Supporting Information 3

Synthesis and Characterization of Bimetallic Nanoclusters Stabilized by Chiral and Achiral Polyvinylpyrrolidinones. Catalytic C(sp^3)-H Oxidation

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X-ray structural information

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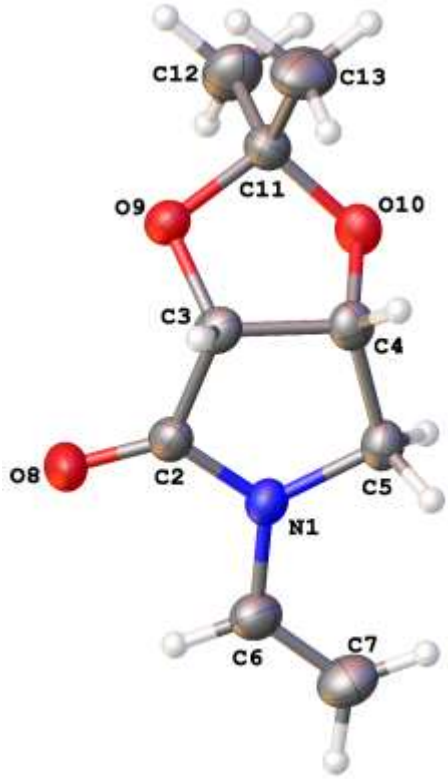

Table SI3-1. Crystal data and structure refinement for compound (-)-6, $C_9H_{13}NO_3$.

Identification code	q69j	
Empirical formula	C9 H13 N O3	
Formula weight	183.20	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 8.4981(2) Å	α= 90°.
	b = 10.0882(2) Å	β= 90°.
	c = 11.2710(2) Å	γ = 90°.
Volume	966.27(3) $Å^3$	
Z	4	
Density (calculated)	1.259 Mg/m^3	
Absorption coefficient	0.788 mm^{-1}	
F(000)	392	
Crystal size	0.240 x 0.185 x 0.125 mm^3	
Theta range for data collection	5.886 to 70.234°.	
Index ranges	-6<=h<=10, -12<=k<=8, -13<=l<=13	
Reflections collected	3636	
Independent reflections	1595 [R(int) = 0.0161]	
Completeness to theta = 66.000°	99.2 %	
Absorption correction	Multi-scan	
Max. and min. transmission	0.7533 and 0.6898	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1595 / 0 / 171	
Goodness-of-fit on F^2	1.063	

Final R indices [I>2sigma(I)]	R1 = 0.0255, wR2 = 0.0674
R indices (all data)	R1 = 0.0256, wR2 = 0.0674
Absolute structure parameter	0.14(7)
Extinction coefficient	0.0177(14)
Largest diff. peak and hole	0.156 and -0.133 e.Å^{-3}

Table SI3-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for C9H13NO3. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	3061(2)	41(1)	4401(1)	29(1)
C(2)	2042(2)	809(2)	5028(1)	31(1)
C(3)	2353(2)	2248(2)	4700(1)	31(1)
C(4)	3461(2)	2186(2)	3635(1)	30(1)
C(5)	4037(2)	760(2)	3556(2)	30(1)
C(6)	3240(2)	-1322(2)	4618(2)	36(1)
C(7)	4265(3)	-2074(2)	4063(2)	44(1)
O(8)	1065(2)	407(1)	5731(1)	49(1)
O(9)	953(1)	2875(1)	4289(1)	35(1)
O(10)	2436(1)	2503(1)	2666(1)	35(1)
C(11)	1314(2)	3403(2)	3135(2)	32(1)
C(12)	-150(3)	3366(3)	2392(2)	49(1)
C(13)	1981(3)	4788(2)	3277(3)	55(1)

Table SI3-3. Bond lengths [Å] and angles [°] for C9H13NO3.

N(1)-C(2)	1.360(2)
N(1)-C(6)	1.405(2)
N(1)-C(5)	1.457(2)
C(2)-O(8)	1.217(2)
C(2)-C(3)	1.521(2)
C(3)-O(9)	1.4250(19)
C(3)-C(4)	1.527(2)
C(3)-H(3)	0.954(19)
C(4)-O(10)	1.4323(19)
C(4)-C(5)	1.521(2)
C(4)-H(4)	0.92(2)
C(5)-H(5A)	0.97(2)
C(5)-H(5B)	1.01(2)
C(6)-C(7)	1.313(3)
C(6)-H(6)	0.95(2)
C(7)-H(7A)	0.97(2)
C(7)-H(7B)	0.92(3)
O(9)-C(11)	1.4377(19)
O(10)-C(11)	1.419(2)
C(11)-C(12)	1.500(3)
C(11)-C(13)	1.517(3)
C(12)-H(12A)	0.99(3)
C(12)-H(12B)	0.97(3)
C(12)-H(12C)	0.97(3)
C(13)-H(13A)	0.95(3)
C(13)-H(13B)	0.95(3)
C(13)-H(13C)	1.04(3)
C(2)-N(1)-C(6)	122.44(15)
C(2)-N(1)-C(5)	114.74(14)
C(6)-N(1)-C(5)	122.66(14)
O(8)-C(2)-N(1)	125.68(16)
O(8)-C(2)-C(3)	126.48(15)
N(1)-C(2)-C(3)	107.84(14)
O(9)-C(3)-C(2)	110.96(14)
O(9)-C(3)-C(4)	106.13(12)
C(2)-C(3)-C(4)	105.01(13)
O(9)-C(3)-H(3)	111.1(12)
C(2)-C(3)-H(3)	108.9(11)
C(4)-C(3)-H(3)	114.6(12)
O(10)-C(4)-C(5)	111.23(14)
O(10)-C(4)-C(3)	102.41(12)
C(5)-C(4)-C(3)	106.46(13)
O(10)-C(4)-H(4)	111.1(13)
C(5)-C(4)-H(4)	112.2(13)
C(3)-C(4)-H(4)	113.0(13)
N(1)-C(5)-C(4)	104.45(13)
N(1)-C(5)-H(5A)	110.7(12)
C(4)-C(5)-H(5A)	111.1(12)
N(1)-C(5)-H(5B)	108.1(11)
C(4)-C(5)-H(5B)	113.9(12)
H(5A)-C(5)-H(5B)	108.5(17)
C(7)-C(6)-N(1)	123.66(18)
C(7)-C(6)-H(6)	123.3(13)

N(1)-C(6)-H(6)	112.9(12)
C(6)-C(7)-H(7A)	121.0(14)
C(6)-C(7)-H(7B)	123.1(17)
H(7A)-C(7)-H(7B)	116(2)
C(3)-O(9)-C(11)	106.27(12)
C(11)-O(10)-C(4)	105.54(12)
O(10)-C(11)-O(9)	104.08(12)
O(10)-C(11)-C(12)	109.48(15)
O(9)-C(11)-C(12)	108.62(15)
O(10)-C(11)-C(13)	112.17(16)
O(9)-C(11)-C(13)	109.01(16)
C(12)-C(11)-C(13)	113.05(18)
C(11)-C(12)-H(12A)	109.6(15)
C(11)-C(12)-H(12B)	109.5(15)
H(12A)-C(12)-H(12B)	109(2)
C(11)-C(12)-H(12C)	109.1(18)
H(12A)-C(12)-H(12C)	109(2)
H(12B)-C(12)-H(12C)	110(2)
C(11)-C(13)-H(13A)	108.2(17)
C(11)-C(13)-H(13B)	109.6(17)
H(13A)-C(13)-H(13B)	109(2)
C(11)-C(13)-H(13C)	108.2(17)
H(13A)-C(13)-H(13C)	110(2)
H(13B)-C(13)-H(13C)	112(2)

