APPENDIX

APPENDIX I

General X-ray experimental description:

Crystals were mounted on a thin glass fibre using silicon grease and cooled on the diffractometer to 120 K using an Oxford Cryostream low temperature attachment. Approximate unit cell dimensions were determined by the Nonius Collect program[1] from 5 index frames of width 2^o in ϕ using a Nonius ^{Kappa}CCD diffractometer, with a detector to crystal distance of 30 mm□ □The Collect program was then used to calculate a data collection stratgey to 99.5 % completeness for $\theta = 27.5^o$ using a combination of 2^o ϕ and ω scans of 10 - 120 s deg^{-1} exposure time (depending on crystal quality). Crystals were indexed using the DENZO-SMN package[2] and positional data were refined along with diffractometer constants to give the final unit cell parameters. Integration and scaling (DENZO-SMN, Scalepack[2]) resulted in unique data sets corrected for Lorentz and polarisation effects and for the effects of crystal decay and absorption by a combination of averaging of equivalent reflections and an overall volume and scaling correction. Structures were solved using SHELXS-97[3] and developed *via* alternating least squares cycles and difference Fourier synthesis (SHELXL-97[3]) with the aid of the program X-Seed.[4] In general all non-hydrogen atoms were modeled anisotropically, while hydrogen atoms are assigned an isotropic thermal parameter 1.2 times that of the parent atom (1.5 for terminal atoms) and allowed to ride, except for acidic protons which were located on the final difference Fourier map and refined freely.

1. R. Hooft, 'Collect', Nonius B.V., Delft, 1998.

2. Z. Otwinowski and W. Minor, in *Methods in Enzymology*, **276**, 1997, *pp* 307 - 326. C. W. Carter and R. M. Sweet (Eds.), Academic Press, New York.

3. G. M. Sheldrick, 'SHELXL-97', University of Göttingen, 1997.

4. L. J. Barbour, *J. Supramol. Chem.*, 2001, **1**, 189.

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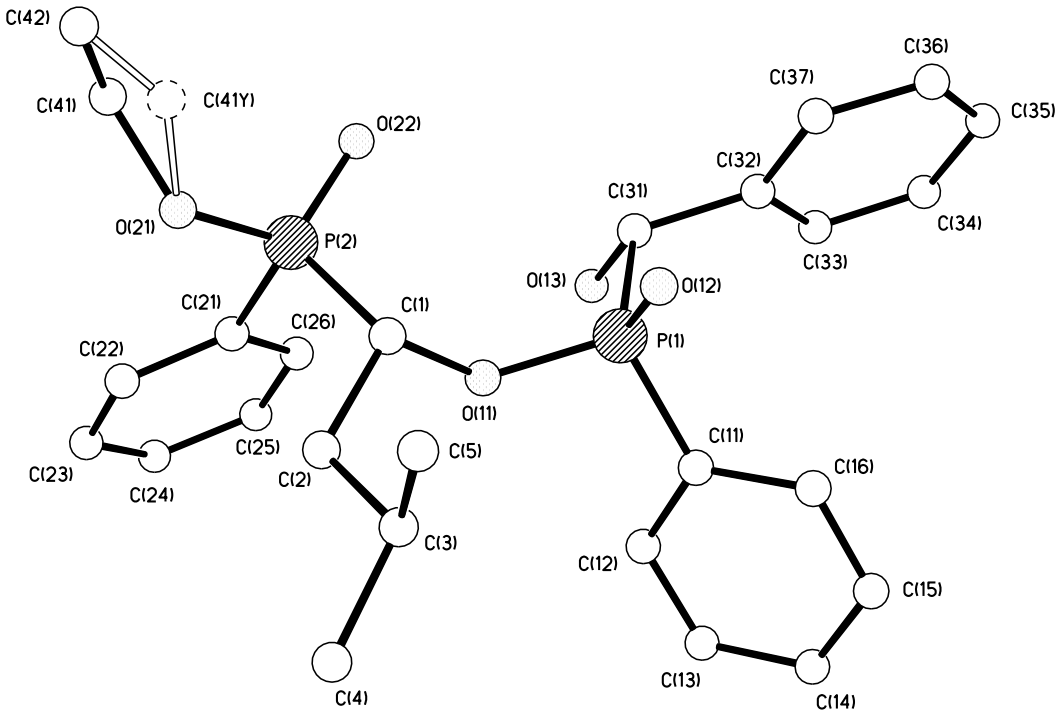

Table 1. Crystal data and structure refinement for MR_MR029d1_0m.

Identification code	mr_mr029d1_0m	
Empirical formula	C24 H36 O5 P2	
Formula weight	466.47	
Temperature	293(2) K	
Wavelength	0.71069 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.644(5) Å	α= 69.369(5)°.
	b = 12.688(5) Å	β= 88.488(5)°.
	c = 13.616(5) Å	γ = 73.101(5)°.
Volume	1332.4(11) Å^3	
Z	2	

Density (calculated)	1.163 Mg/m^3
Absorption coefficient	0.192 mm^{-1}
F(000)	500
Crystal size	0.465 x 0.225 x 0.156 mm^3
Theta range for data collection	2.58 to 28.22°.
Index ranges	-11<=h<=11, -16<=k<=16, -18<=l<=18
Reflections collected	69535
Independent reflections	6482 [R(int) = 0.0339]
Completeness to theta = 28.22°	98.6 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6482 / 0 / 322
Goodness-of-fit on F^2	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0423, wR2 = 0.1004
R indices (all data)	R1 = 0.0681, wR2 = 0.1151
Largest diff. peak and hole	0.247 and -0.272 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for MR_MR029d1_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	2364(1)	3569(1)	2922(1)	36(1)
P(2)	817(1)	2463(1)	979(1)	45(1)
O(11)	2802(1)	2746(1)	2229(1)	42(1)
O(12)	1458(1)	3140(1)	3833(1)	48(1)
O(13)	2234(2)	5293(1)	1126(1)	53(1)

O(21)	79(2)	1431(1)	1084(1)	72(1)
O(22)	-370(2)	3644(1)	753(1)	57(1)
C(1)	1929(2)	1915(1)	2267(1)	42(1)
C(2)	3136(2)	692(2)	2558(1)	54(1)
C(3)	3856(3)	127(2)	3706(2)	60(1)
C(4)	5294(4)	-964(2)	3833(2)	94(1)
C(5)	2598(4)	-170(3)	4461(2)	95(1)
C(11)	4330(2)	3616(1)	3255(1)	39(1)
C(12)	5609(2)	3461(2)	2637(2)	63(1)
C(13)	7122(2)	3459(2)	2956(2)	78(1)
C(14)	7367(3)	3603(2)	3879(2)	70(1)
C(15)	6107(3)	3789(2)	4480(2)	71(1)
C(16)	4581(2)	3799(2)	4171(2)	56(1)
C(21)	2244(2)	2427(2)	6(1)	48(1)
C(22)	2729(3)	1506(2)	-359(2)	83(1)
C(23)	3809(4)	1532(3)	-1126(3)	108(1)
C(24)	4407(3)	2463(3)	-1531(2)	91(1)
C(25)	3966(3)	3363(2)	-1167(2)	86(1)
C(26)	2875(3)	3357(2)	-403(2)	67(1)
C(31)	1262(2)	5034(1)	1985(1)	42(1)
C(32)	874(2)	5953(2)	2502(1)	43(1)
C(33)	1647(3)	6802(2)	2258(2)	72(1)
C(34)	1284(4)	7637(3)	2743(3)	99(1)
C(35)	178(3)	7622(2)	3469(2)	85(1)
C(36)	-567(3)	6783(2)	3723(2)	85(1)
C(37)	-247(3)	5959(2)	3237(2)	73(1)

C(41)	-1442(9)	1575(7)	592(5)	159(3)
C(41Y)	-1447(15)	1395(15)	1419(14)	158(6)
C(42)	-2464(6)	1090(7)	1157(7)	210(3)

Table 3. Bond lengths [Å] and angles [°] for MR_MR029d1_0m.

P(1)-O(12)	1.4729(12)	C(21)-C(26)	1.377(3)
P(1)-O(11)	1.6038(12)	C(21)-C(22)	1.380(3)
P(1)-C(11)	1.7939(18)	C(22)-C(23)	1.381(3)
P(1)-C(31)	1.8313(18)	C(23)-C(24)	1.359(4)
P(2)-O(22)	1.4793(15)	C(24)-C(25)	1.353(4)
P(2)-O(21)	1.5787(15)	C(25)-C(26)	1.385(3)
P(2)-C(21)	1.7898(19)	C(31)-C(32)	1.518(2)
P(2)-C(1)	1.8232(18)	C(32)-C(33)	1.369(3)
O(11)-C(1)	1.4498(19)	C(32)-C(37)	1.375(3)
O(13)-C(31)	1.421(2)	C(33)-C(34)	1.394(3)
O(21)-C(41Y)	1.393(10)	C(34)-C(35)	1.356(4)
O(21)-C(41)	1.425(5)	C(35)-C(36)	1.340(4)
C(1)-C(2)	1.517(2)	C(36)-C(37)	1.384(3)
C(2)-C(3)	1.532(3)	C(41)-C(42)	1.304(9)
C(3)-C(5)	1.512(3)	C(41Y)-C(42)	1.167(10)
C(3)-C(4)	1.527(3)	O(12)-P(1)-O(11)	114.09(7)
C(11)-C(16)	1.380(2)	O(12)-P(1)-C(11)	114.54(8)
C(11)-C(12)	1.382(2)	O(11)-P(1)-C(11)	101.67(7)
C(12)-C(13)	1.388(3)	O(12)-P(1)-C(31)	113.37(8)
C(13)-C(14)	1.363(3)	O(11)-P(1)-C(31)	104.64(8)
C(14)-C(15)	1.361(3)	C(11)-P(1)-C(31)	107.41(8)
C(15)-C(16)	1.390(3)	O(22)-P(2)-O(21)	115.89(9)

O(22)-P(2)-C(21)	113.26(8)	C(26)-C(21)-C(22)	118.53(19)
O(21)-P(2)-C(21)	105.18(9)	C(26)-C(21)-P(2)	118.96(14)
O(22)-P(2)-C(1)	111.66(8)	C(22)-C(21)-P(2)	122.51(16)
O(21)-P(2)-C(1)	101.22(8)	C(21)-C(22)-C(23)	120.2(2)
C(21)-P(2)-C(1)	108.71(9)	C(24)-C(23)-C(22)	120.6(2)
C(1)-O(11)-P(1)	121.91(10)	C(25)-C(24)-C(23)	119.9(2)
C(41Y)-O(21)-C(41)	44.5(6)	C(24)-C(25)-C(26)	120.4(2)
C(41Y)-O(21)-P(2)	124.7(5)	C(21)-C(26)-C(25)	120.4(2)
C(41)-O(21)-P(2)	125.1(3)	O(13)-C(31)-C(32)	112.99(14)
O(11)-C(1)-C(2)	108.79(14)	O(13)-C(31)-P(1)	106.80(11)
O(11)-C(1)-P(2)	106.26(10)	C(32)-C(31)-P(1)	111.41(12)
C(2)-C(1)-P(2)	114.20(12)	C(33)-C(32)-C(37)	117.43(18)
C(1)-C(2)-C(3)	114.85(15)	C(33)-C(32)-C(31)	120.90(16)
C(5)-C(3)-C(4)	111.5(2)	C(37)-C(32)-C(31)	121.66(17)
C(5)-C(3)-C(2)	111.89(19)	C(32)-C(33)-C(34)	120.3(2)
C(4)-C(3)-C(2)	109.33(17)	C(35)-C(34)-C(33)	121.2(2)
C(16)-C(11)-C(12)	118.77(16)	C(36)-C(35)-C(34)	118.9(2)
C(16)-C(11)-P(1)	118.70(13)	C(35)-C(36)-C(37)	120.8(2)
C(12)-C(11)-P(1)	122.52(14)	C(32)-C(37)-C(36)	121.3(2)
C(11)-C(12)-C(13)	120.0(2)	C(42)-C(41)-O(21)	119.2(5)
C(14)-C(13)-C(12)	120.7(2)	C(42)-C(41Y)-O(21)	133.5(11)
C(15)-C(14)-C(13)	119.86(19)	C(41Y)-C(42)-C(41)	50.8(7)
C(14)-C(15)-C(16)	120.3(2)		
C(11)-C(16)-C(15)	120.38(19)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for MR_MR029d1_0m. The anisotropic

displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	32(1)	40(1)	37(1)	-16(1)	3(1)	-10(1)
P(2)	43(1)	54(1)	41(1)	-17(1)	0(1)	-16(1)
O(11)	43(1)	45(1)	47(1)	-23(1)	9(1)	-17(1)
O(12)	45(1)	57(1)	47(1)	-20(1)	12(1)	-20(1)
O(13)	59(1)	57(1)	37(1)	-13(1)	1(1)	-12(1)
O(21)	65(1)	83(1)	82(1)	-31(1)	-1(1)	-41(1)
O(22)	47(1)	66(1)	45(1)	-17(1)	-1(1)	-3(1)
C(1)	46(1)	42(1)	41(1)	-16(1)	3(1)	-18(1)
C(2)	69(1)	43(1)	49(1)	-18(1)	-7(1)	-12(1)
C(3)	80(1)	45(1)	49(1)	-13(1)	-12(1)	-12(1)
C(4)	119(2)	60(1)	74(2)	-20(1)	-30(2)	12(1)
C(5)	122(2)	91(2)	61(2)	-6(1)	2(2)	-40(2)
C(11)	34(1)	38(1)	43(1)	-12(1)	-1(1)	-9(1)
C(12)	43(1)	87(2)	63(1)	-34(1)	11(1)	-20(1)
C(13)	40(1)	102(2)	93(2)	-34(2)	16(1)	-25(1)
C(14)	44(1)	69(1)	90(2)	-14(1)	-12(1)	-24(1)
C(15)	65(1)	83(2)	73(1)	-32(1)	-13(1)	-30(1)
C(16)	47(1)	71(1)	57(1)	-29(1)	1(1)	-21(1)
C(21)	49(1)	53(1)	41(1)	-20(1)	0(1)	-12(1)
C(22)	102(2)	89(2)	97(2)	-63(2)	40(2)	-49(2)
C(23)	122(2)	129(3)	129(3)	-101(2)	61(2)	-57(2)

C(24)	92(2)	118(2)	83(2)	-56(2)	43(2)	-41(2)
C(25)	91(2)	81(2)	89(2)	-31(1)	41(2)	-36(1)
C(26)	75(1)	57(1)	73(1)	-28(1)	26(1)	-20(1)
C(31)	36(1)	45(1)	44(1)	-17(1)	-2(1)	-9(1)
C(32)	36(1)	42(1)	46(1)	-16(1)	-4(1)	-3(1)
C(33)	68(1)	76(2)	98(2)	-52(1)	25(1)	-35(1)
C(34)	97(2)	94(2)	152(3)	-84(2)	26(2)	-47(2)
C(35)	83(2)	84(2)	102(2)	-65(2)	-2(2)	-4(1)
C(36)	91(2)	76(2)	86(2)	-44(1)	31(1)	-6(1)
C(37)	73(1)	58(1)	92(2)	-35(1)	34(1)	-18(1)
C(41)	190(6)	175(6)	112(4)	17(4)	-69(5)	-133(5)
C(41Y)	130(9)	241(15)	222(14)	-169(14)	78(10)	-126(10)
C(42)	116(4)	277(7)	325(9)	-158(7)	39(5)	-126(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for MR_MR029d1_0m.

	x	y	z	U(eq)
H(1)	1155	1911	2806	50
H(2A)	4017	739	2104	65
H(2B)	2601	178	2418	65
H(3)	4262	697	3868	73
H(4A)	5760	-1311	4549	141
H(4B)	6095	-740	3371	141

H(4C)	4930	-1528	3658	141
H(5A)	1755	542	4402	143
H(5B)	3100	-544	5168	143
H(5C)	2140	-696	4292	143
H(12)	5456	3357	2008	75
H(13A)	7977	3359	2535	94
H(14)	8394	3575	4097	84
H(15)	6267	3910	5100	85
H(16)	3724	3931	4584	67
H(22)	2326	864	-87	100
H(23)	4131	908	-1368	130
H(24)	5117	2482	-2058	109
H(25)	4399	3989	-1430	103
H(26)	2566	3986	-165	80
H(31)	240	4997	1725	50
H(33)	2418	6823	1768	87
H(34)	1810	8215	2564	119
H(35)	-59	8185	3785	102
H(36)	-1309	6754	4231	102
H(37)	-801	5399	3411	88
H(41A)	-1987	2416	273	190
H(41B)	-1219	1273	23	190
H(41C)	-1232	942	2169	190
H(41D)	-1997	2201	1363	190
H(42A)	-1400(90)	240(70)	1180(70)	315

H(42B)	-3350(90)	1130(70)	940(70)	315
H(42C)	-2130(100)	950(70)	2160(60)	315
H(13)	1650(30)	5550(20)	560(20)	83(8)

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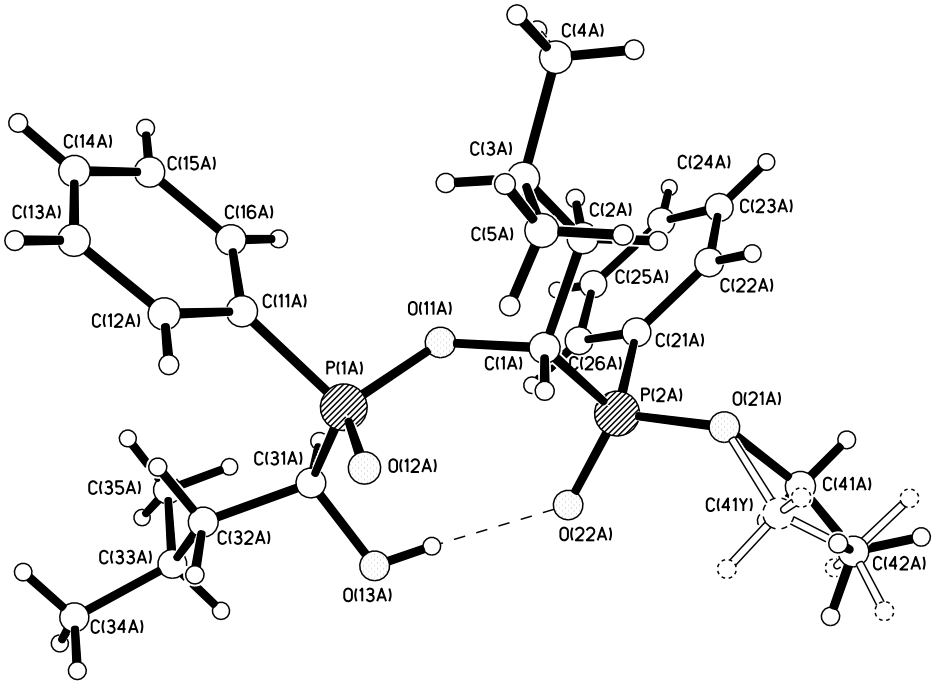

Table 1. Crystal data and structure refinement for MR029.

