	147(2)
P(2)#6-K(4)-K(2)	60.17(3)
P(2)#8-K(4)-K(2)	102.75(5)
P(2)-K(4)-K(2)	50.89(3)
K(2)#6-K(4)-K(2)	59.01(4)
O(12)#6-K(4)-K(2)#8	89.16(9)
O(12)#8-K(4)-K(2)#8	45.05(7)
O(12)-K(4)-K(2)#8	44.62(7)
O(50)-K(4)-K(2)#8	141.9(6)
O(50)#6-K(4)-K(2)#8	147(2)
O(50)#8-K(4)-K(2)#8	147(2)
P(2)#6-K(4)-K(2)#8	102.75(5)
P(2)#8-K(4)-K(2)#8	50.89(3)
P(2)-K(4)-K(2)#8	60.17(3)
K(2)#6-K(4)-K(2)#8	59.01(4)
K(2)-K(4)-K(2)#8	59.01(4)
P(2)#5-O(11)-Ga(2)	130.5(2)
P(2)#5-O(11)-K(2)	98.56(16)
Ga(2)-O(11)-K(2)	104.33(14)
P(2)-O(12)-K(4)	135.8(2)
P(2)-O(12)-K(2)#8	128.08(19)
K(4)-O(12)-K(2)#8	94.73(10)
P(2)-O(12)-K(2)	96.96(17)
K(4)-O(12)-K(2)	94.28(10)
K(2)#8-O(12)-K(2)	88.28(10)
P(2)#6-O(13)-Ga(2)	138.1(2)
C(14)-C(11)-C(12)	109.4(6)
C(14)-C(11)-C(13)	109.3(5)
C(12)-C(11)-C(13)	111.2(7)
C(14)-C(11)-P(2)	109.6(5)
C(12)-C(11)-P(2)	109.5(4)
C(13)-C(11)-P(2)	107.7(4)
O(20')#9-K(5)-O(20')	69.1(8)
O(20')#9-K(5)-O(20')#10	69.1(8)
O(20')-K(5)-O(20')#10	69.1(8)
O(20')#9-K(5)-O(20)#9	12.1(9)
O(20')-K(5)-O(20)#9	72.3(7)
O(20')#10-K(5)-O(20)#9	81.3(6)

O(20')#9-K(5)-O(20)#10	72.3(7)
O(20')-K(5)-O(20)#10	81.3(6)
O(20')#10-K(5)-O(20)#10	12.1(9)
O(20)#9-K(5)-O(20)#10	84.3(5)
O(20')#9-K(5)-O(20)	81.3(6)
O(20')-K(5)-O(20)	12.1(9)
O(20')#10-K(5)-O(20)	72.3(7)
O(20)#9-K(5)-O(20)	84.3(5)
O(20)#10-K(5)-O(20)	84.3(5)
O(20')#9-K(5)-O(30)	111.3(5)
O(20')-K(5)-O(30)	156.3(5)
O(20')#10-K(5)-O(30)	88.6(6)
O(20)#9-K(5)-O(30)	113.4(4)
O(20)#10-K(5)-O(30)	76.7(4)
O(20)-K(5)-O(30)	152.1(4)
O(20')#9-K(5)-O(30)#10	88.6(6)
O(20')-K(5)-O(30)#10	111.3(5)
O(20')#10-K(5)-O(30)#10	156.3(5)
O(20)#9-K(5)-O(30)#10	76.7(4)
O(20)#10-K(5)-O(30)#10	152.1(4)
O(20)-K(5)-O(30)#10	113.4(4)
O(30)-K(5)-O(30)#10	92.31(17)
O(20')#9-K(5)-O(30)#9	156.3(5)
O(20')-K(5)-O(30)#9	88.6(6)
O(20')#10-K(5)-O(30)#9	111.3(5)
O(20)#9-K(5)-O(30)#9	152.1(4)
O(20)#10-K(5)-O(30)#9	113.4(4)
O(20)-K(5)-O(30)#9	76.7(4)
O(30)-K(5)-O(30)#9	92.31(17)
O(30)#10-K(5)-O(30)#9	92.31(17)
O(20')#9-K(5)-C(21')#9	22.7(4)
O(20')-K(5)-C(21')#9	91.7(7)
O(20')#10-K(5)-C(21')#9	74.0(8)
O(20)#9-K(5)-C(21')#9	24.4(6)
O(20)#10-K(5)-C(21')#9	72.1(7)
O(20)-K(5)-C(21')#9	103.8(5)
O(30)-K(5)-C(21')#9	89.7(4)
O(30)#10-K(5)-C(21')#9	82.4(6)
O(30)#9-K(5)-C(21')#9	174.4(6)
O(20')#9-K(5)-C(21')#10	91.7(7)
O(20')-K(5)-C(21')#10	74.0(8)
