Vinyl Oxidative Coupling as a Synthetic Route to Catalytically Active Monovalent Chromium

Khalid Albahily,[a] Yacoob Shaikh, [a] Elena Sebastiao, [a] Sandro Gambarotta,[a] Ilia Korobkov[b] and Serge I. Gorelsky[a,c]*

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Frisch, M. J.; G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *Gaussian 09*, Inc., Wallingford CT, 2009 and Revision A.02

Table 1. Crystal data and structure refinement for **2.**

Identification code	**2**
Empirical formula	C36.80 H83.20 Cl2 Cr2 N8 P4
Formula weight	936.69
Temperature	200(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C2/m
Unit cell dimensions	a = 24.9305(9) A alpha = 90 deg. b = 11.2301(4) A beta = 109.799(2) deg. c = 9.7869(4) A gamma = 90 deg.
Volume	2578.08(17) A^3
Z, Calculated density	2, 1.207 Mg/m^3
Absorption coefficient	0.682 mm^-1
F(000)	1004
Crystal size	0.16 x 0.14 x 0.04 mm
Theta range for data collection	2.21 to 28.33 deg.
Limiting indices	-33<=h<=33, -14<=k<=14, -13<=l<=13
Reflections collected / unique	31048 / 3239 [R(int) = 0.0452]
Completeness to theta = 25.00	96.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9732 and 0.8988
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3239 / 9 / 148
Goodness-of-fit on F^2	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0717, wR2 = 0.1849
R indices (all data)	R1 = 0.0871, wR2 = 0.1968
Largest diff. peak and hole	0.622 and -0.666 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)
Cr(1)	4248(1)	5000	3821(1)	45(1)
P(1)	3305(1)	3825(1)	1911(1)	34(1)
Cl(1)	4803(1)	5392(2)	6322(2)	46(1)
N(1)	3772(1)	3599(3)	3584(3)	42(1)
N(2)	3747(2)	5000	1646(4)	30(1)
N(3)	2867(2)	5000	1921(4)	37(1)
C(1)	3697(3)	2643(4)	4547(5)	68(1)
C(2)	3233(4)	1762(5)	3722(7)	117(3)
C(3)	3525(3)	3199(5)	5761(5)	76(2)
C(4)	4270(5)	1997(9)	5206(9)	146(4)
C(5)	3888(2)	5000	271(5)	41(1)
C(6)	3331(3)	5000	-1044(6)	58(2)
C(7)	4230(2)	3881(5)	241(4)	54(1)
C(8)	2245(2)	5000	1662(7)	49(1)
C(9)	2150(4)	5000	3135(11)	99(3)
C(10)	1980(3)	3873(9)	897(13)	162(5)
C(11)	4697(13)	10310(30)	1860(30)	85(9)
C(12)	4607(19)	9140(40)	1080(50)	132(17)
C(13)	5100(20)	8970(50)	520(50)	150(20)
C(14)	4870(20)	9240(50)	-1090(40)	150(20)
C(15)	5213(19)	10330(40)	-1220(40)	113(14)
C(16)	5310(20)	10790(50)	320(50)	126(15)

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

Cr(1)-N(1)#1	1.938(3)
Cr(1)-N(1)	1.938(3)
Cr(1)-N(2)	2.071(4)
Cr(1)-Cl(1)#1	2.4094(17)
Cr(1)-Cl(1)	2.4094(17)
Cr(1)-Cl(1)#2	2.4559(19)
Cr(1)-Cl(1)#3	2.4559(19)
Cr(1)-P(1)	2.7915(11)
Cr(1)-P(1)#1	2.7916(11)
P(1)-N(1)	1.676(3)
P(1)-N(3)	1.715(3)
P(1)-N(2)	1.794(3)
P(1)-P(1)#1	2.6401(18)
Cl(1)-Cr(1)#3	2.4559(19)
N(1)-C(1)	1.482(5)
N(2)-C(5)	1.501(6)
N(2)-P(1)#1	1.794(3)
N(3)-C(8)	1.486(7)
N(3)-P(1)#1	1.715(3)
C(1)-C(2)	1.528(9)
C(1)-C(3)	1.526(6)
C(1)-C(4)	1.537(9)
C(5)-C(7)	1.525(5)
C(5)-C(7)#1	1.525(5)
C(5)-C(6)	1.540(7)
C(8)-C(10)#1	1.505(8)
C(8)-C(10)	1.505(8)
C(8)-C(9)	1.537(11)
C(11)-C(12)	1.50(2)
C(12)-C(13)	1.51(2)
C(13)-C(14)	1.52(2)
C(14)-C(15)	1.519(19)
C(15)-C(16)	1.53(2)
N(1)#1-Cr(1)-N(1)	108.56(19)
N(1)#1-Cr(1)-N(2)	75.22(10)
N(1)-Cr(1)-N(2)	75.22(10)
N(1)#1-Cr(1)-Cl(1)#1	112.81(10)
N(1)-Cr(1)-Cl(1)#1	95.20(10)
N(2)-Cr(1)-Cl(1)#1	169.38(5)
N(1)#1-Cr(1)-Cl(1)	95.20(10)
N(1)-Cr(1)-Cl(1)	112.81(10)
N(2)-Cr(1)-Cl(1)	169.38(5)
Cl(1)#1-Cr(1)-Cl(1)	21.08(9)
N(1)#1-Cr(1)-Cl(1)#2	114.26(11)
N(1)-Cr(1)-Cl(1)#2	134.62(11)
N(2)-Cr(1)-Cl(1)#2	101.47(11)
Cl(1)#1-Cr(1)-Cl(1)#2	81.88(6)
Cl(1)-Cr(1)-Cl(1)#2	78.06(7)
N(1)#1-Cr(1)-Cl(1)#3	134.62(11)

N(1)-Cr(1)-Cl(1)#3	114.26(11)
N(2)-Cr(1)-Cl(1)#3	101.47(11)
Cl(1)#1-Cr(1)-Cl(1)#3	78.06(7)
Cl(1)-Cr(1)-Cl(1)#3	81.88(6)
Cl(1)#2-Cr(1)-Cl(1)#3	20.68(9)
N(1)#1-Cr(1)-P(1)	87.71(9)
N(1)-Cr(1)-P(1)	36.12(9)
N(2)-Cr(1)-P(1)	39.97(7)
Cl(1)#1-Cr(1)-P(1)	131.08(5)
Cl(1)-Cr(1)-P(1)	146.12(6)
Cl(1)#2-Cr(1)-P(1)	131.00(5)
Cl(1)#3-Cr(1)-P(1)	119.10(5)
N(1)#1-Cr(1)-P(1)#1	36.12(9)
N(1)-Cr(1)-P(1)#1	87.71(9)
N(2)-Cr(1)-P(1)#1	39.97(7)
Cl(1)#1-Cr(1)-P(1)#1	146.12(6)
Cl(1)-Cr(1)-P(1)#1	131.08(5)
Cl(1)#2-Cr(1)-P(1)#1	119.10(5)
Cl(1)#3-Cr(1)-P(1)#1	131.00(5)
P(1)-Cr(1)-P(1)#1	56.44(4)
N(1)-P(1)-N(3)	110.08(18)
N(1)-P(1)-N(2)	89.71(17)
N(3)-P(1)-N(2)	81.83(14)
N(1)-P(1)-P(1)#1	98.71(11)
N(3)-P(1)-P(1)#1	39.65(11)
N(2)-P(1)-P(1)#1	42.64(9)
N(1)-P(1)-Cr(1)	42.99(12)
N(3)-P(1)-Cr(1)	91.46(13)
N(2)-P(1)-Cr(1)	47.85(12)
P(1)#1-P(1)-Cr(1)	61.78(2)
Cr(1)-Cl(1)-Cr(1)#3	98.12(6)
C(1)-N(1)-P(1)	122.4(3)
C(1)-N(1)-Cr(1)	135.8(3)
P(1)-N(1)-Cr(1)	100.88(15)
C(5)-N(2)-P(1)	118.07(19)
C(5)-N(2)-P(1)#1	118.07(19)
P(1)-N(2)-P(1)#1	94.72(18)
C(5)-N(2)-Cr(1)	132.8(3)
P(1)-N(2)-Cr(1)	92.19(14)
P(1)#1-N(2)-Cr(1)	92.19(14)
C(8)-N(3)-P(1)#1	128.97(12)
C(8)-N(3)-P(1)	128.97(12)
P(1)#1-N(3)-P(1)	100.7(2)
N(1)-C(1)-C(2)	111.6(4)
N(1)-C(1)-C(3)	109.2(4)
C(2)-C(1)-C(3)	108.4(5)
N(1)-C(1)-C(4)	108.0(5)
C(2)-C(1)-C(4)	110.2(6)
C(3)-C(1)-C(4)	109.4(5)
N(2)-C(5)-C(7)	108.6(3)
N(2)-C(5)-C(7)#1	108.6(3)
C(7)-C(5)-C(7)#1	111.0(5)
N(2)-C(5)-C(6)	109.4(4)
C(7)-C(5)-C(6)	109.6(3)

C(7)#1-C(5)-C(6)	109.6(3)
C(10)#1-C(8)-C(10)	114.6(10)
C(10)#1-C(8)-N(3)	110.0(4)
C(10)-C(8)-N(3)	110.0(4)
C(10)#1-C(8)-C(9)	106.6(6)
C(10)-C(8)-C(9)	106.6(6)
N(3)-C(8)-C(9)	108.8(5)
C(11)-C(12)-C(13)	108(3)
C(12)-C(13)-C(14)	107(3)
C(13)-C(14)-C(15)	103(3)
C(14)-C(15)-C(16)	96(2)

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1,z #2 -x+1,y,-z+1 #3 -x+1,-y+1,-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
Cr(1)	34(1)	77(1)	22(1)	0	7(1)	0
P(1)	46(1)	28(1)	30(1)	-1(1)	15(1)	0(1)
Cl(1)	41(1)	65(1)	27(1)	-8(1)	6(1)	14(1)
N(1)	55(2)	37(2)	32(1)	7(1)	13(1)	10(1)
N(2)	33(2)	34(2)	23(2)	0	12(1)	0
N(3)	34(2)	45(2)	34(2)	0	14(2)	0
C(1)	120(4)	44(2)	50(2)	20(2)	42(3)	27(3)
C(2)	246(10)	36(3)	89(4)	7(3)	85(6)	-30(4)
C(3)	119(5)	68(3)	57(3)	12(2)	53(3)	0(3)
C(4)	204(9)	140(7)	112(6)	89(6)	77(6)	123(7)
C(5)	45(3)	59(3)	21(2)	0	15(2)	0
C(6)	55(3)	96(5)	22(2)	0	11(2)	0
C(7)	55(2)	72(3)	38(2)	-13(2)	21(2)	7(2)
C(8)	37(3)	58(3)	51(3)	0	13(2)	0
C(9)	70(5)	144(10)	103(7)	0	55(5)	0
C(10)	62(4)	169(9)	254(12)	-138(9)	52(6)	-51(5)

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

	x	y	z	U(eq)
H(2A)	2871	2184	3300	175
H(2B)	3193	1147	4391	175
H(2C)	3339	1389	2944	175
H(3A)	3164	3630	5339	113
H(3B)	3822	3753	6317	113
H(3C)	3477	2570	6405	113
H(4A)	4379	1635	4428	219
H(4B)	4234	1375	5872	219
H(4C)	4563	2570	5740	219
H(6A)	3111	5718	-1021	87
H(6B)	3106	4294	-1006	87
H(6C)	3422	4988	-1943	87
H(7A)	4584	3882	1079	81
H(7B)	4321	3866	-657	81
H(7C)	4004	3175	282	81
H(9A)	2315	5724	3672	149
H(9B)	2335	4299	3695	149
H(9C)	1741	4977	2976	149
H(10A)	2174	3183	1466	243
H(10B)	2018	3848	-66	243
H(10C)	1575	3853	794	243
H(11A)	4409	10407	2333	127
H(11B)	4662	10959	1170	127
H(11C)	5078	10325	2601	127
H(12A)	4241	9150	257	159
H(12B)	4596	8486	1742	159
H(13A)	5238	8136	687	180
H(13B)	5415	9509	1025	180
H(14A)	4458	9415	-1427	182
H(14B)	4941	8566	-1667	182
H(15A)	4988	10890	-1975	136
H(15B)	5572	10119	-1381	136
H(16A)	5553	11511	486	189
H(16B)	5508	10182	1029	189
H(16C)	4948	10989	430	189

Table 6. Torsion angles [deg] for **2**.

N(1)#1-Cr(1)-P(1)-N(1)	-126.5(2)
N(2)-Cr(1)-P(1)-N(1)	164.0(2)
Cl(1)#1-Cr(1)-P(1)-N(1)	-7.84(17)
Cl(1)-Cr(1)-P(1)-N(1)	-30.59(18)
Cl(1)#2-Cr(1)-P(1)-N(1)	112.80(17)
Cl(1)#3-Cr(1)-P(1)-N(1)	92.01(17)
P(1)#1-Cr(1)-P(1)-N(1)	-145.86(16)
N(1)#1-Cr(1)-P(1)-N(3)	-8.07(15)
N(1)-Cr(1)-P(1)-N(3)	118.4(2)
N(2)-Cr(1)-P(1)-N(3)	-77.59(17)
Cl(1)#1-Cr(1)-P(1)-N(3)	110.61(15)
Cl(1)-Cr(1)-P(1)-N(3)	87.86(15)
Cl(1)#2-Cr(1)-P(1)-N(3)	-128.75(14)
Cl(1)#3-Cr(1)-P(1)-N(3)	-149.54(13)
P(1)#1-Cr(1)-P(1)-N(3)	-27.41(13)
N(1)#1-Cr(1)-P(1)-N(2)	69.52(15)
N(1)-Cr(1)-P(1)-N(2)	-164.0(2)
Cl(1)#1-Cr(1)-P(1)-N(2)	-171.80(14)
Cl(1)-Cr(1)-P(1)-N(2)	165.45(14)
Cl(1)#2-Cr(1)-P(1)-N(2)	-51.16(14)
Cl(1)#3-Cr(1)-P(1)-N(2)	-71.95(13)
P(1)#1-Cr(1)-P(1)-N(2)	50.18(12)
N(1)#1-Cr(1)-P(1)-P(1)#1	19.34(9)
N(1)-Cr(1)-P(1)-P(1)#1	145.86(16)
N(2)-Cr(1)-P(1)-P(1)#1	-50.18(12)
Cl(1)#1-Cr(1)-P(1)-P(1)#1	138.02(8)
Cl(1)-Cr(1)-P(1)-P(1)#1	115.26(9)
Cl(1)#2-Cr(1)-P(1)-P(1)#1	-101.34(7)
Cl(1)#3-Cr(1)-P(1)-P(1)#1	-122.13(6)
N(1)#1-Cr(1)-Cl(1)-Cr(1)#3	-134.38(11)
N(1)-Cr(1)-Cl(1)-Cr(1)#3	112.97(12)
N(2)-Cr(1)-Cl(1)-Cr(1)#3	-109.2(6)
Cl(1)#1-Cr(1)-Cl(1)-Cr(1)#3	77.82(6)
Cl(1)#2-Cr(1)-Cl(1)-Cr(1)#3	-20.65(9)
Cl(1)#3-Cr(1)-Cl(1)-Cr(1)#3	0.0
P(1)-Cr(1)-Cl(1)-Cr(1)#3	131.97(6)
P(1)#1-Cr(1)-Cl(1)-Cr(1)#3	-139.01(5)
N(3)-P(1)-N(1)-C(1)	101.1(3)
N(2)-P(1)-N(1)-C(1)	-177.7(3)
P(1)#1-P(1)-N(1)-C(1)	140.4(3)
Cr(1)-P(1)-N(1)-C(1)	170.4(4)
N(3)-P(1)-N(1)-Cr(1)	-69.37(18)
N(2)-P(1)-N(1)-Cr(1)	11.82(15)
P(1)#1-P(1)-N(1)-Cr(1)	-30.02(13)
N(1)#1-Cr(1)-N(1)-C(1)	-110.5(4)
N(2)-Cr(1)-N(1)-C(1)	-179.0(4)
Cl(1)#1-Cr(1)-N(1)-C(1)	5.7(4)
Cl(1)-Cr(1)-N(1)-C(1)	-6.3(4)
Cl(1)#2-Cr(1)-N(1)-C(1)	89.4(4)
Cl(1)#3-Cr(1)-N(1)-C(1)	84.9(4)