Identification code	mr_mr029d2_0m
Empirical formula	C24 H36 O5 P2
Formula weight	466.47
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic

Space group	P2(1)/n
Unit cell dimensions	a = 24.1936(6) Å □= 90°.
	b = 9.7612(2) Å □= 114.9020(10)°.
	c = 24.6066(6) Å □ = 90°.
Volume	5270.8(2) $Å^3$
Z	8
Density (calculated)	1.176 Mg/m^3
Absorption coefficient	0.194 mm^{-1}
F(000)	2000
Crystal size	0.48 x 0.29 x 0.19 mm^3
Theta range for data collection	0.99 to 27.50°.
Index ranges	-31<=h<=31, -8<=k<=12, -31<=l<=31
Reflections collected	83462
Independent reflections	12029 [R(int) = 0.0448]
Completeness to theta = 27.50°	99.3 %
Max. and min. transmission	0.9631 and 0.9121
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12029 / 0 / 579
Goodness-of-fit on F^2	1.100
Final R indices [I>2sigma(I)]	R1 = 0.0514, wR2 = 0.1416
R indices (all data)	R1 = 0.0941, wR2 = 0.1573
Largest diff. peak and hole	0.384 and -0.294 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)

for MR029. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1A)	8507(1)	1710(1)	5132(1)	47(1)
P(2A)	7552(1)	2047(1)	3448(1)	54(1)
O(11A)	8428(1)	1285(1)	4472(1)	48(1)
O(12A)	7987(1)	1355(2)	5262(1)	71(1)
O(13A)	8141(1)	4297(2)	4859(1)	94(1)
O(21A)	6919(1)	1388(2)	3044(1)	76(1)
O(22A)	7533(1)	3400(2)	3703(1)	73(1)
C(1A)	7864(1)	724(2)	4024(1)	47(1)
C(2A)	7992(1)	-637(2)	3807(1)	52(1)
C(3A)	8205(1)	-1772(2)	4280(1)	61(1)
C(4A)	8430(1)	-2999(2)	4045(1)	83(1)
C(5A)	7714(2)	-2182(3)	4478(1)	95(1)
C(11A)	9203(1)	897(2)	5616(1)	54(1)
C(12A)	9270(2)	360(3)	6158(1)	83(1)
C(13A)	9844(2)	-170(3)	6565(1)	108(1)
C(14A)	10315(2)	-154(4)	6397(2)	126(2)
C(15A)	10259(2)	361(4)	5875(2)	119(1)
C(16A)	9706(1)	890(3)	5482(1)	81(1)

C(21A)	7973(1)	2095(2)	3001(1)	50(1)
C(22A)	7876(1)	1155(2)	2543(1)	59(1)
C(23A)	8208(1)	1230(3)	2204(1)	74(1)
C(24A)	8632(1)	2234(3)	2317(1)	83(1)
C(25A)	8742(1)	3154(3)	2766(1)	81(1)
C(26A)	8412(1)	3102(2)	3108(1)	67(1)
C(31A)	8678(1)	3530(2)	5158(1)	56(1)
C(32A)	8994(1)	4084(2)	5794(1)	60(1)
C(33A)	9248(1)	5526(2)	5843(1)	71(1)
C(34A)	9438(2)	6067(3)	6475(1)	96(1)
C(35A)	9771(2)	5610(4)	5670(2)	141(2)
C(41A)	6472(2)	2166(5)	2564(2)	94(2)
C(41Y)	6325(4)	1688(10)	2954(4)	86(2)
C(42A)	5935(2)	2156(6)	2502(3)	229(3)
P(1B)	4818(1)	1675(1)	6458(1)	46(1)
P(2B)	6518(1)	2105(1)	7462(1)	50(1)
O(11B)	5509(1)	1307(1)	6579(1)	46(1)
O(12B)	4636(1)	1199(2)	6925(1)	63(1)
O(13B)	5054(1)	4219(2)	6898(1)	80(1)
O(21B)	6929(1)	1449(2)	8087(1)	66(1)
O(22B)	6250(1)	3442(2)	7489(1)	68(1)
C(1B)	5945(1)	762(2)	7149(1)	47(1)
C(2B)	6179(1)	-610(2)	7044(1)	53(1)
C(3B)	5706(1)	-1758(2)	6845(1)	62(1)
C(4B)	5513(2)	-2161(3)	7333(2)	99(1)

C(5B)	5953(1)	-3000(2)	6639(1)	83(1)
C(11B)	4383(1)	941(2)	5733(1)	50(1)
C(12B)	4557(1)	1103(3)	5270(1)	70(1)
C(13B)	4202(1)	604(3)	4706(1)	89(1)
C(14B)	3671(1)	-50(3)	4599(1)	91(1)
C(15B)	3483(1)	-224(3)	5046(2)	84(1)
C(16B)	3844(1)	273(2)	5620(1)	67(1)
C(21B)	6967(1)	2182(2)	7045(1)	50(1)
C(22B)	6839(1)	3179(3)	6605(1)	70(1)
C(23B)	7171(2)	3198(3)	6262(1)	95(1)
C(24B)	7624(2)	2258(4)	6361(2)	94(1)
C(25B)	7759(1)	1298(3)	6796(1)	83(1)
C(26B)	7433(1)	1248(2)	7134(1)	63(1)
C(31B)	4786(1)	3523(2)	6341(1)	55(1)
C(32B)	4140(1)	4050(2)	6006(1)	63(1)
C(33B)	4085(1)	5522(3)	5780(1)	80(1)
C(34B)	4315(2)	5710(4)	5312(2)	147(2)
C(35B)	3418(2)	5961(3)	5537(2)	112(1)
C(41B)	7415(2)	2220(4)	8544(1)	108(1)
C(42B)	7415(3)	2170(6)	9080(2)	196(3)

Table 3. Bond lengths [Å] and angles [°] for MR029.

P(1A)-O(12A)	1.4645(16)	P(1A)-C(31A)	1.819(2)
P(1A)-O(11A)	1.6090(14)	P(2A)-O(22A)	1.4713(16)
P(1A)-C(11A)	1.789(2)	P(2A)-O(21A)	1.5699(17)

P(2A)-C(21A)	1.788(2)	C(13A)-C(14A)	1.367(5)
P(2A)-C(1A)	1.828(2)	C(13A)-H(13A)	0.9300
O(11A)-C(1A)	1.453(2)	C(14A)-C(15A)	1.330(6)
O(13A)-C(31A)	1.409(3)	C(14A)-H(14A)	0.9300
O(13A)-H(13B)	0.8200	C(15A)-C(16A)	1.380(4)
O(21A)-C(41Y)	1.390(8)	C(15A)-H(15A)	0.9300
O(21A)-C(41A)	1.437(4)	C(16A)-H(16A)	0.9300
C(1A)-C(2A)	1.512(3)	C(21A)-C(26A)	1.388(3)
C(1A)-H(1A)	0.9800	C(21A)-C(22A)	1.395(3)
C(2A)-C(3A)	1.532(3)	C(22A)-C(23A)	1.381(3)
C(2A)-H(2A1)	0.9700	C(22A)-H(22A)	0.9300
C(2A)-H(2A2)	0.9700	C(23A)-C(24A)	1.359(4)
C(3A)-C(5A)	1.516(4)	C(23A)-H(23A)	0.9300
C(3A)-C(4A)	1.528(3)	C(24A)-C(25A)	1.361(4)
C(3A)-H(3A)	0.9800	C(24A)-H(24A)	0.9300
C(4A)-H(4A1)	0.9600	C(25A)-C(26A)	1.383(4)
C(4A)-H(4A2)	0.9600	C(25A)-H(25A)	0.9300
C(4A)-H(4A3)	0.9600	C(26A)-H(26A)	0.9300
C(5A)-H(5A1)	0.9600	C(31A)-C(32A)	1.521(3)
C(5A)-H(5A2)	0.9600	C(31A)-H(31A)	0.9800
C(5A)-H(5A3)	0.9600	C(32A)-C(33A)	1.520(3)
C(11A)-C(12A)	1.377(3)	C(32A)-H(32A)	0.9700
C(11A)-C(16A)	1.387(3)	C(32A)-H(32B)	0.9700
C(12A)-C(13A)	1.426(4)	C(33A)-C(35A)	1.498(4)
C(12A)-H(12A)	0.9300	C(33A)-C(34A)	1.517(3)

C(33A)-H(33A)	0.9800	P(1B)-C(31B)	1.823(2)
C(34A)-H(34A)	0.9600	P(2B)-O(22B)	1.4718(16)
C(34A)-H(34B)	0.9600	P(2B)-O(21B)	1.5726(15)
C(34A)-H(34C)	0.9600	P(2B)-C(21B)	1.782(2)
C(35A)-H(35D)	0.9600	P(2B)-C(1B)	1.827(2)
C(35A)-H(35E)	0.9600	O(11B)-C(1B)	1.455(2)
C(35A)-H(35F)	0.9600	O(13B)-C(31B)	1.419(3)
C(41A)-C(42A)	1.243(6)	O(13B)-H(13C)	0.8200
C(41A)-H(411)	0.9700	O(21B)-C(41B)	1.449(3)
C(41A)-H(412)	0.9700	C(1B)-C(2B)	1.519(3)
C(41A)-H(425)	1.503(4)	C(1B)-H(1B)	0.9800
C(41A)-H(426)	1.206(5)	C(2B)-C(3B)	1.528(3)
C(41Y)-C(42A)	1.205(10)	C(2B)-H(2B1)	0.9700
C(41Y)-H(421)	0.935(8)	C(2B)-H(2B2)	0.9700
C(41Y)-H(413)	0.9700	C(3B)-C(4B)	1.511(4)
C(41Y)-H(414)	0.9700	C(3B)-C(5B)	1.530(3)
C(42A)-H(421)	0.999(7)	C(3B)-H(3B)	0.9800
C(42A)-H(422)	0.909(8)	C(4B)-H(4B1)	0.9600
C(42A)-H(423)	0.938(7)	C(4B)-H(4B2)	0.9600
C(42A)-H(424)	0.944(6)	C(4B)-H(4B3)	0.9600
C(42A)-H(425)	1.003(8)	C(5B)-H(5B1)	0.9600
C(42A)-H(426)	0.973(6)	C(5B)-H(5B2)	0.9600
P(1B)-O(12B)	1.4679(15)	C(5B)-H(5B3)	0.9600
P(1B)-O(11B)	1.6097(14)	C(11B)-C(16B)	1.376(3)
P(1B)-C(11B)	1.795(2)	C(11B)-C(12B)	1.381(3)

C(12B)-C(13B)	1.378(3)	C(33B)-C(34B)	1.487(4)
C(12B)-H(12B)	0.9300	C(33B)-C(35B)	1.528(4)
C(13B)-C(14B)	1.357(4)	C(33B)-H(33B)	0.9800
C(13B)-H(13D)	0.9300	C(34B)-H(34D)	0.9600
C(14B)-C(15B)	1.368(4)	C(34B)-H(34E)	0.9600
C(14B)-H(14B)	0.9300	C(34B)-H(34F)	0.9600
C(15B)-C(16B)	1.398(4)	C(35B)-H(35A)	0.9600
C(15B)-H(15B)	0.9300	C(35B)-H(35B)	0.9600
C(16B)-H(16B)	0.9300	C(35B)-H(35C)	0.9600
C(21B)-C(22B)	1.390(3)	C(41B)-C(42B)	1.319(4)
C(21B)-C(26B)	1.395(3)	C(41B)-H(41A)	0.9700
C(22B)-C(23B)	1.390(4)	C(41B)-H(41B)	0.9700
C(22B)-H(22B)	0.9300	C(42B)-H(42A)	0.9600
C(23B)-C(24B)	1.370(5)	C(42B)-H(42B)	0.9600
C(23B)-H(23B)	0.9300	C(42B)-H(42C)	0.9600
C(24B)-C(25B)	1.354(4)	O(12A)-P(1A)-O(11A)	114.38(9)
C(24B)-H(24B)	0.9300	O(12A)-P(1A)-C(11A)	113.87(11)
C(25B)-C(26B)	1.365(3)	O(11A)-P(1A)-C(11A)	103.62(9)
C(25B)-H(25B)	0.9300	O(12A)-P(1A)-C(31A)	115.31(11)
C(26B)-H(26B)	0.9300	O(11A)-P(1A)-C(31A)	102.47(9)
C(31B)-C(32B)	1.516(3)	C(11A)-P(1A)-C(31A)	105.84(10)
C(31B)-H(31B)	0.9800	O(22A)-P(2A)-O(21A)	116.17(10)
C(32B)-C(33B)	1.527(3)	O(22A)-P(2A)-C(21A)	111.51(10)
C(32B)-H(32C)	0.9700	O(21A)-P(2A)-C(21A)	106.07(10)
C(32B)-H(32D)	0.9700	O(22A)-P(2A)-C(1A)	112.35(9)

O(21A)-P(2A)-C(1A)	100.15(9)	C(3A)-C(4A)-H(4A1)	109.5
C(21A)-P(2A)-C(1A)	109.86(10)	C(3A)-C(4A)-H(4A2)	109.5
C(1A)-O(11A)-P(1A)	122.41(12)	H(4A1)-C(4A)-H(4A2)	109.5
C(31A)-O(13A)-H(13B)	109.5	C(3A)-C(4A)-H(4A3)	109.5
C(41Y)-O(21A)-C(41A)	52.3(4)	H(4A1)-C(4A)-H(4A3)	109.5
C(41Y)-O(21A)-P(2A)	133.0(4)	H(4A2)-C(4A)-H(4A3)	109.5
C(41A)-O(21A)-P(2A)	120.0(2)	C(3A)-C(5A)-H(5A1)	109.5
O(11A)-C(1A)-C(2A)	109.35(16)	C(3A)-C(5A)-H(5A2)	109.5
O(11A)-C(1A)-P(2A)	105.72(12)	H(5A1)-C(5A)-H(5A2)	109.5
C(2A)-C(1A)-P(2A)	115.16(14)	C(3A)-C(5A)-H(5A3)	109.5
O(11A)-C(1A)-H(1A)	108.8	H(5A1)-C(5A)-H(5A3)	109.5
C(2A)-C(1A)-H(1A)	108.8	H(5A2)-C(5A)-H(5A3)	109.5
P(2A)-C(1A)-H(1A)	108.8	C(12A)-C(11A)-C(16A)	118.1(2)
C(1A)-C(2A)-C(3A)	114.81(17)	C(12A)-C(11A)-P(1A)	120.5(2)
C(1A)-C(2A)-H(2A1)	108.6	C(16A)-C(11A)-P(1A)	121.21(18)
C(3A)-C(2A)-H(2A1)	108.6	C(11A)-C(12A)-C(13A)	120.1(3)
C(1A)-C(2A)-H(2A2)	108.6	C(11A)-C(12A)-H(12A)	120.0
C(3A)-C(2A)-H(2A2)	108.6	C(13A)-C(12A)-H(12A)	120.0
H(2A1)-C(2A)-H(2A2)	107.5	C(14A)-C(13A)-C(12A)	118.2(3)
C(5A)-C(3A)-C(4A)	111.6(2)	C(14A)-C(13A)-H(13A)	120.9
C(5A)-C(3A)-C(2A)	112.2(2)	C(12A)-C(13A)-H(13A)	120.9
C(4A)-C(3A)-C(2A)	109.77(19)	C(15A)-C(14A)-C(13A)	122.5(4)
C(5A)-C(3A)-H(3A)	107.7	C(15A)-C(14A)-H(14A)	118.7
C(4A)-C(3A)-H(3A)	107.7	C(13A)-C(14A)-H(14A)	118.7
C(2A)-C(3A)-H(3A)	107.7	C(14A)-C(15A)-C(16A)	119.5(4)

C(14A)-C(15A)-H(15A)	120.3	C(32A)-C(31A)-P(1A)	113.06(15)
C(16A)-C(15A)-H(15A)	120.3	O(13A)-C(31A)-H(31A)	108.4
C(15A)-C(16A)-C(11A)	121.6(3)	C(32A)-C(31A)-H(31A)	108.4
C(15A)-C(16A)-H(16A)	119.2	P(1A)-C(31A)-H(31A)	108.4
C(11A)-C(16A)-H(16A)	119.2	C(31A)-C(32A)-C(33A)	115.02(19)
C(26A)-C(21A)-C(22A)	118.3(2)	C(31A)-C(32A)-H(32A)	108.5
C(26A)-C(21A)-P(2A)	119.31(18)	C(33A)-C(32A)-H(32A)	108.5
C(22A)-C(21A)-P(2A)	122.39(17)	C(31A)-C(32A)-H(32B)	108.5
C(23A)-C(22A)-C(21A)	120.7(2)	C(33A)-C(32A)-H(32B)	108.5
C(23A)-C(22A)-H(22A)	119.6	H(32A)-C(32A)-H(32B)	107.5
C(21A)-C(22A)-H(22A)	119.6	C(35A)-C(33A)-C(34A)	110.2(2)
C(24A)-C(23A)-C(22A)	119.6(3)	C(35A)-C(33A)-C(32A)	112.9(2)
C(24A)-C(23A)-H(23A)	120.2	C(34A)-C(33A)-C(32A)	110.0(2)
C(22A)-C(23A)-H(23A)	120.2	C(35A)-C(33A)-H(33A)	107.9
C(23A)-C(24A)-C(25A)	121.0(3)	C(34A)-C(33A)-H(33A)	107.9
C(23A)-C(24A)-H(24A)	119.5	C(32A)-C(33A)-H(33A)	107.9
C(25A)-C(24A)-H(24A)	119.5	C(33A)-C(34A)-H(34A)	109.5
C(24A)-C(25A)-C(26A)	120.3(3)	C(33A)-C(34A)-H(34B)	109.5
C(24A)-C(25A)-H(25A)	119.8	H(34A)-C(34A)-H(34B)	109.5
C(26A)-C(25A)-H(25A)	119.8	C(33A)-C(34A)-H(34C)	109.5
C(25A)-C(26A)-C(21A)	120.1(2)	H(34A)-C(34A)-H(34C)	109.5
C(25A)-C(26A)-H(26A)	120.0	H(34B)-C(34A)-H(34C)	109.5
C(21A)-C(26A)-H(26A)	120.0	C(33A)-C(35A)-H(35D)	109.5
O(13A)-C(31A)-C(32A)	107.59(18)	C(33A)-C(35A)-H(35E)	109.5
O(13A)-C(31A)-P(1A)	110.73(16)	H(35D)-C(35A)-H(35E)	109.5

