Supporting information

Absolute configuration of 3,3'-Diphenyl-[2,2'-binaphthalene]-1,1'-diol revisited

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(A). *X-ray Structure of the Dextrorotary salt from (±)-VANOL Hydrogen Phosphate and Brucine*

Experimental Section:

A colorless block crystal with dimensions 0.56 x 0.51 x 0.39 mm was mounted on a Nylon loop using very small amount of paratone oil.

Data were collected using a Bruker CCD (charge coupled device) based diffractometer equipped with an Oxford Cryostream low-temperature apparatus operating at 173 K. Data were measured using omega and phi scans of 0.5° per frame for 30 s. The total number of images was based on results from the program COSMO[1] where redundancy was expected to be 4.0 and completeness to 0.83 Å to 100%. Cell parameters were retrieved using APEX II software[2] and refined using SAINT on all observed reflections. Data reduction was performed using the SAINT software[3] which corrects for Lp. Scaling and absorption corrections were applied using SADABS[4] multi-scan technique, supplied by George Sheldrick. The structures are solved by the direct method using the SHELXS-97 program and refined by least squares method on F^2, SHELXL- 97, which are incorporated in SHELXTL-PC V 6.10.[5]

The structure was solved in the space group $P2_12_12_1$ (# 19). All non-hydrogen atoms are refined anisotropically. Hydrogens were calculated by geometrical methods and refined as a riding model. The Flack[6] parameter is used to determine chirality of the crystal studied, the value should be near zero, a value of one is the other enantiomer and a value of 0.5 is racemic. The Flack parameter was refined to 0.03(3), confirming the absolute stereochemistry. Determination of absolute structure using Bayesian statistics on Bijvoet differences using the program within Platon[7] also report

that we have the correct enantiomer based on this comparison.[8] All drawings are done at 50% ellipsoids.

References

1. COSMO V1.56, *Software for the CCD Detector Systems for Determining Data Collection Parameters.* Bruker Analytical X-ray Systems, Madison, WI (2006).

2. APEX2 V 1.2-0 Software *for the CCD Detector System*; Bruker Analytical X-ray Systems, Madison, WI (2006).

3. SAINT V 7.34 Software *for the Integration of CCD Detector System* Bruker Analytical X-ray Systems, Madison, WI (2001).

4. SADABS V2.10 Program for absorption corrections using Bruker-AXS CCD based on the method of Robert Blessing; Blessing, R.H. Acta Cryst. A51, 1995, 33-38.

5. Sheldrick, G.M. "A short history of SHELX". *Acta Cryst*. **A64**, 2008, 112-122.

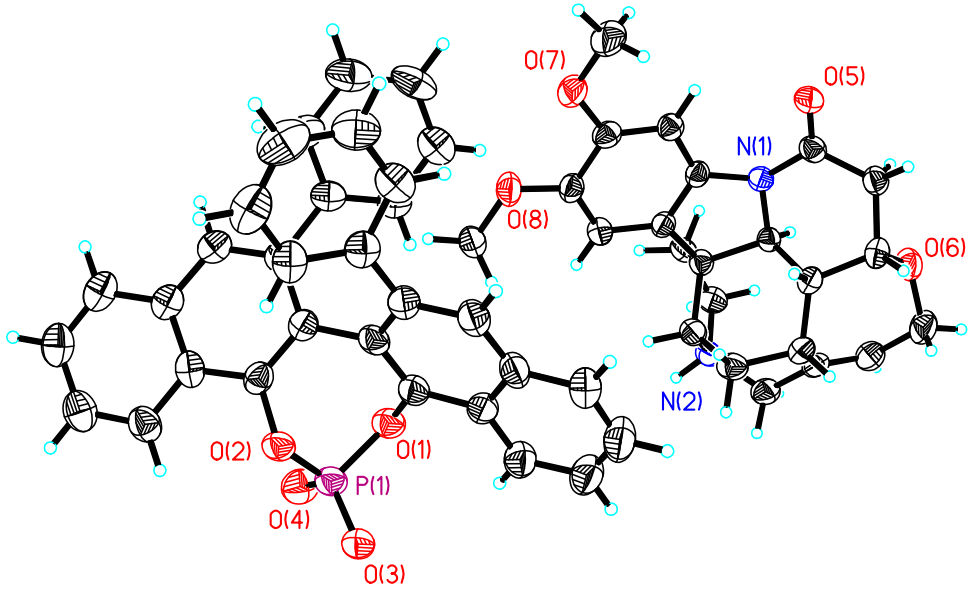
6. Flack, H. D. *Acta Cryst*. **A39**, 1983, 876-881.

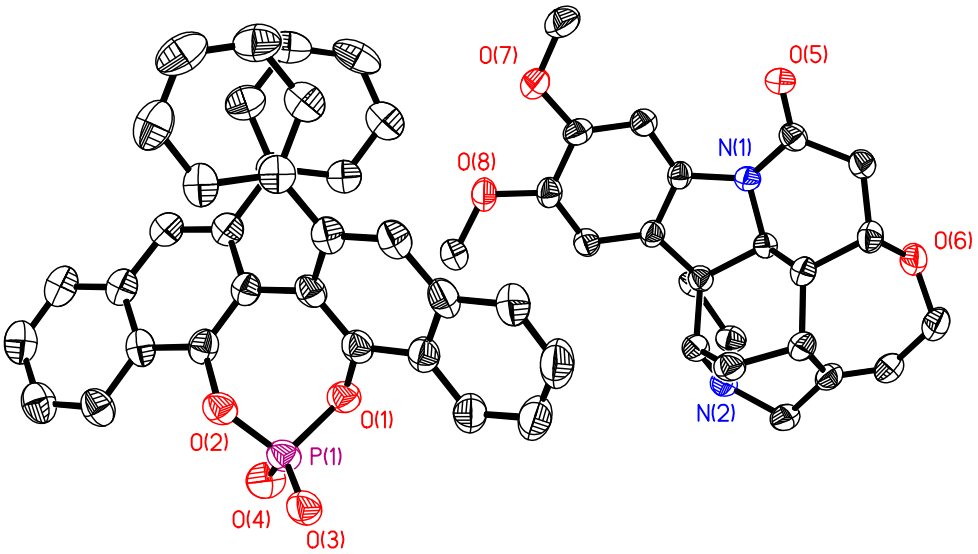
7. Spek, A.L. (2003), J.Appl.Cryst. **36**, 7-13.

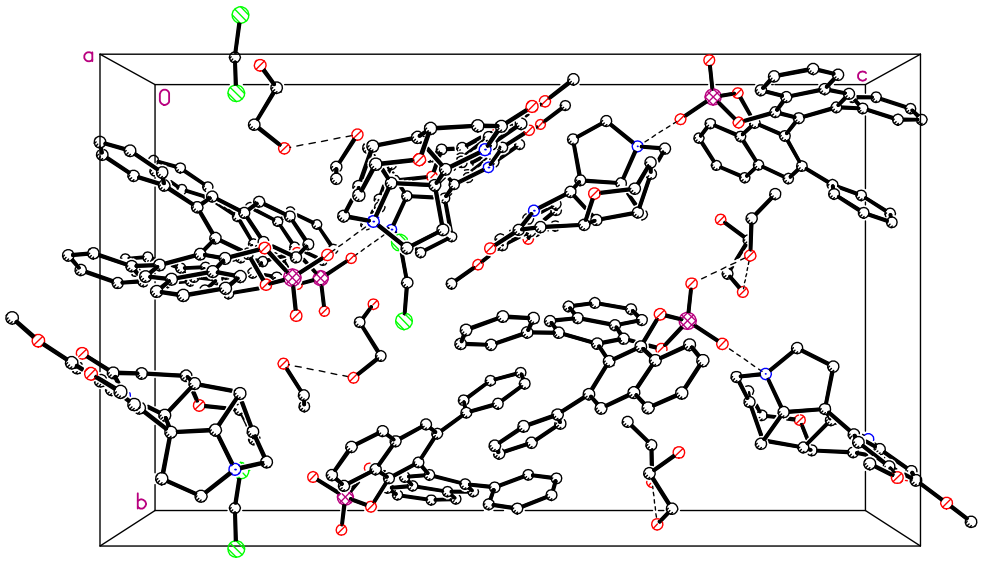
8. Hooft, R.W.W.; Straver, L.H. & A. L. Spek, A.L.. *J. Appl. Cryst.* **41**, *2008,* 96-103

[a] Obtained with graphite monochromated Cu Kα (λ = 1.54178Å) radiation.
[b] $R1 = \sum||F_o| - |F_c||/\sum|F_o|$. [c] $wR_2 = \{\sum[w(F_o^2 - F_c^2)^2/\{\sum[w(F_o^2)^2]\}^{1/2}$.