Table SI3-4. Anisotropic displacement parameters ($Å^2$x 10^3) for C9H13NO3. 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}
N(1)	26(1)	31(1)	30(1)	0(1)	3(1)	2(1)
C(2)	31(1)	36(1)	26(1)	4(1)	2(1)	7(1)
C(3)	33(1)	33(1)	26(1)	-4(1)	-2(1)	5(1)
C(4)	24(1)	34(1)	31(1)	0(1)	-2(1)	-3(1)
C(5)	27(1)	36(1)	28(1)	-2(1)	2(1)	0(1)
C(6)	32(1)	33(1)	43(1)	3(1)	-1(1)	2(1)
C(7)	47(1)	34(1)	52(1)	-5(1)	-1(1)	7(1)
O(8)	49(1)	48(1)	50(1)	18(1)	24(1)	17(1)
O(9)	34(1)	38(1)	32(1)	6(1)	5(1)	10(1)
O(10)	32(1)	46(1)	27(1)	4(1)	1(1)	4(1)
C(11)	32(1)	33(1)	32(1)	5(1)	1(1)	2(1)
C(12)	41(1)	62(1)	44(1)	4(1)	-7(1)	10(1)
C(13)	51(1)	33(1)	81(2)	12(1)	3(1)	0(1)

Table SI3-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for C9H13NO3.

	x	y	z	U(eq)
H(3)	2770(20)	2697(19)	5374(17)	33(5)
H(4)	4280(30)	2780(20)	3684(18)	38(5)
H(5A)	3900(20)	410(20)	2759(19)	35(5)
H(5B)	5170(20)	640(20)	3793(17)	30(5)
H(6)	2580(30)	-1640(20)	5245(19)	40(5)
H(7A)	4370(30)	-3010(20)	4260(20)	49(6)
H(7B)	4910(30)	-1760(30)	3460(20)	58(7)
H(12A)	-960(30)	3960(20)	2740(20)	56(7)
H(12B)	-550(30)	2470(30)	2360(20)	56(7)
H(12C)	100(40)	3670(30)	1600(30)	74(9)
H(13A)	2210(30)	5130(30)	2510(30)	68(8)
H(13B)	1210(30)	5350(30)	3640(20)	66(8)
H(13C)	3000(40)	4720(30)	3780(30)	86(9)

Table SI3-6. Torsion angles [°] for C9H13NO3.

C(6)-N(1)-C(2)-O(8)	-8.7(3)
C(5)-N(1)-C(2)-O(8)	175.85(17)
C(6)-N(1)-C(2)-C(3)	170.84(15)
C(5)-N(1)-C(2)-C(3)	-4.62(19)
O(8)-C(2)-C(3)-O(9)	-55.7(2)
N(1)-C(2)-C(3)-O(9)	124.75(14)
O(8)-C(2)-C(3)-C(4)	-169.97(17)
N(1)-C(2)-C(3)-C(4)	10.50(17)
O(9)-C(3)-C(4)-O(10)	-13.03(16)
C(2)-C(3)-C(4)-O(10)	104.55(14)
O(9)-C(3)-C(4)-C(5)	-129.87(13)
C(2)-C(3)-C(4)-C(5)	-12.29(16)
C(2)-N(1)-C(5)-C(4)	-3.31(18)
C(6)-N(1)-C(5)-C(4)	-178.76(15)
O(10)-C(4)-C(5)-N(1)	-101.08(15)
C(3)-C(4)-C(5)-N(1)	9.72(16)
C(2)-N(1)-C(6)-C(7)	-176.85(18)
C(5)-N(1)-C(6)-C(7)	-1.7(3)
C(2)-C(3)-O(9)-C(11)	-124.66(13)
C(4)-C(3)-O(9)-C(11)	-11.12(16)
C(5)-C(4)-O(10)-C(11)	146.13(14)
C(3)-C(4)-O(10)-C(11)	32.76(16)
C(4)-O(10)-C(11)-O(9)	-40.82(15)
C(4)-O(10)-C(11)-C(12)	-156.79(15)
C(4)-O(10)-C(11)-C(13)	76.87(19)
C(3)-O(9)-C(11)-O(10)	31.65(16)
C(3)-O(9)-C(11)-C(12)	148.22(15)
C(3)-O(9)-C(11)-C(13)	-88.21(17)

Table SI3-7. Hydrogen bonds for C9H13NO3 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(4)-H(4)...O(8)#1	0.92(2)	2.47(2)	3.362(2)	164.8(18)
C(5)-H(5A)...O(8)#2	0.97(2)	2.43(2)	3.396(2)	172.2(17)
C(13)-H(13C)...O(8)#1	1.04(3)	2.67(4)	3.651(3)	159(2)

Symmetry transformations used to generate equivalent atoms:
#1 x+1/2,-y+1/2,-z+1 #2 -x+1/2,-y,z-1/2

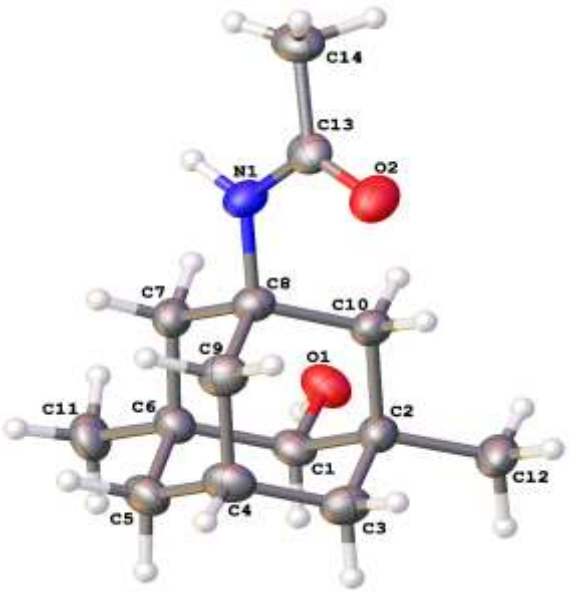

Table SI3-8. Crystal data and structure refinement for compound 35, $C_{14}H_{23}NO_2$.

Identification code	v04e	
Empirical formula	C14 H23 N O2	
Formula weight	237.33	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 8.5906(4) Å	α= 90°.
	b = 8.2369(4) Å	β= 94.514(3)°.
	c = 18.0620(9) Å	γ = 90°.
Volume	1274.10(11) $Å^3$	
Z	4	
Density (calculated)	1.237 Mg/m^3	
Absorption coefficient	0.645 mm^{-1}	
F(000)	520	
Crystal size	0.090 x 0.080 x 0.070 mm^3	
Theta range for data collection	4.912 to 68.315°.	
Index ranges	-10<=h<=10, -7<=k<=9, -20<=l<=21	
Reflections collected	6644	
Independent reflections	2236 [R(int) = 0.0600]	
Completeness to theta = 66.000°	98.1 %	
Absorption correction	Multi-scan	
Max. and min. transmission	0.7531 and 0.6183	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2236 / 0 / 247	
Goodness-of-fit on F^2	1.049	
Final R indices [I>2sigma(I)]	R1 = 0.0851, wR2 = 0.2294	
R indices (all data)	R1 = 0.0987, wR2 = 0.2422	
Extinction coefficient	0.008(2)	
Largest diff. peak and hole	0.412 and -0.597 $e.Å^{-3}$	

Table SI3-9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for C14H23NO2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	424(3)	4347(3)	1772(1)	36(1)
O(2)	7297(3)	3728(3)	1808(1)	41(1)
N(1)	5336(3)	2234(3)	2216(1)	31(1)
C(1)	975(3)	3694(3)	1104(2)	29(1)
C(2)	2446(3)	4635(3)	915(2)	30(1)
C(3)	2942(4)	3973(4)	174(2)	36(1)
C(4)	3340(4)	2175(4)	238(2)	37(1)
C(5)	1881(4)	1254(4)	433(2)	36(1)
C(6)	1342(3)	1858(3)	1178(2)	30(1)
C(7)	2679(3)	1617(3)	1780(2)	30(1)
C(8)	4159(3)	2522(3)	1588(2)	28(1)
C(9)	4679(4)	1889(4)	844(2)	36(1)
C(10)	3771(4)	4333(3)	1515(2)	29(1)
C(11)	-95(4)	902(4)	1368(2)	39(1)
C(12)	2114(4)	6458(4)	846(2)	39(1)
C(13)	6764(3)	2916(3)	2300(2)	32(1)
C(14)	7668(4)	2649(4)	3038(2)	41(1)

Table SI3-10. Bond lengths [Å] and angles [°] for C14H23NO2.