O(20')#10-K(5)-C(21')#10	22.7(4)
O(20)#9-K(5)-C(21')#10	103.8(5)
O(20)#10-K(5)-C(21')#10	24.4(6)
O(20)-K(5)-C(21')#10	72.1(7)
O(30)-K(5)-C(21')#10	82.4(6)
O(30)#10-K(5)-C(21')#10	174.4(6)
O(30)#9-K(5)-C(21')#10	89.7(4)
C(21')#9-K(5)-C(21')#10	95.8(7)
O(20')#9-K(5)-C(21')	73.9(8)
O(20')-K(5)-C(21')	22.7(4)
O(20')#10-K(5)-C(21')	91.7(7)
O(20)#9-K(5)-C(21')	72.1(7)
O(20)#10-K(5)-C(21')	103.8(5)
O(20)-K(5)-C(21')	24.4(6)
O(30)-K(5)-C(21')	174.4(6)
O(30)#10-K(5)-C(21')	89.7(4)
O(30)#9-K(5)-C(21')	82.4(6)
C(21')#9-K(5)-C(21')	95.8(7)
C(21')#10-K(5)-C(21')	95.8(7)
C(21)-O(20)-C(24)	105.9(10)
C(21)-O(20)-K(5)	115.9(10)
C(24)-O(20)-K(5)	134.1(11)
O(20)-C(21)-C(22)	109.8(12)
O(20)-C(21)-K(5)	43.8(7)
C(22)-C(21)-K(5)	146.4(14)
C(21)-C(22)-C(23)	103.1(11)

C(24)-C(23)-C(22)	101.8(11)
C(23)-C(24)-O(20)	106.8(11)
C(21')-O(20')-C(24')	111.0(13)
C(21')-O(20')-K(5)	108.6(15)
C(24')-O(20')-K(5)	126.6(18)
O(20')-C(21')-C(22')	108.7(14)
O(20')-C(21')-K(5)	48.6(11)
C(22')-C(21')-K(5)	137(2)
C(21')-C(22')-C(23')	105.5(12)
C(24')-C(23')-C(22')	106.7(12)
C(23')-C(24')-O(20')	107.3(13)
C(34)-O(30)-C(31)	108.1(6)
C(34)-O(30)-K(5)	116.6(4)
C(31)-O(30)-K(5)	134.5(5)
O(30)-C(31)-C(32')	110.9(8)
O(30)-C(31)-C(32)	106.0(8)
C(32')-C(31)-C(32)	31.2(11)
C(31)-C(32)-C(33)	104.7(9)
C(34)-C(33)-C(32)	102.3(7)
C(34)-C(33)-C(32')	104.2(7)
C(32)-C(33)-C(32')	29.0(10)
O(30)-C(34)-C(33)	108.4(6)
C(31)-C(32')-C(33)	104.1(9)
C(44)-O(40)-C(41)	108.1(10)
C(44)-O(40)-K(3)	130.1(14)
C(41)-O(40)-K(3)	121.6(14)
C(42)-C(41)-O(40)	105.6(15)
C(41)-C(42)-C(43)	101.9(17)
C(44)-C(43)-C(42)	102.0(17)
C(43)-C(44)-O(40)	107.6(14)
C(54)-O(50)-C(51)	107.1(15)
C(54)-O(50)-K(4)	128.0(15)
C(51)-O(50)-K(4)	124.4(14)
C(52)-C(51)-O(50)	106.2(19)
C(51)-C(52)-C(53)	105.2(14)
C(54)-C(53)-C(52)	105.1(12)
C(53)-C(54)-O(50)	108.0(15)

Symmetry transformations used to generate equivalent atoms:
#1 x-y,-y,-z-1 #2 y,x,-z-1 #3 -y,x-y,z
#4 -x+y,-x,z #5 x,x-y,-z-1/2 #6 -x+y-1,-x-1,z
#7 -x+y-1,y,-z-1/2 #8 -y-1,x-y,z
#9 -x+y-1,-x,z #10 -y,x-y+1,z

Table 9. Anisotropic displacement parameters (A^2 x 10^3) for **3**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ga(1)	29(1)	38(1)	44(1)	-5(1)	-1(1)	12(1)
K(1)	35(1)	35(1)	29(1)	1(1)	-1(1)	20(1)
P(1)	38(1)	35(1)	28(1)	-5(1)	-8(1)	21(1)
