Addition Reactions of a Phosphorus Triamide to Nitrosoarenes and Acylpyridines

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Supporting Information

Crystallography data

X-ray diffraction data for **4** was acquired using a Bruker SMART APEX CCD area detector system equipped with a graphite monochromator and a MoKα fine-focus sealed tube (λ = 0.71073 Å). Raw data integration and reduction were performed with the SAINT 3 and SADABS 4 programs. Compound **6** was measured on a Bruker D8 Quest Eco diffractometer equipped with a Triumph monochromator (λ= 0.71073 Å) and a CMOS Photon 50 detector at a temperature of 150(2) K. Intensity data were integrated with the Bruker APEX2 software. Absorption correction and scaling was performed with SADABS. The structures were solved using intrinsic phasing with the program SHELXT. Least-squares refinement was performed with SHELXL-2013 against F2 of all reflections. Non-hydrogen atoms were refined with anisotropic displacement parameters. The H atoms were placed at calculated positions using the instructions AFIX 13, AFIX 43 or AFIX 137 with isotropic displacement parameters having values 1.2 or 1.5 times Ueq of the attached C atoms. CCDC 1993347and CCDC 1993348 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_ request/cif.

Compound **4**

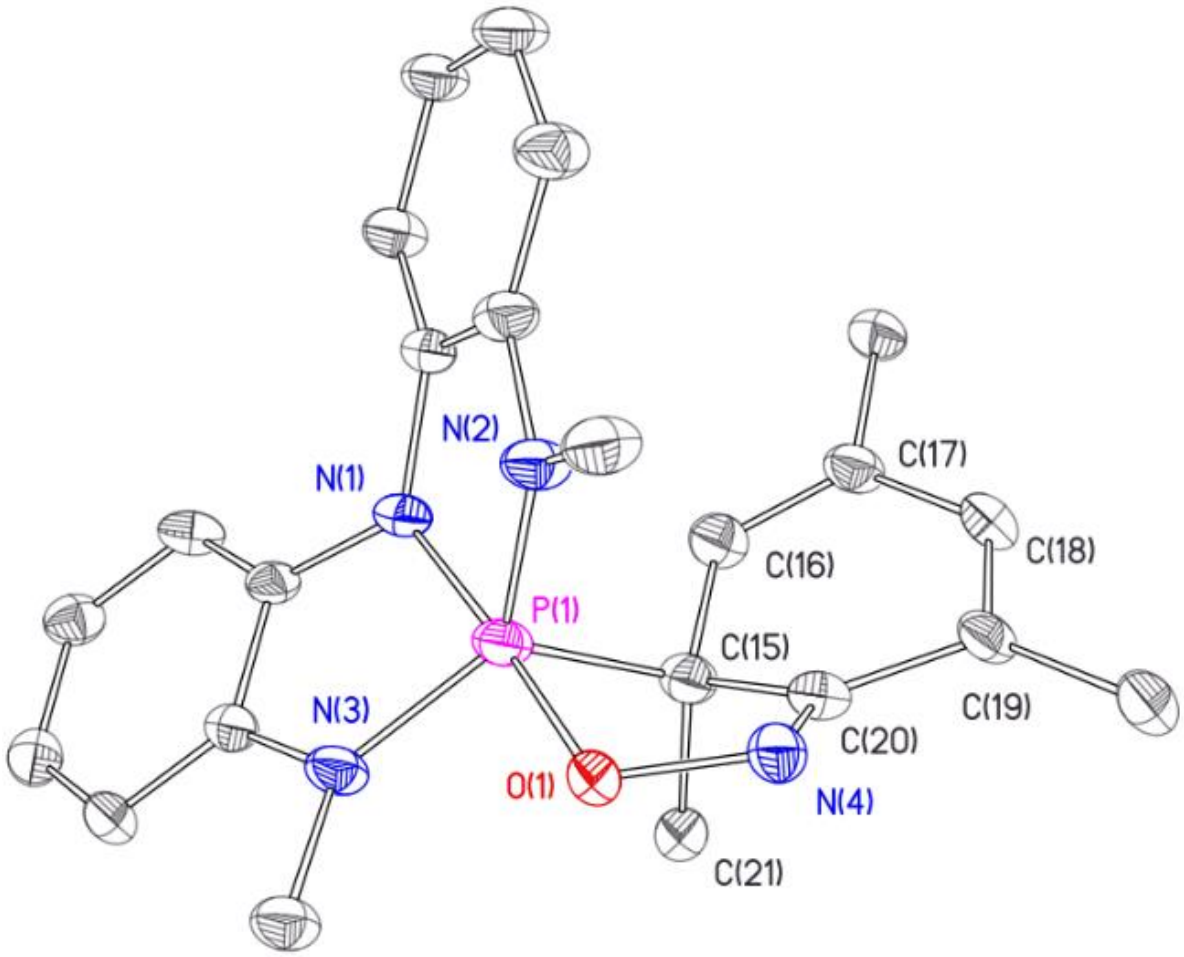

Table D1. Crystal data and structure refinement for **4**.

Empirical formula	C21.50 H28.83 N2.50 O0.67 P0.67	
Formula weight	353.62	
Temperature	288.15 K	
Wavelength	0.24797 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 17.505(4) Å	□= 116.803(3)°.
	b = 19.629(4) Å	□= 103.405(4)°.
	c = 19.682(4) Å	□ = 90.032(5)°.
Volume	5829(2) Å^3	
Z	12	
Density (calculated)	1.209 Mg/m^3	

Absorption coefficient	0.007 mm^{-1}
F(000)	2288
Theta range for data collection	0.838 to 8.505°.
Index ranges	-20<=h<=20, -23<=k<=23, -23<=l<=23
Reflections collected	126864
Independent reflections	20318 [R(int) = 0.0745]
Completeness to theta = 8.505°	98.0 %
Absorption correction	None
Max. and min. transmission	0.7433 and 0.6667
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	20318 / 0 / 1413
Goodness-of-fit on F^2	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0653, wR2 = 0.1631
R indices (all data)	R1 = 0.0852, wR2 = 0.1773
Extinction coefficient	n/a
Largest diff. peak and hole	1.520 and -0.813 e.$Å^{-3}$

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

	x	y	z	U(eq)
P(1)	865(1)	3710(1)	3425(1)	22(1)
O(1)	-113(1)	3761(1)	3411(1)	21(1)
N(1)	1893(2)	3701(1)	3520(2)	23(1)
N(2)	906(2)	2992(2)	3693(2)	26(1)
N(3)	1052(1)	4675(1)	3996(2)	24(1)
N(4)	-593(1)	3104(1)	2756(2)	24(1)
C(1)	2184(2)	3051(2)	3561(2)	24(1)
C(2)	2912(2)	2792(2)	3510(2)	27(1)
C(3)	3048(2)	2111(2)	3557(2)	29(1)
C(4)	2476(2)	1705(2)	3647(2)	33(1)
C(5)	1740(2)	1964(2)	3696(2)	31(1)
C(6)	1605(2)	2641(2)	3653(2)	27(1)
C(7)	2319(2)	4426(2)	3855(2)	20(1)
C(8)	1823(2)	4996(2)	4142(2)	21(1)
C(9)	2104(2)	5767(2)	4480(2)	22(1)
C(10)	2890(2)	5970(2)	4548(2)	25(1)
C(11)	3383(2)	5418(2)	4293(2)	26(1)
C(12)	3104(2)	4638(2)	3930(2)	25(1)
C(13)	306(2)	2687(2)	3924(2)	29(1)
C(14)	527(2)	5221(2)	4391(2)	26(1)
C(15)	522(2)	3257(2)	2303(2)	24(1)
C(16)	1076(2)	2710(2)	1918(2)	26(1)
C(17)	832(2)	1973(2)	1385(2)	26(1)
C(18)	-2(2)	1685(2)	1144(2)	25(1)
C(19)	-558(2)	2083(2)	1481(2)	24(1)
C(20)	-250(2)	2828(2)	2185(2)	24(1)
C(21)	367(2)	3857(2)	1949(2)	25(1)
C(22)	-7(2)	3398(2)	1054(2)	30(1)
C(23)	-207(2)	4423(2)	2300(2)	28(1)
C(24)	1147(2)	4312(2)	2084(2)	28(1)
C(25)	-1437(2)	1772(2)	1211(2)	26(1)

C(26)	-1633(2)	1466(2)	1754(2)	33(1)
C(27)	-1657(2)	1114(2)	361(2)	35(1)
C(28)	-1953(2)	2406(2)	1213(2)	33(1)
C(29)	1398(2)	1400(2)	1020(2)	28(1)
C(30)	1395(2)	785(2)	1305(2)	32(1)
C(31)	1115(2)	1010(2)	110(2)	32(1)
C(32)	2240(2)	1783(2)	1265(2)	36(1)
P(2)	4187(1)	6428(1)	6733(1)	15(1)
O(2)	5179(1)	6439(1)	6770(1)	18(1)
N(5)	3148(1)	6440(1)	6633(1)	16(1)
N(6)	3997(1)	5459(1)	6152(1)	17(1)
N(7)	4160(1)	7126(1)	6448(1)	17(1)
N(8)	5578(1)	6120(1)	7256(1)	19(1)
C(014)	3236(2)	5143(2)	6042(2)	19(1)
C(33)	2737(2)	5703(2)	6328(2)	18(1)
C(34)	1966(2)	5495(2)	6280(2)	25(1)
C(35)	1686(2)	4712(2)	5921(2)	28(1)
C(36)	2176(2)	4152(2)	5626(2)	28(1)
C(37)	2953(2)	4360(2)	5683(2)	23(1)
C(38)	2836(2)	7021(2)	6462(2)	17(1)
C(39)	3432(2)	7416(2)	6360(2)	18(1)
C(40)	3265(2)	8016(2)	6176(2)	24(1)
C(41)	2494(2)	8204(2)	6088(2)	25(1)
C(42)	1907(2)	7811(2)	6184(2)	23(1)
C(43)	2074(2)	7219(2)	6383(2)	20(1)
C(44)	4540(2)	4919(2)	5805(2)	20(1)
C(45)	4776(2)	7428(2)	6219(2)	22(1)
C(46)	4488(2)	6636(2)	7805(2)	16(1)
C(47)	3870(2)	6282(2)	8011(2)	17(1)
C(48)	4026(2)	5785(2)	8310(2)	19(1)
C(49)	4839(2)	5612(2)	8493(2)	20(1)
C(50)	5439(2)	5832(2)	8289(2)	19(1)
C(51)	5211(2)	6212(2)	7786(2)	17(1)
C(52)	4724(2)	7537(2)	8421(2)	19(1)
C(53)	4942(2)	7621(2)	9260(2)	23(1)
C(54)	5435(2)	7896(2)	8315(2)	23(1)

C(55)	4022(2)	7991(2)	8350(2)	22(1)
C(56)	3388(2)	5368(2)	8457(2)	23(1)
C(57)	3265(2)	4519(2)	7824(2)	29(1)
C(58)	3645(2)	5418(2)	9283(2)	30(1)
C(59)	2599(2)	5696(2)	8386(2)	29(1)
C(60)	6292(2)	5664(2)	8504(2)	23(1)
C(61)	6489(2)	5009(2)	7776(2)	28(1)
C(62)	6415(2)	5420(2)	9161(2)	26(1)
C(63)	6869(2)	6388(2)	8799(2)	27(1)
P(3)	5877(1)	8637(1)	13374(1)	17(1)
O(3)	6852(1)	8647(1)	13356(1)	22(1)
N(9)	4889(1)	8605(1)	13463(1)	18(1)
N(10)	5957(1)	9610(1)	13915(1)	19(1)
N(11)	6017(1)	7972(1)	13708(1)	20(1)
N(12)	6997(1)	8923(1)	12835(1)	21(1)
C(64)	4611(2)	9329(2)	13737(2)	17(1)
C(65)	3853(2)	9511(2)	13764(2)	23(1)
C(66)	3735(2)	10290(2)	14078(2)	28(1)
C(67)	4351(2)	10861(2)	14341(2)	26(1)
C(68)	5115(2)	10678(2)	14310(2)	23(1)
C(69)	5239(2)	9909(2)	14003(2)	18(1)
C(70)	4673(2)	8033(2)	13648(2)	17(1)
C(71)	5337(2)	7669(2)	13791(2)	20(1)
C(72)	5271(2)	7077(2)	13985(2)	25(1)
C(73)	4541(2)	6860(2)	14038(2)	26(1)
C(74)	3890(2)	7217(2)	13893(2)	23(1)
C(75)	3951(2)	7810(2)	13692(2)	21(1)
C(76)	6660(2)	10171(2)	14228(2)	26(1)
C(77)	6761(2)	7698(2)	13962(2)	26(1)
C(78)	5630(2)	8387(2)	12284(2)	17(1)
C(79)	4898(2)	8728(2)	12058(2)	18(1)
C(80)	4903(2)	9197(2)	11728(2)	20(1)
C(81)	5619(2)	9352(2)	11530(2)	20(1)
C(82)	6328(2)	9142(2)	11753(2)	21(1)
C(83)	6358(2)	8800(2)	12289(2)	20(1)
C(84)	5548(2)	7482(2)	11695(2)	19(1)

C(85)	5336(2)	7361(2)	10848(2)	24(1)
C(86)	6324(2)	7140(2)	11834(2)	25(1)
C(87)	4890(2)	7039(2)	11789(2)	23(1)
C(88)	4195(2)	9610(2)	11557(2)	20(1)
C(89)	4420(2)	10472(2)	12136(2)	26(1)
C(90)	4010(2)	9494(2)	10706(2)	29(1)
C(91)	3448(2)	9329(2)	11681(2)	26(1)
C(92)	7068(2)	9287(2)	11520(2)	24(1)
C(93)	6847(2)	9484(2)	10830(2)	30(1)
C(94)	7641(2)	9960(2)	12218(2)	28(1)
C(95)	7492(2)	8559(2)	11260(2)	30(1)
P(4)	10880(1)	8689(1)	13380(1)	21(1)
O(4)	11856(1)	8736(1)	13386(1)	21(1)
N(13)	9890(2)	8696(1)	13451(2)	22(1)
N(14)	11010(1)	9652(1)	13972(2)	23(1)
N(15)	10940(1)	7951(1)	13622(2)	23(1)
N(16)	12007(2)	8084(1)	12733(2)	24(1)
C(96)	9663(2)	9434(2)	13814(2)	20(1)
C(97)	8927(2)	9657(2)	13896(2)	27(1)
C(98)	8859(2)	10440(2)	14285(2)	29(1)
C(99)	9508(2)	10983(2)	14564(2)	26(1)
C(100)	10251(2)	10764(2)	14489(2)	24(1)
C(101)	10321(2)	9988(2)	14118(2)	21(1)
C(102)	9591(2)	8041(2)	13469(2)	22(1)
C(103)	10205(2)	7609(2)	13559(2)	24(1)
C(104)	10060(2)	6931(2)	13593(2)	28(1)
C(105)	9296(2)	6687(2)	13533(2)	31(1)
C(106)	8685(2)	7113(2)	13444(2)	31(1)
C(107)	8827(2)	7798(2)	13408(2)	27(1)
C(108)	11754(2)	10178(2)	14384(2)	25(1)
C(109)	11645(2)	7613(2)	13842(2)	27(1)
C(110)	10661(2)	8247(2)	12260(2)	23(1)
C(111)	9908(2)	7696(2)	11859(2)	25(1)
C(112)	9880(2)	6958(2)	11321(2)	24(1)
C(113)	10594(2)	6677(2)	11099(2)	24(1)
C(114)	11324(2)	7080(2)	11449(2)	23(1)

C(115)	11374(2)	7821(2)	12154(2)	22(1)
C(116)	12068(2)	6779(2)	11193(2)	26(1)
C(117)	11861(2)	6114(2)	10350(2)	35(1)
C(118)	12539(2)	6474(2)	11746(2)	33(1)
C(119)	12593(2)	7416(2)	11207(2)	31(1)
C(120)	10650(2)	8858(2)	11918(2)	25(1)
C(121)	11408(2)	9420(2)	12284(2)	27(1)
C(122)	9941(2)	9314(2)	12051(2)	28(1)
C(123)	10565(2)	8411(2)	11024(2)	30(1)
C(124)	9128(2)	6382(2)	10959(2)	27(1)
C(125)	8403(2)	6762(2)	11188(2)	36(1)
C(126)	8949(2)	5976(2)	10055(2)	29(1)
C(127)	9276(2)	5780(2)	11267(2)	33(1)

Table 3. Bond lengths [Å] and angles [°] for **4**.