O(1)-C(1)	1.435(3)
O(1)-H(1O)	1.03(8)
O(2)-C(13)	1.230(4)
N(1)-C(13)	1.347(4)
N(1)-C(8)	1.477(4)
N(1)-H(1N)	0.92(4)
C(1)-C(2)	1.543(4)
C(1)-C(6)	1.548(4)
C(1)-H(1)	0.97(3)
C(2)-C(10)	1.529(4)
C(2)-C(12)	1.532(4)
C(2)-C(3)	1.537(4)
C(3)-C(4)	1.522(4)
C(3)-H(3A)	0.91(4)
C(3)-H(3B)	1.01(4)
C(4)-C(5)	1.530(5)
C(4)-C(9)	1.542(4)
C(4)-H(4)	1.04(4)
C(5)-C(6)	1.540(4)
C(5)-H(5A)	1.08(4)
C(5)-H(5B)	1.04(4)
C(6)-C(11)	1.526(4)
C(6)-C(7)	1.531(4)
C(7)-C(8)	1.537(4)
C(7)-H(7A)	0.97(4)
C(7)-H(7B)	1.01(4)
C(8)-C(10)	1.531(4)
C(8)-C(9)	1.541(4)
C(9)-H(9A)	0.99(4)
C(9)-H(9B)	0.99(4)
C(10)-H(10B)	0.96(4)
C(10)-H(10A)	1.06(3)
C(11)-H(11A)	0.99(4)
C(11)-H(11B)	0.97(4)
C(11)-H(11C)	1.10(4)
C(12)-H(12A)	0.92(4)
C(12)-H(12B)	1.05(5)
C(12)-H(12C)	1.06(5)
C(13)-C(14)	1.504(4)
C(14)-H(14A)	0.85(7)
C(14)-H(14B)	0.98(7)
C(14)-H(14C)	1.02(8)

C(1)-O(1)-H(1O)	114(4)
C(13)-N(1)-C(8)	125.6(3)
C(13)-N(1)-H(1N)	116(2)
C(8)-N(1)-H(1N)	118(2)
O(1)-C(1)-C(2)	109.1(2)
O(1)-C(1)-C(6)	111.8(2)
C(2)-C(1)-C(6)	110.2(2)
O(1)-C(1)-H(1)	110.4(19)
C(2)-C(1)-H(1)	105.9(19)
C(6)-C(1)-H(1)	109.2(18)
C(10)-C(2)-C(12)	109.9(2)

C(10)-C(2)-C(3)	108.5(2)
C(12)-C(2)-C(3)	109.8(3)
C(10)-C(2)-C(1)	109.8(2)
C(12)-C(2)-C(1)	111.1(3)
C(3)-C(2)-C(1)	107.6(2)
C(4)-C(3)-C(2)	110.8(2)
C(4)-C(3)-H(3A)	111(3)
C(2)-C(3)-H(3A)	109(3)
C(4)-C(3)-H(3B)	111(2)
C(2)-C(3)-H(3B)	114(2)
H(3A)-C(3)-H(3B)	100(3)
C(3)-C(4)-C(5)	108.4(3)
C(3)-C(4)-C(9)	110.7(3)
C(5)-C(4)-C(9)	109.8(3)
C(3)-C(4)-H(4)	115(2)
C(5)-C(4)-H(4)	111(2)
C(9)-C(4)-H(4)	101(2)
C(4)-C(5)-C(6)	110.5(2)
C(4)-C(5)-H(5A)	110(2)
C(6)-C(5)-H(5A)	112(2)
C(4)-C(5)-H(5B)	107(2)
C(6)-C(5)-H(5B)	111.2(19)
H(5A)-C(5)-H(5B)	107(3)
C(11)-C(6)-C(7)	110.4(3)
C(11)-C(6)-C(5)	109.5(2)
C(7)-C(6)-C(5)	108.6(2)
C(11)-C(6)-C(1)	111.1(2)
C(7)-C(6)-C(1)	108.9(2)
C(5)-C(6)-C(1)	108.2(2)
C(6)-C(7)-C(8)	111.4(2)
C(6)-C(7)-H(7A)	112(2)
C(8)-C(7)-H(7A)	108(2)
C(6)-C(7)-H(7B)	117(2)
C(8)-C(7)-H(7B)	104(2)
H(7A)-C(7)-H(7B)	103(3)
N(1)-C(8)-C(10)	110.7(2)
N(1)-C(8)-C(7)	106.1(2)
C(10)-C(8)-C(7)	108.3(2)
N(1)-C(8)-C(9)	112.8(2)
C(10)-C(8)-C(9)	109.3(2)
C(7)-C(8)-C(9)	109.5(2)
C(8)-C(9)-C(4)	108.5(2)
C(8)-C(9)-H(9A)	112(2)
C(4)-C(9)-H(9A)	112(2)
C(8)-C(9)-H(9B)	107(2)
C(4)-C(9)-H(9B)	111(2)
H(9A)-C(9)-H(9B)	106(3)
C(2)-C(10)-C(8)	111.4(2)
C(2)-C(10)-H(10B)	108(2)
C(8)-C(10)-H(10B)	111(2)
C(2)-C(10)-H(10A)	109.5(17)
C(8)-C(10)-H(10A)	112.0(16)
H(10B)-C(10)-H(10A)	105(3)
C(6)-C(11)-H(11A)	107(2)
C(6)-C(11)-H(11B)	109(2)
H(11A)-C(11)-H(11B)	110(3)

C(6)-C(11)-H(11C)	110(2)
H(11A)-C(11)-H(11C)	105(3)
H(11B)-C(11)-H(11C)	115(3)
C(2)-C(12)-H(12A)	111(2)
C(2)-C(12)-H(12B)	113(2)
H(12A)-C(12)-H(12B)	110(3)
C(2)-C(12)-H(12C)	109(3)
H(12A)-C(12)-H(12C)	103(4)
H(12B)-C(12)-H(12C)	110(4)
O(2)-C(13)-N(1)	122.2(3)
O(2)-C(13)-C(14)	121.6(3)
N(1)-C(13)-C(14)	116.2(3)
C(13)-C(14)-H(14A)	113(4)
C(13)-C(14)-H(14B)	111(4)
H(14A)-C(14)-H(14B)	102(5)
C(13)-C(14)-H(14C)	103(4)
H(14A)-C(14)-H(14C)	126(6)
H(14B)-C(14)-H(14C)	101(5)