P(1)-Cr(1)-N(1)-C(1)	-168.4(5)
P(1)#1-Cr(1)-N(1)-C(1)	-140.5(4)
N(1)#1-Cr(1)-N(1)-P(1)	57.9(2)
N(2)-Cr(1)-N(1)-P(1)	-10.58(14)
Cl(1)#1-Cr(1)-N(1)-P(1)	174.08(13)
Cl(1)-Cr(1)-N(1)-P(1)	162.07(11)
Cl(1)#2-Cr(1)-N(1)-P(1)	-102.21(16)
Cl(1)#3-Cr(1)-N(1)-P(1)	-106.70(13)
P(1)#1-Cr(1)-N(1)-P(1)	27.91(13)
N(1)-P(1)-N(2)-C(5)	131.4(3)
N(3)-P(1)-N(2)-C(5)	-118.3(3)
P(1)#1-P(1)-N(2)-C(5)	-125.4(4)
Cr(1)-P(1)-N(2)-C(5)	142.2(3)
N(1)-P(1)-N(2)-P(1)#1	-103.24(17)
N(3)-P(1)-N(2)-P(1)#1	7.10(18)
Cr(1)-P(1)-N(2)-P(1)#1	-92.38(15)
N(1)-P(1)-N(2)-Cr(1)	-10.86(13)
N(3)-P(1)-N(2)-Cr(1)	99.48(16)
P(1)#1-P(1)-N(2)-Cr(1)	92.38(15)
N(1)#1-Cr(1)-N(2)-C(5)	122.90(10)
N(1)-Cr(1)-N(2)-C(5)	-122.89(10)
Cl(1)#1-Cr(1)-N(2)-C(5)	-96.9(6)
Cl(1)-Cr(1)-N(2)-C(5)	96.9(6)
Cl(1)#2-Cr(1)-N(2)-C(5)	10.55(5)
Cl(1)#3-Cr(1)-N(2)-C(5)	-10.55(5)
P(1)-Cr(1)-N(2)-C(5)	-132.59(9)
P(1)#1-Cr(1)-N(2)-C(5)	132.59(9)
N(1)#1-Cr(1)-N(2)-P(1)	-104.51(15)
N(1)-Cr(1)-N(2)-P(1)	9.70(12)
Cl(1)#1-Cr(1)-N(2)-P(1)	35.7(7)
Cl(1)-Cr(1)-N(2)-P(1)	-130.5(5)
Cl(1)#2-Cr(1)-N(2)-P(1)	143.14(10)
Cl(1)#3-Cr(1)-N(2)-P(1)	122.04(11)
P(1)#1-Cr(1)-N(2)-P(1)	-94.81(19)
N(1)#1-Cr(1)-N(2)-P(1)#1	-9.70(12)
N(1)-Cr(1)-N(2)-P(1)#1	104.51(15)
Cl(1)#1-Cr(1)-N(2)-P(1)#1	130.5(5)
Cl(1)-Cr(1)-N(2)-P(1)#1	-35.7(7)
Cl(1)#2-Cr(1)-N(2)-P(1)#1	-122.04(11)
Cl(1)#3-Cr(1)-N(2)-P(1)#1	-143.15(10)
P(1)-Cr(1)-N(2)-P(1)#1	94.81(19)
N(1)-P(1)-N(3)-C(8)	-113.4(4)
N(2)-P(1)-N(3)-C(8)	159.9(5)
P(1)#1-P(1)-N(3)-C(8)	167.4(6)
Cr(1)-P(1)-N(3)-C(8)	-153.1(4)
N(1)-P(1)-N(3)-P(1)#1	79.1(2)
N(2)-P(1)-N(3)-P(1)#1	-7.54(19)
Cr(1)-P(1)-N(3)-P(1)#1	39.47(18)
P(1)-N(1)-C(1)-C(2)	12.5(6)
Cr(1)-N(1)-C(1)-C(2)	179.0(4)
P(1)-N(1)-C(1)-C(3)	-107.3(5)
Cr(1)-N(1)-C(1)-C(3)	59.1(6)
P(1)-N(1)-C(1)-C(4)	133.8(5)
Cr(1)-N(1)-C(1)-C(4)	-59.8(6)

P(1)-N(2)-C(5)-C(7)	-63.1(4)
P(1)#1-N(2)-C(5)-C(7)	-176.1(3)
Cr(1)-N(2)-C(5)-C(7)	60.4(3)
P(1)-N(2)-C(5)-C(7)#1	176.1(3)
P(1)#1-N(2)-C(5)-C(7)#1	63.1(4)
Cr(1)-N(2)-C(5)-C(7)#1	-60.4(3)
P(1)-N(2)-C(5)-C(6)	56.5(2)
P(1)#1-N(2)-C(5)-C(6)	-56.5(2)
Cr(1)-N(2)-C(5)-C(6)	180.0
P(1)#1-N(3)-C(8)-C(10)#1	18.5(8)
P(1)-N(3)-C(8)-C(10)#1	-145.6(6)
P(1)#1-N(3)-C(8)-C(10)	145.6(6)
P(1)-N(3)-C(8)-C(10)	-18.5(8)
P(1)#1-N(3)-C(8)-C(9)	-98.0(4)
P(1)-N(3)-C(8)-C(9)	98.0(4)
C(11)-C(12)-C(13)-C(14)	-103(5)
C(12)-C(13)-C(14)-C(15)	115(4)
C(13)-C(14)-C(15)-C(16)	-28(4)

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1,z #2 -x+1,y,-z+1 #3 -x+1,-y+1,-z+1

Table 7. Crystal data and structure refinement for **3**.

Identification code	**3**
Empirical formula	C24 H50 Cr Li N4 O P2
Formula weight	531.56
Temperature	200(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 16.3492(8) A alpha = 90 deg. b = 9.8141(5) A beta = 110.647(3) deg. c = 19.5718(10) A gamma = 90 deg.
Volume	2938.6(3) A^3
Z, Calculated density	4, 1.201 Mg/m^3
Absorption coefficient	0.520 mm^-1
F(000)	1148
Crystal size	0.17 x 0.15 x 0.04 mm
Theta range for data collection	2.15 to 28.33 deg.
Limiting indices	-21<=h<=21, -12<=k<=12, -23<=l<=26
Reflections collected / unique	28818 / 7172 [R(int) = 0.0814]
Completeness to theta = 28.33	97.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9795 and 0.9168
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7172 / 0 / 298
Goodness-of-fit on F^2	1.029
Final R indices [I>2sigma(I)]	R1 = 0.0524, wR2 = 0.1238
R indices (all data)	R1 = 0.0947, wR2 = 0.1422

Largest diff. peak and hole 0.967 and -0.614 e.A^-3

Table 8. 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)
Cr(1)	2730(1)	5777(1)	4121(1)	26(1)
Li(1)	2997(3)	3436(5)	4964(3)	31(1)
N(1)	1348(1)	5237(2)	3860(1)	24(1)
N(2)	1568(1)	3226(2)	4566(1)	24(1)
N(3)	2537(1)	5372(2)	5142(1)	26(1)
N(4)	2587(1)	3690(2)	3813(1)	25(1)
O(1)	3836(1)	2217(2)	5642(1)	40(1)
P(1)	1480(1)	4930(1)	4799(1)	24(1)
P(2)	1525(1)	3503(1)	3670(1)	23(1)
C(1)	532(2)	5953(3)	3381(2)	30(1)
C(2)	525(2)	5974(4)	2601(2)	45(1)
C(3)	556(2)	7402(3)	3665(2)	43(1)
C(4)	-287(2)	5231(4)	3392(2)	44(1)
C(5)	1136(2)	2053(3)	4793(2)	28(1)
C(6)	146(2)	2171(3)	4501(2)	40(1)
C(7)	1472(2)	2014(3)	5624(2)	41(1)
C(8)	1405(2)	744(3)	4501(2)	39(1)
C(9)	2805(2)	6168(3)	5844(2)	31(1)
C(10)	2397(2)	7582(3)	5725(2)	43(1)
C(11)	3801(2)	6288(4)	6141(2)	43(1)
C(12)	2530(2)	5427(4)	6418(2)	44(1)
C(13)	2914(2)	2949(3)	3289(2)	30(1)
C(14)	2459(2)	3443(4)	2505(2)	42(1)
C(15)	3894(2)	3206(4)	3511(2)	41(1)
C(16)	2759(2)	1421(3)	3318(2)	40(1)
C(17)	4103(2)	6279(3)	4477(2)	47(1)
C(18)	3599(3)	7507(4)	4424(2)	60(1)
C(19)	2940(3)	7808(4)	3755(3)	65(1)
C(20)	2829(3)	6923(5)	3185(2)	69(1)
C(21)	4204(2)	1052(4)	5407(2)	50(1)
C(22)	4747(3)	317(4)	6082(2)	69(1)
C(23)	4539(4)	936(5)	6671(2)	101(2)
C(24)	4205(3)	2306(4)	6418(2)	53(1)

Table 9. Bond lengths [A] and angles [deg] for **3.**

Cr(1)-N(4)	2.125(2)
Cr(1)-C(17)	2.160(3)
Cr(1)-C(18)	2.158(4)
Cr(1)-N(3)	2.167(2)
Cr(1)-C(19)	2.186(3)
Cr(1)-C(20)	2.204(4)
Cr(1)-N(1)	2.198(2)
Cr(1)-Li(1)	2.771(5)
Li(1)-O(1)	1.947(5)
Li(1)-N(3)	2.116(5)
Li(1)-N(4)	2.126(5)
Li(1)-N(2)	2.196(5)
Li(1)-P(1)	2.799(5)
Li(1)-P(2)	2.812(5)
N(1)-C(1)	1.507(3)
N(1)-P(2)	1.788(2)
N(1)-P(1)	1.799(2)
N(2)-C(5)	1.498(3)
N(2)-P(2)	1.751(2)
N(2)-P(1)	1.753(2)
N(3)-C(9)	1.504(3)
N(3)-P(1)	1.675(2)
N(4)-C(13)	1.502(3)
N(4)-P(2)	1.668(2)
O(1)-C(24)	1.426(4)
O(1)-C(21)	1.441(4)
P(1)-P(2)	2.6388(9)
C(1)-C(3)	1.522(4)
C(1)-C(4)	1.523(4)
C(1)-C(2)	1.523(4)
C(5)-C(6)	1.518(4)
C(5)-C(7)	1.522(4)
C(5)-C(8)	1.533(4)
C(9)-C(10)	1.522(4)
C(9)-C(11)	1.528(4)
C(9)-C(12)	1.534(4)
C(13)-C(15)	1.525(4)
C(13)-C(16)	1.526(4)
C(13)-C(14)	1.529(4)
C(17)-C(18)	1.444(5)
C(18)-C(19)	1.402(5)
C(19)-C(20)	1.375(6)
C(21)-C(22)	1.493(5)
C(22)-C(23)	1.446(6)
C(23)-C(24)	1.470(6)
N(4)-Cr(1)-C(17)	108.02(11)
N(4)-Cr(1)-C(18)	146.36(12)
C(17)-Cr(1)-C(18)	39.07(14)
N(4)-Cr(1)-N(3)	92.71(8)

C(17)-Cr(1)-N(3)	102.55(11)
C(18)-Cr(1)-N(3)	100.74(13)
N(4)-Cr(1)-C(19)	143.21(15)
C(17)-Cr(1)-C(19)	68.43(14)
C(18)-Cr(1)-C(19)	37.67(15)
N(3)-Cr(1)-C(19)	124.05(15)
N(4)-Cr(1)-C(20)	106.83(15)
C(17)-Cr(1)-C(20)	77.25(15)
C(18)-Cr(1)-C(20)	65.99(17)
N(3)-Cr(1)-C(20)	159.62(15)
C(19)-Cr(1)-C(20)	36.51(16)
N(4)-Cr(1)-N(1)	72.57(8)
C(17)-Cr(1)-N(1)	174.98(11)
C(18)-Cr(1)-N(1)	140.90(13)
N(3)-Cr(1)-N(1)	72.43(8)
C(19)-Cr(1)-N(1)	114.24(12)
C(20)-Cr(1)-N(1)	107.47(12)
N(4)-Cr(1)-Li(1)	49.32(11)
C(17)-Cr(1)-Li(1)	94.00(14)
C(18)-Cr(1)-Li(1)	122.58(15)
N(3)-Cr(1)-Li(1)	48.89(11)
C(19)-Cr(1)-Li(1)	160.23(15)
C(20)-Cr(1)-Li(1)	151.14(17)
N(1)-Cr(1)-Li(1)	82.62(11)
O(1)-Li(1)-N(3)	130.2(3)
O(1)-Li(1)-N(4)	132.6(3)
N(3)-Li(1)-N(4)	94.1(2)
O(1)-Li(1)-N(2)	126.1(3)
N(3)-Li(1)-N(2)	75.40(17)
N(4)-Li(1)-N(2)	74.73(17)
O(1)-Li(1)-Cr(1)	147.2(2)
N(3)-Li(1)-Cr(1)	50.49(12)
N(4)-Li(1)-Cr(1)	49.29(12)
N(2)-Li(1)-Cr(1)	86.70(16)
O(1)-Li(1)-P(1)	141.5(2)
N(3)-Li(1)-P(1)	36.64(9)
N(4)-Li(1)-P(1)	83.18(16)
N(2)-Li(1)-P(1)	38.77(9)
Cr(1)-Li(1)-P(1)	63.28(10)
O(1)-Li(1)-P(2)	143.2(2)
N(3)-Li(1)-P(2)	83.51(16)
N(4)-Li(1)-P(2)	36.23(9)
N(2)-Li(1)-P(2)	38.50(9)
Cr(1)-Li(1)-P(2)	62.60(10)
P(1)-Li(1)-P(2)	56.10(9)
C(1)-N(1)-P(2)	119.15(17)
C(1)-N(1)-P(1)	118.39(16)
P(2)-N(1)-P(1)	94.75(10)
C(1)-N(1)-Cr(1)	130.10(17)
P(2)-N(1)-Cr(1)	92.82(9)
P(1)-N(1)-Cr(1)	93.42(9)
C(5)-N(2)-P(2)	124.07(17)
C(5)-N(2)-P(1)	124.43(16)
P(2)-N(2)-P(1)	97.74(11)

