

SUPPORTING INFORMATION_II

Dearomatizing Anionic Cyclization of Phosphonamides. A Route to Phosphonic Acid Derivatives with Antitumor Properties

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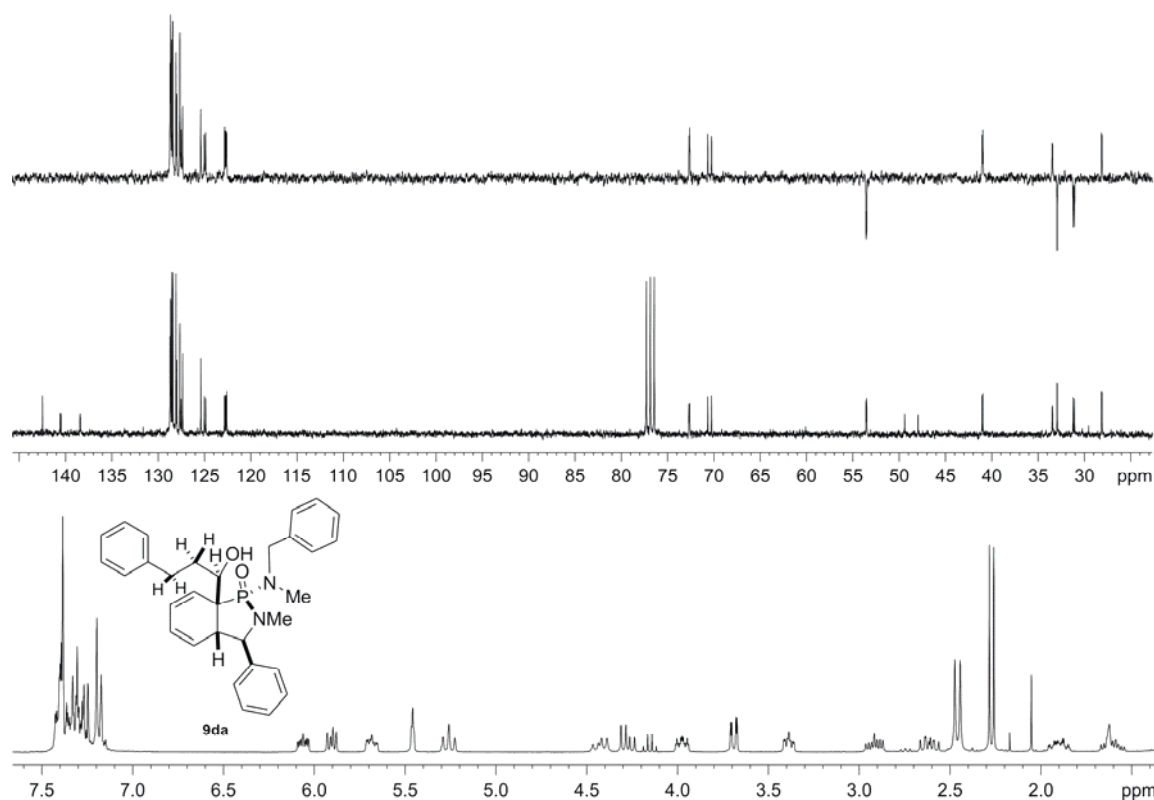


Figure S24. ^1H NMR (bottom) (300.13 MHz) and $^{13}\text{C}\{^1\text{H}\}$ (middle) and DEPT-135 (top) NMR spectra (75.47 MHz) of **9da** measured in CDCl_3 at 50 °C.

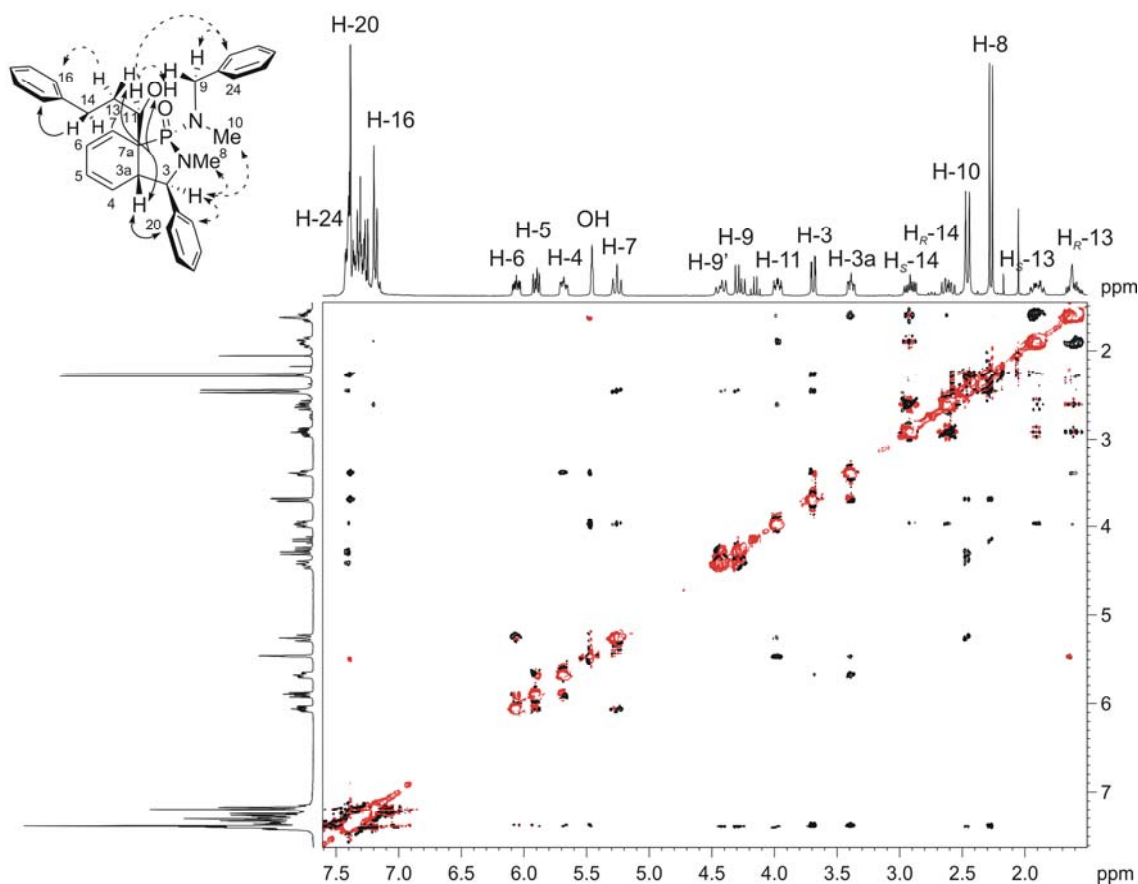


Figure S25. 2D gNOESY spectrum (300.13 MHz, mixing time 0.5 s) at 50 °C of **9da** and selected NOEs observed that confirm the assignment of the relative configuration of the stereogenic centers.

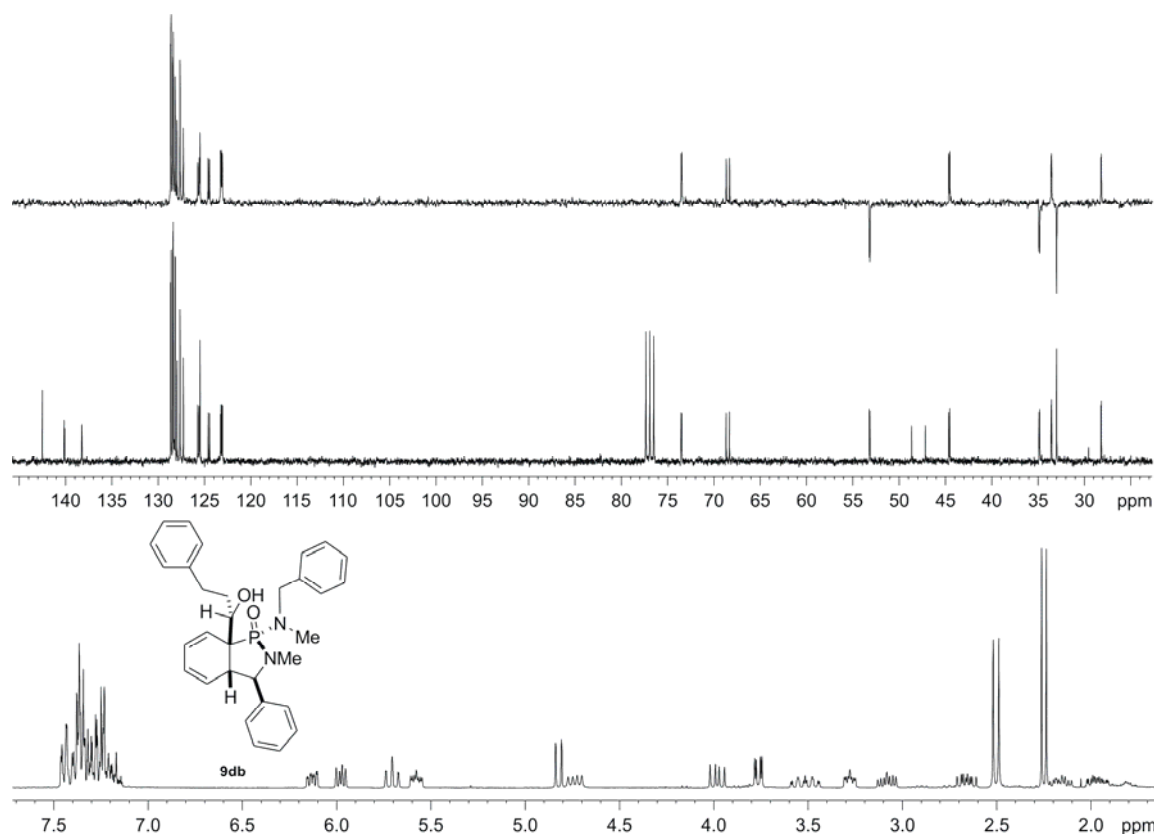


Figure S26. ¹H NMR (bottom) (300.13 MHz) and ¹³C{¹H} (middle) and DEPT-135 (top) NMR spectra (75.47 MHz) of **9db** measured in CDCl₃ at 50 °C.

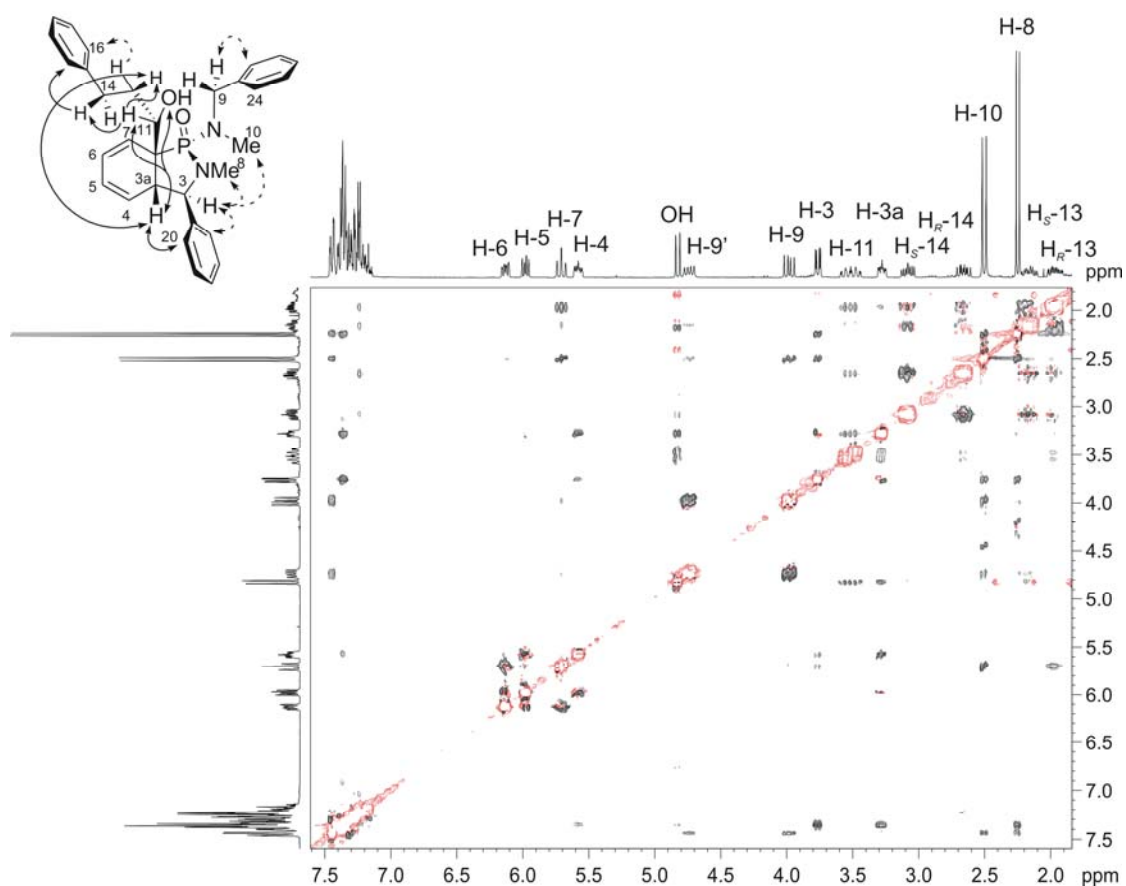


Figure S27. 2D gNOESY spectrum (300.13 MHz, mixing time 0.5 s) at 50 °C of **9db** and selected NOEs observed that confirm the assignment of the relative configuration of the stereogenic centers.

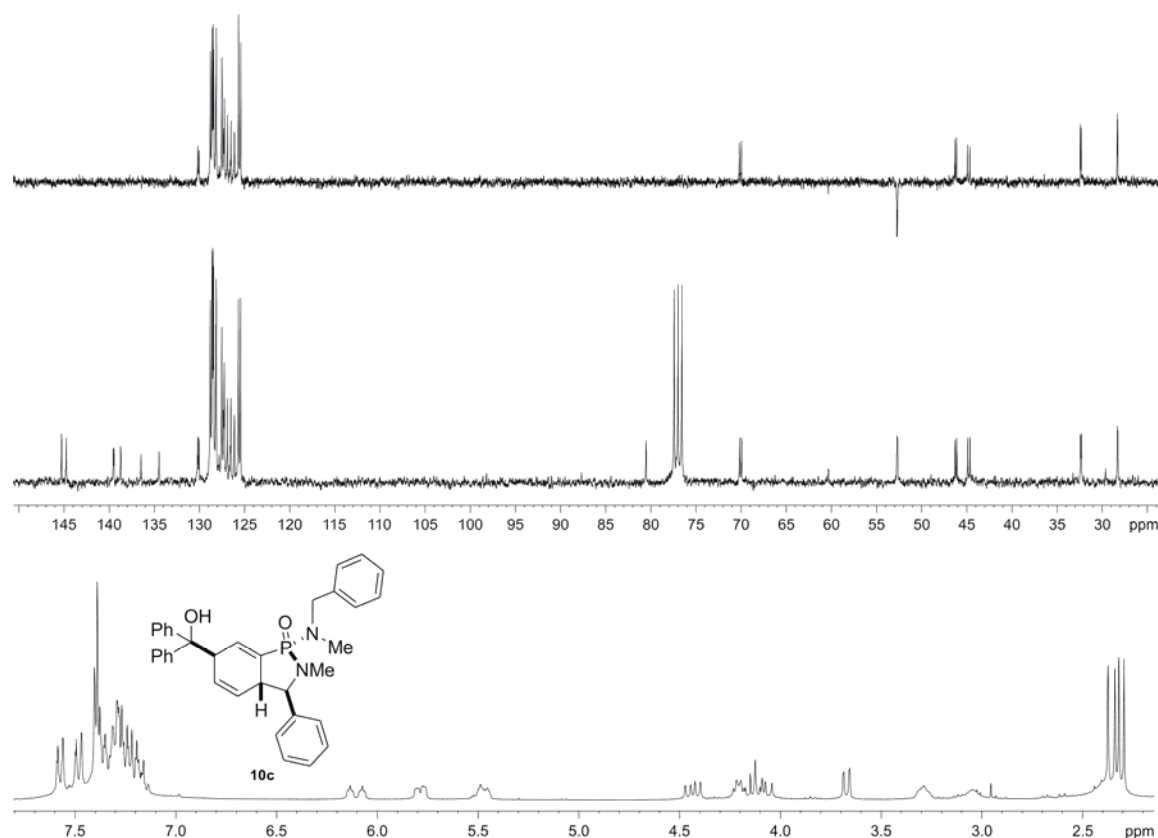


Figure S28. ^1H NMR (bottom) (300.13 MHz) and $^{13}\text{C}\{^1\text{H}\}$ (middle) and DEPT-135 (top) NMR spectra (75.47 MHz) of **10c** measured in CDCl_3 .

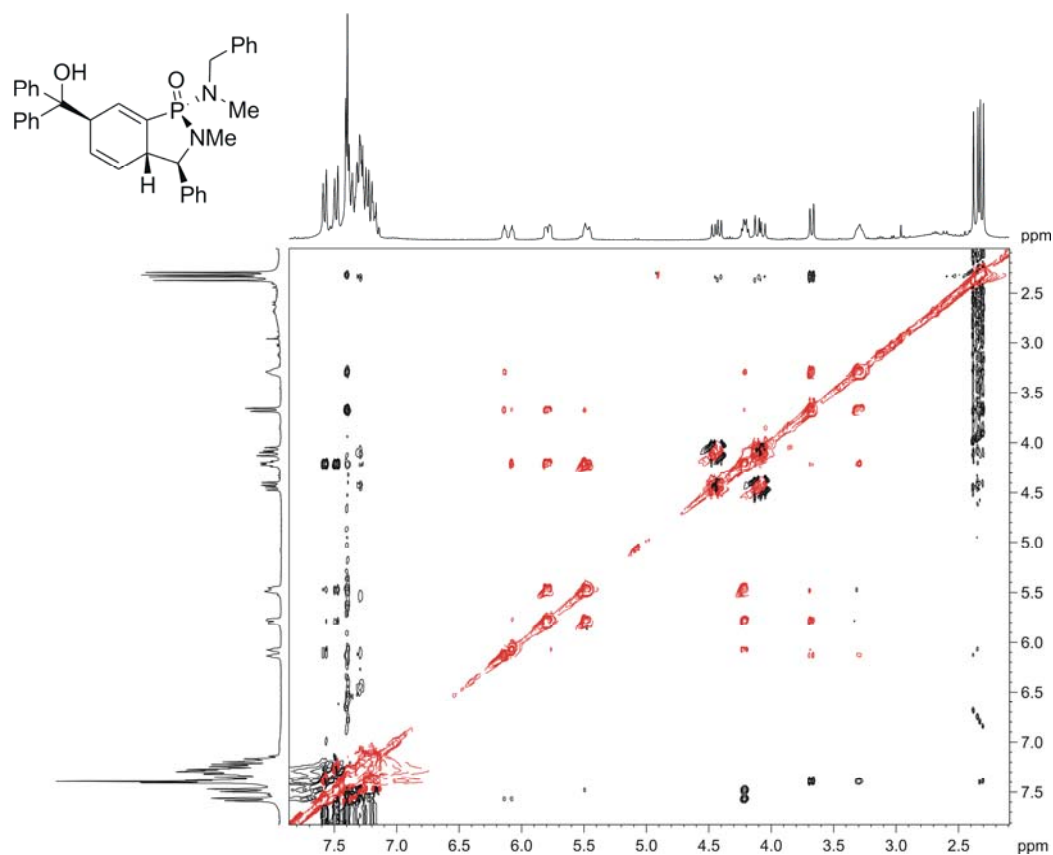


Figure S29. 2D ROESY spectrum (300.13 MHz, mixing time 0.2 s) of **10c** measured in CDCl_3 .