C(33A)-C(35A)-H(35F)	109.5	O(21A)-C(41Y)-H(414)	105.9
H(35D)-C(35A)-H(35F)	109.5	H(421)-C(41Y)-H(414)	102.3
H(35E)-C(35A)-H(35F)	109.5	H(413)-C(41Y)-H(414)	106.2
C(42A)-C(41A)-O(21A)	118.8(5)	C(41Y)-C(42A)-C(41A)	61.2(5)
C(42A)-C(41A)-H(411)	107.6	C(41Y)-C(42A)-H(421)	49.1(5)
O(21A)-C(41A)-H(411)	107.6	C(41A)-C(42A)-H(421)	106.6(5)
C(42A)-C(41A)-H(412)	107.6	C(41Y)-C(42A)-H(422)	139.3(8)
O(21A)-C(41A)-H(412)	107.6	C(41A)-C(42A)-H(422)	107.0(8)
H(411)-C(41A)-H(412)	107.0	H(421)-C(42A)-H(422)	110.5(6)
C(42A)-C(41A)-H(425)	41.5(4)	C(41Y)-C(42A)-H(423)	104.3(8)
O(21A)-C(41A)-H(425)	120.7(3)	C(41A)-C(42A)-H(423)	108.1(6)
H(411)-C(41A)-H(425)	130.9	H(421)-C(42A)-H(423)	108.0(8)
H(412)-C(41A)-H(425)	67.9	H(422)-C(42A)-H(423)	116.2(5)
C(42A)-C(41A)-H(426)	46.8(3)	C(41Y)-C(42A)-H(424)	115.3(9)
O(21A)-C(41A)-H(426)	148.5(5)	C(41A)-C(42A)-H(424)	169.4(9)
H(411)-C(41A)-H(426)	64.2	H(421)-C(42A)-H(424)	74.2(5)
H(412)-C(41A)-H(426)	103.8	H(422)-C(42A)-H(424)	82.2(4)
H(425)-C(41A)-H(426)	69.8(2)	H(423)-C(42A)-H(424)	62.2(4)
C(42A)-C(41Y)-O(21A)	125.6(8)	C(41Y)-C(42A)-H(425)	109.3(6)
C(42A)-C(41Y)-H(421)	53.9(5)	C(41A)-C(42A)-H(425)	83.2(6)
O(21A)-C(41Y)-H(421)	149.8(9)	H(421)-C(42A)-H(425)	98.7(5)
C(42A)-C(41Y)-H(413)	105.9	H(422)-C(42A)-H(425)	31.6(3)
O(21A)-C(41Y)-H(413)	105.9	H(423)-C(42A)-H(425)	145.8(7)
H(421)-C(41Y)-H(413)	55.0	H(424)-C(42A)-H(425)	107.2(6)
C(42A)-C(41Y)-H(414)	105.9	C(41Y)-C(42A)-H(426)	109.7(7)

C(41A)-C(42A)-H(426)	64.6(4)	C(2B)-C(1B)-H(1B)	109.0
H(421)-C(42A)-H(426)	153.1(9)	P(2B)-C(1B)-H(1B)	109.0
H(422)-C(42A)-H(426)	96.4(7)	C(1B)-C(2B)-C(3B)	114.68(18)
H(423)-C(42A)-H(426)	56.3(3)	C(1B)-C(2B)-H(2B1)	108.6
H(424)-C(42A)-H(426)	109.7(5)	C(3B)-C(2B)-H(2B1)	108.6
H(425)-C(42A)-H(426)	105.0(7)	C(1B)-C(2B)-H(2B2)	108.6
O(12B)-P(1B)-O(11B)	114.43(8)	C(3B)-C(2B)-H(2B2)	108.6
O(12B)-P(1B)-C(11B)	114.04(10)	H(2B1)-C(2B)-H(2B2)	107.6
O(11B)-P(1B)-C(11B)	102.99(8)	C(4B)-C(3B)-C(5B)	110.6(2)
O(12B)-P(1B)-C(31B)	115.45(10)	C(4B)-C(3B)-C(2B)	112.2(2)
O(11B)-P(1B)-C(31B)	102.83(9)	C(5B)-C(3B)-C(2B)	110.0(2)
C(11B)-P(1B)-C(31B)	105.68(10)	C(4B)-C(3B)-H(3B)	108.0
O(22B)-P(2B)-O(21B)	115.28(9)	C(5B)-C(3B)-H(3B)	108.0
O(22B)-P(2B)-C(21B)	112.06(10)	C(2B)-C(3B)-H(3B)	108.0
O(21B)-P(2B)-C(21B)	106.96(10)	C(3B)-C(4B)-H(4B1)	109.5
O(22B)-P(2B)-C(1B)	112.60(9)	C(3B)-C(4B)-H(4B2)	109.5
O(21B)-P(2B)-C(1B)	100.10(9)	H(4B1)-C(4B)-H(4B2)	109.5
C(21B)-P(2B)-C(1B)	109.03(9)	C(3B)-C(4B)-H(4B3)	109.5
C(1B)-O(11B)-P(1B)	122.34(12)	H(4B1)-C(4B)-H(4B3)	109.5
C(31B)-O(13B)-H(13C)	109.5	H(4B2)-C(4B)-H(4B3)	109.5
C(41B)-O(21B)-P(2B)	121.34(17)	C(3B)-C(5B)-H(5B1)	109.5
O(11B)-C(1B)-C(2B)	109.21(16)	C(3B)-C(5B)-H(5B2)	109.5
O(11B)-C(1B)-P(2B)	104.89(12)	H(5B1)-C(5B)-H(5B2)	109.5
C(2B)-C(1B)-P(2B)	115.64(14)	C(3B)-C(5B)-H(5B3)	109.5
O(11B)-C(1B)-H(1B)	109.0	H(5B1)-C(5B)-H(5B3)	109.5

H(5B2)-C(5B)-H(5B3)	109.5	C(24B)-C(23B)-C(22B)	120.3(3)
C(16B)-C(11B)-C(12B)	118.7(2)	C(24B)-C(23B)-H(23B)	119.8
C(16B)-C(11B)-P(1B)	119.93(19)	C(22B)-C(23B)-H(23B)	119.8
C(12B)-C(11B)-P(1B)	121.24(17)	C(25B)-C(24B)-C(23B)	120.9(3)
C(13B)-C(12B)-C(11B)	120.8(2)	C(25B)-C(24B)-H(24B)	119.5
C(13B)-C(12B)-H(12B)	119.6	C(23B)-C(24B)-H(24B)	119.5
C(11B)-C(12B)-H(12B)	119.6	C(24B)-C(25B)-C(26B)	119.7(3)
C(14B)-C(13B)-C(12B)	120.0(3)	C(24B)-C(25B)-H(25B)	120.1
C(14B)-C(13B)-H(13D)	120.0	C(26B)-C(25B)-H(25B)	120.1
C(12B)-C(13B)-H(13D)	120.0	C(25B)-C(26B)-C(21B)	121.2(3)
C(13B)-C(14B)-C(15B)	120.7(3)	C(25B)-C(26B)-H(26B)	119.4
C(13B)-C(14B)-H(14B)	119.7	C(21B)-C(26B)-H(26B)	119.4
C(15B)-C(14B)-H(14B)	119.7	O(13B)-C(31B)-C(32B)	107.99(18)
C(14B)-C(15B)-C(16B)	119.5(3)	O(13B)-C(31B)-P(1B)	110.46(15)
C(14B)-C(15B)-H(15B)	120.2	C(32B)-C(31B)-P(1B)	112.79(15)
C(16B)-C(15B)-H(15B)	120.2	O(13B)-C(31B)-H(31B)	108.5
C(11B)-C(16B)-C(15B)	120.2(3)	C(32B)-C(31B)-H(31B)	108.5
C(11B)-C(16B)-H(16B)	119.9	P(1B)-C(31B)-H(31B)	108.5
C(15B)-C(16B)-H(16B)	119.9	C(31B)-C(32B)-C(33B)	115.4(2)
C(22B)-C(21B)-C(26B)	118.7(2)	C(31B)-C(32B)-H(32C)	108.4
C(22B)-C(21B)-P(2B)	119.22(18)	C(33B)-C(32B)-H(32C)	108.4
C(26B)-C(21B)-P(2B)	122.11(17)	C(31B)-C(32B)-H(32D)	108.4
C(21B)-C(22B)-C(23B)	119.1(3)	C(33B)-C(32B)-H(32D)	108.4
C(21B)-C(22B)-H(22B)	120.4	H(32C)-C(32B)-H(32D)	107.5
C(23B)-C(22B)-H(22B)	120.4	C(34B)-C(33B)-C(32B)	113.3(3)

C(34B)-C(33B)-C(35B)	109.9(3)	H(35A)-C(35B)-H(35C)	109.5
C(32B)-C(33B)-C(35B)	108.8(2)	H(35B)-C(35B)-H(35C)	109.5
C(34B)-C(33B)-H(33B)	108.2	C(42B)-C(41B)-O(21B)	114.6(3)
C(32B)-C(33B)-H(33B)	108.2	C(42B)-C(41B)-H(41A)	108.6
C(35B)-C(33B)-H(33B)	108.2	O(21B)-C(41B)-H(41A)	108.6
C(33B)-C(34B)-H(34D)	109.5	C(42B)-C(41B)-H(41B)	108.6
C(33B)-C(34B)-H(34E)	109.5	O(21B)-C(41B)-H(41B)	108.6
H(34D)-C(34B)-H(34E)	109.5	H(41A)-C(41B)-H(41B)	107.6
C(33B)-C(34B)-H(34F)	109.5	C(41B)-C(42B)-H(42A)	109.5
H(34D)-C(34B)-H(34F)	109.5	C(41B)-C(42B)-H(42B)	109.5
H(34E)-C(34B)-H(34F)	109.5	H(42A)-C(42B)-H(42B)	109.5
C(33B)-C(35B)-H(35A)	109.5	C(41B)-C(42B)-H(42C)	109.5
C(33B)-C(35B)-H(35B)	109.5	H(42A)-C(42B)-H(42C)	109.5
H(35A)-C(35B)-H(35B)	109.5	H(42B)-C(42B)-H(42C)	109.5
C(33B)-C(35B)-H(35C)	109.5		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for MR029. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1A)	45(1)	51(1)	45(1)	-5(1)	19(1)	0(1)
P(2A)	46(1)	58(1)	49(1)	3(1)	11(1)	8(1)

O(11A)	41(1)	57(1)	41(1)	-3(1)	15(1)	-2(1)
O(12A)	61(1)	95(1)	71(1)	-20(1)	40(1)	-19(1)
O(13A)	93(1)	62(1)	83(1)	-13(1)	-6(1)	29(1)
O(21A)	42(1)	93(1)	76(1)	4(1)	7(1)	3(1)
O(22A)	80(1)	64(1)	62(1)	1(1)	18(1)	25(1)
C(1A)	42(1)	56(1)	40(1)	-2(1)	13(1)	-4(1)
C(2A)	58(1)	51(1)	42(1)	-1(1)	16(1)	-2(1)
C(3A)	76(2)	54(1)	45(1)	3(1)	19(1)	3(1)
C(4A)	111(2)	58(2)	76(2)	4(1)	36(2)	12(1)
C(5A)	131(3)	78(2)	92(2)	21(2)	63(2)	3(2)
C(11A)	63(2)	47(1)	43(1)	-2(1)	12(1)	4(1)
C(12A)	122(2)	62(2)	56(1)	7(1)	27(2)	5(2)
C(13A)	161(4)	65(2)	54(2)	9(1)	3(2)	13(2)
C(14A)	132(4)	95(3)	87(3)	-14(2)	-16(3)	36(2)
C(15A)	65(2)	139(3)	115(3)	-29(2)	-1(2)	27(2)
C(16A)	52(2)	102(2)	71(2)	-4(1)	9(1)	16(1)
C(21A)	46(1)	48(1)	44(1)	9(1)	8(1)	1(1)
C(22A)	61(1)	61(1)	48(1)	4(1)	15(1)	-5(1)
C(23A)	80(2)	86(2)	56(1)	2(1)	30(1)	2(2)
C(24A)	84(2)	99(2)	76(2)	20(2)	44(2)	7(2)
C(25A)	65(2)	74(2)	102(2)	19(2)	34(2)	-12(1)
C(26A)	61(2)	56(1)	71(2)	1(1)	14(1)	-4(1)
C(31A)	59(1)	50(1)	51(1)	-2(1)	14(1)	2(1)
C(32A)	69(2)	57(1)	51(1)	-8(1)	22(1)	-3(1)
C(33A)	85(2)	66(2)	61(1)	-11(1)	28(1)	-18(1)

C(34A)	125(3)	89(2)	75(2)	-32(2)	44(2)	-31(2)
C(35A)	148(4)	182(4)	128(3)	-78(3)	92(3)	-98(3)
C(41A)	48(3)	128(4)	81(3)	35(3)	4(2)	-3(2)
C(41Y)	54(5)	125(7)	88(6)	-8(5)	38(5)	-17(5)
C(42A)	74(3)	186(5)	340(9)	80(5)	1(4)	30(3)
P(1B)	41(1)	50(1)	46(1)	0(1)	18(1)	3(1)
P(2B)	45(1)	56(1)	44(1)	-6(1)	13(1)	-4(1)
O(11B)	38(1)	57(1)	40(1)	1(1)	14(1)	4(1)
O(12B)	60(1)	79(1)	60(1)	11(1)	34(1)	8(1)
O(13B)	72(1)	64(1)	83(1)	-23(1)	13(1)	13(1)
O(21B)	59(1)	81(1)	43(1)	0(1)	8(1)	-13(1)
O(22B)	57(1)	62(1)	76(1)	-22(1)	21(1)	-4(1)
C(1B)	39(1)	55(1)	41(1)	2(1)	12(1)	0(1)
C(2B)	44(1)	51(1)	57(1)	1(1)	15(1)	1(1)
C(3B)	44(1)	51(1)	81(2)	-3(1)	17(1)	-4(1)
C(4B)	106(2)	76(2)	140(3)	-4(2)	75(2)	-22(2)
C(5B)	75(2)	57(1)	105(2)	-10(1)	27(2)	3(1)
C(11B)	40(1)	50(1)	54(1)	-2(1)	14(1)	4(1)
C(12B)	53(2)	96(2)	55(1)	-13(1)	18(1)	-7(1)
C(13B)	76(2)	121(2)	57(2)	-19(2)	17(2)	4(2)
C(14B)	74(2)	96(2)	73(2)	-22(2)	2(2)	4(2)
C(15B)	48(2)	69(2)	102(2)	-11(2)	-1(2)	-12(1)
C(16B)	50(1)	66(1)	78(2)	1(1)	19(1)	-5(1)
C(21B)	45(1)	54(1)	45(1)	-6(1)	15(1)	-10(1)
C(22B)	78(2)	69(2)	61(1)	2(1)	28(1)	-9(1)

C(23B)	124(3)	100(2)	66(2)	1(2)	46(2)	-36(2)
C(24B)	93(2)	121(3)	90(2)	-42(2)	62(2)	-43(2)
C(25B)	62(2)	104(2)	92(2)	-29(2)	41(2)	-20(2)
C(26B)	48(1)	71(2)	63(1)	-8(1)	18(1)	-9(1)
C(31B)	51(1)	51(1)	61(1)	-1(1)	21(1)	2(1)
C(32B)	54(1)	60(1)	72(2)	9(1)	24(1)	12(1)
C(33B)	78(2)	67(2)	91(2)	20(1)	33(2)	19(1)
C(34B)	124(3)	170(4)	171(4)	103(3)	85(3)	53(3)
C(35B)	95(2)	100(2)	138(3)	38(2)	46(2)	48(2)
C(41B)	99(2)	134(3)	58(2)	2(2)	-1(2)	-43(2)
C(42B)	276(7)	223(5)	72(2)	-57(3)	57(3)	-115(5)

366d

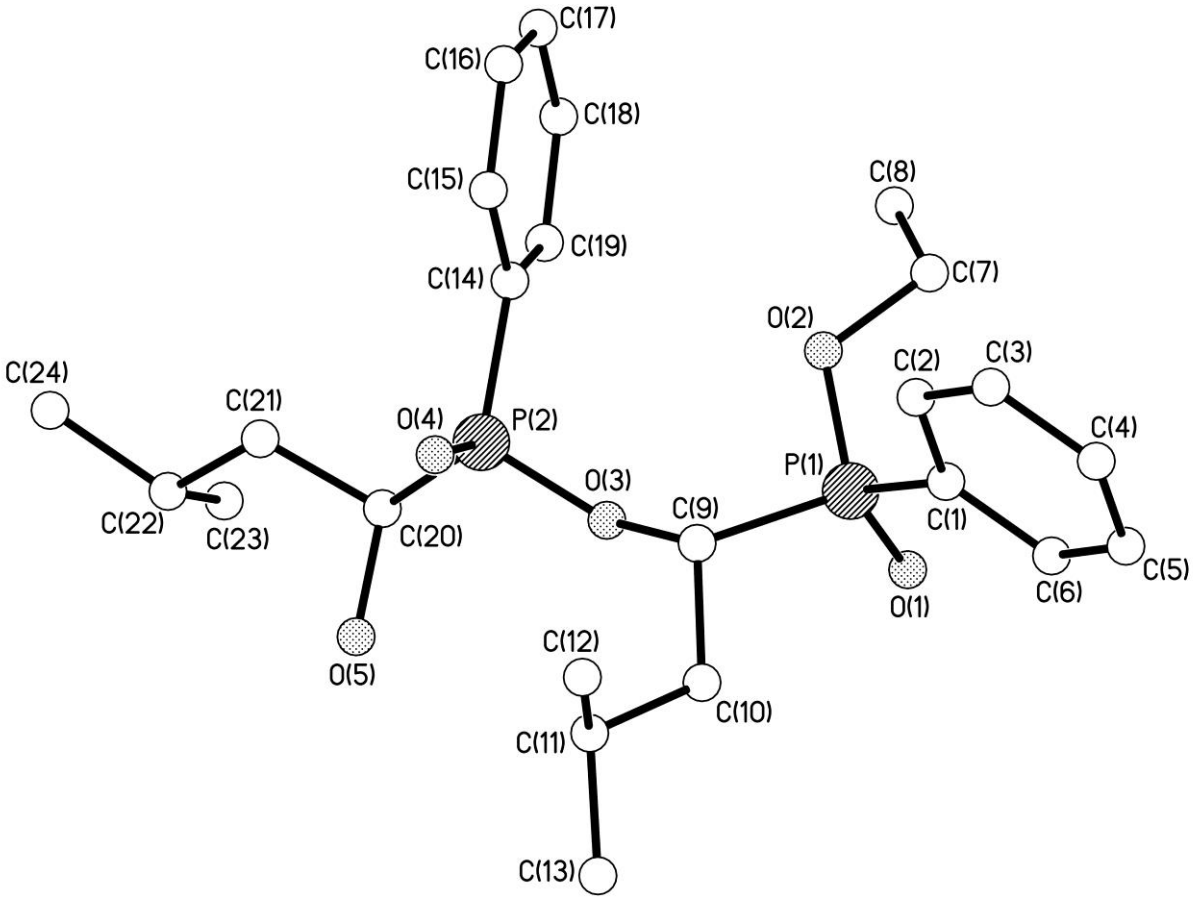

Table 1. Crystal data and structure refinement for 6d.