C(5)-N(2)-Li(1)	121.4(2)
P(2)-N(2)-Li(1)	90.14(15)
P(1)-N(2)-Li(1)	89.54(15)
C(9)-N(3)-P(1)	115.30(16)
C(9)-N(3)-Li(1)	127.6(2)
P(1)-N(3)-Li(1)	94.44(16)
C(9)-N(3)-Cr(1)	131.01(17)
P(1)-N(3)-Cr(1)	98.21(10)
Li(1)-N(3)-Cr(1)	80.62(15)
C(13)-N(4)-P(2)	115.64(17)
C(13)-N(4)-Cr(1)	129.05(17)
P(2)-N(4)-Cr(1)	99.08(10)
C(13)-N(4)-Li(1)	127.8(2)
P(2)-N(4)-Li(1)	94.91(16)
Cr(1)-N(4)-Li(1)	81.39(15)
C(24)-O(1)-C(21)	108.8(2)
C(24)-O(1)-Li(1)	128.3(2)
C(21)-O(1)-Li(1)	122.9(2)
N(3)-P(1)-N(2)	100.62(11)
N(3)-P(1)-N(1)	95.83(10)
N(2)-P(1)-N(1)	83.41(10)
N(3)-P(1)-P(2)	98.27(8)
N(2)-P(1)-P(2)	41.10(7)
N(1)-P(1)-P(2)	42.47(7)
N(3)-P(1)-Li(1)	48.93(13)
N(2)-P(1)-Li(1)	51.69(12)
N(1)-P(1)-Li(1)	89.32(12)
P(2)-P(1)-Li(1)	62.20(10)
N(4)-P(2)-N(2)	100.21(10)
N(4)-P(2)-N(1)	95.48(11)
N(2)-P(2)-N(1)	83.79(10)
N(4)-P(2)-P(1)	97.78(8)
N(2)-P(2)-P(1)	41.16(7)
N(1)-P(2)-P(1)	42.78(7)
N(4)-P(2)-Li(1)	48.86(12)
N(2)-P(2)-Li(1)	51.36(12)
N(1)-P(2)-Li(1)	89.12(12)
P(1)-P(2)-Li(1)	61.70(10)
N(1)-C(1)-C(3)	107.7(2)
N(1)-C(1)-C(4)	111.3(2)
C(3)-C(1)-C(4)	109.8(2)
N(1)-C(1)-C(2)	108.8(2)
C(3)-C(1)-C(2)	110.2(3)
C(4)-C(1)-C(2)	109.0(3)
N(2)-C(5)-C(6)	112.4(2)
N(2)-C(5)-C(7)	107.8(2)
C(6)-C(5)-C(7)	109.9(2)
N(2)-C(5)-C(8)	107.8(2)
C(6)-C(5)-C(8)	109.4(2)
C(7)-C(5)-C(8)	109.5(2)
N(3)-C(9)-C(10)	111.4(2)
N(3)-C(9)-C(11)	108.4(2)
C(10)-C(9)-C(11)	109.8(3)
N(3)-C(9)-C(12)	110.9(2)

C(10)-C(9)-C(12)	108.5(3)
C(11)-C(9)-C(12)	107.8(3)
N(4)-C(13)-C(15)	108.5(2)
N(4)-C(13)-C(16)	110.3(2)
C(15)-C(13)-C(16)	108.9(2)
N(4)-C(13)-C(14)	111.6(2)
C(15)-C(13)-C(14)	108.9(2)
C(16)-C(13)-C(14)	108.7(3)
C(18)-C(17)-Cr(1)	70.39(19)
C(19)-C(18)-C(17)	118.3(4)
C(19)-C(18)-Cr(1)	72.2(2)
C(17)-C(18)-Cr(1)	70.54(19)
C(18)-C(19)-C(20)	117.6(4)
C(18)-C(19)-Cr(1)	70.1(2)
C(20)-C(19)-Cr(1)	72.5(2)
C(19)-C(20)-Cr(1)	71.0(2)
O(1)-C(21)-C(22)	106.6(3)
C(23)-C(22)-C(21)	105.6(3)
C(22)-C(23)-C(24)	106.3(4)
O(1)-C(24)-C(23)	105.6(3)

Symmetry transformations used to generate equivalent atoms:

Table 10. 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
Cr(1)	28(1)	27(1)	25(1)	2(1)	10(1)	-3(1)
Li(1)	33(2)	34(3)	25(2)	2(2)	9(2)	3(2)
N(1)	24(1)	27(1)	20(1)	3(1)	8(1)	2(1)
N(2)	28(1)	28(1)	18(1)	0(1)	10(1)	-2(1)
N(3)	30(1)	26(1)	20(1)	-3(1)	7(1)	-1(1)
N(4)	28(1)	32(1)	17(1)	-3(1)	10(1)	0(1)
O(1)	41(1)	45(1)	32(1)	5(1)	11(1)	11(1)
P(1)	25(1)	28(1)	20(1)	-2(1)	9(1)	0(1)
P(2)	25(1)	27(1)	18(1)	-1(1)	8(1)	-1(1)
C(1)	30(1)	32(2)	25(2)	4(1)	6(1)	7(1)
C(2)	48(2)	57(2)	25(2)	9(2)	8(1)	12(2)
C(3)	44(2)	36(2)	46(2)	4(2)	12(2)	13(1)
C(4)	26(1)	49(2)	49(2)	7(2)	4(1)	1(1)
C(5)	33(1)	29(1)	25(1)	0(1)	13(1)	-5(1)
C(6)	38(2)	46(2)	39(2)	-1(2)	18(1)	-9(1)
C(7)	51(2)	45(2)	27(2)	7(1)	14(1)	-8(1)
C(8)	57(2)	26(2)	40(2)	0(1)	24(2)	-4(1)
C(9)	34(2)	34(2)	23(1)	-6(1)	8(1)	-2(1)
C(10)	50(2)	35(2)	42(2)	-11(2)	14(2)	-1(1)
C(11)	36(2)	51(2)	33(2)	-10(2)	0(1)	-6(1)
C(12)	54(2)	54(2)	24(2)	-7(2)	14(1)	-12(2)
C(13)	32(1)	40(2)	21(1)	-1(1)	11(1)	4(1)
C(14)	45(2)	63(2)	22(2)	1(2)	15(1)	5(2)
C(15)	36(2)	54(2)	40(2)	-4(2)	20(1)	2(1)
C(16)	49(2)	37(2)	35(2)	-11(1)	18(1)	4(1)
C(17)	34(2)	45(2)	56(2)	-4(2)	11(2)	-11(1)
C(18)	59(2)	50(2)	75(3)	-9(2)	30(2)	-19(2)
C(19)	58(2)	39(2)	86(3)	26(2)	12(2)	-16(2)
C(20)	65(3)	78(3)	62(3)	37(2)	21(2)	-8(2)
C(21)	58(2)	43(2)	43(2)	-2(2)	12(2)	11(2)
C(22)	82(3)	55(2)	57(3)	7(2)	8(2)	29(2)
C(23)	163(5)	86(4)	38(2)	18(2)	18(3)	54(4)
C(24)	60(2)	63(3)	34(2)	2(2)	14(2)	17(2)

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **3.**

	x	y	z	U(eq)
H(2A)	1051	6437	2589	67
H(2B)	5	6461	2287	67
H(2C)	515	5037	2425	67
H(3A)	561	7377	4167	64
H(3B)	39	7900	3355	64
H(3C)	1085	7862	3657	64
H(4A)	-289	5219	3893	66
H(4B)	-294	4294	3218	66
H(4C)	-806	5716	3074	66
H(6A)	-27	3006	4689	60
H(6B)	-107	1380	4660	60
H(6C)	-66	2203	3967	60
H(7A)	1302	2853	5810	62
H(7B)	2111	1937	5809	62
H(7C)	1220	1228	5787	62
H(8A)	2043	668	4688	59
H(8B)	1190	772	3966	59
H(8C)	1153	-45	4662	59
H(10A)	2559	8065	5354	64
H(10B)	2608	8094	6185	64
H(10C)	1759	7500	5562	64
H(11A)	4060	5375	6216	65
H(11B)	3988	6778	6607	65
H(11C)	3993	6788	5791	65
H(12A)	2784	4511	6497	66
H(12B)	1891	5360	6246	66
H(12C)	2738	5937	6877	66
H(14A)	2553	4425	2479	64
H(14B)	1831	3257	2353	64
H(14C)	2701	2962	2180	64
H(15A)	4000	4185	3493	62
H(15B)	4118	2727	3174	62
H(15C)	4193	2869	4008	62
H(16A)	3053	1090	3817	59
H(16B)	2994	946	2986	59
H(16C)	2130	1245	3169	59
H(17A)	3985	5698	4065	56
H(17B)	4554	6051	4924	56
H(18A)	3710	8096	4832	72
H(19A)	2584	8595	3698	78
H(20A)	3191	6142	3252	83
H(20B)	2389	7094	2723	83
H(21A)	4569	1347	5124	60
H(21B)	3734	451	5095	60
H(22A)	4602	-666	6044	83

H(22B)	5377	422	6163	83
H(23A)	5067	993	7118	121
H(23B)	4090	394	6782	121
H(24A)	3755	2579	6623	64
H(24B)	4685	2983	6569	64

Table 12. Torsion angles [deg] for **3.**

N(4)-Cr(1)-Li(1)-O(1)	108.3(5)
C(17)-Cr(1)-Li(1)-O(1)	-2.1(4)
C(18)-Cr(1)-Li(1)-O(1)	-30.6(5)
N(3)-Cr(1)-Li(1)-O(1)	-105.3(5)
C(19)-Cr(1)-Li(1)-O(1)	-28.6(8)
C(20)-Cr(1)-Li(1)-O(1)	68.5(6)
N(1)-Cr(1)-Li(1)-O(1)	-178.4(4)
N(4)-Cr(1)-Li(1)-N(3)	-146.40(19)
C(17)-Cr(1)-Li(1)-N(3)	103.18(15)
C(18)-Cr(1)-Li(1)-N(3)	74.70(19)
C(19)-Cr(1)-Li(1)-N(3)	76.7(5)
C(20)-Cr(1)-Li(1)-N(3)	173.8(3)
N(1)-Cr(1)-Li(1)-N(3)	-73.08(13)
C(17)-Cr(1)-Li(1)-N(4)	-110.42(15)
C(18)-Cr(1)-Li(1)-N(4)	-138.90(16)
N(3)-Cr(1)-Li(1)-N(4)	146.40(19)
C(19)-Cr(1)-Li(1)-N(4)	-136.9(5)
C(20)-Cr(1)-Li(1)-N(4)	-39.8(4)
N(1)-Cr(1)-Li(1)-N(4)	73.32(12)
N(4)-Cr(1)-Li(1)-N(2)	-72.64(15)
C(17)-Cr(1)-Li(1)-N(2)	176.94(16)
C(18)-Cr(1)-Li(1)-N(2)	148.45(16)
N(3)-Cr(1)-Li(1)-N(2)	73.76(15)
C(19)-Cr(1)-Li(1)-N(2)	150.4(4)
C(20)-Cr(1)-Li(1)-N(2)	-112.4(3)
N(1)-Cr(1)-Li(1)-N(2)	0.68(13)
N(4)-Cr(1)-Li(1)-P(1)	-104.93(14)
C(17)-Cr(1)-Li(1)-P(1)	144.65(11)
C(18)-Cr(1)-Li(1)-P(1)	116.16(14)
N(3)-Cr(1)-Li(1)-P(1)	41.47(9)
C(19)-Cr(1)-Li(1)-P(1)	118.1(5)
C(20)-Cr(1)-Li(1)-P(1)	-144.7(3)
N(1)-Cr(1)-Li(1)-P(1)	-31.61(8)
N(4)-Cr(1)-Li(1)-P(2)	-41.19(9)
C(17)-Cr(1)-Li(1)-P(2)	-151.61(11)
C(18)-Cr(1)-Li(1)-P(2)	179.91(13)
N(3)-Cr(1)-Li(1)-P(2)	105.21(14)
C(19)-Cr(1)-Li(1)-P(2)	-178.1(4)
C(20)-Cr(1)-Li(1)-P(2)	-81.0(3)
N(1)-Cr(1)-Li(1)-P(2)	32.13(7)
N(4)-Cr(1)-N(1)-C(1)	-131.2(2)
C(17)-Cr(1)-N(1)-C(1)	131.2(12)
C(18)-Cr(1)-N(1)-C(1)	44.6(3)
N(3)-Cr(1)-N(1)-C(1)	130.1(2)
C(19)-Cr(1)-N(1)-C(1)	10.0(3)
C(20)-Cr(1)-N(1)-C(1)	-28.6(3)
Li(1)-Cr(1)-N(1)-C(1)	179.2(2)
N(4)-Cr(1)-N(1)-P(2)	1.54(8)
C(17)-Cr(1)-N(1)-P(2)	-96.0(13)
C(18)-Cr(1)-N(1)-P(2)	177.39(18)

N(3)-Cr(1)-N(1)-P(2)	-97.17(10)
C(19)-Cr(1)-N(1)-P(2)	142.72(16)
C(20)-Cr(1)-N(1)-P(2)	104.21(16)
Li(1)-Cr(1)-N(1)-P(2)	-48.05(12)
N(4)-Cr(1)-N(1)-P(1)	96.47(10)
C(17)-Cr(1)-N(1)-P(1)	-1.1(13)
C(18)-Cr(1)-N(1)-P(1)	-87.7(2)
N(3)-Cr(1)-N(1)-P(1)	-2.24(8)
C(19)-Cr(1)-N(1)-P(1)	-122.35(16)
C(20)-Cr(1)-N(1)-P(1)	-160.86(16)
Li(1)-Cr(1)-N(1)-P(1)	46.88(12)
O(1)-Li(1)-N(2)-C(5)	-1.4(4)
N(3)-Li(1)-N(2)-C(5)	-130.8(2)
N(4)-Li(1)-N(2)-C(5)	130.6(2)
Cr(1)-Li(1)-N(2)-C(5)	179.23(18)
P(1)-Li(1)-N(2)-C(5)	-131.1(2)
P(2)-Li(1)-N(2)-C(5)	131.1(2)
O(1)-Li(1)-N(2)-P(2)	-132.5(3)
N(3)-Li(1)-N(2)-P(2)	98.03(14)
N(4)-Li(1)-N(2)-P(2)	-0.50(13)
Cr(1)-Li(1)-N(2)-P(2)	48.09(12)
P(1)-Li(1)-N(2)-P(2)	97.74(11)
O(1)-Li(1)-N(2)-P(1)	129.7(3)
N(3)-Li(1)-N(2)-P(1)	0.29(13)
N(4)-Li(1)-N(2)-P(1)	-98.24(14)
Cr(1)-Li(1)-N(2)-P(1)	-49.65(11)
P(2)-Li(1)-N(2)-P(1)	-97.74(11)
O(1)-Li(1)-N(3)-C(9)	1.4(5)
N(4)-Li(1)-N(3)-C(9)	-160.3(2)
N(2)-Li(1)-N(3)-C(9)	126.7(2)
Cr(1)-Li(1)-N(3)-C(9)	-135.4(2)
P(1)-Li(1)-N(3)-C(9)	127.0(3)
P(2)-Li(1)-N(3)-C(9)	165.0(2)
O(1)-Li(1)-N(3)-P(1)	-125.6(3)
N(4)-Li(1)-N(3)-P(1)	72.74(17)
N(2)-Li(1)-N(3)-P(1)	-0.31(13)
Cr(1)-Li(1)-N(3)-P(1)	97.61(10)
P(2)-Li(1)-N(3)-P(1)	38.04(12)
O(1)-Li(1)-N(3)-Cr(1)	136.8(3)
N(4)-Li(1)-N(3)-Cr(1)	-24.87(14)
N(2)-Li(1)-N(3)-Cr(1)	-97.92(12)
P(1)-Li(1)-N(3)-Cr(1)	-97.61(10)
P(2)-Li(1)-N(3)-Cr(1)	-59.57(9)
N(4)-Cr(1)-N(3)-C(9)	157.4(2)
C(17)-Cr(1)-N(3)-C(9)	48.3(2)
C(18)-Cr(1)-N(3)-C(9)	8.4(2)
C(19)-Cr(1)-N(3)-C(9)	-24.0(3)
C(20)-Cr(1)-N(3)-C(9)	-38.9(5)
N(1)-Cr(1)-N(3)-C(9)	-131.8(2)
Li(1)-Cr(1)-N(3)-C(9)	132.6(3)
N(4)-Cr(1)-N(3)-P(1)	-68.33(11)
C(17)-Cr(1)-N(3)-P(1)	-177.47(12)
C(18)-Cr(1)-N(3)-P(1)	142.65(14)
C(19)-Cr(1)-N(3)-P(1)	110.24(15)