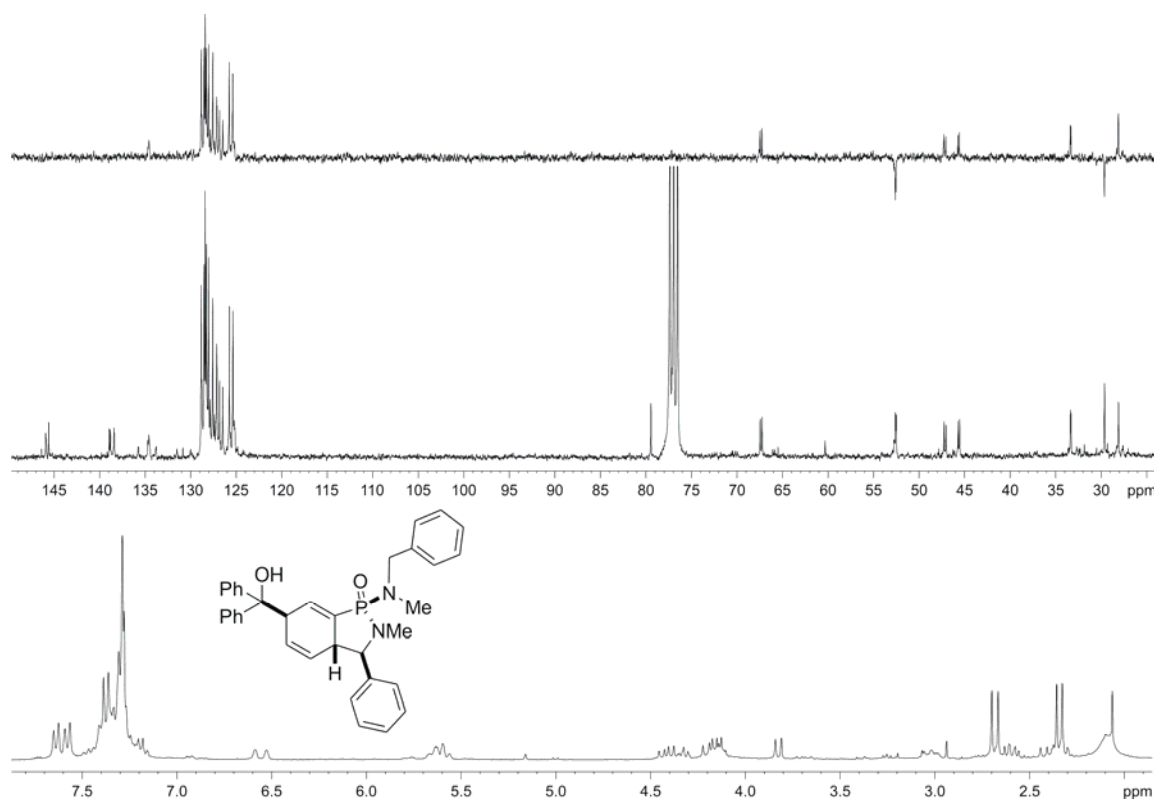


Figure S30. ^1H NMR (bottom) (300.13 MHz) and $^{13}\text{C}\{^1\text{H}\}$ (middle) and DEPT-135 (top) NMR spectra (75.47 MHz) of the epimer of **10c** at the phosphorus atom measured in CDCl_3 .

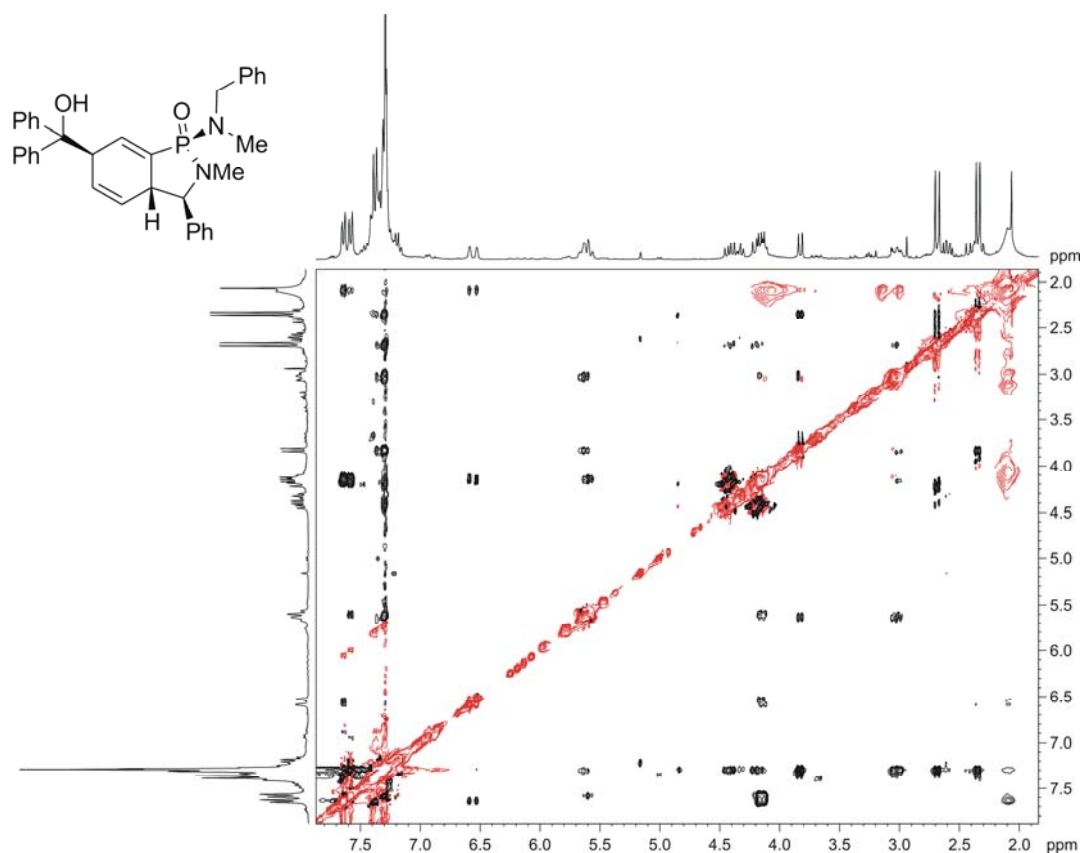


Figure S31. 2D gNOESY spectrum (300.13 MHz, mixing time 0.5 s) of the epimer of **10c** at the phosphorus atom measured in CDCl_3 .

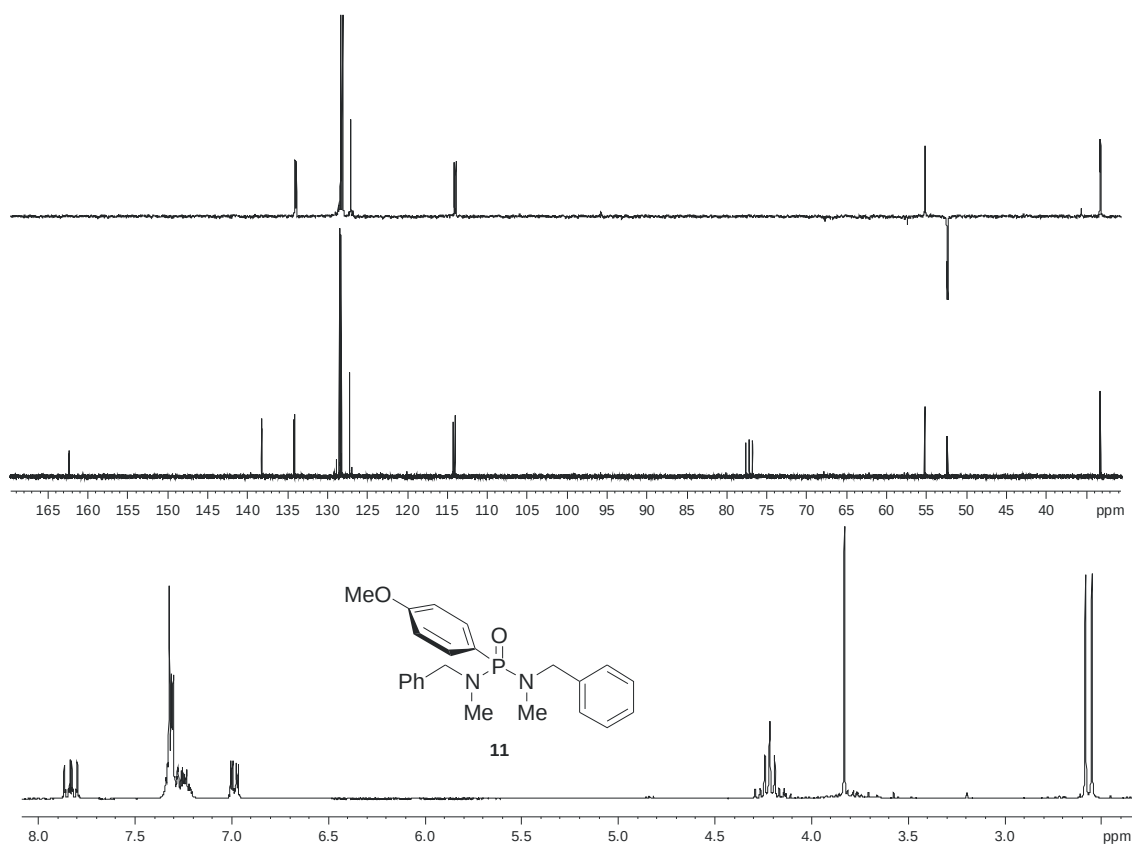


Figure S32. ^1H NMR (bottom) (300.13 MHz) and $^{13}\text{C}\{^1\text{H}\}$ (middle) and DEPT-135 (top) NMR spectra (75.47 MHz) of **11** measured in CDCl_3 .

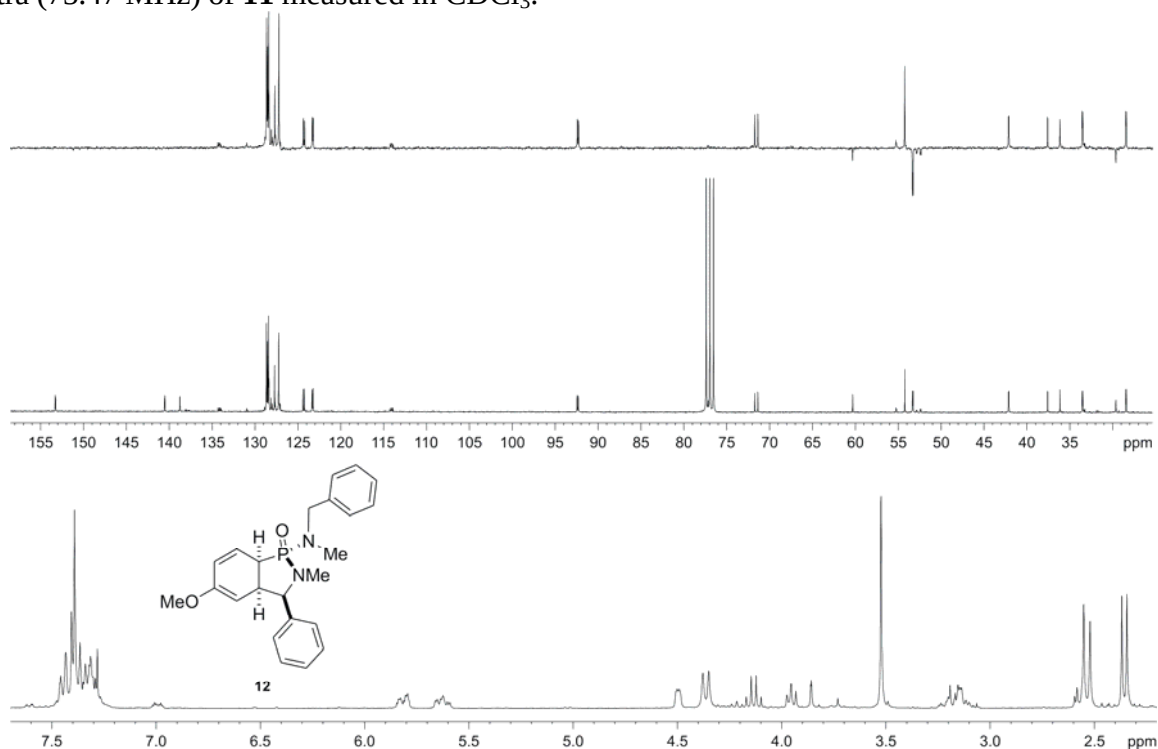


Figure S33. ^1H NMR (bottom) (300.13 MHz) and $^{13}\text{C}\{^1\text{H}\}$ (middle) and DEPT-135 (top) NMR spectra (75.47 MHz) of **12** measured in CDCl_3 .

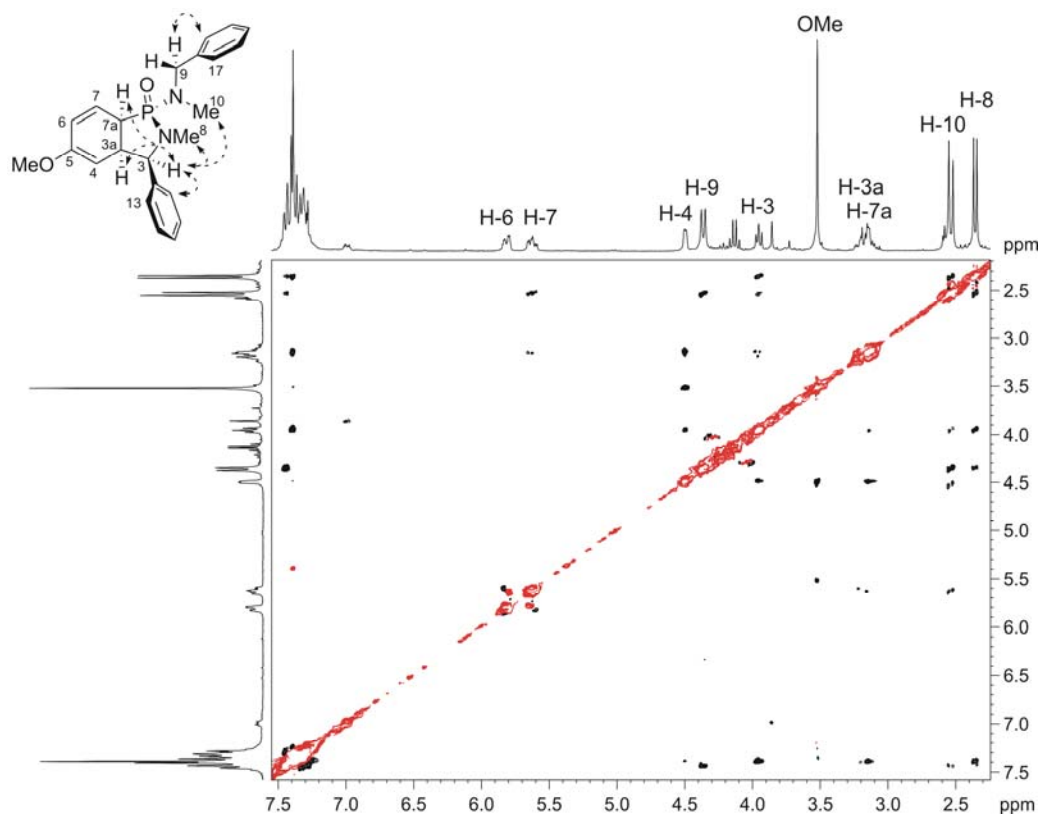


Figure S34. 2D gNOESY spectrum (300.13 MHz, mixing time 0.5 s) of **12** and selected NOEs observed that confirm the assignment of the relative configuration of the stereogenic centers.

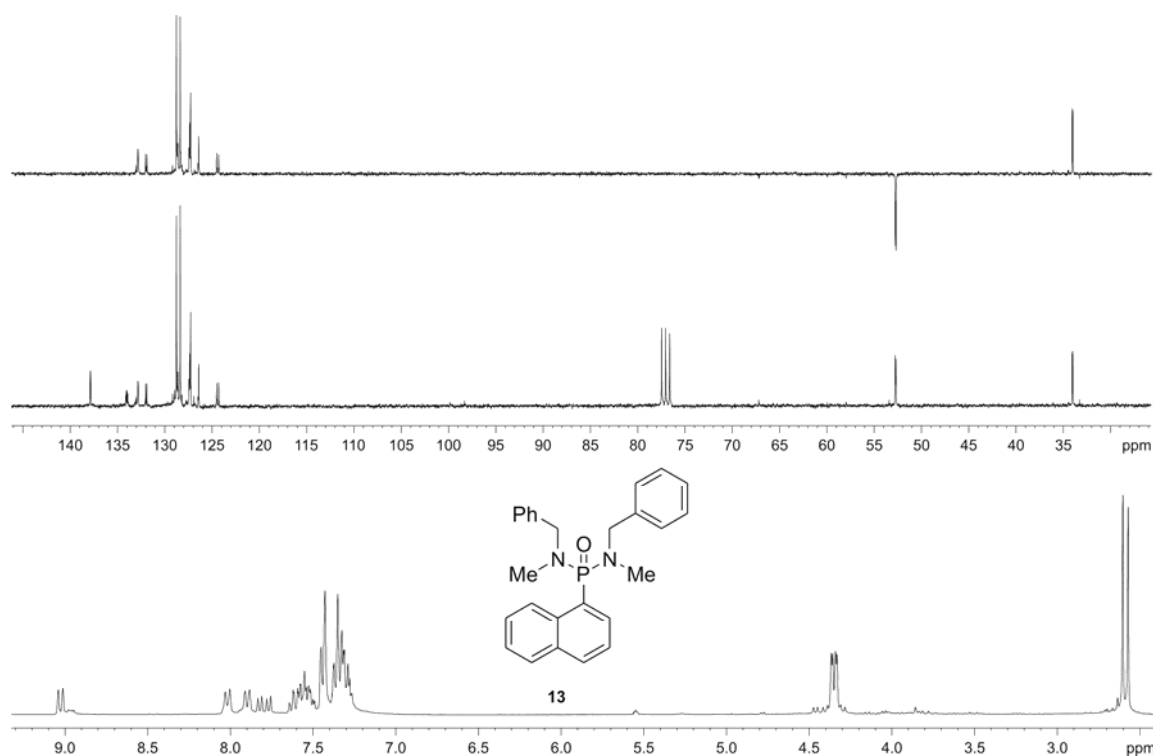


Figure S35. ^1H NMR (bottom) (300.13 MHz) and $^{13}\text{C}\{^1\text{H}\}$ (middle) and DEPT-135 (top) NMR spectra (75.47 MHz) of **13** measured in CDCl_3 .