Table SI3-11. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for C14H23NO2. 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}
O(1)	28(1)	39(1)	40(1)	-10(1)	1(1)	1(1)
O(2)	27(1)	41(1)	53(1)	9(1)	-1(1)	1(1)
N(1)	27(1)	32(1)	33(1)	7(1)	-3(1)	1(1)
C(1)	22(2)	32(1)	33(2)	-4(1)	-4(1)	1(1)
C(2)	28(2)	26(1)	33(2)	2(1)	-3(1)	-1(1)
C(3)	33(2)	42(2)	31(2)	5(1)	2(1)	-1(1)
C(4)	38(2)	44(2)	30(2)	-6(1)	2(1)	5(1)
C(5)	39(2)	33(2)	36(2)	-9(1)	-4(1)	2(1)
C(6)	28(2)	28(1)	33(2)	-3(1)	-1(1)	-2(1)
C(7)	28(2)	25(1)	35(2)	3(1)	-1(1)	-2(1)
C(8)	27(2)	30(1)	28(1)	2(1)	-1(1)	2(1)
C(9)	36(2)	37(2)	35(2)	-2(1)	3(1)	7(1)
C(10)	30(2)	28(1)	29(1)	4(1)	-1(1)	-1(1)
C(11)	32(2)	31(2)	53(2)	-1(1)	-1(2)	-8(1)
C(12)	39(2)	29(2)	48(2)	5(1)	-8(2)	2(1)
C(13)	25(2)	29(1)	41(2)	-1(1)	-1(1)	7(1)
C(14)	35(2)	43(2)	44(2)	-1(1)	-11(2)	5(1)

Table SI3-12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10 ^{3}) for C14H23NO2.

	x	y	z	U(eq)
H(1O)	-760(100)	4220(90)	1810(40)	150(30)
H(1N)	5080(40)	1540(40)	2585(18)	28(8)
H(1)	210(40)	3860(40)	686(18)	25(8)
H(3A)	3760(50)	4560(50)	30(20)	53(11)
H(3B)	2150(40)	4180(40)	-260(20)	38(9)
H(4)	3810(50)	1680(50)	-220(20)	42(9)
H(5A)	970(50)	1370(40)	-10(20)	42(10)
H(5B)	2180(40)	40(50)	460(20)	38(9)
H(7A)	2940(40)	480(50)	1850(20)	38(9)
H(7B)	2510(40)	2000(40)	2300(20)	38(9)
H(9A)	5660(50)	2410(50)	720(20)	47(10)
H(9B)	4910(40)	710(50)	910(20)	37(9)
H(10B)	4660(40)	4950(40)	1385(19)	33(8)
H(10A)	3470(40)	4840(40)	2025(17)	21(7)
H(11A)	180(40)	-260(40)	1350(20)	38(9)
H(11B)	-950(50)	1130(40)	1000(20)	38(9)
H(11C)	-330(50)	1130(50)	1950(30)	55(11)
H(12A)	1960(50)	6910(50)	1300(20)	45(10)
H(12B)	1160(50)	6720(50)	460(20)	60(12)
H(12C)	3130(60)	7060(60)	690(30)	68(14)
H(14A)	7400(70)	1780(80)	3250(30)	92(19)
H(14B)	8770(80)	2450(70)	2970(30)	100(20)
H(14C)	7730(90)	3790(100)	3260(40)	130(20)

Table SI3-13. Torsion angles [°] for C14H23NO2.

O(1)-C(1)-C(2)-C(10)	65.5(3)
C(6)-C(1)-C(2)-C(10)	-57.6(3)
O(1)-C(1)-C(2)-C(12)	-56.3(3)
C(6)-C(1)-C(2)-C(12)	-179.5(2)
O(1)-C(1)-C(2)-C(3)	-176.6(2)
C(6)-C(1)-C(2)-C(3)	60.3(3)
C(10)-C(2)-C(3)-C(4)	57.6(3)
C(12)-C(2)-C(3)-C(4)	177.8(3)
C(1)-C(2)-C(3)-C(4)	-61.2(3)
C(2)-C(3)-C(4)-C(5)	61.3(3)
C(2)-C(3)-C(4)-C(9)	-59.2(4)
C(3)-C(4)-C(5)-C(6)	-60.3(3)
C(9)-C(4)-C(5)-C(6)	60.7(3)
C(4)-C(5)-C(6)-C(11)	-179.0(3)
C(4)-C(5)-C(6)-C(7)	-58.4(3)
C(4)-C(5)-C(6)-C(1)	59.7(3)
O(1)-C(1)-C(6)-C(11)	58.2(3)
C(2)-C(1)-C(6)-C(11)	179.8(2)
O(1)-C(1)-C(6)-C(7)	-63.7(3)
C(2)-C(1)-C(6)-C(7)	57.9(3)
O(1)-C(1)-C(6)-C(5)	178.5(2)
C(2)-C(1)-C(6)-C(5)	-59.9(3)
C(11)-C(6)-C(7)-C(8)	178.1(2)
C(5)-C(6)-C(7)-C(8)	58.0(3)
C(1)-C(6)-C(7)-C(8)	-59.6(3)
C(13)-N(1)-C(8)-C(10)	-57.2(4)
C(13)-N(1)-C(8)-C(7)	-174.5(3)
C(13)-N(1)-C(8)-C(9)	65.6(4)
C(6)-C(7)-C(8)-N(1)	178.4(2)
C(6)-C(7)-C(8)-C(10)	59.5(3)
C(6)-C(7)-C(8)-C(9)	-59.5(3)
N(1)-C(8)-C(9)-C(4)	177.3(2)
C(10)-C(8)-C(9)-C(4)	-59.1(3)
C(7)-C(8)-C(9)-C(4)	59.3(3)
C(3)-C(4)-C(9)-C(8)	59.2(3)
C(5)-C(4)-C(9)-C(8)	-60.5(3)
C(12)-C(2)-C(10)-C(8)	-178.8(3)
C(3)-C(2)-C(10)-C(8)	-58.6(3)
C(1)-C(2)-C(10)-C(8)	58.7(3)
N(1)-C(8)-C(10)-C(2)	-174.7(2)
C(7)-C(8)-C(10)-C(2)	-58.7(3)
C(9)-C(8)-C(10)-C(2)	60.5(3)
C(8)-N(1)-C(13)-O(2)	-8.3(5)
C(8)-N(1)-C(13)-C(14)	170.8(3)

Table SI3-14. Hydrogen bonds for C14H23NO2 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1O)...O(2)#1	1.03(8)	1.72(8)	2.740(3)	172(7)
N(1)-H(1N)...O(1)#2	0.92(4)	2.21(4)	3.101(3)	164(3)
C(9)-H(9A)...O(2)	0.99(4)	2.57(4)	3.126(4)	115(3)
C(10)-H(10B)...O(2)	0.96(4)	2.54(3)	3.074(4)	115(2)
C(14)-H(14A)...O(2)#3	0.85(7)	2.53(7)	3.241(4)	141(5)

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z #2 -x+1/2,y-1/2,-z+1/2 #3 -x+3/2,y-1/2,-z+1/2

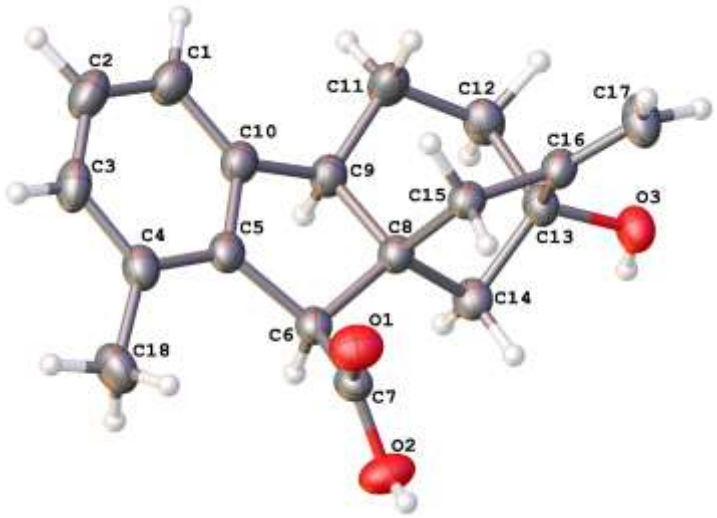

Table SI3-15. Crystal data and structure refinement for compound 46, $C_{18}H_{22}O_4$.