C(20)-Cr(1)-N(3)-P(1)	95.4(4)
N(1)-Cr(1)-N(3)-P(1)	2.43(9)
Li(1)-Cr(1)-N(3)-P(1)	-93.17(17)
N(4)-Cr(1)-N(3)-Li(1)	24.84(15)
C(17)-Cr(1)-N(3)-Li(1)	-84.30(17)
C(18)-Cr(1)-N(3)-Li(1)	-124.18(18)
C(19)-Cr(1)-N(3)-Li(1)	-156.59(19)
C(20)-Cr(1)-N(3)-Li(1)	-171.4(4)
N(1)-Cr(1)-N(3)-Li(1)	95.60(15)
C(17)-Cr(1)-N(4)-C(13)	-53.0(2)
C(18)-Cr(1)-N(4)-C(13)	-43.0(3)
N(3)-Cr(1)-N(4)-C(13)	-157.1(2)
C(19)-Cr(1)-N(4)-C(13)	24.9(3)
C(20)-Cr(1)-N(4)-C(13)	28.8(3)
N(1)-Cr(1)-N(4)-C(13)	132.3(2)
Li(1)-Cr(1)-N(4)-C(13)	-132.4(3)
C(17)-Cr(1)-N(4)-P(2)	173.10(12)
C(18)-Cr(1)-N(4)-P(2)	-176.9(2)
N(3)-Cr(1)-N(4)-P(2)	68.96(10)
C(19)-Cr(1)-N(4)-P(2)	-109.1(2)
C(20)-Cr(1)-N(4)-P(2)	-105.18(14)
N(1)-Cr(1)-N(4)-P(2)	-1.67(9)
Li(1)-Cr(1)-N(4)-P(2)	93.64(16)
C(17)-Cr(1)-N(4)-Li(1)	79.46(17)
C(18)-Cr(1)-N(4)-Li(1)	89.4(3)
N(3)-Cr(1)-N(4)-Li(1)	-24.67(15)
C(19)-Cr(1)-N(4)-Li(1)	157.3(2)
C(20)-Cr(1)-N(4)-Li(1)	161.18(17)
N(1)-Cr(1)-N(4)-Li(1)	-95.30(15)
O(1)-Li(1)-N(4)-C(13)	-2.1(5)
N(3)-Li(1)-N(4)-C(13)	158.9(2)
N(2)-Li(1)-N(4)-C(13)	-127.5(2)
Cr(1)-Li(1)-N(4)-C(13)	133.5(3)
P(1)-Li(1)-N(4)-C(13)	-166.1(2)
P(2)-Li(1)-N(4)-C(13)	-128.0(3)
O(1)-Li(1)-N(4)-P(2)	125.9(3)
N(3)-Li(1)-N(4)-P(2)	-73.12(17)
N(2)-Li(1)-N(4)-P(2)	0.52(14)
Cr(1)-Li(1)-N(4)-P(2)	-98.46(11)
P(1)-Li(1)-N(4)-P(2)	-38.10(13)
O(1)-Li(1)-N(4)-Cr(1)	-135.6(3)
N(3)-Li(1)-N(4)-Cr(1)	25.34(14)
N(2)-Li(1)-N(4)-Cr(1)	98.98(13)
P(1)-Li(1)-N(4)-Cr(1)	60.37(9)
P(2)-Li(1)-N(4)-Cr(1)	98.46(11)
N(3)-Li(1)-O(1)-C(24)	10.5(5)
N(4)-Li(1)-O(1)-C(24)	165.3(3)
N(2)-Li(1)-O(1)-C(24)	-91.5(4)
Cr(1)-Li(1)-O(1)-C(24)	87.4(5)
P(1)-Li(1)-O(1)-C(24)	-40.8(5)
P(2)-Li(1)-O(1)-C(24)	-141.5(4)
N(3)-Li(1)-O(1)-C(21)	-167.7(3)
N(4)-Li(1)-O(1)-C(21)	-12.9(5)
N(2)-Li(1)-O(1)-C(21)	90.3(4)

Cr(1)-Li(1)-O(1)-C(21)	-90.8(5)
P(1)-Li(1)-O(1)-C(21)	141.1(3)
P(2)-Li(1)-O(1)-C(21)	40.3(5)
C(9)-N(3)-P(1)-N(2)	-135.20(19)
Li(1)-N(3)-P(1)-N(2)	0.38(16)
Cr(1)-N(3)-P(1)-N(2)	81.52(11)
C(9)-N(3)-P(1)-N(1)	140.43(19)
Li(1)-N(3)-P(1)-N(1)	-83.99(16)
Cr(1)-N(3)-P(1)-N(1)	-2.84(11)
C(9)-N(3)-P(1)-P(2)	-176.83(18)
Li(1)-N(3)-P(1)-P(2)	-41.25(15)
Cr(1)-N(3)-P(1)-P(2)	39.90(8)
C(9)-N(3)-P(1)-Li(1)	-135.6(3)
Cr(1)-N(3)-P(1)-Li(1)	81.14(15)
C(5)-N(2)-P(1)-N(3)	128.4(2)
P(2)-N(2)-P(1)-N(3)	-90.44(12)
Li(1)-N(2)-P(1)-N(3)	-0.37(16)
C(5)-N(2)-P(1)-N(1)	-136.9(2)
P(2)-N(2)-P(1)-N(1)	4.28(10)
Li(1)-N(2)-P(1)-N(1)	94.35(15)
C(5)-N(2)-P(1)-P(2)	-141.1(3)
Li(1)-N(2)-P(1)-P(2)	90.08(15)
C(5)-N(2)-P(1)-Li(1)	128.8(3)
P(2)-N(2)-P(1)-Li(1)	-90.08(15)
C(1)-N(1)-P(1)-N(3)	-137.2(2)
P(2)-N(1)-P(1)-N(3)	95.90(11)
Cr(1)-N(1)-P(1)-N(3)	2.78(10)
C(1)-N(1)-P(1)-N(2)	122.7(2)
P(2)-N(1)-P(1)-N(2)	-4.16(10)
Cr(1)-N(1)-P(1)-N(2)	-97.28(9)
C(1)-N(1)-P(1)-P(2)	126.9(2)
Cr(1)-N(1)-P(1)-P(2)	-93.12(10)
C(1)-N(1)-P(1)-Li(1)	174.2(2)
P(2)-N(1)-P(1)-Li(1)	47.33(12)
Cr(1)-N(1)-P(1)-Li(1)	-45.79(12)
O(1)-Li(1)-P(1)-N(3)	92.6(4)
N(4)-Li(1)-P(1)-N(3)	-106.4(2)
N(2)-Li(1)-P(1)-N(3)	179.5(2)
Cr(1)-Li(1)-P(1)-N(3)	-58.88(12)
P(2)-Li(1)-P(1)-N(3)	-132.48(16)
O(1)-Li(1)-P(1)-N(2)	-86.9(4)
N(3)-Li(1)-P(1)-N(2)	-179.5(2)
N(4)-Li(1)-P(1)-N(2)	74.06(16)
Cr(1)-Li(1)-P(1)-N(2)	121.60(15)
P(2)-Li(1)-P(1)-N(2)	48.00(10)
O(1)-Li(1)-P(1)-N(1)	-169.0(4)
N(3)-Li(1)-P(1)-N(1)	98.34(15)
N(4)-Li(1)-P(1)-N(1)	-8.08(15)
N(2)-Li(1)-P(1)-N(1)	-82.14(13)
Cr(1)-Li(1)-P(1)-N(1)	39.46(9)
P(2)-Li(1)-P(1)-N(1)	-34.14(9)
O(1)-Li(1)-P(1)-P(2)	-134.9(4)
N(3)-Li(1)-P(1)-P(2)	132.48(16)
N(4)-Li(1)-P(1)-P(2)	26.06(10)

N(2)-Li(1)-P(1)-P(2)	-48.00(10)
Cr(1)-Li(1)-P(1)-P(2)	73.59(7)
C(13)-N(4)-P(2)-N(2)	135.65(19)
Cr(1)-N(4)-P(2)-N(2)	-82.69(11)
Li(1)-N(4)-P(2)-N(2)	-0.64(17)
C(13)-N(4)-P(2)-N(1)	-139.70(19)
Cr(1)-N(4)-P(2)-N(1)	1.97(10)
Li(1)-N(4)-P(2)-N(1)	84.01(16)
C(13)-N(4)-P(2)-P(1)	177.28(18)
Cr(1)-N(4)-P(2)-P(1)	-41.06(8)
Li(1)-N(4)-P(2)-P(1)	40.98(15)
C(13)-N(4)-P(2)-Li(1)	136.3(3)
Cr(1)-N(4)-P(2)-Li(1)	-82.05(16)
C(5)-N(2)-P(2)-N(4)	-128.5(2)
P(1)-N(2)-P(2)-N(4)	90.17(12)
Li(1)-N(2)-P(2)-N(4)	0.62(16)
C(5)-N(2)-P(2)-N(1)	137.0(2)
P(1)-N(2)-P(2)-N(1)	-4.30(10)
Li(1)-N(2)-P(2)-N(1)	-93.85(15)
C(5)-N(2)-P(2)-P(1)	141.3(2)
Li(1)-N(2)-P(2)-P(1)	-89.55(16)
C(5)-N(2)-P(2)-Li(1)	-129.1(3)
P(1)-N(2)-P(2)-Li(1)	89.55(16)
C(1)-N(1)-P(2)-N(4)	138.11(19)
P(1)-N(1)-P(2)-N(4)	-95.55(10)
Cr(1)-N(1)-P(2)-N(4)	-1.88(10)
C(1)-N(1)-P(2)-N(2)	-122.17(19)
P(1)-N(1)-P(2)-N(2)	4.16(10)
Cr(1)-N(1)-P(2)-N(2)	97.84(9)
C(1)-N(1)-P(2)-P(1)	-126.3(2)
Cr(1)-N(1)-P(2)-P(1)	93.67(10)
C(1)-N(1)-P(2)-Li(1)	-173.4(2)
P(1)-N(1)-P(2)-Li(1)	-47.04(12)
Cr(1)-N(1)-P(2)-Li(1)	46.63(11)
N(3)-P(1)-P(2)-N(4)	0.06(12)
N(2)-P(1)-P(2)-N(4)	-96.63(13)
N(1)-P(1)-P(2)-N(4)	89.66(13)
Li(1)-P(1)-P(2)-N(4)	-34.12(14)
N(3)-P(1)-P(2)-N(2)	96.70(13)
N(1)-P(1)-P(2)-N(2)	-173.70(15)
Li(1)-P(1)-P(2)-N(2)	62.51(15)
N(3)-P(1)-P(2)-N(1)	-89.60(13)
N(2)-P(1)-P(2)-N(1)	173.70(15)
Li(1)-P(1)-P(2)-N(1)	-123.79(15)
N(3)-P(1)-P(2)-Li(1)	34.19(14)
N(2)-P(1)-P(2)-Li(1)	-62.51(15)
N(1)-P(1)-P(2)-Li(1)	123.79(15)
O(1)-Li(1)-P(2)-N(4)	-95.0(4)
N(3)-Li(1)-P(2)-N(4)	106.1(2)
N(2)-Li(1)-P(2)-N(4)	-179.2(2)
Cr(1)-Li(1)-P(2)-N(4)	57.62(13)
P(1)-Li(1)-P(2)-N(4)	132.44(17)
O(1)-Li(1)-P(2)-N(2)	84.2(4)
N(3)-Li(1)-P(2)-N(2)	-74.67(16)

N(4)-Li(1)-P(2)-N(2)	179.2(2)
Cr(1)-Li(1)-P(2)-N(2)	-123.19(15)
P(1)-Li(1)-P(2)-N(2)	-48.37(11)
O(1)-Li(1)-P(2)-N(1)	166.9(4)
N(3)-Li(1)-P(2)-N(1)	8.08(14)
N(4)-Li(1)-P(2)-N(1)	-98.06(15)
N(2)-Li(1)-P(2)-N(1)	82.75(14)
Cr(1)-Li(1)-P(2)-N(1)	-40.44(9)
P(1)-Li(1)-P(2)-N(1)	34.37(8)
O(1)-Li(1)-P(2)-P(1)	132.6(4)
N(3)-Li(1)-P(2)-P(1)	-26.29(9)
N(4)-Li(1)-P(2)-P(1)	-132.44(17)
N(2)-Li(1)-P(2)-P(1)	48.37(11)
Cr(1)-Li(1)-P(2)-P(1)	-74.82(7)
P(2)-N(1)-C(1)-C(3)	-179.80(18)
P(1)-N(1)-C(1)-C(3)	66.1(3)
Cr(1)-N(1)-C(1)-C(3)	-56.9(3)
P(2)-N(1)-C(1)-C(4)	59.8(3)
P(1)-N(1)-C(1)-C(4)	-54.4(3)
Cr(1)-N(1)-C(1)-C(4)	-177.33(19)
P(2)-N(1)-C(1)-C(2)	-60.4(3)
P(1)-N(1)-C(1)-C(2)	-174.6(2)
Cr(1)-N(1)-C(1)-C(2)	62.5(3)
P(2)-N(2)-C(5)-C(6)	-69.9(3)
P(1)-N(2)-C(5)-C(6)	61.5(3)
Li(1)-N(2)-C(5)-C(6)	175.5(2)
P(2)-N(2)-C(5)-C(7)	168.87(19)
P(1)-N(2)-C(5)-C(7)	-59.8(3)
Li(1)-N(2)-C(5)-C(7)	54.3(3)
P(2)-N(2)-C(5)-C(8)	50.7(3)
P(1)-N(2)-C(5)-C(8)	-177.93(19)
Li(1)-N(2)-C(5)-C(8)	-63.9(3)
P(1)-N(3)-C(9)-C(10)	-68.0(3)
Li(1)-N(3)-C(9)-C(10)	173.8(2)
Cr(1)-N(3)-C(9)-C(10)	60.4(3)
P(1)-N(3)-C(9)-C(11)	171.1(2)
Li(1)-N(3)-C(9)-C(11)	52.9(3)
Cr(1)-N(3)-C(9)-C(11)	-60.6(3)
P(1)-N(3)-C(9)-C(12)	52.9(3)
Li(1)-N(3)-C(9)-C(12)	-65.3(3)
Cr(1)-N(3)-C(9)-C(12)	-178.73(19)
P(2)-N(4)-C(13)-C(15)	-178.7(2)
Cr(1)-N(4)-C(13)-C(15)	53.4(3)
Li(1)-N(4)-C(13)-C(15)	-59.2(3)
P(2)-N(4)-C(13)-C(16)	-59.5(3)
Cr(1)-N(4)-C(13)-C(16)	172.54(19)
Li(1)-N(4)-C(13)-C(16)	59.9(3)
P(2)-N(4)-C(13)-C(14)	61.3(3)
Cr(1)-N(4)-C(13)-C(14)	-66.6(3)
Li(1)-N(4)-C(13)-C(14)	-179.2(2)
N(4)-Cr(1)-C(17)-C(18)	171.3(2)
N(3)-Cr(1)-C(17)-C(18)	-91.7(2)
C(19)-Cr(1)-C(17)-C(18)	30.3(2)
C(20)-Cr(1)-C(17)-C(18)	67.5(3)