Identification code	c:~1~16srv092m	
Empirical formula	C24 H36 O5 P2	
Formula weight	466.47	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	?	
Space group	?	
Unit cell dimensions	a = 13.0290(13) Å	α= 90°.
	b = 12.6029(13) Å	β= 101.187(2)°.
	c = 15.4649(16) Å	γ = 90°.
Volume	2491.1(4) $Å^3$	
Z	4	
Density (calculated)	1.244 Mg/m^3	
Absorption coefficient	0.206 mm^{-1}	
F(000)	1000	
Crystal size	0.30 x 0.20 x 0.20 mm^3	
Theta range for data collection	2.27 to 23.28°.	

Index ranges	-14<=h<=14, -14<=k<=13, -17<=l<=17
Reflections collected	22487
Independent reflections	3578 [R(int) = 0.0570]
Completeness to theta = 23.28°	99.9 %
Max. and min. transmission	0.9600 and 0.9409
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3578 / 0 / 290
Goodness-of-fit on F^2	0.886
Final R indices [I>2sigma(I)]	R1 = 0.0341, wR2 = 0.0680
R indices (all data)	R1 = 0.0543, wR2 = 0.0725
Extinction coefficient	0.0000(3)
Largest diff. peak and hole	0.263 and -0.295 e.$Å^{-3}$

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

	x	y	z	U(eq)
P(1)	3012(1)	4533(1)	614(1)	21(1)
P(2)	2910(1)	3908(1)	-1921(1)	22(1)
O(1)	3763(1)	5354(1)	1017(1)	27(1)
O(2)	1946(1)	4971(1)	66(1)	25(1)
O(3)	3498(1)	4317(1)	-972(1)	21(1)
O(4)	2849(1)	2749(1)	-2005(1)	29(1)
O(5)	4732(1)	4133(1)	-2438(1)	33(1)
C(1)	2656(2)	3648(2)	1414(1)	20(1)
C(2)	1845(2)	2917(2)	1172(2)	26(1)
C(3)	1549(2)	2257(2)	1788(2)	30(1)
C(4)	2060(2)	2308(2)	2656(2)	32(1)
C(5)	2874(2)	3014(2)	2903(2)	32(1)
C(6)	3168(2)	3689(2)	2287(1)	25(1)
C(7)	1293(2)	5625(2)	524(2)	34(1)
C(8)	947(2)	6577(2)	-27(2)	42(1)
C(9)	3472(2)	3694(2)	-189(1)	21(1)
C(10)	4559(2)	3280(2)	199(1)	25(1)
C(11)	4943(2)	2370(2)	-309(2)	30(1)
C(12)	4293(2)	1371(2)	-291(2)	38(1)
C(13)	6092(2)	2154(2)	72(2)	49(1)

C(14)	1630(2)	4500(2)	-2155(1)	20(1)
C(15)	767(2)	3831(2)	-2364(1)	27(1)
C(16)	-229(2)	4250(2)	-2586(2)	32(1)
C(17)	-372(2)	5328(2)	-2616(2)	31(1)
C(18)	476(2)	6004(2)	-2420(1)	29(1)
C(19)	1473(2)	5591(2)	-2191(1)	25(1)
C(20)	3711(2)	4596(2)	-2597(1)	26(1)
C(21)	3245(2)	4494(2)	-3563(1)	28(1)
C(22)	3887(2)	4991(2)	-4185(2)	29(1)
C(23)	4124(2)	6172(2)	-3992(2)	35(1)
C(24)	3314(2)	4846(2)	-5136(2)	38(1)

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

P(1)-O(1)	1.4761(15)	C(7)-H(7A)	0.9900
P(1)-O(2)	1.5802(15)	C(7)-H(7B)	0.9900
P(1)-C(1)	1.793(2)	C(8)-H(8A)	0.9800
P(1)-C(9)	1.819(2)	C(8)-H(8B)	0.9800
P(2)-O(4)	1.4677(15)	C(8)-H(8C)	0.9800
P(2)-O(3)	1.6032(15)	C(9)-C(10)	1.520(3)
P(2)-C(14)	1.799(2)	C(9)-H(9)	1.0000
P(2)-C(20)	1.832(2)	C(10)-C(11)	1.528(3)
O(2)-C(7)	1.463(3)	C(10)-H(10A)	0.9900
O(3)-C(9)	1.449(2)	C(10)-H(10B)	0.9900
O(5)-C(20)	1.429(3)	C(11)-C(12)	1.521(3)
O(5)-H(5O)	0.83(3)	C(11)-C(13)	1.524(3)
C(1)-C(6)	1.385(3)	C(11)-H(11)	1.0000
C(1)-C(2)	1.397(3)	C(12)-H(12A)	0.9800
C(2)-C(3)	1.375(3)	C(12)-H(12B)	0.9800
C(2)-H(2)	0.9500	C(12)-H(12C)	0.9800
C(3)-C(4)	1.380(3)	C(13)-H(13A)	0.9800
C(3)-H(3)	0.9500	C(13)-H(13B)	0.9800
C(4)-C(5)	1.380(3)	C(13)-H(13C)	0.9800
C(4)-H(4)	0.9500	C(14)-C(19)	1.389(3)
C(5)-C(6)	1.385(3)	C(14)-C(15)	1.393(3)
C(5)-H(5)	0.9500	C(15)-C(16)	1.381(3)
C(6)-H(6)	0.9500	C(15)-H(15)	0.9500
C(7)-C(8)	1.489(3)	C(16)-C(17)	1.371(3)

C(16)-H(16)	0.9500	C(2)-C(1)-P(1)	120.59(17)
C(17)-C(18)	1.381(3)	C(3)-C(2)-C(1)	120.8(2)
C(17)-H(17)	0.9500	C(3)-C(2)-H(2)	119.6
C(18)-C(19)	1.380(3)	C(1)-C(2)-H(2)	119.6
C(18)-H(18)	0.9500	C(2)-C(3)-C(4)	119.9(2)
C(19)-H(19)	0.9500	C(2)-C(3)-H(3)	120.0
C(20)-C(21)	1.504(3)	C(4)-C(3)-H(3)	120.0
C(20)-H(20)	1.0000	C(3)-C(4)-C(5)	119.9(2)
C(21)-C(22)	1.527(3)	C(3)-C(4)-H(4)	120.0
C(21)-H(21A)	0.9900	C(5)-C(4)-H(4)	120.0
C(21)-H(21B)	0.9900	C(4)-C(5)-C(6)	120.4(2)
C(22)-C(24)	1.525(3)	C(4)-C(5)-H(5)	119.8
C(22)-C(23)	1.537(3)	C(6)-C(5)-H(5)	119.8
C(22)-H(22)	1.0000	C(1)-C(6)-C(5)	120.1(2)
C(23)-H(23A)	0.9800	C(1)-C(6)-H(6)	119.9
C(23)-H(23B)	0.9800	C(5)-C(6)-H(6)	119.9
C(23)-H(23C)	0.9800	O(2)-C(7)-C(8)	108.45(19)
C(24)-H(24A)	0.9800	O(2)-C(7)-H(7A)	110.0
C(24)-H(24B)	0.9800	C(8)-C(7)-H(7A)	110.0
C(24)-H(24C)	0.9800	O(2)-C(7)-H(7B)	110.0
		C(8)-C(7)-H(7B)	110.0
O(1)-P(1)-O(2)	115.06(9)	H(7A)-C(7)-H(7B)	108.4
O(1)-P(1)-C(1)	112.58(9)	C(7)-C(8)-H(8A)	109.5
O(2)-P(1)-C(1)	105.65(9)	C(7)-C(8)-H(8B)	109.5
O(1)-P(1)-C(9)	114.62(9)	H(8A)-C(8)-H(8B)	109.5
O(2)-P(1)-C(9)	101.99(9)	C(7)-C(8)-H(8C)	109.5
C(1)-P(1)-C(9)	105.85(10)	H(8A)-C(8)-H(8C)	109.5
O(4)-P(2)-O(3)	114.14(8)	H(8B)-C(8)-H(8C)	109.5
O(4)-P(2)-C(14)	111.31(10)	O(3)-C(9)-C(10)	110.12(16)
O(3)-P(2)-C(14)	108.13(9)	O(3)-C(9)-P(1)	108.67(14)
O(4)-P(2)-C(20)	116.53(10)	C(10)-C(9)-P(1)	109.57(14)
O(3)-P(2)-C(20)	98.40(9)	O(3)-C(9)-H(9)	109.5
C(14)-P(2)-C(20)	107.34(10)	C(10)-C(9)-H(9)	109.5
C(7)-O(2)-P(1)	118.01(13)	P(1)-C(9)-H(9)	109.5
C(9)-O(3)-P(2)	120.40(12)	C(9)-C(10)-C(11)	115.30(18)
C(20)-O(5)-H(5O)	113.1(18)	C(9)-C(10)-H(10A)	108.4
C(6)-C(1)-C(2)	118.8(2)	C(11)-C(10)-H(10A)	108.4
C(6)-C(1)-P(1)	120.59(17)	C(9)-C(10)-H(10B)	108.4

C(11)-C(10)-H(10B)	108.4	C(18)-C(19)-C(14)	120.4(2)
H(10A)-C(10)-H(10B)	107.5	C(18)-C(19)-H(19)	119.8
C(12)-C(11)-C(13)	110.7(2)	C(14)-C(19)-H(19)	119.8
C(12)-C(11)-C(10)	111.89(19)	O(5)-C(20)-C(21)	108.64(18)
C(13)-C(11)-C(10)	109.3(2)	O(5)-C(20)-P(2)	108.83(15)
C(12)-C(11)-H(11)	108.3	C(21)-C(20)-P(2)	111.15(15)
C(13)-C(11)-H(11)	108.3	O(5)-C(20)-H(20)	109.4
C(10)-C(11)-H(11)	108.3	C(21)-C(20)-H(20)	109.4
C(11)-C(12)-H(12A)	109.5	P(2)-C(20)-H(20)	109.4
C(11)-C(12)-H(12B)	109.5	C(20)-C(21)-C(22)	115.17(18)
H(12A)-C(12)-H(12B)	109.5	C(20)-C(21)-H(21A)	108.5
C(11)-C(12)-H(12C)	109.5	C(22)-C(21)-H(21A)	108.5
H(12A)-C(12)-H(12C)	109.5	C(20)-C(21)-H(21B)	108.5
H(12B)-C(12)-H(12C)	109.5	C(22)-C(21)-H(21B)	108.5
C(11)-C(13)-H(13A)	109.5	H(21A)-C(21)-H(21B)	107.5
C(11)-C(13)-H(13B)	109.5	C(24)-C(22)-C(21)	109.41(18)
H(13A)-C(13)-H(13B)	109.5	C(24)-C(22)-C(23)	110.28(19)
C(11)-C(13)-H(13C)	109.5	C(21)-C(22)-C(23)	112.90(19)
H(13A)-C(13)-H(13C)	109.5	C(24)-C(22)-H(22)	108.0
H(13B)-C(13)-H(13C)	109.5	C(21)-C(22)-H(22)	108.0
C(19)-C(14)-C(15)	119.0(2)	C(23)-C(22)-H(22)	108.0
C(19)-C(14)-P(2)	122.77(16)	C(22)-C(23)-H(23A)	109.5
C(15)-C(14)-P(2)	118.08(17)	C(22)-C(23)-H(23B)	109.5
C(16)-C(15)-C(14)	120.2(2)	H(23A)-C(23)-H(23B)	109.5
C(16)-C(15)-H(15)	119.9	C(22)-C(23)-H(23C)	109.5
C(14)-C(15)-H(15)	119.9	H(23A)-C(23)-H(23C)	109.5
C(17)-C(16)-C(15)	120.2(2)	H(23B)-C(23)-H(23C)	109.5
C(17)-C(16)-H(16)	119.9	C(22)-C(24)-H(24A)	109.5
C(15)-C(16)-H(16)	119.9	C(22)-C(24)-H(24B)	109.5
C(16)-C(17)-C(18)	120.4(2)	H(24A)-C(24)-H(24B)	109.5
C(16)-C(17)-H(17)	119.8	C(22)-C(24)-H(24C)	109.5
C(18)-C(17)-H(17)	119.8	H(24A)-C(24)-H(24C)	109.5
C(19)-C(18)-C(17)	119.8(2)	H(24B)-C(24)-H(24C)	109.5
C(19)-C(18)-H(18)	120.1		
C(17)-C(18)-H(18)	120.1		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 6d. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	20(1)	23(1)	21(1)	-2(1)	5(1)	-1(1)
P(2)	22(1)	23(1)	21(1)	-1(1)	4(1)	5(1)
O(1)	27(1)	28(1)	27(1)	-7(1)	7(1)	-6(1)
O(2)	25(1)	27(1)	23(1)	-2(1)	5(1)	7(1)
O(3)	24(1)	21(1)	19(1)	2(1)	6(1)	1(1)
O(4)	32(1)	22(1)	31(1)	-3(1)	1(1)	5(1)
O(5)	18(1)	55(1)	25(1)	-8(1)	2(1)	8(1)
C(1)	17(1)	23(1)	21(1)	-1(1)	5(1)	4(1)
C(2)	26(1)	27(1)	26(1)	-5(1)	8(1)	-1(1)
C(3)	29(1)	25(1)	40(2)	-2(1)	14(1)	-4(1)
C(4)	36(2)	28(2)	38(2)	11(1)	20(1)	12(1)
C(5)	35(2)	36(2)	24(1)	6(1)	5(1)	10(1)
C(6)	22(1)	28(1)	27(2)	-3(1)	5(1)	2(1)
C(7)	26(1)	39(2)	37(2)	-12(1)	8(1)	5(1)
C(8)	37(2)	37(2)	49(2)	-11(1)	0(1)	12(1)
C(9)	22(1)	21(1)	19(1)	4(1)	5(1)	-2(1)
C(10)	21(1)	32(1)	23(1)	3(1)	5(1)	3(1)
C(11)	30(1)	34(2)	29(1)	6(1)	12(1)	12(1)
C(12)	47(2)	29(2)	41(2)	6(1)	12(1)	14(1)
C(13)	33(2)	54(2)	62(2)	12(2)	13(1)	21(1)
C(14)	21(1)	23(1)	16(1)	3(1)	8(1)	2(1)
C(15)	30(1)	24(1)	29(1)	3(1)	10(1)	1(1)
C(16)	21(1)	40(2)	36(2)	2(1)	7(1)	-5(1)
C(17)	22(1)	45(2)	29(2)	9(1)	10(1)	11(1)
C(18)	30(2)	25(1)	33(2)	6(1)	12(1)	8(1)
C(19)	23(1)	26(2)	27(1)	1(1)	10(1)	-1(1)
C(20)	17(1)	36(2)	26(1)	-4(1)	5(1)	3(1)
C(21)	24(1)	29(1)	30(1)	1(1)	7(1)	1(1)
C(22)	21(1)	32(1)	36(2)	12(1)	14(1)	5(1)
C(23)	31(1)	38(2)	35(2)	3(1)	4(1)	-4(1)
C(24)	38(2)	44(2)	36(2)	-3(1)	16(1)	-8(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for 6d.

	x	y	z	U(eq)
H(2)	1494	2875	574	31
H(3)	992	1768	1616	36
H(4)	1853	1857	3084	39
H(5)	3235	3038	3499	38
H(6)	3722	4180	2463	30
H(7A)	1698	5846	1106	41
H(7B)	677	5215	620	41
H(8A)	1560	6992	-100	63
H(8B)	491	7013	263	63
H(8C)	562	6351	-606	63
H(9)	2981	3083	-345	25
H(10A)	4565	3039	809	30
H(10B)	5061	3876	232	30
H(11)	4882	2596	-937	36
H(12A)	4578	800	-604	58
H(12B)	3567	1512	-579	58
H(12C)	4315	1158	322	58
H(13A)	6167	1928	688	74
H(13B)	6500	2802	43	74
H(13C)	6349	1592	-269	74
H(15)	863	3083	-2353	32
H(16)	-817	3791	-2718	39
H(17)	-1058	5612	-2773	38
H(18)	374	6750	-2443	34
H(19)	2057	6056	-2058	30
H(20)	3767	5363	-2431	32
H(21A)	2543	4827	-3673	33
H(21B)	3148	3731	-3708	33
H(22)	4568	4604	-4111	34
H(23A)	3468	6557	-4006	53
H(23B)	4485	6464	-4439	53
H(23C)	4572	6246	-3408	53
H(24A)	3147	4093	-5245	57
H(24B)	3761	5089	-5537	57
H(24C)	2665	5261	-5235	57

H(5O)	5090(20)	4290(20)	-1946(17)	56(10)

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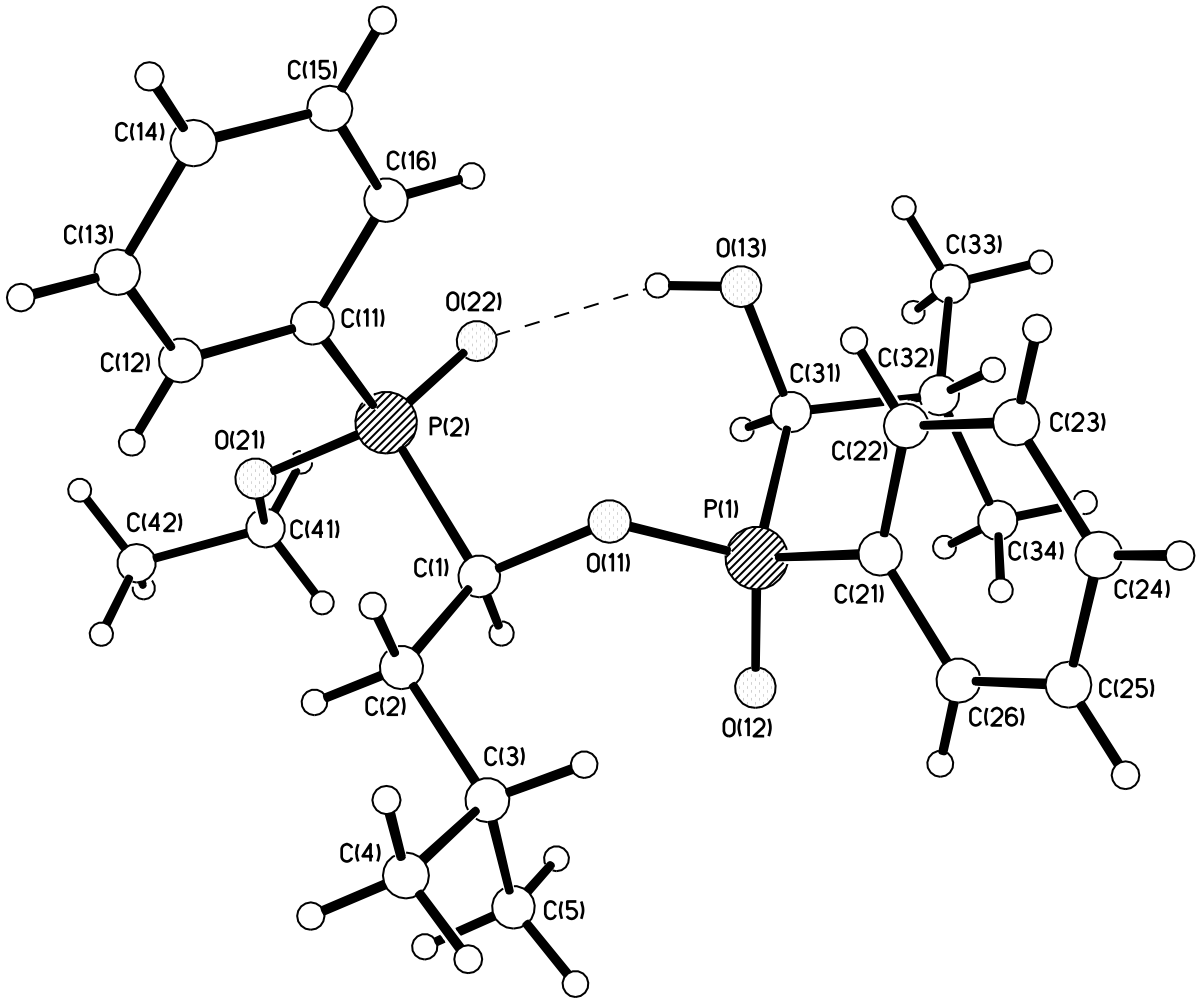

Table 1. Crystal data and structure refinement for MR048_d1_0m.