The following are 50% thermal ellipsoidal drawings of the molecule in the asymmetric cell with various amount of labeling.


O(7)
O(5)
N(1)
O(8)
O(6)
N(2)
O(2)
O(1)
P(1)
O(4)
O(3)


O(7)
O(5)
N(1)
O(8)
O(6)
N(2)
O(2)
O(1)
P(1)
O(4)
O(3)



This is a drawing of the packing along the a-axis where the dotted line represent potential hydrogen bonding.

Table S1. Crystal data and structure refinement for ww05_0m.

Identification code	ww05_0m	
Empirical formula	C62 H67 Cl2 N2 O11 P	
Formula weight	1118.05	
Temperature	173(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 12.3355(2) Å	α= 90°.
	b = 16.4408(2) Å	β= 90°.
	c = 27.3926(4) Å	γ = 90°.
Volume	5555.37(14) $Å^3$	
Z	4	
Density (calculated)	1.337 Mg/m^3	
Absorption coefficient	1.848 mm^{-1}	
F(000)	2360	
Crystal size	0.56 x 0.51 x 0.39 mm^3	
Theta range for data collection	3.13 to 67.69°.	
Index ranges	-14<=h<=12, -19<=k<=19, -31<=l<=32	
Reflections collected	49513	
Independent reflections	9705 [R(int) = 0.0524]	
Completeness to theta = 67.50°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.5326 and 0.4226	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9705 / 0 / 729	
Goodness-of-fit on F^2	1.048	
Final R indices [I>2sigma(I)]	R1 = 0.0701, wR2 = 0.1803	
R indices (all data)	R1 = 0.0848, wR2 = 0.1918	
Absolute structure parameter	0.03(3)	
Largest diff. peak and hole	0.889 and -0.594 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ww05_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	7905(1)	4542(1)	2257(1)	40(1)
O(1)	6920(2)	4691(2)	1881(1)	41(1)
O(2)	8667(2)	3929(2)	1945(1)	41(1)
O(3)	7544(3)	4061(2)	2686(1)	47(1)
O(4)	8428(3)	5333(2)	2328(1)	54(1)
C(1)	6496(3)	4025(3)	1627(2)	39(1)
C(2)	7066(3)	3702(2)	1243(2)	37(1)
C(3)	6579(3)	3031(3)	982(2)	39(1)
C(4)	5553(4)	2776(3)	1116(2)	46(1)
C(5)	4969(4)	3118(3)	1505(2)	47(1)
C(6)	3940(4)	2849(4)	1652(2)	58(1)
C(7)	3431(4)	3163(4)	2039(2)	68(2)
C(8)	3905(4)	3795(4)	2307(2)	63(1)
C(9)	4905(4)	4093(3)	2181(2)	51(1)
C(10)	5456(4)	3763(3)	1780(2)	42(1)
C(11)	8912(3)	4146(2)	1465(2)	38(1)
C(12)	8150(3)	4051(2)	1111(2)	34(1)
C(13)	8425(3)	4280(2)	622(2)	38(1)
C(14)	9468(4)	4520(2)	518(2)	40(1)
C(15)	10279(3)	4575(2)	888(2)	40(1)
C(16)	11352(4)	4820(2)	780(2)	47(1)
C(17)	12099(4)	4896(3)	1144(2)	53(1)
C(18)	11804(4)	4756(3)	1626(2)	54(1)
C(19)	10771(4)	4523(3)	1746(2)	48(1)
C(20)	9990(3)	4421(2)	1374(2)	40(1)
C(21)	7154(4)	2583(2)	595(2)	42(1)
C(22)	6597(4)	2359(3)	167(2)	50(1)
C(23)	7122(5)	1929(3)	-195(2)	61(1)
C(24)	8179(6)	1709(3)	-143(2)	70(2)
C(25)	8731(5)	1910(3)	275(2)	61(1)
C(26)	8235(4)	2346(3)	641(2)	46(1)

C(27)	7612(4)	4299(2)	214(2)	38(1)
C(28)	6572(4)	4613(2)	290(2)	41(1)
C(29)	5837(4)	4654(3)	-93(2)	50(1)
C(30)	6135(5)	4376(3)	-549(2)	60(2)
C(31)	7156(5)	4068(3)	-625(2)	60(1)
C(32)	7906(5)	4031(3)	-246(2)	51(1)
O(5)	-562(2)	6096(2)	-263(1)	41(1)
O(6)	-2405(2)	7236(2)	1066(1)	46(1)
O(7)	3464(2)	5763(2)	-446(1)	47(1)
O(8)	4584(2)	6366(2)	251(1)	44(1)
N(1)	166(3)	6936(2)	310(1)	30(1)
N(2)	1019(3)	8383(2)	1696(1)	36(1)
C(33)	-669(3)	6499(2)	109(2)	34(1)
C(34)	-1729(3)	6542(3)	386(2)	36(1)
C(35)	-1682(3)	6590(3)	946(2)	38(1)
C(36)	-517(3)	6715(2)	1122(2)	33(1)
C(37)	10(3)	7341(2)	790(1)	29(1)
C(38)	1173(3)	7632(2)	937(2)	31(1)
C(39)	1883(3)	7119(2)	611(1)	31(1)
C(40)	1291(3)	6775(2)	237(1)	30(1)
C(41)	1775(3)	6327(2)	-134(2)	33(1)
C(42)	2879(3)	6201(2)	-109(2)	36(1)
C(43)	3503(3)	6529(2)	276(2)	35(1)
C(44)	3008(3)	7007(2)	627(2)	34(1)
C(45)	1417(3)	7576(2)	1484(2)	36(1)
C(46)	900(4)	6868(3)	1751(2)	40(1)
C(47)	-325(3)	6882(3)	1667(2)	37(1)
C(48)	1317(3)	8551(2)	838(2)	35(1)
C(49)	779(4)	8935(2)	1275(2)	39(1)
C(50)	56(4)	8291(3)	2033(2)	42(1)
C(51)	-752(3)	7711(3)	1826(2)	37(1)
C(52)	-1790(4)	7918(3)	1794(2)	47(1)
C(53)	-2613(4)	7336(4)	1574(2)	55(1)
C(54)	2863(4)	5329(4)	-803(2)	60(1)
C(55)	5241(4)	6686(3)	634(2)	48(1)
C(1S)	5880(6)	4648(5)	3663(3)	84(2)

Cl(1)	5145(4)	3772(2)	3551(1)	180(2)
Cl(2)	5121(4)	5491(2)	3605(2)	209(2)
O(1S)	9284(7)	5943(4)	3118(3)	148(3)
C(2S)	9303(8)	7274(4)	3444(3)	103(3)
C(3S)	8829(9)	6735(5)	3117(3)	107(3)
O(2S)	4127(5)	6444(3)	1983(2)	114(2)
C(4S)	3382(8)	7422(5)	2232(4)	110(3)
C(5S)	4355(9)	7136(6)	2263(6)	163(6)
O(3SA)	7051(9)	1793(8)	2120(3)	98(3)
C(6SA)	7643(9)	1316(5)	1766(3)	81(6)
C(7SA)	7887(8)	552(5)	2059(3)	65(4)
O(3SB)	8844(6)	146(3)	1897(3)	48(2)
C(7SB)	7643(9)	1316(5)	1766(3)	176(8)
C(6SB)	7887(8)	552(5)	2059(3)	184(9)

Table S3. Bond lengths [Å] and angles [°] for ww05_0m.