N(1)-Cr(1)-C(17)-C(18)	-92.8(13)
Li(1)-Cr(1)-C(17)-C(18)	-140.4(2)
Cr(1)-C(17)-C(18)-C(19)	-56.1(3)
N(4)-Cr(1)-C(18)-C(19)	114.8(3)
C(17)-Cr(1)-C(18)-C(19)	129.9(4)
N(3)-Cr(1)-C(18)-C(19)	-133.4(3)
C(20)-Cr(1)-C(18)-C(19)	30.4(3)
N(1)-Cr(1)-C(18)-C(19)	-58.1(3)
Li(1)-Cr(1)-C(18)-C(19)	178.9(3)
N(4)-Cr(1)-C(18)-C(17)	-15.1(4)
N(3)-Cr(1)-C(18)-C(17)	96.7(2)
C(19)-Cr(1)-C(18)-C(17)	-129.9(4)
C(20)-Cr(1)-C(18)-C(17)	-99.5(3)
N(1)-Cr(1)-C(18)-C(17)	172.03(18)
Li(1)-Cr(1)-C(18)-C(17)	49.0(3)
C(17)-C(18)-C(19)-C(20)	-1.3(5)
Cr(1)-C(18)-C(19)-C(20)	-56.6(3)
C(17)-C(18)-C(19)-Cr(1)	55.3(3)
N(4)-Cr(1)-C(19)-C(18)	-122.9(3)
C(17)-Cr(1)-C(19)-C(18)	-31.3(2)
N(3)-Cr(1)-C(19)-C(18)	59.5(3)
C(20)-Cr(1)-C(19)-C(18)	-129.1(4)
N(1)-Cr(1)-C(19)-C(18)	144.0(2)
Li(1)-Cr(1)-C(19)-C(18)	-2.7(6)
N(4)-Cr(1)-C(19)-C(20)	6.2(4)
C(17)-Cr(1)-C(19)-C(20)	97.8(3)
C(18)-Cr(1)-C(19)-C(20)	129.1(4)
N(3)-Cr(1)-C(19)-C(20)	-171.4(2)
N(1)-Cr(1)-C(19)-C(20)	-86.8(3)
Li(1)-Cr(1)-C(19)-C(20)	126.4(5)
C(18)-C(19)-C(20)-Cr(1)	55.4(3)
N(4)-Cr(1)-C(20)-C(19)	-176.1(2)
C(17)-Cr(1)-C(20)-C(19)	-70.9(3)
C(18)-Cr(1)-C(20)-C(19)	-31.3(2)
N(3)-Cr(1)-C(20)-C(19)	20.9(5)
N(1)-Cr(1)-C(20)-C(19)	107.4(2)
Li(1)-Cr(1)-C(20)-C(19)	-145.7(3)
C(24)-O(1)-C(21)-C(22)	6.5(4)
Li(1)-O(1)-C(21)-C(22)	-175.0(3)
O(1)-C(21)-C(22)-C(23)	10.6(5)
C(21)-C(22)-C(23)-C(24)	-23.2(6)
C(21)-O(1)-C(24)-C(23)	-20.8(4)
Li(1)-O(1)-C(24)-C(23)	160.8(4)
C(22)-C(23)-C(24)-O(1)	27.4(6)

Symmetry transformations used to generate equivalent atoms:

Table 13. Crystal data and structure refinement for **4**.

Identification code	**4**
Empirical formula	C15 H33 Cr N2 P2
Formula weight	355.37
Temperature	200(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pnma
Unit cell dimensions	a = 13.5057(6) A alpha = 90 deg. b = 16.7235(8) A beta = 90 deg. c = 8.9182(4) A gamma = 90 deg.
Volume	2014.29(16) A^3
Z, Calculated density	4, 1.172 Mg/m^3
Absorption coefficient	0.721 mm^-1
F(000)	764
Crystal size	0.21 x 0.07 x 0.05 mm
Theta range for data collection	2.44 to 26.35 deg.
Limiting indices	-16<=h<=16, -20<=k<=20, -11<=l<=11
Reflections collected / unique	43166 / 2031 [R(int) = 0.1177]
Completeness to theta = 26.35	95.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9648 and 0.8633
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2031 / 0 / 97
Goodness-of-fit on F^2	1.086
Final R indices [I>2sigma(I)]	R1 = 0.0741, wR2 = 0.1053
R indices (all data)	R1 = 0.1182, wR2 = 0.1158
Largest diff. peak and hole	0.379 and -0.527 e.A^-3

Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **4.**
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cr(1)	9329(1)	7500	661(1)	25(1)
P(1)	8774(1)	7500	3632(2)	33(1)
P(2)	7709(1)	7500	-537(2)	30(1)
N(1)	8999(2)	6780(2)	2495(3)	28(1)
C(1)	8946(3)	5921(2)	2891(4)	40(1)
C(2)	8304(3)	5503(2)	1730(5)	64(1)
C(3)	9986(3)	5580(2)	2816(6)	61(1)
C(4)	8529(3)	5789(3)	4463(5)	65(1)
C(5)	6643(4)	7500	684(8)	77(2)
C(6)	7450(4)	6669(3)	-1752(5)	73(2)
C(7)	10039(3)	6677(3)	-909(5)	59(1)
C(8)	10761(3)	7090(3)	-83(5)	55(1)

Table 15. Bond lengths [A] and angles [deg] for **4.**

Cr(1)-N(1)#1	2.080(3)
Cr(1)-N(1)	2.080(3)
Cr(1)-C(8)#1	2.156(3)
Cr(1)-C(8)	2.156(3)
Cr(1)-C(7)#1	2.185(4)
Cr(1)-C(7)	2.185(4)
Cr(1)-P(2)	2.4348(14)
Cr(1)-P(1)	2.7538(16)
P(1)-N(1)#1	1.603(3)
P(1)-N(1)	1.603(3)
P(2)-C(5)	1.805(6)
P(2)-C(6)	1.797(4)
P(2)-C(6)#1	1.797(4)
N(1)-C(1)	1.482(4)
C(1)-C(3)	1.518(5)
C(1)-C(2)	1.520(5)
C(1)-C(4)	1.527(5)
C(7)-C(8)	1.404(6)
C(8)-C(8)#1	1.373(8)
N(1)#1-Cr(1)-N(1)	70.76(15)
N(1)#1-Cr(1)-C(8)#1	104.48(13)
N(1)-Cr(1)-C(8)#1	128.21(14)
N(1)#1-Cr(1)-C(8)	128.21(14)
N(1)-Cr(1)-C(8)	104.48(13)
C(8)#1-Cr(1)-C(8)	37.1(2)
N(1)#1-Cr(1)-C(7)#1	103.49(15)
N(1)-Cr(1)-C(7)#1	164.35(15)
C(8)#1-Cr(1)-C(7)#1	37.72(15)
C(8)-Cr(1)-C(7)#1	67.05(16)
N(1)#1-Cr(1)-C(7)	164.35(15)
N(1)-Cr(1)-C(7)	103.49(15)
C(8)#1-Cr(1)-C(7)	67.05(16)
C(8)-Cr(1)-C(7)	37.72(15)
C(7)#1-Cr(1)-C(7)	78.1(2)
N(1)#1-Cr(1)-P(2)	98.78(8)
N(1)-Cr(1)-P(2)	98.78(8)
C(8)#1-Cr(1)-P(2)	132.11(13)
C(8)-Cr(1)-P(2)	132.12(13)
C(7)#1-Cr(1)-P(2)	96.48(13)
C(7)-Cr(1)-P(2)	96.48(13)
N(1)#1-Cr(1)-P(1)	35.38(7)
N(1)-Cr(1)-P(1)	35.39(7)
C(8)#1-Cr(1)-P(1)	122.69(12)
C(8)-Cr(1)-P(1)	122.69(12)
C(7)#1-Cr(1)-P(1)	137.39(13)
C(7)-Cr(1)-P(1)	137.39(13)
P(2)-Cr(1)-P(1)	100.25(5)
N(1)#1-P(1)-N(1)	97.4(2)
N(1)#1-P(1)-Cr(1)	48.69(10)

N(1)-P(1)-Cr(1)	48.69(10)
C(5)-P(2)-C(6)	102.0(2)
C(5)-P(2)-C(6)#1	102.0(2)
C(6)-P(2)-C(6)#1	101.4(3)
C(5)-P(2)-Cr(1)	116.9(2)
C(6)-P(2)-Cr(1)	116.10(16)
C(6)#1-P(2)-Cr(1)	116.10(16)
C(1)-N(1)-P(1)	124.7(2)
C(1)-N(1)-Cr(1)	139.4(2)
P(1)-N(1)-Cr(1)	95.92(12)
N(1)-C(1)-C(3)	108.0(3)
N(1)-C(1)-C(2)	108.1(3)
C(3)-C(1)-C(2)	109.0(3)
N(1)-C(1)-C(4)	112.1(3)
C(3)-C(1)-C(4)	109.1(3)
C(2)-C(1)-C(4)	110.4(3)
C(8)-C(7)-Cr(1)	70.0(2)
C(8)#1-C(8)-C(7)	119.5(2)
C(8)#1-C(8)-Cr(1)	71.44(11)
C(7)-C(8)-Cr(1)	72.2(2)

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+3/2,z

Table 16. Anisotropic displacement parameters (A^2 x 10^3) for **4**. 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
Cr(1)	24(1)	27(1)	26(1)	0	2(1)	0
P(1)	37(1)	36(1)	25(1)	0	0(1)	0
P(2)	31(1)	32(1)	27(1)	0	-6(1)	0
N(1)	29(2)	26(2)	29(2)	6(1)	-3(1)	0(1)
C(1)	46(2)	26(2)	47(3)	11(2)	-11(2)	-1(2)
C(2)	84(3)	30(2)	78(4)	16(2)	-34(3)	-16(2)
C(3)	70(3)	33(2)	79(4)	6(2)	-18(2)	15(2)
C(4)	82(3)	49(3)	63(4)	32(2)	3(2)	-3(2)
C(5)	28(3)	137(7)	67(5)	0	1(3)	0
C(6)	90(4)	60(3)	68(4)	-29(3)	-47(3)	10(3)
C(7)	51(3)	61(3)	64(3)	-17(2)	15(2)	18(2)
C(8)	30(2)	83(3)	52(3)	-1(2)	17(2)	19(2)

Table 17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **4.**

	x	y	z	U(eq)
H(2A)	7629	5717	1779	96
H(2B)	8291	4928	1936	96
H(2C)	8577	5596	727	96
H(3A)	10405	5847	3559	91
H(3B)	10260	5667	1811	91
H(3C)	9965	5005	3028	91
H(4A)	8950	6060	5199	97
H(4B)	8512	5215	4683	97
H(4C)	7856	6006	4517	97
H(5A)	6703	7063	1411	116
H(5B)	6042	7425	86	116
H(5C)	6607	8011	1217	116
H(6A)	6784	6727	-2174	109
H(6B)	7488	6170	-1178	109
H(6C)	7936	6656	-2567	109
H(7A)	9555	6966	-1462	70
H(7B)	10033	6109	-915	70
H(8A)	11246	6803	471	66

Table 18. Torsion angles [deg] for **4.**

N(1)-Cr(1)-P(1)-N(1)#1	178.5(3)
C(8)#1-Cr(1)-P(1)-N(1)#1	67.01(18)
C(8)-Cr(1)-P(1)-N(1)#1	111.45(19)
C(7)#1-Cr(1)-P(1)-N(1)#1	20.7(2)
C(7)-Cr(1)-P(1)-N(1)#1	157.8(2)
P(2)-Cr(1)-P(1)-N(1)#1	-90.77(13)
N(1)#1-Cr(1)-P(1)-N(1)	-178.5(3)
C(8)#1-Cr(1)-P(1)-N(1)	-111.45(19)
C(8)-Cr(1)-P(1)-N(1)	-67.01(18)
C(7)#1-Cr(1)-P(1)-N(1)	-157.8(2)
C(7)-Cr(1)-P(1)-N(1)	-20.7(2)
P(2)-Cr(1)-P(1)-N(1)	90.77(13)
N(1)#1-Cr(1)-P(2)-C(5)	-35.86(7)
N(1)-Cr(1)-P(2)-C(5)	35.87(7)
C(8)#1-Cr(1)-P(2)-C(5)	-154.59(15)
C(8)-Cr(1)-P(2)-C(5)	154.59(15)
C(7)#1-Cr(1)-P(2)-C(5)	-140.64(12)
C(7)-Cr(1)-P(2)-C(5)	140.64(12)
P(1)-Cr(1)-P(2)-C(5)	0.0
N(1)#1-Cr(1)-P(2)-C(6)	-156.4(2)
N(1)-Cr(1)-P(2)-C(6)	-84.7(2)
C(8)#1-Cr(1)-P(2)-C(6)	84.9(3)
C(8)-Cr(1)-P(2)-C(6)	34.1(3)
C(7)#1-Cr(1)-P(2)-C(6)	98.8(2)
C(7)-Cr(1)-P(2)-C(6)	20.1(2)
P(1)-Cr(1)-P(2)-C(6)	-120.5(2)
N(1)#1-Cr(1)-P(2)-C(6)#1	84.7(2)
N(1)-Cr(1)-P(2)-C(6)#1	156.4(2)
C(8)#1-Cr(1)-P(2)-C(6)#1	-34.1(3)
C(8)-Cr(1)-P(2)-C(6)#1	-84.9(3)
C(7)#1-Cr(1)-P(2)-C(6)#1	-20.1(2)
C(7)-Cr(1)-P(2)-C(6)#1	-98.8(2)
P(1)-Cr(1)-P(2)-C(6)#1	120.5(2)
N(1)#1-P(1)-N(1)-C(1)	178.48(19)
Cr(1)-P(1)-N(1)-C(1)	179.6(3)
N(1)#1-P(1)-N(1)-Cr(1)	-1.16(19)
N(1)#1-Cr(1)-N(1)-C(1)	-178.6(3)
C(8)#1-Cr(1)-N(1)-C(1)	-85.0(4)
C(8)-Cr(1)-N(1)-C(1)	-52.7(4)
C(7)#1-Cr(1)-N(1)-C(1)	-107.9(6)
C(7)-Cr(1)-N(1)-C(1)	-13.8(4)
P(2)-Cr(1)-N(1)-C(1)	85.1(3)
P(1)-Cr(1)-N(1)-C(1)	-179.6(4)
N(1)#1-Cr(1)-N(1)-P(1)	0.94(16)
C(8)#1-Cr(1)-N(1)-P(1)	94.51(19)
C(8)-Cr(1)-N(1)-P(1)	126.85(16)
C(7)#1-Cr(1)-N(1)-P(1)	71.7(5)
C(7)-Cr(1)-N(1)-P(1)	165.76(16)
P(2)-Cr(1)-N(1)-P(1)	-95.36(11)
P(1)-N(1)-C(1)-C(3)	-113.3(3)

Cr(1)-N(1)-C(1)-C(3)	66.1(4)
P(1)-N(1)-C(1)-C(2)	128.9(3)
Cr(1)-N(1)-C(1)-C(2)	-51.7(5)
P(1)-N(1)-C(1)-C(4)	7.0(4)
Cr(1)-N(1)-C(1)-C(4)	-173.6(3)
N(1)#1-Cr(1)-C(7)-C(8)	-29.9(7)
N(1)-Cr(1)-C(7)-C(8)	-96.3(3)
C(8)#1-Cr(1)-C(7)-C(8)	29.8(2)
C(7)#1-Cr(1)-C(7)-C(8)	67.7(3)
P(2)-Cr(1)-C(7)-C(8)	163.0(2)
P(1)-Cr(1)-C(7)-C(8)	-84.2(3)
Cr(1)-C(7)-C(8)-C(8)#1	-55.61(16)
N(1)#1-Cr(1)-C(8)-C(8)#1	-59.14(12)
N(1)-Cr(1)-C(8)-C(8)#1	-135.85(10)
C(7)#1-Cr(1)-C(8)-C(8)#1	30.24(16)
C(7)-Cr(1)-C(8)-C(8)#1	130.7(2)
P(2)-Cr(1)-C(8)-C(8)#1	107.67(12)
P(1)-Cr(1)-C(8)-C(8)#1	-102.44(9)
N(1)#1-Cr(1)-C(8)-C(7)	170.1(2)
N(1)-Cr(1)-C(8)-C(7)	93.4(3)
C(8)#1-Cr(1)-C(8)-C(7)	-130.7(2)
C(7)#1-Cr(1)-C(8)-C(7)	-100.5(4)
P(2)-Cr(1)-C(8)-C(7)	-23.0(3)
P(1)-Cr(1)-C(8)-C(7)	126.8(2)

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+3/2,z

Table 19. Crystal data and structure refinement for **5**.