O(1)	36(2)	36(2)	31(2)	-7(1)	-4(1)	19(2)
C(1)	53(3)	55(3)	35(3)	-16(2)	-18(2)	32(3)
O(2)	38(2)	38(2)	25(2)	0(2)	-2(1)	19(2)
C(2)	93(5)	69(4)	36(3)	2(3)	-16(3)	44(4)
Ga(2)	23(1)	37(1)	96(1)	-1(1)	-6(1)	17(1)
K(2)	25(1)	23(1)	38(1)	-2(1)	0	13(1)
P(2)	30(1)	30(1)	54(1)	-18(1)	-11(1)	14(1)
C(3)	66(4)	54(4)	40(3)	-19(3)	-16(3)	35(3)
K(3)	43(1)	43(1)	23(1)	0	0	22(1)
O(3)	50(2)	44(2)	38(2)	-9(2)	-12(2)	31(2)
K(4)	47(1)	47(1)	25(1)	0	0	24(1)
C(4)	63(4)	94(5)	67(4)	-38(4)	-43(3)	52(4)
C(5)	22(3)	74(4)	83(4)	-13(4)	-9(3)	21(3)
O(11)	26(2)	25(2)	66(2)	-3(2)	10(2)	13(2)
C(6)	61(4)	45(3)	52(3)	7(3)	12(3)	23(3)
O(12)	31(2)	28(2)	38(2)	-10(1)	-7(2)	15(2)
O(13)	33(2)	44(2)	81(3)	6(2)	-10(2)	25(2)
C(11)	56(4)	56(4)	60(4)	-36(3)	-23(3)	26(3)
C(12)	77(5)	88(5)	67(4)	-34(4)	-46(4)	44(4)
C(13)	71(4)	72(5)	56(4)	-39(4)	-14(3)	25(4)
C(14)	57(4)	71(4)	97(6)	-55(4)	-31(4)	20(3)
C(15)	45(4)	73(5)	178(8)	10(6)	7(5)	46(4)
C(16)	48(4)	51(4)	87(5)	-4(3)	-19(4)	16(3)
K(5)	104(2)	104(2)	45(1)	0	0	52(1)
O(20)	141(7)	108(5)	107(6)	-21(5)	48(6)	28(5)
C(21)	138(7)	108(5)	111(6)	-15(5)	56(6)	28(5)
C(22)	131(7)	103(5)	121(7)	-20(5)	44(7)	36(5)
C(23)	138(7)	107(6)	112(7)	-21(6)	50(7)	38(5)
C(24)	136(7)	107(5)	114(7)	-15(5)	55(6)	33(5)
O(20')	135(7)	105(5)	114(6)	-23(5)	53(6)	35(5)
C(21')	132(7)	101(5)	112(7)	-16(5)	53(6)	38(5)
C(22')	136(7)	101(5)	111(8)	-12(6)	56(7)	39(5)
C(23')	132(7)	103(5)	118(7)	-13(6)	53(7)	41(5)
C(24')	133(7)	107(5)	115(7)	-21(6)	56(6)	35(5)
O(30)	80(3)	79(3)	81(3)	8(3)	-13(3)	35(3)
C(31)	84(5)	88(4)	97(5)	16(4)	-13(4)	42(4)
C(32)	75(6)	87(5)	95(6)	19(5)	-8(5)	25(5)
C(33)	68(4)	92(5)	86(4)	10(4)	-11(3)	28(4)
C(34)	61(4)	83(4)	76(4)	8(3)	-10(3)	37(3)
C(32')	79(6)	82(5)	94(6)	11(5)	-4(5)	24(5)
O(40)	110(2)	220(2)	23(3)	16(17)	10(10)	120(2)
C(41)	114(19)	270(3)	41(8)	-35(19)	-12(11)	140(2)
C(42)	140(3)	270(3)	66(11)	30(2)	-20(13)	140(2)
C(43)	130(2)	250(3)	54(9)	-21(19)	15(12)	130(2)
C(44)	101(17)	220(3)	37(8)	43(16)	23(10)	120(2)
O(50)	119(17)	137(16)	38(4)	12(10)	15(10)	89(14)
C(51)	130(2)	140(2)	51(9)	-7(12)	17(14)	88(16)
C(52)	109(18)	150(2)	60(12)	5(14)	33(15)	52(16)
C(53)	116(18)	180(3)	58(8)	48(18)	18(17)	61(18)
C(54)	109(19)	200(3)	50(8)	25(17)	5(12)	91(15)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **3**.