P(1)-O(4)	1.466(3)
P(1)-O(3)	1.485(3)
P(1)-O(1)	1.613(3)
P(1)-O(2)	1.620(3)
O(1)-C(1)	1.398(5)
O(2)-C(11)	1.398(5)
C(1)-C(2)	1.373(6)
C(1)-C(10)	1.417(6)
C(2)-C(3)	1.445(6)
C(2)-C(12)	1.499(6)
C(3)-C(4)	1.383(6)
C(3)-C(21)	1.472(6)
C(4)-C(5)	1.404(7)
C(4)-H(4)	0.9500
C(5)-C(6)	1.403(7)
C(5)-C(10)	1.432(7)
C(6)-C(7)	1.336(8)
C(6)-H(6)	0.9500
C(7)-C(8)	1.399(9)
C(7)-H(7)	0.9500
C(8)-C(9)	1.371(7)
C(8)-H(8)	0.9500
C(9)-C(10)	1.402(7)
C(9)-H(9)	0.9500
C(11)-C(12)	1.358(6)
C(11)-C(20)	1.427(6)
C(12)-C(13)	1.434(6)
C(13)-C(14)	1.375(6)
C(13)-C(27)	1.501(6)
C(14)-C(15)	1.428(6)
C(14)-H(14)	0.9500
C(15)-C(20)	1.400(6)
C(15)-C(16)	1.415(6)
C(16)-C(17)	1.362(7)

C(16)-H(16)	0.9500
C(17)-C(18)	1.390(8)
C(17)-H(17)	0.9500
C(18)-C(19)	1.370(7)
C(18)-H(18)	0.9500
C(19)-C(20)	1.413(6)
C(19)-H(19)	0.9500
C(21)-C(26)	1.396(6)
C(21)-C(22)	1.409(7)
C(22)-C(23)	1.379(8)
C(22)-H(22)	0.9500
C(23)-C(24)	1.362(9)
C(23)-H(23)	0.9500
C(24)-C(25)	1.372(9)
C(24)-H(24)	0.9500
C(25)-C(26)	1.376(7)
C(25)-H(25)	0.9500
C(26)-H(26)	0.9500
C(27)-C(32)	1.384(7)
C(27)-C(28)	1.399(6)
C(28)-C(29)	1.387(7)
C(28)-H(28)	0.9500
C(29)-C(30)	1.380(8)
C(29)-H(29)	0.9500
C(30)-C(31)	1.374(9)
C(30)-H(30)	0.9500
C(31)-C(32)	1.392(8)
C(31)-H(31)	0.9500
C(32)-H(32)	0.9500
O(5)-C(33)	1.224(5)
O(6)-C(53)	1.425(6)
O(6)-C(35)	1.425(5)
O(7)-C(42)	1.375(5)
O(7)-C(54)	1.421(6)
O(8)-C(43)	1.362(5)
O(8)-C(55)	1.427(5)

N(1)-C(33)	1.370(5)
N(1)-C(40)	1.427(5)
N(1)-C(37)	1.487(5)
N(2)-C(49)	1.497(5)
N(2)-C(50)	1.512(6)
N(2)-C(45)	1.528(5)
N(2)-H(2A)	0.9601
C(33)-C(34)	1.513(6)
C(34)-C(35)	1.538(6)
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900
C(35)-C(36)	1.529(6)
C(35)-H(35)	1.0000
C(36)-C(37)	1.521(5)
C(36)-C(47)	1.535(6)
C(36)-H(36)	1.0000
C(37)-C(38)	1.565(5)
C(37)-H(37)	1.0000
C(38)-C(39)	1.509(5)
C(38)-C(45)	1.532(6)
C(38)-C(48)	1.545(5)
C(39)-C(40)	1.378(6)
C(39)-C(44)	1.401(5)
C(40)-C(41)	1.390(6)
C(41)-C(42)	1.380(6)
C(41)-H(41)	0.9500
C(42)-C(43)	1.412(6)
C(43)-C(44)	1.386(6)
C(44)-H(44)	0.9500
C(45)-C(46)	1.516(6)
C(45)-H(45)	1.0000
C(46)-C(47)	1.530(6)
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(47)-C(51)	1.525(6)
C(47)-H(47)	1.0000

C(48)-C(49)	1.506(6)
C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900
C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900
C(50)-C(51)	1.491(6)
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
C(51)-C(52)	1.328(6)
C(52)-C(53)	1.519(7)
C(52)-H(52)	0.9500
C(53)-H(53A)	0.9900
C(53)-H(53B)	0.9900
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
C(55)-H(55A)	0.9800
C(55)-H(55B)	0.9800
C(55)-H(55C)	0.9800
C(1S)-Cl(2)	1.681(8)
C(1S)-Cl(1)	1.729(8)
C(1S)-H(1S1)	0.9900
C(1S)-H(1S2)	0.9900
O(1S)-C(3S)	1.419(10)
O(1S)-H(1S)	0.8400
C(2S)-C(3S)	1.390(11)
C(2S)-H(2S1)	0.9800
C(2S)-H(2S2)	0.9800
C(2S)-H(2S3)	0.9800
C(3S)-H(3SC)	0.9900
C(3S)-H(3SD)	0.9900
O(2S)-C(5S)	1.400(11)
O(2S)-H(2S)	0.8400
C(4S)-C(5S)	1.292(12)
C(4S)-H(4S1)	0.9800
C(4S)-H(4S2)	0.9800

C(4S)-H(4S3)	0.9800
C(5S)-H(5S1)	0.9900
C(5S)-H(5S2)	0.9900
O(3SA)-C(6SA)	1.445(13)
O(3SA)-H(3SA)	0.8399
C(6SA)-C(7SA)	1.522(11)
C(6SA)-H(6SA)	0.9900
C(6SA)-H(6SB)	0.9900
C(7SA)-H(7SA)	0.9800
C(7SA)-H(7SB)	0.9800
C(7SA)-H(7SC)	0.9800
O(3SB)-H(3SB)	0.8400

O(4)-P(1)-O(3)	120.0(2)
O(4)-P(1)-O(1)	106.31(18)
O(3)-P(1)-O(1)	111.17(17)
O(4)-P(1)-O(2)	111.51(18)
O(3)-P(1)-O(2)	105.04(17)
O(1)-P(1)-O(2)	101.26(16)
C(1)-O(1)-P(1)	118.6(3)
C(11)-O(2)-P(1)	117.6(3)
C(2)-C(1)-O(1)	119.5(4)
C(2)-C(1)-C(10)	124.9(4)
O(1)-C(1)-C(10)	115.5(4)
C(1)-C(2)-C(3)	117.5(4)
C(1)-C(2)-C(12)	119.5(4)
C(3)-C(2)-C(12)	123.0(4)
C(4)-C(3)-C(2)	118.7(4)
C(4)-C(3)-C(21)	118.7(4)
C(2)-C(3)-C(21)	122.5(4)
C(3)-C(4)-C(5)	123.3(4)
C(3)-C(4)-H(4)	118.3
C(5)-C(4)-H(4)	118.3
C(6)-C(5)-C(4)	123.7(5)
C(6)-C(5)-C(10)	117.5(5)
C(4)-C(5)-C(10)	118.7(4)

C(7)-C(6)-C(5)	122.0(5)
C(7)-C(6)-H(6)	119.0
C(5)-C(6)-H(6)	119.0
C(6)-C(7)-C(8)	120.5(5)
C(6)-C(7)-H(7)	119.8
C(8)-C(7)-H(7)	119.8
C(9)-C(8)-C(7)	120.7(5)
C(9)-C(8)-H(8)	119.7
C(7)-C(8)-H(8)	119.7
C(8)-C(9)-C(10)	119.6(5)
C(8)-C(9)-H(9)	120.2
C(10)-C(9)-H(9)	120.2
C(9)-C(10)-C(1)	123.6(5)
C(9)-C(10)-C(5)	119.7(4)
C(1)-C(10)-C(5)	116.7(4)
C(12)-C(11)-O(2)	119.5(4)
C(12)-C(11)-C(20)	123.9(4)
O(2)-C(11)-C(20)	116.5(4)
C(11)-C(12)-C(13)	118.2(4)
C(11)-C(12)-C(2)	119.3(4)
C(13)-C(12)-C(2)	122.4(4)
C(14)-C(13)-C(12)	119.3(4)
C(14)-C(13)-C(27)	117.7(4)
C(12)-C(13)-C(27)	122.9(4)
C(13)-C(14)-C(15)	121.8(4)
C(13)-C(14)-H(14)	119.1
C(15)-C(14)-H(14)	119.1
C(20)-C(15)-C(16)	119.2(4)
C(20)-C(15)-C(14)	119.0(4)
C(16)-C(15)-C(14)	121.6(4)
C(17)-C(16)-C(15)	120.4(5)
C(17)-C(16)-H(16)	119.8
C(15)-C(16)-H(16)	119.8
C(16)-C(17)-C(18)	120.2(5)
C(16)-C(17)-H(17)	119.9
C(18)-C(17)-H(17)	119.9