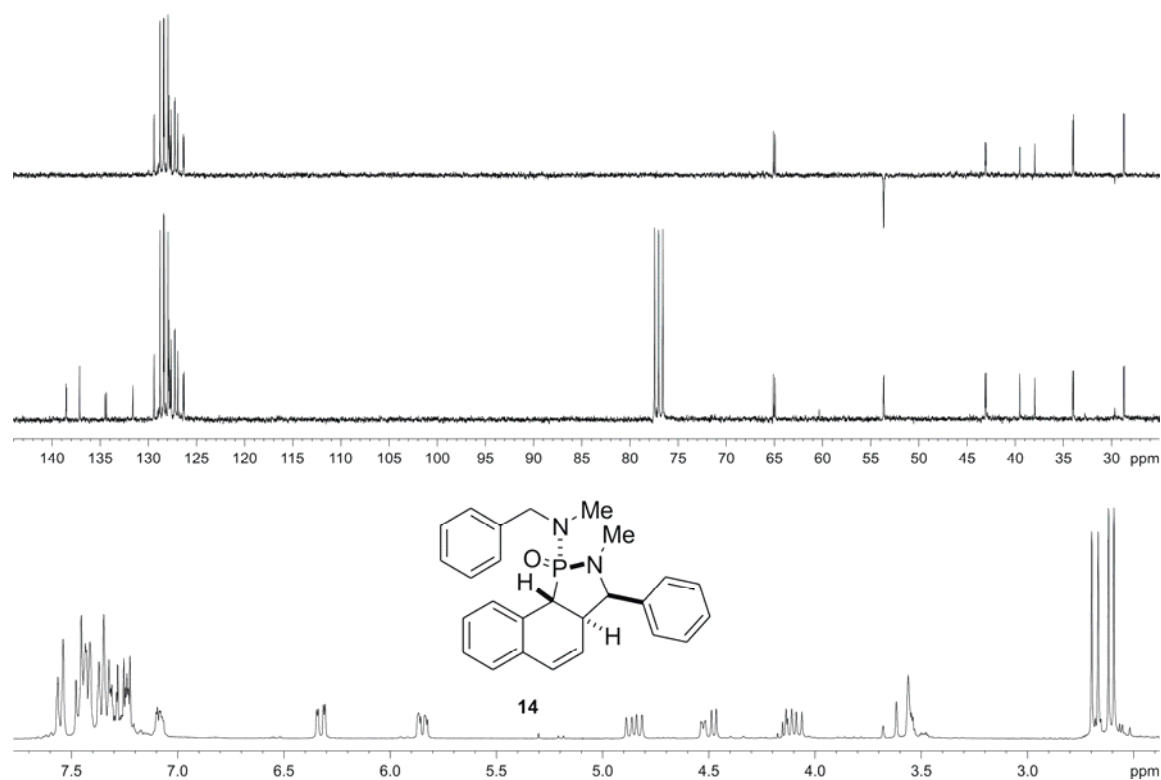


Figure S36. ¹H NMR (bottom) (300.13 MHz) and ¹³C{¹H}(middle) and DEPT-135 (top) NMR spectra (75.47 MHz) of **14** measured in CDCl₃.

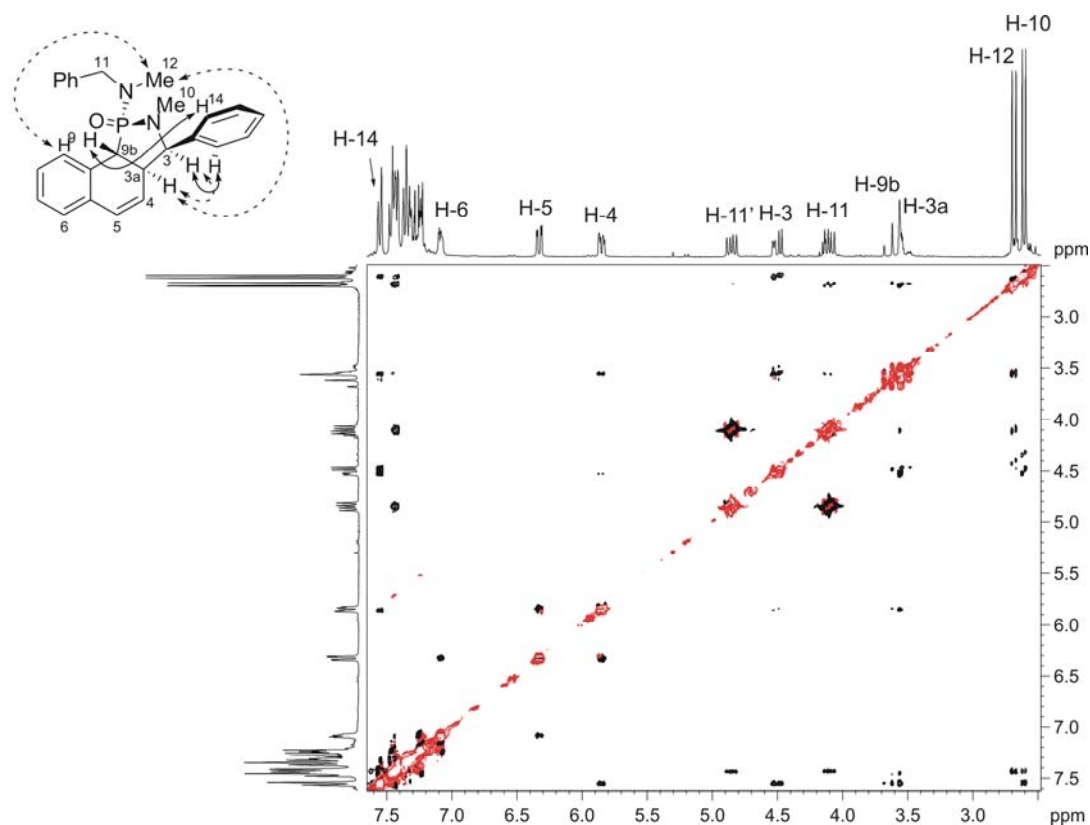


Figure S37. 2D gNOESY spectrum (300.13 MHz, mixing time 0.5 s) of **14** and selected NOEs observed that confirm the assignment of the relative configuration of the stereogenic centers.

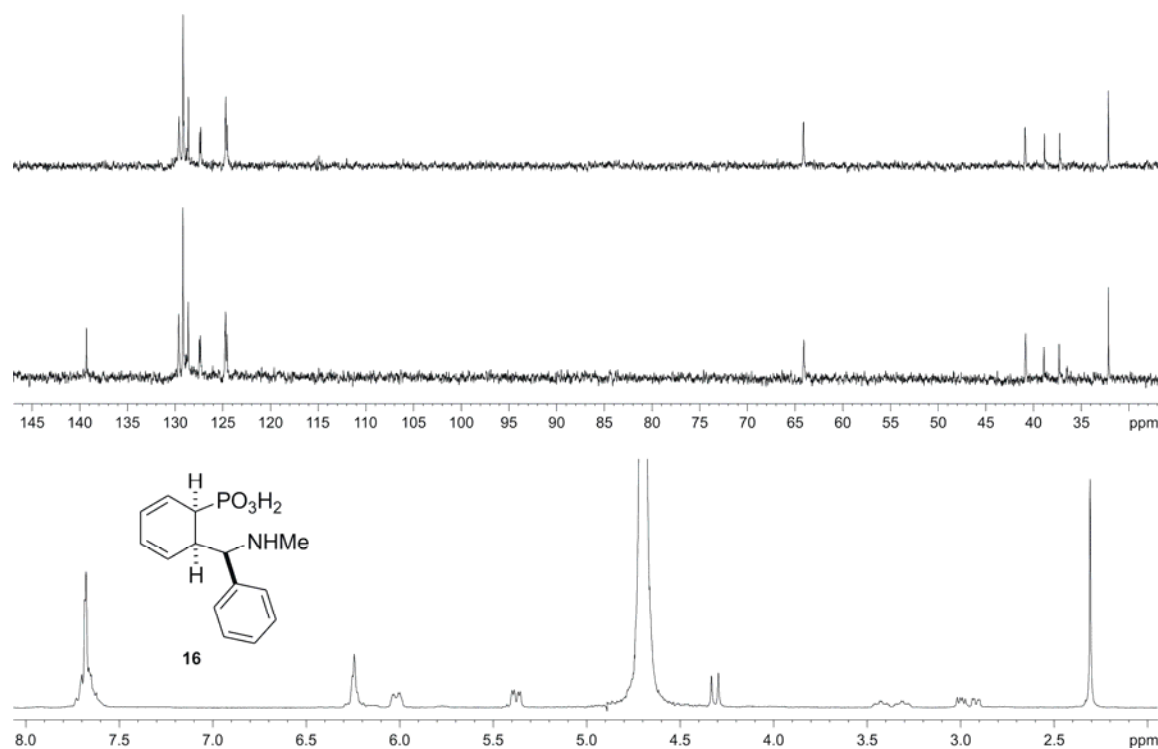


Figure S38. ¹H NMR (bottom) (300.13 MHz) and ¹³C{¹H} (middle) and DEPT-135 (top) NMR spectra (75.47 MHz) of **16** measured in D₂O.

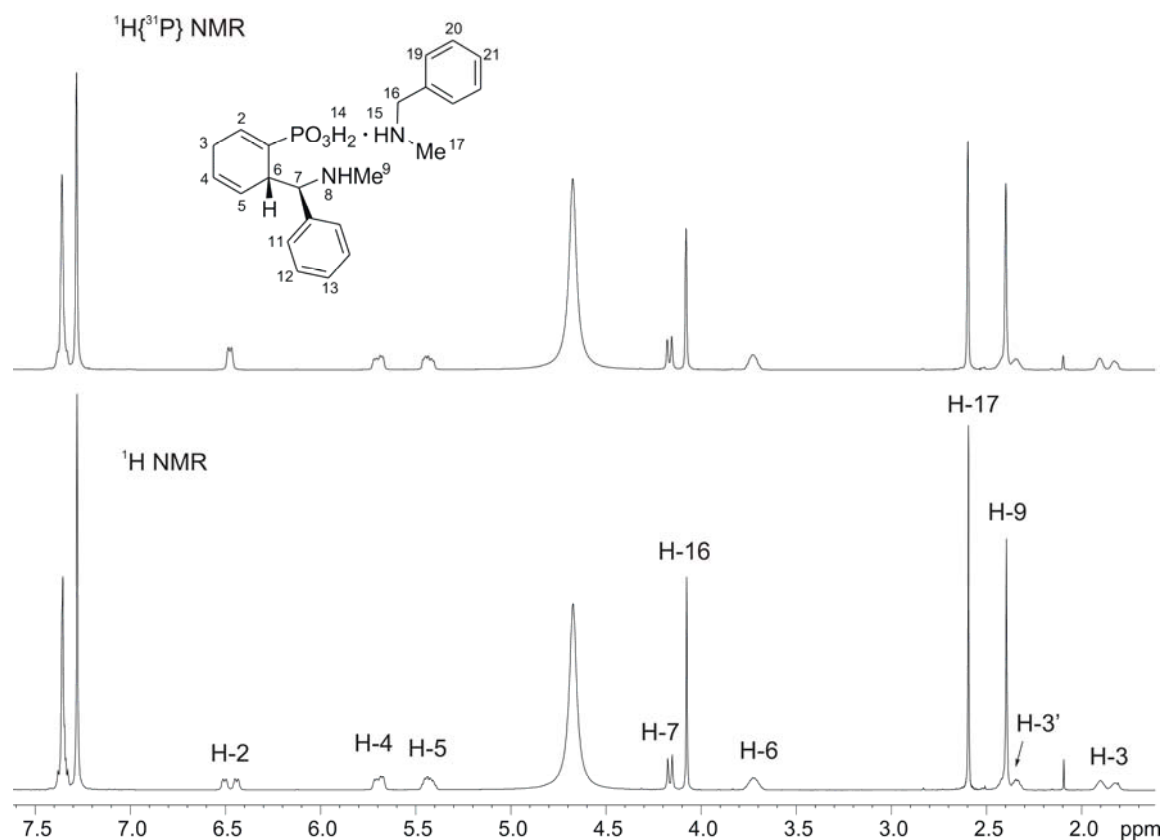


Figure S39. ¹H and ¹H{³¹P} NMR spectra (300.13 MHz) of phosphonic acid **17a** measured in D₂O.

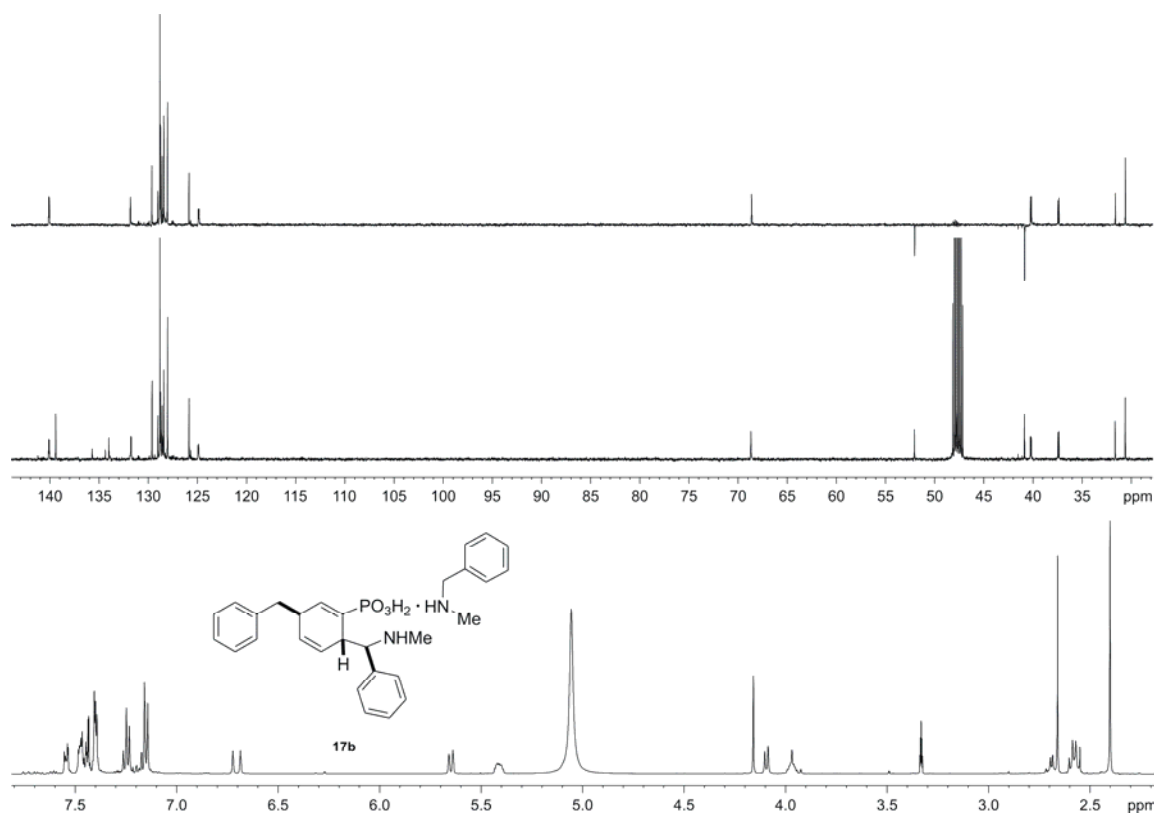


Figure S40. ¹H NMR (bottom) (500.13 MHz) and ¹³C{¹H} (middle) and DEPT-135 (top) NMR spectra (125.76 MHz) of **17b** measured in MeOH-*d*₄.

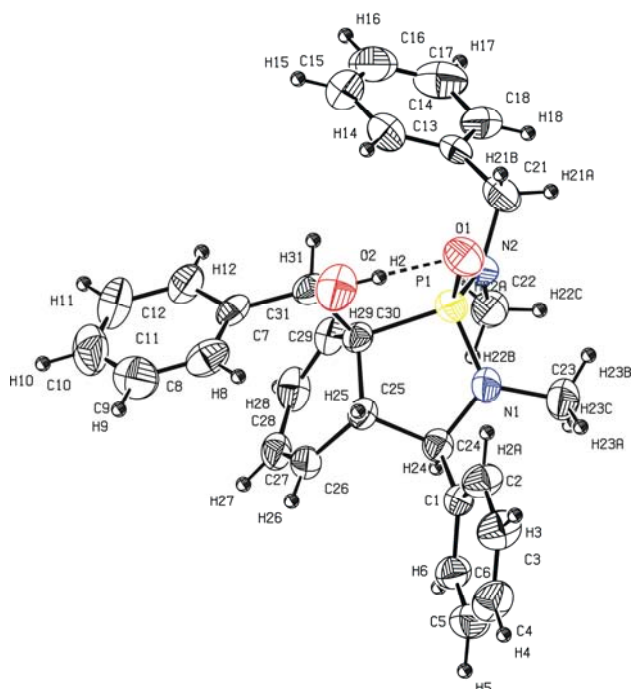


Figure S41. ORTEP view (40% anisotropic displacement) of **9aa**.