P(1)-O(1)	1.708(2)	C(11)-C(12)	1.394(4)
P(1)-N(1)	1.767(3)	C(12)-H(12)	0.9300
P(1)-N(2)	1.709(3)	C(13)-H(13A)	0.9600
P(1)-N(3)	1.694(3)	C(13)-H(13B)	0.9600
P(1)-C(15)	1.908(3)	C(13)-H(13C)	0.9600
O(1)-N(4)	1.425(3)	C(14)-H(14A)	0.9600
N(1)-C(1)	1.404(4)	C(14)-H(14B)	0.9600
N(1)-C(7)	1.393(4)	C(14)-H(14C)	0.9600
N(2)-C(6)	1.405(4)	C(15)-C(16)	1.508(4)
N(2)-C(13)	1.463(4)	C(15)-C(20)	1.504(4)
N(3)-C(8)	1.400(4)	C(15)-C(21)	1.612(4)
N(3)-C(14)	1.475(4)	C(16)-H(16)	0.9300
N(4)-H(4)	0.8600	C(16)-C(17)	1.341(4)
N(4)-C(20)	1.297(4)	C(17)-C(18)	1.453(4)
C(1)-C(2)	1.380(4)	C(17)-C(29)	1.538(4)
C(1)-C(6)	1.387(4)	C(18)-H(18)	0.9300
C(2)-H(2)	0.9300	C(18)-C(19)	1.353(4)
C(2)-C(3)	1.398(4)	C(19)-C(20)	1.475(4)
C(3)-H(3)	0.9300	C(19)-C(25)	1.532(4)
C(3)-C(4)	1.370(5)	C(21)-C(22)	1.543(4)
C(4)-H(4A)	0.9300	C(21)-C(23)	1.533(4)
C(4)-C(5)	1.394(4)	C(21)-C(24)	1.535(4)
C(5)-H(5)	0.9300	C(22)-H(22A)	0.9600
C(5)-C(6)	1.387(4)	C(22)-H(22B)	0.9600
C(7)-C(8)	1.408(4)	C(22)-H(22C)	0.9600
C(7)-C(12)	1.389(4)	C(23)-H(23A)	0.9600
C(8)-C(9)	1.383(4)	C(23)-H(23B)	0.9600
C(9)-H(9)	0.9300	C(23)-H(23C)	0.9600
C(9)-C(10)	1.391(4)	C(24)-H(24A)	0.9600
C(10)-H(10)	0.9300	C(24)-H(24B)	0.9600
C(10)-C(11)	1.372(4)	C(24)-H(24C)	0.9600
C(11)-H(11)	0.9300	C(25)-C(26)	1.540(4)
		C(25)-C(27)	1.538(4)
		C(25)-C(28)	1.538(4)
		C(26)-H(26A)	0.9600

C(26)-H(26B)	0.9600	C(34)-H(34)	0.9300
C(26)-H(26C)	0.9600	C(34)-C(35)	1.401(4)
C(27)-H(27A)	0.9600	C(35)-H(35)	0.9300
C(27)-H(27B)	0.9600	C(35)-C(36)	1.391(5)
C(27)-H(27C)	0.9600	C(36)-H(36)	0.9300
C(28)-H(28A)	0.9600	C(36)-C(37)	1.384(4)
C(28)-H(28B)	0.9600	C(37)-H(37)	0.9300
C(28)-H(28C)	0.9600	C(38)-C(39)	1.403(4)
C(29)-C(30)	1.544(5)	C(38)-C(43)	1.382(4)
C(29)-C(31)	1.546(5)	C(39)-C(40)	1.392(4)
C(29)-C(32)	1.521(5)	C(40)-H(40)	0.9300
C(30)-H(30A)	0.9600	C(40)-C(41)	1.392(4)
C(30)-H(30B)	0.9600	C(41)-H(41)	0.9300
C(30)-H(30C)	0.9600	C(41)-C(42)	1.380(4)
C(31)-H(31A)	0.9600	C(42)-H(42)	0.9300
C(31)-H(31B)	0.9600	C(42)-C(43)	1.396(4)
C(31)-H(31C)	0.9600	C(43)-H(43)	0.9300
C(32)-H(32A)	0.9600	C(44)-H(44A)	0.9600
C(32)-H(32B)	0.9600	C(44)-H(44B)	0.9600
C(32)-H(32C)	0.9600	C(44)-H(44C)	0.9600
P(2)-O(2)	1.721(2)	C(45)-H(45A)	0.9600
P(2)-N(5)	1.784(2)	C(45)-H(45B)	0.9600
P(2)-N(6)	1.701(2)	C(45)-H(45C)	0.9600
P(2)-N(7)	1.696(2)	C(46)-C(47)	1.508(4)
P(2)-C(46)	1.899(3)	C(46)-C(51)	1.514(4)
O(2)-N(8)	1.424(3)	C(46)-C(52)	1.613(4)
N(5)-C(33)	1.409(3)	C(47)-H(47)	0.9300
N(5)-C(38)	1.406(3)	C(47)-C(48)	1.346(4)
N(6)-C(014)	1.396(4)	C(48)-C(49)	1.464(4)
N(6)-C(44)	1.464(3)	C(48)-C(56)	1.536(4)
N(7)-C(39)	1.403(4)	C(49)-H(49)	0.9300
N(7)-C(45)	1.477(4)	C(49)-C(50)	1.342(4)
N(8)-C(51)	1.293(4)	C(50)-C(51)	1.477(4)
C(014)-C(33)	1.399(4)	C(50)-C(60)	1.533(4)
C(014)-C(37)	1.402(4)	C(52)-C(53)	1.536(4)
C(33)-C(34)	1.380(4)	C(52)-C(54)	1.530(4)

C(52)-C(55)	1.535(4)	P(3)-N(10)	1.702(2)
C(53)-H(53A)	0.9600	P(3)-N(11)	1.702(2)
C(53)-H(53B)	0.9600	P(3)-C(78)	1.910(3)
C(53)-H(53C)	0.9600	O(3)-N(12)	1.424(3)
C(54)-H(54A)	0.9600	N(9)-C(64)	1.406(4)
C(54)-H(54B)	0.9600	N(9)-C(70)	1.403(4)
C(54)-H(54C)	0.9600	N(10)-C(69)	1.402(4)
C(55)-H(55A)	0.9600	N(10)-C(76)	1.463(4)
C(55)-H(55B)	0.9600	N(11)-C(71)	1.406(4)
C(55)-H(55C)	0.9600	N(11)-C(77)	1.474(4)
C(56)-C(57)	1.542(4)	N(12)-C(83)	1.293(4)
C(56)-C(58)	1.540(4)	C(64)-C(65)	1.380(4)
C(56)-C(59)	1.529(4)	C(64)-C(69)	1.404(4)
C(57)-H(57A)	0.9600	C(65)-H(65)	0.9300
C(57)-H(57B)	0.9600	C(65)-C(66)	1.403(4)
C(57)-H(57C)	0.9600	C(66)-H(66)	0.9300
C(58)-H(58A)	0.9600	C(66)-C(67)	1.381(5)
C(58)-H(58B)	0.9600	C(67)-H(67)	0.9300
C(58)-H(58C)	0.9600	C(67)-C(68)	1.393(4)
C(59)-H(59A)	0.9600	C(68)-H(68)	0.9300
C(59)-H(59B)	0.9600	C(68)-C(69)	1.390(4)
C(59)-H(59C)	0.9600	C(70)-C(71)	1.404(4)
C(60)-C(61)	1.546(4)	C(70)-C(75)	1.372(4)
C(60)-C(62)	1.541(4)	C(71)-C(72)	1.389(4)
C(60)-C(63)	1.536(4)	C(72)-H(72)	0.9300
C(61)-H(61A)	0.9600	C(72)-C(73)	1.388(4)
C(61)-H(61B)	0.9600	C(73)-H(73)	0.9300
C(61)-H(61C)	0.9600	C(73)-C(74)	1.379(4)
C(62)-H(62A)	0.9600	C(74)-H(74)	0.9300
C(62)-H(62B)	0.9600	C(74)-C(75)	1.398(4)
C(62)-H(62C)	0.9600	C(75)-H(75)	0.9300
C(63)-H(63A)	0.9600	C(76)-H(76A)	0.9600
C(63)-H(63B)	0.9600	C(76)-H(76B)	0.9600
C(63)-H(63C)	0.9600	C(76)-H(76C)	0.9600
P(3)-O(3)	1.715(2)	C(77)-H(77A)	0.9600
P(3)-N(9)	1.782(2)	C(77)-H(77B)	0.9600

C(77)-H(77C)	0.9600	C(92)-C(93)	1.540(4)
C(78)-C(79)	1.514(4)	C(92)-C(94)	1.536(4)
C(78)-C(83)	1.506(4)	C(92)-C(95)	1.540(4)
C(78)-C(84)	1.609(4)	C(93)-H(93A)	0.9600
C(79)-H(79)	0.9300	C(93)-H(93B)	0.9600
C(79)-C(80)	1.346(4)	C(93)-H(93C)	0.9600
C(80)-C(81)	1.466(4)	C(94)-H(94A)	0.9600
C(80)-C(88)	1.536(4)	C(94)-H(94B)	0.9600
C(81)-H(81)	0.9300	C(94)-H(94C)	0.9600
C(81)-C(82)	1.347(4)	C(95)-H(95A)	0.9600
C(82)-C(83)	1.477(4)	C(95)-H(95B)	0.9600
C(82)-C(92)	1.536(4)	C(95)-H(95C)	0.9600
C(84)-C(85)	1.526(4)	P(4)-O(4)	1.707(2)
C(84)-C(86)	1.537(4)	P(4)-N(13)	1.770(3)
C(84)-C(87)	1.536(4)	P(4)-N(14)	1.695(3)
C(85)-H(85A)	0.9600	P(4)-N(15)	1.712(3)
C(85)-H(85B)	0.9600	P(4)-C(110)	1.909(3)
C(85)-H(85C)	0.9600	O(4)-N(16)	1.427(3)
C(86)-H(86A)	0.9600	N(13)-C(96)	1.402(4)
C(86)-H(86B)	0.9600	N(13)-C(102)	1.407(4)
C(86)-H(86C)	0.9600	N(14)-C(101)	1.402(4)
C(87)-H(87A)	0.9600	N(14)-C(108)	1.474(4)
C(87)-H(87B)	0.9600	N(15)-C(103)	1.403(4)
C(87)-H(87C)	0.9600	N(15)-C(109)	1.471(4)
C(88)-C(89)	1.538(4)	N(16)-C(115)	1.294(4)
C(88)-C(90)	1.537(4)	C(96)-C(97)	1.382(4)
C(88)-C(91)	1.532(4)	C(96)-C(101)	1.400(4)
C(89)-H(89A)	0.9600	C(97)-H(97)	0.9300
C(89)-H(89B)	0.9600	C(97)-C(98)	1.395(4)
C(89)-H(89C)	0.9600	C(98)-H(98)	0.9300
C(90)-H(90A)	0.9600	C(98)-C(99)	1.381(4)
C(90)-H(90B)	0.9600	C(99)-H(99)	0.9300
C(90)-H(90C)	0.9600	C(99)-C(100)	1.390(4)
C(91)-H(91A)	0.9600	C(100)-H(100)	0.9300
C(91)-H(91B)	0.9600	C(100)-C(101)	1.381(4)
C(91)-H(91C)	0.9600	C(102)-C(103)	1.399(4)

C(102)-C(107)	1.379(4)	C(119)-H(11H)	0.9600
C(103)-C(104)	1.389(4)	C(119)-H(11I)	0.9600
C(104)-H(104)	0.9300	C(120)-C(121)	1.527(4)
C(104)-C(105)	1.381(5)	C(120)-C(122)	1.534(4)
C(105)-H(105)	0.9300	C(120)-C(123)	1.541(4)
C(105)-C(106)	1.386(5)	C(121)-H(12A)	0.9600
C(106)-H(106)	0.9300	C(121)-H(12B)	0.9600
C(106)-C(107)	1.404(4)	C(121)-H(12C)	0.9600
C(107)-H(107)	0.9300	C(122)-H(12D)	0.9600
C(108)-H(10A)	0.9600	C(122)-H(12E)	0.9600
C(108)-H(10B)	0.9600	C(122)-H(12F)	0.9600
C(108)-H(10C)	0.9600	C(123)-H(12G)	0.9600
C(109)-H(10D)	0.9600	C(123)-H(12H)	0.9600
C(109)-H(10E)	0.9600	C(123)-H(12I)	0.9600
C(109)-H(10F)	0.9600	C(124)-C(125)	1.526(4)
C(110)-C(111)	1.508(4)	C(124)-C(126)	1.538(4)
C(110)-C(115)	1.505(4)	C(124)-C(127)	1.550(5)
C(110)-C(120)	1.614(4)	C(125)-H(12J)	0.9600
C(111)-H(111)	0.9300	C(125)-H(12K)	0.9600
C(111)-C(112)	1.347(4)	C(125)-H(12L)	0.9600
C(112)-C(113)	1.448(4)	C(126)-H(12M)	0.9600
C(112)-C(124)	1.535(4)	C(126)-H(12N)	0.9600
C(113)-H(113)	0.9300	C(126)-H(12O)	0.9600
C(113)-C(114)	1.353(4)	C(127)-H(12P)	0.9600
C(114)-C(115)	1.475(4)	C(127)-H(12Q)	0.9600
C(114)-C(116)	1.529(4)	C(127)-H(12R)	0.9600
C(116)-C(117)	1.536(5)		
C(116)-C(118)	1.546(4)	O(1)-P(1)-N(1)	175.48(12)
C(116)-C(119)	1.538(4)	O(1)-P(1)-N(2)	92.20(11)
C(117)-H(11A)	0.9600	O(1)-P(1)-C(15)	86.42(11)
C(117)-H(11B)	0.9600	N(1)-P(1)-C(15)	98.04(13)
C(117)-H(11C)	0.9600	N(2)-P(1)-N(1)	87.06(12)
C(118)-H(11D)	0.9600	N(2)-P(1)-C(15)	108.56(13)
C(118)-H(11E)	0.9600	N(3)-P(1)-O(1)	89.57(11)
C(118)-H(11F)	0.9600	N(3)-P(1)-N(1)	87.46(12)
C(119)-H(11G)	0.9600	N(3)-P(1)-N(2)	129.61(14)

N(3)-P(1)-C(15)	121.80(13)	C(9)-C(8)-N(3)	127.6(3)
N(4)-O(1)-P(1)	110.87(16)	C(9)-C(8)-C(7)	120.6(3)
C(1)-N(1)-P(1)	114.0(2)	C(8)-C(9)-H(9)	120.6
C(7)-N(1)-P(1)	114.48(19)	C(8)-C(9)-C(10)	118.8(3)
C(7)-N(1)-C(1)	125.9(2)	C(10)-C(9)-H(9)	120.6
C(6)-N(2)-P(1)	114.2(2)	C(9)-C(10)-H(10)	119.6
C(6)-N(2)-C(13)	117.1(2)	C(11)-C(10)-C(9)	120.8(3)
C(13)-N(2)-P(1)	128.6(2)	C(11)-C(10)-H(10)	119.6
C(8)-N(3)-P(1)	115.44(19)	C(10)-C(11)-H(11)	119.5
C(8)-N(3)-C(14)	115.3(2)	C(10)-C(11)-C(12)	121.1(3)
C(14)-N(3)-P(1)	129.2(2)	C(12)-C(11)-H(11)	119.5
O(1)-N(4)-H(4)	125.0	C(7)-C(12)-C(11)	118.7(3)
C(20)-N(4)-O(1)	110.1(2)	C(7)-C(12)-H(12)	120.6
C(20)-N(4)-H(4)	125.0	C(11)-C(12)-H(12)	120.6
C(2)-C(1)-N(1)	129.8(3)	N(2)-C(13)-H(13A)	109.5
C(2)-C(1)-C(6)	120.5(3)	N(2)-C(13)-H(13B)	109.5
C(6)-C(1)-N(1)	109.7(3)	N(2)-C(13)-H(13C)	109.5
C(1)-C(2)-H(2)	120.9	H(13A)-C(13)-H(13B)	109.5
C(1)-C(2)-C(3)	118.2(3)	H(13A)-C(13)-H(13C)	109.5
C(3)-C(2)-H(2)	120.9	H(13B)-C(13)-H(13C)	109.5
C(2)-C(3)-H(3)	119.3	N(3)-C(14)-H(14A)	109.5
C(4)-C(3)-C(2)	121.3(3)	N(3)-C(14)-H(14B)	109.5
C(4)-C(3)-H(3)	119.3	N(3)-C(14)-H(14C)	109.5
C(3)-C(4)-H(4A)	119.7	H(14A)-C(14)-H(14B)	109.5
C(3)-C(4)-C(5)	120.5(3)	H(14A)-C(14)-H(14C)	109.5
C(5)-C(4)-H(4A)	119.7	H(14B)-C(14)-H(14C)	109.5
C(4)-C(5)-H(5)	120.9	C(16)-C(15)-P(1)	111.7(2)
C(6)-C(5)-C(4)	118.2(3)	C(16)-C(15)-C(21)	109.9(2)
C(6)-C(5)-H(5)	120.9	C(20)-C(15)-P(1)	98.3(2)
C(1)-C(6)-N(2)	112.4(3)	C(20)-C(15)-C(16)	111.1(2)
C(5)-C(6)-N(2)	126.5(3)	C(20)-C(15)-C(21)	110.1(2)
C(5)-C(6)-C(1)	121.1(3)	C(21)-C(15)-P(1)	115.2(2)
N(1)-C(7)-C(8)	109.5(3)	C(15)-C(16)-H(16)	118.6
C(12)-C(7)-N(1)	130.6(3)	C(17)-C(16)-C(15)	122.7(3)
C(12)-C(7)-C(8)	119.9(3)	C(17)-C(16)-H(16)	118.6
N(3)-C(8)-C(7)	111.8(3)	C(16)-C(17)-C(18)	119.4(3)