Identification code	mr048_d1_0m	
Empirical formula	C23 H34 O5 P2	
Formula weight	452.44	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.1386(2) Å	α= 113.9030(10)°.
	b = 11.9523(2) Å	β= 96.4940(10)°.
	c = 12.7388(3) Å	γ = 91.6580(10)°.
Volume	1259.64(5) $Å^3$	
Z	2	
Density (calculated)	1.193 Mg/m^3	
Absorption coefficient	0.201 mm^{-1}	
F(000)	484	
Crystal size	0.44 x 0.35 x 0.16 mm^3	
Theta range for data collection	2.66 to 29.94°.	
Index ranges	-12<=h<=12, -16<=k<=16, -17<=l<=17	
Reflections collected	88980	
Independent reflections	7245 [R(int) = 0.0336]	
Completeness to theta = 29.94°	99.1 %	
Absorption correction	Multiscan	
Max. and min. transmission	0.9689 and 0.9175	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	7245 / 0 / 280
Goodness-of-fit on F^2	1.047
Final R indices [I>2sigma(I)]	R1 = 0.0404, wR2 = 0.1037
R indices (all data)	R1 = 0.0665, wR2 = 0.1227
Largest diff. peak and hole	0.304 and -0.261 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for MR048_d1_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	5600(1)	6510(1)	7627(1)	40(1)
P(2)	8572(1)	7386(1)	6124(1)	39(1)
O(11)	6372(1)	7527(1)	7304(1)	41(1)
O(12)	4557(1)	5610(1)	6677(1)	54(1)
O(13)	8377(1)	6663(1)	8676(1)	59(1)
O(21)	8819(1)	7087(1)	4840(1)	47(1)
O(22)	9264(1)	6600(1)	6654(1)	53(1)
C(1)	6563(2)	7287(1)	6115(1)	39(1)
C(2)	5751(2)	8212(2)	5779(2)	49(1)
C(3)	4092(2)	8202(2)	5859(2)	54(1)
C(4)	3488(3)	9326(2)	5739(2)	88(1)
C(5)	3234(2)	7039(2)	4984(2)	84(1)
C(11)	9282(2)	8961(1)	6859(1)	42(1)
C(12)	9218(2)	9765(2)	6324(2)	57(1)

C(13)	9788(3)	10977(2)	6932(2)	77(1)
C(14)	10403(2)	11386(2)	8069(2)	81(1)
C(15)	10464(2)	10609(2)	8608(2)	78(1)
C(16)	9911(2)	9390(2)	8008(2)	61(1)
C(21)	4773(2)	7468(2)	8862(1)	48(1)
C(22)	5607(3)	8292(2)	9857(2)	88(1)
C(23)	4918(4)	9009(3)	10800(2)	114(1)
C(24)	3416(3)	8885(3)	10734(2)	94(1)
C(25)	2585(3)	8070(2)	9757(2)	81(1)
C(26)	3253(2)	7365(2)	8817(2)	63(1)
C(31)	7135(2)	5796(2)	8114(1)	46(1)
C(32)	6729(2)	5195(2)	8915(2)	64(1)
C(33)	8048(3)	4599(3)	9233(3)	116(1)
C(34)	5384(3)	4288(2)	8406(2)	90(1)
C(41)	8749(2)	5819(2)	3981(2)	61(1)
C(42)	9092(3)	5826(2)	2889(2)	74(1)

Table 3. Bond lengths [Å] and angles [°] for MR048_d1_0m.

P(1)-O(12)	1.4680(12)	P(2)-C(1)	1.8351(14)
P(1)-O(11)	1.6023(10)	O(11)-C(1)	1.4542(16)
P(1)-C(21)	1.7940(16)	O(13)-C(31)	1.422(2)
P(1)-C(31)	1.8395(16)	O(13)-H(13O)	0.83(3)
P(2)-O(22)	1.4792(11)	O(21)-C(41)	1.4610(19)
P(2)-O(21)	1.5713(11)	C(1)-C(2)	1.522(2)
P(2)-C(11)	1.7909(15)	C(1)-H(1)	0.9800

C(2)-C(3)	1.532(2)	C(22)-C(23)	1.394(3)
C(2)-H(2A)	0.9700	C(22)-H(22)	0.9300
C(2)-H(2B)	0.9700	C(23)-C(24)	1.365(4)
C(3)-C(5)	1.508(3)	C(23)-H(23)	0.9300
C(3)-C(4)	1.524(3)	C(24)-C(25)	1.355(4)
C(3)-H(3)	0.9800	C(24)-H(24)	0.9300
C(4)-H(4A)	0.9600	C(25)-C(26)	1.376(3)
C(4)-H(4B)	0.9600	C(25)-H(25)	0.9300
C(4)-H(4C)	0.9600	C(26)-H(26)	0.9300
C(5)-H(5A)	0.9600	C(31)-C(32)	1.536(2)
C(5)-H(5B)	0.9600	C(31)-H(31)	0.9800
C(5)-H(5C)	0.9600	C(32)-C(34)	1.509(3)
C(11)-C(12)	1.384(2)	C(32)-C(33)	1.516(3)
C(11)-C(16)	1.385(2)	C(32)-H(32)	0.9800
C(12)-C(13)	1.387(3)	C(33)-H(33A)	0.9600
C(12)-H(12)	0.9300	C(33)-H(33B)	0.9600
C(13)-C(14)	1.370(3)	C(33)-H(33C)	0.9600
C(13)-H(13A)	0.9300	C(34)-H(34A)	0.9600
C(14)-C(15)	1.359(4)	C(34)-H(34B)	0.9600
C(14)-H(14)	0.9300	C(34)-H(34C)	0.9600
C(15)-C(16)	1.389(3)	C(41)-C(42)	1.463(3)
C(15)-H(15)	0.9300	C(41)-H(41A)	0.9700
C(16)-H(16)	0.9300	C(41)-H(41B)	0.9700
C(21)-C(22)	1.372(3)	C(42)-H(42A)	0.9600
C(21)-C(26)	1.383(2)	C(42)-H(42B)	0.9600

C(42)-H(42C)	0.9600	C(1)-C(2)-H(2B)	108.4
O(12)-P(1)-O(11)	114.04(6)	C(3)-C(2)-H(2B)	108.4
O(12)-P(1)-C(21)	114.58(7)	H(2A)-C(2)-H(2B)	107.5
O(11)-P(1)-C(21)	100.65(7)	C(5)-C(3)-C(4)	110.89(17)
O(12)-P(1)-C(31)	112.59(7)	C(5)-C(3)-C(2)	112.95(16)
O(11)-P(1)-C(31)	105.11(6)	C(4)-C(3)-C(2)	109.72(16)
C(21)-P(1)-C(31)	108.85(7)	C(5)-C(3)-H(3)	107.7
O(22)-P(2)-O(21)	116.55(6)	C(4)-C(3)-H(3)	107.7
O(22)-P(2)-C(11)	112.61(7)	C(2)-C(3)-H(3)	107.7
O(21)-P(2)-C(11)	101.96(6)	C(3)-C(4)-H(4A)	109.5
O(22)-P(2)-C(1)	110.18(6)	C(3)-C(4)-H(4B)	109.5
O(21)-P(2)-C(1)	105.92(6)	H(4A)-C(4)-H(4B)	109.5
C(11)-P(2)-C(1)	109.05(7)	C(3)-C(4)-H(4C)	109.5
C(1)-O(11)-P(1)	121.67(9)	H(4A)-C(4)-H(4C)	109.5
C(31)-O(13)-H(13O)	107.4(17)	H(4B)-C(4)-H(4C)	109.5
C(41)-O(21)-P(2)	120.90(10)	C(3)-C(5)-H(5A)	109.5
O(11)-C(1)-C(2)	108.46(12)	C(3)-C(5)-H(5B)	109.5
O(11)-C(1)-P(2)	104.57(9)	H(5A)-C(5)-H(5B)	109.5
C(2)-C(1)-P(2)	115.15(10)	C(3)-C(5)-H(5C)	109.5
O(11)-C(1)-H(1)	109.5	H(5A)-C(5)-H(5C)	109.5
C(2)-C(1)-H(1)	109.5	H(5B)-C(5)-H(5C)	109.5
P(2)-C(1)-H(1)	109.5	C(12)-C(11)-C(16)	118.98(16)
C(1)-C(2)-C(3)	115.49(13)	C(12)-C(11)-P(2)	122.45(13)
C(1)-C(2)-H(2A)	108.4	C(16)-C(11)-P(2)	118.57(13)
C(3)-C(2)-H(2A)	108.4	C(11)-C(12)-C(13)	120.17(18)

C(11)-C(12)-H(12)	119.9	C(23)-C(24)-H(24)	119.7
C(13)-C(12)-H(12)	119.9	C(24)-C(25)-C(26)	120.0(2)
C(14)-C(13)-C(12)	120.1(2)	C(24)-C(25)-H(25)	120.0
C(14)-C(13)-H(13A)	120.0	C(26)-C(25)-H(25)	120.0
C(12)-C(13)-H(13A)	120.0	C(25)-C(26)-C(21)	120.6(2)
C(15)-C(14)-C(13)	120.41(19)	C(25)-C(26)-H(26)	119.7
C(15)-C(14)-H(14)	119.8	C(21)-C(26)-H(26)	119.7
C(13)-C(14)-H(14)	119.8	O(13)-C(31)-C(32)	109.29(14)
C(14)-C(15)-C(16)	120.2(2)	O(13)-C(31)-P(1)	110.85(11)
C(14)-C(15)-H(15)	119.9	C(32)-C(31)-P(1)	113.90(12)
C(16)-C(15)-H(15)	119.9	O(13)-C(31)-H(31)	107.5
C(11)-C(16)-C(15)	120.14(19)	C(32)-C(31)-H(31)	107.5
C(11)-C(16)-H(16)	119.9	P(1)-C(31)-H(31)	107.5
C(15)-C(16)-H(16)	119.9	C(34)-C(32)-C(33)	111.2(2)
C(22)-C(21)-C(26)	119.00(17)	C(34)-C(32)-C(31)	113.06(16)
C(22)-C(21)-P(1)	121.84(14)	C(33)-C(32)-C(31)	109.68(16)
C(26)-C(21)-P(1)	119.16(14)	C(34)-C(32)-H(32)	107.6
C(21)-C(22)-C(23)	119.9(2)	C(33)-C(32)-H(32)	107.6
C(21)-C(22)-H(22)	120.1	C(31)-C(32)-H(32)	107.6
C(23)-C(22)-H(22)	120.1	C(32)-C(33)-H(33A)	109.5
C(24)-C(23)-C(22)	119.9(2)	C(32)-C(33)-H(33B)	109.5
C(24)-C(23)-H(23)	120.0	H(33A)-C(33)-H(33B)	109.5
C(22)-C(23)-H(23)	120.0	C(32)-C(33)-H(33C)	109.5
C(25)-C(24)-C(23)	120.6(2)	H(33A)-C(33)-H(33C)	109.5
C(25)-C(24)-H(24)	119.7	H(33B)-C(33)-H(33C)	109.5

C(32)-C(34)-H(34A)	109.5	C(42)-C(41)-H(41B)	110.0
C(32)-C(34)-H(34B)	109.5	H(41A)-C(41)-H(41B)	108.4
H(34A)-C(34)-H(34B)	109.5	C(41)-C(42)-H(42A)	109.5
C(32)-C(34)-H(34C)	109.5	C(41)-C(42)-H(42B)	109.5
H(34A)-C(34)-H(34C)	109.5	H(42A)-C(42)-H(42B)	109.5
H(34B)-C(34)-H(34C)	109.5	C(41)-C(42)-H(42C)	109.5
O(21)-C(41)-C(42)	108.58(14)	H(42A)-C(42)-H(42C)	109.5
O(21)-C(41)-H(41A)	110.0	H(42B)-C(42)-H(42C)	109.5
C(42)-C(41)-H(41A)	110.0		
O(21)-C(41)-H(41B)	110.0		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for MR048_d1_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	36(1)	43(1)	42(1)	17(1)	8(1)	1(1)
P(2)	36(1)	39(1)	49(1)	21(1)	13(1)	8(1)
O(11)	39(1)	42(1)	42(1)	18(1)	7(1)	1(1)
O(12)	48(1)	56(1)	54(1)	20(1)	3(1)	-9(1)
O(13)	48(1)	74(1)	54(1)	29(1)	0(1)	2(1)
O(21)	56(1)	37(1)	50(1)	16(1)	19(1)	7(1)
O(22)	47(1)	58(1)	72(1)	40(1)	19(1)	20(1)
C(1)	36(1)	42(1)	43(1)	19(1)	8(1)	2(1)
C(2)	39(1)	57(1)	58(1)	32(1)	7(1)	8(1)

C(3)	39(1)	69(1)	56(1)	30(1)	7(1)	13(1)
C(4)	63(1)	100(2)	118(2)	60(2)	14(1)	36(1)
C(5)	53(1)	95(2)	91(2)	31(1)	-15(1)	-4(1)
C(11)	31(1)	44(1)	50(1)	16(1)	9(1)	5(1)
C(12)	59(1)	44(1)	65(1)	22(1)	2(1)	-2(1)
C(13)	81(1)	47(1)	99(2)	28(1)	6(1)	-7(1)
C(14)	67(1)	52(1)	94(2)	1(1)	12(1)	-14(1)
C(15)	60(1)	86(2)	59(1)	4(1)	-1(1)	-12(1)
C(16)	53(1)	72(1)	55(1)	23(1)	3(1)	0(1)
C(21)	47(1)	52(1)	50(1)	21(1)	15(1)	7(1)
C(22)	62(1)	103(2)	65(1)	-3(1)	15(1)	4(1)
C(23)	107(2)	121(2)	64(2)	-15(2)	19(1)	13(2)
C(24)	99(2)	107(2)	78(2)	27(1)	47(2)	45(2)
C(25)	68(1)	99(2)	84(2)	37(1)	38(1)	31(1)
C(26)	51(1)	72(1)	68(1)	27(1)	21(1)	11(1)
C(31)	47(1)	52(1)	45(1)	24(1)	12(1)	8(1)
C(32)	73(1)	81(1)	62(1)	47(1)	26(1)	20(1)
C(33)	101(2)	172(3)	148(3)	135(3)	33(2)	42(2)
C(34)	98(2)	97(2)	108(2)	70(2)	34(2)	-1(1)
C(41)	80(1)	39(1)	57(1)	11(1)	19(1)	-6(1)
C(42)	102(2)	54(1)	55(1)	11(1)	21(1)	-6(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for MR048_d1_0m.

	x	y	z	U(eq)
H(1)	6144	6454	5600	47
H(2A)	5888	8057	4989	58
H(2B)	6207	9028	6275	58
H(3)	3961	8263	6633	64
H(4A)	3558	9270	4974	132
H(4B)	4054	10054	6300	132
H(4C)	2473	9362	5869	132
H(5A)	2221	7046	5121	127
H(5B)	3653	6342	5057	127
H(5C)	3280	6987	4217	127
H(12)	8791	9492	5555	68
H(13A)	9752	11513	6568	92
H(14)	10780	12199	8474	97
H(15)	10879	10894	9380	93
H(16)	9962	8860	8379	74
H(22)	6630	8372	9901	106
H(23)	5480	9571	11474	137
H(24)	2960	9365	11365	113
H(25)	1564	7986	9723	97
H(26)	2677	6815	8145	76
H(31)	7432	5150	7423	55
H(32)	6503	5849	9632	77

H(33A)	7866	4378	9855	173
H(33B)	8911	5166	9474	173
H(33C)	8203	3875	8571	173
H(34A)	5542	3672	7668	135
H(34B)	4538	4710	8304	135
H(34C)	5217	3906	8920	135
H(41A)	7768	5420	3869	73
H(41B)	9455	5368	4247	73
H(42A)	8353	6229	2607	110
H(42B)	9104	4996	2329	110
H(42C)	10042	6257	3016	110
H(13O)	8810(30)	6730(20)	8160(20)	83(8)

367b

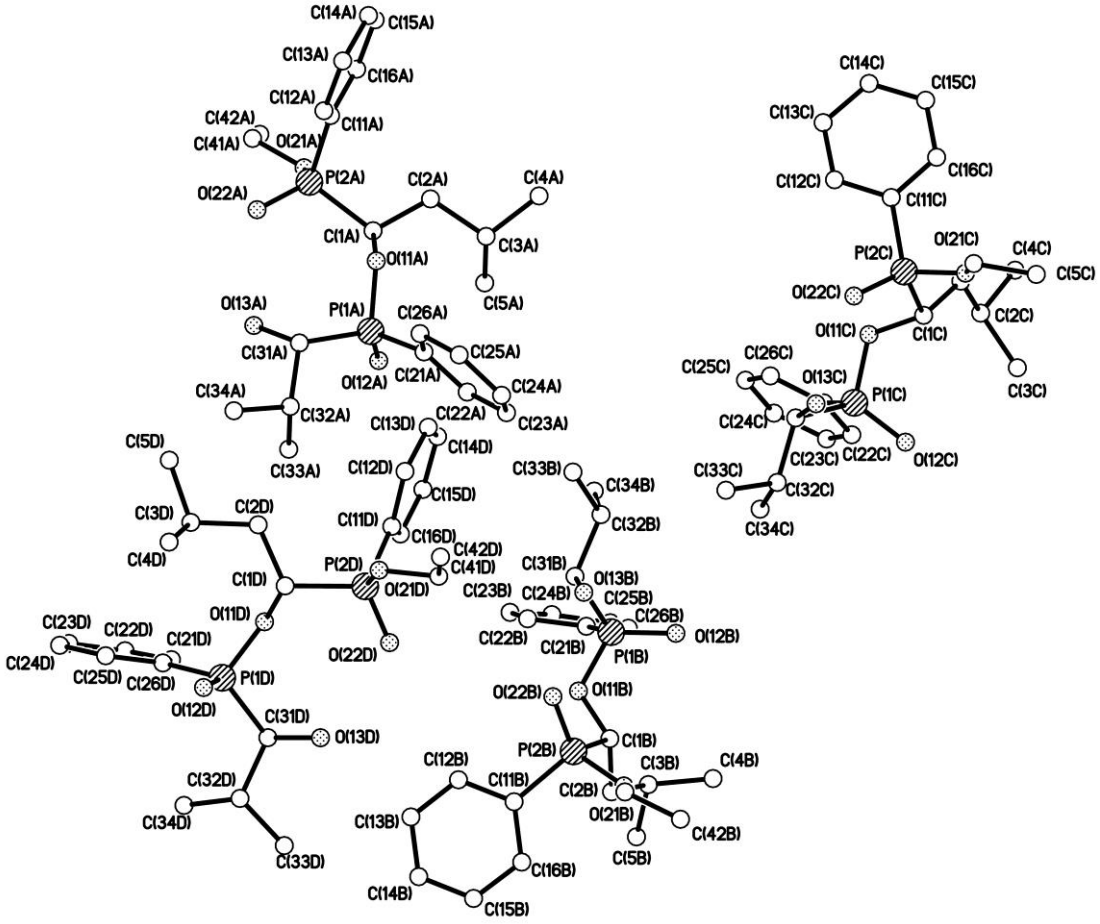

Table 1. Crystal data and structure refinement for MR048d2.