Table S1. Crystal data and structure refinement for **9aa** = r280fr1m:

Identification code	r280fr1m		
Empirical formula	C29 H32 N2 O2.50 P		
Formula weight	479.53		
Temperature	293(2) K		
Wavelength	0.71069 Å		
Crystal system	Triclinic		
Space group	P-1		
Unit cell dimensions	a = 7.249(5)Å	α = 83.225(5)°	
	b = 10.825(5)Å	β = 89.079(5)°	
	c = 16.951(5)Å	γ = 79.998(5)°	
Volume	1300.8(11) Å³		
Z	2		
Density (calculated)	1.222 Mg/m³		
Absorption coefficient	0.136 mm⁻¹		
F(000)	508		
Crystal size	? x ? x ? mm		
Theta range for data collection	1.92 to 23.26°		
Limiting indices	-7=<h<=8, -11=<k<=12, -18=<l<=15		
Reflections collected	5906		
Independent reflections	3615 [R(int) = 0.0305]		
Completeness to theta = 23.26°	97.2 %		
Absorption correction	None		
Refinement method	Full-matrix least-squares on F²		
Data / restraints / parameters	3615 / 0 / 319		
Goodness-of-fit on F²	1.264		
Final R indices [I>2sigma(I)]	R1 = 0.0810, wR2 = 0.2015		
R indices (all data)	R1 = 0.0994, wR2 = 0.2170		
Largest diff. peak and hole	0.289 and -0.368 e. Å⁻³		

Table S2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for **9aa** = r280fr1m. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1w)	3407(12)	764(8)	9933(4)	100(3)
P(1)	7564(2)	1202(1)	8220(1)	53(1)
O(1)	5926(5)	825(3)	8653(2)	77(1)
O(2)	4101(4)	852(4)	7299(2)	81(1)
N(1)	9319(5)	99(3)	8074(2)	56(1)
N(2)	8357(6)	2236(4)	8687(2)	63(1)
C(1)	10198(6)	-1493(4)	7143(2)	46(1)
C(2)	9130(7)	-2334(4)	7504(3)	63(1)

C(3)	9465(8)	-3575(5)	7380(3)	73(2)
C(4)	10875(8)	-4016(5)	6888(3)	75(2)
C(5)	11952(8)	-3199(5)	6525(3)	71(1)
C(6)	11649(6)	-1948(4)	6651(3)	58(1)
C(7)	4281(5)	2335(4)	6168(3)	49(1)
C(8)	4066(6)	1456(5)	5661(3)	69(1)
C(9)	3561(7)	1848(7)	4871(4)	89(2)
C(10)	3269(8)	3111(8)	4595(4)	94(2)
C(11)	3446(8)	3961(6)	5090(4)	89(2)
C(12)	3968(6)	3587(5)	5868(3)	68(1)
C(13)	6681(7)	4234(5)	9163(3)	62(1)
C(14)	5273(8)	4742(6)	8622(3)	86(2)
C(15)	4675(9)	6039(7)	8473(4)	97(2)
C(16)	5488(11)	6826(6)	8869(4)	97(2)
C(17)	6847(10)	6348(7)	9399(4)	98(2)
C(18)	7439(8)	5060(6)	9541(3)	81(2)
C(21)	7320(9)	2835(5)	9342(3)	82(2)
C(22)	10167(7)	2616(5)	8515(3)	72(2)
C(23)	10663(8)	-525(5)	8701(3)	82(2)
C(24)	9781(6)	-116(4)	7257(2)	47(1)
C(25)	8038(5)	576(4)	6751(2)	44(1)
C(26)	8640(6)	914(5)	5915(3)	55(1)
C(27)	9019(6)	2045(5)	5682(3)	62(1)
C(28)	8739(6)	3019(5)	6207(3)	61(1)
C(29)	7813(6)	2891(4)	6873(3)	53(1)
C(30)	7046(5)	1710(4)	7154(2)	44(1)
C(31)	4869(6)	1935(4)	7023(3)	54(1)

Table S3. Bond lengths [Å] and angles [°] for **9aa** = r280fr1m.

P(1)-O(1)	1.478(3)
P(1)-N(1)	1.624(4)
P(1)-N(2)	1.631(4)
P(1)-C(30)	1.850(4)
O(2)-C(31)	1.412(5)
O(2)-H(2)	0.8200
N(1)-C(24)	1.454(5)
N(1)-C(23)	1.473(6)
N(2)-C(22)	1.457(6)
N(2)-C(21)	1.481(6)
C(1)-C(2)	1.378(6)
C(1)-C(6)	1.391(6)
C(1)-C(24)	1.504(6)
C(2)-C(3)	1.364(6)
C(2)-H(2A)	0.9300
C(3)-C(4)	1.365(7)
C(3)-H(3)	0.9300
C(4)-C(5)	1.366(7)
C(4)-H(4)	0.9300
C(5)-C(6)	1.375(6)
C(5)-H(5)	0.9300
C(6)-H(6)	0.9300
C(7)-C(12)	1.371(6)
C(7)-C(8)	1.385(6)
C(7)-C(31)	1.509(6)
C(8)-C(9)	1.392(8)
C(8)-H(8)	0.9300
C(9)-C(10)	1.372(9)
C(9)-H(9)	0.9300
C(10)-C(11)	1.339(8)
C(10)-H(10)	0.9300
C(11)-C(12)	1.371(7)
C(11)-H(11)	0.9300
C(12)-H(12)	0.9300
C(13)-C(18)	1.351(7)
C(13)-C(14)	1.379(7)
C(13)-C(21)	1.501(7)
C(14)-C(15)	1.390(8)
C(14)-H(14)	0.9300
C(15)-C(16)	1.358(9)
C(15)-H(15)	0.9300
C(16)-C(17)	1.336(9)
C(16)-H(16)	0.9300
C(17)-C(18)	1.379(8)
C(17)-H(17)	0.9300
C(18)-H(18)	0.9300
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(24)-C(25)	1.564(5)
C(24)-H(24)	0.9800
C(25)-C(26)	1.498(6)
C(25)-C(30)	1.539(5)
C(25)-H(25)	0.9800

C(26)-C(27)	1.316(6)
C(26)-H(26)	0.9300
C(27)-C(28)	1.444(7)
C(27)-H(27)	0.9300
C(28)-C(29)	1.310(6)
C(28)-H(28)	0.9300
C(29)-C(30)	1.505(6)
C(29)-H(29)	0.9300
C(30)-C(31)	1.570(6)
C(31)-H(31)	0.9800
O(1)-P(1)-N(1)	117.9(2)
O(1)-P(1)-N(2)	108.9(2)
N(1)-P(1)-N(2)	107.7(2)
O(1)-P(1)-C(30)	112.05(19)
N(1)-P(1)-C(30)	95.43(17)
N(2)-P(1)-C(30)	114.6(2)
C(31)-O(2)-H(2)	109.5
C(24)-N(1)-C(23)	117.9(3)
C(24)-N(1)-P(1)	117.7(3)
C(23)-N(1)-P(1)	123.5(3)
C(22)-N(2)-C(21)	114.4(4)
C(22)-N(2)-P(1)	123.0(3)
C(21)-N(2)-P(1)	122.5(4)
C(2)-C(1)-C(6)	118.1(4)
C(2)-C(1)-C(24)	121.3(4)
C(6)-C(1)-C(24)	120.6(4)
C(3)-C(2)-C(1)	121.4(5)
C(3)-C(2)-H(2A)	119.3
C(1)-C(2)-H(2A)	119.3
C(2)-C(3)-C(4)	120.4(5)
C(2)-C(3)-H(3)	119.8
C(4)-C(3)-H(3)	119.8
C(3)-C(4)-C(5)	119.1(5)
C(3)-C(4)-H(4)	120.4
C(5)-C(4)-H(4)	120.4
C(4)-C(5)-C(6)	121.2(5)
C(4)-C(5)-H(5)	119.4
C(6)-C(5)-H(5)	119.4
C(5)-C(6)-C(1)	119.7(4)
C(5)-C(6)-H(6)	120.1
C(1)-C(6)-H(6)	120.1
C(12)-C(7)-C(8)	117.9(5)
C(12)-C(7)-C(31)	120.7(4)
C(8)-C(7)-C(31)	121.4(4)
C(7)-C(8)-C(9)	120.2(5)
C(7)-C(8)-H(8)	119.9
C(9)-C(8)-H(8)	119.9
C(10)-C(9)-C(8)	119.8(5)
C(10)-C(9)-H(9)	120.1
C(8)-C(9)-H(9)	120.1
C(11)-C(10)-C(9)	119.9(6)
C(11)-C(10)-H(10)	120.0
C(9)-C(10)-H(10)	120.0
C(10)-C(11)-C(12)	120.9(6)
C(10)-C(11)-H(11)	119.5
C(12)-C(11)-H(11)	119.5
C(11)-C(12)-C(7)	121.2(5)
C(11)-C(12)-H(12)	119.4
C(7)-C(12)-H(12)	119.4
C(18)-C(13)-C(14)	116.7(5)
C(18)-C(13)-C(21)	121.3(5)

C(14)-C(13)-C(21)	122.1(5)
C(13)-C(14)-C(15)	121.4(6)
C(13)-C(14)-H(14)	119.3
C(15)-C(14)-H(14)	119.3
C(16)-C(15)-C(14)	119.5(6)
C(16)-C(15)-H(15)	120.3
C(14)-C(15)-H(15)	120.3
C(17)-C(16)-C(15)	119.9(6)
C(17)-C(16)-H(16)	120.1
C(15)-C(16)-H(16)	120.1
C(16)-C(17)-C(18)	120.3(6)
C(16)-C(17)-H(17)	119.8
C(18)-C(17)-H(17)	119.8
C(13)-C(18)-C(17)	122.3(6)
C(13)-C(18)-H(18)	118.8
C(17)-C(18)-H(18)	118.8
N(2)-C(21)-C(13)	114.3(4)
N(2)-C(21)-H(21A)	108.7
C(13)-C(21)-H(21A)	108.7
N(2)-C(21)-H(21B)	108.7
C(13)-C(21)-H(21B)	108.7
H(21A)-C(21)-H(21B)	107.6
N(2)-C(22)-H(22A)	109.5
N(2)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
N(2)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
N(1)-C(23)-H(23A)	109.5
N(1)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
N(1)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
N(1)-C(24)-C(1)	113.1(3)
N(1)-C(24)-C(25)	105.6(3)
C(1)-C(24)-C(25)	110.7(3)
N(1)-C(24)-H(24)	109.1
C(1)-C(24)-H(24)	109.1
C(25)-C(24)-H(24)	109.1
C(26)-C(25)-C(30)	114.1(3)
C(26)-C(25)-C(24)	109.3(3)
C(30)-C(25)-C(24)	109.7(3)
C(26)-C(25)-H(25)	107.9
C(30)-C(25)-H(25)	107.9
C(24)-C(25)-H(25)	107.9
C(27)-C(26)-C(25)	120.7(4)
C(27)-C(26)-H(26)	119.6
C(25)-C(26)-H(26)	119.6
C(26)-C(27)-C(28)	120.9(4)
C(26)-C(27)-H(27)	119.5
C(28)-C(27)-H(27)	119.5
C(29)-C(28)-C(27)	121.5(4)
C(29)-C(28)-H(28)	119.2
C(27)-C(28)-H(28)	119.2
C(28)-C(29)-C(30)	122.4(4)
C(28)-C(29)-H(29)	118.8
C(30)-C(29)-H(29)	118.8
C(29)-C(30)-C(25)	111.5(3)
C(29)-C(30)-C(31)	110.4(3)
C(25)-C(30)-C(31)	111.6(3)
C(29)-C(30)-P(1)	111.3(3)
C(25)-C(30)-P(1)	103.0(3)

C(31)-C(30)-P(1)	108.9(3)
O(2)-C(31)-C(7)	108.3(4)
O(2)-C(31)-C(30)	111.8(3)
C(7)-C(31)-C(30)	113.6(3)
O(2)-C(31)-H(31)	107.6
C(7)-C(31)-H(31)	107.6
C(30)-C(31)-H(31)	107.6

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **9aa** = r280fr1m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$.

	U11	U22	U33	U23	U13	U12
O(1W)	118(7)	110(6)	67(5)	12(4)	14(5)	-23(5)
P(1)	59(1)	54(1)	43(1)	2(1)	8(1)	-4(1)
O(1)	75(2)	89(3)	62(2)	9(2)	21(2)	-15(2)
O(2)	47(2)	99(3)	93(3)	22(2)	4(2)	-28(2)
N(1)	68(2)	51(2)	45(2)	0(2)	-8(2)	2(2)
N(2)	69(3)	64(3)	52(2)	-13(2)	8(2)	6(2)
C(1)	49(2)	41(2)	45(2)	-1(2)	-1(2)	-4(2)
C(2)	61(3)	48(3)	78(3)	-4(2)	13(3)	-8(2)
C(3)	77(4)	49(3)	94(4)	-5(3)	10(3)	-16(3)
C(4)	87(4)	47(3)	93(4)	-20(3)	-16(3)	-4(3)
C(5)	79(4)	64(4)	67(3)	-16(3)	9(3)	-2(3)
C(6)	54(3)	56(3)	60(3)	-2(2)	7(2)	-4(2)
C(7)	29(2)	47(3)	67(3)	-1(2)	-1(2)	0(2)
C(8)	46(3)	62(3)	103(4)	-19(3)	-5(3)	-9(2)
C(9)	59(3)	129(6)	90(5)	-41(4)	-12(3)	-24(3)
C(10)	66(4)	138(6)	76(4)	7(4)	-25(3)	-22(4)
C(11)	80(4)	83(4)	97(5)	15(4)	-34(3)	-10(3)
C(12)	59(3)	59(3)	82(4)	-7(3)	-17(3)	2(2)
C(13)	78(3)	67(3)	36(2)	-13(2)	8(2)	10(3)
C(14)	100(4)	96(5)	57(3)	-24(3)	-7(3)	5(4)
C(15)	94(4)	101(5)	77(4)	1(4)	-1(3)	26(4)
C(16)	108(5)	81(5)	92(5)	-9(4)	36(4)	10(4)
C(17)	94(5)	96(5)	112(5)	-47(4)	23(4)	-16(4)
C(18)	75(4)	87(4)	75(4)	-29(3)	4(3)	11(3)
C(21)	114(5)	75(4)	48(3)	-9(2)	10(3)	5(3)
C(22)	74(4)	72(4)	69(3)	-19(3)	-11(3)	1(3)
C(23)	103(4)	68(3)	63(3)	-2(3)	-19(3)	11(3)
C(24)	45(2)	48(3)	46(3)	3(2)	3(2)	-11(2)
C(25)	39(2)	43(2)	47(2)	0(2)	-3(2)	-8(2)
C(26)	46(3)	68(3)	45(3)	0(2)	1(2)	-1(2)
C(27)	42(3)	86(4)	49(3)	19(3)	5(2)	-4(2)
C(28)	55(3)	64(3)	65(3)	19(2)	-8(2)	-28(2)
C(29)	53(3)	48(3)	55(3)	4(2)	-10(2)	-9(2)
C(30)	36(2)	47(3)	47(2)	1(2)	3(2)	-5(2)
C(31)	43(2)	52(3)	64(3)	-1(2)	10(2)	-3(2)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **9aa** = r280fr1m.

	x	y	z	U(eq)
H(2)	4430	611	7760	121
H(2A)	8160	-2049	7839	76
H(3)	8729	-4125	7632	88
H(4)	11099	-4861	6801	90
H(5)	12907	-3494	6186	85
H(6)	12411	-1408	6407	69
H(8)	4260	601	5849	83
H(9)	3421	1257	4530	107
H(10)	2948	3376	4066	113
H(11)	3213	4817	4904	107
H(12)	4111	4193	6197	82
H(14)	4713	4205	8351	103
H(15)	3725	6366	8106	116
H(16)	5101	7695	8771	117
H(17)	7395	6887	9673	118
H(18)	8393	4749	9909	97
H(21A)	8117	2674	9810	98
H(21B)	6232	2439	9467	98
H(22A)	9998	3518	8395	108
H(22B)	10721	2226	8068	108
H(22C)	10975	2355	8969	108
H(23A)	10789	-1425	8713	122
H(23B)	10217	-281	9206	122
H(23C)	11859	-277	8592	122
H(24)	10869	275	7092	56
H(25)	7163	-17	6739	52
H(26)	8746	317	5557	66
H(27)	9474	2220	5172	74
H(28)	9227	3754	6068	73
H(29)	7623	3555	7184	63
H(31)	4311	2614	7333	65

Table S6. Torsion angles [°] for **9aa** = r280fr1m.

