X-Ray Data for compound 5c

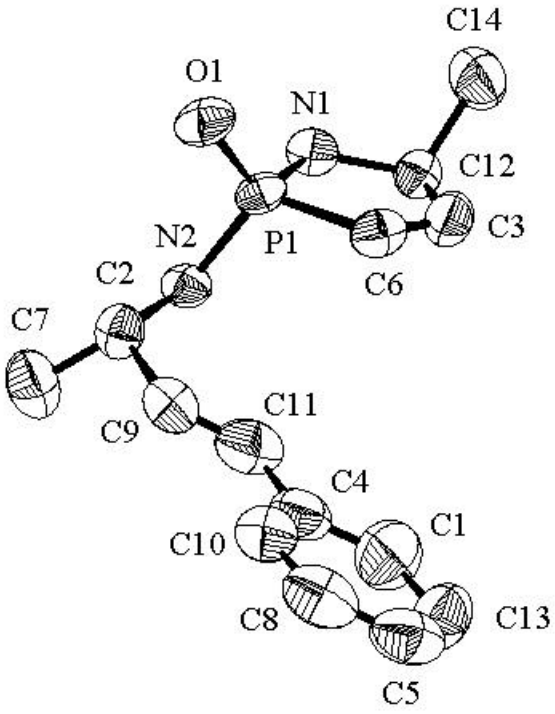

Figure 1. X-ray structure for compound **5c** (50% thermal ellipsoids, hydrogen atoms are omitted for clarity).

Table 1. Crystal data and structure refinement for **5c**.

Empirical formula	$C_{14}H_{19}N_2OP$	
Formula weight	262.28	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 9.5311(12) Å b = 5.0488(6) Å c = 16.058(2) Å	α = 90 deg. β = 105.548(2) deg. γ = 90 deg.
Volume, Z	744.5(2) $Å^3$, 2	
Density (calculated)	1.170 g/cm^3	
Absorption coefficient	0.176 mm^{-1}	
F(000)	280	
Crystal size	0.20 x 0.18 x 0.15 mm	
θ range for data collection	1.32 to 23.28 deg.	
Index ranges	-10<=h<=8, -5<=k<=5, -17<=l<=17	
Reflections collected	3116	
Independent reflections	1973 [R(int) = 0.0434]	
Refinement method	Full-matrix least-squares on F^2	
Data / parameters	1973 / 168	
Goodness-of-fit on F^2	1.097	
Final R indices [I>2σ(I)]	R1 = 0.0469, wR2 = 0.1397	
R indices (all data)	R1 = 0.05045, wR2 = 0.1481	
Largest diff. peak and hole	0.265 and -0.226 e. $Å^{-3}$	

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

Atom	x	y	z	U(eq)
P(1)	8072(2)	6640(3)	3969(1)	48(1)
O(1)	8369(5)	9465(9)	3834(3)	68(1)
N(1)	8684(6)	5383(10)	4935(3)	52(1)
N(2)	8723(6)	4851(10)	3309(3)	52(2)
C(1)	3740(11)	1355(30)	1578(7)	112(3)
C(2)	8527(8)	5613(14)	2413(5)	63(2)
C(3)	6189(8)	4572(17)	4632(5)	71(2)
C(4)	4559(9)	3209(27)	1337(6)	90(3)
C(5)	1726(11)	2211(25)	381(8)	104(4)
C(6)	6247(8)	5857(15)	3940(5)	64(2)
C(7)	9702(9)	4305(21)	2061(5)	89(3)
C(8)	2485(14)	4077(28)	103(6)	114(4)
C(9)	7026(11)	5047(22)	1821(6)	96(3)
C(10)	3933(13)	4620(24)	594(7)	106(3)
C(11)	6082(13)	3601(22)	1912(6)	104(3)
C(12)	7625(8)	4020(14)	5277(5)	61(2)
C(13)	2336(12)	831(24)	1108(8)	115(4)
C(14)	7652(10)	5081(21)	6184(5)	95(3)
H(1)	4135(11)	392(30)	2080(7)	135
H(3)	5310(8)	4026(17)	4723(5)	85
H(5)	771(11)	1859(25)	71(8)	125
H(6)	5440(8)	6304(15)	3492(5)	77
H(7A)	10645(9)	4665(21)	2443(5)	134
H(7B)	9654(9)	5006(21)	1498(5)	134
H(7C)	9544(9)	2426(21)	2020(5)	134
H(8)	2072(14)	5006(28)	9597(6)	137
H(9)	6802(11)	5976(22)	1302(6)	116
H(10)	4465(13)	5941(24)	413(7)	127
H(11)	6321(13)	2569(22)	2410(6)	124
H(13)	1802(12)	9520(24)	1292(8)	138
H(14A)	8577(10)	4683(21)	6580(5)	143
H(14B)	6890(10)	4254(21)	6379(5)	143
H(14C)	7507(10)	6964(21)	6156(5)	143
H(15)	9794(10)	5181(21)	5206(5)	98(26)
H(16)	8794(10)	2923(21)	3404(5)	61(19)
H(17)	8602(10)	7904(21)	2373(5)	103(26)
H(18)	7802(10)	1644(21)	5282(5)	90(21)

Table 3. Bond lengths [Å] and angles [deg] for **5c**.