Identification code	**5**
Empirical formula	C24 H52 Li2 N4 O2 P2
Formula weight	504.52
Temperature	201(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 10.635(5) A alpha = 90 deg. b = 15.822(7) A beta = 105.545(7) deg. c = 19.350(8) A gamma = 90 deg.
Volume	3137(2) A^3
Z, Calculated density	4, 1.068 Mg/m^3
Absorption coefficient	0.163 mm^-1
F(000)	1104

Crystal size	0.23 x 0.21 x 0.16 mm
Theta range for data collection	1.99 to 25.55 deg.
Limiting indices	-12<=h<=12, -18<=k<=18, -22<=l<=23
Reflections collected / unique	21916 / 5385 [R(int) = 0.0639]
Completeness to theta = 25.00	96.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9744 and 0.9635
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5385 / 0 / 307
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0521, wR2 = 0.1287
R indices (all data)	R1 = 0.1037, wR2 = 0.1566
Largest diff. peak and hole	0.359 and -0.221 e.A^-3

Table 20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5.**
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Li(1)	1551(4)	2723(3)	679(3)	36(1)
Li(2)	3730(4)	2291(3)	1530(3)	37(1)
P(1)	1578(1)	2157(1)	2034(1)	36(1)
P(2)	2533(1)	3686(1)	1889(1)	33(1)
N(1)	1032(2)	3135(1)	1607(1)	33(1)
N(2)	3045(2)	2741(1)	2389(1)	35(1)
N(3)	1933(2)	1672(1)	1353(1)	34(1)
N(4)	3083(2)	3505(1)	1183(1)	31(1)
O(1)	473(2)	2768(1)	-309(1)	53(1)
O(2)	5315(2)	1730(1)	1425(1)	54(1)
C(1)	-248(3)	3515(2)	1587(2)	41(1)
C(2)	-371(4)	3726(3)	2333(2)	77(1)
C(3)	-400(3)	4320(2)	1140(2)	64(1)
C(4)	-1302(3)	2891(2)	1220(3)	84(2)
C(5)	3723(3)	2759(2)	3166(2)	46(1)
C(6)	2849(4)	3112(2)	3614(2)	58(1)
C(7)	4935(3)	3307(3)	3273(2)	65(1)

C(8)	4109(4)	1853(2)	3408(2)	65(1)
C(9)	1715(3)	747(2)	1259(2)	39(1)
C(10)	2036(4)	501(2)	564(2)	60(1)
C(11)	299(3)	510(2)	1209(2)	59(1)
C(12)	2607(3)	249(2)	1872(2)	57(1)
C(13)	3855(3)	4158(2)	931(2)	37(1)
C(14)	4122(4)	3828(2)	250(2)	59(1)
C(15)	3103(4)	4992(2)	766(2)	63(1)
C(16)	5160(3)	4321(2)	1485(2)	65(1)
C(17)	307(4)	3503(2)	-755(2)	59(1)
C(18)	-766(3)	3324(2)	-1417(2)	61(1)
C(19)	-1496(3)	2607(3)	-1181(2)	76(1)
C(20)	-439(3)	2138(2)	-660(2)	61(1)
C(21)	6273(4)	1357(3)	2003(2)	77(1)
C(22)	7056(4)	753(3)	1710(2)	75(1)
C(23)	6293(5)	658(3)	944(3)	88(1)
C(24)	5564(4)	1471(2)	770(2)	65(1)

Table 21. Bond lengths [A] and angles [deg] for **5.**

Li(1)-O(1)	1.950(5)
Li(1)-N(4)	2.070(5)
Li(1)-N(3)	2.085(5)
Li(1)-N(1)	2.119(6)
Li(1)-Li(2)	2.550(6)
Li(1)-P(2)	2.753(5)
Li(1)-P(1)	2.763(5)
Li(2)-O(2)	1.964(5)
Li(2)-N(4)	2.090(5)
Li(2)-N(3)	2.092(5)
Li(2)-N(2)	2.108(5)
Li(2)-P(1)	2.725(5)
Li(2)-P(2)	2.728(5)
P(1)-N(3)	1.654(2)
P(1)-N(1)	1.776(2)
P(1)-N(2)	1.785(2)
P(1)-P(2)	2.6666(13)
P(2)-N(4)	1.649(2)
P(2)-N(1)	1.771(2)
P(2)-N(2)	1.784(2)
N(1)-C(1)	1.478(3)
N(2)-C(5)	1.483(4)
N(3)-C(9)	1.484(3)

N(4)-C(13)	1.481(3)
O(1)-C(20)	1.429(4)
O(1)-C(17)	1.432(4)
O(2)-C(24)	1.423(4)
O(2)-C(21)	1.423(4)
C(1)-C(4)	1.518(5)
C(1)-C(3)	1.524(4)
C(1)-C(2)	1.521(5)
C(5)-C(8)	1.529(4)
C(5)-C(7)	1.521(5)
C(5)-C(6)	1.536(5)
C(9)-C(10)	1.525(4)
C(9)-C(12)	1.525(4)
C(9)-C(11)	1.530(4)
C(13)-C(14)	1.514(4)
C(13)-C(15)	1.532(4)
C(13)-C(16)	1.531(4)
C(17)-C(18)	1.496(4)
C(18)-C(19)	1.512(5)
C(19)-C(20)	1.492(5)
C(21)-C(22)	1.476(5)
C(22)-C(23)	1.495(6)
C(23)-C(24)	1.494(5)

O(1)-Li(1)-N(4)	128.4(3)
O(1)-Li(1)-N(3)	127.4(2)
N(4)-Li(1)-N(3)	100.7(2)

O(1)-Li(1)-N(1)	127.0(2)
N(4)-Li(1)-N(1)	76.59(18)
N(3)-Li(1)-N(1)	76.53(19)
O(1)-Li(1)-Li(2)	146.8(3)
N(4)-Li(1)-Li(2)	52.54(16)
N(3)-Li(1)-Li(2)	52.50(16)
N(1)-Li(1)-Li(2)	86.2(2)
O(1)-Li(1)-P(2)	143.4(2)
N(4)-Li(1)-P(2)	36.65(10)
N(3)-Li(1)-P(2)	86.78(18)
N(1)-Li(1)-P(2)	40.04(10)
Li(2)-Li(1)-P(2)	61.78(15)
O(1)-Li(1)-P(1)	142.8(2)
N(4)-Li(1)-P(1)	86.59(17)
N(3)-Li(1)-P(1)	36.65(10)
N(1)-Li(1)-P(1)	40.01(10)
Li(2)-Li(1)-P(1)	61.56(16)
P(2)-Li(1)-P(1)	57.82(10)
O(2)-Li(2)-N(4)	126.8(3)
O(2)-Li(2)-N(3)	122.9(2)
N(4)-Li(2)-N(3)	99.8(2)
O(2)-Li(2)-N(2)	136.2(3)
N(4)-Li(2)-N(2)	77.87(18)
N(3)-Li(2)-N(2)	78.15(19)
O(2)-Li(2)-Li(1)	135.3(3)
N(4)-Li(2)-Li(1)	51.83(15)
N(3)-Li(2)-Li(1)	52.24(15)

N(2)-Li(2)-Li(1)	88.4(2)
O(2)-Li(2)-P(1)	146.0(2)
N(4)-Li(2)-P(1)	87.20(16)
N(3)-Li(2)-P(1)	37.34(10)
N(2)-Li(2)-P(1)	40.90(11)
Li(1)-Li(2)-P(1)	63.07(16)
O(2)-Li(2)-P(2)	149.8(2)
N(4)-Li(2)-P(2)	37.14(10)
N(3)-Li(2)-P(2)	87.30(16)
N(2)-Li(2)-P(2)	40.82(10)
Li(1)-Li(2)-P(2)	62.77(15)
P(1)-Li(2)-P(2)	58.55(10)
N(3)-P(1)-N(1)	98.65(12)
N(3)-P(1)-N(2)	100.60(12)
N(1)-P(1)-N(2)	82.59(10)
N(3)-P(1)-P(2)	99.35(8)
N(1)-P(1)-P(2)	41.19(7)
N(2)-P(1)-P(2)	41.64(7)
N(3)-P(1)-Li(2)	50.08(12)
N(1)-P(1)-Li(2)	88.14(12)
N(2)-P(1)-Li(2)	50.65(13)
P(2)-P(1)-Li(2)	60.78(10)
N(3)-P(1)-Li(1)	48.78(12)
N(1)-P(1)-Li(1)	50.07(12)
N(2)-P(1)-Li(1)	89.02(12)
P(2)-P(1)-Li(1)	60.90(9)
Li(2)-P(1)-Li(1)	55.37(14)

N(4)-P(2)-N(1)	98.67(11)
N(4)-P(2)-N(2)	100.33(11)
N(1)-P(2)-N(2)	82.76(10)
N(4)-P(2)-P(1)	99.19(8)
N(1)-P(2)-P(1)	41.34(7)
N(2)-P(2)-P(1)	41.66(8)
N(4)-P(2)-Li(2)	49.90(13)
N(1)-P(2)-Li(2)	88.15(12)
N(2)-P(2)-Li(2)	50.57(13)
P(1)-P(2)-Li(2)	60.67(11)
N(4)-P(2)-Li(1)	48.51(12)
N(1)-P(2)-Li(1)	50.32(13)
N(2)-P(2)-Li(1)	89.35(12)
P(1)-P(2)-Li(1)	61.28(10)
Li(2)-P(2)-Li(1)	55.45(13)
C(1)-N(1)-P(2)	123.80(18)
C(1)-N(1)-P(1)	123.37(18)
P(2)-N(1)-P(1)	97.47(11)
C(1)-N(1)-Li(1)	123.3(2)
P(2)-N(1)-Li(1)	89.65(15)
P(1)-N(1)-Li(1)	89.92(15)
C(5)-N(2)-P(1)	122.47(19)
C(5)-N(2)-P(2)	121.91(18)
P(1)-N(2)-P(2)	96.70(11)
C(5)-N(2)-Li(2)	128.9(2)
P(1)-N(2)-Li(2)	88.46(16)
P(2)-N(2)-Li(2)	88.61(16)

C(9)-N(3)-P(1)	119.53(19)
C(9)-N(3)-Li(1)	135.4(2)
P(1)-N(3)-Li(1)	94.57(17)
C(9)-N(3)-Li(2)	126.0(2)
P(1)-N(3)-Li(2)	92.59(17)
Li(1)-N(3)-Li(2)	75.26(19)
C(13)-N(4)-P(2)	120.12(18)
C(13)-N(4)-Li(1)	134.3(2)
P(2)-N(4)-Li(1)	94.83(17)
C(13)-N(4)-Li(2)	125.7(2)
P(2)-N(4)-Li(2)	92.96(17)
Li(1)-N(4)-Li(2)	75.63(18)
C(20)-O(1)-C(17)	108.8(2)
C(20)-O(1)-Li(1)	125.9(2)
C(17)-O(1)-Li(1)	124.5(2)
C(24)-O(2)-C(21)	108.4(3)
C(24)-O(2)-Li(2)	126.3(2)
C(21)-O(2)-Li(2)	124.0(3)
N(1)-C(1)-C(4)	107.9(2)
N(1)-C(1)-C(3)	108.2(2)
C(4)-C(1)-C(3)	109.0(3)
N(1)-C(1)-C(2)	112.1(3)
C(4)-C(1)-C(2)	110.2(3)
C(3)-C(1)-C(2)	109.3(3)
N(2)-C(5)-C(8)	108.1(2)
N(2)-C(5)-C(7)	108.2(3)
C(8)-C(5)-C(7)	110.2(3)

N(2)-C(5)-C(6)	112.1(3)
C(8)-C(5)-C(6)	108.7(3)
C(7)-C(5)-C(6)	109.5(3)
N(3)-C(9)-C(10)	107.1(2)
N(3)-C(9)-C(12)	111.7(2)
C(10)-C(9)-C(12)	108.3(3)
N(3)-C(9)-C(11)	111.6(2)
C(10)-C(9)-C(11)	109.3(3)
C(12)-C(9)-C(11)	108.6(3)
N(4)-C(13)-C(14)	107.1(2)
N(4)-C(13)-C(15)	111.4(2)
C(14)-C(13)-C(15)	109.0(3)
N(4)-C(13)-C(16)	111.5(3)
C(14)-C(13)-C(16)	108.8(3)
C(15)-C(13)-C(16)	109.0(3)
O(1)-C(17)-C(18)	107.7(3)
C(17)-C(18)-C(19)	102.7(3)
C(20)-C(19)-C(18)	102.9(3)
O(1)-C(20)-C(19)	105.4(3)
O(2)-C(21)-C(22)	109.0(3)
C(21)-C(22)-C(23)	103.6(3)
C(24)-C(23)-C(22)	104.3(3)
O(2)-C(24)-C(23)	104.8(3)

Symmetry transformations used to generate equivalent atoms:

Table 22. Anisotropic displacement parameters (A^2 x 10^3) for **5.** 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
Li(1)	35(2)	32(2)	37(3)	1(2)	3(2)	-2(2)
Li(2)	34(2)	36(3)	39(3)	-1(2)	6(2)	5(2)
P(1)	40(1)	28(1)	43(1)	5(1)	17(1)	2(1)
P(2)	36(1)	27(1)	34(1)	-1(1)	9(1)	-2(1)
N(1)	33(1)	25(1)	44(2)	4(1)	13(1)	3(1)
N(2)	41(1)	34(1)	29(2)	5(1)	7(1)	3(1)
N(3)	38(1)	26(1)	39(2)	0(1)	13(1)	0(1)
N(4)	35(1)	28(1)	31(1)	0(1)	11(1)	-7(1)
O(1)	61(1)	42(1)	43(1)	4(1)	-9(1)	-7(1)
O(2)	43(1)	68(2)	50(2)	-4(1)	10(1)	16(1)
C(1)	36(2)	31(2)	61(2)	2(1)	19(2)	7(1)
C(2)	81(3)	85(3)	81(3)	8(2)	47(2)	34(2)
C(3)	50(2)	55(2)	88(3)	26(2)	22(2)	20(2)
C(4)	32(2)	58(2)	160(5)	-18(2)	24(2)	1(2)
C(5)	54(2)	49(2)	31(2)	1(1)	6(2)	8(2)
C(6)	75(2)	66(2)	36(2)	-2(2)	20(2)	7(2)