O(1)-P(1)-N(1)-C(24)	116.5(3)
N(2)-P(1)-N(1)-C(24)	-120.0(3)
C(30)-P(1)-N(1)-C(24)	-2.0(3)
O(1)-P(1)-N(1)-C(23)	-75.2(4)
N(2)-P(1)-N(1)-C(23)	48.4(4)
C(30)-P(1)-N(1)-C(23)	166.4(4)
O(1)-P(1)-N(2)-C(22)	167.4(4)
N(1)-P(1)-N(2)-C(22)	38.5(4)
C(30)-P(1)-N(2)-C(22)	-66.3(4)
O(1)-P(1)-N(2)-C(21)	-10.4(4)
N(1)-P(1)-N(2)-C(21)	-139.2(4)
C(30)-P(1)-N(2)-C(21)	116.0(4)
C(6)-C(1)-C(2)-C(3)	-0.5(7)
C(24)-C(1)-C(2)-C(3)	177.7(4)
C(1)-C(2)-C(3)-C(4)	-0.3(8)
C(2)-C(3)-C(4)-C(5)	0.4(8)
C(3)-C(4)-C(5)-C(6)	0.5(8)
C(4)-C(5)-C(6)-C(1)	-1.3(7)
C(2)-C(1)-C(6)-C(5)	1.3(6)
C(24)-C(1)-C(6)-C(5)	-176.9(4)
C(12)-C(7)-C(8)-C(9)	0.5(7)
C(31)-C(7)-C(8)-C(9)	-178.6(4)
C(7)-C(8)-C(9)-C(10)	-0.2(8)
C(8)-C(9)-C(10)-C(11)	-0.9(9)
C(9)-C(10)-C(11)-C(12)	1.8(10)
C(10)-C(11)-C(12)-C(7)	-1.6(9)
C(8)-C(7)-C(12)-C(11)	0.4(7)
C(31)-C(7)-C(12)-C(11)	179.5(4)
C(18)-C(13)-C(14)-C(15)	0.2(8)
C(21)-C(13)-C(14)-C(15)	178.9(5)
C(13)-C(14)-C(15)-C(16)	-0.1(9)
C(14)-C(15)-C(16)-C(17)	-0.3(10)
C(15)-C(16)-C(17)-C(18)	0.6(10)
C(14)-C(13)-C(18)-C(17)	0.1(8)
C(21)-C(13)-C(18)-C(17)	-178.6(5)
C(16)-C(17)-C(18)-C(13)	-0.5(9)
C(22)-N(2)-C(21)-C(13)	66.8(6)
P(1)-N(2)-C(21)-C(13)	-115.3(5)
C(18)-C(13)-C(21)-N(2)	-111.2(6)
C(14)-C(13)-C(21)-N(2)	70.2(7)
C(23)-N(1)-C(24)-C(1)	54.5(5)
P(1)-N(1)-C(24)-C(1)	-136.4(3)
C(23)-N(1)-C(24)-C(25)	175.7(4)
P(1)-N(1)-C(24)-C(25)	-15.2(4)
C(2)-C(1)-C(24)-N(1)	42.1(5)
C(6)-C(1)-C(24)-N(1)	-139.8(4)
C(2)-C(1)-C(24)-C(25)	-76.2(5)
C(6)-C(1)-C(24)-C(25)	102.0(4)
N(1)-C(24)-C(25)-C(26)	154.9(4)
C(1)-C(24)-C(25)-C(26)	-82.4(4)
N(1)-C(24)-C(25)-C(30)	29.1(4)
C(1)-C(24)-C(25)-C(30)	151.8(3)
C(30)-C(25)-C(26)-C(27)	27.3(5)
C(24)-C(25)-C(26)-C(27)	-95.9(5)
C(25)-C(26)-C(27)-C(28)	-4.5(6)
C(26)-C(27)-C(28)-C(29)	-11.8(7)
C(27)-C(28)-C(29)-C(30)	2.5(7)
C(28)-C(29)-C(30)-C(25)	20.0(5)
C(28)-C(29)-C(30)-C(31)	-104.6(5)

C(28)-C(29)-C(30)-P(1)	134.4(4)
C(26)-C(25)-C(30)-C(29)	-33.1(5)
C(24)-C(25)-C(30)-C(29)	89.9(4)
C(26)-C(25)-C(30)-C(31)	90.8(4)
C(24)-C(25)-C(30)-C(31)	-146.2(3)
C(26)-C(25)-C(30)-P(1)	-152.5(3)
C(24)-C(25)-C(30)-P(1)	-29.5(4)
O(1)-P(1)-C(30)-C(29)	136.0(3)
N(1)-P(1)-C(30)-C(29)	-101.0(3)
N(2)-P(1)-C(30)-C(29)	11.3(4)
O(1)-P(1)-C(30)-C(25)	-104.5(3)
N(1)-P(1)-C(30)-C(25)	18.6(3)
N(2)-P(1)-C(30)-C(25)	130.8(3)
O(1)-P(1)-C(30)-C(31)	14.1(3)
N(1)-P(1)-C(30)-C(31)	137.1(3)
N(2)-P(1)-C(30)-C(31)	-110.7(3)
C(12)-C(7)-C(31)-O(2)	147.1(4)
C(8)-C(7)-C(31)-O(2)	-33.8(5)
C(12)-C(7)-C(31)-C(30)	-88.1(5)
C(8)-C(7)-C(31)-C(30)	91.0(5)
C(29)-C(30)-C(31)-O(2)	-178.6(4)
C(25)-C(30)-C(31)-O(2)	56.8(5)
P(1)-C(30)-C(31)-O(2)	-56.2(4)
C(29)-C(30)-C(31)-C(7)	58.5(5)
C(25)-C(30)-C(31)-C(7)	-66.1(5)
P(1)-C(30)-C(31)-C(7)	-179.1(3)

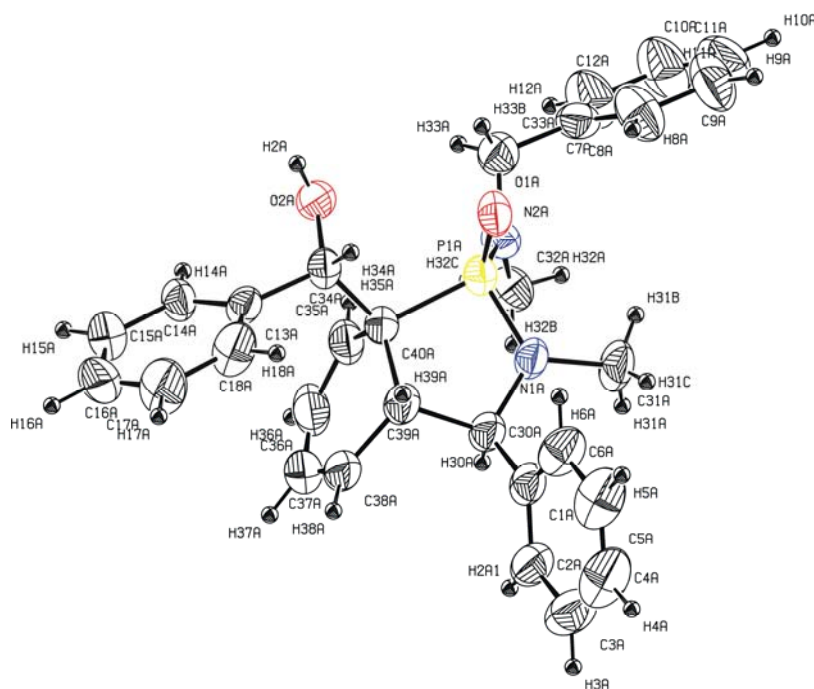


Figure S42. ORTEP view (40% anisotropic displacement) of **9ab**.

Table S7. Crystal data and structure refinement for **9ab** = r280fr2s:

Identification code	r280fr2s
Empirical formula	C _{29.25} H ₃₁ N ₂ O _{2.25} P
Formula weight	477.53
Temperature	293(2) K
Wavelength	0.71073
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 11.6003(12) Å α = 107.273(3)° b = 13.1387(13) Å β = 93.096(3)° c = 19.295(2) Å γ = 109.039(3)°
Volume	2617.2(5) Å ³
Z	4
Density (calculated)	1.212 Mg/m ³
Absorption coefficient	0.134 mm ⁻¹
F(000)	1014
Crystal size	0.350 x 0.155 x 0.140 mm
Theta range for data collection	1.12 to 23.27°
Limiting indices	-11=<h<=12, -14=<k<=11, -18=<l<=21
Reflections collected	12505
Independent reflections	7488 [R(int) = 0.0400]
Completeness to theta = 23.27°	99.4 %
Absorption correction	Empirical
Max. and min. transmission	0.984 and 0.852
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	7488 / 0 / 627
Goodness-of-fit on F ²	1.013
Final R indices [I>2sigma(I)]	R1 = 0.0705, wR2 = 0.1716
R indices (all data)	R1 = 0.1200, wR2 = 0.2025
Largest diff. peak and hole	0.560 and -0.188 e.Å ⁻³

Table S8. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **9ab** = r280fr2s. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
P(1A)	2028(1)	6434(1)	4333(1)	52(1)
P(1B)	5833(1)	8054(1)	218(1)	52(1)
O(1A)	1581(3)	5209(2)	4240(2)	61(1)
O(2A)	71(3)	6347(3)	5305(2)	60(1)
O(1B)	6576(3)	9184(2)	189(2)	59(1)
O(2B)	3740(3)	8915(2)	-1(2)	65(1)
N(1A)	3481(3)	7026(3)	4284(2)	57(1)
N(2A)	1240(3)	6649(3)	3695(2)	57(1)
N(1B)	6484(3)	7521(3)	727(2)	54(1)
N(2B)	5436(4)	7111(3)	-611(2)	65(1)
C(1A)	5521(5)	7794(5)	5079(2)	63(1)
C(2A)	6579(5)	8738(5)	5299(3)	85(2)
C(3A)	7731(6)	8623(8)	5414(3)	110(2)
C(4A)	7791(7)	7551(9)	5296(4)	112(3)
C(5A)	6745(7)	6632(7)	5086(3)	102(2)
C(6A)	5614(5)	6740(6)	4974(3)	82(2)
C(7A)	-113(4)	5336(4)	2512(3)	66(1)
C(8A)	415(6)	4536(5)	2240(3)	94(2)
C(9A)	311(7)	4043(5)	1480(4)	112(2)
C(10A)	-310(6)	4367(6)	1005(3)	100(2)
C(11A)	-803(7)	5156(7)	1273(4)	117(2)
C(12A)	-700(6)	5651(6)	2026(4)	107(2)
C(13A)	1393(4)	7289(4)	6499(2)	53(1)
C(14A)	689(4)	7929(4)	6770(2)	60(1)
C(15A)	837(5)	8507(4)	7508(3)	78(2)
C(16A)	1711(6)	8484(5)	7993(3)	91(2)
C(17A)	2421(6)	7855(6)	7745(3)	106(2)
C(18A)	2252(5)	7260(5)	7007(3)	84(2)
C(30A)	4277(4)	7908(4)	4944(2)	58(1)
C(31A)	3979(5)	6874(5)	3591(3)	76(2)
C(32A)	1619(5)	7697(4)	3512(3)	69(1)
C(33A)	-9(4)	5855(5)	3335(3)	73(1)
C(34A)	1273(4)	6664(4)	5686(2)	53(1)
C(35A)	1771(5)	8367(4)	5285(3)	66(1)
C(36A)	2375(7)	9411(5)	5715(4)	96(2)
C(37A)	3435(8)	9686(7)	6225(5)	126(3)
C(38A)	3983(6)	8949(7)	6202(3)	112(3)
C(39A)	3527(4)	7795(5)	5585(3)	70(1)
C(40A)	2146(4)	7381(4)	5279(2)	51(1)
C(1B)	6738(4)	7556(4)	2024(2)	51(1)
C(2B)	6432(5)	6859(4)	2459(2)	61(1)
C(3B)	7175(5)	7116(5)	3112(3)	72(2)
C(4B)	8244(6)	8066(6)	3340(3)	77(2)
C(5B)	8566(5)	8749(5)	2920(3)	75(2)
C(6B)	7821(5)	8504(4)	2268(3)	68(1)
C(7B)	5683(6)	7020(4)	-1892(3)	71(2)
C(8B)	6915(7)	7347(6)	-1837(4)	104(2)
C(9B)	7456(10)	6996(9)	-2431(7)	151(4)
C(10B)	6735(15)	6295(11)	-3090(7)	174(6)
C(11B)	5486(13)	5977(8)	-3163(4)	162(4)
C(12B)	4932(7)	6312(5)	-2547(3)	109(2)
C(13B)	3325(4)	9348(4)	1261(3)	58(1)
C(14B)	2054(5)	8788(5)	1051(4)	92(2)

C(15B)	1277(6)	8985(8)	1570(6)	129(3)
C(16B)	1775(9)	9726(9)	2261(5)	131(3)
C(17B)	2999(7)	10304(6)	2469(3)	99(2)
C(18B)	3778(5)	10109(5)	1968(3)	71(1)
C(30B)	5870(4)	7318(3)	1339(2)	50(1)
C(31B)	7425(5)	7024(4)	510(3)	76(2)
C(32B)	4985(6)	5883(4)	-764(3)	91(2)
C(33B)	5109(6)	7440(5)	-1239(3)	83(2)
C(34B)	4210(4)	9120(3)	739(2)	50(1)
C(35B)	3421(4)	6984(4)	379(3)	61(1)
C(36B)	2763(5)	6420(4)	775(3)	72(1)
C(37B)	3034(5)	6819(4)	1567(3)	71(1)
C(38B)	4100(5)	7647(4)	1910(3)	62(1)
C(39B)	5073(4)	8082(3)	1481(2)	47(1)
C(40B)	4537(4)	8056(3)	727(2)	48(1)
C(1E)	846(15)	10291(13)	9382(9)	138(5)
O(2M)	-52(11)	9554(8)	9684(6)	149(4)

Table S9. Bond lengths [Å] and angles [°] for **9ab** = r280fr2s.

P(1A)-O(1A)	1.472(3)
P(1A)-N(1A)	1.631(4)
P(1A)-N(2A)	1.637(4)
P(1A)-C(40A)	1.848(4)
P(1B)-O(1B)	1.473(3)
P(1B)-N(2B)	1.636(4)
P(1B)-N(1B)	1.642(3)
P(1B)-C(40B)	1.840(4)
O(2A)-C(34A)	1.410(5)
O(2A)-H(2A)	0.8200
O(2B)-C(34B)	1.415(5)
O(2B)-H(2B)	0.8200
N(1A)-C(30A)	1.455(5)
N(1A)-C(31A)	1.469(5)
N(2A)-C(32A)	1.458(5)
N(2A)-C(33A)	1.465(6)
N(1B)-C(30B)	1.459(5)
N(1B)-C(31B)	1.465(5)
N(2B)-C(32B)	1.454(6)
N(2B)-C(33B)	1.470(6)
C(1A)-C(2A)	1.365(7)
C(1A)-C(6A)	1.380(7)
C(1A)-C(30A)	1.516(6)
C(2A)-C(3A)	1.406(8)
C(2A)-H(2A1)	0.9300
C(3A)-C(4A)	1.383(9)
C(3A)-H(3A)	0.9300
C(4A)-C(5A)	1.340(9)
C(4A)-H(4A)	0.9300
C(5A)-C(6A)	1.377(7)
C(5A)-H(5A)	0.9300
C(6A)-H(6A)	0.9300
C(7A)-C(12A)	1.365(7)
C(7A)-C(8A)	1.372(7)
C(7A)-C(33A)	1.511(6)
C(8A)-C(9A)	1.396(8)
C(8A)-H(8A)	0.9300
C(9A)-C(10A)	1.379(8)
C(9A)-H(9A)	0.9300
C(10A)-C(11A)	1.330(8)
C(10A)-H(10A)	0.9300
C(11A)-C(12A)	1.385(8)
C(11A)-H(11A)	0.9300
C(12A)-H(12A)	0.9300
C(13A)-C(14A)	1.371(6)
C(13A)-C(18A)	1.377(6)
C(13A)-C(34A)	1.513(6)
C(14A)-C(15A)	1.371(6)
C(14A)-H(14A)	0.9300
C(15A)-C(16A)	1.358(8)
C(15A)-H(15A)	0.9300
C(16A)-C(17A)	1.357(8)
C(16A)-H(16A)	0.9300
C(17A)-C(18A)	1.374(7)
C(17A)-H(17A)	0.9300
C(18A)-H(18A)	0.9300
C(30A)-C(39A)	1.564(6)
C(30A)-H(30A)	0.9800

C(31A)-H(31A)	0.9600
C(31A)-H(31B)	0.9600
C(31A)-H(31C)	0.9600
C(32A)-H(32A)	0.9600
C(32A)-H(32B)	0.9600
C(32A)-H(32C)	0.9600
C(33A)-H(33A)	0.9700
C(33A)-H(33B)	0.9700
C(34A)-C(40A)	1.560(6)
C(34A)-H(34A)	0.9800
C(35A)-C(36A)	1.302(7)
C(35A)-C(40A)	1.493(6)
C(35A)-H(35A)	0.9300
C(36A)-C(37A)	1.406(10)
C(36A)-H(36A)	0.9300
C(37A)-C(38A)	1.312(10)
C(37A)-H(37A)	0.9300
C(38A)-C(39A)	1.528(8)
C(38A)-H(38A)	0.9300
C(39A)-C(40A)	1.532(6)
C(39A)-H(39A)	0.9800
C(1B)-C(6B)	1.385(6)
C(1B)-C(2B)	1.396(6)
C(1B)-C(30B)	1.504(6)
C(2B)-C(3B)	1.373(6)
C(2B)-H(2B1)	0.9300
C(3B)-C(4B)	1.377(7)
C(3B)-H(3B)	0.9300
C(4B)-C(5B)	1.359(7)
C(4B)-H(4B)	0.9300
C(5B)-C(6B)	1.377(7)
C(5B)-H(5B)	0.9300
C(6B)-H(6B)	0.9300
C(7B)-C(8B)	1.339(8)
C(7B)-C(12B)	1.370(7)
C(7B)-C(33B)	1.501(7)
C(8B)-C(9B)	1.369(11)
C(8B)-H(8B)	0.9300
C(9B)-C(10B)	1.361(14)
C(9B)-H(9B)	0.9300
C(10B)-C(11B)	1.357(14)
C(10B)-H(10B)	0.9300
C(11B)-C(12B)	1.406(10)
C(11B)-H(11B)	0.9300
C(12B)-H(12B)	0.9300
C(13B)-C(18B)	1.380(6)
C(13B)-C(14B)	1.389(7)
C(13B)-C(34B)	1.514(6)
C(14B)-C(15B)	1.406(9)
C(14B)-H(14B)	0.9300
C(15B)-C(16B)	1.357(10)
C(15B)-H(15B)	0.9300
C(16B)-C(17B)	1.345(10)
C(16B)-H(16B)	0.9300
C(17B)-C(18B)	1.383(7)
C(17B)-H(17B)	0.9300
C(18B)-H(18B)	0.9300
C(30B)-C(39B)	1.551(5)
C(30B)-H(30B)	0.9800
C(31B)-H(31D)	0.9600
C(31B)-H(31E)	0.9600
C(31B)-H(31F)	0.9600
C(32B)-H(32D)	0.9600

C(32B)-H(32E)	0.9600
C(32B)-H(32F)	0.9600
C(33B)-H(33C)	0.9700
C(33B)-H(33D)	0.9700
C(34B)-C(40B)	1.558(5)
C(34B)-H(34B)	0.9800
C(35B)-C(36B)	1.321(6)
C(35B)-C(40B)	1.505(6)
C(35B)-H(35B)	0.9300
C(36B)-C(37B)	1.441(7)
C(36B)-H(36B)	0.9300
C(37B)-C(38B)	1.326(6)
C(37B)-H(37B)	0.9300
C(38B)-C(39B)	1.500(6)
C(38B)-H(38B)	0.9300
C(39B)-C(40B)	1.536(5)
C(39B)-H(39B)	0.9800
C(1E)-O(2M)	1.451(17)
O(2M)-O(2M)#1	1.386(18)