C(19)-C(18)-C(17)	121.2(5)
C(19)-C(18)-H(18)	119.4
C(17)-C(18)-H(18)	119.4
C(18)-C(19)-C(20)	119.6(5)
C(18)-C(19)-H(19)	120.2
C(20)-C(19)-H(19)	120.2
C(15)-C(20)-C(19)	119.4(4)
C(15)-C(20)-C(11)	117.4(4)
C(19)-C(20)-C(11)	123.2(4)
C(26)-C(21)-C(22)	117.9(5)
C(26)-C(21)-C(3)	122.3(4)
C(22)-C(21)-C(3)	119.8(4)
C(23)-C(22)-C(21)	120.3(5)
C(23)-C(22)-H(22)	119.9
C(21)-C(22)-H(22)	119.9
C(24)-C(23)-C(22)	120.7(5)
C(24)-C(23)-H(23)	119.6
C(22)-C(23)-H(23)	119.6
C(25)-C(24)-C(23)	119.9(5)
C(25)-C(24)-H(24)	120.0
C(23)-C(24)-H(24)	120.0
C(24)-C(25)-C(26)	120.9(5)
C(24)-C(25)-H(25)	119.5
C(26)-C(25)-H(25)	119.5
C(25)-C(26)-C(21)	120.3(5)
C(25)-C(26)-H(26)	119.9
C(21)-C(26)-H(26)	119.9
C(32)-C(27)-C(28)	119.5(4)
C(32)-C(27)-C(13)	119.8(4)
C(28)-C(27)-C(13)	120.7(4)
C(29)-C(28)-C(27)	120.4(4)
C(29)-C(28)-H(28)	119.8
C(27)-C(28)-H(28)	119.8
C(28)-C(29)-C(30)	119.5(5)
C(28)-C(29)-H(29)	120.2
C(30)-C(29)-H(29)	120.2

C(31)-C(30)-C(29)	120.3(5)
C(31)-C(30)-H(30)	119.9
C(29)-C(30)-H(30)	119.9
C(30)-C(31)-C(32)	120.8(5)
C(30)-C(31)-H(31)	119.6
C(32)-C(31)-H(31)	119.6
C(27)-C(32)-C(31)	119.5(5)
C(27)-C(32)-H(32)	120.3
C(31)-C(32)-H(32)	120.3
C(53)-O(6)-C(35)	115.1(4)
C(42)-O(7)-C(54)	116.9(3)
C(43)-O(8)-C(55)	116.5(3)
C(33)-N(1)-C(40)	125.4(3)
C(33)-N(1)-C(37)	119.5(3)
C(40)-N(1)-C(37)	109.4(3)
C(49)-N(2)-C(50)	112.0(3)
C(49)-N(2)-C(45)	107.3(3)
C(50)-N(2)-C(45)	113.4(3)
C(49)-N(2)-H(2A)	108.0
C(50)-N(2)-H(2A)	108.0
C(45)-N(2)-H(2A)	108.0
O(5)-C(33)-N(1)	122.5(4)
O(5)-C(33)-C(34)	122.4(4)
N(1)-C(33)-C(34)	115.1(4)
C(33)-C(34)-C(35)	118.0(3)
C(33)-C(34)-H(34A)	107.8
C(35)-C(34)-H(34A)	107.8
C(33)-C(34)-H(34B)	107.8
C(35)-C(34)-H(34B)	107.8
H(34A)-C(34)-H(34B)	107.1
O(6)-C(35)-C(36)	114.5(3)
O(6)-C(35)-C(34)	104.2(3)
C(36)-C(35)-C(34)	110.9(3)
O(6)-C(35)-H(35)	109.0
C(36)-C(35)-H(35)	109.0
C(34)-C(35)-H(35)	109.0

C(37)-C(36)-C(35)	107.7(3)
C(37)-C(36)-C(47)	113.3(3)
C(35)-C(36)-C(47)	118.4(3)
C(37)-C(36)-H(36)	105.5
C(35)-C(36)-H(36)	105.5
C(47)-C(36)-H(36)	105.5
N(1)-C(37)-C(36)	106.4(3)
N(1)-C(37)-C(38)	104.3(3)
C(36)-C(37)-C(38)	116.4(3)
N(1)-C(37)-H(37)	109.8
C(36)-C(37)-H(37)	109.8
C(38)-C(37)-H(37)	109.8
C(39)-C(38)-C(45)	115.6(3)
C(39)-C(38)-C(48)	112.1(3)
C(45)-C(38)-C(48)	102.0(3)
C(39)-C(38)-C(37)	102.0(3)
C(45)-C(38)-C(37)	114.5(3)
C(48)-C(38)-C(37)	111.0(3)
C(40)-C(39)-C(44)	119.7(4)
C(40)-C(39)-C(38)	111.2(3)
C(44)-C(39)-C(38)	129.0(4)
C(39)-C(40)-C(41)	122.2(4)
C(39)-C(40)-N(1)	109.7(3)
C(41)-C(40)-N(1)	128.1(4)
C(42)-C(41)-C(40)	117.8(4)
C(42)-C(41)-H(41)	121.1
C(40)-C(41)-H(41)	121.1
C(41)-C(42)-O(7)	124.3(4)
C(41)-C(42)-C(43)	121.3(4)
O(7)-C(42)-C(43)	114.5(4)
O(8)-C(43)-C(44)	125.3(4)
O(8)-C(43)-C(42)	115.0(4)
C(44)-C(43)-C(42)	119.7(4)
C(43)-C(44)-C(39)	119.2(4)
C(43)-C(44)-H(44)	120.4
C(39)-C(44)-H(44)	120.4

C(46)-C(45)-N(2)	110.5(3)
C(46)-C(45)-C(38)	115.8(3)
N(2)-C(45)-C(38)	104.9(3)
C(46)-C(45)-H(45)	108.5
N(2)-C(45)-H(45)	108.5
C(38)-C(45)-H(45)	108.5
C(45)-C(46)-C(47)	109.3(3)
C(45)-C(46)-H(46A)	109.8
C(47)-C(46)-H(46A)	109.8
C(45)-C(46)-H(46B)	109.8
C(47)-C(46)-H(46B)	109.8
H(46A)-C(46)-H(46B)	108.3
C(46)-C(47)-C(51)	108.2(3)
C(46)-C(47)-C(36)	107.2(3)
C(51)-C(47)-C(36)	112.6(3)
C(46)-C(47)-H(47)	109.6
C(51)-C(47)-H(47)	109.6
C(36)-C(47)-H(47)	109.6
C(49)-C(48)-C(38)	102.7(3)
C(49)-C(48)-H(48A)	111.2
C(38)-C(48)-H(48A)	111.2
C(49)-C(48)-H(48B)	111.2
C(38)-C(48)-H(48B)	111.2
H(48A)-C(48)-H(48B)	109.1
N(2)-C(49)-C(48)	105.7(3)
N(2)-C(49)-H(49A)	110.6
C(48)-C(49)-H(49A)	110.6
N(2)-C(49)-H(49B)	110.6
C(48)-C(49)-H(49B)	110.6
H(49A)-C(49)-H(49B)	108.7
C(51)-C(50)-N(2)	110.9(3)
C(51)-C(50)-H(50A)	109.5
N(2)-C(50)-H(50A)	109.5
C(51)-C(50)-H(50B)	109.5
N(2)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	108.0

C(52)-C(51)-C(50)	120.4(4)
C(52)-C(51)-C(47)	122.9(4)
C(50)-C(51)-C(47)	116.7(4)
C(51)-C(52)-C(53)	120.6(4)
C(51)-C(52)-H(52)	119.7
C(53)-C(52)-H(52)	119.7
O(6)-C(53)-C(52)	109.9(4)
O(6)-C(53)-H(53A)	109.7
C(52)-C(53)-H(53A)	109.7
O(6)-C(53)-H(53B)	109.7
C(52)-C(53)-H(53B)	109.7
H(53A)-C(53)-H(53B)	108.2
O(7)-C(54)-H(54A)	109.5
O(7)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
O(7)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
O(8)-C(55)-H(55A)	109.5
O(8)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	109.5
O(8)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5
Cl(2)-C(1S)-Cl(1)	112.2(4)
Cl(2)-C(1S)-H(1S1)	109.2
Cl(1)-C(1S)-H(1S1)	109.2
Cl(2)-C(1S)-H(1S2)	109.2
Cl(1)-C(1S)-H(1S2)	109.2
H(1S1)-C(1S)-H(1S2)	107.9
C(3S)-O(1S)-H(1S)	108.3
C(3S)-C(2S)-H(2S1)	109.5
C(3S)-C(2S)-H(2S2)	109.5
H(2S1)-C(2S)-H(2S2)	109.5
C(3S)-C(2S)-H(2S3)	109.5
H(2S1)-C(2S)-H(2S3)	109.5