P(1)-O(1)	1.481(5)
P(1)-N(2)	1.636(5)
P(1)-N(1)	1.633(5)
P(1)-C(6)	1.772(8)
N(1)-C(12)	1.446(8)
N(2)-C(2)	1.452(9)
C(1)-C(4)	1.34(2)
C(1)-C(13)	1.375(13)
C(2)-C(7)	1.533(10)
C(2)-C(9)	1.518(12)
C(3)-C(6)	1.300(10)
C(3)-C(12)	1.505(10)
C(4)-C(10)	1.38(2)
C(4)-C(11)	1.510(13)
C(5)-C(8)	1.335(14)
C(5)-C(13)	1.350(14)
C(8)-C(10)	1.421(14)
C(9)-C(11)	1.198(12)
C(12)-C(14)	1.545(10)
O(1)-P(1)-N(2)	108.4(3)
O(1)-P(1)-N(1)	118.7(3)
N(2)-P(1)-N(1)	107.5(3)
O(1)-P(1)-C(6)	115.9(3)
N(2)-P(1)-C(6)	113.6(3)
N(1)-P(1)-C(6)	92.1(3)
C(12)-N(1)-P(1)	116.0(4)
C(2)-N(2)-P(1)	121.7(5)
C(4)-C(1)-C(13)	122.1(11)
N(2)-C(2)-C(7)	109.8(6)
N(2)-C(2)-C(9)	114.9(6)
C(7)-C(2)-C(9)	110.3(7)
C(6)-C(3)-C(12)	116.2(7)
C(1)-C(4)-C(10)	117.4(9)
C(1)-C(4)-C(11)	116.9(11)
C(10)-C(4)-C(11)	125.7(11)
C(8)-C(5)-C(13)	120.4(11)
C(3)-C(6)-P(1)	110.8(6)
C(5)-C(8)-C(10)	118.9(11)
C(11)-C(9)-C(2)	130.6(11)
C(4)-C(10)-C(8)	120.7(11)
C(9)-C(11)-C(4)	129.4(12)
N(1)-C(12)-C(3)	104.4(6)
N(1)-C(12)-C(14)	110.8(6)
C(3)-C(12)-C(14)	111.6(7)
C(5)-C(13)-C(1)	120.4(12)

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **5c**.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [h^2 a^{*2} U11 + ... + 2 h k a* b* U12]

Atom	U11	U22	U33	U23	U13	U12
P(1)	53(1)	30(1)	57(1)	1(1)	7(1)	-1(1)
O(1)	88(4)	33(2)	80(3)	3(3)	15(3)	-5(2)
N(1)	51(3)	51(3)	52(3)	2(3)	11(3)	1(3)
N(2)	69(4)	35(3)	52(3)	4(3)	16(3)	3(3)
C(1)	81(7)	136(10)	113(7)	-12(8)	14(6)	-4(8)
C(2)	68(5)	57(4)	62(4)	8(4)	15(4)	-1(3)
C(3)	52(4)	77(5)	85(6)	-6(5)	19(4)	-10(4)
C(4)	65(6)	128(8)	76(6)	-46(6)	16(5)	-7(6)
C(5)	88(7)	115(11)	102(8)	-34(7)	15(6)	4(7)
C(6)	54(4)	62(5)	71(5)	-2(4)	6(4)	9(3)
C(7)	85(6)	121(8)	68(5)	5(5)	32(4)	9(5)
C(8)	130(10)	126(10)	78(7)	-20(7)	15(7)	10(8)
C(9)	112(8)	112(8)	78(6)	-20(6)	47(6)	-20(7)
C(10)	112(8)	117(8)	93(7)	-32(7)	35(6)	-23(7)
C(11)	133(9)	88(8)	97(7)	-24(6)	44(7)	-2(7)
C(12)	67(5)	53(4)	67(5)	-6(4)	24(4)	-1(3)
C(13)	89(8)	120(11)	140(10)	-11(8)	39(7)	-18(6)
C(14)	99(6)	120(8)	74(6)	-4(5)	36(5)	-6(6)