O(1A)-P(1A)-N(1A)	116.76(19)
O(1A)-P(1A)-N(2A)	109.61(19)
N(1A)-P(1A)-N(2A)	105.87(19)
O(1A)-P(1A)-C(40A)	114.46(18)
N(1A)-P(1A)-C(40A)	94.63(19)
N(2A)-P(1A)-C(40A)	114.70(19)
O(1B)-P(1B)-N(2B)	109.80(18)
O(1B)-P(1B)-N(1B)	117.00(19)
N(2B)-P(1B)-N(1B)	105.86(18)
O(1B)-P(1B)-C(40B)	114.01(17)
N(2B)-P(1B)-C(40B)	114.2(2)
N(1B)-P(1B)-C(40B)	95.19(18)
C(34A)-O(2A)-H(2A)	109.5
C(34B)-O(2B)-H(2B)	109.5
C(30A)-N(1A)-C(31A)	117.8(4)
C(30A)-N(1A)-P(1A)	117.4(3)
C(31A)-N(1A)-P(1A)	123.8(3)
C(32A)-N(2A)-C(33A)	113.9(4)
C(32A)-N(2A)-P(1A)	124.0(3)
C(33A)-N(2A)-P(1A)	121.5(3)
C(30B)-N(1B)-C(31B)	119.3(3)
C(30B)-N(1B)-P(1B)	115.3(3)
C(31B)-N(1B)-P(1B)	124.0(3)
C(32B)-N(2B)-C(33B)	113.4(4)
C(32B)-N(2B)-P(1B)	124.0(3)
C(33B)-N(2B)-P(1B)	119.5(3)
C(2A)-C(1A)-C(6A)	118.5(5)
C(2A)-C(1A)-C(30A)	120.3(5)
C(6A)-C(1A)-C(30A)	121.1(5)
C(1A)-C(2A)-C(3A)	120.0(6)
C(1A)-C(2A)-H(2A1)	120.0
C(3A)-C(2A)-H(2A1)	120.0
C(4A)-C(3A)-C(2A)	119.9(7)
C(4A)-C(3A)-H(3A)	120.0
C(2A)-C(3A)-H(3A)	120.0
C(5A)-C(4A)-C(3A)	119.5(7)
C(5A)-C(4A)-H(4A)	120.3
C(3A)-C(4A)-H(4A)	120.3
C(4A)-C(5A)-C(6A)	120.8(7)
C(4A)-C(5A)-H(5A)	119.6
C(6A)-C(5A)-H(5A)	119.6
C(5A)-C(6A)-C(1A)	121.2(6)

C(5A)-C(6A)-H(6A)	119.4
C(1A)-C(6A)-H(6A)	119.4
C(12A)-C(7A)-C(8A)	118.4(5)
C(12A)-C(7A)-C(33A)	122.1(5)
C(8A)-C(7A)-C(33A)	119.4(5)
C(7A)-C(8A)-C(9A)	119.8(6)
C(7A)-C(8A)-H(8A)	120.1
C(9A)-C(8A)-H(8A)	120.1
C(10A)-C(9A)-C(8A)	120.1(6)
C(10A)-C(9A)-H(9A)	120.0
C(8A)-C(9A)-H(9A)	120.0
C(11A)-C(10A)-C(9A)	119.8(6)
C(11A)-C(10A)-H(10A)	120.1
C(9A)-C(10A)-H(10A)	120.1
C(10A)-C(11A)-C(12A)	120.4(6)
C(10A)-C(11A)-H(11A)	119.8
C(12A)-C(11A)-H(11A)	119.8
C(7A)-C(12A)-C(11A)	121.4(6)
C(7A)-C(12A)-H(12A)	119.3
C(11A)-C(12A)-H(12A)	119.3
C(14A)-C(13A)-C(18A)	116.5(4)
C(14A)-C(13A)-C(34A)	122.7(4)
C(18A)-C(13A)-C(34A)	120.8(4)
C(13A)-C(14A)-C(15A)	121.5(5)
C(13A)-C(14A)-H(14A)	119.3
C(15A)-C(14A)-H(14A)	119.3
C(16A)-C(15A)-C(14A)	120.6(5)
C(16A)-C(15A)-H(15A)	119.7
C(14A)-C(15A)-H(15A)	119.7
C(17A)-C(16A)-C(15A)	119.5(6)
C(17A)-C(16A)-H(16A)	120.3
C(15A)-C(16A)-H(16A)	120.3
C(16A)-C(17A)-C(18A)	119.5(5)
C(16A)-C(17A)-H(17A)	120.2
C(18A)-C(17A)-H(17A)	120.2
C(17A)-C(18A)-C(13A)	122.4(5)
C(17A)-C(18A)-H(18A)	118.8
C(13A)-C(18A)-H(18A)	118.8
N(1A)-C(30A)-C(1A)	112.5(4)
N(1A)-C(30A)-C(39A)	105.3(3)
C(1A)-C(30A)-C(39A)	112.3(4)
N(1A)-C(30A)-H(30A)	108.9
C(1A)-C(30A)-H(30A)	108.9
C(39A)-C(30A)-H(30A)	108.9
N(1A)-C(31A)-H(31A)	109.5
N(1A)-C(31A)-H(31B)	109.5
H(31A)-C(31A)-H(31B)	109.5
N(1A)-C(31A)-H(31C)	109.5
H(31A)-C(31A)-H(31C)	109.5
H(31B)-C(31A)-H(31C)	109.5
N(2A)-C(32A)-H(32A)	109.5
N(2A)-C(32A)-H(32B)	109.5
H(32A)-C(32A)-H(32B)	109.5
N(2A)-C(32A)-H(32C)	109.5
H(32A)-C(32A)-H(32C)	109.5
H(32B)-C(32A)-H(32C)	109.5
N(2A)-C(33A)-C(7A)	113.0(4)
N(2A)-C(33A)-H(33A)	109.0
C(7A)-C(33A)-H(33A)	109.0
N(2A)-C(33A)-H(33B)	109.0
C(7A)-C(33A)-H(33B)	109.0
H(33A)-C(33A)-H(33B)	107.8
O(2A)-C(34A)-C(13A)	112.1(3)

O(2A)-C(34A)-C(40A)	105.0(3)
C(13A)-C(34A)-C(40A)	114.0(3)
O(2A)-C(34A)-H(34A)	108.5
C(13A)-C(34A)-H(34A)	108.5
C(40A)-C(34A)-H(34A)	108.5
C(36A)-C(35A)-C(40A)	123.5(6)
C(36A)-C(35A)-H(35A)	118.3
C(40A)-C(35A)-H(35A)	118.3
C(35A)-C(36A)-C(37A)	121.6(7)
C(35A)-C(36A)-H(36A)	119.2
C(37A)-C(36A)-H(36A)	119.2
C(38A)-C(37A)-C(36A)	121.3(7)
C(38A)-C(37A)-H(37A)	119.4
C(36A)-C(37A)-H(37A)	119.4
C(37A)-C(38A)-C(39A)	120.2(7)
C(37A)-C(38A)-H(38A)	119.9
C(39A)-C(38A)-H(38A)	119.9
C(38A)-C(39A)-C(40A)	112.8(4)
C(38A)-C(39A)-C(30A)	108.5(4)
C(40A)-C(39A)-C(30A)	108.6(4)
C(38A)-C(39A)-H(39A)	108.9
C(40A)-C(39A)-H(39A)	108.9
C(30A)-C(39A)-H(39A)	108.9
C(35A)-C(40A)-C(39A)	110.5(4)
C(35A)-C(40A)-C(34A)	109.0(3)
C(39A)-C(40A)-C(34A)	114.7(4)
C(35A)-C(40A)-P(1A)	111.8(3)
C(39A)-C(40A)-P(1A)	102.7(3)
C(34A)-C(40A)-P(1A)	108.0(3)
C(6B)-C(1B)-C(2B)	117.9(4)
C(6B)-C(1B)-C(30B)	121.6(4)
C(2B)-C(1B)-C(30B)	120.4(4)
C(3B)-C(2B)-C(1B)	120.9(5)
C(3B)-C(2B)-H(2B1)	119.6
C(1B)-C(2B)-H(2B1)	119.6
C(2B)-C(3B)-C(4B)	119.8(5)
C(2B)-C(3B)-H(3B)	120.1
C(4B)-C(3B)-H(3B)	120.1
C(5B)-C(4B)-C(3B)	120.2(5)
C(5B)-C(4B)-H(4B)	119.9
C(3B)-C(4B)-H(4B)	119.9
C(4B)-C(5B)-C(6B)	120.3(5)
C(4B)-C(5B)-H(5B)	119.8
C(6B)-C(5B)-H(5B)	119.8
C(5B)-C(6B)-C(1B)	120.9(5)
C(5B)-C(6B)-H(6B)	119.6
C(1B)-C(6B)-H(6B)	119.6
C(8B)-C(7B)-C(12B)	120.5(6)
C(8B)-C(7B)-C(33B)	120.3(6)
C(12B)-C(7B)-C(33B)	119.2(6)
C(7B)-C(8B)-C(9B)	121.2(8)
C(7B)-C(8B)-H(8B)	119.4
C(9B)-C(8B)-H(8B)	119.4
C(10B)-C(9B)-C(8B)	119.8(10)
C(10B)-C(9B)-H(9B)	120.1
C(8B)-C(9B)-H(9B)	120.1
C(11B)-C(10B)-C(9B)	120.0(9)
C(11B)-C(10B)-H(10B)	120.0
C(9B)-C(10B)-H(10B)	120.0
C(10B)-C(11B)-C(12B)	120.1(9)
C(10B)-C(11B)-H(11B)	119.9
C(12B)-C(11B)-H(11B)	119.9
C(7B)-C(12B)-C(11B)	118.3(8)

C(7B)-C(12B)-H(12B)	120.8
C(11B)-C(12B)-H(12B)	120.8
C(18B)-C(13B)-C(14B)	118.6(5)
C(18B)-C(13B)-C(34B)	120.0(4)
C(14B)-C(13B)-C(34B)	121.4(5)
C(13B)-C(14B)-C(15B)	119.2(6)
C(13B)-C(14B)-H(14B)	120.4
C(15B)-C(14B)-H(14B)	120.4
C(16B)-C(15B)-C(14B)	119.7(7)
C(16B)-C(15B)-H(15B)	120.2
C(14B)-C(15B)-H(15B)	120.2
C(17B)-C(16B)-C(15B)	122.1(7)
C(17B)-C(16B)-H(16B)	119.0
C(15B)-C(16B)-H(16B)	119.0
C(16B)-C(17B)-C(18B)	118.9(7)
C(16B)-C(17B)-H(17B)	120.6
C(18B)-C(17B)-H(17B)	120.6
C(13B)-C(18B)-C(17B)	121.5(6)
C(13B)-C(18B)-H(18B)	119.2
C(17B)-C(18B)-H(18B)	119.2
N(1B)-C(30B)-C(1B)	114.3(4)
N(1B)-C(30B)-C(39B)	105.5(3)
C(1B)-C(30B)-C(39B)	111.6(3)
N(1B)-C(30B)-H(30B)	108.4
C(1B)-C(30B)-H(30B)	108.4
C(39B)-C(30B)-H(30B)	108.4
N(1B)-C(31B)-H(31D)	109.5
N(1B)-C(31B)-H(31E)	109.5
H(31D)-C(31B)-H(31E)	109.5
N(1B)-C(31B)-H(31F)	109.5
H(31D)-C(31B)-H(31F)	109.5
H(31E)-C(31B)-H(31F)	109.5
N(2B)-C(32B)-H(32D)	109.5
N(2B)-C(32B)-H(32E)	109.5
H(32D)-C(32B)-H(32E)	109.5
N(2B)-C(32B)-H(32F)	109.5
H(32D)-C(32B)-H(32F)	109.5
H(32E)-C(32B)-H(32F)	109.5
N(2B)-C(33B)-C(7B)	112.8(4)
N(2B)-C(33B)-H(33C)	109.0
C(7B)-C(33B)-H(33C)	109.0
N(2B)-C(33B)-H(33D)	109.0
C(7B)-C(33B)-H(33D)	109.0
H(33C)-C(33B)-H(33D)	107.8
O(2B)-C(34B)-C(13B)	113.0(4)
O(2B)-C(34B)-C(40B)	105.2(3)
C(13B)-C(34B)-C(40B)	113.5(3)
O(2B)-C(34B)-H(34B)	108.3
C(13B)-C(34B)-H(34B)	108.3
C(40B)-C(34B)-H(34B)	108.3
C(36B)-C(35B)-C(40B)	121.9(4)
C(36B)-C(35B)-H(35B)	119.0
C(40B)-C(35B)-H(35B)	119.0
C(35B)-C(36B)-C(37B)	122.2(5)
C(35B)-C(36B)-H(36B)	118.9
C(37B)-C(36B)-H(36B)	118.9
C(38B)-C(37B)-C(36B)	119.4(5)
C(38B)-C(37B)-H(37B)	120.3
C(36B)-C(37B)-H(37B)	120.3
C(37B)-C(38B)-C(39B)	120.5(4)
C(37B)-C(38B)-H(38B)	119.8
C(39B)-C(38B)-H(38B)	119.8
C(38B)-C(39B)-C(40B)	113.3(4)

C(38B)-C(39B)-C(30B)	108.8(3)
C(40B)-C(39B)-C(30B)	107.3(3)
C(38B)-C(39B)-H(39B)	109.1
C(40B)-C(39B)-H(39B)	109.1
C(30B)-C(39B)-H(39B)	109.1
C(35B)-C(40B)-C(39B)	110.0(3)
C(35B)-C(40B)-C(34B)	110.0(3)
C(39B)-C(40B)-C(34B)	114.9(3)
C(35B)-C(40B)-P(1B)	111.5(3)
C(39B)-C(40B)-P(1B)	101.9(3)
C(34B)-C(40B)-P(1B)	108.3(3)
O(2M)#1-O(2M)-C(1E)	92.9(12)

Table S10. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **9ab** = r280fr2s The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U11	U22	U33	U23	U13	U12
P(1A)	57(1)	59(1)	42(1)	16(1)	13(1)	24(1)
P(1B)	73(1)	49(1)	40(1)	18(1)	14(1)	26(1)
O(1A)	79(2)	58(2)	50(2)	17(2)	24(2)	29(2)
O(2A)	54(2)	70(2)	52(2)	21(2)	8(2)	17(2)
O(1B)	75(2)	49(2)	62(2)	28(2)	25(2)	25(2)
O(2B)	93(2)	60(2)	48(2)	25(2)	5(2)	31(2)
N(1A)	48(2)	82(3)	42(2)	20(2)	14(2)	23(2)
N(2A)	58(2)	60(2)	47(2)	16(2)	3(2)	16(2)
N(1B)	71(3)	64(2)	42(2)	22(2)	16(2)	38(2)
N(2B)	109(3)	51(2)	40(2)	15(2)	13(2)	37(2)
C(1A)	58(3)	87(4)	45(3)	26(3)	15(2)	23(3)
C(2A)	55(4)	114(5)	71(4)	23(3)	14(3)	18(4)
C(3A)	62(4)	168(7)	78(5)	45(5)	7(3)	12(5)
C(4A)	77(5)	204(9)	82(5)	72(6)	14(4)	63(6)
C(5A)	97(5)	162(7)	89(5)	75(5)	24(4)	69(5)
C(6A)	65(4)	116(5)	81(4)	51(4)	16(3)	38(3)
C(7A)	54(3)	68(3)	60(3)	16(3)	-1(3)	7(3)
C(8A)	141(6)	77(4)	65(4)	21(3)	7(4)	44(4)
C(9A)	155(6)	82(4)	83(5)	0(4)	28(5)	47(4)
C(10A)	109(5)	101(5)	54(4)	12(4)	-13(4)	8(4)
C(11A)	132(6)	147(6)	68(5)	12(4)	-16(4)	72(5)
C(12A)	112(5)	139(6)	68(4)	14(4)	-15(4)	68(5)
C(13A)	45(3)	70(3)	46(3)	24(2)	11(2)	20(2)
C(14A)	62(3)	75(3)	40(3)	13(2)	10(2)	27(3)
C(15A)	87(4)	82(4)	61(4)	14(3)	21(3)	32(3)
C(16A)	95(5)	102(5)	47(3)	9(3)	7(3)	13(4)
C(17A)	87(4)	180(7)	52(4)	38(4)	0(3)	51(5)
C(18A)	72(4)	138(5)	65(4)	47(4)	15(3)	53(4)
C(30A)	52(3)	74(3)	47(3)	21(3)	12(2)	18(2)
C(31A)	78(4)	111(4)	49(3)	35(3)	29(3)	37(3)
C(32A)	81(4)	70(3)	56(3)	21(3)	4(3)	29(3)
C(33A)	64(3)	91(4)	60(3)	18(3)	9(3)	26(3)
C(34A)	56(3)	62(3)	44(3)	16(2)	13(2)	27(2)
C(35A)	81(4)	61(3)	53(3)	14(3)	25(3)	23(3)
C(36A)	131(6)	62(4)	82(5)	12(4)	59(4)	21(4)
C(37A)	105(6)	106(6)	95(6)	-21(5)	53(5)	-12(5)

C(38A)	60(4)	154(7)	55(4)	-11(4)	17(3)	-5(4)
C(39A)	57(3)	96(4)	45(3)	19(3)	14(2)	16(3)
C(40A)	49(3)	56(3)	46(3)	13(2)	11(2)	19(2)
C(1B)	56(3)	57(3)	45(3)	17(2)	10(2)	26(2)
C(2B)	78(3)	72(3)	51(3)	30(3)	19(3)	38(3)
C(3B)	86(4)	105(4)	54(3)	41(3)	22(3)	57(4)
C(4B)	80(4)	117(5)	47(3)	18(3)	6(3)	61(4)
C(5B)	59(3)	94(4)	63(4)	15(3)	4(3)	26(3)
C(6B)	65(3)	74(3)	65(3)	25(3)	13(3)	24(3)
C(7B)	110(5)	78(4)	43(3)	24(3)	15(3)	52(3)
C(8B)	112(6)	109(5)	97(5)	37(4)	32(4)	45(4)
C(9B)	177(9)	164(9)	181(10)	102(8)	101(9)	100(8)
C(10B)	313(18)	217(12)	138(9)	120(9)	152(12)	209(13)
C(11B)	314(14)	188(9)	42(4)	20(5)	35(7)	180(11)
C(12B)	167(6)	128(5)	52(4)	14(4)	1(4)	94(5)
C(13B)	61(3)	73(3)	63(3)	38(3)	18(3)	36(3)
C(14B)	63(4)	114(5)	113(5)	55(4)	16(4)	33(4)
C(15B)	59(4)	200(9)	161(8)	92(7)	41(5)	55(5)
C(16B)	114(7)	224(10)	137(7)	106(7)	78(6)	113(7)
C(17B)	122(6)	151(6)	75(4)	51(4)	48(4)	95(5)
C(18B)	84(4)	99(4)	60(3)	40(3)	31(3)	57(3)
C(30B)	66(3)	42(2)	38(3)	13(2)	6(2)	18(2)
C(31B)	99(4)	88(4)	64(3)	33(3)	30(3)	52(3)
C(32B)	143(5)	68(4)	59(4)	14(3)	12(3)	43(4)
C(33B)	132(5)	96(4)	43(3)	21(3)	13(3)	69(4)
C(34B)	59(3)	52(3)	38(3)	16(2)	7(2)	19(2)
C(35B)	66(3)	58(3)	52(3)	21(3)	5(2)	13(3)
C(36B)	70(3)	62(3)	71(4)	29(3)	-1(3)	1(3)
C(37B)	60(3)	77(4)	77(4)	45(3)	12(3)	10(3)
C(38B)	78(4)	73(3)	47(3)	30(3)	15(3)	34(3)
C(39B)	51(3)	49(2)	42(3)	20(2)	7(2)	15(2)
C(40B)	57(3)	44(2)	41(3)	16(2)	3(2)	14(2)