H(2S2)-C(2S)-H(2S3)	109.5
C(2S)-C(3S)-O(1S)	114.6(8)
C(2S)-C(3S)-H(3SC)	108.6
O(1S)-C(3S)-H(3SC)	108.6
C(2S)-C(3S)-H(3SD)	108.6
O(1S)-C(3S)-H(3SD)	108.6
H(3SC)-C(3S)-H(3SD)	107.6
C(5S)-O(2S)-H(2S)	112.3
C(5S)-C(4S)-H(4S1)	109.5
C(5S)-C(4S)-H(4S2)	109.5
H(4S1)-C(4S)-H(4S2)	109.5
C(5S)-C(4S)-H(4S3)	109.5
H(4S1)-C(4S)-H(4S3)	109.5
H(4S2)-C(4S)-H(4S3)	109.5
C(4S)-C(5S)-O(2S)	94.2(8)
C(4S)-C(5S)-H(5S1)	112.9
O(2S)-C(5S)-H(5S1)	112.9
C(4S)-C(5S)-H(5S2)	112.9
O(2S)-C(5S)-H(5S2)	112.9
H(5S1)-C(5S)-H(5S2)	110.3
C(6SA)-O(3SA)-H(3SA)	110.3
O(3SA)-C(6SA)-C(7SA)	101.1(7)
O(3SA)-C(6SA)-H(6SA)	111.6
C(7SA)-C(6SA)-H(6SA)	111.6
O(3SA)-C(6SA)-H(6SB)	111.6
C(7SA)-C(6SA)-H(6SB)	111.6
H(6SA)-C(6SA)-H(6SB)	109.4
C(6SA)-C(7SA)-H(7SA)	109.5
C(6SA)-C(7SA)-H(7SB)	109.5
H(7SA)-C(7SA)-H(7SB)	109.5
C(6SA)-C(7SA)-H(7SC)	109.5
H(7SA)-C(7SA)-H(7SC)	109.5
H(7SB)-C(7SA)-H(7SC)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for ww05_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)	43(1)	43(1)	35(1)	7(1)	-2(1)	-4(1)
O(1)	46(2)	42(2)	37(2)	2(1)	-2(1)	6(1)
O(2)	43(2)	43(2)	35(2)	10(1)	-4(1)	-2(1)
O(3)	42(2)	59(2)	39(2)	13(1)	-2(1)	-2(1)
O(4)	60(2)	52(2)	51(2)	0(2)	2(2)	-8(2)
C(1)	37(2)	42(2)	38(2)	7(2)	-3(2)	1(2)
C(2)	37(2)	38(2)	36(2)	9(2)	-7(2)	2(2)
C(3)	38(2)	36(2)	43(2)	13(2)	-1(2)	-1(2)
C(4)	38(2)	48(2)	51(3)	5(2)	-5(2)	-4(2)
C(5)	33(2)	57(3)	51(3)	12(2)	-7(2)	-2(2)
C(6)	37(2)	77(3)	61(3)	-1(3)	2(2)	-3(2)
C(7)	39(3)	86(4)	79(4)	6(3)	10(3)	-1(3)
C(8)	44(3)	81(4)	63(3)	7(3)	13(3)	9(3)
C(9)	41(2)	58(3)	54(3)	5(2)	2(2)	4(2)
C(10)	37(2)	51(2)	39(2)	13(2)	0(2)	6(2)
C(11)	36(2)	36(2)	42(2)	6(2)	6(2)	3(2)
C(12)	35(2)	29(2)	39(2)	5(2)	3(2)	4(2)
C(13)	43(2)	32(2)	39(2)	7(2)	1(2)	4(2)
C(14)	48(2)	30(2)	42(2)	5(2)	6(2)	2(2)
C(15)	43(2)	28(2)	49(3)	8(2)	8(2)	2(2)
C(16)	49(3)	29(2)	62(3)	7(2)	16(2)	0(2)
C(17)	43(3)	38(2)	77(4)	3(2)	5(3)	-4(2)
C(18)	46(3)	45(2)	71(4)	0(2)	-7(2)	-6(2)
C(19)	43(2)	46(2)	54(3)	11(2)	-6(2)	-3(2)
C(20)	33(2)	30(2)	55(3)	4(2)	-2(2)	0(2)
C(21)	46(2)	32(2)	48(3)	6(2)	2(2)	-4(2)
C(22)	55(3)	38(2)	56(3)	4(2)	-9(2)	-2(2)
C(23)	81(4)	46(3)	56(3)	-12(2)	-3(3)	0(3)
C(24)	97(5)	47(3)	67(4)	-13(3)	21(3)	1(3)
C(25)	63(3)	39(2)	80(4)	4(3)	18(3)	7(2)
C(26)	42(2)	35(2)	62(3)	8(2)	2(2)	0(2)

C(27)	49(2)	29(2)	36(2)	4(2)	-1(2)	-1(2)
C(28)	48(2)	33(2)	41(2)	4(2)	0(2)	0(2)
C(29)	57(3)	34(2)	59(3)	8(2)	-11(2)	-2(2)
C(30)	81(4)	49(3)	49(3)	15(2)	-28(3)	-21(3)
C(31)	84(4)	53(3)	43(3)	-3(2)	-8(3)	-14(3)
C(32)	64(3)	47(2)	42(3)	5(2)	6(2)	-3(2)
O(5)	39(2)	50(2)	34(2)	-10(1)	-1(1)	-2(1)
O(6)	32(2)	56(2)	51(2)	-12(2)	2(1)	3(1)
O(7)	39(2)	57(2)	46(2)	-13(1)	7(1)	1(1)
O(8)	28(1)	52(2)	53(2)	-6(2)	3(1)	2(1)
N(1)	31(2)	31(2)	29(2)	-4(1)	0(1)	-2(1)
N(2)	35(2)	41(2)	32(2)	-4(2)	-4(1)	4(2)
C(33)	34(2)	35(2)	34(2)	4(2)	-5(2)	0(2)
C(34)	32(2)	38(2)	40(2)	-3(2)	-1(2)	-4(2)
C(35)	31(2)	37(2)	45(2)	-1(2)	5(2)	-4(2)
C(36)	30(2)	33(2)	35(2)	3(2)	5(2)	1(2)
C(37)	26(2)	31(2)	29(2)	-1(2)	0(2)	2(2)
C(38)	29(2)	31(2)	33(2)	-1(2)	0(2)	-2(2)
C(39)	28(2)	34(2)	31(2)	2(2)	4(2)	-1(2)
C(40)	28(2)	31(2)	32(2)	4(2)	3(2)	-2(2)
C(41)	33(2)	31(2)	34(2)	0(2)	2(2)	-2(2)
C(42)	40(2)	35(2)	33(2)	-5(2)	5(2)	-2(2)
C(43)	29(2)	37(2)	39(2)	5(2)	4(2)	-3(2)
C(44)	30(2)	35(2)	36(2)	-1(2)	-1(2)	-1(2)
C(45)	34(2)	39(2)	36(2)	-5(2)	-2(2)	3(2)
C(46)	45(2)	42(2)	34(2)	2(2)	-2(2)	8(2)
C(47)	36(2)	40(2)	34(2)	3(2)	6(2)	-2(2)
C(48)	37(2)	33(2)	34(2)	-1(2)	-7(2)	-3(2)
C(49)	45(2)	34(2)	37(2)	-2(2)	-4(2)	2(2)
C(50)	43(2)	48(2)	34(2)	-6(2)	2(2)	5(2)
C(51)	37(2)	47(2)	28(2)	4(2)	6(2)	2(2)
C(52)	42(2)	56(3)	41(2)	-10(2)	8(2)	6(2)
C(53)	38(2)	74(3)	53(3)	-16(3)	14(2)	-3(2)
C(54)	56(3)	69(3)	57(3)	-27(3)	12(3)	-4(3)
C(55)	33(2)	65(3)	47(3)	-8(2)	-4(2)	1(2)
C(1S)	67(4)	103(5)	84(5)	10(4)	4(3)	1(4)

Cl(1)	270(4)	181(3)	87(2)	-2(2)	-19(2)	-116(3)
Cl(2)	201(4)	163(3)	262(5)	27(3)	-86(3)	69(3)
O(1S)	177(7)	127(5)	140(6)	-44(4)	-51(5)	-6(5)
C(2S)	127(7)	68(4)	114(6)	2(4)	-41(5)	-14(4)
C(3S)	162(8)	67(4)	90(5)	-13(4)	3(5)	24(5)
O(2S)	147(5)	98(4)	95(4)	-40(3)	45(4)	-42(4)
C(4S)	109(6)	81(5)	140(8)	-11(5)	-46(6)	-2(5)
C(5S)	119(8)	89(6)	280(17)	-28(8)	-69(10)	2(6)
O(3SA)	91(6)	142(9)	61(5)	1(6)	3(5)	39(7)
C(6SA)	127(15)	44(6)	72(10)	8(9)	-43(13)	18(10)
C(7SA)	94(10)	68(7)	35(5)	9(7)	30(8)	51(10)
O(3SB)	49(4)	31(3)	63(4)	-17(3)	-25(3)	11(3)
C(7SB)	185(17)	175(11)	167(7)	100(20)	70(30)	30(30)
C(6SB)	184(19)	184(13)	184(8)	0(40)	0(40)	0(40)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ww05_0m.