Identification code	mr_048d2_3_0m	
Empirical formula	C23 H34 O5 P2	
Formula weight	452.44	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.6935(7) Å	α= 73.726(5)°.
	b = 23.972(2) Å	β= 88.844(5)°.
	c = 24.195(2) Å	γ = 88.865(5)°.
Volume	4838.6(7) $Å^3$	
Z	8	
Density (calculated)	1.242 Mg/m^3	
Absorption coefficient	0.210 mm^{-1}	
F(000)	1936	

Crystal size	0.39 x 0.15 x 0.06 mm^3
Theta range for data collection	1.41 to 25.00°.
Index ranges	-10<=h<=10, -28<=k<=28, -28<=l<=28
Reflections collected	249416
Independent reflections	17037 [R(int) = 0.2501]
Completeness to theta = 25.00°	99.9 %
Absorption correction	None
Max. and min. transmission	0.9881 and 0.9219
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	17037 / 0 / 1114
Goodness-of-fit on F^2	0.989
Final R indices [I>2sigma(I)]	R1 = 0.0698, wR2 = 0.1404
R indices (all data)	R1 = 0.1964, wR2 = 0.1694
Largest diff. peak and hole	0.530 and -0.496 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for MR048d2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1A)	8189(1)	2944(1)	5784(1)	26(1)
P(2A)	5496(1)	3461(1)	6852(1)	30(1)
O(11A)	7900(3)	3348(1)	6208(1)	26(1)
O(12A)	7195(3)	3105(1)	5276(1)	33(1)
O(13A)	6404(3)	2119(2)	6432(2)	39(1)
O(21A)	3913(3)	3781(1)	6661(1)	34(1)
O(22A)	5451(3)	2817(1)	7077(1)	38(1)
C(1A)	6527(4)	3713(2)	6165(2)	23(1)
C(2A)	6966(5)	4348(2)	6015(2)	31(1)
C(3A)	7869(5)	4588(2)	5454(2)	36(1)
C(4A)	8280(6)	5216(2)	5402(2)	54(2)
C(5A)	7020(7)	4552(2)	4928(2)	58(2)
C(11A)	6310(5)	3790(2)	7354(2)	26(1)
C(12A)	7497(5)	3504(2)	7705(2)	34(1)
C(13A)	8194(6)	3763(2)	8076(2)	45(1)
C(14A)	7729(6)	4307(3)	8101(2)	42(1)
C(15A)	6548(6)	4594(2)	7755(2)	41(1)
C(16A)	5860(5)	4339(2)	7387(2)	37(1)

C(21A)	10188(5)	3009(2)	5610(2)	28(1)
C(22A)	10648(5)	3199(2)	5037(2)	33(1)
C(23A)	12193(5)	3211(2)	4883(2)	45(2)
C(24A)	13290(5)	3012(2)	5296(3)	41(1)
C(25A)	12864(5)	2825(2)	5870(2)	39(1)
C(26A)	11322(5)	2817(2)	6029(2)	35(1)
C(31A)	7959(5)	2207(2)	6251(2)	30(1)
C(32A)	8516(6)	1741(2)	5967(2)	40(1)
C(33A)	7592(7)	1734(3)	5455(3)	71(2)
C(34A)	8480(7)	1149(2)	6406(3)	68(2)
C(41A)	2540(5)	3645(2)	7022(2)	44(1)
C(42A)	1225(5)	4000(3)	6705(2)	54(2)
P(1B)	8825(1)	4064(1)	1594(1)	25(1)
P(2B)	11338(1)	2685(1)	1555(1)	29(1)
O(11B)	9059(3)	3438(1)	1475(1)	26(1)
O(12B)	9891(3)	4513(1)	1267(1)	32(1)
O(13B)	10526(4)	3605(2)	2499(2)	36(1)
O(21B)	12892(3)	2752(2)	1204(1)	42(1)
O(22B)	11442(3)	2675(1)	2169(1)	35(1)
C(1B)	10316(4)	3315(2)	1121(2)	25(1)
C(2B)	9693(5)	3239(2)	567(2)	29(1)
C(3B)	8996(5)	3788(2)	157(2)	39(1)
C(4B)	10196(7)	4240(2)	-85(2)	58(2)
C(5B)	8150(6)	3621(3)	-323(2)	55(2)
C(11B)	10450(5)	2042(2)	1484(2)	26(1)
C(12B)	9274(5)	1794(2)	1867(2)	30(1)
C(13B)	8575(5)	1291(2)	1837(2)	39(1)
C(14B)	9039(6)	1034(2)	1418(2)	41(1)
C(15B)	10174(6)	1284(2)	1034(2)	42(1)
C(16B)	10888(5)	1787(2)	1056(2)	35(1)
C(21B)	6855(5)	4225(2)	1420(2)	25(1)
C(22B)	5658(5)	3890(2)	1715(2)	31(1)
C(23B)	4129(5)	4040(2)	1581(2)	35(1)
C(24B)	3810(5)	4526(2)	1139(2)	36(1)
C(25B)	4962(5)	4865(2)	831(2)	38(1)
C(26B)	6491(5)	4723(2)	969(2)	33(1)
C(31B)	9055(5)	3873(2)	2375(2)	24(1)
C(32B)	9042(5)	4397(2)	2620(2)	31(1)

C(33B)	9404(6)	4210(2)	3261(2)	43(1)
C(34B)	7519(6)	4728(2)	2525(2)	47(2)
C(41B)	14280(5)	2461(2)	1451(2)	46(2)
C(42B)	15605(5)	2656(3)	1060(2)	54(2)
P(1C)	6953(1)	7885(1)	862(1)	28(1)
P(2C)	9337(1)	8460(1)	1955(1)	37(1)
O(11C)	7123(3)	8282(1)	1294(1)	29(1)
O(12C)	7992(3)	8044(1)	355(1)	34(1)
O(13C)	8767(4)	7124(2)	1575(2)	41(1)
O(21C)	10900(3)	8774(2)	1762(2)	57(1)
O(22C)	9439(4)	7823(1)	2218(2)	45(1)
C(1C)	8417(5)	8666(2)	1257(2)	30(1)
C(2C)	7881(5)	9297(2)	1083(2)	37(1)
C(3C)	7108(6)	9525(2)	503(2)	46(1)
C(4C)	6597(7)	10158(2)	426(3)	70(2)
C(5C)	8111(8)	9479(3)	-5(3)	88(2)
C(11C)	8381(5)	8822(2)	2419(2)	32(1)
C(12C)	7212(5)	8544(2)	2781(2)	39(1)
C(13C)	6432(6)	8817(2)	3141(2)	44(1)
C(14C)	6831(6)	9371(3)	3136(2)	45(1)
C(15C)	7990(6)	9654(2)	2780(2)	49(2)
C(16C)	8756(6)	9380(2)	2421(2)	40(1)
C(21C)	4977(5)	7964(2)	692(2)	31(1)
C(22C)	4559(5)	8206(2)	120(2)	37(1)
C(23C)	3041(6)	8233(2)	-28(2)	45(2)
C(24C)	1904(5)	8023(2)	367(3)	48(2)
C(25C)	2285(6)	7789(2)	942(3)	45(2)
C(26C)	3810(5)	7758(2)	1095(2)	35(1)
C(31C)	7302(5)	7149(2)	1322(2)	28(1)
C(32C)	7353(5)	6684(2)	999(2)	39(1)
C(33C)	7582(6)	6077(2)	1426(2)	45(1)
C(34C)	5967(7)	6675(3)	640(3)	67(2)
C(41C)	12297(5)	8621(3)	2068(2)	54(2)
C(42C)	13583(6)	8963(3)	1735(3)	75(2)
P(1D)	3634(1)	902(1)	3422(1)	24(1)
P(2D)	6108(1)	2258(1)	3439(1)	25(1)
O(11D)	3822(3)	1531(1)	3528(1)	22(1)
O(12D)	4717(3)	454(1)	3742(1)	29(1)

O(13D)	5394(3)	1319(2)	2514(1)	36(1)
O(21D)	7659(3)	2157(1)	3782(1)	30(1)
O(22D)	6233(3)	2254(1)	2832(1)	30(1)
C(1D)	5019(4)	1652(2)	3886(2)	21(1)
C(2D)	4297(5)	1768(2)	4422(2)	25(1)
C(3D)	3439(5)	1255(2)	4826(2)	34(1)
C(4D)	4485(6)	741(2)	5089(2)	53(2)
C(5D)	2600(6)	1456(2)	5299(2)	50(2)
C(11D)	5327(5)	2934(2)	3499(2)	22(1)
C(12D)	4196(5)	3217(2)	3122(2)	29(1)
C(13D)	3611(5)	3749(2)	3142(2)	30(1)
C(14D)	4165(5)	4006(2)	3540(2)	33(1)
C(15D)	5261(5)	3730(2)	3928(2)	33(1)
C(16D)	5839(5)	3193(2)	3916(2)	30(1)
C(21D)	1664(5)	745(2)	3610(2)	25(1)
C(22D)	1289(5)	259(2)	4069(2)	30(1)
C(23D)	-231(5)	132(2)	4207(2)	37(1)
C(24D)	-1390(5)	466(2)	3892(2)	38(1)
C(25D)	-1039(5)	945(2)	3435(2)	35(1)
C(26D)	457(5)	1088(2)	3299(2)	28(1)
C(31D)	3903(4)	1074(2)	2637(2)	26(1)
C(32D)	3866(5)	545(2)	2405(2)	32(1)
C(33D)	4305(6)	721(2)	1765(2)	47(2)
C(34D)	2309(5)	250(2)	2488(2)	47(2)
C(41D)	9019(5)	2475(2)	3525(2)	40(1)
C(42D)	10307(5)	2316(2)	3937(2)	53(2)

Table 3. Bond lengths [Å] and angles [°] for MR048d2.

P(1A)-O(12A)	1.472(3)	O(21A)-C(41A)	1.451(5)
P(1A)-O(11A)	1.610(3)	C(1A)-C(2A)	1.517(6)
P(1A)-C(21A)	1.780(5)	C(2A)-C(3A)	1.526(6)
P(1A)-C(31A)	1.822(5)	C(3A)-C(5A)	1.507(7)
P(2A)-O(22A)	1.487(3)	C(3A)-C(4A)	1.526(6)
P(2A)-O(21A)	1.574(3)	C(11A)-C(16A)	1.389(6)
P(2A)-C(11A)	1.786(5)	C(11A)-C(12A)	1.391(6)
P(2A)-C(1A)	1.825(4)	C(12A)-C(13A)	1.380(7)
O(11A)-C(1A)	1.453(4)	C(13A)-C(14A)	1.376(7)
O(13A)-C(31A)	1.414(5)	C(14A)-C(15A)	1.382(7)

C(15A)-C(16A)	1.367(6)	C(31B)-C(32B)	1.531(6)
C(21A)-C(22A)	1.384(6)	C(32B)-C(34B)	1.517(6)
C(21A)-C(26A)	1.405(6)	C(32B)-C(33B)	1.526(6)
C(22A)-C(23A)	1.385(6)	C(41B)-C(42B)	1.473(6)
C(23A)-C(24A)	1.374(7)	P(1C)-O(12C)	1.474(3)
C(24A)-C(25A)	1.380(7)	P(1C)-O(11C)	1.609(3)
C(25A)-C(26A)	1.386(6)	P(1C)-C(21C)	1.769(5)
C(31A)-C(32A)	1.533(6)	P(1C)-C(31C)	1.827(5)
C(32A)-C(33A)	1.495(7)	P(2C)-O(22C)	1.483(3)
C(32A)-C(34A)	1.514(7)	P(2C)-O(21C)	1.565(3)
C(41A)-C(42A)	1.499(7)	P(2C)-C(11C)	1.784(5)
P(1B)-O(12B)	1.475(3)	P(2C)-C(1C)	1.819(5)
P(1B)-O(11B)	1.611(3)	O(11C)-C(1C)	1.453(5)
P(1B)-C(21B)	1.780(4)	O(13C)-C(31C)	1.418(5)
P(1B)-C(31B)	1.830(4)	O(21C)-C(41C)	1.423(6)
P(2B)-O(22B)	1.484(3)	C(1C)-C(2C)	1.520(6)
P(2B)-O(21B)	1.568(3)	C(2C)-C(3C)	1.521(7)
P(2B)-C(11B)	1.788(5)	C(3C)-C(5C)	1.520(7)
P(2B)-C(1B)	1.807(4)	C(3C)-C(4C)	1.534(7)
O(11B)-C(1B)	1.452(5)	C(11C)-C(12C)	1.382(6)
O(13B)-C(31B)	1.419(5)	C(11C)-C(16C)	1.384(6)
O(21B)-C(41B)	1.436(5)	C(12C)-C(13C)	1.388(7)
C(1B)-C(2B)	1.514(6)	C(13C)-C(14C)	1.376(7)
C(2B)-C(3B)	1.530(6)	C(14C)-C(15C)	1.372(7)
C(3B)-C(4B)	1.507(7)	C(15C)-C(16C)	1.382(7)
C(3B)-C(5B)	1.537(7)	C(21C)-C(26C)	1.391(6)
C(11B)-C(16B)	1.386(6)	C(21C)-C(22C)	1.394(6)
C(11B)-C(12B)	1.391(6)	C(22C)-C(23C)	1.370(6)
C(12B)-C(13B)	1.383(6)	C(23C)-C(24C)	1.362(7)
C(13B)-C(14B)	1.376(7)	C(24C)-C(25C)	1.389(7)
C(14B)-C(15B)	1.367(7)	C(25C)-C(26C)	1.379(6)
C(15B)-C(16B)	1.383(7)	C(31C)-C(32C)	1.529(6)
C(21B)-C(22B)	1.387(6)	C(32C)-C(34C)	1.503(7)
C(21B)-C(26B)	1.408(6)	C(32C)-C(33C)	1.542(7)
C(22B)-C(23B)	1.390(6)	C(41C)-C(42C)	1.484(7)
C(23B)-C(24B)	1.370(7)	P(1D)-O(12D)	1.471(3)
C(24B)-C(25B)	1.371(6)	P(1D)-O(11D)	1.611(3)
C(25B)-C(26B)	1.390(6)	P(1D)-C(21D)	1.784(4)

P(1D)-C(31D)	1.836(4)	O(22A)-P(2A)-C(1A)	113.27(19)
P(2D)-O(22D)	1.474(3)	O(21A)-P(2A)-C(1A)	98.11(18)
P(2D)-O(21D)	1.577(3)	C(11A)-P(2A)-C(1A)	108.8(2)
P(2D)-C(11D)	1.786(4)	C(1A)-O(11A)-P(1A)	121.2(3)
P(2D)-C(1D)	1.819(4)	C(41A)-O(21A)-P(2A)	121.6(3)
O(11D)-C(1D)	1.452(5)	O(11A)-C(1A)-C(2A)	110.2(3)
O(13D)-C(31D)	1.424(5)	O(11A)-C(1A)-P(2A)	106.6(3)
O(21D)-C(41D)	1.450(5)	C(2A)-C(1A)-P(2A)	113.5(3)
C(1D)-C(2D)	1.521(6)	C(1A)-C(2A)-C(3A)	116.8(4)
C(2D)-C(3D)	1.535(6)	C(5A)-C(3A)-C(2A)	113.5(4)
C(3D)-C(4D)	1.512(6)	C(5A)-C(3A)-C(4A)	110.3(4)
C(3D)-C(5D)	1.527(6)	C(2A)-C(3A)-C(4A)	108.5(4)
C(11D)-C(12D)	1.386(6)	C(16A)-C(11A)-C(12A)	118.2(4)
C(11D)-C(16D)	1.407(6)	C(16A)-C(11A)-P(2A)	122.2(4)
C(12D)-C(13D)	1.377(6)	C(12A)-C(11A)-P(2A)	119.5(4)
C(13D)-C(14D)	1.379(6)	C(13A)-C(12A)-C(11A)	120.4(5)
C(14D)-C(15D)	1.375(6)	C(14A)-C(13A)-C(12A)	120.4(5)
C(15D)-C(16D)	1.380(6)	C(13A)-C(14A)-C(15A)	119.7(5)
C(21D)-C(22D)	1.403(6)	C(16A)-C(15A)-C(14A)	120.0(5)
C(21D)-C(26D)	1.412(6)	C(15A)-C(16A)-C(11A)	121.4(5)
C(22D)-C(23D)	1.376(6)	C(22A)-C(21A)-C(26A)	118.4(4)
C(23D)-C(24D)	1.376(7)	C(22A)-C(21A)-P(1A)	119.2(4)
C(24D)-C(25D)	1.387(7)	C(26A)-C(21A)-P(1A)	122.0(4)
C(25D)-C(26D)	1.362(6)	C(21A)-C(22A)-C(23A)	120.7(5)
C(31D)-C(32D)	1.526(6)	C(24A)-C(23A)-C(22A)	120.3(5)
C(32D)-C(34D)	1.524(6)	C(23A)-C(24A)-C(25A)	120.1(4)
C(32D)-C(33D)	1.527(6)	C(24A)-C(25A)-C(26A)	120.0(5)
C(4D)-C(42D)	1.485(6)	C(25A)-C(26A)-C(21A)	120.4(5)
		O(13A)-C(31A)-C(32A)	110.7(4)
O(12A)-P(1A)-O(11A)	112.85(16)	O(13A)-C(31A)-P(1A)	109.7(3)
O(12A)-P(1A)-C(21A)	113.6(2)	C(32A)-C(31A)-P(1A)	113.0(3)
O(11A)-P(1A)-C(21A)	104.46(18)	C(33A)-C(32A)-C(34A)	110.0(5)
O(12A)-P(1A)-C(31A)	115.5(2)	C(33A)-C(32A)-C(31A)	112.8(4)
O(11A)-P(1A)-C(31A)	103.96(19)	C(34A)-C(32A)-C(31A)	109.6(4)
C(21A)-P(1A)-C(31A)	105.4(2)	O(21A)-C(41A)-C(42A)	108.3(4)
O(22A)-P(2A)-O(21A)	116.31(18)	O(12B)-P(1B)-O(11B)	114.46(16)
O(22A)-P(2A)-C(11A)	112.2(2)	O(12B)-P(1B)-C(21B)	113.8(2)
O(21A)-P(2A)-C(11A)	107.05(19)	O(11B)-P(1B)-C(21B)	102.13(18)