C(7)	53(2)	89(3)	42(2)	-2(2)	-6(2)	-2(2)
C(8)	90(3)	64(2)	35(2)	12(2)	7(2)	26(2)
C(9)	39(2)	27(1)	51(2)	-2(1)	13(1)	-2(1)
C(10)	79(3)	35(2)	70(3)	-12(2)	29(2)	-6(2)
C(11)	48(2)	35(2)	91(3)	-4(2)	16(2)	-8(1)
C(12)	61(2)	34(2)	74(3)	9(2)	13(2)	9(2)
C(13)	38(2)	33(2)	40(2)	-1(1)	11(1)	-8(1)
C(14)	73(2)	63(2)	50(2)	-4(2)	33(2)	-26(2)
C(15)	74(2)	37(2)	87(3)	15(2)	37(2)	-2(2)
C(16)	48(2)	78(3)	66(3)	-3(2)	13(2)	-30(2)
C(17)	68(2)	49(2)	49(2)	12(2)	-4(2)	-3(2)
C(18)	63(2)	54(2)	52(2)	4(2)	-6(2)	11(2)
C(19)	48(2)	93(3)	75(3)	-13(2)	-5(2)	-10(2)
C(20)	68(2)	50(2)	53(3)	-2(2)	-1(2)	-18(2)
C(21)	49(2)	111(3)	65(3)	7(2)	2(2)	26(2)
C(22)	64(2)	68(2)	101(4)	25(2)	33(2)	22(2)
C(23)	98(3)	73(3)	101(4)	-11(3)	40(3)	23(2)
C(24)	57(2)	82(3)	58(3)	-4(2)	18(2)	0(2)

Table 23. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **5.**

	x	y	z	U(eq)
H(2A)	-280	3208	2620	116
H(2B)	-1228	3979	2294	116
H(2C)	315	4127	2564	116
H(3A)	-324	4185	659	95
H(3B)	285	4723	1371	95
H(3C)	-1257	4571	1105	95
H(4A)	-1213	2761	740	126
H(4B)	-2163	3140	1179	126
H(4C)	-1210	2371	1504	126
H(6A)	2068	2759	3544	87
H(6B)	2592	3692	3461	87
H(6C)	3332	3111	4122	87
H(7A)	4676	3886	3118	97
H(7B)	5493	3080	2988	97
H(7C)	5416	3308	3782	97
H(8A)	3321	1506	3339	97
H(8B)	4590	1853	3916	97
H(8C)	4663	1620	3123	97

H(10A)	2943	651	595	90
H(10B)	1453	803	161	90
H(10C)	1917	-110	488	90
H(11A)	-286	822	814	88
H(11B)	97	654	1661	88
H(11C)	177	-98	1121	88
H(12A)	3519	391	1907	85
H(12B)	2469	-358	1780	85
H(12C)	2406	394	2323	85
H(14A)	4606	3295	351	88
H(14B)	4639	4243	69	88
H(14C)	3292	3731	-112	88
H(15A)	2268	4893	411	95
H(15B)	3618	5400	576	95
H(15C)	2943	5217	1207	95
H(16A)	5651	3791	1590	97
H(16B)	4998	4542	1927	97
H(16C)	5665	4735	1294	97
H(17A)	1126	3632	-885	71
H(17B)	77	3996	-499	71
H(18A)	-413	3150	-1819	73
H(18B)	-1336	3824	-1564	73
H(19A)	-2155	2823	-948	91
H(19B)	-1933	2244	-1592	91
H(20A)	-794	1830	-308	73
H(20B)	-17	1726	-912	73
H(21A)	5843	1059	2327	93

H(21B)	6847	1801	2282	93
H(22A)	7140	206	1966	90
H(22B)	7939	981	1746	90
H(23A)	6882	571	631	106
H(23B)	5684	174	885	106
H(24A)	6095	1899	602	78
H(24B)	4737	1387	393	78

Table 24. Torsion angles [deg] for **5**.

O(1)-Li(1)-Li(2)-O(2)	-1.8(7)
N(4)-Li(1)-Li(2)-O(2)	-106.8(4)
N(3)-Li(1)-Li(2)-O(2)	101.2(4)
N(1)-Li(1)-Li(2)-O(2)	177.1(3)
P(2)-Li(1)-Li(2)-O(2)	-149.5(4)
P(1)-Li(1)-Li(2)-O(2)	143.9(4)
O(1)-Li(1)-Li(2)-N(4)	105.0(5)
N(3)-Li(1)-Li(2)-N(4)	-152.0(3)
N(1)-Li(1)-Li(2)-N(4)	-76.03(18)
P(2)-Li(1)-Li(2)-N(4)	-42.62(11)
P(1)-Li(1)-Li(2)-N(4)	-109.25(18)
O(1)-Li(1)-Li(2)-N(3)	-103.0(5)
N(4)-Li(1)-Li(2)-N(3)	152.0(3)
N(1)-Li(1)-Li(2)-N(3)	75.95(18)
P(2)-Li(1)-Li(2)-N(3)	109.36(19)
P(1)-Li(1)-Li(2)-N(3)	42.73(12)
O(1)-Li(1)-Li(2)-N(2)	-179.2(4)
N(4)-Li(1)-Li(2)-N(2)	75.78(18)
N(3)-Li(1)-Li(2)-N(2)	-76.20(19)
N(1)-Li(1)-Li(2)-N(2)	-0.25(18)
P(2)-Li(1)-Li(2)-N(2)	33.16(11)
P(1)-Li(1)-Li(2)-N(2)	-33.47(11)
O(1)-Li(1)-Li(2)-P(1)	-145.7(4)

N(4)-Li(1)-Li(2)-P(1)	109.25(18)
N(3)-Li(1)-Li(2)-P(1)	-42.73(12)
N(1)-Li(1)-Li(2)-P(1)	33.22(11)
P(2)-Li(1)-Li(2)-P(1)	66.63(10)
O(1)-Li(1)-Li(2)-P(2)	147.6(5)
N(4)-Li(1)-Li(2)-P(2)	42.62(11)
N(3)-Li(1)-Li(2)-P(2)	-109.36(19)
N(1)-Li(1)-Li(2)-P(2)	-33.41(11)
P(1)-Li(1)-Li(2)-P(2)	-66.63(10)
O(2)-Li(2)-P(1)-N(3)	-70.1(4)
N(4)-Li(2)-P(1)-N(3)	110.2(2)
N(2)-Li(2)-P(1)-N(3)	-175.2(2)
Li(1)-Li(2)-P(1)-N(3)	62.20(17)
P(2)-Li(2)-P(1)-N(3)	135.29(16)
O(2)-Li(2)-P(1)-N(1)	-173.0(4)
N(4)-Li(2)-P(1)-N(1)	7.29(15)
N(3)-Li(2)-P(1)-N(1)	-102.91(15)
N(2)-Li(2)-P(1)-N(1)	81.93(14)
Li(1)-Li(2)-P(1)-N(1)	-40.71(15)
P(2)-Li(2)-P(1)-N(1)	32.38(9)
O(2)-Li(2)-P(1)-N(2)	105.1(4)
N(4)-Li(2)-P(1)-N(2)	-74.64(16)
N(3)-Li(2)-P(1)-N(2)	175.2(2)
Li(1)-Li(2)-P(1)-N(2)	-122.64(19)
P(2)-Li(2)-P(1)-N(2)	-49.55(11)
O(2)-Li(2)-P(1)-P(2)	154.7(5)
N(4)-Li(2)-P(1)-P(2)	-25.09(10)

N(3)-Li(2)-P(1)-P(2)	-135.29(16)
N(2)-Li(2)-P(1)-P(2)	49.55(11)
Li(1)-Li(2)-P(1)-P(2)	-73.09(13)
O(2)-Li(2)-P(1)-Li(1)	-132.3(5)
N(4)-Li(2)-P(1)-Li(1)	48.00(16)
N(3)-Li(2)-P(1)-Li(1)	-62.20(17)
N(2)-Li(2)-P(1)-Li(1)	122.64(19)
P(2)-Li(2)-P(1)-Li(1)	73.09(13)
O(1)-Li(1)-P(1)-N(3)	85.0(4)
N(4)-Li(1)-P(1)-N(3)	-113.1(2)
N(1)-Li(1)-P(1)-N(3)	173.8(2)
Li(2)-Li(1)-P(1)-N(3)	-64.41(17)
P(2)-Li(1)-P(1)-N(3)	-137.28(16)
O(1)-Li(1)-P(1)-N(1)	-88.8(4)
N(4)-Li(1)-P(1)-N(1)	73.12(16)
N(3)-Li(1)-P(1)-N(1)	-173.8(2)
Li(2)-Li(1)-P(1)-N(1)	121.78(19)
P(2)-Li(1)-P(1)-N(1)	48.91(11)
O(1)-Li(1)-P(1)-N(2)	-170.0(4)
N(4)-Li(1)-P(1)-N(2)	-8.02(15)
N(3)-Li(1)-P(1)-N(2)	105.05(15)
N(1)-Li(1)-P(1)-N(2)	-81.14(14)
Li(2)-Li(1)-P(1)-N(2)	40.63(15)
P(2)-Li(1)-P(1)-N(2)	-32.24(9)
O(1)-Li(1)-P(1)-P(2)	-137.7(4)
N(4)-Li(1)-P(1)-P(2)	24.21(10)
N(3)-Li(1)-P(1)-P(2)	137.28(16)

N(1)-Li(1)-P(1)-P(2)	-48.91(11)
Li(2)-Li(1)-P(1)-P(2)	72.87(14)
O(1)-Li(1)-P(1)-Li(2)	149.4(4)
N(4)-Li(1)-P(1)-Li(2)	-48.65(16)
N(3)-Li(1)-P(1)-Li(2)	64.41(17)
N(1)-Li(1)-P(1)-Li(2)	-121.77(19)
P(2)-Li(1)-P(1)-Li(2)	-72.87(14)
N(3)-P(1)-P(2)-N(4)	-0.22(11)
N(1)-P(1)-P(2)-N(4)	-92.71(14)
N(2)-P(1)-P(2)-N(4)	95.25(15)
Li(2)-P(1)-P(2)-N(4)	32.93(14)
Li(1)-P(1)-P(2)-N(4)	-31.36(13)
N(3)-P(1)-P(2)-N(1)	92.49(14)
N(2)-P(1)-P(2)-N(1)	-172.04(17)
Li(2)-P(1)-P(2)-N(1)	125.64(17)
Li(1)-P(1)-P(2)-N(1)	61.35(16)
N(3)-P(1)-P(2)-N(2)	-95.47(15)
N(1)-P(1)-P(2)-N(2)	172.04(17)
Li(2)-P(1)-P(2)-N(2)	-62.33(16)
Li(1)-P(1)-P(2)-N(2)	-126.61(16)
N(3)-P(1)-P(2)-Li(2)	-33.15(14)
N(1)-P(1)-P(2)-Li(2)	-125.64(17)
N(2)-P(1)-P(2)-Li(2)	62.33(16)
Li(1)-P(1)-P(2)-Li(2)	-64.29(16)
N(3)-P(1)-P(2)-Li(1)	31.14(13)
N(1)-P(1)-P(2)-Li(1)	-61.35(16)
N(2)-P(1)-P(2)-Li(1)	126.61(16)

Li(2)-P(1)-P(2)-Li(1)	64.29(16)
O(2)-Li(2)-P(2)-N(4)	73.0(5)
N(3)-Li(2)-P(2)-N(4)	-110.2(2)
N(2)-Li(2)-P(2)-N(4)	174.9(2)
Li(1)-Li(2)-P(2)-N(4)	-61.86(17)
P(1)-Li(2)-P(2)-N(4)	-135.45(16)
O(2)-Li(2)-P(2)-N(1)	175.9(5)
N(4)-Li(2)-P(2)-N(1)	102.96(15)
N(3)-Li(2)-P(2)-N(1)	-7.20(16)
N(2)-Li(2)-P(2)-N(1)	-82.14(14)
Li(1)-Li(2)-P(2)-N(1)	41.11(16)
P(1)-Li(2)-P(2)-N(1)	-32.49(10)
O(2)-Li(2)-P(2)-N(2)	-101.9(5)
N(4)-Li(2)-P(2)-N(2)	-174.9(2)
N(3)-Li(2)-P(2)-N(2)	74.94(18)
Li(1)-Li(2)-P(2)-N(2)	123.2(2)
P(1)-Li(2)-P(2)-N(2)	49.65(11)
O(2)-Li(2)-P(2)-P(1)	-151.6(5)
N(4)-Li(2)-P(2)-P(1)	135.45(16)
N(3)-Li(2)-P(2)-P(1)	25.29(11)
N(2)-Li(2)-P(2)-P(1)	-49.65(11)
Li(1)-Li(2)-P(2)-P(1)	73.60(14)
O(2)-Li(2)-P(2)-Li(1)	134.8(6)
N(4)-Li(2)-P(2)-Li(1)	61.86(17)
N(3)-Li(2)-P(2)-Li(1)	-48.31(16)
N(2)-Li(2)-P(2)-Li(1)	-123.2(2)
P(1)-Li(2)-P(2)-Li(1)	-73.60(14)

O(1)-Li(1)-P(2)-N(4)	-86.4(4)
N(3)-Li(1)-P(2)-N(4)	112.8(2)
N(1)-Li(1)-P(2)-N(4)	-174.4(2)
Li(2)-Li(1)-P(2)-N(4)	64.21(18)
P(1)-Li(1)-P(2)-N(4)	136.70(16)
O(1)-Li(1)-P(2)-N(1)	88.1(4)
N(4)-Li(1)-P(2)-N(1)	174.4(2)
N(3)-Li(1)-P(2)-N(1)	-72.80(17)
Li(2)-Li(1)-P(2)-N(1)	-121.4(2)
P(1)-Li(1)-P(2)-N(1)	-48.87(11)
O(1)-Li(1)-P(2)-N(2)	169.2(4)
N(4)-Li(1)-P(2)-N(2)	-104.45(15)
N(3)-Li(1)-P(2)-N(2)	8.32(16)
N(1)-Li(1)-P(2)-N(2)	81.12(14)
Li(2)-Li(1)-P(2)-N(2)	-40.24(16)
P(1)-Li(1)-P(2)-N(2)	32.25(9)
O(1)-Li(1)-P(2)-P(1)	136.9(4)
N(4)-Li(1)-P(2)-P(1)	-136.70(16)
N(3)-Li(1)-P(2)-P(1)	-23.93(10)
N(1)-Li(1)-P(2)-P(1)	48.87(11)
Li(2)-Li(1)-P(2)-P(1)	-72.49(15)
O(1)-Li(1)-P(2)-Li(2)	-150.6(5)
N(4)-Li(1)-P(2)-Li(2)	-64.21(18)
N(3)-Li(1)-P(2)-Li(2)	48.56(17)
N(1)-Li(1)-P(2)-Li(2)	121.4(2)
P(1)-Li(1)-P(2)-Li(2)	72.49(15)
N(4)-P(2)-N(1)-C(1)	-126.9(2)

N(2)-P(2)-N(1)-C(1)	133.7(2)
P(1)-P(2)-N(1)-C(1)	139.1(3)
Li(2)-P(2)-N(1)-C(1)	-175.8(2)
Li(1)-P(2)-N(1)-C(1)	-131.1(3)
N(4)-P(2)-N(1)-P(1)	94.09(12)
N(2)-P(2)-N(1)-P(1)	-5.33(11)
Li(2)-P(2)-N(1)-P(1)	45.14(14)
Li(1)-P(2)-N(1)-P(1)	89.87(16)
N(4)-P(2)-N(1)-Li(1)	4.22(15)
N(2)-P(2)-N(1)-Li(1)	-95.19(15)
P(1)-P(2)-N(1)-Li(1)	-89.87(16)
Li(2)-P(2)-N(1)-Li(1)	-44.72(17)
N(3)-P(1)-N(1)-C(1)	126.4(2)
N(2)-P(1)-N(1)-C(1)	-134.0(2)
P(2)-P(1)-N(1)-C(1)	-139.3(3)
Li(2)-P(1)-N(1)-C(1)	175.5(2)
Li(1)-P(1)-N(1)-C(1)	131.1(3)
N(3)-P(1)-N(1)-P(2)	-94.34(12)
N(2)-P(1)-N(1)-P(2)	5.33(11)
Li(2)-P(1)-N(1)-P(2)	-45.21(13)
Li(1)-P(1)-N(1)-P(2)	-89.63(16)
N(3)-P(1)-N(1)-Li(1)	-4.70(16)
N(2)-P(1)-N(1)-Li(1)	94.96(15)
P(2)-P(1)-N(1)-Li(1)	89.63(16)
Li(2)-P(1)-N(1)-Li(1)	44.42(16)
O(1)-Li(1)-N(1)-C(1)	-0.3(4)
N(4)-Li(1)-N(1)-C(1)	128.0(2)