	x	y	z	U(eq)
H(4)	5226	2348	936	55
H(6)	3594	2431	1470	70
H(7)	2743	2957	2133	82
H(8)	3531	4018	2578	76
H(9)	5222	4522	2365	61
H(14)	9654	4652	191	48
H(16)	11553	4932	452	56
H(17)	12823	5044	1067	63
H(18)	12328	4824	1877	65
H(19)	10582	4431	2078	57
H(22)	5857	2504	127	60
H(23)	6741	1786	-484	73
H(24)	8535	1416	-396	84
H(25)	9465	1747	311	73
H(26)	8631	2486	926	56
H(28)	6368	4800	605	49
H(29)	5133	4873	-41	60
H(30)	5631	4397	-811	72
H(31)	7353	3878	-941	72
H(32)	8613	3823	-303	61
H(2A)	1603	8618	1880	43
H(34A)	-2161	6056	298	44
H(34B)	-2131	7023	267	44
H(35)	-1968	6072	1087	45
H(36)	-135	6192	1053	39
H(37)	-480	7822	751	34
H(41)	1358	6114	-396	39
H(44)	3427	7257	877	41
H(45)	2220	7544	1529	43
H(46A)	1057	6907	2105	48

H(46B)	1206	6349	1629	48
H(47)	-677	6446	1866	44
H(48A)	2093	8700	820	42
H(48B)	954	8714	531	42
H(49A)	1076	9485	1335	47
H(49B)	-13	8980	1223	47
H(50A)	305	8090	2355	50
H(50B)	-290	8827	2082	50
H(52)	-2021	8434	1911	56
H(53A)	-2568	6803	1740	66
H(53B)	-3354	7554	1622	66
H(54A)	2371	4947	-642	91
H(54B)	3363	5029	-1015	91
H(54C)	2441	5713	-1000	91
H(55A)	5196	7281	633	73
H(55B)	5995	6518	585	73
H(55C)	4982	6478	949	73
H(1S1)	6180	4624	3998	101
H(1S2)	6496	4676	3432	101
H(1S)	9934	5978	3030	222
H(2S1)	9323	7026	3770	154
H(2S2)	8876	7776	3457	154
H(2S3)	10043	7399	3338	154
H(3SC)	8894	6964	2784	128
H(3SD)	8046	6692	3193	128
H(2S)	4474	6034	2079	170
H(4S1)	2873	6974	2175	165
H(4S2)	3341	7808	1960	165
H(4S3)	3194	7700	2537	165
H(5S1)	4569	7004	2602	195
H(5S2)	4903	7495	2110	195
H(3SA)	7481	2014	2317	147
H(6SA)	8316	1594	1661	97
H(6SB)	7194	1194	1475	97
H(7SA)	8306	172	1858	98
H(7SB)	7205	295	2159	98

H(7SC)	8308	698	2350	98
H(3SB)	9331	490	1840	72
H(7SD)	6982	1573	1892	263
H(7SE)	7538	1171	1422	263
H(7SF)	8251	1697	1794	263
H(6SC)	7974	701	2407	221
H(6SD)	7264	175	2034	221

Table S6. Torsion angles [°] for ww05_0m.

O(4)-P(1)-O(1)-C(1)	160.0(3)
O(3)-P(1)-O(1)-C(1)	-67.8(3)
O(2)-P(1)-O(1)-C(1)	43.4(3)
O(4)-P(1)-O(2)-C(11)	-63.6(3)
O(3)-P(1)-O(2)-C(11)	164.9(3)
O(1)-P(1)-O(2)-C(11)	49.1(3)
P(1)-O(1)-C(1)-C(2)	-75.6(4)
P(1)-O(1)-C(1)-C(10)	107.8(4)
O(1)-C(1)-C(2)-C(3)	-178.0(3)
C(10)-C(1)-C(2)-C(3)	-1.8(6)
O(1)-C(1)-C(2)-C(12)	2.1(6)
C(10)-C(1)-C(2)-C(12)	178.4(4)
C(1)-C(2)-C(3)-C(4)	3.2(6)
C(12)-C(2)-C(3)-C(4)	-177.0(4)
C(1)-C(2)-C(3)-C(21)	-173.9(4)
C(12)-C(2)-C(3)-C(21)	5.9(6)
C(2)-C(3)-C(4)-C(5)	-2.3(6)
C(21)-C(3)-C(4)-C(5)	174.9(4)
C(3)-C(4)-C(5)-C(6)	-178.3(5)
C(3)-C(4)-C(5)-C(10)	-0.2(7)
C(4)-C(5)-C(6)-C(7)	176.7(5)
C(10)-C(5)-C(6)-C(7)	-1.5(8)
C(5)-C(6)-C(7)-C(8)	1.7(9)
C(6)-C(7)-C(8)-C(9)	-0.9(9)
C(7)-C(8)-C(9)-C(10)	0.0(8)
C(8)-C(9)-C(10)-C(1)	-179.1(5)
C(8)-C(9)-C(10)-C(5)	0.1(7)
C(2)-C(1)-C(10)-C(9)	178.6(4)
O(1)-C(1)-C(10)-C(9)	-4.9(6)
C(2)-C(1)-C(10)-C(5)	-0.7(6)
O(1)-C(1)-C(10)-C(5)	175.8(4)
C(6)-C(5)-C(10)-C(9)	0.5(7)
C(4)-C(5)-C(10)-C(9)	-177.7(4)
C(6)-C(5)-C(10)-C(1)	179.9(4)

C(4)-C(5)-C(10)-C(1)	1.7(6)
P(1)-O(2)-C(11)-C(12)	-76.3(4)
P(1)-O(2)-C(11)-C(20)	106.7(4)
O(2)-C(11)-C(12)-C(13)	180.0(3)
C(20)-C(11)-C(12)-C(13)	-3.2(6)
O(2)-C(11)-C(12)-C(2)	-1.1(6)
C(20)-C(11)-C(12)-C(2)	175.7(4)
C(1)-C(2)-C(12)-C(11)	50.9(5)
C(3)-C(2)-C(12)-C(11)	-128.9(4)
C(1)-C(2)-C(12)-C(13)	-130.2(4)
C(3)-C(2)-C(12)-C(13)	50.0(5)
C(11)-C(12)-C(13)-C(14)	5.4(6)
C(2)-C(12)-C(13)-C(14)	-173.6(4)
C(11)-C(12)-C(13)-C(27)	-172.4(4)
C(2)-C(12)-C(13)-C(27)	8.7(6)
C(12)-C(13)-C(14)-C(15)	-2.2(6)
C(27)-C(13)-C(14)-C(15)	175.6(4)
C(13)-C(14)-C(15)-C(20)	-3.3(6)
C(13)-C(14)-C(15)-C(16)	179.8(4)
C(20)-C(15)-C(16)-C(17)	0.7(6)
C(14)-C(15)-C(16)-C(17)	177.7(4)
C(15)-C(16)-C(17)-C(18)	-1.9(7)
C(16)-C(17)-C(18)-C(19)	1.6(7)
C(17)-C(18)-C(19)-C(20)	0.0(7)
C(16)-C(15)-C(20)-C(19)	0.9(6)
C(14)-C(15)-C(20)-C(19)	-176.2(4)
C(16)-C(15)-C(20)-C(11)	-177.6(4)
C(14)-C(15)-C(20)-C(11)	5.3(6)
C(18)-C(19)-C(20)-C(15)	-1.2(7)
C(18)-C(19)-C(20)-C(11)	177.2(4)
C(12)-C(11)-C(20)-C(15)	-2.2(6)
O(2)-C(11)-C(20)-C(15)	174.7(3)
C(12)-C(11)-C(20)-C(19)	179.4(4)
O(2)-C(11)-C(20)-C(19)	-3.7(6)
C(4)-C(3)-C(21)-C(26)	-133.5(4)
C(2)-C(3)-C(21)-C(26)	43.6(6)