Identification code	exp_290	
Empirical formula	C18 H22 O4	
Formula weight	302.35	
Temperature	210.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 7.39013(18) Å	α= 90°.
	b = 6.96698(16) Å	β= 96.278(2)°.
	c = 15.1801(4) Å	γ = 90°.
Volume	776.89(3) Å^3	
Z	2	
Density (calculated)	1.293 Mg/m^3	
Absorption coefficient	0.733 mm^{-1}	
F(000)	324	
Crystal size	0.21 x 0.02 x 0.02 mm^3	
Theta range for data collection	2.929 to 77.693°.	
Index ranges	-9<=h<=9, -8<=k<=8, -19<=l<=19	
Reflections collected	11480	
Independent reflections	3219 [R(int) = 0.0377]	
Completeness to theta = 67.684°	99.9 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.707	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3219 / 1 / 274	
Goodness-of-fit on F^2	1.097	
Final R indices [I>2sigma(I)]	R1 = 0.0406, wR2 = 0.1139	
R indices (all data)	R1 = 0.0424, wR2 = 0.1156	
Absolute structure parameter	0.12(12)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.245 and -0.252 e.Å^{-3}	

Table SI3-16. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $C_{18}H_{22}O_4$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	8018(3)	5459(3)	8216(1)	41(1)
O(2)	5992(3)	7788(3)	8259(2)	42(1)
O(3)	269(2)	2684(3)	8967(1)	34(1)
C(1)	5617(4)	1227(4)	5698(2)	39(1)
C(2)	7181(4)	1646(5)	5297(2)	42(1)
C(3)	8117(4)	3349(5)	5483(2)	39(1)
C(4)	7581(4)	4679(4)	6093(2)	34(1)
C(5)	6081(3)	4182(3)	6532(2)	30(1)
C(6)	5225(3)	5297(3)	7239(2)	27(1)
C(7)	6565(3)	6179(3)	7946(2)	29(1)
C(8)	3980(3)	3764(3)	7618(2)	27(1)
C(9)	3386(4)	2547(4)	6784(2)	32(1)
C(10)	5073(3)	2517(4)	6311(2)	32(1)
C(11)	2425(4)	696(4)	6993(2)	37(1)
C(12)	927(4)	1150(4)	7594(2)	36(1)
C(13)	1626(3)	2485(4)	8362(2)	30(1)
C(14)	2274(3)	4419(4)	8021(2)	31(1)
C(15)	4919(3)	2493(3)	8365(2)	28(1)
C(16)	3389(3)	1681(3)	8830(2)	30(1)
C(17)	3515(4)	517(5)	9522(2)	42(1)
C(18)	8511(4)	6592(4)	6207(2)	43(1)
O(1W)	8197(3)	9509(3)	9453(2)	48(1)

Table SI3-17. Bond lengths [Å] and angles [°] for $C_{18}H_{22}O_4$.

O(1)-C(7)	1.215(3)
O(2)-C(7)	1.306(3)
O(3)-C(13)	1.438(3)
C(1)-C(2)	1.395(4)
C(1)-C(10)	1.384(4)
C(2)-C(3)	1.387(5)
C(3)-C(4)	1.397(4)
C(4)-C(5)	1.398(3)
C(4)-C(18)	1.501(4)
C(5)-C(6)	1.518(3)
C(5)-C(10)	1.399(4)
C(6)-C(7)	1.509(4)
C(6)-C(8)	1.560(3)
C(8)-C(9)	1.547(3)
C(8)-C(14)	1.529(3)
C(8)-C(15)	1.543(3)
C(9)-C(10)	1.506(3)
C(9)-C(11)	1.521(4)
C(11)-C(12)	1.542(4)
C(12)-C(13)	1.537(4)
C(13)-C(14)	1.539(4)
C(13)-C(16)	1.521(3)
C(15)-C(16)	1.507(3)
C(16)-C(17)	1.323(4)
C(10)-C(1)-C(2)	118.2(3)
C(3)-C(2)-C(1)	120.6(3)
C(2)-C(3)-C(4)	122.1(2)
C(3)-C(4)-C(5)	116.7(2)
C(3)-C(4)-C(18)	120.4(2)
C(5)-C(4)-C(18)	122.8(2)
C(4)-C(5)-C(6)	128.6(2)
C(4)-C(5)-C(10)	121.3(2)
C(10)-C(5)-C(6)	110.0(2)
C(5)-C(6)-C(8)	102.61(19)
C(7)-C(6)-C(5)	114.8(2)
C(7)-C(6)-C(8)	112.55(19)
O(1)-C(7)-O(2)	122.7(2)
O(1)-C(7)-C(6)	124.0(2)
O(2)-C(7)-C(6)	113.3(2)
C(9)-C(8)-C(6)	101.51(18)
C(14)-C(8)-C(6)	119.2(2)
C(14)-C(8)-C(9)	108.5(2)
C(14)-C(8)-C(15)	101.64(18)
C(15)-C(8)-C(6)	115.35(19)
C(15)-C(8)-C(9)	110.6(2)
C(10)-C(9)-C(8)	102.8(2)
C(10)-C(9)-C(11)	121.1(2)
C(11)-C(9)-C(8)	113.0(2)
C(1)-C(10)-C(5)	120.9(2)
C(1)-C(10)-C(9)	130.2(3)
C(5)-C(10)-C(9)	108.7(2)
C(9)-C(11)-C(12)	109.3(2)
C(13)-C(12)-C(11)	111.7(2)

O(3)-C(13)-C(12)	110.0(2)
O(3)-C(13)-C(14)	113.3(2)
O(3)-C(13)-C(16)	111.03(19)
C(12)-C(13)-C(14)	111.4(2)
C(16)-C(13)-C(12)	109.3(2)
C(16)-C(13)-C(14)	101.4(2)
C(8)-C(14)-C(13)	100.02(19)
C(16)-C(15)-C(8)	105.04(18)
C(15)-C(16)-C(13)	106.93(19)
C(17)-C(16)-C(13)	125.4(2)
C(17)-C(16)-C(15)	127.6(2)

Table SI3-18. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $C_{18}H_{22}O_4$. 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}
O(1)	31(1)	40(1)	50(1)	-2(1)	-3(1)	8(1)
O(2)	42(1)	35(1)	49(1)	-11(1)	-4(1)	11(1)
O(3)	29(1)	39(1)	35(1)	6(1)	9(1)	6(1)
C(1)	46(2)	42(1)	30(1)	-5(1)	5(1)	3(1)
C(2)	46(2)	50(2)	31(1)	-5(1)	8(1)	10(1)
C(3)	36(1)	54(2)	29(1)	6(1)	11(1)	9(1)
C(4)	33(1)	38(1)	30(1)	8(1)	7(1)	6(1)
C(5)	32(1)	31(1)	25(1)	4(1)	4(1)	6(1)
C(6)	29(1)	27(1)	27(1)	3(1)	5(1)	5(1)
C(7)	29(1)	26(1)	32(1)	3(1)	7(1)	3(1)
C(8)	28(1)	28(1)	26(1)	1(1)	4(1)	4(1)
C(9)	34(1)	35(1)	26(1)	0(1)	4(1)	1(1)
C(10)	34(1)	35(1)	26(1)	1(1)	4(1)	4(1)
C(11)	41(1)	39(1)	32(1)	-8(1)	6(1)	-7(1)
C(12)	34(1)	40(1)	32(1)	2(1)	2(1)	-6(1)
C(13)	27(1)	33(1)	29(1)	4(1)	7(1)	2(1)
C(14)	28(1)	32(1)	33(1)	4(1)	6(1)	6(1)
C(15)	29(1)	28(1)	27(1)	1(1)	3(1)	6(1)
C(16)	32(1)	32(1)	26(1)	1(1)	6(1)	5(1)
C(17)	39(1)	52(2)	36(1)	15(1)	11(1)	12(1)
C(18)	41(2)	43(2)	47(2)	11(1)	14(1)	-2(1)
O(1W)	51(1)	45(1)	45(1)	10(1)	-7(1)	-13(1)