O(12B)-P(1B)-C(31B)	114.0(2)	C(34B)-C(32B)-C(31B)	112.2(4)
O(11B)-P(1B)-C(31B)	101.27(18)	C(33B)-C(32B)-C(31B)	110.9(4)
C(21B)-P(1B)-C(31B)	109.8(2)	O(21B)-C(41B)-C(42B)	110.7(4)
O(22B)-P(2B)-O(21B)	116.34(18)	O(12C)-P(1C)-O(11C)	114.11(17)
O(22B)-P(2B)-C(11B)	111.1(2)	O(12C)-P(1C)-C(21C)	113.9(2)
O(21B)-P(2B)-C(11B)	107.0(2)	O(11C)-P(1C)-C(21C)	102.78(18)
O(22B)-P(2B)-C(1B)	113.35(19)	O(12C)-P(1C)-C(31C)	113.06(19)
O(21B)-P(2B)-C(1B)	99.12(18)	O(11C)-P(1C)-C(31C)	103.38(19)
C(11B)-P(2B)-C(1B)	109.1(2)	C(21C)-P(1C)-C(31C)	108.6(2)
C(1B)-O(11B)-P(1B)	122.4(3)	O(22C)-P(2C)-O(21C)	116.0(2)
C(41B)-O(21B)-P(2B)	121.7(3)	O(22C)-P(2C)-C(11C)	112.0(2)
O(11B)-C(1B)-C(2B)	109.8(3)	O(21C)-P(2C)-C(11C)	107.2(2)
O(11B)-C(1B)-P(2B)	106.9(3)	O(22C)-P(2C)-C(1C)	113.5(2)
C(2B)-C(1B)-P(2B)	114.2(3)	O(21C)-P(2C)-C(1C)	97.8(2)
C(1B)-C(2B)-C(3B)	115.3(4)	C(11C)-P(2C)-C(1C)	109.3(2)
C(4B)-C(3B)-C(2B)	111.9(4)	C(1C)-O(11C)-P(1C)	122.0(3)
C(4B)-C(3B)-C(5B)	111.4(4)	C(41C)-O(21C)-P(2C)	124.1(4)
C(2B)-C(3B)-C(5B)	109.1(4)	O(11C)-C(1C)-C(2C)	110.6(3)
C(16B)-C(11B)-C(12B)	119.0(5)	O(11C)-C(1C)-P(2C)	107.2(3)
C(16B)-C(11B)-P(2B)	122.0(4)	C(2C)-C(1C)-P(2C)	112.3(3)
C(12B)-C(11B)-P(2B)	118.9(4)	C(1C)-C(2C)-C(3C)	117.4(4)
C(13B)-C(12B)-C(11B)	121.0(5)	C(2C)-C(3C)-C(5C)	113.9(5)
C(14B)-C(13B)-C(12B)	119.5(5)	C(2C)-C(3C)-C(4C)	108.8(4)
C(15B)-C(14B)-C(13B)	119.6(5)	C(5C)-C(3C)-C(4C)	110.3(5)
C(14B)-C(15B)-C(16B)	121.9(5)	C(12C)-C(11C)-C(16C)	118.7(5)
C(15B)-C(16B)-C(11B)	119.0(5)	C(12C)-C(11C)-P(2C)	119.4(4)
C(22B)-C(21B)-C(26B)	118.3(4)	C(16C)-C(11C)-P(2C)	121.9(4)
C(22B)-C(21B)-P(1B)	123.1(4)	C(11C)-C(12C)-C(13C)	120.8(5)
C(26B)-C(21B)-P(1B)	118.6(3)	C(14C)-C(13C)-C(12C)	119.4(5)
C(21B)-C(22B)-C(23B)	121.6(5)	C(15C)-C(14C)-C(13C)	120.7(5)
C(24B)-C(23B)-C(22B)	118.8(5)	C(14C)-C(15C)-C(16C)	119.6(5)
C(23B)-C(24B)-C(25B)	121.4(4)	C(15C)-C(16C)-C(11C)	120.9(5)
C(24B)-C(25B)-C(26B)	120.1(5)	C(26C)-C(21C)-C(22C)	117.8(4)
C(25B)-C(26B)-C(21B)	119.8(4)	C(26C)-C(21C)-P(1C)	123.1(4)
O(13B)-C(31B)-C(32B)	106.0(3)	C(22C)-C(21C)-P(1C)	118.9(4)
O(13B)-C(31B)-P(1B)	107.3(3)	C(23C)-C(22C)-C(21C)	119.9(5)
C(32B)-C(31B)-P(1B)	114.0(3)	C(24C)-C(23C)-C(22C)	122.1(5)
C(34B)-C(32B)-C(33B)	109.7(4)	C(23C)-C(24C)-C(25C)	119.2(5)

C(26C)-C(25C)-C(24C)	119.2(5)	C(4D)-C(3D)-C(5D)	110.3(4)
C(25C)-C(26C)-C(21C)	121.8(5)	C(4D)-C(3D)-C(2D)	113.0(4)
O(13C)-C(31C)-C(32C)	105.5(4)	C(5D)-C(3D)-C(2D)	109.6(4)
O(13C)-C(31C)-P(1C)	108.9(3)	C(12D)-C(11D)-C(16D)	118.7(4)
C(32C)-C(31C)-P(1C)	114.1(3)	C(12D)-C(11D)-P(2D)	119.4(4)
C(34C)-C(32C)-C(31C)	114.9(4)	C(16D)-C(11D)-P(2D)	121.9(3)
C(34C)-C(32C)-C(33C)	108.9(4)	C(13D)-C(12D)-C(11D)	121.0(4)
C(31C)-C(32C)-C(33C)	110.2(4)	C(12D)-C(13D)-C(14D)	119.5(4)
O(21C)-C(41C)-C(42C)	110.0(5)	C(15D)-C(14D)-C(13D)	120.9(5)
O(12D)-P(1D)-O(11D)	114.54(16)	C(14D)-C(15D)-C(16D)	119.9(5)
O(12D)-P(1D)-C(21D)	113.9(2)	C(15D)-C(16D)-C(11D)	120.0(4)
O(11D)-P(1D)-C(21D)	102.55(18)	C(22D)-C(21D)-C(26D)	118.6(4)
O(12D)-P(1D)-C(31D)	113.16(19)	C(22D)-C(21D)-P(1D)	119.6(3)
O(11D)-P(1D)-C(31D)	101.64(18)	C(26D)-C(21D)-P(1D)	121.8(4)
C(21D)-P(1D)-C(31D)	109.9(2)	C(23D)-C(22D)-C(21D)	119.6(4)
O(22D)-P(2D)-O(21D)	115.83(17)	C(22D)-C(23D)-C(24D)	120.8(5)
O(22D)-P(2D)-C(11D)	111.08(19)	C(23D)-C(24D)-C(25D)	120.3(4)
O(21D)-P(2D)-C(11D)	106.07(19)	C(26D)-C(25D)-C(24D)	119.9(5)
O(22D)-P(2D)-C(1D)	113.18(19)	C(25D)-C(26D)-C(21D)	120.7(5)
O(21D)-P(2D)-C(1D)	99.24(18)	O(13D)-C(31D)-C(32D)	107.4(3)
C(11D)-P(2D)-C(1D)	110.7(2)	O(13D)-C(31D)-P(1D)	106.2(3)
C(1D)-O(11D)-P(1D)	122.5(2)	C(32D)-C(31D)-P(1D)	114.0(3)
C(41D)-O(21D)-P(2D)	119.6(3)	C(34D)-C(32D)-C(31D)	113.2(4)
O(11D)-C(1D)-C(2D)	109.7(3)	C(34D)-C(32D)-C(33D)	109.3(4)
O(11D)-C(1D)-P(2D)	106.8(3)	C(31D)-C(32D)-C(33D)	109.9(4)
C(2D)-C(1D)-P(2D)	114.0(3)	O(21D)-C(41D)-C(42D)	109.2(4)
C(1D)-C(2D)-C(3D)	115.4(4)	:	

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for MR048d2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1A)	24(1)	29(1)	29(1)	-12(1)	-2(1)	3(1)
P(2A)	27(1)	31(1)	31(1)	-9(1)	3(1)	0(1)
O(11A)	23(2)	29(2)	28(2)	-13(2)	-5(1)	5(1)
O(12A)	30(2)	35(2)	36(2)	-14(2)	-7(2)	4(2)
O(13A)	31(2)	29(2)	57(3)	-14(2)	4(2)	-4(2)

O(21A)	22(2)	45(2)	33(2)	-9(2)	3(1)	2(2)
O(22A)	42(2)	28(2)	42(2)	-5(2)	5(2)	-3(2)
C(1A)	15(2)	28(3)	27(3)	-10(2)	1(2)	3(2)
C(2A)	34(3)	25(3)	36(3)	-10(2)	2(2)	4(2)
C(3A)	44(3)	31(3)	32(3)	-9(3)	8(2)	-1(2)
C(4A)	77(4)	37(4)	46(4)	-11(3)	21(3)	-15(3)
C(5A)	94(4)	43(4)	33(4)	-5(3)	-3(3)	-5(3)
C(11A)	23(2)	26(3)	27(3)	-6(2)	4(2)	3(2)
C(12A)	40(3)	32(3)	30(3)	-8(3)	-4(2)	6(2)
C(13A)	45(3)	48(4)	39(4)	-8(3)	-13(3)	9(3)
C(14A)	49(3)	57(4)	20(3)	-10(3)	-6(2)	-9(3)
C(15A)	55(3)	35(3)	36(3)	-16(3)	-3(3)	3(3)
C(16A)	40(3)	36(3)	34(3)	-9(3)	-6(2)	14(2)
C(21A)	43(3)	18(3)	29(3)	-16(2)	-8(2)	5(2)
C(22A)	37(3)	26(3)	31(3)	-1(2)	-2(2)	-2(2)
C(23A)	35(3)	44(4)	54(4)	-12(3)	13(3)	-7(3)
C(24A)	22(3)	43(4)	63(4)	-25(3)	9(3)	-5(2)
C(25A)	22(3)	46(4)	56(4)	-27(3)	-12(3)	5(2)
C(26A)	31(3)	44(4)	31(3)	-15(3)	-1(2)	-3(2)
C(31A)	29(3)	25(3)	36(3)	-9(2)	-2(2)	0(2)
C(32A)	45(3)	31(3)	44(4)	-12(3)	-6(3)	0(2)
C(33A)	121(5)	48(4)	50(4)	-25(4)	-8(4)	3(4)
C(34A)	108(5)	33(4)	67(5)	-17(3)	-23(4)	19(3)
C(41A)	27(3)	58(4)	49(4)	-21(3)	11(3)	1(3)
C(42A)	31(3)	64(4)	69(4)	-25(4)	0(3)	6(3)
P(1B)	23(1)	27(1)	24(1)	-3(1)	2(1)	-3(1)
P(2B)	27(1)	34(1)	23(1)	-2(1)	-2(1)	2(1)
O(11B)	26(2)	25(2)	24(2)	-3(2)	7(1)	-3(1)
O(12B)	30(2)	28(2)	34(2)	-5(2)	6(2)	-5(1)
O(13B)	33(2)	51(3)	31(2)	-22(2)	-10(2)	5(2)
O(21B)	22(2)	56(3)	40(2)	1(2)	1(2)	4(2)
O(22B)	45(2)	36(2)	24(2)	-8(2)	-9(2)	8(2)
C(1B)	19(2)	25(3)	24(3)	1(2)	6(2)	1(2)
C(2B)	35(3)	31(3)	20(3)	-4(2)	2(2)	3(2)
C(3B)	49(3)	42(4)	21(3)	-4(3)	1(2)	18(3)
C(4B)	105(5)	33(4)	31(4)	0(3)	2(3)	1(3)
C(5B)	65(4)	67(4)	28(3)	-5(3)	-16(3)	16(3)
C(11B)	30(3)	28(3)	15(3)	1(2)	1(2)	4(2)

C(12B)	33(3)	32(3)	24(3)	-7(2)	1(2)	6(2)
C(13B)	38(3)	41(4)	33(3)	-3(3)	-2(2)	6(3)
C(14B)	47(3)	31(3)	44(4)	-9(3)	-8(3)	-5(3)
C(15B)	49(3)	43(4)	39(4)	-23(3)	-3(3)	11(3)
C(16B)	40(3)	41(4)	22(3)	-5(3)	2(2)	9(3)
C(21B)	27(3)	28(3)	21(3)	-9(2)	9(2)	-6(2)
C(22B)	33(3)	36(3)	25(3)	-10(2)	1(2)	-7(2)
C(23B)	32(3)	47(4)	28(3)	-16(3)	4(2)	-9(2)
C(24B)	27(3)	43(4)	44(4)	-22(3)	-4(3)	9(3)
C(25B)	41(3)	34(3)	37(3)	-8(3)	-15(3)	5(3)
C(26B)	37(3)	28(3)	32(3)	-4(3)	0(2)	-3(2)
C(31B)	24(3)	27(3)	18(3)	-3(2)	-1(2)	0(2)
C(32B)	32(3)	33(3)	26(3)	-7(3)	3(2)	-6(2)
C(33B)	48(3)	47(4)	37(3)	-17(3)	-2(3)	6(3)
C(34B)	61(4)	43(4)	41(4)	-20(3)	-6(3)	9(3)
C(41B)	36(3)	46(4)	50(4)	-4(3)	-8(3)	10(3)
C(42B)	36(3)	64(4)	68(4)	-29(4)	4(3)	7(3)
P(1C)	22(1)	31(1)	33(1)	-11(1)	1(1)	0(1)
P(2C)	30(1)	35(1)	47(1)	-11(1)	-8(1)	0(1)
O(11C)	26(2)	30(2)	34(2)	-11(2)	2(1)	-2(1)
O(12C)	27(2)	47(2)	30(2)	-14(2)	6(2)	-2(2)
O(13C)	34(2)	35(2)	57(3)	-20(2)	-11(2)	12(2)
O(21C)	19(2)	67(3)	80(3)	-12(2)	-8(2)	-2(2)
O(22C)	53(2)	30(2)	53(3)	-10(2)	-14(2)	5(2)
C(1C)	25(3)	28(3)	38(3)	-10(3)	4(2)	-6(2)
C(2C)	42(3)	30(3)	40(3)	-11(3)	-2(2)	2(2)
C(3C)	71(4)	32(3)	33(3)	-4(3)	-4(3)	-4(3)
C(4C)	111(5)	36(4)	57(4)	-7(3)	-27(4)	20(4)
C(5C)	167(7)	56(5)	33(4)	-2(3)	28(4)	5(4)
C(11C)	28(3)	29(3)	41(3)	-13(3)	-13(2)	-4(2)
C(12C)	47(3)	32(3)	35(3)	-4(3)	-11(3)	-5(3)
C(13C)	58(4)	39(4)	34(3)	-9(3)	-2(3)	-5(3)
C(14C)	57(4)	48(4)	28(3)	-9(3)	-7(3)	8(3)
C(15C)	73(4)	38(4)	41(4)	-17(3)	-19(3)	-7(3)
C(16C)	47(3)	37(4)	35(3)	-8(3)	-9(3)	-9(3)
C(21C)	35(3)	28(3)	35(3)	-16(3)	4(2)	1(2)
C(22C)	29(3)	40(3)	43(4)	-10(3)	-1(2)	0(2)
C(23C)	41(3)	48(4)	47(4)	-14(3)	-12(3)	11(3)

C(24C)	21(3)	49(4)	80(5)	-30(4)	-14(3)	8(3)
C(25C)	33(3)	35(4)	62(4)	-6(3)	8(3)	0(2)
C(26C)	34(3)	34(3)	34(3)	-5(3)	2(2)	3(2)
C(31C)	29(3)	23(3)	31(3)	-6(2)	4(2)	3(2)
C(32C)	39(3)	31(3)	49(4)	-14(3)	0(3)	-2(2)
C(33C)	62(4)	31(3)	45(4)	-15(3)	-3(3)	0(3)
C(34C)	82(4)	57(4)	69(5)	-29(4)	-32(4)	16(3)
C(41C)	31(3)	77(5)	61(4)	-34(4)	-8(3)	3(3)
C(42C)	29(3)	97(6)	123(6)	-71(5)	8(3)	-14(3)
P(1D)	25(1)	21(1)	23(1)	-4(1)	-3(1)	1(1)
P(2D)	26(1)	25(1)	22(1)	-3(1)	-1(1)	-1(1)
O(11D)	30(2)	17(2)	19(2)	-2(1)	-3(1)	-1(1)
O(12D)	30(2)	24(2)	31(2)	-3(2)	-8(1)	5(1)
O(13D)	35(2)	43(2)	34(2)	-20(2)	9(2)	-6(2)
O(21D)	24(2)	30(2)	30(2)	1(2)	-1(1)	-2(1)
O(22D)	40(2)	29(2)	21(2)	-6(2)	6(1)	-6(2)
C(1D)	25(2)	17(3)	21(3)	-3(2)	-9(2)	0(2)
C(2D)	36(3)	17(3)	20(3)	-3(2)	-1(2)	-7(2)
C(3D)	57(3)	21(3)	21(3)	-4(2)	5(2)	-9(2)
C(4D)	90(4)	30(3)	34(4)	1(3)	9(3)	3(3)
C(5D)	76(4)	41(4)	29(3)	-5(3)	14(3)	-16(3)
C(11D)	24(2)	18(3)	19(3)	5(2)	-1(2)	-1(2)
C(12D)	29(3)	31(3)	25(3)	-7(2)	2(2)	-5(2)
C(13D)	28(3)	27(3)	31(3)	-3(3)	-3(2)	2(2)
C(14D)	40(3)	20(3)	37(3)	-6(3)	10(3)	3(2)
C(15D)	34(3)	38(3)	31(3)	-18(3)	3(2)	-7(2)
C(16D)	29(3)	31(3)	26(3)	-3(2)	1(2)	-7(2)
C(21D)	38(3)	20(3)	19(3)	-6(2)	-4(2)	0(2)
C(22D)	34(3)	26(3)	31(3)	-8(3)	-6(2)	-2(2)
C(23D)	39(3)	36(3)	33(3)	-7(3)	5(2)	-12(3)
C(24D)	23(3)	48(4)	53(4)	-31(3)	7(3)	-9(3)
C(25D)	29(3)	45(4)	38(3)	-21(3)	-2(2)	6(2)
C(26D)	35(3)	29(3)	20(3)	-7(2)	2(2)	0(2)
C(31D)	18(2)	32(3)	26(3)	-8(2)	-1(2)	2(2)
C(32D)	32(3)	34(3)	35(3)	-17(3)	-6(2)	6(2)
C(33D)	54(3)	54(4)	40(4)	-26(3)	10(3)	-5(3)
C(34D)	53(3)	49(4)	50(4)	-32(3)	13(3)	-16(3)
C(41D)	31(3)	38(3)	53(4)	-16(3)	2(3)	-8(2)