C(4)-C(3)-C(21)-C(22)	44.6(6)
C(2)-C(3)-C(21)-C(22)	-138.3(4)
C(26)-C(21)-C(22)-C(23)	-0.9(6)
C(3)-C(21)-C(22)-C(23)	-179.1(4)
C(21)-C(22)-C(23)-C(24)	0.6(8)
C(22)-C(23)-C(24)-C(25)	0.4(8)
C(23)-C(24)-C(25)-C(26)	-1.1(8)
C(24)-C(25)-C(26)-C(21)	0.7(7)
C(22)-C(21)-C(26)-C(25)	0.3(6)
C(3)-C(21)-C(26)-C(25)	178.4(4)
C(14)-C(13)-C(27)-C(32)	41.8(6)
C(12)-C(13)-C(27)-C(32)	-140.4(4)
C(14)-C(13)-C(27)-C(28)	-135.7(4)
C(12)-C(13)-C(27)-C(28)	42.0(6)
C(32)-C(27)-C(28)-C(29)	0.2(6)
C(13)-C(27)-C(28)-C(29)	177.8(4)
C(27)-C(28)-C(29)-C(30)	0.6(7)
C(28)-C(29)-C(30)-C(31)	-0.7(7)
C(29)-C(30)-C(31)-C(32)	0.0(8)
C(28)-C(27)-C(32)-C(31)	-0.9(6)
C(13)-C(27)-C(32)-C(31)	-178.5(4)
C(30)-C(31)-C(32)-C(27)	0.7(7)
C(40)-N(1)-C(33)-O(5)	-23.4(6)
C(37)-N(1)-C(33)-O(5)	-173.7(4)
C(40)-N(1)-C(33)-C(34)	155.7(4)
C(37)-N(1)-C(33)-C(34)	5.5(5)
O(5)-C(33)-C(34)-C(35)	144.2(4)
N(1)-C(33)-C(34)-C(35)	-35.0(5)
C(53)-O(6)-C(35)-C(36)	-66.4(5)
C(53)-O(6)-C(35)-C(34)	172.3(3)
C(33)-C(34)-C(35)-O(6)	132.3(4)
C(33)-C(34)-C(35)-C(36)	8.5(5)
O(6)-C(35)-C(36)-C(37)	-75.0(4)
C(34)-C(35)-C(36)-C(37)	42.6(4)
O(6)-C(35)-C(36)-C(47)	55.1(5)
C(34)-C(35)-C(36)-C(47)	172.7(3)

C(33)-N(1)-C(37)-C(36)	46.5(4)
C(40)-N(1)-C(37)-C(36)	-108.1(3)
C(33)-N(1)-C(37)-C(38)	170.1(3)
C(40)-N(1)-C(37)-C(38)	15.5(4)
C(35)-C(36)-C(37)-N(1)	-70.6(4)
C(47)-C(36)-C(37)-N(1)	156.5(3)
C(35)-C(36)-C(37)-C(38)	173.7(3)
C(47)-C(36)-C(37)-C(38)	40.8(4)
N(1)-C(37)-C(38)-C(39)	-18.1(4)
C(36)-C(37)-C(38)-C(39)	98.7(4)
N(1)-C(37)-C(38)-C(45)	-143.7(3)
C(36)-C(37)-C(38)-C(45)	-26.9(5)
N(1)-C(37)-C(38)-C(48)	101.5(3)
C(36)-C(37)-C(38)-C(48)	-141.7(3)
C(45)-C(38)-C(39)-C(40)	140.6(3)
C(48)-C(38)-C(39)-C(40)	-103.1(4)
C(37)-C(38)-C(39)-C(40)	15.8(4)
C(45)-C(38)-C(39)-C(44)	-43.8(6)
C(48)-C(38)-C(39)-C(44)	72.5(5)
C(37)-C(38)-C(39)-C(44)	-168.7(4)
C(44)-C(39)-C(40)-C(41)	-1.1(6)
C(38)-C(39)-C(40)-C(41)	174.9(3)
C(44)-C(39)-C(40)-N(1)	177.2(3)
C(38)-C(39)-C(40)-N(1)	-6.8(4)
C(33)-N(1)-C(40)-C(39)	-158.8(4)
C(37)-N(1)-C(40)-C(39)	-6.0(4)
C(33)-N(1)-C(40)-C(41)	19.4(6)
C(37)-N(1)-C(40)-C(41)	172.1(4)
C(39)-C(40)-C(41)-C(42)	2.8(6)
N(1)-C(40)-C(41)-C(42)	-175.2(4)
C(40)-C(41)-C(42)-O(7)	179.3(4)
C(40)-C(41)-C(42)-C(43)	-1.2(6)
C(54)-O(7)-C(42)-C(41)	-8.6(6)
C(54)-O(7)-C(42)-C(43)	171.8(4)
C(55)-O(8)-C(43)-C(44)	3.3(6)
C(55)-O(8)-C(43)-C(42)	-179.8(4)

C(41)-C(42)-C(43)-O(8)	-179.1(4)
O(7)-C(42)-C(43)-O(8)	0.5(5)
C(41)-C(42)-C(43)-C(44)	-2.0(6)
O(7)-C(42)-C(43)-C(44)	177.6(4)
O(8)-C(43)-C(44)-C(39)	-179.5(4)
C(42)-C(43)-C(44)-C(39)	3.7(6)
C(40)-C(39)-C(44)-C(43)	-2.2(6)
C(38)-C(39)-C(44)-C(43)	-177.4(4)
C(49)-N(2)-C(45)-C(46)	-136.6(4)
C(50)-N(2)-C(45)-C(46)	-12.4(5)
C(49)-N(2)-C(45)-C(38)	-11.2(4)
C(50)-N(2)-C(45)-C(38)	113.1(4)
C(39)-C(38)-C(45)-C(46)	-83.7(4)
C(48)-C(38)-C(45)-C(46)	154.4(3)
C(37)-C(38)-C(45)-C(46)	34.4(5)
C(39)-C(38)-C(45)-N(2)	154.3(3)
C(48)-C(38)-C(45)-N(2)	32.4(4)
C(37)-C(38)-C(45)-N(2)	-87.6(4)
N(2)-C(45)-C(46)-C(47)	63.9(4)
C(38)-C(45)-C(46)-C(47)	-55.1(5)
C(45)-C(46)-C(47)-C(51)	-55.5(4)
C(45)-C(46)-C(47)-C(36)	66.2(4)
C(37)-C(36)-C(47)-C(46)	-60.0(4)
C(35)-C(36)-C(47)-C(46)	172.5(4)
C(37)-C(36)-C(47)-C(51)	58.9(4)
C(35)-C(36)-C(47)-C(51)	-68.6(5)
C(39)-C(38)-C(48)-C(49)	-166.1(3)
C(45)-C(38)-C(48)-C(49)	-41.8(4)
C(37)-C(38)-C(48)-C(49)	80.5(4)
C(50)-N(2)-C(49)-C(48)	-140.4(3)
C(45)-N(2)-C(49)-C(48)	-15.3(4)
C(38)-C(48)-C(49)-N(2)	35.5(4)
C(49)-N(2)-C(50)-C(51)	78.5(4)
C(45)-N(2)-C(50)-C(51)	-43.1(5)
N(2)-C(50)-C(51)-C(52)	-129.5(4)
N(2)-C(50)-C(51)-C(47)	51.8(5)

C(46)-C(47)-C(51)-C(52)	179.4(4)
C(36)-C(47)-C(51)-C(52)	61.1(5)
C(46)-C(47)-C(51)-C(50)	-1.8(5)
C(36)-C(47)-C(51)-C(50)	-120.2(4)
C(50)-C(51)-C(52)-C(53)	178.7(4)
C(47)-C(51)-C(52)-C(53)	-2.6(7)
C(35)-O(6)-C(53)-C(52)	89.8(5)
C(51)-C(52)-C(53)-O(6)	-67.2(6)

Symmetry transformations used to generate equivalent atoms:

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Space Group P212121
Wavelength 1.54178

Bijvoet Pairs 4185
Coverage ... 93.2
DiffCalcMax. 1185.77
Outlier Crit 2371.54
Sigma Crit.. 0.25
Select Pairs 2534
Number Plus 1937
Number Minus 597
Aver. Ratio 0.966
RC 0.939

Normal Prob. Plot
Sample Size. 4185
Corr. Coeff. 0.996
Intercept .. 0.075
Slope 1.115

Bayesian Statistics
Type ..... Gaussian
Select Pairs 4185
P2(true).... 1.000
P3(true).... 1.000
P3(rac-twin) 0.0E+00
P3(false) .. 0.0E+00
G 0.9392
G (su) 0.0142
Hooft y 0.030
Hooft (su) . 0.007

Space Group P212121
Wavelength 1.54178

Bijvoet Pairs 4185
Coverage ... 93.2
DiffCalcMax. 1185.77
Outlier Crit 2371.54
Sigma Crit.. 0.25
Select Pairs 2534
Number Plus 1937
Number Minus 597
Aver. Ratio 0.966
RC 0.939