	x	y	z	U(eq)
H(2A)	-1362	285	-6128	97
H(2B)	-2070	581	-6086	97
H(2C)	-2164	-68	-6386	97
H(3A)	-2730	-1929	-5852	77
H(3B)	-1782	-1271	-5995	77
H(3C)	-2606	-1629	-6242	77
H(4A)	-3680	-1152	-6165	103
H(4B)	-3525	-426	-5889	103
H(4C)	-3800	-1388	-5768	103
H(5A)	-4651	-1139	-4808	92
H(5B)	-4877	-1893	-5080	92
H(5C)	-4287	-900	-5189	92
H(6A)	-3243	-2654	-4785	81
H(6B)	-3959	-2701	-4526	81
H(6C)	-2951	-2093	-4443	81
H(12A)	-9030	-5319	-3746	113
H(12B)	-8416	-4631	-3466	113
H(12C)	-9367	-5384	-3363	113
H(13A)	-7941	-5827	-3881	107
H(13B)	-7470	-5995	-3567	107
H(13C)	-7295	-5038	-3642	107
H(14A)	-9702	-6873	-3303	121
H(14B)	-8986	-7146	-3373	121
H(14C)	-9396	-6894	-3684	121
H(15A)	-9624	-1808	-2384	138
H(15B)	-10495	-2724	-2344	138
H(15C)	-10264	-2225	-2702	138
H(16A)	-10254	-4032	-3079	99
H(16B)	-10256	-4527	-2738	99
H(16C)	-9428	-4122	-2984	99
H(21A)	-2681	5671	-3525	161
H(21B)	-2024	5329	-3435	161
H(22A)	-2116	6455	-3087	154
H(22B)	-1847	5793	-2923	154
H(23A)	-3039	5470	-2599	155
H(23B)	-3527	5636	-2912	155
H(24A)	-4133	4249	-2935	158
H(24B)	-3285	4248	-2796	158
H(21A)	-2163	5208	-3541	148
H(21B)	-1813	5225	-3163	148
H(22A)	-2473	6159	-3420	150
H(22B)	-1976	6284	-3064	150
H(23A)	-3217	5612	-2782	151
H(23B)	-3696	5628	-3127	151
H(24A)	-4201	4313	-3191	156
H(24B)	-3793	4285	-2830	156
H(31A)	-4737	857	-3814	108
H(31B)	-4241	786	-4144	108
H(31C)	-5021	817	-3859	108
H(31D)	-4166	858	-4011	108
H(32A)	-5900	554	-4101	111
H(32B)	-5578	-14	-4309	111
H(33A)	-5051	947	-4745	104
H(33B)	-5793	1152	-4620	104
H(33C)	-5197	1081	-4798	104
H(33D)	-5849	1056	-4508	104
H(34A)	-4121	2267	-4599	87
H(34B)	-4845	2377	-4398	87

H(32A)	-5667	-1	-4276	111
H(32B)	-4776	303	-4480	111
H(41A)	-1107	-802	-6712	146
H(41B)	-935	154	-6625	146
H(42A)	-103	728	-7068	166
H(42B)	-794	-216	-7215	166
H(43A)	133	-764	-7115	155
H(43B)	818	214	-7232	155
H(44A)	1221	640	-6722	122
H(44B)	904	-367	-6662	122
H(51A)	-5642	-3621	-4104	121
H(51B)	-6564	-4383	-4238	121
H(52A)	-6057	-3777	-4717	133
H(52B)	-5428	-2846	-4548	133
H(53A)	-6438	-2508	-4682	149
H(53B)	-7145	-3505	-4759	149
H(54A)	-7691	-3634	-4274	134
H(54B)	-7034	-2620	-4209	134