Table S11. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **9ab** = r280fr2s.

	x	y	z	U(eq)
H(2A)	-407	5826	5415	90
H(2B)	3695	9505	-44	97
H(2A1)	6539	9456	5371	102
H(3A)	8452	9266	5570	132
H(4A)	8552	7469	5361	134
H(5A)	6782	5913	5016	122
H(6A)	4900	6090	4824	98
H(8A)	841	4323	2560	113
H(9A)	661	3495	1294	134
H(10A)	-384	4035	499	120
H(11A)	-1220	5376	952	140
H(12A)	-1038	6211	2204	128
H(14A)	97	7971	6445	72
H(15A)	333	8920	7677	94
H(16A)	1823	8895	8491	110
H(17A)	3019	7827	8073	127
H(18A)	2734	6821	6845	101
H(30A)	4410	8657	4894	70
H(31A)	4347	7603	3530	114

H(31B)	3321	6386	3187	114
H(31C)	4593	6533	3605	114
H(32A)	1598	7513	2990	104
H(32B)	2445	8173	3763	104
H(32C)	1065	8096	3663	104
H(33A)	-582	6257	3434	88
H(33B)	-247	5247	3546	88
H(34A)	1460	5971	5630	63
H(35A)	1068	8229	4963	80
H(36A)	2100	9989	5685	115
H(37A)	3753	10403	6586	152
H(38A)	4650	9130	6563	134
H(39A)	3680	7227	5773	84
H(2B1)	5715	6212	2305	74
H(3B)	6957	6649	3400	86
H(4B)	8747	8242	3782	92
H(5B)	9294	9386	3074	91
H(6B)	8047	8981	1987	81
H(8B)	7411	7821	-1387	125
H(9B)	8313	7235	-2384	181
H(10B)	7098	6034	-3491	208
H(11B)	4997	5536	-3620	194
H(12B)	4075	6059	-2583	131
H(14B)	1722	8289	574	111
H(15B)	425	8608	1439	155
H(16B)	1253	9839	2602	157
H(17B)	3318	10825	2942	119
H(18B)	4626	10499	2111	85
H(30B)	5315	6518	1181	59
H(31D)	8150	7405	883	114
H(31E)	7636	7116	52	114
H(31F)	7106	6226	452	114
H(32D)	4124	5563	-977	136
H(32E)	5089	5727	-314	136
H(32F)	5444	5550	-1103	136
H(33C)	5378	8266	-1087	100
H(33D)	4217	7134	-1381	100
H(34B)	4977	9790	893	60
H(35B)	3189	6710	-130	73
H(36B)	2103	5743	534	87
H(37B)	2466	6499	1836	85
H(38B)	4246	7961	2421	74
H(39B)	5603	8867	1769	56

Table S12. Torsion angles [°] for **9ab** = r280fr2s.

O(1A)-P(1A)-N(1A)-C(30A)	-115.6(3)
N(2A)-P(1A)-N(1A)-C(30A)	122.1(3)
C(40A)-P(1A)-N(1A)-C(30A)	4.8(3)
O(1A)-P(1A)-N(1A)-C(31A)	75.9(4)
N(2A)-P(1A)-N(1A)-C(31A)	-46.4(4)
C(40A)-P(1A)-N(1A)-C(31A)	-163.7(4)
O(1A)-P(1A)-N(2A)-C(32A)	-164.8(3)
N(1A)-P(1A)-N(2A)-C(32A)	-38.0(4)
C(40A)-P(1A)-N(2A)-C(32A)	64.8(4)
O(1A)-P(1A)-N(2A)-C(33A)	24.6(4)
N(1A)-P(1A)-N(2A)-C(33A)	151.3(3)
C(40A)-P(1A)-N(2A)-C(33A)	-105.8(4)
O(1B)-P(1B)-N(1B)-C(30B)	118.3(3)
N(2B)-P(1B)-N(1B)-C(30B)	-119.0(3)

C(40B)-P(1B)-N(1B)-C(30B)	-2.0(3)
O(1B)-P(1B)-N(1B)-C(31B)	-75.7(4)
N(2B)-P(1B)-N(1B)-C(31B)	47.0(4)
C(40B)-P(1B)-N(1B)-C(31B)	164.0(4)
O(1B)-P(1B)-N(2B)-C(32B)	163.5(4)
N(1B)-P(1B)-N(2B)-C(32B)	36.3(5)
C(40B)-P(1B)-N(2B)-C(32B)	-67.0(5)
O(1B)-P(1B)-N(2B)-C(33B)	-37.8(4)
N(1B)-P(1B)-N(2B)-C(33B)	-165.0(4)
C(40B)-P(1B)-N(2B)-C(33B)	91.7(4)
C(6A)-C(1A)-C(2A)-C(3A)	-0.3(8)
C(30A)-C(1A)-C(2A)-C(3A)	-179.2(5)
C(1A)-C(2A)-C(3A)-C(4A)	0.9(9)
C(2A)-C(3A)-C(4A)-C(5A)	-1.4(10)
C(3A)-C(4A)-C(5A)-C(6A)	1.3(10)
C(4A)-C(5A)-C(6A)-C(1A)	-0.6(9)
C(2A)-C(1A)-C(6A)-C(5A)	0.1(8)
C(30A)-C(1A)-C(6A)-C(5A)	179.1(5)
C(12A)-C(7A)-C(8A)-C(9A)	-1.9(9)
C(33A)-C(7A)-C(8A)-C(9A)	179.3(5)
C(7A)-C(8A)-C(9A)-C(10A)	0.7(10)
C(8A)-C(9A)-C(10A)-C(11A)	0.4(10)
C(9A)-C(10A)-C(11A)-C(12A)	-0.2(11)
C(8A)-C(7A)-C(12A)-C(11A)	2.1(10)
C(33A)-C(7A)-C(12A)-C(11A)	-179.1(6)
C(10A)-C(11A)-C(12A)-C(7A)	-1.1(11)
C(18A)-C(13A)-C(14A)-C(15A)	0.0(7)
C(34A)-C(13A)-C(14A)-C(15A)	-178.5(4)
C(13A)-C(14A)-C(15A)-C(16A)	1.5(8)
C(14A)-C(15A)-C(16A)-C(17A)	-1.8(9)
C(15A)-C(16A)-C(17A)-C(18A)	0.5(10)
C(16A)-C(17A)-C(18A)-C(13A)	1.0(10)
C(14A)-C(13A)-C(18A)-C(17A)	-1.3(8)
C(34A)-C(13A)-C(18A)-C(17A)	177.2(5)
C(31A)-N(1A)-C(30A)-C(1A)	-53.4(5)
P(1A)-N(1A)-C(30A)-C(1A)	137.4(3)
C(31A)-N(1A)-C(30A)-C(39A)	-176.0(4)
P(1A)-N(1A)-C(30A)-C(39A)	14.7(5)
C(2A)-C(1A)-C(30A)-N(1A)	137.5(4)
C(6A)-C(1A)-C(30A)-N(1A)	-41.4(6)
C(2A)-C(1A)-C(30A)-C(39A)	-103.8(5)
C(6A)-C(1A)-C(30A)-C(39A)	77.2(6)
C(32A)-N(2A)-C(33A)-C(7A)	68.4(5)
P(1A)-N(2A)-C(33A)-C(7A)	-120.1(4)
C(12A)-C(7A)-C(33A)-N(2A)	-106.8(6)
C(8A)-C(7A)-C(33A)-N(2A)	72.0(6)
C(14A)-C(13A)-C(34A)-O(2A)	-28.5(6)
C(18A)-C(13A)-C(34A)-O(2A)	153.0(4)
C(14A)-C(13A)-C(34A)-C(40A)	90.5(5)
C(18A)-C(13A)-C(34A)-C(40A)	-87.9(5)
C(40A)-C(35A)-C(36A)-C(37A)	-1.1(8)
C(35A)-C(36A)-C(37A)-C(38A)	12.0(10)
C(36A)-C(37A)-C(38A)-C(39A)	4.0(10)
C(37A)-C(38A)-C(39A)-C(40A)	-28.1(8)
C(37A)-C(38A)-C(39A)-C(30A)	92.4(7)
N(1A)-C(30A)-C(39A)-C(38A)	-154.9(5)
C(1A)-C(30A)-C(39A)-C(38A)	82.3(6)
N(1A)-C(30A)-C(39A)-C(40A)	-31.9(5)
C(1A)-C(30A)-C(39A)-C(40A)	-154.7(4)
C(36A)-C(35A)-C(40A)-C(39A)	-22.9(6)
C(36A)-C(35A)-C(40A)-C(34A)	104.0(5)
C(36A)-C(35A)-C(40A)-P(1A)	-136.7(4)
C(38A)-C(39A)-C(40A)-C(35A)	34.9(6)

C(30A)-C(39A)-C(40A)-C(35A)	-85.5(5)
C(38A)-C(39A)-C(40A)-C(34A)	-88.7(5)
C(30A)-C(39A)-C(40A)-C(34A)	150.8(4)
C(38A)-C(39A)-C(40A)-P(1A)	154.4(4)
C(30A)-C(39A)-C(40A)-P(1A)	33.9(4)
O(2A)-C(34A)-C(40A)-C(35A)	57.4(4)
C(13A)-C(34A)-C(40A)-C(35A)	-65.6(5)
O(2A)-C(34A)-C(40A)-C(39A)	-178.1(3)
C(13A)-C(34A)-C(40A)-C(39A)	58.9(5)
O(2A)-C(34A)-C(40A)-P(1A)	-64.3(4)
C(13A)-C(34A)-C(40A)-P(1A)	172.7(3)
O(1A)-P(1A)-C(40A)-C(35A)	-142.0(3)
N(1A)-P(1A)-C(40A)-C(35A)	95.8(3)
N(2A)-P(1A)-C(40A)-C(35A)	-14.0(4)
O(1A)-P(1A)-C(40A)-C(39A)	99.5(3)
N(1A)-P(1A)-C(40A)-C(39A)	-22.8(3)
N(2A)-P(1A)-C(40A)-C(39A)	-132.6(3)
O(1A)-P(1A)-C(40A)-C(34A)	-22.1(3)
N(1A)-P(1A)-C(40A)-C(34A)	-144.3(3)
N(2A)-P(1A)-C(40A)-C(34A)	105.9(3)
C(6B)-C(1B)-C(2B)-C(3B)	0.8(6)
C(30B)-C(1B)-C(2B)-C(3B)	-175.3(4)
C(1B)-C(2B)-C(3B)-C(4B)	-0.7(7)
C(2B)-C(3B)-C(4B)-C(5B)	-0.1(7)
C(3B)-C(4B)-C(5B)-C(6B)	0.7(8)
C(4B)-C(5B)-C(6B)-C(1B)	-0.6(7)
C(2B)-C(1B)-C(6B)-C(5B)	-0.2(7)
C(30B)-C(1B)-C(6B)-C(5B)	175.9(4)
C(12B)-C(7B)-C(8B)-C(9B)	0.7(10)
C(33B)-C(7B)-C(8B)-C(9B)	-178.4(6)
C(7B)-C(8B)-C(9B)-C(10B)	-0.5(12)
C(8B)-C(9B)-C(10B)-C(11B)	2.1(15)
C(9B)-C(10B)-C(11B)-C(12B)	-3.9(15)
C(8B)-C(7B)-C(12B)-C(11B)	-2.5(9)
C(33B)-C(7B)-C(12B)-C(11B)	176.6(5)
C(10B)-C(11B)-C(12B)-C(7B)	4.1(12)
C(18B)-C(13B)-C(14B)-C(15B)	-2.0(8)
C(34B)-C(13B)-C(14B)-C(15B)	176.5(5)
C(13B)-C(14B)-C(15B)-C(16B)	0.9(10)
C(14B)-C(15B)-C(16B)-C(17B)	1.2(13)
C(15B)-C(16B)-C(17B)-C(18B)	-2.0(11)
C(14B)-C(13B)-C(18B)-C(17B)	1.2(7)
C(34B)-C(13B)-C(18B)-C(17B)	-177.3(4)
C(16B)-C(17B)-C(18B)-C(13B)	0.8(9)
C(31B)-N(1B)-C(30B)-C(1B)	49.9(5)
P(1B)-N(1B)-C(30B)-C(1B)	-143.4(3)
C(31B)-N(1B)-C(30B)-C(39B)	172.9(4)
P(1B)-N(1B)-C(30B)-C(39B)	-20.4(4)
C(6B)-C(1B)-C(30B)-N(1B)	41.9(5)
C(2B)-C(1B)-C(30B)-N(1B)	-142.2(4)
C(6B)-C(1B)-C(30B)-C(39B)	-77.8(5)
C(2B)-C(1B)-C(30B)-C(39B)	98.1(4)
C(32B)-N(2B)-C(33B)-C(7B)	-63.4(6)
P(1B)-N(2B)-C(33B)-C(7B)	135.8(4)
C(8B)-C(7B)-C(33B)-N(2B)	-60.1(7)
C(12B)-C(7B)-C(33B)-N(2B)	120.8(5)
C(18B)-C(13B)-C(34B)-O(2B)	-145.6(4)
C(14B)-C(13B)-C(34B)-O(2B)	35.9(6)
C(18B)-C(13B)-C(34B)-C(40B)	94.6(5)
C(14B)-C(13B)-C(34B)-C(40B)	-83.8(5)
C(40B)-C(35B)-C(36B)-C(37B)	2.8(8)
C(35B)-C(36B)-C(37B)-C(38B)	-13.2(8)
C(36B)-C(37B)-C(38B)-C(39B)	-6.4(7)

C(37B)-C(38B)-C(39B)-C(40B)	33.3(6)
C(37B)-C(38B)-C(39B)-C(30B)	-86.0(5)
N(1B)-C(30B)-C(39B)-C(38B)	160.9(4)
C(1B)-C(30B)-C(39B)-C(38B)	-74.4(4)
N(1B)-C(30B)-C(39B)-C(40B)	38.0(4)
C(1B)-C(30B)-C(39B)-C(40B)	162.7(3)
C(36B)-C(35B)-C(40B)-C(39B)	23.6(6)
C(36B)-C(35B)-C(40B)-C(34B)	-103.9(5)
C(36B)-C(35B)-C(40B)-P(1B)	136.0(4)
C(38B)-C(39B)-C(40B)-C(35B)	-39.5(5)
C(30B)-C(39B)-C(40B)-C(35B)	80.7(4)
C(38B)-C(39B)-C(40B)-C(34B)	85.3(4)
C(30B)-C(39B)-C(40B)-C(34B)	-154.6(3)
C(38B)-C(39B)-C(40B)-P(1B)	-157.9(3)
C(30B)-C(39B)-C(40B)-P(1B)	-37.8(3)
O(2B)-C(34B)-C(40B)-C(35B)	-55.2(4)
C(13B)-C(34B)-C(40B)-C(35B)	68.8(5)
O(2B)-C(34B)-C(40B)-C(39B)	180.0(3)
C(13B)-C(34B)-C(40B)-C(39B)	-55.9(5)
O(2B)-C(34B)-C(40B)-P(1B)	66.8(4)
C(13B)-C(34B)-C(40B)-P(1B)	-169.1(3)
O(1B)-P(1B)-C(40B)-C(35B)	143.5(3)
N(2B)-P(1B)-C(40B)-C(35B)	16.2(4)
N(1B)-P(1B)-C(40B)-C(35B)	-93.8(3)
O(1B)-P(1B)-C(40B)-C(39B)	-99.1(3)
N(2B)-P(1B)-C(40B)-C(39B)	133.5(3)
N(1B)-P(1B)-C(40B)-C(39B)	23.6(3)
O(1B)-P(1B)-C(40B)-C(34B)	22.4(3)
N(2B)-P(1B)-C(40B)-C(34B)	-104.9(3)
N(1B)-P(1B)-C(40B)-C(34B)	145.1(3)

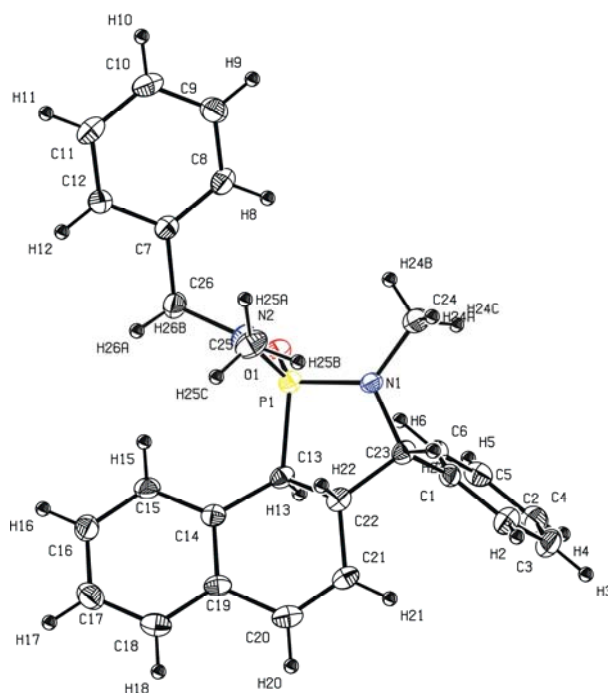


Figure S43. ORTEP view (40% anisotropic displacement) of **14**.