C(16)-C(17)-C(29)	123.1(3)	C(19)-C(25)-C(27)	111.3(2)
C(18)-C(17)-C(29)	117.4(3)	C(19)-C(25)-C(28)	110.3(2)
C(17)-C(18)-H(18)	117.6	C(27)-C(25)-C(26)	108.5(3)
C(19)-C(18)-C(17)	124.7(3)	C(28)-C(25)-C(26)	110.0(3)
C(19)-C(18)-H(18)	117.6	C(28)-C(25)-C(27)	106.5(3)
C(18)-C(19)-C(20)	114.9(3)	C(25)-C(26)-H(26A)	109.5
C(18)-C(19)-C(25)	123.8(3)	C(25)-C(26)-H(26B)	109.5
C(20)-C(19)-C(25)	121.1(3)	C(25)-C(26)-H(26C)	109.5
N(4)-C(20)-C(15)	117.4(3)	H(26A)-C(26)-H(26B)	109.5
N(4)-C(20)-C(19)	121.4(3)	H(26A)-C(26)-H(26C)	109.5
C(19)-C(20)-C(15)	120.9(3)	H(26B)-C(26)-H(26C)	109.5
C(22)-C(21)-C(15)	108.3(2)	C(25)-C(27)-H(27A)	109.5
C(23)-C(21)-C(15)	113.0(2)	C(25)-C(27)-H(27B)	109.5
C(23)-C(21)-C(22)	107.3(3)	C(25)-C(27)-H(27C)	109.5
C(23)-C(21)-C(24)	108.9(3)	H(27A)-C(27)-H(27B)	109.5
C(24)-C(21)-C(15)	110.7(2)	H(27A)-C(27)-H(27C)	109.5
C(24)-C(21)-C(22)	108.4(3)	H(27B)-C(27)-H(27C)	109.5
C(21)-C(22)-H(22A)	109.5	C(25)-C(28)-H(28A)	109.5
C(21)-C(22)-H(22B)	109.5	C(25)-C(28)-H(28B)	109.5
C(21)-C(22)-H(22C)	109.5	C(25)-C(28)-H(28C)	109.5
H(22A)-C(22)-H(22B)	109.5	H(28A)-C(28)-H(28B)	109.5
H(22A)-C(22)-H(22C)	109.5	H(28A)-C(28)-H(28C)	109.5
H(22B)-C(22)-H(22C)	109.5	H(28B)-C(28)-H(28C)	109.5
C(21)-C(23)-H(23A)	109.5	C(17)-C(29)-C(30)	107.5(3)
C(21)-C(23)-H(23B)	109.5	C(17)-C(29)-C(31)	110.4(3)
C(21)-C(23)-H(23C)	109.5	C(30)-C(29)-C(31)	109.5(3)
H(23A)-C(23)-H(23B)	109.5	C(32)-C(29)-C(17)	112.5(3)
H(23A)-C(23)-H(23C)	109.5	C(32)-C(29)-C(30)	108.9(3)
H(23B)-C(23)-H(23C)	109.5	C(32)-C(29)-C(31)	108.0(3)
C(21)-C(24)-H(24A)	109.5	C(29)-C(30)-H(30A)	109.5
C(21)-C(24)-H(24B)	109.5	C(29)-C(30)-H(30B)	109.5
C(21)-C(24)-H(24C)	109.5	C(29)-C(30)-H(30C)	109.5
H(24A)-C(24)-H(24B)	109.5	H(30A)-C(30)-H(30B)	109.5
H(24A)-C(24)-H(24C)	109.5	H(30A)-C(30)-H(30C)	109.5
H(24B)-C(24)-H(24C)	109.5	H(30B)-C(30)-H(30C)	109.5
C(19)-C(25)-C(26)	110.2(3)	C(29)-C(31)-H(31A)	109.5

C(29)-C(31)-H(31B)	109.5	C(34)-C(33)-N(5)	129.7(3)
C(29)-C(31)-H(31C)	109.5	C(34)-C(33)-C(014)	120.7(3)
H(31A)-C(31)-H(31B)	109.5	C(33)-C(34)-H(34)	120.7
H(31A)-C(31)-H(31C)	109.5	C(33)-C(34)-C(35)	118.7(3)
H(31B)-C(31)-H(31C)	109.5	C(35)-C(34)-H(34)	120.7
C(29)-C(32)-H(32A)	109.5	C(34)-C(35)-H(35)	119.6
C(29)-C(32)-H(32B)	109.5	C(36)-C(35)-C(34)	120.9(3)
C(29)-C(32)-H(32C)	109.5	C(36)-C(35)-H(35)	119.6
H(32A)-C(32)-H(32B)	109.5	C(35)-C(36)-H(36)	119.7
H(32A)-C(32)-H(32C)	109.5	C(37)-C(36)-C(35)	120.5(3)
H(32B)-C(32)-H(32C)	109.5	C(37)-C(36)-H(36)	119.7
O(2)-P(2)-N(5)	175.32(10)	C(014)-C(37)-H(37)	120.6
O(2)-P(2)-C(46)	86.75(11)	C(36)-C(37)-C(014)	118.9(3)
N(5)-P(2)-C(46)	97.39(11)	C(36)-C(37)-H(37)	120.6
N(6)-P(2)-O(2)	93.18(10)	C(39)-C(38)-N(5)	109.5(2)
N(6)-P(2)-N(5)	87.57(11)	C(43)-C(38)-N(5)	129.7(3)
N(6)-P(2)-C(46)	108.86(12)	C(43)-C(38)-C(39)	120.7(3)
N(7)-P(2)-O(2)	88.12(10)	C(38)-C(39)-N(7)	112.7(2)
N(7)-P(2)-N(5)	87.78(11)	C(40)-C(39)-N(7)	126.9(3)
N(7)-P(2)-N(6)	128.07(12)	C(40)-C(39)-C(38)	120.4(3)
N(7)-P(2)-C(46)	123.03(12)	C(39)-C(40)-H(40)	120.8
N(8)-O(2)-P(2)	111.12(15)	C(39)-C(40)-C(41)	118.4(3)
C(33)-N(5)-P(2)	113.01(18)	C(41)-C(40)-H(40)	120.8
C(38)-N(5)-P(2)	114.19(18)	C(40)-C(41)-H(41)	119.4
C(38)-N(5)-C(33)	123.6(2)	C(42)-C(41)-C(40)	121.1(3)
C(014)-N(6)-P(2)	114.70(18)	C(42)-C(41)-H(41)	119.4
C(014)-N(6)-C(44)	116.7(2)	C(41)-C(42)-H(42)	119.6
C(44)-N(6)-P(2)	128.46(19)	C(41)-C(42)-C(43)	120.8(3)
C(39)-N(7)-P(2)	115.45(18)	C(43)-C(42)-H(42)	119.6
C(39)-N(7)-C(45)	115.3(2)	C(38)-C(43)-C(42)	118.6(3)
C(45)-N(7)-P(2)	129.02(19)	C(38)-C(43)-H(43)	120.7
C(51)-N(8)-O(2)	109.9(2)	C(42)-C(43)-H(43)	120.7
N(6)-C(014)-C(33)	112.7(2)	N(6)-C(44)-H(44A)	109.5
N(6)-C(014)-C(37)	126.9(3)	N(6)-C(44)-H(44B)	109.5
C(33)-C(014)-C(37)	120.3(3)	N(6)-C(44)-H(44C)	109.5
C(014)-C(33)-N(5)	109.6(2)	H(44A)-C(44)-H(44B)	109.5

H(44A)-C(44)-H(44C)	109.5	C(52)-C(53)-H(53B)	109.5
H(44B)-C(44)-H(44C)	109.5	C(52)-C(53)-H(53C)	109.5
N(7)-C(45)-H(45A)	109.5	H(53A)-C(53)-H(53B)	109.5
N(7)-C(45)-H(45B)	109.5	H(53A)-C(53)-H(53C)	109.5
N(7)-C(45)-H(45C)	109.5	H(53B)-C(53)-H(53C)	109.5
H(45A)-C(45)-H(45B)	109.5	C(52)-C(54)-H(54A)	109.5
H(45A)-C(45)-H(45C)	109.5	C(52)-C(54)-H(54B)	109.5
H(45B)-C(45)-H(45C)	109.5	C(52)-C(54)-H(54C)	109.5
C(47)-C(46)-P(2)	111.91(19)	H(54A)-C(54)-H(54B)	109.5
C(47)-C(46)-C(51)	110.3(2)	H(54A)-C(54)-H(54C)	109.5
C(47)-C(46)-C(52)	110.8(2)	H(54B)-C(54)-H(54C)	109.5
C(51)-C(46)-P(2)	98.61(18)	C(52)-C(55)-H(55A)	109.5
C(51)-C(46)-C(52)	110.7(2)	C(52)-C(55)-H(55B)	109.5
C(52)-C(46)-P(2)	113.94(18)	C(52)-C(55)-H(55C)	109.5
C(46)-C(47)-H(47)	118.5	H(55A)-C(55)-H(55B)	109.5
C(48)-C(47)-C(46)	123.0(2)	H(55A)-C(55)-H(55C)	109.5
C(48)-C(47)-H(47)	118.5	H(55B)-C(55)-H(55C)	109.5
C(47)-C(48)-C(49)	119.2(3)	C(48)-C(56)-C(57)	107.1(2)
C(47)-C(48)-C(56)	123.5(2)	C(48)-C(56)-C(58)	111.5(2)
C(49)-C(48)-C(56)	117.3(2)	C(58)-C(56)-C(57)	109.5(2)
C(48)-C(49)-H(49)	117.7	C(59)-C(56)-C(48)	112.5(2)
C(50)-C(49)-C(48)	124.7(3)	C(59)-C(56)-C(57)	108.6(3)
C(50)-C(49)-H(49)	117.7	C(59)-C(56)-C(58)	107.7(2)
C(49)-C(50)-C(51)	114.8(2)	C(56)-C(57)-H(57A)	109.5
C(49)-C(50)-C(60)	124.0(3)	C(56)-C(57)-H(57B)	109.5
C(51)-C(50)-C(60)	121.1(2)	C(56)-C(57)-H(57C)	109.5
N(8)-C(51)-C(46)	118.1(2)	H(57A)-C(57)-H(57B)	109.5
N(8)-C(51)-C(50)	120.2(2)	H(57A)-C(57)-H(57C)	109.5
C(50)-C(51)-C(46)	121.3(2)	H(57B)-C(57)-H(57C)	109.5
C(53)-C(52)-C(46)	108.3(2)	C(56)-C(58)-H(58A)	109.5
C(54)-C(52)-C(46)	112.8(2)	C(56)-C(58)-H(58B)	109.5
C(54)-C(52)-C(53)	107.8(2)	C(56)-C(58)-H(58C)	109.5
C(54)-C(52)-C(55)	109.0(2)	H(58A)-C(58)-H(58B)	109.5
C(55)-C(52)-C(46)	110.9(2)	H(58A)-C(58)-H(58C)	109.5
C(55)-C(52)-C(53)	107.8(2)	H(58B)-C(58)-H(58C)	109.5
C(52)-C(53)-H(53A)	109.5	C(56)-C(59)-H(59A)	109.5

C(56)-C(59)-H(59B)	109.5	N(11)-P(3)-O(3)	88.27(11)
C(56)-C(59)-H(59C)	109.5	N(11)-P(3)-N(9)	87.26(11)
H(59A)-C(59)-H(59B)	109.5	N(11)-P(3)-C(78)	123.73(12)
H(59A)-C(59)-H(59C)	109.5	N(12)-O(3)-P(3)	111.76(15)
H(59B)-C(59)-H(59C)	109.5	C(64)-N(9)-P(3)	113.22(18)
C(50)-C(60)-C(61)	110.4(2)	C(70)-N(9)-P(3)	114.77(18)
C(50)-C(60)-C(62)	110.8(2)	C(70)-N(9)-C(64)	123.4(2)
C(50)-C(60)-C(63)	109.8(2)	C(69)-N(10)-P(3)	114.83(19)
C(62)-C(60)-C(61)	108.4(2)	C(69)-N(10)-C(76)	116.4(2)
C(63)-C(60)-C(61)	108.9(3)	C(76)-N(10)-P(3)	128.5(2)
C(63)-C(60)-C(62)	108.4(2)	C(71)-N(11)-P(3)	115.60(18)
C(60)-C(61)-H(61A)	109.5	C(71)-N(11)-C(77)	115.3(2)
C(60)-C(61)-H(61B)	109.5	C(77)-N(11)-P(3)	129.0(2)
C(60)-C(61)-H(61C)	109.5	C(83)-N(12)-O(3)	110.2(2)
H(61A)-C(61)-H(61B)	109.5	C(65)-C(64)-N(9)	129.5(3)
H(61A)-C(61)-H(61C)	109.5	C(65)-C(64)-C(69)	120.6(3)
H(61B)-C(61)-H(61C)	109.5	C(69)-C(64)-N(9)	109.9(2)
C(60)-C(62)-H(62A)	109.5	C(64)-C(65)-H(65)	120.9
C(60)-C(62)-H(62B)	109.5	C(64)-C(65)-C(66)	118.1(3)
C(60)-C(62)-H(62C)	109.5	C(66)-C(65)-H(65)	120.9
H(62A)-C(62)-H(62B)	109.5	C(65)-C(66)-H(66)	119.3
H(62A)-C(62)-H(62C)	109.5	C(67)-C(66)-C(65)	121.5(3)
H(62B)-C(62)-H(62C)	109.5	C(67)-C(66)-H(66)	119.3
C(60)-C(63)-H(63A)	109.5	C(66)-C(67)-H(67)	119.7
C(60)-C(63)-H(63B)	109.5	C(66)-C(67)-C(68)	120.6(3)
C(60)-C(63)-H(63C)	109.5	C(68)-C(67)-H(67)	119.7
H(63A)-C(63)-H(63B)	109.5	C(67)-C(68)-H(68)	120.8
H(63A)-C(63)-H(63C)	109.5	C(69)-C(68)-C(67)	118.4(3)
H(63B)-C(63)-H(63C)	109.5	C(69)-C(68)-H(68)	120.8
O(3)-P(3)-N(9)	174.87(11)	N(10)-C(69)-C(64)	112.2(2)
O(3)-P(3)-C(78)	86.77(11)	C(68)-C(69)-N(10)	126.9(3)
N(9)-P(3)-C(78)	97.80(12)	C(68)-C(69)-C(64)	120.9(3)
N(10)-P(3)-O(3)	93.14(11)	N(9)-C(70)-C(71)	109.3(2)
N(10)-P(3)-N(9)	87.64(11)	C(75)-C(70)-N(9)	129.8(3)
N(10)-P(3)-N(11)	127.91(12)	C(75)-C(70)-C(71)	120.9(3)
N(10)-P(3)-C(78)	108.33(12)	C(70)-C(71)-N(11)	112.4(2)