Normal Prob. Plot
Sample Size. 4185
Corr. Coeff. 0.996
Intercept .. 0.075
Slope 1.115

Bayesian Statistics
Type ..... Gaussian
Select Pairs 4185
P2(true).... 1.000
P3(true).... 1.000
P3(rac-twin) 0.0E+00
P3(false) .. 0.0E+00
G 0.9392
G (su) 0.0142
Hooft y 0.030
Hooft (su) . 0.007

(B). Cartesian coordinates, and intensities for vibrational and electronic transitions

Table S7. Cartesian coordinates for cis-cis conformer of (aS)-Vanol

Atom	X	Y	Z
O	-1.31356	1.11515	-2.43191
H	-1.42208	0.16318	-2.30091
C	0.20121	0.72193	-0.61201
C	-0.09596	2.95852	-1.59087
C	0.8225	3.48235	-0.63946
C	1.14032	1.26402	0.3264
C	1.41827	2.61119	0.30288
H	2.13492	3.01659	1.00421
C	-0.38732	1.56726	-1.53923
C	-0.38732	5.1596	-2.54488
C	-0.69359	3.82216	-2.53819
C	0.52555	5.68621	-1.60654
H	0.75922	6.74234	-1.62277
C	1.82994	0.40577	1.33026
C	2.60914	-0.69023	0.94512
H	2.70386	-0.94166	-0.10181
C	1.11576	4.8678	-0.67808
H	1.81659	5.27094	0.04149
C	1.74961	0.71913	2.69095
H	1.13661	1.55286	3.00459
C	3.28749	-1.44701	1.89212
H	3.89102	-2.28592	1.57245
C	3.19739	-1.12653	3.24248
H	3.72455	-1.71824	3.97871
C	2.42585	-0.04026	3.63863
H	2.34505	0.21544	4.68677
C	-0.20121	-0.72193	-0.61201
O	1.31356	-1.11515	-2.43191
H	1.42208	-0.16318	-2.30091
C	0.09596	-2.95852	-1.59087
C	-0.8225	-3.48235	-0.63946
C	-1.14032	-1.26402	0.3264
C	-1.41827	-2.61119	0.30288
H	-2.13492	-3.01659	1.00421
C	0.38732	-1.56726	-1.53923
C	0.38732	-5.1596	-2.54488
C	0.69359	-3.82216	-2.53819
C	-0.52555	-5.68621	-1.60654
H	-0.75922	-6.74234	-1.62277
C	-1.82994	-0.40577	1.33026
C	-2.60914	0.69023	0.94512
H	-2.70386	0.94166	-0.10181
C	-1.11576	-4.8678	-0.67808
H	-1.81659	-5.27094	0.04149
C	-1.74961	-0.71913	2.69095
H	-1.13661	-1.55286	3.00459
C	-3.28749	1.44701	1.89212
H	-3.89102	2.28592	1.57245

C	-3.19739	1.12653	3.24248
H	-3.72455	1.71824	3.97871
C	-2.42585	0.04026	3.63863
H	-2.34505	-0.21544	4.68677
H	0.84586	-5.81559	-3.27226
H	1.39023	-3.41021	-3.25269
H	-0.84586	5.81559	-3.27226
H	-1.39023	3.41021	-3.25269

Table S8. Vibrational frequencies and intensities for (aR)-(+)-VANOL in the mid-infared region.

B3LYP/6-311G(2d,2p)

Symmetry	Wavenumber (cm^{-1})	Absorption (km/mol)	Rotational Strength[a]
A	865.6421	0.0111	-1.2027
A	871.4675	4.8645	-26.3132
B	871.8404	6.7748	24.6781
B	877.7299	7.7919	-35.794
B	904.5151	10.9654	73.209
A	904.6109	9.1582	-50.7117
A	909.785	0.019	-2.7692
B	930.7033	26.0895	67.9585
A	945.3238	2.9226	-5.0005
B	949.7567	2.3343	-5.2679
A	967.2147	29.3	37.4337
B	978.1241	1.0133	5.0854
A	978.1436	1.3866	-5.6859
A	993.3482	0.433	-1.2669
B	993.539	0.3408	-2.772
B	1002.1631	0.0013	-0.0086
A	1002.1726	0.0012	-0.0117
A	1008.5462	0.0021	0.1543
B	1008.5726	1.2102	2.0445
A	1020.6731	2.2001	6.7353
B	1020.7071	1.1046	2.425
B	1041.6975	8.3836	5.163
A	1044.6648	4.5621	3.2711
B	1053.0479	6.1862	-14.1493
A	1053.7981	1.1378	2.8568

B	1088.487	26.9001	-52.7905
B	1105.0746	4.4075	2.7517
A	1105.3745	7.5657	6.7794
A	1117.3512	12.7126	60.1682
B	1133.3858	25.8157	-69.0371
A	1165.3943	11.0257	47.9494
B	1173.7763	18.6193	-76.8837
B	1175.1181	7.7829	-10.7929
A	1175.5154	3.8691	16.7086
A	1183.8287	0.0011	0.0209
B	1183.8605	0.029	-0.0291
B	1209.9313	0.4882	-1.1943
A	1210.34	0.3499	2.0293
A	1216.7938	11.8672	-29.1752
B	1218.9784	23.4495	22.3229
A	1247.8252	6.3106	29.7377
B	1253.01	26.1765	-84.62
A	1264.3253	40.0841	24.2861
B	1283.0708	53.3019	39.3425
A	1303.4608	22.7659	-12.9443
B	1304.75	0.3363	2.9607
A	1308.7954	19.0692	-101.0014
A	1324.1934	2.3387	22.5075
B	1327.0251	5.0236	28.8045
A	1358.3814	0.0044	1.3428
B	1358.8699	2.8025	40.6357
A	1375.7659	0.6431	-25.6566
B	1378.0984	3.2938	42.6968
A	1388.4892	7.1254	13.3386
B	1389.7609	29.525	-17.1999
B	1408.2222	123.6869	-14.0011
A	1411.2193	35.0677	169.8819
B	1466.9515	3.369	-7.208
A	1474.1757	7.9541	-13.2032
A	1481.1945	0.0782	-6.9401
B	1483.7682	4.7509	-11.092
B	1485.7823	18.5235	11.3111
A	1496.5867	0.0076	2.5319
A	1528.6299	36.57	128.6933
B	1529.7301	28.9237	-132.1189
A	1536.2854	9.0532	3.5198
B	1536.5871	9.7869	-4.1063
B	1601.4729	22.2742	-17.3655

A	1602.3194	26.7937	23.8155
A	1615.5558	2.5428	9.2874
B	1615.7454	12.3443	-11.7689
B	1630.9929	19.0712	-58.3227
A	1632.6641	33.5129	66.0446
B	1642.629	2.854	-11.9158
A	1642.7462	1.407	8.2281
A	1663.7756	10.77	14.5768
B	1664.2956	34.3682	-19.674

[a] $10^{-44} esu^2 cm^2$

Table S9: Electronic transition wavelengths, oscillator strengths and rotational strengths of (aR)-(+)-VANOL

B3LYP/6-311G(2d,2p)

Symmetry	Wavelength (nm)	Oscillator strength	Rotational strength[a]
A	320.26	0.0027	3.4077
B	315.85	0.075	10.3585
B	309.48	0.0325	-41.7889
A	307.66	0.0124	50.872
B	299.14	0.0761	-26.4901
A	295.8	0.0065	19.8943
A	285.84	0.0005	-0.748
B	283.91	0.0193	-15.4888
A	267.8	0.1639	345.7138
B	263.91	0.1419	18.9711
B	259.52	0.2285	-106.3627
A	254.39	0.0075	16.24
B	252.47	0.137	-151.7852
A	251.52	0.1245	249.3029
B	249.61	0.0647	-163.9362
A	249.26	0.0033	-7.3375
B	248.24	0.0386	-54.5203
B	246.45	0.116	-123.9641
A	245.73	0.0021	1.277
B	244.45	0.0283	-26.2095
A	243.38	0.0024	-13.6895
A	242.69	0.0204	17.8628
A	240.25	0.0099	15.5526

B	236.94	0.0061	-8.9222
A	236.89	0.0913	177.1756
B	236.24	0.0073	-2.1281
A	236.09	0.0019	4.1265
B	233.61	0.0596	-164.6821
A	231.43	0.0612	94.5211
B	230.3	0.1743	-70.3867

[a] 10^{-40} erg•esu•cm/Gauss