C(42D)	35(3)	55(4)	75(5)	-24(4)	-7(3)	-8(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for MR048d2.

	x	y	z	U(eq)
H(13O)	6140(50)	2360(20)	6630(20)	41(16)
H(1A)	5868	3653	5854	28
H(2A1)	7583	4405	6333	37
H(2A2)	6010	4583	5997	37
H(3A)	8847	4357	5476	43
H(4A1)	8924	5368	5057	80
H(4A2)	8846	5233	5743	80
H(4A3)	7336	5452	5372	80
H(5A1)	6783	4145	4963	87
H(5A2)	7665	4706	4584	87
H(5A3)	6062	4780	4895	87
H(12A)	7830	3129	7689	41
H(13B)	9000	3564	8315	54
H(14A)	8217	4485	8354	50
H(15A)	6215	4969	7773	49
H(16A)	5057	4541	7148	44
H(22A)	9896	3322	4747	39
H(23A)	12495	3357	4490	54
H(24A)	14343	3003	5186	49
H(25A)	13627	2702	6156	47
H(26A)	11030	2680	6424	41
H(31A)	8592	2167	6601	36
H(32A)	9608	1824	5837	48
H(33J)	7974	1422	5297	106
H(33K)	7688	2108	5160	106
H(33L)	6509	1668	5570	106
H(34J)	7410	1038	6505	103
H(34K)	9019	1166	6753	103
H(34L)	8990	862	6243	103
H(41A)	2694	3738	7390	52

H(41B)	2316	3226	7107	52
H(42A)	1465	4414	6614	80
H(42B)	292	3922	6947	80
H(42C)	1058	3896	6347	80
H(13P)	10700(50)	3360(20)	2343(19)	23(15)
H(1B)	11029	3652	1023	29
H(2B1)	8896	2937	666	35
H(2B2)	10539	3095	361	35
H(3B)	8223	3956	380	46
H(4B1)	10678	4351	230	87
H(4B2)	9708	4583	-347	87
H(4B3)	10980	4080	-297	87
H(5B1)	7690	3970	-585	83
H(5B2)	7339	3344	-153	83
H(5B3)	8881	3441	-538	83
H(12B)	8947	1974	2154	36
H(13C)	7779	1124	2103	47
H(14B)	8575	686	1396	49
H(15B)	10480	1106	743	50
H(16B)	11666	1955	783	42
H(22B)	5886	3550	2017	37
H(23B)	3321	3810	1792	42
H(24B)	2769	4630	1044	43
H(25B)	4714	5197	524	45
H(26B)	7289	4961	760	40
H(31B)	8237	3596	2570	29
H(32B)	9865	4667	2416	37
H(33A)	8546	3986	3476	65
H(33B)	9557	4555	3394	65
H(33C)	10343	3968	3324	65
H(34A)	7361	4896	2111	70
H(34B)	7532	5040	2714	70
H(34C)	6681	4462	2689	70
H(41C)	14167	2036	1526	55
H(41D)	14461	2543	1823	55
H(42D)	15460	2549	703	81
H(42E)	16549	2471	1246	81
H(42F)	15687	3080	972	81

H(13Q)	8770(50)	7340(20)	1750(20)	24(16)
H(1C)	9167	8604	959	36
H(2C1)	8784	9542	1085	45
H(2C2)	7153	9353	1384	45
H(3C)	6165	9291	510	55
H(4C1)	5943	10181	754	104
H(4C2)	6018	10298	69	104
H(4C3)	7505	10399	406	104
H(5C1)	9088	9674	1	132
H(5C2)	7580	9665	-364	132
H(5C3)	8311	9068	22	132
H(12C)	6940	8161	2784	47
H(13D)	5629	8623	3389	53
H(14C)	6299	9559	3382	54
H(15C)	8265	10035	2781	59
H(16C)	9551	9578	2171	48
H(22C)	5326	8353	-167	45
H(23C)	2773	8402	-418	54
H(24C)	863	8037	251	57
H(25C)	1505	7652	1225	54
H(26C)	4071	7592	1487	42
H(31C)	6492	7050	1631	34
H(32C)	8271	6761	734	47
H(33D)	8430	6088	1683	68
H(33E)	7825	5794	1212	68
H(33F)	6635	5964	1654	68
H(34G)	5032	6657	877	100
H(34H)	6028	6333	494	100
H(34I)	5938	7028	316	100
H(41G)	12516	8201	2133	64
H(41H)	12193	8698	2448	64
H(42J)	13679	8887	1359	112
H(42K)	14543	8850	1946	112
H(42L)	13376	9378	1682	112
H(13R)	5472	1595	2662	53
H(1D)	5717	1305	4007	26
H(2D1)	3567	2100	4300	30
H(2D2)	5119	1885	4642	30

H(3D)	2650	1125	4596	40
H(4D1)	5304	863	5300	80
H(4D2)	4941	593	4783	80
H(4D3)	3887	434	5354	80
H(5D1)	2032	1130	5550	75
H(5D2)	1880	1772	5124	75
H(5D3)	3351	1593	5526	75
H(12D)	3820	3042	2846	34
H(13F)	2831	3938	2883	35
H(14D)	3784	4378	3547	40
H(15D)	5621	3908	4205	39
H(16D)	6582	2999	4188	36
H(22D)	2080	20	4282	36
H(23D)	-484	-190	4525	44
H(24D)	-2434	367	3987	46
H(25D)	-1841	1174	3217	42
H(26D)	692	1421	2991	34
H(31D)	3107	1366	2442	31
H(32D)	4650	257	2615	39
H(33G)	3546	1003	1551	70
H(33H)	4325	376	1623	70
H(33I)	5325	897	1712	70
H(34D)	2048	120	2900	70
H(34E)	2356	-85	2332	70
H(34F)	1520	526	2287	70
H(41E)	8805	2898	3432	48
H(41F)	9302	2379	3164	48
H(42G)	10034	2424	4288	80
H(42H)	11235	2521	3761	80
H(42I)	10500	1895	4033	80

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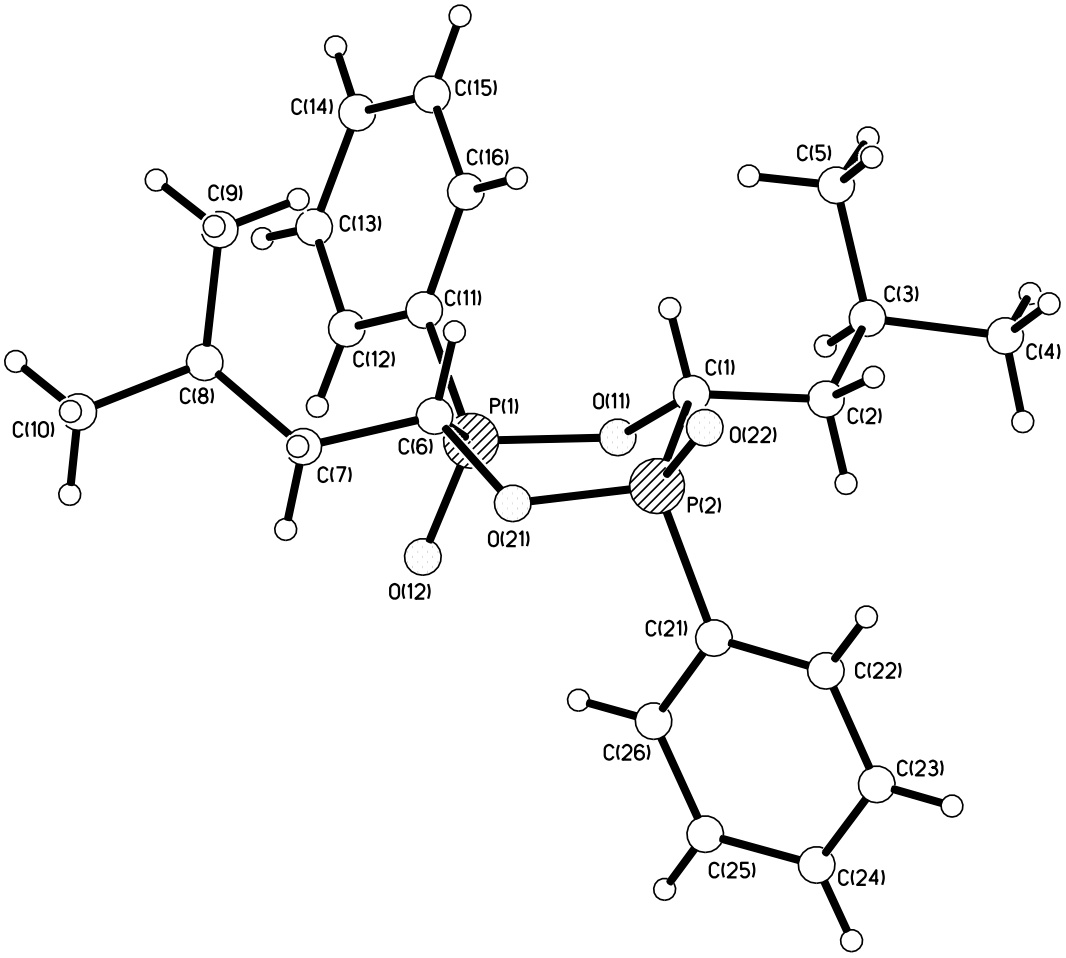

Table 1. Crystal data and structure refinement for MR226.

Identification code	mr_mr226_0m	
Empirical formula	C22 H30 O4 P2	
Formula weight	420.40	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.5472(6) Å	α= 70.696(3)°.
	b = 11.5689(9) Å	β= 79.604(2)°.
	c = 11.7515(9) Å	γ = 74.616(2)°.

Volume	1174.94(15) $Å^3$
Z	2
Density (calculated)	1.188 Mg/m^3
Absorption coefficient	0.208 mm^{-1}
F(000)	448
Crystal size	0.23 x 0.21 x 0.19 mm^3
Theta range for data collection	1.85 to 28.69°.
Index ranges	-12<=h<=10, -15<=k<=14, -15<=l<=13
Reflections collected	10825
Independent reflections	5486 [R(int) = 0.0290]
Completeness to theta = 28.69°	90.4 %
Absorption correction	None
Max. and min. transmission	0.9623 and 0.9531
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5486 / 0 / 257
Goodness-of-fit on F^2	0.877
Final R indices [I>2sigma(I)]	R1 = 0.0479, wR2 = 0.1260
R indices (all data)	R1 = 0.0894, wR2 = 0.1747
Largest diff. peak and hole	0.404 and -0.431 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for MR226. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)

P(1)	7943(1)	2800(1)	7816(1)	38(1)
P(2)	8131(1)	5747(1)	6243(1)	35(1)
C(11)	9174(3)	1289(3)	8012(2)	44(1)
C(16)	10585(3)	1146(3)	7411(3)	55(1)
C(12)	8714(4)	235(3)	8817(3)	63(1)
C(15)	11520(4)	-28(4)	7631(4)	74(1)
C(14)	11076(6)	-1058(4)	8429(4)	86(1)
C(13)	9694(6)	-941(3)	9012(4)	87(1)
C(1)	9517(2)	4588(2)	7167(2)	36(1)
C(2)	10293(3)	5188(3)	7758(3)	45(1)
C(3)	11552(3)	4325(3)	8476(3)	56(1)
C(5)	12706(4)	3627(5)	7739(5)	108(2)
C(4)	12196(4)	5099(4)	8996(4)	86(1)
C(6)	7702(3)	3572(2)	6195(2)	38(1)
C(7)	6568(3)	3178(3)	5732(3)	53(1)
C(8)	6957(4)	1842(3)	5658(3)	63(1)
C(10)	5655(5)	1571(5)	5274(5)	107(2)
C(9)	8333(5)	1585(4)	4801(5)	98(2)
C(21)	6939(3)	6649(2)	7159(2)	36(1)
C(26)	5872(3)	6165(3)	8038(2)	42(1)
C(25)	5049(3)	6848(3)	8795(3)	50(1)
C(24)	5286(3)	8002(3)	8690(3)	60(1)
C(22)	7156(3)	7823(3)	7052(3)	55(1)
C(23)	6328(4)	8490(3)	7828(4)	68(1)
O(21)	7136(2)	4914(2)	6091(2)	42(1)

O(22)	8810(2)	6515(2)	5117(2)	50(1)
O(11)	8824(2)	3652(2)	8107(2)	40(1)
O(12)	6555(2)	2743(2)	8590(2)	57(1)

Table 3. Bond lengths [Å] and angles [°] for MR226.

P(1)-O(12)	1.4701(19)	C(7)-C(8)	1.519(5)
P(1)-O(11)	1.601(2)	C(8)-C(9)	1.530(5)
P(1)-C(11)	1.797(3)	C(8)-C(10)	1.533(5)
P(1)-C(6)	1.845(3)	C(21)-C(22)	1.390(4)
P(2)-O(22)	1.4764(19)	C(21)-C(26)	1.399(3)
P(2)-O(21)	1.589(2)	C(26)-C(25)	1.384(4)
P(2)-C(21)	1.792(2)	C(25)-C(24)	1.375(5)
P(2)-C(1)	1.828(2)	C(24)-C(23)	1.375(5)
C(11)-C(12)	1.395(4)	C(22)-C(23)	1.390(5)
C(11)-C(16)	1.399(4)	O(12)-P(1)-O(11)	112.04(12)
C(16)-C(15)	1.384(4)	O(12)-P(1)-C(11)	112.96(13)
C(12)-C(13)	1.405(5)	O(11)-P(1)-C(11)	105.22(12)
C(15)-C(14)	1.366(6)	O(12)-P(1)-C(6)	113.21(12)
C(14)-C(13)	1.367(6)	O(11)-P(1)-C(6)	102.69(11)
C(1)-O(11)	1.468(3)	C(11)-P(1)-C(6)	109.96(12)
C(1)-C(2)	1.512(4)	O(22)-P(2)-O(21)	116.58(12)
C(2)-C(3)	1.526(4)	O(22)-P(2)-C(21)	113.78(12)
C(3)-C(5)	1.504(5)	O(21)-P(2)-C(21)	103.03(11)
C(3)-C(4)	1.530(5)	O(22)-P(2)-C(1)	111.12(11)
C(6)-O(21)	1.472(3)	O(21)-P(2)-C(1)	103.04(11)
C(6)-C(7)	1.521(4)	C(21)-P(2)-C(1)	108.38(12)

C(12)-C(11)-C(16)	119.3(3)	O(21)-C(6)-P(1)	104.92(16)
C(12)-C(11)-P(1)	118.6(2)	C(7)-C(6)-P(1)	114.7(2)
C(16)-C(11)-P(1)	122.0(2)	C(8)-C(7)-C(6)	116.2(2)
C(15)-C(16)-C(11)	120.1(3)	C(7)-C(8)-C(9)	112.8(3)
C(11)-C(12)-C(13)	118.8(4)	C(7)-C(8)-C(10)	109.3(3)
C(14)-C(15)-C(16)	120.6(4)	C(9)-C(8)-C(10)	110.7(4)
C(15)-C(14)-C(13)	120.2(4)	C(22)-C(21)-C(26)	119.2(3)
C(14)-C(13)-C(12)	121.0(4)	C(22)-C(21)-P(2)	118.8(2)
O(11)-C(1)-C(2)	109.5(2)	C(26)-C(21)-P(2)	121.8(2)
O(11)-C(1)-P(2)	109.28(15)	C(25)-C(26)-C(21)	120.2(3)
C(2)-C(1)-P(2)	112.02(18)	C(24)-C(25)-C(26)	120.0(3)
C(1)-C(2)-C(3)	116.7(2)	C(25)-C(24)-C(23)	120.4(3)
C(5)-C(3)-C(2)	112.8(3)	C(23)-C(22)-C(21)	119.7(3)
C(5)-C(3)-C(4)	111.4(3)	C(24)-C(23)-C(22)	120.5(3)
C(2)-C(3)-C(4)	108.9(3)	C(6)-O(21)-P(2)	121.67(15)
O(21)-C(6)-C(7)	106.1(2)	C(1)-O(11)-P(1)	123.47(16)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for MR226. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	38(1)	41(1)	33(1)	-12(1)	3(1)	-12(1)
P(2)	34(1)	40(1)	28(1)	-9(1)	2(1)	-7(1)
C(11)	57(2)	41(2)	37(1)	-10(1)	-10(1)	-12(1)
C(16)	58(2)	46(2)	56(2)	-15(1)	-6(1)	-2(1)

C(12)	84(2)	48(2)	60(2)	-5(2)	-12(2)	-28(2)
C(15)	72(2)	61(2)	82(3)	-27(2)	-18(2)	9(2)
C(14)	105(3)	51(2)	98(3)	-24(2)	-41(3)	11(2)
C(13)	135(4)	37(2)	87(3)	3(2)	-39(3)	-25(2)
C(1)	31(1)	42(1)	34(1)	-11(1)	2(1)	-8(1)
C(2)	41(1)	47(2)	47(2)	-12(1)	-7(1)	-12(1)
C(3)	49(2)	56(2)	58(2)	-6(2)	-17(1)	-13(1)
C(5)	55(2)	141(4)	131(4)	-65(4)	-34(2)	21(2)
C(4)	79(3)	98(3)	92(3)	-21(2)	-43(2)	-27(2)
C(6)	36(1)	44(2)	38(1)	-18(1)	-1(1)	-7(1)
C(7)	50(2)	59(2)	56(2)	-22(2)	-12(1)	-11(1)
C(8)	83(2)	51(2)	64(2)	-11(2)	-32(2)	-20(2)
C(10)	120(4)	89(3)	144(5)	-37(3)	-69(3)	-36(3)
C(9)	110(3)	87(3)	117(4)	-70(3)	-14(3)	-7(3)
C(21)	34(1)	37(1)	34(1)	-12(1)	-2(1)	-4(1)
C(26)	37(1)	44(2)	42(2)	-12(1)	3(1)	-8(1)
C(25)	41(1)	59(2)	46(2)	-20(1)	6(1)	-6(1)
C(24)	57(2)	62(2)	61(2)	-33(2)	6(2)	-3(2)
C(22)	57(2)	47(2)	61(2)	-18(2)	10(1)	-18(1)
C(23)	81(2)	44(2)	82(3)	-28(2)	4(2)	-15(2)
O(21)	41(1)	44(1)	44(1)	-16(1)	-11(1)	-4(1)
O(22)	52(1)	52(1)	35(1)	-6(1)	8(1)	-10(1)
O(11)	50(1)	40(1)	30(1)	-8(1)	-3(1)	-14(1)
O(12)	48(1)	72(2)	48(1)	-17(1)	13(1)	-23(1)