Table S13. Crystal data and structure refinement for **14** = r685_2m:

Identification code	r685_2m
Empirical formula	C ₂₆ H ₂₇ N ₂ O P
Formula weight	414.47
Temperature	150(2) K
Wavelength	0.71069 Å
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 16.5336(13)Å α = 90° b = 6.9286(5)Å β = 93.033(2)° c = 18.8474(14)Å γ = 90°
Volume	2156.0(3) Å ³
Z	4
Density (calculated)	1.277 Mg/m ³
Absorption coefficient	0.148 mm ⁻¹
F(000)	880
Crystal size	0.210 x 0.110 x 0.085 mm
Crystal description	prismatic colorless
Theta range for data collection	1.23 to 23.26°
Limiting indices	-17=<h<=18, -7=<k<=7, -15=<l<= 20
Reflections collected	9066
Independent reflections	3094 [R(int) = 0.0543]
Completeness to theta = 23.26°	99.9 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3094 / 0 / 273
Goodness-of-fit on F ²	0.895
Final R indices [I>2sigma(I)]	R1 = 0.0409, wR2 = 0.0713
R indices (all data)	R1 = 0.0628, wR2 = 0.0763
Largest diff. peak and hole	0.287 and -0.268 e.Å ⁻³

Table S14. Atomic coordinates (× 10⁴) and equivalent isotropic displacement parameters (Å² × 10³) for **14** = r685_2m. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
P(1)	7250(1)	1514(1)	4951(1)	23(1)
O(1)	7319(1)	3380(2)	5337(1)	29(1)
N(1)	6804(1)	-318(3)	5326(1)	23(1)
N(2)	6740(1)	1877(3)	4190(1)	25(1)
C(1)	7633(1)	-1940(4)	6295(1)	24(1)

C(2)	7815(1)	-3661(4)	6653(1)	33(1)
C(3)	8114(2)	-3636(4)	7355(2)	38(1)
C(4)	8228(1)	-1906(4)	7710(2)	35(1)
C(5)	8048(1)	-197(4)	7357(1)	31(1)
C(6)	7748(1)	-217(4)	6661(1)	26(1)
C(7)	5983(1)	4651(3)	3610(1)	25(1)
C(8)	5322(1)	4501(4)	4026(1)	31(1)
C(9)	4592(2)	5385(4)	3825(2)	35(1)
C(10)	4522(2)	6438(4)	3202(2)	37(1)
C(11)	5183(2)	6637(4)	2791(1)	33(1)
C(12)	5905(1)	5733(3)	2988(1)	26(1)
C(13)	8204(1)	229(3)	4912(1)	24(1)
C(14)	8810(1)	585(4)	4361(1)	23(1)
C(15)	8874(1)	2316(4)	3990(1)	28(1)
C(16)	9476(1)	2577(4)	3520(1)	33(1)
C(17)	10023(2)	1123(4)	3406(2)	38(1)
C(18)	9976(1)	-597(4)	3777(1)	34(1)
C(19)	9379(1)	-887(4)	4257(1)	26(1)
C(20)	9352(2)	-2655(4)	4682(1)	33(1)
C(21)	8709(1)	-3135(4)	5040(1)	28(1)
C(22)	7980(1)	-1875(3)	4977(1)	26(1)
C(23)	7320(1)	-1981(3)	5522(1)	25(1)
C(24)	5986(1)	-278(4)	5570(1)	36(1)
C(25)	6453(2)	294(4)	3724(1)	38(1)
C(26)	6790(1)	3749(4)	3825(1)	34(1)

Table S15. Bond lengths [Å] and angles [°] for **14** = r685_2m.

P(1)-O(1)	1.4845(16)
P(1)-N(2)	1.644(2)
P(1)-N(1)	1.6463(19)
P(1)-C(13)	1.816(2)
N(1)-C(24)	1.450(3)
N(1)-C(23)	1.469(3)
N(2)-C(25)	1.468(3)
N(2)-C(26)	1.473(3)
C(1)-C(6)	1.387(3)
C(1)-C(2)	1.395(3)
C(1)-C(23)	1.521(3)
C(2)-C(3)	1.389(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.380(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.383(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.378(3)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-C(8)	1.382(3)
C(7)-C(12)	1.392(3)
C(7)-C(26)	1.509(3)
C(8)-C(9)	1.389(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.383(3)
C(9)-H(9)	0.9500
C(10)-C(11)	1.379(3)
C(10)-H(10)	0.9500
C(11)-C(12)	1.381(3)
C(11)-H(11)	0.9500

C(12)-H(12)	0.9500
C(13)-C(14)	1.501(3)
C(13)-C(22)	1.511(3)
C(13)-H(13)	1.0000
C(14)-C(15)	1.395(3)
C(14)-C(19)	1.408(3)
C(15)-C(16)	1.378(3)
C(15)-H(15)	0.9500
C(16)-C(17)	1.378(3)
C(16)-H(16)	0.9500
C(17)-C(18)	1.386(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.389(3)
C(18)-H(18)	0.9500
C(19)-C(20)	1.466(3)
C(20)-C(21)	1.331(3)
C(20)-H(20)	0.9500
C(21)-C(22)	1.488(3)
C(21)-H(21)	0.9500
C(22)-C(23)	1.541(3)
C(22)-H(22)	1.0000
C(23)-H(23)	1.0000
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900

O(1)-P(1)-N(2)	108.43(10)
O(1)-P(1)-N(1)	119.05(10)
N(2)-P(1)-N(1)	105.73(10)
O(1)-P(1)-C(13)	113.77(10)
N(2)-P(1)-C(13)	116.47(11)
N(1)-P(1)-C(13)	92.88(10)
C(24)-N(1)-C(23)	118.29(19)
C(24)-N(1)-P(1)	124.60(16)
C(23)-N(1)-P(1)	116.40(14)
C(25)-N(2)-C(26)	113.7(2)
C(25)-N(2)-P(1)	122.88(17)
C(26)-N(2)-P(1)	120.21(16)
C(6)-C(1)-C(2)	118.4(2)
C(6)-C(1)-C(23)	121.5(2)
C(2)-C(1)-C(23)	120.1(2)
C(3)-C(2)-C(1)	120.5(3)
C(3)-C(2)-H(2)	119.8
C(1)-C(2)-H(2)	119.8
C(4)-C(3)-C(2)	120.3(3)
C(4)-C(3)-H(3)	119.8
C(2)-C(3)-H(3)	119.8
C(3)-C(4)-C(5)	119.4(3)
C(3)-C(4)-H(4)	120.3
C(5)-C(4)-H(4)	120.3
C(6)-C(5)-C(4)	120.4(3)
C(6)-C(5)-H(5)	119.8
C(4)-C(5)-H(5)	119.8
C(5)-C(6)-C(1)	121.0(2)
C(5)-C(6)-H(6)	119.5
C(1)-C(6)-H(6)	119.5
C(8)-C(7)-C(12)	118.5(2)

C(8)-C(7)-C(26)	122.0(2)
C(12)-C(7)-C(26)	119.4(2)
C(7)-C(8)-C(9)	121.0(2)
C(7)-C(8)-H(8)	119.5
C(9)-C(8)-H(8)	119.5
C(10)-C(9)-C(8)	119.7(3)
C(10)-C(9)-H(9)	120.1
C(8)-C(9)-H(9)	120.1
C(11)-C(10)-C(9)	119.8(3)
C(11)-C(10)-H(10)	120.1
C(9)-C(10)-H(10)	120.1
C(10)-C(11)-C(12)	120.3(3)
C(10)-C(11)-H(11)	119.9
C(12)-C(11)-H(11)	119.9
C(11)-C(12)-C(7)	120.7(2)
C(11)-C(12)-H(12)	119.7
C(7)-C(12)-H(12)	119.7
C(14)-C(13)-C(22)	113.0(2)
C(14)-C(13)-P(1)	124.09(17)
C(22)-C(13)-P(1)	104.61(15)
C(14)-C(13)-H(13)	104.4
C(22)-C(13)-H(13)	104.4
P(1)-C(13)-H(13)	104.4
C(15)-C(14)-C(19)	119.0(2)
C(15)-C(14)-C(13)	124.0(2)
C(19)-C(14)-C(13)	116.9(2)
C(16)-C(15)-C(14)	120.8(2)
C(16)-C(15)-H(15)	119.6
C(14)-C(15)-H(15)	119.6
C(17)-C(16)-C(15)	120.4(3)
C(17)-C(16)-H(16)	119.8
C(15)-C(16)-H(16)	119.8
C(16)-C(17)-C(18)	119.7(3)
C(16)-C(17)-H(17)	120.1
C(18)-C(17)-H(17)	120.1
C(17)-C(18)-C(19)	120.9(3)
C(17)-C(18)-H(18)	119.6
C(19)-C(18)-H(18)	119.6
C(18)-C(19)-C(14)	119.3(2)
C(18)-C(19)-C(20)	121.3(2)
C(14)-C(19)-C(20)	119.3(2)
C(21)-C(20)-C(19)	122.3(2)
C(21)-C(20)-H(20)	118.9
C(19)-C(20)-H(20)	118.9
C(20)-C(21)-C(22)	118.5(2)
C(20)-C(21)-H(21)	120.7
C(22)-C(21)-H(21)	120.7
C(21)-C(22)-C(13)	111.80(19)
C(21)-C(22)-C(23)	121.2(2)
C(13)-C(22)-C(23)	106.58(19)
C(21)-C(22)-H(22)	105.3
C(13)-C(22)-H(22)	105.3
C(23)-C(22)-H(22)	105.3
N(1)-C(23)-C(1)	113.0(2)
N(1)-C(23)-C(22)	102.59(19)
C(1)-C(23)-C(22)	114.9(2)
N(1)-C(23)-H(23)	108.7
C(1)-C(23)-H(23)	108.7
C(22)-C(23)-H(23)	108.7
N(1)-C(24)-H(24A)	109.5
N(1)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
N(1)-C(24)-H(24C)	109.5

H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
N(2)-C(25)-H(25A)	109.5
N(2)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
N(2)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
N(2)-C(26)-C(7)	114.82(19)
N(2)-C(26)-H(26A)	108.6
C(7)-C(26)-H(26A)	108.6
N(2)-C(26)-H(26B)	108.6
C(7)-C(26)-H(26B)	108.6
H(26A)-C(26)-H(26B)	107.5

Table S16. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **14** = r685_2m The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U11	U22	U33	U23	U13	U12
P(1)	23(1)	20(1)	25(1)	0(1)	-2(1)	0(1)
O(1)	34(1)	19(1)	35(1)	-5(1)	-4(1)	-1(1)
N(1)	20(1)	19(1)	28(1)	3(1)	-1(1)	1(1)
N(2)	29(1)	20(1)	23(1)	2(1)	-7(1)	0(1)
C(1)	21(1)	26(2)	23(2)	3(1)	0(1)	-2(1)
C(2)	36(2)	28(2)	34(2)	4(1)	-2(2)	0(1)
C(3)	38(2)	39(2)	34(2)	12(2)	-3(2)	3(2)
C(4)	30(2)	50(2)	24(2)	2(2)	-1(1)	1(2)
C(5)	27(2)	38(2)	30(2)	-5(2)	2(1)	2(1)
C(6)	25(2)	29(2)	24(2)	3(1)	2(1)	1(1)
C(7)	24(2)	23(2)	28(2)	1(1)	-5(1)	-3(1)
C(8)	34(2)	29(2)	31(2)	6(1)	-3(1)	0(1)
C(9)	30(2)	34(2)	43(2)	0(2)	6(2)	1(1)
C(10)	32(2)	28(2)	48(2)	2(2)	-7(2)	7(1)
C(11)	40(2)	23(2)	34(2)	2(1)	-10(2)	1(1)
C(12)	25(2)	22(2)	30(2)	-2(1)	-1(1)	-4(1)
C(13)	24(1)	22(2)	27(2)	1(1)	-5(1)	0(1)
C(14)	20(1)	28(2)	20(2)	-3(1)	-6(1)	-1(1)
C(15)	20(1)	30(2)	33(2)	3(1)	-3(1)	2(1)
C(16)	25(2)	37(2)	36(2)	10(1)	-3(2)	-5(1)
C(17)	27(2)	52(2)	35(2)	3(2)	4(1)	-1(2)
C(18)	23(2)	39(2)	40(2)	-5(2)	-2(2)	4(1)
C(19)	20(1)	28(2)	28(2)	-4(1)	-7(1)	1(1)
C(20)	28(2)	28(2)	41(2)	-5(1)	-5(2)	6(1)
C(21)	31(2)	22(2)	30(2)	-1(1)	-4(1)	5(1)
C(22)	30(2)	23(2)	25(2)	-1(1)	-2(1)	2(1)
C(23)	27(1)	18(2)	30(2)	0(1)	-2(1)	-2(1)
C(24)	29(2)	32(2)	48(2)	11(2)	0(2)	2(1)
C(25)	44(2)	36(2)	34(2)	-3(2)	-12(2)	6(1)
C(26)	30(2)	33(2)	39(2)	13(1)	1(1)	-3(1)

Table S17. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **14** = r685_2m.

	x	y	z	U(eq)
H(2)	7733	-4859	6414	40
H(3)	8240	-4815	7593	45
H(4)	8429	-1890	8192	42
H(5)	8132	999	7596	38
H(6)	7619	967	6428	31
H(8)	5369	3782	4455	38
H(9)	4142	5267	4115	42
H(10)	4020	7022	3056	44
H(11)	5142	7398	2372	39
H(12)	6353	5852	2695	31
H(13)	8503	539	5373	29
H(15)	8499	3326	4061	34
H(16)	9514	3767	3273	40
H(17)	10429	1298	3074	45
H(18)	10358	-1591	3702	41
H(20)	9809	-3487	4703	39
H(21)	8715	-4257	5330	34
H(22)	7701	-2222	4510	31
H(23)	6999	-3190	5437	30
H(24A)	5671	-1332	5346	54
H(24B)	5732	960	5441	54
H(24C)	6004	-434	6087	54
H(25A)	5925	636	3497	57
H(25B)	6399	-884	4006	57
H(25C)	6842	74	3358	57
H(26A)	7100	3571	3394	41
H(26B)	7098	4657	4142	41

Table S18. Torsion angles [$^\circ$] for **14** = r685_2m.

O(1)-P(1)-N(1)-C(24)	56.3(2)
N(2)-P(1)-N(1)-C(24)	-65.8(2)
C(13)-P(1)-N(1)-C(24)	175.7(2)
O(1)-P(1)-N(1)-C(23)	-113.81(17)
N(2)-P(1)-N(1)-C(23)	124.04(17)
C(13)-P(1)-N(1)-C(23)	5.50(19)
O(1)-P(1)-N(2)-C(25)	-170.38(18)
N(1)-P(1)-N(2)-C(25)	-41.7(2)
C(13)-P(1)-N(2)-C(25)	59.8(2)
O(1)-P(1)-N(2)-C(26)	31.1(2)
N(1)-P(1)-N(2)-C(26)	159.80(18)
C(13)-P(1)-N(2)-C(26)	-98.75(19)
C(6)-C(1)-C(2)-C(3)	-0.9(4)
C(23)-C(1)-C(2)-C(3)	179.0(2)
C(1)-C(2)-C(3)-C(4)	0.6(4)
C(2)-C(3)-C(4)-C(5)	-0.5(4)

C(3)-C(4)-C(5)-C(6)	0.7(4)
C(4)-C(5)-C(6)-C(1)	-1.1(4)
C(2)-C(1)-C(6)-C(5)	1.1(4)
C(23)-C(1)-C(6)-C(5)	-178.7(2)
C(12)-C(7)-C(8)-C(9)	0.8(4)
C(26)-C(7)-C(8)-C(9)	178.3(2)
C(7)-C(8)-C(9)-C(10)	-0.2(4)
C(8)-C(9)-C(10)-C(11)	-1.4(4)
C(9)-C(10)-C(11)-C(12)	2.3(4)
C(10)-C(11)-C(12)-C(7)	-1.6(4)
C(8)-C(7)-C(12)-C(11)	0.0(4)
C(26)-C(7)-C(12)-C(11)	-177.5(2)
O(1)-P(1)-C(13)-C(14)	-84.9(2)
N(2)-P(1)-C(13)-C(14)	42.3(2)
N(1)-P(1)-C(13)-C(14)	151.4(2)
O(1)-P(1)-C(13)-C(22)	143.51(15)
N(2)-P(1)-C(13)-C(22)	-89.26(18)
N(1)-P(1)-C(13)-C(22)	19.90(17)
C(22)-C(13)-C(14)-C(15)	152.6(2)
P(1)-C(13)-C(14)-C(15)	24.4(3)
C(22)-C(13)-C(14)-C(19)	-32.1(3)
P(1)-C(13)-C(14)-C(19)	-160.27(18)
C(19)-C(14)-C(15)-C(16)	1.0(4)
C(13)-C(14)-C(15)-C(16)	176.2(2)
C(14)-C(15)-C(16)-C(17)	0.4(4)
C(15)-C(16)-C(17)-C(18)	-1.4(4)
C(16)-C(17)-C(18)-C(19)	0.9(4)
C(17)-C(18)-C(19)-C(14)	0.6(4)
C(17)-C(18)-C(19)-C(20)	-176.5(2)
C(15)-C(14)-C(19)-C(18)	-1.5(4)
C(13)-C(14)-C(19)-C(18)	-177.1(2)
C(15)-C(14)-C(19)-C(20)	175.6(2)
C(13)-C(14)-C(19)-C(20)	0.0(3)
C(18)-C(19)-C(20)-C(21)	-166.8(2)
C(14)-C(19)-C(20)-C(21)	16.1(4)
C(19)-C(20)-C(21)-C(22)	3.0(4)
C(20)-C(21)-C(22)-C(13)	-35.3(3)
C(20)-C(21)-C(22)-C(23)	-162.3(2)
C(14)-C(13)-C(22)-C(21)	49.1(3)
P(1)-C(13)-C(22)-C(21)	-173.22(18)
C(14)-C(13)-C(22)-C(23)	-176.36(19)
P(1)-C(13)-C(22)-C(23)	-38.7(2)
C(24)-N(1)-C(23)-C(1)	-74.8(3)
P(1)-N(1)-C(23)-C(1)	96.0(2)
C(24)-N(1)-C(23)-C(22)	160.9(2)
P(1)-N(1)-C(23)-C(22)	-28.3(2)
C(6)-C(1)-C(23)-N(1)	-28.1(3)
C(2)-C(1)-C(23)-N(1)	152.0(2)
C(6)-C(1)-C(23)-C(22)	89.1(3)
C(2)-C(1)-C(23)-C(22)	-90.8(3)
C(21)-C(22)-C(23)-N(1)	171.1(2)
C(13)-C(22)-C(23)-N(1)	41.8(2)
C(21)-C(22)-C(23)-C(1)	48.1(3)
C(13)-C(22)-C(23)-C(1)	-81.2(2)
C(25)-N(2)-C(26)-C(7)	70.7(3)
P(1)-N(2)-C(26)-C(7)	-128.9(2)
C(8)-C(7)-C(26)-N(2)	36.4(4)
C(12)-C(7)-C(26)-N(2)	-146.2(2)