C(72)-C(71)-N(11)	127.4(3)	C(79)-C(80)-C(88)	123.7(3)
C(72)-C(71)-C(70)	120.1(3)	C(81)-C(80)-C(88)	116.4(2)
C(71)-C(72)-H(72)	120.7	C(80)-C(81)-H(81)	117.8
C(73)-C(72)-C(71)	118.7(3)	C(82)-C(81)-C(80)	124.3(3)
C(73)-C(72)-H(72)	120.7	C(82)-C(81)-H(81)	117.8
C(72)-C(73)-H(73)	119.5	C(81)-C(82)-C(83)	114.5(3)
C(74)-C(73)-C(72)	121.0(3)	C(81)-C(82)-C(92)	123.7(3)
C(74)-C(73)-H(73)	119.5	C(83)-C(82)-C(92)	121.7(2)
C(73)-C(74)-H(74)	119.7	N(12)-C(83)-C(78)	118.1(3)
C(73)-C(74)-C(75)	120.7(3)	N(12)-C(83)-C(82)	120.0(3)
C(75)-C(74)-H(74)	119.7	C(82)-C(83)-C(78)	121.5(2)
C(70)-C(75)-C(74)	118.7(3)	C(85)-C(84)-C(78)	108.8(2)
C(70)-C(75)-H(75)	120.7	C(85)-C(84)-C(86)	108.0(2)
C(74)-C(75)-H(75)	120.7	C(85)-C(84)-C(87)	108.3(2)
N(10)-C(76)-H(76A)	109.5	C(86)-C(84)-C(78)	112.0(2)
N(10)-C(76)-H(76B)	109.5	C(87)-C(84)-C(78)	110.9(2)
N(10)-C(76)-H(76C)	109.5	C(87)-C(84)-C(86)	108.7(2)
H(76A)-C(76)-H(76B)	109.5	C(84)-C(85)-H(85A)	109.5
H(76A)-C(76)-H(76C)	109.5	C(84)-C(85)-H(85B)	109.5
H(76B)-C(76)-H(76C)	109.5	C(84)-C(85)-H(85C)	109.5
N(11)-C(77)-H(77A)	109.5	H(85A)-C(85)-H(85B)	109.5
N(11)-C(77)-H(77B)	109.5	H(85A)-C(85)-H(85C)	109.5
N(11)-C(77)-H(77C)	109.5	H(85B)-C(85)-H(85C)	109.5
H(77A)-C(77)-H(77B)	109.5	C(84)-C(86)-H(86A)	109.5
H(77A)-C(77)-H(77C)	109.5	C(84)-C(86)-H(86B)	109.5
H(77B)-C(77)-H(77C)	109.5	C(84)-C(86)-H(86C)	109.5
C(79)-C(78)-P(3)	111.23(19)	H(86A)-C(86)-H(86B)	109.5
C(79)-C(78)-C(84)	110.7(2)	H(86A)-C(86)-H(86C)	109.5
C(83)-C(78)-P(3)	99.01(18)	H(86B)-C(86)-H(86C)	109.5
C(83)-C(78)-C(79)	110.5(2)	C(84)-C(87)-H(87A)	109.5
C(83)-C(78)-C(84)	110.7(2)	C(84)-C(87)-H(87B)	109.5
C(84)-C(78)-P(3)	114.13(18)	C(84)-C(87)-H(87C)	109.5
C(78)-C(79)-H(79)	118.9	H(87A)-C(87)-H(87B)	109.5
C(80)-C(79)-C(78)	122.2(3)	H(87A)-C(87)-H(87C)	109.5
C(80)-C(79)-H(79)	118.9	H(87B)-C(87)-H(87C)	109.5
C(79)-C(80)-C(81)	119.8(3)	C(80)-C(88)-C(89)	107.2(2)

C(80)-C(88)-C(90)	111.1(2)	C(92)-C(94)-H(94B)	109.5
C(90)-C(88)-C(89)	109.5(2)	C(92)-C(94)-H(94C)	109.5
C(91)-C(88)-C(80)	112.1(2)	H(94A)-C(94)-H(94B)	109.5
C(91)-C(88)-C(89)	108.5(2)	H(94A)-C(94)-H(94C)	109.5
C(91)-C(88)-C(90)	108.4(2)	H(94B)-C(94)-H(94C)	109.5
C(88)-C(89)-H(89A)	109.5	C(92)-C(95)-H(95A)	109.5
C(88)-C(89)-H(89B)	109.5	C(92)-C(95)-H(95B)	109.5
C(88)-C(89)-H(89C)	109.5	C(92)-C(95)-H(95C)	109.5
H(89A)-C(89)-H(89B)	109.5	H(95A)-C(95)-H(95B)	109.5
H(89A)-C(89)-H(89C)	109.5	H(95A)-C(95)-H(95C)	109.5
H(89B)-C(89)-H(89C)	109.5	H(95B)-C(95)-H(95C)	109.5
C(88)-C(90)-H(90A)	109.5	O(4)-P(4)-N(13)	175.49(12)
C(88)-C(90)-H(90B)	109.5	O(4)-P(4)-N(15)	92.96(11)
C(88)-C(90)-H(90C)	109.5	O(4)-P(4)-C(110)	86.36(12)
H(90A)-C(90)-H(90B)	109.5	N(13)-P(4)-C(110)	97.83(13)
H(90A)-C(90)-H(90C)	109.5	N(14)-P(4)-O(4)	88.87(11)
H(90B)-C(90)-H(90C)	109.5	N(14)-P(4)-N(13)	87.46(12)
C(88)-C(91)-H(91A)	109.5	N(14)-P(4)-N(15)	129.77(13)
C(88)-C(91)-H(91B)	109.5	N(14)-P(4)-C(110)	122.50(13)
C(88)-C(91)-H(91C)	109.5	N(15)-P(4)-N(13)	87.38(12)
H(91A)-C(91)-H(91B)	109.5	N(15)-P(4)-C(110)	107.71(13)
H(91A)-C(91)-H(91C)	109.5	N(16)-O(4)-P(4)	111.33(16)
H(91B)-C(91)-H(91C)	109.5	C(96)-N(13)-P(4)	114.21(19)
C(82)-C(92)-C(93)	111.1(2)	C(96)-N(13)-C(102)	125.5(3)
C(82)-C(92)-C(95)	109.6(2)	C(102)-N(13)-P(4)	113.8(2)
C(94)-C(92)-C(82)	110.7(3)	C(101)-N(14)-P(4)	115.6(2)
C(94)-C(92)-C(93)	108.1(2)	C(101)-N(14)-C(108)	115.5(2)
C(94)-C(92)-C(95)	109.1(3)	C(108)-N(14)-P(4)	128.8(2)
C(95)-C(92)-C(93)	108.3(3)	C(103)-N(15)-P(4)	114.2(2)
C(92)-C(93)-H(93A)	109.5	C(103)-N(15)-C(109)	117.0(2)
C(92)-C(93)-H(93B)	109.5	C(109)-N(15)-P(4)	128.7(2)
C(92)-C(93)-H(93C)	109.5	C(115)-N(16)-O(4)	109.4(2)
H(93A)-C(93)-H(93B)	109.5	C(97)-C(96)-N(13)	130.0(3)
H(93A)-C(93)-H(93C)	109.5	C(97)-C(96)-C(101)	120.1(3)
H(93B)-C(93)-H(93C)	109.5	C(101)-C(96)-N(13)	109.8(3)
C(92)-C(94)-H(94A)	109.5	C(96)-C(97)-H(97)	120.7

C(96)-C(97)-C(98)	118.5(3)	H(10A)-C(108)-H(10C)	109.5
C(98)-C(97)-H(97)	120.7	H(10B)-C(108)-H(10C)	109.5
C(97)-C(98)-H(98)	119.6	N(15)-C(109)-H(10D)	109.5
C(99)-C(98)-C(97)	120.9(3)	N(15)-C(109)-H(10E)	109.5
C(99)-C(98)-H(98)	119.6	N(15)-C(109)-H(10F)	109.5
C(98)-C(99)-H(99)	119.5	H(10D)-C(109)-H(10E)	109.5
C(98)-C(99)-C(100)	121.0(3)	H(10D)-C(109)-H(10F)	109.5
C(100)-C(99)-H(99)	119.5	H(10E)-C(109)-H(10F)	109.5
C(99)-C(100)-H(100)	121.0	C(111)-C(110)-P(4)	111.5(2)
C(101)-C(100)-C(99)	118.0(3)	C(111)-C(110)-C(120)	110.4(2)
C(101)-C(100)-H(100)	121.0	C(115)-C(110)-P(4)	98.19(19)
C(96)-C(101)-N(14)	111.8(3)	C(115)-C(110)-C(111)	110.9(2)
C(100)-C(101)-N(14)	126.8(3)	C(115)-C(110)-C(120)	110.1(2)
C(100)-C(101)-C(96)	121.4(3)	C(120)-C(110)-P(4)	115.1(2)
C(103)-C(102)-N(13)	109.6(3)	C(110)-C(111)-H(111)	118.6
C(107)-C(102)-N(13)	129.9(3)	C(112)-C(111)-C(110)	122.9(3)
C(107)-C(102)-C(103)	120.5(3)	C(112)-C(111)-H(111)	118.6
C(102)-C(103)-N(15)	112.4(3)	C(111)-C(112)-C(113)	119.2(3)
C(104)-C(103)-N(15)	126.9(3)	C(111)-C(112)-C(124)	122.8(3)
C(104)-C(103)-C(102)	120.7(3)	C(113)-C(112)-C(124)	117.9(3)
C(103)-C(104)-H(104)	120.5	C(112)-C(113)-H(113)	117.6
C(105)-C(104)-C(103)	118.9(3)	C(114)-C(113)-C(112)	124.8(3)
C(105)-C(104)-H(104)	120.5	C(114)-C(113)-H(113)	117.6
C(104)-C(105)-H(105)	119.7	C(113)-C(114)-C(115)	115.1(3)
C(104)-C(105)-C(106)	120.5(3)	C(113)-C(114)-C(116)	123.9(3)
C(106)-C(105)-H(105)	119.7	C(115)-C(114)-C(116)	120.8(3)
C(105)-C(106)-H(106)	119.6	N(16)-C(115)-C(110)	118.1(3)
C(105)-C(106)-C(107)	120.9(3)	N(16)-C(115)-C(114)	120.9(3)
C(107)-C(106)-H(106)	119.6	C(114)-C(115)-C(110)	120.7(3)
C(102)-C(107)-C(106)	118.4(3)	C(114)-C(116)-C(117)	111.4(2)
C(102)-C(107)-H(107)	120.8	C(114)-C(116)-C(118)	109.8(3)
C(106)-C(107)-H(107)	120.8	C(114)-C(116)-C(119)	110.8(2)
N(14)-C(108)-H(10A)	109.5	C(117)-C(116)-C(118)	107.7(3)
N(14)-C(108)-H(10B)	109.5	C(117)-C(116)-C(119)	107.3(3)
N(14)-C(108)-H(10C)	109.5	C(119)-C(116)-C(118)	109.8(3)
H(10A)-C(108)-H(10B)	109.5	C(116)-C(117)-H(11A)	109.5

C(116)-C(117)-H(11B)	109.5
C(116)-C(117)-H(11C)	109.5
H(11A)-C(117)-H(11B)	109.5
H(11A)-C(117)-H(11C)	109.5
H(11B)-C(117)-H(11C)	109.5
C(116)-C(118)-H(11D)	109.5
C(116)-C(118)-H(11E)	109.5
C(116)-C(118)-H(11F)	109.5
H(11D)-C(118)-H(11E)	109.5
H(11D)-C(118)-H(11F)	109.5
H(11E)-C(118)-H(11F)	109.5
C(116)-C(119)-H(11G)	109.5
C(116)-C(119)-H(11H)	109.5
C(116)-C(119)-H(11I)	109.5
H(11G)-C(119)-H(11H)	109.5
H(11G)-C(119)-H(11I)	109.5
H(11H)-C(119)-H(11I)	109.5
C(121)-C(120)-C(110)	113.1(2)
C(121)-C(120)-C(122)	109.0(3)
C(121)-C(120)-C(123)	107.5(3)
C(122)-C(120)-C(110)	110.3(2)
C(122)-C(120)-C(123)	108.3(3)
C(123)-C(120)-C(110)	108.5(2)
C(120)-C(121)-H(12A)	109.5
C(120)-C(121)-H(12B)	109.5
C(120)-C(121)-H(12C)	109.5
H(12A)-C(121)-H(12B)	109.5
H(12A)-C(121)-H(12C)	109.5
H(12B)-C(121)-H(12C)	109.5
C(120)-C(122)-H(12D)	109.5
C(120)-C(122)-H(12E)	109.5
C(120)-C(122)-H(12F)	109.5
H(12D)-C(122)-H(12E)	109.5
H(12D)-C(122)-H(12F)	109.5
H(12E)-C(122)-H(12F)	109.5
C(120)-C(123)-H(12G)	109.5
C(120)-C(123)-H(12H)	109.5
C(120)-C(123)-H(12I)	109.5
H(12G)-C(123)-H(12H)	109.5
H(12G)-C(123)-H(12I)	109.5
H(12H)-C(123)-H(12I)	109.5
C(112)-C(124)-C(126)	110.4(3)
C(112)-C(124)-C(127)	107.5(3)
C(125)-C(124)-C(112)	112.7(3)
C(125)-C(124)-C(126)	108.1(3)
C(125)-C(124)-C(127)	108.5(3)
C(126)-C(124)-C(127)	109.6(3)
C(124)-C(125)-H(12J)	109.5
C(124)-C(125)-H(12K)	109.5
C(124)-C(125)-H(12L)	109.5
H(12J)-C(125)-H(12K)	109.5
H(12J)-C(125)-H(12L)	109.5
H(12K)-C(125)-H(12L)	109.5
C(124)-C(126)-H(12M)	109.5
C(124)-C(126)-H(12N)	109.5
C(124)-C(126)-H(12O)	109.5
H(12M)-C(126)-H(12N)	109.5
H(12M)-C(126)-H(12O)	109.5
H(12N)-C(126)-H(12O)	109.5
C(124)-C(127)-H(12P)	109.5
C(124)-C(127)-H(12Q)	109.5
C(124)-C(127)-H(12R)	109.5
H(12P)-C(127)-H(12Q)	109.5
H(12P)-C(127)-H(12R)	109.5
H(12Q)-C(127)-H(12R)	109.5

Symmetry transformations used to generate equivalent atoms

Compound **6**

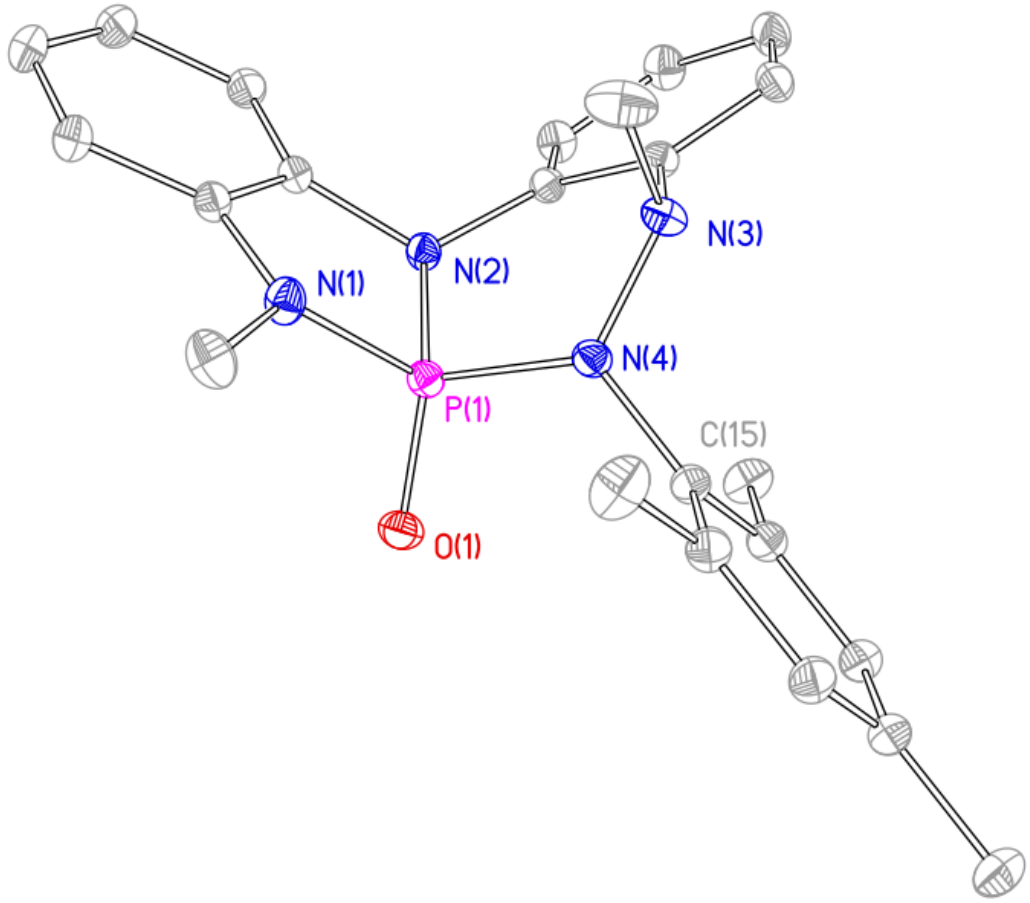

Table 1. Crystal data and structure refinement for **6**.

Empirical formula	C23 H25 N4 O P	
Formula weight	404.44	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 11.3284(11) Å	α= 90°.
	b = 11.8731(10) Å	β= 90°.
	c = 15.1405(12) Å	γ = 90°.
Volume	2036.4(3) $Å^3$	
Z	4	
Density (calculated)	1.319 Mg/m^3	
Absorption coefficient	0.157 mm^{-1}	
F(000)	856	
Crystal size	0.510 x 0.400 x 0.050 mm^3	
Theta range for data collection	2.180 to 32.073°.	
Index ranges	-24<=h<=24, -14<=k<=14, -30<=l<=30	
Reflections collected	7123	
Independent reflections	7123 [R(int) = 0.0490]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7462 and 0.6900	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7123 / 0 / 267	
Goodness-of-fit on F^2	1.057	
Final R indices [I>2sigma(I)]	R1 = 0.0344, wR2 = 0.0908	
R indices (all data)	R1 = 0.0358, wR2 = 0.0924	
Absolute structure parameter	0.06(2)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.692 and -0.353 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	511(1)	9289(1)	1302(1)	12(1)
N(1)	454(1)	10691(1)	1200(1)	16(1)
O(1)	-188(1)	8842(1)	2041(1)	17(1)
N(4)	1857(1)	8758(1)	1317(1)	13(1)
N(2)	95(1)	9076(1)	248(1)	12(1)
C(20)	2005(1)	6892(1)	2026(1)	14(1)
C(1)	-415(1)	10077(1)	-104(1)	13(1)
C(13)	1951(1)	8219(1)	-203(1)	12(1)
N(3)	2549(1)	8723(1)	527(1)	14(1)
C(17)	3373(1)	7820(1)	3377(1)	17(1)
C(9)	171(1)	7747(1)	-1002(1)	15(1)
C(6)	-212(1)	10996(1)	458(1)	14(1)
C(19)	2428(1)	6229(1)	2716(1)	16(1)
C(12)	2614(1)	7591(1)	-802(1)	16(1)
C(5)	-667(2)	12054(1)	263(1)	19(1)
C(11)	2064(2)	7074(1)	-1515(1)	18(1)
C(23)	1258(1)	6351(1)	1317(1)	19(1)
C(2)	-1050(1)	10203(1)	-878(1)	17(1)
C(15)	2278(1)	8049(1)	2024(1)	13(1)
C(16)	2965(1)	8522(1)	2698(1)	15(1)
C(18)	3121(1)	6674(1)	3396(1)	17(1)
C(10)	842(1)	7137(1)	-1607(1)	18(1)
C(8)	729(1)	8326(1)	-319(1)	12(1)
C(4)	-1316(2)	12173(1)	-518(1)	24(1)
C(22)	3560(2)	5928(2)	4128(1)	22(1)
C(14)	3136(2)	9791(2)	313(1)	24(1)
C(7)	728(2)	11502(1)	1894(1)	20(1)
C(21)	3286(2)	9756(1)	2728(1)	23(1)
C(3)	-1499(2)	11270(2)	-1080(1)	22(1)

Table 3. Bond lengths [Å] and angles [°] for **6**.

P(1)-O(1)	1.4704(11)	O(1)-P(1)-N(4)	110.44(7)
P(1)-N(4)	1.6501(13)	O(1)-P(1)-N(1)	114.09(7)
P(1)-N(1)	1.6724(13)	N(4)-P(1)-N(1)	114.67(7)
P(1)-N(2)	1.6826(12)	O(1)-P(1)-N(2)	121.09(7)
N(1)-C(6)	1.4012(19)	N(4)-P(1)-N(2)	102.39(6)
N(1)-C(7)	1.4590(19)	N(1)-P(1)-N(2)	92.97(6)
N(4)-N(3)	1.4306(17)	C(6)-N(1)-C(7)	121.36(12)
N(4)-C(15)	1.4430(18)	C(6)-N(1)-P(1)	110.64(10)
N(2)-C(1)	1.4255(18)	C(7)-N(1)-P(1)	125.65(11)
N(2)-C(8)	1.4314(17)	N(3)-N(4)-C(15)	114.94(11)
C(20)-C(19)	1.393(2)	N(3)-N(4)-P(1)	120.40(10)
C(20)-C(15)	1.408(2)	C(15)-N(4)-P(1)	122.61(10)
C(20)-C(23)	1.509(2)	C(1)-N(2)-C(8)	119.80(11)
C(1)-C(2)	1.383(2)	C(1)-N(2)-P(1)	110.08(9)
C(1)-C(6)	1.404(2)	C(8)-N(2)-P(1)	121.48(10)
C(13)-C(12)	1.3943(19)	C(19)-C(20)-C(15)	118.49(13)
C(13)-C(8)	1.4010(19)	C(19)-C(20)-C(23)	119.04(13)
C(13)-N(3)	1.4281(18)	C(15)-C(20)-C(23)	122.47(13)
N(3)-C(14)	1.468(2)	C(2)-C(1)-C(6)	121.01(13)
C(17)-C(18)	1.390(2)	C(2)-C(1)-N(2)	128.21(13)
C(17)-C(16)	1.402(2)	C(6)-C(1)-N(2)	110.77(12)
C(9)-C(10)	1.393(2)	C(12)-C(13)-C(8)	119.92(13)
C(9)-C(8)	1.3932(19)	C(12)-C(13)-N(3)	118.17(13)
C(6)-C(5)	1.389(2)	C(8)-C(13)-N(3)	121.90(12)
C(19)-C(18)	1.399(2)	C(13)-N(3)-N(4)	113.50(11)
C(12)-C(11)	1.390(2)	C(13)-N(3)-C(14)	113.98(12)
C(5)-C(4)	1.400(2)	N(4)-N(3)-C(14)	114.06(12)
C(11)-C(10)	1.393(2)	C(18)-C(17)-C(16)	122.00(14)
C(2)-C(3)	1.399(2)	C(10)-C(9)-C(8)	119.75(13)
C(15)-C(16)	1.4017(19)	C(5)-C(6)-N(1)	127.20(14)
C(16)-C(21)	1.510(2)	C(5)-C(6)-C(1)	120.87(14)
C(18)-C(22)	1.504(2)	N(1)-C(6)-C(1)	111.92(12)
C(4)-C(3)	1.385(3)	C(20)-C(19)-C(18)	122.12(14)
		C(11)-C(12)-C(13)	120.00(14)

C(6)-C(5)-C(4)	117.74(15)	C(17)-C(18)-C(22)	121.62(14)
C(12)-C(11)-C(10)	119.96(14)	C(19)-C(18)-C(22)	120.36(15)
C(1)-C(2)-C(3)	118.22(14)	C(9)-C(10)-C(11)	120.32(14)
C(16)-C(15)-C(20)	120.80(13)	C(9)-C(8)-C(13)	119.83(13)
C(16)-C(15)-N(4)	119.33(12)	C(9)-C(8)-N(2)	121.63(12)
C(20)-C(15)-N(4)	119.87(13)	C(13)-C(8)-N(2)	118.48(12)
C(17)-C(16)-C(15)	118.57(13)	C(3)-C(4)-C(5)	121.36(15)
C(17)-C(16)-C(21)	118.44(13)	C(4)-C(3)-C(2)	120.79(15)
C(15)-C(16)-C(21)	122.99(13)		
C(17)-C(18)-C(19)	118.02(14)		

Symmetry transformations used to generate equivalent atoms:

DFT calculations

The mechanism of the formation of the various adducts were explored computationally, using DFT. Geometry optimizations were carried out with the Gaussian 09 program. For the mechanism calculated in Figure 1, nitrosobenzene without substituents was used to reduce computation time. We used DFT calculations at the M06-2X level, in combination with the 6-311++G(2d,2p) basis set, expect for the calculation of **3** and **4** where the 6-311+G(d,p) basis set was used to reduce computation time. All minima (no imaginary frequencies) and transition states (one imaginary frequency) were characterized by calculating the Hessian matrix. The nature of the transition states was confirmed by following the intrinsic reaction coordinate. The relative free energies (ΔG°333K in kcal mol-1) obtained from these calculations are reported in the main text.

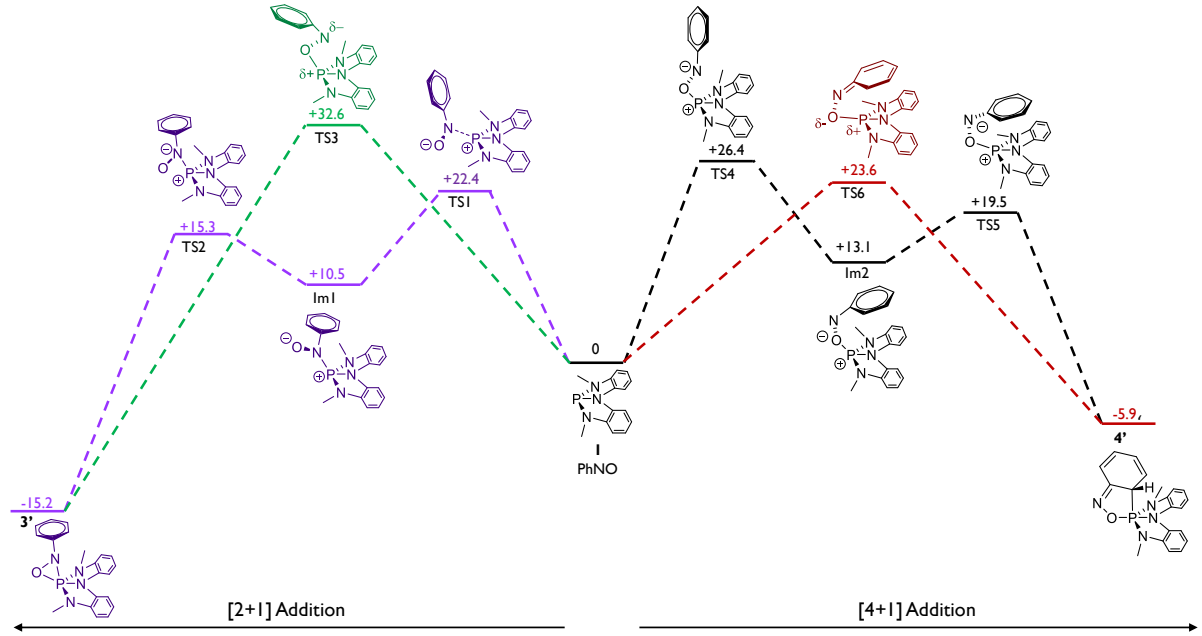

*Figure 1. DFT calculations on formation of oxazaphosphirane **2'** and oximinophosphole **3'** using Gaussian 09 M06-2X /6-311++G(2d,2p). Calculations were run on phosphorus triamide **1**, but the aryl rings were omitted for visual clarity.*

Optimized Geometries

M06-2X/6-311+G(d,p)

Phosphorus triamide **1**

Symbol	X	Y	Z
C	-2.5432960	-2.6068330	0.3730570
C	-3.4580440	-1.6763390	0.8457890
C	-1.3656400	-2.1935870	-0.2575560
C	-1.1186990	-0.8401770	-0.3959480
C	-3.2134890	-0.3077700	0.7094430
C	-2.0431950	0.0981720	0.0864040
C	3.1552740	-2.1167720	-0.1363920
C	1.9129990	-1.8647590	-0.7317700

C	1.2999760	-0.6495910	-0.5107070
C	1.9238770	0.3453540	0.2630930
C	3.7629460	-1.1455330	0.6444870
C	3.1587910	0.0994720	0.8476970
H	-4.3707880	-2.0092390	1.3262280
H	-3.9198610	0.4219550	1.0889780
H	-2.7401930	-3.6662480	0.4872480
N	0.0220350	-0.2290220	-0.9900110
N	-1.6427540	1.4034090	-0.1936330
H	3.6446320	-3.0693190	-0.3003660
H	4.7280740	-1.3434190	1.0973220
H	3.6456330	0.8554520	1.4530280
N	1.2024890	1.5368920	0.2874400
P	-0.0905620	1.5373520	-0.9023190
H	-0.6592280	-2.9239470	-0.6304300
H	1.4476840	-2.6005710	-1.3762740
C	-2.5480430	2.5191970	-0.0237490
C	1.8683010	2.7648300	0.6706720
H	-3.5086630	2.3071980	-0.5018460
H	-2.1149600	3.4046750	-0.4921980
H	-2.7216970	2.7399580	1.0338180
H	2.8497860	2.8564790	0.1917350
H	2.0008130	2.8176330	1.7546210
H	1.2542470	3.6161840	0.3692190

2,4,6-tri-*tert*-butylnitrosobenzene (**2)**

Symbol	X	Y	Z
C	-0.7407040	-1.0749850	0.0014160
C	-1.0980280	0.2908780	0.0521410
C	-0.1466870	1.3378060	-0.0435010
C	1.1932870	0.9713250	-0.0207360
C	1.6061360	-0.3604550	0.0423020
C	0.6305690	-1.3493060	0.0171320
H	1.9520000	1.7401960	-0.0515920
H	0.9495360	-2.3791830	-0.0023260
N	-2.4502770	0.7457220	0.2459140
O	-3.0874130	0.0982880	1.0333080
C	-0.5416430	2.8263710	-0.1403960
C	-1.7148320	-2.2678400	-0.1691450
C	3.1019770	-0.6771270	0.0921400
C	-1.4193370	3.0620190	-1.3834760
H	-2.3564700	2.5122170	-1.3322660
H	-1.6525590	4.1272990	-1.4693900
H	-0.8860240	2.7622190	-2.2897920
C	0.6958560	3.7228410	-0.2965710
H	1.3469320	3.6893730	0.5810370
H	1.2847270	3.4644090	-1.1803400

H	0.3662970	4.7570360	-0.4154330
C	-1.2711550	3.2978550	1.1305480
H	-2.2582130	2.8503660	1.2340130
H	-0.6870960	3.0590240	2.0236450
H	-1.4023570	4.3832100	1.0959490
C	3.7848460	-0.1148540	-1.1654110
H	3.6739350	0.9690090	-1.2396270
H	4.8550730	-0.3390960	-1.1454230
H	3.3602820	-0.5580860	-2.0696440
C	3.7123800	-0.0212740	1.3420220
H	3.2462690	-0.4079450	2.2517000
H	4.7843920	-0.2312670	1.3918910
H	3.5852040	1.0631800	1.3356920
C	3.3799240	-2.1814420	0.1570910
H	2.9272670	-2.6402890	1.0399220
H	3.0127820	-2.7026960	-0.7309350
H	4.4576780	-2.3513990	0.2141870
C	-2.1286630	-2.8324290	1.2005350
H	-2.7569160	-3.7171090	1.0578160
H	-1.2476760	-3.1346170	1.7736690
H	-2.6846390	-2.1007230	1.7832250
C	-2.9654930	-1.9137720	-1.0023200
H	-2.7082000	-1.2789670	-1.8553760
H	-3.4036760	-2.8322900	-1.3980940
H	-3.7440680	-1.4182640	-0.4295300
C	-1.0128150	-3.4086840	-0.9389850
H	-0.5977920	-3.0597880	-1.8883320
H	-0.2152940	-3.8838200	-0.3661460
H	-1.7438490	-4.1899180	-1.1550700

Oxazaphosphirane **3**

Symbol	X	Y	Z
C	5.4209546	-1.4866411	-0.8875067
C	5.9953339	-0.2538870	-0.6179296
C	5.2247137	0.7950633	-0.1077338
C	3.8780636	0.5761478	0.1272632
C	3.2900037	-0.6699174	-0.1552410
C	4.0576385	-1.7033010	-0.6640473
C	0.3382265	-3.8557170	1.2800413
C	1.1910757	-3.0367037	0.5328067
C	1.2004865	-1.6746703	0.7813508
C	0.3719882	-1.1356031	1.7791342
C	-0.4824515	-1.9425655	2.5110309
C	-0.4926578	-3.3151163	2.2500906
N	1.9222811	-0.6484022	0.1495630
N	2.9569526	1.5031646	0.6356821
N	0.5063132	0.2511778	1.8922100

C	3.3873469	2.8710212	0.8777804
C	-0.2789633	0.9501223	2.8941041
H	3.7451790	3.3248872	-0.0505855
H	2.5513997	3.4547291	1.2490972
H	4.1928584	2.8795853	1.6160115
H	-1.3439994	0.9075824	2.6495244
H	0.0272351	1.9898903	2.9445798
H	-0.1066221	0.4851139	3.8678790
H	5.6769714	1.7565513	0.1031813
H	7.0506942	-0.0942589	-0.8053039
H	6.0276718	-2.2928622	-1.2823499
H	3.6179207	-2.6642102	-0.8932281
H	1.8098328	-3.4706059	-0.2399336
H	0.3256572	-4.9219452	1.0870903
H	-1.1584213	-3.9586564	2.8141581
H	-1.1312975	-1.5212512	3.2690600
P	1.3743643	0.9510803	0.6308688
N	0.4538738	1.6510966	-0.6153393
C	-0.8338487	1.0297445	-0.7446155
C	-0.8861482	-0.1900686	-1.4553018
C	-2.9592455	-0.7058167	-0.2561879
C	-1.9441333	-1.0483868	-1.1417433
C	-3.0020867	0.6267472	0.1580336
C	-1.9909182	1.5458130	-0.1169343
H	-1.9668657	-2.0182328	-1.6223125
H	-3.8745124	0.9731466	0.7009657
O	0.5923333	2.4281408	0.6837273
C	-2.2746770	3.0552811	0.0842460
C	-3.7361338	3.3151236	-0.3480564
H	-3.9169971	4.3924068	-0.3805842
H	-3.9337722	2.9046732	-1.3412296
H	-4.4637376	2.8912668	0.3461817
C	-1.4073145	3.9278715	-0.8386677
H	-1.7647551	4.9602741	-0.7922368
H	-0.3569022	3.9285970	-0.5610275
H	-1.4916102	3.5929221	-1.8767498
C	-2.1372587	3.5292414	1.5364330
H	-2.7256225	2.9002422	2.2115561
H	-1.0990066	3.5208528	1.8592410
H	-2.5140789	4.5527735	1.6261483
C	-0.0174042	-0.5492056	-2.6872892
C	0.6218033	-1.9421452	-2.5980464
H	0.9887087	-2.2370855	-3.5856198
H	1.4736186	-1.9276885	-1.9198428
H	-0.0758419	-2.7098341	-2.2575636
C	1.0939784	0.4498174	-3.0352673
H	1.5246884	0.1608618	-3.9983049

H	0.7147166	1.4688275	-3.1241357
H	1.9023469	0.4497936	-2.3036707
C	-1.0021337	-0.5403165	-3.8800522
H	-1.7805096	-1.2976459	-3.7690686
H	-1.4914485	0.4331599	-3.9686980
H	-0.4644543	-0.7415187	-4.8109656
C	-4.0738623	-1.6717374	0.1475819
C	-4.1943447	-1.7069064	1.6788890
H	-4.3848824	-0.7150786	2.0956272
H	-5.0192417	-2.3593409	1.9805205
H	-3.2731810	-2.0902454	2.1237446
C	-5.4060509	-1.2001808	-0.4571787
H	-6.2134765	-1.8888957	-0.1906120
H	-5.6825409	-0.2057093	-0.0984694
H	-5.3405254	-1.1548453	-1.5472966
C	-3.7959337	-3.0984030	-0.3349452
H	-3.8086619	-3.1707732	-1.4257161
H	-2.8270572	-3.4574195	0.0242384
H	-4.5684575	-3.7728446	0.0437958

Oximinophosphole **4**

Symbol	X	Y	Z
C	4.9126699	0.1701388	1.0632974
C	5.1203398	-1.0780468	0.4976994
C	4.0670876	-1.7619366	-0.1154462
C	2.8126153	-1.1714315	-0.1470998
C	2.5986548	0.0891957	0.4301437
C	3.6475899	0.7633298	1.0374318
C	0.6315188	4.1560453	0.1485197
C	1.2144113	2.9626216	0.5894872
C	0.8398846	1.7687463	-0.0035794
C	-0.1228618	1.7558475	-1.0285961
C	-0.7138010	2.9373278	-1.4518443
C	-0.3238848	4.1410667	-0.8550717
N	1.2671181	0.4666380	0.2788385
N	1.6518084	-1.7113162	-0.7183481
N	-0.3869526	0.4721509	-1.5114720
C	1.8375985	-2.9446422	-1.4815139
C	-1.2911741	0.3601039	-2.6478317
H	2.2079227	-3.7370388	-0.8245255
H	0.9060820	-3.2640339	-1.9271286
H	2.5791183	-2.7716638	-2.2661596
H	-2.3159794	0.6200998	-2.3624138
H	-1.2809576	-0.6513037	-3.0375168
H	-0.9534581	1.0424390	-3.4320478
H	4.2410840	-2.7318549	-0.5632452
H	6.1031950	-1.5333793	0.5267835

H	5.7336981	0.6944744	1.5382661
H	3.5010026	1.7319734	1.4922045
H	1.9194709	2.9802347	1.4089632
H	0.9204513	5.0917355	0.6124568
H	-0.7823704	5.0675614	-1.1813956
H	-1.4672511	2.9348465	-2.2296794
P	0.2323708	-0.7840747	-0.5143390
N	-1.9955965	-1.9774837	-1.1018683
C	-2.2162062	-1.4613691	0.0526567
C	-3.5887915	-1.1389231	0.4797822
C	-2.5423584	0.6830881	1.8166098
C	-3.6913188	-0.0832439	1.3085214
C	-1.2997200	0.2169551	1.6269825
C	-1.0209475	-1.0597223	0.8843237
O	-0.6427657	-2.0146653	-1.3831440
H	-4.6754210	0.2434529	1.6198194
H	-0.4458436	0.7308816	2.0449642
C	-0.6114197	-2.2212439	1.8966635
C	-2.8475584	1.9796072	2.5616274
C	-4.7876348	-1.9041470	-0.0768853
C	-1.5765819	2.6702450	3.0569276
H	-1.0234778	2.0442761	3.7632840
H	-0.9145894	2.9285678	2.2273911
H	-1.8415573	3.5965962	3.5732199
C	-3.7450537	1.6895164	3.7757909
H	-3.9432950	2.6155434	4.3227733
H	-4.7113949	1.2659767	3.4941271
H	-3.2576040	0.9905715	4.4611316
C	-3.5657583	2.9373354	1.5964125
H	-4.4993807	2.5147200	1.2161670
H	-3.8088308	3.8750357	2.1047964
H	-2.9223525	3.1671135	0.7422337
C	-6.0620337	-1.5743361	0.7080878
H	-6.8841654	-2.1928350	0.3405145
H	-5.9406823	-1.7747667	1.7762280
H	-6.3632325	-0.5312911	0.5829266
C	-4.5432124	-3.4187653	0.0246804
H	-3.6814819	-3.7269597	-0.5668773
H	-4.3813011	-3.7226545	1.0630274
H	-5.4185827	-3.9588133	-0.3462980
C	-5.0212427	-1.5202951	-1.5502262
H	-5.1796929	-0.4422073	-1.6433368
H	-4.1756308	-1.8026583	-2.1753424
H	-5.9156683	-2.0280079	-1.9240366
C	0.6594148	-1.8338783	2.6635371
H	1.5262802	-1.7167800	2.0105946
H	0.5308437	-0.9101486	3.2315575

H	0.8980830	-2.6269128	3.3776283
C	-0.3764535	-3.5607836	1.1890728
H	-0.2304526	-4.3364605	1.9458555
H	-1.2295506	-3.8534679	0.5730040
H	0.5108808	-3.5431147	0.5602343
C	-1.7445715	-2.4332641	2.9133365
H	-1.4207557	-3.1654992	3.6578099
H	-2.0051832	-1.5125010	3.4378859
H	-2.6463385	-2.8222137	2.4366793

M06-2X/6-311++G(2d,2p)

Phosphorus triamide **1**

Symbol	X	Y	Z
C	-2.5638090	-2.5964140	0.3585960
C	-3.4711560	-1.6623970	0.8378760
C	-1.3827800	-2.1880840	-0.2691040
C	-1.1253150	-0.8358350	-0.3972780
C	-3.2162360	-0.2947260	0.7116310
C	-2.0429920	0.1064980	0.0911320
C	3.1383680	-2.1367400	-0.1223480
C	1.8972740	-1.8791580	-0.7176890
C	1.2952930	-0.6568590	-0.5056610
C	1.9303100	0.3388510	0.2581750
C	3.7563340	-1.1647580	0.6491550
C	3.1635550	0.0870940	0.8435340
H	-4.3857500	-1.9917270	1.3156350
H	-3.9165250	0.4377230	1.0949030
H	-2.7691990	-3.6543110	0.4646050
N	0.0204500	-0.2288540	-0.9854550
N	-1.6335630	1.4102850	-0.1806060
H	3.6187230	-3.0942880	-0.2790710
H	4.7195450	-1.3680100	1.1019550
H	3.6570300	0.8437460	1.4411800
N	1.2201230	1.5369060	0.2729340
P	-0.0851070	1.5384810	-0.9007310
H	-0.6826280	-2.9203410	-0.6476240
H	1.4242750	-2.6160910	-1.3538010
C	-2.5309640	2.5324680	-0.0035360
C	1.8948790	2.7639360	0.6467920
H	-3.4948040	2.3268350	-0.4784220
H	-2.0916830	3.4149600	-0.4724360
H	-2.6976830	2.7507520	1.0558230
H	2.8801880	2.8381960	0.1725140
H	2.0201990	2.8281010	1.7312040
H	1.2892940	3.6156360	0.3287470

2,4,6-trimethylnitrosobenzene (**3**)

Symbol	X	Y	Z
C	-0.3234230	-1.1253290	-0.0017880
C	-0.8149230	0.1988410	0.0032230

C	0.0520220	1.3087610	-0.0000980
C	1.4221040	1.0805850	-0.0086370
C	1.9413320	-0.2128300	-0.0112200
C	1.0578250	-1.2920540	-0.0103430
H	2.1002700	1.9279310	-0.0149270
H	1.4586660	-2.3009360	-0.0181390
N	-2.1973130	0.5677470	0.0091450
O	-2.9995300	-0.3324070	0.0020630
C	-0.4785140	2.7202180	-0.0012580
H	-1.0760160	2.9145550	-0.8930870
H	-1.1260240	2.8994300	0.8574820
H	0.3500770	3.4280250	0.0268170
C	-1.1984600	-2.3500950	-0.0007700
H	-1.8534080	-2.3690410	0.8717690
H	-1.8539980	-2.3703450	-0.8728120
H	-0.5739770	-3.2442960	-0.0001790
C	3.4280330	-0.4433610	0.0113800
H	3.9607650	0.3732500	-0.4776840
H	3.7852240	-0.5039270	1.0434620
H	3.6898840	-1.3780330	-0.4861540

Adduct **6**

Symbol	X	Y	Z
C	-2.0293720	-3.0319760	-1.1248700
C	-3.2397560	-3.5451930	-0.6651770
C	-3.9697510	-2.8889210	0.3169700
C	-3.4836180	-1.6953030	0.8414830
C	-2.2969760	-1.1651920	0.3636930
C	-1.5422110	-1.8242620	-0.6193210
H	-1.4766280	-3.5817790	-1.8736790
H	-3.6025810	-4.4811820	-1.0734910
H	-4.9022010	-3.3033940	0.6789000
H	-4.0152800	-1.1566320	1.6172220
N	-1.8122870	0.0905900	0.8342200
N	-0.3541370	-1.1895010	-1.0616410
P	-0.1844040	0.1811190	1.2657180
C	0.4020210	-1.9355360	-2.0553050
H	-0.2618060	-2.1311820	-2.8960290
H	1.2300020	-1.3313500	-2.4171480
H	0.7966640	-2.8822960	-1.6613730
O	0.3543110	-0.1556310	2.5948930
N	-0.0836550	1.8184950	0.9031020
C	0.9700520	2.6938530	1.3810750
H	1.6740530	2.1015900	1.9658190
H	1.5052420	3.1584410	0.5474610
H	0.5498420	3.4752740	2.0206090
C	-2.2357410	1.2972260	0.2163170
C	-1.2451700	2.2932610	0.2934770
C	-3.4451000	1.5471200	-0.3970960
C	-1.4833870	3.5632860	-0.2007350
C	-3.6790030	2.8280000	-0.9134170
H	-4.1930550	0.7669560	-0.4725340

C	-2.7180200	3.8222930	-0.8073410
H	-0.7239290	4.3328320	-0.1283170
H	-4.6248550	3.0392240	-1.3964140
H	-2.9166970	4.8102740	-1.2041450
N	0.4945860	-0.8525760	0.0956020
C	1.8822620	-0.5461080	-0.1505450
C	2.2756170	0.4985920	-0.9989730
C	3.6390590	0.7814450	-1.1081750
H	3.9507840	1.5847110	-1.7703120
C	4.5976410	0.0735220	-0.3932770
C	4.1728450	-0.9639980	0.4377030
H	4.9106650	-1.5322330	0.9966330
C	2.8294190	-1.2967730	0.5682180
C	1.3015210	1.3049520	-1.8267050
H	1.3004390	2.3519610	-1.5122370
H	1.6071240	1.2855860	-2.8766680
H	0.2809000	0.9340270	-1.7597050
C	2.3949620	-2.4199680	1.4691710
H	3.2601290	-2.9878680	1.8129660
H	1.8533910	-2.0241600	2.3310910
H	1.7110260	-3.0911710	0.9454210
C	6.0642700	0.3941580	-0.5207170
H	6.5236690	0.5115330	0.4631430
H	6.5927250	-0.4118940	-1.0365050
H	6.2210360	1.3150870	-1.0833200

Nitrosobenzene

Symbol	X	Y	Z
C	-0.0957250	1.0967480	0.0000000
C	1.2698530	1.3313980	0.0000000
C	2.1654730	0.2593920	0.0000000
C	1.7018130	-1.0519330	0.0000000
C	0.3326180	-1.2956350	0.0000000
C	-0.5488350	-0.2217370	0.0000000
H	-0.8155600	1.9060630	0.0000000
H	1.6449360	2.3476460	0.0000000
H	3.2318220	0.4523950	0.0000000
H	2.4021940	-1.8778280	0.0000000
H	-0.0713480	-2.3015360	0.0000000
N	-1.9531450	-0.5782080	0.0000010
O	-2.7089010	0.3514140	-0.0000010

TS1

Symbol	X	Y	Z
C	4.4656720	1.6326430	-1.3035440
C	4.2135260	2.6725140	-0.4192370
C	3.0113150	2.7379940	0.2877670
C	2.0698270	1.7350030	0.0989050
C	2.3355970	0.6707460	-0.7814040
C	3.5173450	0.6248870	-1.4976860
C	2.4432700	-3.8173940	-0.4875490
C	2.3717650	-2.5201390	-1.0035190

C	1.4777480	-1.6245400	-0.4459740
C	0.6329410	-2.0223630	0.6054610
C	0.6961810	-3.3132830	1.1106470
C	1.6152860	-4.2071860	0.5548770
N	1.2775750	-0.2701690	-0.7962670
N	0.8145020	1.6530050	0.7050930
N	-0.2343620	-1.0080950	1.0269300
C	0.5336180	2.4492310	1.8919230
C	-1.0511610	-1.2202790	2.2108180
H	0.3197600	3.4882740	1.6357510
H	-0.3363520	2.0487300	2.4064760
H	1.3982610	2.3974940	2.5608860
H	-1.8017260	-2.0008140	2.0451130
H	-1.5690950	-0.2998280	2.4674590
H	-0.4123670	-1.5226480	3.0466330
H	2.8134950	3.5590530	0.9654730
H	4.9517300	3.4532270	-0.2808780
H	5.3966790	1.6026300	-1.8553450
H	3.7019010	-0.1759460	-2.2006690
H	3.0042150	-2.2219540	-1.8283150
H	3.1464230	-4.5220800	-0.9137520
H	1.6734480	-5.2167500	0.9428750
H	0.0513350	-3.6223670	1.9236700
P	-0.1355370	0.3932020	0.0339570
N	-1.9384800	1.2205770	0.5817600
C	-3.0668310	0.6437730	-0.1576210
C	-4.0953780	1.4870860	-0.5642870
C	-5.3409420	-0.4233720	-1.3516850
C	-5.2295180	0.9485910	-1.1624390
C	-4.3078860	-1.2620520	-0.9371880
C	-3.1737980	-0.7366910	-0.3363120
H	-3.9922750	2.5510130	-0.3998570
H	-6.0299540	1.6071860	-1.4781060
H	-6.2256160	-0.8405350	-1.8172700
H	-4.3829340	-2.3322500	-1.0884900
H	-2.3673050	-1.3959810	-0.0435960
O	-1.9315840	2.4559090	0.6135330

Im1

Symbol	X	Y	Z
C	-4.8064220	-0.2221390	-1.0036440
C	-4.8646810	-1.4168300	-0.3005650
C	-3.7221410	-1.9537080	0.2967100
C	-2.5299190	-1.2607720	0.1782600
C	-2.4680690	-0.0535350	-0.5387320
C	-3.5981640	0.4677360	-1.1382160
C	-0.8236410	4.2004540	-0.3248570
C	-1.3095230	2.9725570	-0.7826120
C	-0.8110760	1.8106980	-0.2235650
C	0.1853450	1.8663200	0.7679320
C	0.6865580	3.0816290	1.2032670
C	0.1614940	4.2525220	0.6510100

N	-1.1513190	0.4726260	-0.5288300
N	-1.2882500	-1.6452530	0.7051090
N	0.5969750	0.5924630	1.1881740
C	-1.1015340	-2.9370770	1.3570210
C	1.6999370	0.4356410	2.1248760
H	-1.3523230	-3.7379940	0.6611290
H	-0.0515740	-3.0556180	1.6147650
H	-1.7260680	-2.9804490	2.2530010
H	2.6130670	0.8823890	1.7208650
H	1.8812490	-0.6259640	2.2888210
H	1.4418980	0.9062070	3.0763920
H	-3.7653450	-2.8886690	0.8405630
H	-5.8051930	-1.9469360	-0.2155330
H	-5.6998590	0.1786740	-1.4652120
H	-3.5529910	1.3840770	-1.7095540
H	-2.0488490	2.9337930	-1.5702280
H	-1.2134500	5.1169470	-0.7494730
H	0.5374670	5.2107700	0.9876820
H	1.4618830	3.1245280	1.9577300
P	-0.0746140	-0.6197600	0.2496650
N	1.1305350	-1.5563670	-0.2848990
C	2.4473990	-1.0590920	-0.5160000
C	3.5084230	-1.9344920	-0.2906920
C	5.0638000	-0.1806180	-0.8772380
C	4.8108270	-1.4875860	-0.4641300
C	3.9984200	0.6730130	-1.1422350
C	2.6881040	0.2338800	-0.9796620
H	3.2726880	-2.9505590	-0.0008150
H	5.6355480	-2.1669000	-0.2823390
H	6.0823400	0.1612040	-1.0152920
H	4.1811050	1.6785350	-1.5029430
H	1.8618890	0.8897950	-1.2362840
O	0.8824160	-2.8491650	-0.6170870

TS2

Symbol	X	Y	Z
C	-4.5624930	-0.0461080	-1.4885860
C	-4.8003280	-1.1845630	-0.7314650
C	-3.7944520	-1.7535950	0.0524910
C	-2.5492100	-1.1467010	0.0683290
C	-2.3121430	0.0070830	-0.6949210
C	-3.3019270	0.5558190	-1.4845570
C	-0.6078260	4.1717220	-0.0572830
C	-1.0701120	2.9828740	-0.6274930
C	-0.6463290	1.7833270	-0.0894390
C	0.2426920	1.7598760	0.9983450
C	0.7241900	2.9372260	1.5456890
C	0.2823350	4.1472650	1.0079880
N	-0.9748310	0.4679200	-0.5255970
N	-1.4175230	-1.5852340	0.7807380
N	0.5921800	0.4551680	1.3773530
C	-1.4900960	-2.7823000	1.6187780

C	1.7881820	0.1760950	2.1695890
H	-1.6794710	-3.6575540	0.9955270
H	-0.5341140	-2.9303280	2.1094660
H	-2.2926740	-2.6470950	2.3483850
H	2.6521810	0.6791230	1.7258680
H	1.9689820	-0.9010070	2.1634600
H	1.6421750	0.5105910	3.1983730
H	-3.9830310	-2.6491130	0.6298300
H	-5.7778690	-1.6502390	-0.7530900
H	-5.3509520	0.3738180	-2.0998000
H	-3.1023440	1.4235600	-2.0979780
H	-1.7351010	3.0041450	-1.4795610
H	-0.9398140	5.1186850	-0.4636360
H	0.6447170	5.0772350	1.4285300
H	1.4198930	2.9154270	2.3750440
P	-0.0928420	-0.6820110	0.3641660
N	1.0767080	-1.6541030	-0.2054370
C	2.3109160	-1.1324720	-0.6376590
C	3.4658480	-1.8848470	-0.4190530
C	4.7921370	-0.1181380	-1.4107470
C	4.6961820	-1.3710550	-0.8119680
C	3.6323320	0.6194030	-1.6369400
C	2.3924130	0.1166010	-1.2669880
H	3.3538270	-2.8504250	0.0553030
H	5.5922490	-1.9574580	-0.6425460
H	5.7559330	0.2750260	-1.7097660
H	3.6892500	1.5881730	-2.1197320
H	1.4948140	0.6852860	-1.4909620
O	1.0605480	-2.8736270	0.4688410

oxazaphosphirane **3'**

Symbol	X	Y	Z
C	-4.4225600	1.0012090	-1.3802280
C	-4.9379520	-0.1690520	-0.8445290
C	-4.1092900	-1.0666620	-0.1652820
C	-2.7659350	-0.7589710	-0.0344160
C	-2.2384700	0.4223010	-0.5841930
C	-3.0628730	1.3040290	-1.2602490
C	0.4991720	3.9607520	0.2115570
C	-0.2698460	2.9600750	-0.3906840
C	-0.1906150	1.6694170	0.1008160
C	0.6653660	1.3707310	1.1750860
C	1.4386900	2.3581480	1.7619800
C	1.3427560	3.6630200	1.2707340
N	-0.8608440	0.5118030	-0.3297660
N	-1.7906780	-1.5347020	0.6089220
N	0.6369840	0.0142260	1.5259530
C	-2.1591780	-2.8352070	1.1486360
C	1.5218370	-0.4606520	2.5791670
H	-2.5293860	-3.4837380	0.3497430
H	-1.2882220	-3.3010760	1.5983320
H	-2.9389570	-2.7107740	1.9038600

H	2.5672810	-0.3070270	2.2945900
H	1.3579530	-1.5213770	2.7428810
H	1.3110060	0.0848260	3.5025860
H	-4.5130160	-1.9798500	0.2529880
H	-5.9910320	-0.3968190	-0.9532460
H	-5.0730020	1.6873530	-1.9080620
H	-2.6680340	2.2079230	-1.7005050
H	-0.8966340	3.1955310	-1.2386730
H	0.4400330	4.9737510	-0.1663410
H	1.9411070	4.4445790	1.7224250
H	2.1030730	2.1275420	2.5847040
P	-0.2365980	-0.9346220	0.4453840
N	0.7053010	-1.7829250	-0.6611740
C	2.0142520	-1.3032710	-0.9396790
C	2.1443610	-0.3578760	-1.9590430
C	4.5345140	-0.3452750	-1.6161140
C	3.4052600	0.1192830	-2.2871800
C	4.3914430	-1.2917630	-0.6081100
C	3.1326650	-1.7724950	-0.2588000
H	1.2578040	-0.0094860	-2.4767590
H	3.5072230	0.8592390	-3.0723010
H	5.5165250	0.0275850	-1.8796400
H	5.2657020	-1.6620050	-0.0850280
H	3.0016980	-2.5060830	0.5260010
O	0.5926160	-2.3720030	0.7246670

TS3

Symbol	X	Y	Z
C	0.1290280	3.9442360	-0.0589460
C	-0.8705130	3.7275340	0.8774200
C	-1.1519130	2.4385100	1.3409220
C	-0.4002260	1.3857110	0.8483100
C	0.6177950	1.6044770	-0.0943130
C	0.8785030	2.8760310	-0.5635070
C	4.9793990	0.6092850	-0.6600960
C	3.6528280	1.0203810	-0.8178330
C	2.6389730	0.1765880	-0.4006660
C	2.9512830	-1.0685530	0.1685810
C	4.2635010	-1.4848820	0.3126070
C	5.2825210	-0.6273750	-0.1095670
N	1.2449930	0.3867200	-0.4525630
N	-0.5544850	0.0264490	1.1532350
N	1.7958480	-1.7835940	0.5187130
C	-1.6419290	-0.4137930	2.0116160
C	1.8609480	-3.1775160	0.9171250
H	-1.6570000	-1.5032620	2.0425130
H	-1.4877540	-0.0297350	3.0234460
H	-2.6078870	-0.0707040	1.6284170
H	2.4247180	-3.7570540	0.1812570
H	0.8464500	-3.5750370	0.9761720
H	2.3343010	-3.2797940	1.8968550
H	-1.9409330	2.2674470	2.0624600

H	-1.4521440	4.5624770	1.2487280
H	0.3235390	4.9459230	-0.4210040
H	1.6200630	3.0438140	-1.3315320
H	3.4316700	1.9780490	-1.2653120
H	5.7769860	1.2666050	-0.9829020
H	6.3151850	-0.9353860	-0.0033830
H	4.4932910	-2.4472740	0.7532620
P	0.3557480	-0.9775460	0.1128280
N	-1.4400580	-0.3488600	-1.5994930
C	-2.7049100	-0.6082960	-1.0964060
C	-3.5781620	0.4941070	-1.0210600
C	-5.2283700	-0.8806690	0.0791740
C	-4.8252270	0.3542510	-0.4402880
C	-4.3733130	-1.9750900	-0.0034800
C	-3.1173120	-1.8545860	-0.5886880
O	-0.6480800	-1.3794890	-1.4386090
H	-2.4561340	-2.7069650	-0.6729740
H	-5.4894820	1.2087120	-0.3791300
H	-3.2301590	1.4469470	-1.4044780
H	-4.6918610	-2.9360840	0.3851450
H	-6.2059260	-0.9866970	0.5342410

TS 4

Symbol	X	Y	Z
C	-4.3548560	-1.9383750	-1.3223940
C	-4.1114670	-2.9214040	-0.3730310
C	-2.9774840	-2.8686890	0.4404230
C	-2.0996560	-1.8034290	0.2922520
C	-2.3481540	-0.8079170	-0.6707600
C	-3.4624380	-0.8772810	-1.4880870
C	-2.5189800	3.6983060	-1.0864110
C	-2.4085370	2.3354990	-1.3652680
C	-1.5706540	1.5600210	-0.5808510
C	-0.8128200	2.1416670	0.4517890
C	-0.9200090	3.4994450	0.7225650
C	-1.7845360	4.2703540	-0.0550020
N	-1.3454310	0.1757570	-0.6459670
N	-0.9106930	-1.5934910	0.9988970
N	0.0127650	1.2256510	1.1058220
C	-0.4907430	-2.5791680	1.9863830
C	0.6643900	1.6155530	2.3503940
H	0.3725930	-2.2079210	2.5291580
H	-1.3095060	-2.7494460	2.6905530
H	-0.2281820	-3.5273210	1.5079840
H	1.4532720	2.3466230	2.1648720
H	1.1178120	0.7454910	2.8153760
H	-0.0881040	2.0407910	3.0218100
H	-2.7907910	-3.6457240	1.1703580
H	-4.8027910	-3.7478320	-0.2631360
H	-5.2347280	-1.9965140	-1.9506890
H	-3.6367530	-0.1279710	-2.2471780
H	-2.9657300	1.8959410	-2.1803010

H	-3.1775140	4.3126760	-1.6875670
H	-1.8730640	5.3310570	0.1453720
H	-0.3415820	3.9518980	1.5178630
P	0.0151490	-0.3093340	0.3536070
N	2.6369530	-0.1439410	1.2137770
C	3.5144630	-0.3796910	0.1777760
C	4.6951080	0.3932770	0.1645510
C	5.3217990	-0.5939390	-1.9440750
C	5.5879450	0.2773480	-0.8797730
C	4.1567820	-1.3497870	-1.9427430
C	3.2519340	-1.2611310	-0.8888660
O	1.6032480	-0.9325430	1.1392300
H	2.3639850	-1.8771810	-0.8687800
H	6.4945550	0.8712210	-0.8826020
H	4.8692970	1.0768950	0.9872280
H	3.9519540	-2.0259040	-2.7648860
H	6.0243870	-0.6782280	-2.7643200

Im2

Symbol	X	Y	Z
C	-4.5409570	1.5306760	-0.8796500
C	-5.1383930	0.3546150	-0.4477700
C	-4.3641290	-0.7258000	-0.0196210
C	-2.9874000	-0.5908190	-0.0339210
C	-2.3815670	0.5909730	-0.4882530
C	-3.1497640	1.6566700	-0.9130330
C	0.9260480	3.6291460	0.4126020
C	0.0070630	2.8236410	-0.2636470
C	-0.1205240	1.5071660	0.1273860
C	0.6712820	0.9754060	1.1551320
C	1.6035270	1.7629330	1.8064010
C	1.7129410	3.1019240	1.4275690
N	-0.9620860	0.5035220	-0.4373900
N	-2.0429190	-1.5639060	0.3446410
N	0.4411300	-0.4010240	1.3712920
C	-2.4164740	-2.9601380	0.5382710
C	1.2713930	-1.1543820	2.3091800
H	-1.5122180	-3.5629550	0.6085180
H	-3.0035130	-3.0723130	1.4518670
H	-2.9973200	-3.3068450	-0.3192520
H	2.3198430	-1.0986790	2.0065080
H	0.9727690	-2.1999690	2.2965450
H	1.1314070	-0.7388500	3.3100140
H	-4.8276050	-1.6412910	0.3264760
H	-6.2177620	0.2692940	-0.4382860
H	-5.1553200	2.3610650	-1.2036680
H	-2.6873670	2.5672980	-1.2674620
H	-0.5694580	3.2144990	-1.0912180
H	1.0393790	4.6659280	0.1230500
H	2.4399120	3.7315280	1.9253150
H	2.2432590	1.3479300	2.5741250
P	-0.4960220	-1.0081880	0.1497660

N	1.6656020	-2.4801250	-0.2523410
C	2.4680340	-1.4879150	-0.7117130
C	3.8225470	-1.5691980	-0.2731660
C	4.3617970	0.5451680	-1.3329330
C	4.7302950	-0.5773600	-0.5794010
C	3.0576860	0.6167860	-1.8000400
C	2.1223530	-0.3763400	-1.5173320
O	0.2232530	-2.1393460	-0.6247940
H	1.1360590	-0.3070730	-1.9593240
H	5.7495370	-0.6727710	-0.2192500
H	4.1176230	-2.4313920	0.3153230
H	2.7493590	1.4600050	-2.4103770
H	5.0790800	1.3239980	-1.5568110

TS5

Symbol	X	Y	Z
C	-4.3198640	1.7389260	-0.8187250
C	-4.9663350	0.5545180	-0.4891640
C	-4.2400660	-0.5723490	-0.0997860
C	-2.8590260	-0.4778410	-0.0459780
C	-2.2054000	0.7129940	-0.3950970
C	-2.9269470	1.8272720	-0.7856070
C	1.2732300	3.5649800	0.5087110
C	0.2940470	2.8184760	-0.1469890
C	0.0974440	1.5060260	0.2405570
C	0.8871810	0.9231500	1.2447080
C	1.8759550	1.6574160	1.8798040
C	2.0530410	2.9886460	1.5044950
N	-0.8133820	0.5631160	-0.2783650
N	-1.9566150	-1.4891540	0.3108620
N	0.5903600	-0.4342490	1.4538620
C	-2.4470260	-2.8340220	0.5913610
C	1.3684280	-1.2154720	2.4090340
H	-2.9470740	-3.2406110	-0.2909080
H	-1.6102260	-3.4774910	0.8457380
H	-3.1518750	-2.7978670	1.4252040
H	2.4236720	-1.2187340	2.1258120
H	1.0149420	-2.2435890	2.4066700
H	1.2375840	-0.7796990	3.4033480
H	-4.7458560	-1.4936490	0.1592470
H	-6.0468930	0.4995520	-0.5322760
H	-4.8983130	2.6060550	-1.1119600
H	-2.4265020	2.7478280	-1.0510300
H	-0.2808670	3.2485290	-0.9560750
H	1.4378360	4.5960700	0.2227810
H	2.8228020	3.5752200	1.9907670
H	2.5017800	1.2060360	2.6386280
P	-0.3558940	-1.0160020	0.2070540
N	1.6666700	-2.6234930	-0.0407500
C	2.2349980	-1.6784020	-0.7940060
C	3.6355740	-1.4295580	-0.6109390
C	3.4466330	0.6664480	-1.8361820

C	4.2003700	-0.2846880	-1.1043880
C	2.1314270	0.3845020	-2.1199980
C	1.5078800	-0.7831420	-1.6345270
O	0.2268010	-2.4715630	-0.1823730
H	0.5976080	-1.1193820	-2.1153280
H	5.2536130	-0.0980260	-0.9215900
H	4.2130760	-2.1455020	-0.0372280
H	1.5564690	1.0545960	-2.7518500
H	3.9137190	1.5723780	-2.1997390

Oximinophosphole **4'**

Symbol	X	Y	Z
C	4.4762720	-0.6977780	-1.0004720
C	4.7909530	0.5831360	-0.5755120
C	3.7995470	1.4225110	-0.0580340
C	2.4975760	0.9537910	0.0148930
C	2.1733310	-0.3352770	-0.4384960
C	3.1618110	-1.1692270	-0.9374160
C	-0.3004670	-4.1324580	-0.0482230
C	0.4308320	-3.0405510	-0.5255210
C	0.2126960	-1.7920180	0.0326970
C	-0.7538060	-1.6204590	1.0405200
C	-1.4802170	-2.7037830	1.5099290
C	-1.2397450	-3.9654440	0.9579500
N	0.8130380	-0.5679560	-0.2692850
N	1.3889220	1.6434820	0.5299180
N	-0.8746630	-0.2893190	1.4558510
C	1.6529100	2.9713530	1.0828580
C	-1.7839640	-0.0055100	2.5599100
H	2.0066050	3.6382690	0.2909960
H	0.7549800	3.3832390	1.5219410
H	2.4294260	2.8909270	1.8480970
H	-2.8202500	-0.2071170	2.2719100
H	-1.6969560	1.0344800	2.8539180
H	-1.5154300	-0.6412270	3.4076710
H	4.0547530	2.4162780	0.2848130
H	5.8105140	0.9423870	-0.6384400
H	5.2511540	-1.3454690	-1.3915200
H	2.9313130	-2.1700120	-1.2706980
H	1.1365230	-3.1715850	-1.3335520
H	-0.1349410	-5.1124000	-0.4785840
H	-1.8056970	-4.8167630	1.3159730
H	-2.2246170	-2.5788190	2.2853830
P	-0.0930370	0.8188760	0.4116690
N	-2.2272190	2.2907130	0.7411750
C	-2.3773620	1.7697600	-0.4231450
C	-3.6841040	1.6430270	-1.0435250
C	-2.7272920	-0.0817680	-2.4992050
C	-3.8392790	0.7471380	-2.0331440
C	-1.4774820	0.0956180	-2.0516840
C	-1.1643000	1.1780480	-1.0713590
O	-0.8982130	2.1921330	1.1325560

H	-0.5980200	1.9806370	-1.5728430
H	-4.8134500	0.6038880	-2.4864760
H	-4.5038970	2.2278880	-0.6451120
H	-0.6562350	-0.5041580	-2.4251740
H	-2.9325230	-0.8497530	-3.2355310

TS6

Symbol	X	Y	Z
C	-4.4231250	1.5500030	-0.4966100
C	-4.9606540	0.3171550	-0.1533160
C	-4.1330680	-0.7910630	0.0447670
C	-2.7660680	-0.6308680	-0.1146530
C	-2.2231450	0.6098530	-0.4816490
C	-3.0447630	1.7054890	-0.6702850
C	1.0171910	3.7055510	0.2556900
C	0.1713170	2.8577320	-0.4685940
C	0.0017880	1.5612810	-0.0338910
C	0.6823770	1.0749090	1.0996430
C	1.5201950	1.9167170	1.8193970
C	1.6755920	3.2356160	1.3839580
N	-0.8131290	0.5521030	-0.6281700
N	-1.7756540	-1.6113990	0.0337710
N	0.4299350	-0.2744660	1.3441750
C	-2.1214650	-2.9982980	0.3000690
C	0.9639560	-0.9240850	2.5273750
H	-2.6215870	-3.0890190	1.2690220
H	-2.7885570	-3.3736700	-0.4803680
H	-1.2116480	-3.5954060	0.3157760
H	2.0559560	-0.8646850	2.5591550
H	0.6822770	-1.9761290	2.5181190
H	0.5443060	-0.4499590	3.4203400
H	-4.5481590	-1.7501720	0.3292230
H	-6.0312630	0.2091930	-0.0297960
H	-5.0754240	2.4030000	-0.6362320
H	-2.6250110	2.6661780	-0.9393800
H	-0.3312730	3.1994840	-1.3653270
H	1.1602630	4.7279270	-0.0705050
H	2.3310990	3.8978490	1.9371780
H	2.0451500	1.5580690	2.6959160
P	-0.2042380	-1.0017010	-0.1050490
N	2.1613460	-2.5527410	0.4366980
C	2.5732630	-1.6243330	-0.4698820
C	3.6806950	-0.8120140	-0.1064420
C	3.0921370	0.7257020	-1.8721190
C	3.9298010	0.3450530	-0.7890340
C	2.0413190	-0.0592710	-2.2679480
C	1.7328740	-1.2561710	-1.5619220
O	1.0114040	-3.0116460	0.1731820
H	1.1419560	-2.0319110	-2.0307680
H	4.7549150	0.9845310	-0.5012180
H	4.2751640	-1.1189280	0.7469250
H	1.4328290	0.2271400	-3.1173200

H	3.3025720	1.6469600	-2.4030980

Oximinophosphole **8**

Symbol	X	Y	Z
C	5.0489150	-2.0093340	0.2507250
C	4.4132590	-3.2332680	0.1098150
C	3.0277830	-3.2987730	-0.0636510
C	2.3016750	-2.1182970	-0.0820710
C	2.9417300	-0.8813260	0.0854430
C	4.3174830	-0.8184080	0.2417970
C	3.2644060	3.5718690	-0.7658760
C	3.2658490	2.3104150	-0.1640360
C	2.2232830	1.4404630	-0.4347350
C	1.1626430	1.8297180	-1.2696180
C	1.1554590	3.0877840	-1.8536140
C	2.2240670	3.9518630	-1.6005520
N	2.0030540	0.1439990	0.0388650
N	0.9202630	-1.9834220	-0.2682530
N	0.1790150	0.8433630	-1.3802010
C	0.1629670	-3.2239660	-0.4139530
C	-0.9831720	1.1499450	-2.2062420
H	0.3136400	-3.8483190	0.4711110
H	-0.8913270	-3.0097100	-0.5246600
H	0.5185470	-3.7664150	-1.2941910
H	-1.5872690	1.9442170	-1.7556280
H	-1.5969920	0.2649390	-2.3302270
H	-0.6374310	1.4746860	-3.1905060
H	2.5402980	-4.2561710	-0.1908740
H	4.9896470	-4.1498410	0.1272110
H	6.1240360	-1.9684220	0.3742760
H	4.8254660	0.1284180	0.3491190
H	4.0560270	2.0354850	0.5202940
H	4.0763130	4.2590640	-0.5634660
H	2.2269750	4.9357960	-2.0532640
H	0.3389010	3.4019250	-2.4901910
P	0.3234190	-0.3945500	-0.1999410
C	-2.2020070	-0.2899480	0.2957920
C	-1.6481260	0.3350090	1.3708930
N	-0.2447210	0.2139500	1.3489510
O	-1.2428750	-0.9388760	-0.4713820
C	-2.2492150	1.0512620	2.4641330
C	0.5236150	0.6991380	2.3862150
C	-0.0401480	1.3248660	3.4414680
C	-3.5720930	-0.4142240	-0.1356520
C	-1.4665260	1.5180410	3.4635030
H	-3.3216880	1.1733780	2.4469290
H	0.5859400	1.6812720	4.2463300
H	-1.9175630	2.0447590	4.2961180
H	1.5878680	0.5408820	2.2903360
C	-3.8868350	-1.1805470	-1.2739880
C	-5.2097130	-1.2788180	-1.6674720
H	-5.4758300	-1.8642810	-2.5405180

C	-6.1903030	-0.6217930	-0.9303650
C	-5.7815980	0.1080150	0.1819710
H	-7.2365780	-0.6706050	-1.2017590
N	-4.5198460	0.2205540	0.5797670
H	-6.5149920	0.6348440	0.7863370
H	-3.0970240	-1.6838520	-1.8161040

Oxazaphosphirane **10**

Symbol	X	Y	Z
C	2.0208210	4.1008200	1.4711990
C	2.9728920	3.9193330	0.4803220
C	2.8115730	2.9217070	-0.4873220
C	1.6824550	2.1224300	-0.4355750
C	0.7149250	2.3027090	0.5705340
C	0.8832310	3.2887010	1.5268570
C	-3.7527130	2.5713680	1.3941850
C	-2.3685500	2.3985620	1.5025790
C	-1.7014140	1.7018340	0.5118510
C	-2.4086040	1.1620270	-0.5773120
C	-3.7812140	1.3118300	-0.6723900
C	-4.4488890	2.0332280	0.3236640
N	-0.3386430	1.3970340	0.4071140
N	1.3507940	1.0880170	-1.3204210
N	-1.5813610	0.4709840	-1.4743760
C	2.1879280	0.8541560	-2.4835760
C	-2.2130940	-0.3075590	-2.5270530
H	2.2380410	1.7631160	-3.0900040
H	3.2003470	0.5754460	-2.1748490
H	1.7654810	0.0469060	-3.0757530
H	-2.8608670	-1.0767900	-2.0916940
H	-1.4534330	-0.7887960	-3.1336200
H	-2.8112020	0.3566310	-3.1551500
H	3.5528340	2.7857540	-1.2648020
H	3.8527130	4.5503690	0.4511350
H	2.1569170	4.8731930	2.2181580
H	0.1543080	3.4283030	2.3119020
H	-1.8389070	2.7820460	2.3628020
H	-4.2810250	3.1188030	2.1650640
H	-5.5220450	2.1639410	0.2547670
H	-4.3309100	0.8870510	-1.5023940
P	-0.0262470	0.2202130	-0.8718550
C	0.3617290	-1.4337060	-0.3469470
C	-0.7383000	-2.3300130	0.1533240
N	-1.8863390	-1.7424710	0.4907810
O	0.3260050	-1.1800250	-1.7952130
C	-0.5482280	-3.7103230	0.2190550
C	-2.8892890	-2.5141830	0.9066140
C	-2.7995250	-3.8981010	1.0007850
C	1.7284880	-1.7503750	0.1731310
C	-1.6005020	-4.5058630	0.6465010
H	0.4079790	-4.1394940	-0.0559850
H	-3.6460670	-4.4784660	1.3455090

H	-1.4870310	-5.5821590	0.7067610
H	-3.8035910	-1.9950260	1.1785780
C	2.8048440	-1.9312280	-0.6935290
C	4.0503810	-2.2129570	-0.1470730
H	4.9093610	-2.3687670	-0.7900000
C	4.1753910	-2.2935920	1.2332760
C	3.0348300	-2.1036650	2.0090700
H	5.1274070	-2.5022510	1.7044690
N	1.8335570	-1.8450090	1.5012800
H	3.0904670	-2.1656890	3.0918050
H	2.6438430	-1.8598330	-1.7608580

TS7

Symbol	X	Y	Z
C	-4.1531000	-2.8137820	0.4286340
C	-3.5519130	-3.0615400	1.6545230
C	-2.4859630	-2.2815580	2.1116490
C	-2.0394670	-1.2264220	1.3240160
C	-2.6482860	-0.9847770	0.0774060
C	-3.6867990	-1.7714340	-0.3799320
C	-4.4855990	2.8064720	-1.3462110
C	-3.9825670	1.5057970	-1.2491460
C	-2.7021850	1.3172010	-0.7614520
C	-1.9210630	2.4153300	-0.3651260
C	-2.4134340	3.7085130	-0.4797670
C	-3.7069090	3.8935040	-0.9741900
N	-2.0180660	0.0909940	-0.5966200
N	-0.9906760	-0.3488850	1.6000840
N	-0.6604220	2.0357710	0.0948360
C	-0.1898380	-0.6025390	2.7844890
C	0.3680690	3.0421380	0.2655050
H	0.4367890	-1.4954620	2.6707880
H	0.4498270	0.2517560	2.9867150
H	-0.8628150	-0.7368050	3.6348180
H	0.3898180	3.7090410	-0.6013890
H	1.3354590	2.5544000	0.3605540
H	0.1866730	3.6384180	1.1659900
H	-2.0182790	-2.5063950	3.0610640
H	-3.9022560	-3.8828520	2.2684270
H	-4.9704630	-3.4361480	0.0869030
H	-4.1126500	-1.5927700	-1.3597310
H	-4.5849340	0.6576120	-1.5470660
H	-5.4891770	2.9618670	-1.7222600
H	-4.1033580	4.8977670	-1.0618770
H	-1.8142220	4.5566740	-0.1722400
P	-0.4064840	0.3282280	0.1051490
C	2.3991890	-0.3389730	0.2624890
C	1.9440910	-1.4662000	-0.5031700
N	0.5986640	-1.6655810	-0.3823180
O	1.4915490	0.2986090	0.9005640
C	2.7031660	-2.1900720	-1.4583380
C	0.0014420	-2.5796020	-1.1815390

C	0.6933390	-3.3395410	-2.0907310
C	3.7400560	0.2870420	0.2095920
C	2.0775880	-3.1299350	-2.2361560
H	3.7557580	-1.9770640	-1.5550110
H	0.1755430	-4.0981320	-2.6638590
H	2.6448510	-3.7011620	-2.9610230
H	-1.0652830	-2.7094470	-1.0332120
C	3.9468450	1.4857550	0.9109630
C	5.2016360	2.0698150	0.8880470
H	5.3824670	2.9975030	1.4187070
C	6.2264740	1.4424050	0.1886580
C	5.9352140	0.2437790	-0.4533120
H	7.2251230	1.8575330	0.1481020
N	4.7336190	-0.3234580	-0.4511770
H	6.7101790	-0.2877550	-0.9979370
H	3.1340850	1.9189840	1.4767300

Adduct **11**

Symbol	X	Y	Z
C	1.0507430	2.8168700	0.8495560
C	0.8902470	3.8946840	-0.0130150
C	0.1558020	3.7684600	-1.1874110
C	-0.4508940	2.5523170	-1.4802620
C	-0.3322530	1.4888110	-0.5980390
C	0.4494370	1.5891880	0.5654840
H	1.6692950	2.9209000	1.7309380
H	1.3681690	4.8375560	0.2258780
H	0.0554100	4.6050120	-1.8672080
H	-1.0370250	2.4132000	-2.3813690
N	-1.0611600	0.2774360	-0.8097900
N	0.5498730	0.4586540	1.4000160
C	0.9574730	-0.7792730	0.7537240
H	0.8179170	-1.5893270	1.4802830
P	-0.2623400	-1.1964710	-0.5894650
C	1.1034480	0.6538880	2.7309630
H	0.5751180	1.4731410	3.2209320
H	0.9303960	-0.2544170	3.3107080
H	2.1777710	0.8686070	2.7166120
C	2.4085350	-0.8242870	0.2802460
C	2.9528760	-2.0119900	-0.2150760
C	4.2762960	-2.0148360	-0.6211640
H	2.3375180	-2.8979100	-0.3074560
C	4.3842840	0.2860800	-0.0113280
C	5.0141010	-0.8392810	-0.5219290
H	4.7248940	-2.9180400	-1.0178400
H	4.9209550	1.2249210	0.0854570
H	6.0499780	-0.7937350	-0.8331260
N	3.1107560	0.2992180	0.3875790
O	0.3724250	-1.9459080	-1.6931320
N	-1.6195220	-1.9267540	0.0884420
C	-1.7490730	-3.3568610	0.2944030
H	-0.7868890	-3.8342680	0.1051810

H	-2.0582210	-3.5719380	1.3209180
H	-2.4805680	-3.7811460	-0.3991930
C	-2.4148130	0.1981740	-0.3908550
C	-2.7327390	-1.0804640	0.0940480
C	-3.3646010	1.1988690	-0.4174840
C	-4.0190380	-1.3820820	0.5058810
C	-4.6598710	0.9028670	0.0221680
H	-3.1058180	2.1900900	-0.7682880
C	-4.9845660	-0.3706620	0.4654090
H	-4.2670390	-2.3723360	0.8681720
H	-5.4143340	1.6794550	0.0081960
H	-5.9938280	-0.5881540	0.7926070