Table SI3-19. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $C_{18}H_{22}O_4$.

	x	y	z	U(eq)
H(2)	6785	8226	8635	81(16)
H(3)	-550(60)	3490(70)	8780(30)	62(12)
H(1)	4930(50)	10(60)	5540(30)	44(9)
H(2A)	7600(50)	750(60)	4830(30)	45(9)
H(3A)	9090(50)	3630(60)	5190(20)	42(9)
H(6)	4470(40)	6280(50)	6980(20)	33(7)
H(9)	2420(50)	3400(60)	6420(20)	42(9)
H(11A)	1810(50)	70(60)	6440(30)	46(9)
H(11B)	3360(50)	-220(60)	7320(20)	41(9)
H(12A)	470(50)	-130(60)	7910(30)	53(10)
H(12B)	-60(50)	1860(60)	7310(20)	40(9)
H(14A)	2600(50)	5320(60)	8530(30)	44(9)
H(14B)	1400(50)	5010(50)	7610(20)	36(8)
H(15A)	5700(50)	3230(60)	8770(20)	43(9)
H(15B)	5590(50)	1540(50)	8090(20)	36(8)
H(17A)	2480(50)	150(60)	9830(30)	45(9)
H(17B)	4720(50)	50(50)	9780(20)	42(9)
H(18A)	7621	7607	6085	64
H(18B)	9429	6691	5799	64
H(18C)	9083	6713	6811	64
H(1WA)	9000(60)	10480(70)	9290(30)	59(11)
H(1WB)	8530(60)	8940(70)	9870(30)	52(12)

Table SI3-20. Torsion angles [°] for $C_{18}H_{22}O_4$.

O(3)-C(13)-C(14)-C(8)	166.0(2)
O(3)-C(13)-C(16)-C(15)	-149.5(2)
O(3)-C(13)-C(16)-C(17)	29.5(4)
C(1)-C(2)-C(3)-C(4)	2.0(4)
C(2)-C(1)-C(10)-C(5)	-0.9(4)
C(2)-C(1)-C(10)-C(9)	173.9(3)
C(2)-C(3)-C(4)-C(5)	2.1(4)
C(2)-C(3)-C(4)-C(18)	-173.7(3)
C(3)-C(4)-C(5)-C(6)	178.3(2)
C(3)-C(4)-C(5)-C(10)	-5.7(4)
C(4)-C(5)-C(6)-C(7)	-43.4(3)
C(4)-C(5)-C(6)-C(8)	-165.8(2)
C(4)-C(5)-C(10)-C(1)	5.2(4)
C(4)-C(5)-C(10)-C(9)	-170.6(2)
C(5)-C(6)-C(7)-O(1)	-33.3(3)
C(5)-C(6)-C(7)-O(2)	148.1(2)
C(5)-C(6)-C(8)-C(9)	-33.3(2)
C(5)-C(6)-C(8)-C(14)	-152.3(2)
C(5)-C(6)-C(8)-C(15)	86.3(2)
C(6)-C(5)-C(10)-C(1)	-178.0(2)
C(6)-C(5)-C(10)-C(9)	6.1(3)
C(6)-C(8)-C(9)-C(10)	37.0(2)
C(6)-C(8)-C(9)-C(11)	169.3(2)
C(6)-C(8)-C(14)-C(13)	-175.4(2)
C(6)-C(8)-C(15)-C(16)	160.26(19)
C(7)-C(6)-C(8)-C(9)	-157.18(19)
C(7)-C(6)-C(8)-C(14)	83.8(3)
C(7)-C(6)-C(8)-C(15)	-37.6(3)
C(8)-C(6)-C(7)-O(1)	83.5(3)
C(8)-C(6)-C(7)-O(2)	-95.0(2)
C(8)-C(9)-C(10)-C(1)	157.0(3)
C(8)-C(9)-C(10)-C(5)	-27.6(3)
C(8)-C(9)-C(11)-C(12)	49.2(3)
C(8)-C(15)-C(16)-C(13)	-0.4(3)
C(8)-C(15)-C(16)-C(17)	-179.4(3)
C(9)-C(8)-C(14)-C(13)	69.3(2)
C(9)-C(8)-C(15)-C(16)	-85.3(2)
C(9)-C(11)-C(12)-C(13)	-46.6(3)
C(10)-C(1)-C(2)-C(3)	-2.6(4)
C(10)-C(5)-C(6)-C(7)	140.2(2)
C(10)-C(5)-C(6)-C(8)	17.7(3)
C(10)-C(9)-C(11)-C(12)	171.8(2)
C(11)-C(9)-C(10)-C(1)	29.7(4)
C(11)-C(9)-C(10)-C(5)	-155.0(2)
C(11)-C(12)-C(13)-O(3)	-172.9(2)
C(11)-C(12)-C(13)-C(14)	60.6(3)
C(11)-C(12)-C(13)-C(16)	-50.7(3)
C(12)-C(13)-C(14)-C(8)	-69.3(2)
C(12)-C(13)-C(16)-C(15)	88.9(2)
C(12)-C(13)-C(16)-C(17)	-92.2(3)
C(14)-C(8)-C(9)-C(10)	163.4(2)
C(14)-C(8)-C(9)-C(11)	-64.3(3)
C(14)-C(8)-C(15)-C(16)	29.8(2)
C(14)-C(13)-C(16)-C(15)	-28.9(2)

C(14)-C(13)-C(16)-C(17)	150.1(3)
C(15)-C(8)-C(9)-C(10)	-85.9(2)
C(15)-C(8)-C(9)-C(11)	46.4(3)
C(15)-C(8)-C(14)-C(13)	-47.3(2)
C(16)-C(13)-C(14)-C(8)	47.0(2)
C(18)-C(4)-C(5)-C(6)	-6.1(4)
C(18)-C(4)-C(5)-C(10)	170.0(2)

Table SI3-21. Hydrogen bonds for $C_{18}H_{22}O_4$ [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...O(1W)	0.83	1.77	2.595(3)	169.6
O(3)-H(3)...O(1)#1	0.85(5)	1.88(5)	2.718(3)	168(4)
O(1W)-H(1WA)...O(3)#2	0.95(5)	1.90(5)	2.834(3)	171(4)
O(1W)-H(1WB)...O(3)#3	0.76(5)	2.09(5)	2.839(3)	172(5)

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z #2 x+1,y+1,z #3 -x+1,y+1/2,-z+2

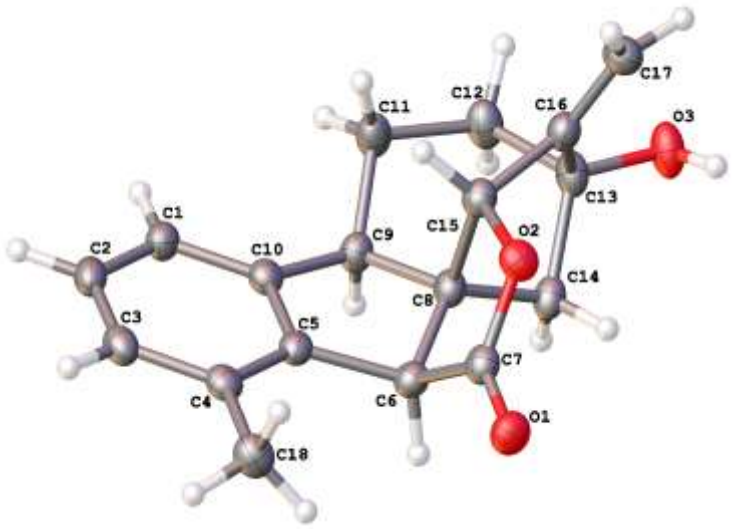

Table SI3-22. Crystal data and structure refinement for compound 47, $C_{18}H_{18}O_3$.

Identification code	exp_312_auto	
Empirical formula	C18 H18 O3	
Formula weight	282.32	
Temperature	130.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 6.16580(5) Å	α= 90°.
	b = 13.22862(9) Å	β= 90°.
	c = 17.33002(12) Å	γ = 90°.
Volume	1413.524(17) $Å^3$	
Z	4	
Density (calculated)	1.327 Mg/m^3	
Absorption coefficient	0.719 mm^{-1}	
F(000)	600	
Crystal size	0.275 x 0.11 x 0.09 mm^3	
Theta range for data collection	4.204 to 77.657°.	
Index ranges	-7<=h<=7, -16<=k<=16, -21<=l<=21	
Reflections collected	53813	
Independent reflections	3008 [R(int) = 0.0362]	
Completeness to theta = 67.684°	100.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.64983	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3008 / 0 / 262	
Goodness-of-fit on F^2	1.059	
Final R indices [I>2sigma(I)]	R1 = 0.0267, wR2 = 0.0730	
R indices (all data)	R1 = 0.0269, wR2 = 0.0732	
Absolute structure parameter	0.02(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.176 and -0.148 $e.Å^{-3}$	

Table SI3-23. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $C_{18}H_{18}O_3$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4196(2)	6078(1)	3870(1)	29(1)
O(2)	4782(2)	6679(1)	5054(1)	25(1)
O(3)	-308(2)	7058(1)	6927(1)	32(1)
C(1)	7194(3)	3420(1)	6332(1)	25(1)
C(2)	8825(3)	3022(1)	5868(1)	26(1)
C(3)	8934(2)	3265(1)	5089(1)	26(1)
C(4)	7416(3)	3907(1)	4740(1)	23(1)
C(5)	5770(2)	4294(1)	5211(1)	21(1)
C(6)	3825(2)	4959(1)	4988(1)	22(1)
C(7)	4305(2)	5930(1)	4556(1)	23(1)
C(8)	3133(2)	5360(1)	5778(1)	22(1)
C(9)	3740(3)	4557(1)	6376(1)	24(1)
C(10)	5672(2)	4061(1)	6000(1)	22(1)
C(11)	3978(3)	5047(1)	7172(1)	28(1)
C(12)	2026(3)	5740(1)	7334(1)	30(1)
C(13)	1416(3)	6447(1)	6656(1)	26(1)
C(14)	881(2)	5796(1)	5937(1)	24(1)
C(15)	4610(2)	6306(1)	5849(1)	23(1)
C(16)	3388(3)	7019(1)	6363(1)	24(1)
C(17)	3895(3)	7980(1)	6492(1)	28(1)
C(18)	7623(3)	4162(1)	3896(1)	29(1)

Table SI3-24. Bond lengths [Å] and angles [°] for $C_{18}H_{18}O_3$.

O(1)-C(7)	1.2065(19)
O(2)-C(7)	1.3468(18)
O(2)-C(15)	1.4675(17)
O(3)-C(13)	1.4154(18)
C(1)-C(2)	1.391(2)
C(1)-C(10)	1.390(2)
C(2)-C(3)	1.388(2)
C(3)-C(4)	1.401(2)
C(4)-C(5)	1.399(2)
C(4)-C(18)	1.506(2)
C(5)-C(6)	1.537(2)
C(5)-C(10)	1.403(2)
C(6)-C(7)	1.516(2)
C(6)-C(8)	1.529(2)
C(8)-C(9)	1.530(2)
C(8)-C(14)	1.529(2)
C(8)-C(15)	1.552(2)
C(9)-C(10)	1.508(2)
C(9)-C(11)	1.532(2)
C(11)-C(12)	1.539(2)
C(12)-C(13)	1.548(2)
C(13)-C(14)	1.551(2)
C(13)-C(16)	1.520(2)
C(15)-C(16)	1.501(2)
C(16)-C(17)	1.328(2)
C(7)-O(2)-C(15)	109.78(11)
C(10)-C(1)-C(2)	118.58(14)
C(3)-C(2)-C(1)	120.66(14)
C(2)-C(3)-C(4)	121.83(14)
C(3)-C(4)-C(18)	119.89(14)
C(5)-C(4)-C(3)	117.03(14)
C(5)-C(4)-C(18)	123.07(14)
C(4)-C(5)-C(6)	128.99(13)
C(4)-C(5)-C(10)	121.28(14)
C(10)-C(5)-C(6)	109.68(13)
C(7)-C(6)-C(5)	117.16(12)
C(7)-C(6)-C(8)	101.74(12)
C(8)-C(6)-C(5)	101.02(11)
O(1)-C(7)-O(2)	121.59(14)
O(1)-C(7)-C(6)	127.86(14)
O(2)-C(7)-C(6)	110.44(12)
C(6)-C(8)-C(9)	107.31(12)
C(6)-C(8)-C(15)	100.74(12)
C(9)-C(8)-C(15)	111.27(12)
C(14)-C(8)-C(6)	123.02(13)
C(14)-C(8)-C(9)	111.26(13)
C(14)-C(8)-C(15)	102.39(11)
C(8)-C(9)-C(11)	109.85(13)
C(10)-C(9)-C(8)	101.65(12)
C(10)-C(9)-C(11)	119.88(13)
C(1)-C(10)-C(5)	120.60(14)
C(1)-C(10)-C(9)	128.24(14)
C(5)-C(10)-C(9)	111.12(13)

C(9)-C(11)-C(12)	109.95(13)
C(11)-C(12)-C(13)	114.32(13)
O(3)-C(13)-C(12)	106.01(13)
O(3)-C(13)-C(14)	115.10(14)
O(3)-C(13)-C(16)	115.28(13)
C(12)-C(13)-C(14)	109.04(13)
C(16)-C(13)-C(12)	111.11(13)
C(16)-C(13)-C(14)	100.26(12)
C(8)-C(14)-C(13)	99.26(12)
O(2)-C(15)-C(8)	103.87(11)
O(2)-C(15)-C(16)	112.47(12)
C(16)-C(15)-C(8)	105.02(12)
C(15)-C(16)-C(13)	106.66(12)
C(17)-C(16)-C(13)	127.53(15)
C(17)-C(16)-C(15)	125.70(15)

Table SI3-25. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $C_{18}H_{18}O_3$. 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}
O(1)	31(1)	29(1)	26(1)	5(1)	-1(1)	1(1)
O(2)	26(1)	23(1)	26(1)	2(1)	4(1)	-3(1)
O(3)	30(1)	27(1)	39(1)	7(1)	12(1)	9(1)
C(1)	26(1)	22(1)	26(1)	1(1)	-3(1)	3(1)
C(2)	23(1)	21(1)	35(1)	-2(1)	-5(1)	2(1)
C(3)	22(1)	21(1)	35(1)	-4(1)	2(1)	-1(1)
C(4)	23(1)	19(1)	27(1)	-2(1)	1(1)	-4(1)
C(5)	20(1)	18(1)	26(1)	0(1)	-2(1)	-2(1)
C(6)	19(1)	23(1)	23(1)	1(1)	-1(1)	-1(1)
C(7)	18(1)	24(1)	27(1)	2(1)	1(1)	0(1)
C(8)	18(1)	22(1)	25(1)	1(1)	1(1)	1(1)
C(9)	23(1)	23(1)	25(1)	4(1)	0(1)	2(1)
C(10)	22(1)	19(1)	25(1)	-1(1)	0(1)	-1(1)
C(11)	33(1)	28(1)	23(1)	3(1)	1(1)	8(1)
C(12)	34(1)	29(1)	27(1)	4(1)	7(1)	7(1)
C(13)	23(1)	23(1)	32(1)	3(1)	6(1)	4(1)
C(14)	18(1)	23(1)	31(1)	5(1)	1(1)	1(1)
C(15)	19(1)	24(1)	25(1)	1(1)	1(1)	0(1)
C(16)	22(1)	25(1)	24(1)	1(1)	-1(1)	3(1)
C(17)	27(1)	27(1)	30(1)	-4(1)	0(1)	-1(1)
C(18)	33(1)	28(1)	28(1)	1(1)	4(1)	0(1)

Table SI3-26. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10 ^{3}) for $C_{18}H_{18}O_3$.

	x	y	z	U(eq)
H(3)	-510(40)	7508(19)	6598(14)	44(6)
H(1)	7150(30)	3242(14)	6872(11)	24(4)
H(2)	9920(40)	2584(17)	6099(13)	40(6)
H(3A)	10110(40)	2983(14)	4781(10)	27(5)
H(6)	2740(40)	4572(15)	4711(12)	35(5)
H(9)	2500(40)	4068(16)	6392(11)	32(5)
H(11A)	4020(40)	4540(16)	7575(12)	30(5)
H(11B)	5390(30)	5432(14)	7184(11)	24(4)
H(12A)	2260(40)	6172(15)	7799(12)	35(5)
H(12B)	740(40)	5321(17)	7443(12)	33(5)
H(14A)	400(30)	6245(15)	5528(11)	27(5)
H(14B)	-260(40)	5283(16)	6034(12)	33(5)
H(15)	6090(30)	6196(13)	6024(10)	19(4)
H(17A)	2960(40)	8448(15)	6794(12)	33(5)
H(17B)	5260(40)	8295(16)	6261(12)	36(5)
H(18A)	8460(40)	3654(19)	3621(14)	49(7)
H(18B)	6230(40)	4228(19)	3637(14)	49(7)
H(18C)	8460(50)	4780(20)	3827(15)	59(8)

Table SI3-27. Torsion angles [°] for $C_{18}H_{18}O_3$.

O(2)-C(15)-C(16)-C(13)	119.02(13)
O(2)-C(15)-C(16)-C(17)	-57.4(2)
O(3)-C(13)-C(14)-C(8)	174.09(12)
O(3)-C(13)-C(16)-C(15)	-159.34(13)
O(3)-C(13)-C(16)-C(17)	17.0(2)
C(1)-C(2)-C(3)-C(4)	-0.6(2)
C(2)-C(1)-C(10)-C(5)	0.6(2)
C(2)-C(1)-C(10)-C(9)	178.13(14)
C(2)-C(3)-C(4)-C(5)	-0.2(2)
C(2)-C(3)-C(4)-C(18)	179.02(14)
C(3)-C(4)-C(5)-C(6)	-176.22(13)
C(3)-C(4)-C(5)-C(10)	1.1(2)
C(4)-C(5)-C(6)-C(7)	-53.9(2)
C(4)-C(5)-C(6)-C(8)	-163.34(14)
C(4)-C(5)-C(10)-C(1)	-1.3(2)
C(4)-C(5)-C(10)-C(9)	-179.26(13)
C(5)-C(6)-C(7)-O(1)	98.52(19)
C(5)-C(6)-C(7)-O(2)	-85.22(16)
C(5)-C(6)-C(8)-C(9)	-29.56(15)
C(5)-C(6)-C(8)-C(14)	-160.51(13)
C(5)-C(6)-C(8)-C(15)	86.92(12)
C(6)-C(5)-C(10)-C(1)	176.46(13)
C(6)-C(5)-C(10)-C(9)	-1.49(16)
C(6)-C(8)-C(9)-C(10)	28.92(15)
C(6)-C(8)-C(9)-C(11)	156.88(12)
C(6)-C(8)-C(14)-C(13)	-157.71(13)
C(6)-C(8)-C(15)-O(2)	34.19(13)
C(6)-C(8)-C(15)-C(16)	152.47(12)
C(7)-O(2)-C(15)-C(8)	-21.02(15)
C(7)-O(2)-C(15)-C(16)	-134.04(13)
C(7)-C(6)-C(8)-C(9)	-150.59(12)
C(7)-C(6)-C(8)-C(14)	78.45(16)
C(7)-C(6)-C(8)-C(15)	-34.11(14)
C(8)-C(6)-C(7)-O(1)	-152.45(16)
C(8)-C(6)-C(7)-O(2)	23.81(15)
C(8)-C(9)-C(10)-C(1)	165.41(15)
C(8)-C(9)-C(10)-C(5)	-16.84(15)
C(8)-C(9)-C(11)-C(12)	47.49(17)
C(8)-C(15)-C(16)-C(13)	6.72(16)
C(8)-C(15)-C(16)-C(17)	-169.69(16)
C(9)-C(8)-C(14)-C(13)	72.98(14)
C(9)-C(8)-C(15)-O(2)	147.69(12)
C(9)-C(8)-C(15)-C(16)	-94.02(14)
C(9)-C(11)-C(12)-C(13)	-46.31(19)
C(10)-C(1)-C(2)-C(3)	0.3(2)
C(10)-C(5)-C(6)-C(7)	128.56(14)
C(10)-C(5)-C(6)-C(8)	19.12(15)
C(10)-C(9)-C(11)-C(12)	164.56(14)
C(11)-C(9)-C(10)-C(1)	44.2(2)
C(11)-C(9)-C(10)-C(5)	-138.06(14)
C(11)-C(12)-C(13)-O(3)	-176.65(14)
C(11)-C(12)-C(13)-C(14)	58.88(19)
C(11)-C(12)-C(13)-C(16)	-50.71(19)
C(12)-C(13)-C(14)-C(8)	-66.96(15)

C(12)-C(13)-C(16)-C(15)	80.04(16)
C(12)-C(13)-C(16)-C(17)	-103.64(18)
C(14)-C(8)-C(9)-C(10)	166.12(12)
C(14)-C(8)-C(9)-C(11)	-65.92(16)
C(14)-C(8)-C(15)-O(2)	-93.37(13)
C(14)-C(8)-C(15)-C(16)	24.92(15)
C(14)-C(13)-C(16)-C(15)	-35.13(15)
C(14)-C(13)-C(16)-C(17)	141.19(16)
C(15)-O(2)-C(7)-O(1)	174.87(14)
C(15)-O(2)-C(7)-C(6)	-1.66(16)
C(15)-C(8)-C(9)-C(10)	-80.40(14)
C(15)-C(8)-C(9)-C(11)	47.56(17)
C(15)-C(8)-C(14)-C(13)	-45.97(14)
C(16)-C(13)-C(14)-C(8)	49.76(13)
C(18)-C(4)-C(5)-C(6)	4.6(2)
C(18)-C(4)-C(5)-C(10)	-178.07(14)