N(3)-Li(1)-N(1)-C(1)	-127.3(2)
Li(2)-Li(1)-N(1)-C(1)	-179.6(2)
P(2)-Li(1)-N(1)-C(1)	131.4(2)
P(1)-Li(1)-N(1)-C(1)	-131.1(2)
O(1)-Li(1)-N(1)-P(2)	-131.8(3)
N(4)-Li(1)-N(1)-P(2)	-3.41(12)
N(3)-Li(1)-N(1)-P(2)	101.26(14)
Li(2)-Li(1)-N(1)-P(2)	48.95(15)
P(1)-Li(1)-N(1)-P(2)	97.47(11)
O(1)-Li(1)-N(1)-P(1)	130.8(3)
N(4)-Li(1)-N(1)-P(1)	-100.89(14)
N(3)-Li(1)-N(1)-P(1)	3.79(13)
Li(2)-Li(1)-N(1)-P(1)	-48.52(15)
P(2)-Li(1)-N(1)-P(1)	-97.47(11)
N(3)-P(1)-N(2)-C(5)	-132.9(2)
N(1)-P(1)-N(2)-C(5)	129.6(2)
P(2)-P(1)-N(2)-C(5)	134.9(3)
Li(2)-P(1)-N(2)-C(5)	-136.7(3)
Li(1)-P(1)-N(2)-C(5)	179.4(2)
N(3)-P(1)-N(2)-P(2)	92.19(12)
N(1)-P(1)-N(2)-P(2)	-5.28(11)
Li(2)-P(1)-N(2)-P(2)	88.41(16)
Li(1)-P(1)-N(2)-P(2)	44.55(13)
N(3)-P(1)-N(2)-Li(2)	3.78(16)
N(1)-P(1)-N(2)-Li(2)	-93.69(16)
P(2)-P(1)-N(2)-Li(2)	-88.41(16)
Li(1)-P(1)-N(2)-Li(2)	-43.87(16)

N(4)-P(2)-N(2)-C(5)	132.5(2)
N(1)-P(2)-N(2)-C(5)	-129.9(2)
P(1)-P(2)-N(2)-C(5)	-135.2(3)
Li(2)-P(2)-N(2)-C(5)	136.5(3)
Li(1)-P(2)-N(2)-C(5)	-180.0(2)
N(4)-P(2)-N(2)-P(1)	-92.25(12)
N(1)-P(2)-N(2)-P(1)	5.29(11)
Li(2)-P(2)-N(2)-P(1)	-88.28(16)
Li(1)-P(2)-N(2)-P(1)	-44.74(13)
N(4)-P(2)-N(2)-Li(2)	-3.97(16)
N(1)-P(2)-N(2)-Li(2)	93.58(16)
P(1)-P(2)-N(2)-Li(2)	88.28(16)
Li(1)-P(2)-N(2)-Li(2)	43.54(17)
O(2)-Li(2)-N(2)-C(5)	3.3(5)
N(4)-Li(2)-N(2)-C(5)	-128.1(3)
N(3)-Li(2)-N(2)-C(5)	129.0(2)
Li(1)-Li(2)-N(2)-C(5)	-179.4(2)
P(1)-Li(2)-N(2)-C(5)	132.0(3)
P(2)-Li(2)-N(2)-C(5)	-131.3(3)
O(2)-Li(2)-N(2)-P(1)	-128.7(3)
N(4)-Li(2)-N(2)-P(1)	99.89(14)
N(3)-Li(2)-N(2)-P(1)	-3.00(13)
Li(1)-Li(2)-N(2)-P(1)	48.68(15)
P(2)-Li(2)-N(2)-P(1)	96.74(11)
O(2)-Li(2)-N(2)-P(2)	134.6(3)
N(4)-Li(2)-N(2)-P(2)	3.15(13)
N(3)-Li(2)-N(2)-P(2)	-99.74(14)

Li(1)-Li(2)-N(2)-P(2)	-48.06(16)
P(1)-Li(2)-N(2)-P(2)	-96.74(11)
N(1)-P(1)-N(3)-C(9)	-145.22(19)
N(2)-P(1)-N(3)-C(9)	130.77(19)
P(2)-P(1)-N(3)-C(9)	173.07(18)
Li(2)-P(1)-N(3)-C(9)	134.6(3)
Li(1)-P(1)-N(3)-C(9)	-150.0(3)
N(1)-P(1)-N(3)-Li(1)	4.80(16)
N(2)-P(1)-N(3)-Li(1)	-79.22(16)
P(2)-P(1)-N(3)-Li(1)	-36.92(14)
Li(2)-P(1)-N(3)-Li(1)	-75.41(19)
N(1)-P(1)-N(3)-Li(2)	80.20(16)
N(2)-P(1)-N(3)-Li(2)	-3.81(16)
P(2)-P(1)-N(3)-Li(2)	38.48(15)
Li(1)-P(1)-N(3)-Li(2)	75.41(19)
O(1)-Li(1)-N(3)-C(9)	11.1(5)
N(4)-Li(1)-N(3)-C(9)	-149.1(3)
N(1)-Li(1)-N(3)-C(9)	137.7(3)
Li(2)-Li(1)-N(3)-C(9)	-126.8(3)
P(2)-Li(1)-N(3)-C(9)	176.8(2)
P(1)-Li(1)-N(3)-C(9)	141.7(3)
O(1)-Li(1)-N(3)-P(1)	-130.7(3)
N(4)-Li(1)-N(3)-P(1)	69.2(2)
N(1)-Li(1)-N(3)-P(1)	-4.09(14)
Li(2)-Li(1)-N(3)-P(1)	91.48(17)
P(2)-Li(1)-N(3)-P(1)	35.10(13)
O(1)-Li(1)-N(3)-Li(2)	137.9(4)

N(4)-Li(1)-N(3)-Li(2)	-22.3(2)
N(1)-Li(1)-N(3)-Li(2)	-95.56(19)
P(2)-Li(1)-N(3)-Li(2)	-56.37(16)
P(1)-Li(1)-N(3)-Li(2)	-91.48(17)
O(2)-Li(2)-N(3)-C(9)	11.2(4)
N(4)-Li(2)-N(3)-C(9)	158.0(2)
N(2)-Li(2)-N(3)-C(9)	-126.8(2)
Li(1)-Li(2)-N(3)-C(9)	135.9(3)
P(1)-Li(2)-N(3)-C(9)	-130.0(3)
P(2)-Li(2)-N(3)-C(9)	-166.9(2)
O(2)-Li(2)-N(3)-P(1)	141.2(3)
N(4)-Li(2)-N(3)-P(1)	-72.0(2)
N(2)-Li(2)-N(3)-P(1)	3.24(14)
Li(1)-Li(2)-N(3)-P(1)	-94.05(17)
P(2)-Li(2)-N(3)-P(1)	-36.93(13)
O(2)-Li(2)-N(3)-Li(1)	-124.7(3)
N(4)-Li(2)-N(3)-Li(1)	22.0(2)
N(2)-Li(2)-N(3)-Li(1)	97.29(19)
P(1)-Li(2)-N(3)-Li(1)	94.05(17)
P(2)-Li(2)-N(3)-Li(1)	57.12(17)
N(1)-P(2)-N(4)-C(13)	145.0(2)
N(2)-P(2)-N(4)-C(13)	-130.9(2)
P(1)-P(2)-N(4)-C(13)	-173.18(18)
Li(2)-P(2)-N(4)-C(13)	-134.9(3)
Li(1)-P(2)-N(4)-C(13)	149.3(3)
N(1)-P(2)-N(4)-Li(1)	-4.33(16)
N(2)-P(2)-N(4)-Li(1)	79.82(16)

P(1)-P(2)-N(4)-Li(1)	37.54(14)
Li(2)-P(2)-N(4)-Li(1)	75.82(19)
N(1)-P(2)-N(4)-Li(2)	-80.15(16)
N(2)-P(2)-N(4)-Li(2)	4.01(16)
P(1)-P(2)-N(4)-Li(2)	-38.28(14)
Li(1)-P(2)-N(4)-Li(2)	-75.82(19)
O(1)-Li(1)-N(4)-C(13)	-11.3(5)
N(3)-Li(1)-N(4)-C(13)	148.6(3)
N(1)-Li(1)-N(4)-C(13)	-138.2(3)
Li(2)-Li(1)-N(4)-C(13)	126.3(3)
P(2)-Li(1)-N(4)-C(13)	-141.9(3)
P(1)-Li(1)-N(4)-C(13)	-177.4(2)
O(1)-Li(1)-N(4)-P(2)	130.6(3)
N(3)-Li(1)-N(4)-P(2)	-69.5(2)
N(1)-Li(1)-N(4)-P(2)	3.68(13)
Li(2)-Li(1)-N(4)-P(2)	-91.83(18)
P(1)-Li(1)-N(4)-P(2)	-35.56(12)
O(1)-Li(1)-N(4)-Li(2)	-137.6(4)
N(3)-Li(1)-N(4)-Li(2)	22.3(2)
N(1)-Li(1)-N(4)-Li(2)	95.51(19)
P(2)-Li(1)-N(4)-Li(2)	91.83(18)
P(1)-Li(1)-N(4)-Li(2)	56.27(17)
O(2)-Li(2)-N(4)-C(13)	-12.0(4)
N(3)-Li(2)-N(4)-C(13)	-156.9(2)
N(2)-Li(2)-N(4)-C(13)	127.6(2)
Li(1)-Li(2)-N(4)-C(13)	-134.8(3)
P(1)-Li(2)-N(4)-C(13)	167.8(2)

P(2)-Li(2)-N(4)-C(13)	131.0(3)
O(2)-Li(2)-N(4)-P(2)	-143.0(3)
N(3)-Li(2)-N(4)-P(2)	72.1(2)
N(2)-Li(2)-N(4)-P(2)	-3.41(14)
Li(1)-Li(2)-N(4)-P(2)	94.24(18)
P(1)-Li(2)-N(4)-P(2)	36.81(12)
O(2)-Li(2)-N(4)-Li(1)	122.8(3)
N(3)-Li(2)-N(4)-Li(1)	-22.1(2)
N(2)-Li(2)-N(4)-Li(1)	-97.6(2)
P(1)-Li(2)-N(4)-Li(1)	-57.43(17)
P(2)-Li(2)-N(4)-Li(1)	-94.24(18)
N(4)-Li(1)-O(1)-C(20)	169.8(3)
N(3)-Li(1)-O(1)-C(20)	15.0(5)
N(1)-Li(1)-O(1)-C(20)	-87.0(4)
Li(2)-Li(1)-O(1)-C(20)	91.6(5)
P(2)-Li(1)-O(1)-C(20)	-140.7(4)
P(1)-Li(1)-O(1)-C(20)	-33.4(5)
N(4)-Li(1)-O(1)-C(17)	-21.7(5)
N(3)-Li(1)-O(1)-C(17)	-176.5(3)
N(1)-Li(1)-O(1)-C(17)	81.4(4)
Li(2)-Li(1)-O(1)-C(17)	-99.9(5)
P(2)-Li(1)-O(1)-C(17)	27.8(5)
P(1)-Li(1)-O(1)-C(17)	135.0(3)
N(4)-Li(2)-O(2)-C(24)	-66.8(4)
N(3)-Li(2)-O(2)-C(24)	70.8(4)
N(2)-Li(2)-O(2)-C(24)	179.5(3)
Li(1)-Li(2)-O(2)-C(24)	3.3(5)

P(1)-Li(2)-O(2)-C(24)	113.5(4)
P(2)-Li(2)-O(2)-C(24)	-113.0(5)
N(4)-Li(2)-O(2)-C(21)	127.5(4)
N(3)-Li(2)-O(2)-C(21)	-95.0(4)
N(2)-Li(2)-O(2)-C(21)	13.7(5)
Li(1)-Li(2)-O(2)-C(21)	-162.5(3)
P(1)-Li(2)-O(2)-C(21)	-52.2(5)
P(2)-Li(2)-O(2)-C(21)	81.3(6)
P(2)-N(1)-C(1)-C(4)	172.1(3)
P(1)-N(1)-C(1)-C(4)	-59.0(4)
Li(1)-N(1)-C(1)-C(4)	56.5(4)
P(2)-N(1)-C(1)-C(3)	54.3(3)
P(1)-N(1)-C(1)-C(3)	-176.8(2)
Li(1)-N(1)-C(1)-C(3)	-61.3(3)
P(2)-N(1)-C(1)-C(2)	-66.3(3)
P(1)-N(1)-C(1)-C(2)	62.6(3)
Li(1)-N(1)-C(1)-C(2)	178.2(3)
P(1)-N(2)-C(5)-C(8)	60.2(3)
P(2)-N(2)-C(5)-C(8)	-175.8(2)
Li(2)-N(2)-C(5)-C(8)	-58.0(4)
P(1)-N(2)-C(5)-C(7)	179.5(2)
P(2)-N(2)-C(5)-C(7)	-56.5(3)
Li(2)-N(2)-C(5)-C(7)	61.3(3)
P(1)-N(2)-C(5)-C(6)	-59.6(3)
P(2)-N(2)-C(5)-C(6)	64.3(3)
Li(2)-N(2)-C(5)-C(6)	-177.9(3)
P(1)-N(3)-C(9)-C(10)	176.0(2)

Li(1)-N(3)-C(9)-C(10)	41.2(4)
Li(2)-N(3)-C(9)-C(10)	-65.6(3)
P(1)-N(3)-C(9)-C(12)	-65.6(3)
Li(1)-N(3)-C(9)-C(12)	159.6(3)
Li(2)-N(3)-C(9)-C(12)	52.9(4)
P(1)-N(3)-C(9)-C(11)	56.3(3)
Li(1)-N(3)-C(9)-C(11)	-78.5(4)
Li(2)-N(3)-C(9)-C(11)	174.7(3)
P(2)-N(4)-C(13)-C(14)	-175.8(2)
Li(1)-N(4)-C(13)-C(14)	-41.2(4)
Li(2)-N(4)-C(13)-C(14)	64.8(3)
P(2)-N(4)-C(13)-C(15)	-56.8(3)
Li(1)-N(4)-C(13)-C(15)	77.9(4)
Li(2)-N(4)-C(13)-C(15)	-176.1(3)
P(2)-N(4)-C(13)-C(16)	65.2(3)
Li(1)-N(4)-C(13)-C(16)	-160.1(3)
Li(2)-N(4)-C(13)-C(16)	-54.1(4)
C(20)-O(1)-C(17)-C(18)	0.2(4)
Li(1)-O(1)-C(17)-C(18)	-170.0(3)
O(1)-C(17)-C(18)-C(19)	20.9(4)
C(17)-C(18)-C(19)-C(20)	-33.0(4)
C(17)-O(1)-C(20)-C(19)	-21.7(4)
Li(1)-O(1)-C(20)-C(19)	148.2(3)
C(18)-C(19)-C(20)-O(1)	34.1(4)
C(24)-O(2)-C(21)-C(22)	-7.5(4)
Li(2)-O(2)-C(21)-C(22)	160.4(3)
O(2)-C(21)-C(22)-C(23)	-12.6(5)

C(21)-C(22)-C(23)-C(24)	26.8(4)
C(21)-O(2)-C(24)-C(23)	24.5(4)
Li(2)-O(2)-C(24)-C(23)	-143.1(3)
C(22)-C(23)-C(24)-O(2)	-31.9(4)

Symmetry transformations used to generate equivalent atoms: