Supplementary Information

Nucleation control and separation of vanillin polymorphs I and II through Swift cooling crystallization process

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Table S1: Data collection conditions and results of SCXRD analysis of vanillin polymorphs

Identification Code	Form-I [17]	Form-II
Chemical formula	$C_8H_8O_3$	$C_8H_8O_3$
Formula weight	152.14 g/mol	152.14 g/mol
Temperature	296(2) K	296(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal size	0.200 x 0.200 x 0.300 mm	0.100 x 0.100 x 0.300 mm
Crystal habit	clear intense white PLATY	clear intense white NEEDLE
Crystal system	Monoclinic	Orthorhombic
Space group	P 2_1	P n a 2_1
Unit cell dimensions	a = 14.0276(8) Å b = 7.8650(4) Å c = 14.9871(8) Å α = 90° β = 115.475(2)° γ = 90°	a = 16.4359(13) Å b = 3.8887(3) Å c = 45.843(4) Å α = 90° β = 90° γ = 90°
Volume	1492.72(14) $Å^3$	2930.0(4) $Å^3$
Z	8	16
Density (calculated)	1.354 g/cm3	1.380 g/cm^3
Absorption coefficient	0.104 mm^{-1}	0.106 mm^{-1}
F(000)	640	1280
Theta range for data collection	2.63 to 27.19°	2.48 to 27.13°
Index ranges	-18<=h<=18,-10<=k<=10,-19<=l<=19	-21<=h<=21, -4<=k<=4, -58<=l<=58
Reflections collected	43087	75071
Independent reflections	6592 [R(int) = 0.0446]	6393 [R(int) = 0.1905]
Absorption correction	multi-scan	multi-scan
Max. and min. transmission	0.9790 and 0.9690	0.9890 and 0.9690
Refinement method	Full-matrix least-squares on F2	Full-matrix least-squares on F2
Refinement program	SHELXL-2016/6 (Sheldrick, 2016)	SHELXL-2016/6 (Sheldrick, 2016)
Data/restraints/ parameters	6592 / 1 / 406	6393 / 1 / 406
Goodness-of-fit on F2	1.105	1.014
Final R indices I>2σ(I)	R1 = 0.0457, wR2 = 0.1072	R1 = 0.0597, wR2 = 0.0845
R for all	R1 = 0.0633, wR2 = 0.1137	R1 = 0.1558, wR2 = 0.1040
Extinction coefficient	0.0250(20)	0.0044(5)
Largest diff. peak and hole	0.184 and -0.177 $eÅ^{-3}$	0.155 and -0.156 $eÅ^{-3}$
Reference	CCDC-1948418	CCDC-1990284

Form-I (CCDC-1948418)

Table S2: Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2)

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

	x/a	y/b	z/c	U(eq)
O3	0.18272(16)	0.0873(3)	0.77753(14)	0.0488(6)
O9	0.79955(16)	0.1421(3)	0.27477(14)	0.0502(6)
O2	0.05881(16)	0.1027(4)	0.58379(15)	0.0570(6)
O8	0.71468(18)	0.0617(4)	0.08350(16)	0.0607(7)
O6	0.63785(16)	0.6092(3)	0.69675(15)	0.0563(6)
O5	0.70716(18)	0.5730(4)	0.89226(16)	0.0633(7)
O12	0.26410(18)	0.6527(4)	0.19431(15)	0.0614(7)
O4	0.95543(19)	0.9139(4)	0.66826(18)	0.0653(7)
O1	0.52626(19)	0.3898(4)	0.8080(2)	0.0673(7)
O10	0.91447(19)	0.9405(4)	0.1608(2)	0.0690(7)
O7	0.4924(2)	0.4724(4)	0.3086(2)	0.0706(8)
O11	0.3770(2)	0.6351(5)	0.38884(18)	0.0785(9)
C5	0.1565(2)	0.1689(4)	0.6198(2)	0.0409(7)
C29	0.6584(2)	0.1522(4)	0.1203(2)	0.0436(7)
C3	0.3224(2)	0.2371(4)	0.7551(2)	0.0406(7)
C30	0.6986(2)	0.1959(4)	0.2205(2)	0.0398(7)
C6	0.1899(3)	0.2428(5)	0.5548(2)	0.0520(8)
C31	0.6377(2)	0.2853(4)	0.2548(2)	0.0420(7)
C4	0.2244(2)	0.1655(4)	0.7217(2)	0.0374(6)
C13	0.7685(2)	0.6485(4)	0.8557(2)	0.0455(7)
C15	0.8015(2)	0.7495(4)	0.7204(2)	0.0432(7)
C2	0.3562(2)	0.3102(4)	0.6886(2)	0.0462(7)
C10	0.9008(2)	0.8070(4)	0.7872(2)	0.0470(8)
C14	0.7360(2)	0.6715(4)	0.7539(2)	0.0407(7)
C21	0.2803(3)	0.7030(5)	0.3525(2)	0.0526(8)
C20	0.2176(2)	0.7154(4)	0.2495(2)	0.0454(7)
C19	0.1192(2)	0.7861(4)	0.2150(2)	0.0452(7)
C8	0.2461(3)	0.0842(5)	0.8819(2)	0.0554(9)
C26	0.5358(2)	0.3338(4)	0.1899(3)	0.0487(8)
C27	0.4971(2)	0.2938(5)	0.0911(3)	0.0559(9)
C18	0.0810(3)	0.8459(4)	0.2819(3)	0.0470(8)
C23	0.1429(3)	0.8336(5)	0.3821(3)	0.0599(10)
C28	0.5576(3)	0.2035(5)	0.0556(2)	0.0567(9)
C7	0.2896(3)	0.3127(5)	0.5895(3)	0.0556(9)
C1	0.4611(3)	0.3862(5)	0.7243(3)	0.0594(9)
C32	0.8466(3)	0.1821(5)	0.3768(2)	0.0556(9)
C22	0.2419(3)	0.7652(6)	0.4163(3)	0.0649(11)
C16	0.5956(3)	0.6406(6)	0.5930(2)	0.0710(12)

	x/a	y/b	z/c	U(eq)
C12	0.8664(3)	0.7073(5)	0.9209(2)	0.0615(10)
C9	0.9722(3)	0.8903(5)	0.7532(3)	0.0593(9)
C17	0.9759(3)	0.9206(5)	0.2462(3)	0.0585(9)
C25	0.4689(3)	0.4296(5)	0.2247(3)	0.0586(9)
C11	0.9320(3)	0.7863(6)	0.8871(2)	0.0627(10)
C24	0.2067(3)	0.6658(6)	0.0891(2)	0.0707(11)

Table S3: Bond lengths (Å)

O3-C4	1.356(3)	**O3-C8**	1.428(3)
O9-C30	1.362(3)	**O9-C32**	1.416(4)
O2-C5	1.344(4)	**O2-H2**	0.82
O8-C29	1.345(4)	**O8-H8**	0.82
O6-C14	1.362(3)	**O6-C16**	1.427(4)
O5-C13	1.341(4)	**O5-H5**	0.82
O12-C20	1.347(4)	**O12-C24**	1.433(4)
O4-C9	1.205(4)	**O1-C1**	1.193(4)
O10-C17	1.207(4)	**O7-C25**	1.202(5)
O11-C21	1.336(4)	**O11-H11**	0.82
C5-C6	1.378(4)	**C5-C4**	1.410(4)
C29-C28	1.387(4)	**C29-C30**	1.401(4)
C3-C4	1.366(4)	**C3-C2**	1.398(4)
C3-H3	0.93	**C30-C31**	1.366(4)
C6-C7	1.380(5)	**C6-H6**	0.93
C31-C26	1.393(4)	**C31-H31**	0.93
C13-C12	1.379(4)	**C13-C14**	1.404(4)
C15-C14	1.367(4)	**C15-C10**	1.395(4)
C15-H15	0.93	**C2-C7**	1.374(5)
C2-C1	1.460(5)	**C10-C11**	1.377(5)
C10-C9	1.460(5)	**C21-C22**	1.374(5)
C21-C20	1.414(4)	**C20-C19**	1.368(4)
C19-C18	1.405(4)	**C19-H19**	0.93
C8-H8A	0.96	**C8-H8B**	0.96
C8-H8C	0.96	**C26-C27**	1.376(5)
C26-C25	1.464(5)	**C27-C28**	1.376(5)
C27-H27	0.93	**C18-C23**	1.377(5)
C18-C17	1.458(5)	**C23-C22**	1.367(5)
C23-H23	0.93	**C28-H28**	0.93
C7-H7	0.93	**C1-H1**	0.93
C32-H32A	0.96	**C32-H32B**	0.96
C32-H32C	0.96	**C22-H22**	0.93
C16-H16A	0.96	**C16-H16B**	0.96
C16-H16C	0.96	**C12-C11**	1.375(5)
C12-H12	0.93	**C9-H9**	0.93
C17-H17	0.93	**C25-H25**	0.93
C11-H11A	0.93	**C24-H24A**	0.96

C24-H24B	0.96	**C24-H24C**	0.96

Table S4: Bond angles (°)

C4-O3-C8	116.9(2)	**C30-O9-C32**	117.2(2)
C5-O2-H2	109.5	**C29-O8-H8**	109.5
C14-O6-C16	117.1(2)	**C13-O5-H5**	109.5
C20-O12-C24	117.2(3)	**C21-O11-H11**	109.5
O2-C5-C6	118.5(3)	**O2-C5-C4**	121.7(3)
C6-C5-C4	119.9(3)	**O8-C29-C28**	118.0(3)
O8-C29-C30	122.2(3)	**C28-C29-C30**	119.8(3)
C4-C3-C2	120.4(3)	**C4-C3-H3**	119.8
C2-C3-H3	119.8	**O9-C30-C31**	126.4(3)
O9-C30-C29	113.5(3)	**C31-C30-C29**	120.1(3)
C5-C6-C7	119.9(3)	**C5-C6-H6**	120.0
C7-C6-H6	120.0	**C30-C31-C26**	119.9(3)
C30-C31-H31	120.1	**C26-C31-H31**	120.1
O3-C4-C3	126.4(3)	**O3-C4-C5**	114.0(2)
C3-C4-C5	119.5(3)	**O5-C13-C12**	118.5(3)
O5-C13-C14	122.4(3)	**C12-C13-C14**	119.0(3)
C14-C15-C10	120.2(3)	**C14-C15-H15**	119.9
C10-C15-H15	119.9	**C7-C2-C3**	119.7(3)
C7-C2-C1	119.9(3)	**C3-C2-C1**	120.4(3)
C11-C10-C15	119.6(3)	**C11-C10-C9**	119.2(3)
C15-C10-C9	121.2(3)	**O6-C14-C15**	126.0(3)
O6-C14-C13	113.8(3)	**C15-C14-C13**	120.1(3)
O11-C21-C22	119.5(3)	**O11-C21-C20**	121.2(3)
C22-C21-C20	119.4(3)	**O12-C20-C19**	126.4(3)
O12-C20-C21	114.1(3)	**C19-C20-C21**	119.5(3)
C20-C19-C18	120.0(3)	**C20-C19-H19**	120.0
C18-C19-H19	120.0	**O3-C8-H8A**	109.5
O3-C8-H8B	109.5	**H8A-C8-H8B**	109.5
O3-C8-H8C	109.5	**H8A-C8-H8C**	109.5
H8B-C8-H8C	109.5	**C27-C26-C31**	120.0(3)
C27-C26-C25	119.0(3)	**C31-C26-C25**	121.0(3)
C26-C27-C28	120.7(3)	**C26-C27-H27**	119.7
C28-C27-H27	119.7	**C23-C18-C19**	120.0(3)
C23-C18-C17	119.5(3)	**C19-C18-C17**	120.5(3)
C22-C23-C18	119.9(3)	**C22-C23-H23**	120.0
C18-C23-H23	120.0	**C27-C28-C29**	119.5(3)
C27-C28-H28	120.2	**C29-C28-H28**	120.2
C2-C7-C6	120.6(3)	**C2-C7-H7**	119.7
C6-C7-H7	119.7	**O1-C1-C2**	126.2(4)
O1-C1-H1	116.9	**C2-C1-H1**	116.9
O9-C32-H32A	109.5	**O9-C32-H32B**	109.5
H32A-C32-H32B	109.5	**O9-C32-H32C**	109.5
H32A-C32-H32C	109.5	**H32B-C32-H32C**	109.5

C23-C22-C21	121.2(3)	**C23-C22-H22**	119.4
C21-C22-H22	119.4	**O6-C16-H16A**	109.5
O6-C16-H16B	109.5	**H16A-C16-H16B**	109.5
O6-C16-H16C	109.5	**H16A-C16-H16C**	109.5
H16B-C16-H16C	109.5	**C11-C12-C13**	120.8(3)
C11-C12-H12	119.6	**C13-C12-H12**	119.6
O4-C9-C10	125.9(3)	**O4-C9-H9**	117.0
C10-C9-H9	117.0	**O10-C17-C18**	126.2(3)
O10-C17-H17	116.9	**C18-C17-H17**	116.9
O7-C25-C26	125.9(3)	**O7-C25-H25**	117.0
C26-C25-H25	117.0	**C12-C11-C10**	120.2(3)
C12-C11-H11A	119.9	**C10-C11-H11A**	119.9
O12-C24-H24A	109.5	**O12-C24-H24B**	109.5
H24A-C24-H24B	109.5	**O12-C24-H24C**	109.5
H24A-C24-H24C	109.5	**H24B-C24-H24C**	109.5

Table S5: Torsion angles (°)

C32-O9-C30-C31	0.1(5)	**C32-O9-C30-C29**	179.6(3)
O8-C29-C30-O9	1.7(4)	**C28-C29-C30-O9**	-177.9(3)
O8-C29-C30-C31	-178.8(3)	**C28-C29-C30-C31**	1.6(5)
O2-C5-C6-C7	179.7(3)	**C4-C5-C6-C7**	0.2(5)
O9-C30-C31-C26	179.1(3)	**C29-C30-C31-C26**	-0.4(5)
C8-O3-C4-C3	2.1(5)	**C8-O3-C4-C5**	-178.0(3)
C2-C3-C4-O3	178.5(3)	**C2-C3-C4-C5**	-1.3(5)
O2-C5-C4-O3	1.3(4)	**C6-C5-C4-O3**	-179.2(3)
O2-C5-C4-C3	-178.9(3)	**C6-C5-C4-C3**	0.7(5)
C4-C3-C2-C7	1.2(5)	**C4-C3-C2-C1**	-179.8(3)
C14-C15-C10-C11	-0.7(5)	**C14-C15-C10-C9**	179.8(3)
C16-O6-C14-C15	-5.6(5)	**C16-O6-C14-C13**	174.8(3)
C10-C15-C14-O6	-179.7(3)	**C10-C15-C14-C13**	-0.1(5)
O5-C13-C14-O6	-0.5(5)	**C12-C13-C14-O6**	-179.7(3)
O5-C13-C14-C15	179.9(3)	**C12-C13-C14-C15**	0.7(5)
C24-O12-C20-C19	2.2(6)	**C24-O12-C20-C21**	-178.1(3)
O11-C21-C20-O12	0.4(5)	**C22-C21-C20-O12**	179.0(4)
O11-C21-C20-C19	-179.8(4)	**C22-C21-C20-C19**	-1.3(6)
O12-C20-C19-C18	179.8(3)	**C21-C20-C19-C18**	0.1(5)
C30-C31-C26-C27	-1.0(5)	**C30-C31-C26-C25**	180.0(3)
C31-C26-C27-C28	1.1(5)	**C25-C26-C27-C28**	-179.8(3)
C20-C19-C18-C23	0.2(5)	**C20-C19-C18-C17**	-179.6(3)

C19-C18-C23-C22	0.8(6)	**C17-C18-C23-C22**	-179.4(4)
C26-C27-C28-C29	0.1(6)	**O8-C29-C28-C27**	178.9(3)
C30-C29-C28-C27	-1.4(5)	**C3-C2-C7-C6**	-0.4(5)
C1-C2-C7-C6	-179.4(4)	**C5-C6-C7-C2**	-0.3(6)
C7-C2-C1-O1	-178.8(4)	**C3-C2-C1-O1**	2.1(6)
C18-C23-C22-C21	-2.1(6)	**O11-C21-C22-C23**	-179.2(4)
C20-C21-C22-C23	2.3(6)	**O5-C13-C12-C11**	-179.7(4)
C14-C13-C12-C11	-0.4(6)	**C11-C10-C9-O4**	178.7(4)
C15-C10-C9-O4	-1.8(6)	**C23-C18-C17-O10**	179.1(4)
C19-C18-C17-O10	-1.1(6)	**C27-C26-C25-O7**	179.7(4)
C31-C26-C25-O7	-1.2(6)	**C13-C12-C11-C10**	-0.3(6)
C15-C10-C11-C12	0.9(6)	**C9-C10-C11-C12**	-179.6(4)

Table S6: Anisotropic atomic displacement parameters (Å²)

The anisotropic atomic 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}
O3	0.0402(11)	0.0699(15)	0.0323(10)	0.0011(10)	0.0116(9)	-0.0138(11)
O9	0.0354(10)	0.0702(16)	0.0370(11)	-0.0030(11)	0.0079(9)	0.0127(11)
O2	0.0414(11)	0.0802(18)	0.0389(11)	0.0054(12)	0.0075(9)	-0.0137(12)
O8	0.0482(13)	0.0890(19)	0.0414(12)	-0.0070(13)	0.0161(10)	0.0152(14)
O6	0.0385(11)	0.0809(18)	0.0398(11)	0.0051(12)	0.0077(9)	-0.0164(12)
O5	0.0495(13)	0.094(2)	0.0436(12)	0.0036(13)	0.0177(10)	-0.0216(14)
O12	0.0532(13)	0.0929(19)	0.0413(12)	0.0034(13)	0.0234(10)	0.0248(14)
O4	0.0567(14)	0.0872(19)	0.0578(15)	-0.0112(14)	0.0300(12)	-0.0251(14)
O1	0.0450(13)	0.0807(19)	0.0713(18)	-0.0027(15)	0.0205(13)	-0.0146(13)
O10	0.0458(13)	0.087(2)	0.0722(18)	0.0039(15)	0.0240(13)	0.0162(13)
O7	0.0610(16)	0.074(2)	0.087(2)	-0.0061(15)	0.0415(15)	0.0109(14)
O11	0.0560(15)	0.121(3)	0.0481(14)	-0.0017(16)	0.0122(11)	0.0349(16)
C5	0.0378(15)	0.0451(17)	0.0359(15)	0.0013(13)	0.0123(12)	-0.0007(14)
C29	0.0393(15)	0.0497(19)	0.0396(15)	0.0017(14)	0.0148(13)	0.0037(14)
C3	0.0371(15)	0.0435(17)	0.0371(15)	-0.0007(13)	0.0120(12)	-0.0005(13)
C30	0.0331(14)	0.0423(18)	0.0413(15)	0.0033(13)	0.0134(12)	0.0027(13)
C6	0.0546(19)	0.061(2)	0.0336(15)	0.0031(15)	0.0129(14)	-0.0054(17)
C31	0.0381(15)	0.0441(17)	0.0424(16)	0.0012(14)	0.0160(13)	0.0019(13)
C4	0.0350(14)	0.0419(17)	0.0364(15)	-0.0006(13)	0.0162(12)	-0.0001(13)
C13	0.0382(15)	0.054(2)	0.0421(16)	-0.0002(15)	0.0153(13)	-0.0049(15)
C15	0.0390(15)	0.0500(19)	0.0399(15)	-0.0016(14)	0.0163(13)	-0.0012(14)
C2	0.0411(16)	0.0454(18)	0.0563(19)	-0.0023(15)	0.0249(15)	-0.0024(14)
C10	0.0385(16)	0.055(2)	0.0473(18)	-0.0017(15)	0.0181(14)	-0.0067(15)
C14	0.0308(13)	0.0457(18)	0.0423(16)	0.0002(14)	0.0124(12)	-0.0015(13)
C21	0.0444(17)	0.065(2)	0.0460(17)	0.0047(16)	0.0174(14)	0.0140(16)
C20	0.0393(15)	0.053(2)	0.0470(17)	0.0011(15)	0.0219(14)	0.0044(15)
C19	0.0420(16)	0.0504(19)	0.0434(17)	0.0026(15)	0.0186(14)	0.0021(15)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C8	0.0523(18)	0.076(3)	0.0304(15)	0.0049(16)	0.0107(13)	-0.0095(18)
C26	0.0359(16)	0.0433(19)	0.068(2)	0.0020(16)	0.0232(15)	0.0026(14)
C27	0.0343(16)	0.059(2)	0.058(2)	0.0014(17)	0.0050(15)	0.0074(15)
C18	0.0423(16)	0.0485(19)	0.0565(19)	0.0012(15)	0.0270(15)	0.0020(14)
C23	0.063(2)	0.076(3)	0.053(2)	-0.0032(18)	0.0367(18)	0.012(2)
C28	0.0474(18)	0.066(2)	0.0430(17)	-0.0036(16)	0.0065(14)	0.0059(17)
C7	0.064(2)	0.060(2)	0.0494(19)	0.0041(16)	0.0309(17)	-0.0075(18)
C1	0.0500(19)	0.066(2)	0.068(2)	-0.0022(19)	0.0307(19)	-0.0101(18)
C32	0.0469(18)	0.068(2)	0.0415(17)	-0.0023(16)	0.0089(14)	0.0085(17)
C22	0.065(2)	0.090(3)	0.0411(18)	0.0029(19)	0.0245(16)	0.020(2)
C16	0.0511(19)	0.107(3)	0.0393(18)	0.002(2)	0.0042(15)	-0.024(2)
C12	0.0497(18)	0.089(3)	0.0352(16)	0.0069(18)	0.0078(14)	-0.0152(19)
C9	0.0434(18)	0.076(3)	0.057(2)	-0.0093(19)	0.0203(16)	-0.0181(18)
C17	0.055(2)	0.058(2)	0.076(3)	-0.002(2)	0.040(2)	0.0065(18)
C25	0.0417(18)	0.053(2)	0.080(3)	0.002(2)	0.0259(18)	0.0077(16)
C11	0.0388(17)	0.084(3)	0.0493(19)	-0.0001(19)	0.0034(15)	-0.0208(18)
C24	0.069(2)	0.101(3)	0.0454(19)	0.001(2)	0.0278(17)	0.020(2)

Table S7: Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å²)

	x/a	y/b	z/c	U(eq)
H2	0.0498	0.0562	0.6285	0.085
H8	0.7765	0.0574	0.1245	0.091
H5	0.6549	0.5327	0.8468	0.095
H11	0.3886	0.5979	0.3433	0.118
H3	0.3668	0.2372	0.8224	0.049
H6	0.1452	0.2455	0.4876	0.062
H31	0.6643	0.3138	0.3214	0.05
H15	0.7798	0.7643	0.6529	0.052
H19	0.0775	0.7947	0.1473	0.054
H8A	0.3135	0.0345	0.8955	0.083
H8B	0.2114	0.0178	0.9129	0.083
H8C	0.2561	0.1982	0.9072	0.083
H27	0.4294	0.3282	0.0479	0.067
H23	0.1174	0.8718	0.4264	0.072
H28	0.5310	0.1771	-0.0112	0.068
H7	0.3120	0.3619	0.5453	0.067
H1	0.4788	0.4365	0.6773	0.071

	x/a	y/b	z/c	U(eq)
H32A	0.8461	0.3031	0.3850	0.083
H32B	0.9181	0.1416	0.4063	0.083
H32C	0.8075	0.1286	0.4082	0.083
H22	0.2840	0.7608	0.4840	0.078
H16A	0.5907	0.7610	0.5813	0.106
H16B	0.5266	0.5908	0.5608	0.106
H16C	0.6411	0.5912	0.5671	0.106
H12	0.8884	0.6933	0.9885	0.074
H9	1.0364	0.9286	0.8014	0.071
H17	-0.0458	0.9562	0.2937	0.07
H25	0.4021	0.4602	0.1776	0.07
H11A	0.9977	0.8259	0.9319	0.075
H24A	0.1406	0.6069	0.0680	0.106
H24B	0.2473	0.6160	0.0581	0.106
H24C	0.1936	0.7834	0.0707	0.106

Form-II (CCDC-1990284)

Table S8: Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2)

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

	x/a	y/b	z/c	U(eq)
O9	0.18553(18)	0.2395(10)	0.53470(7)	0.0477(10)
O12	0.14976(18)	0.1753(10)	0.65851(7)	0.0539(11)
O3	0.5972(2)	0.2564(9)	0.34097(7)	0.0497(10)
O5	0.22561(18)	0.7404(11)	0.44957(8)	0.0541(11)
O6	0.53826(18)	0.7600(9)	0.46860(7)	0.0471(10)
O8	0.49795(19)	0.2922(11)	0.55401(8)	0.0583(12)
O7	0.12892(18)	0.9620(11)	0.58346(7)	0.0536(11)
O10	0.0216(2)	0.9057(12)	0.63173(7)	0.0576(11)
O1	0.7092(2)	0.9504(11)	0.37369(7)	0.0565(11)
O4	0.59579(18)	0.0322(12)	0.41984(7)	0.0552(12)
O11	0.0333(3)	0.4647(13)	0.76201(8)	0.0776(14)
C22	0.2431(3)	0.1453(13)	0.55449(10)	0.0332(12)
C9	0.5141(3)	0.0104(14)	0.42371(11)	0.0352(13)
C13	0.3990(3)	0.8354(13)	0.45168(10)	0.0361(13)
C21	0.3247(3)	0.1850(13)	0.55179(10)	0.0333(12)
C12	0.3485(3)	0.9588(13)	0.42956(10)	0.0324(13)
C10	0.4648(3)	0.1347(14)	0.40222(10)	0.0422(14)
C30	0.0786(3)	0.1612(14)	0.67451(10)	0.0394(14)
C14	0.4818(3)	0.8667(13)	0.44873(10)	0.0321(12)
C15	0.2604(3)	0.9063(15)	0.43129(11)	0.0397(14)
C25	0.0138(3)	0.0166(13)	0.65968(11)	0.0413(14)

	x/a	y/b	z/c	U(eq)
C2	0.7978(3)	0.8977(14)	0.33407(10)	0.0426(14)
C6	0.6672(3)	0.1617(13)	0.32716(11)	0.0387(14)
O2	0.7367(3)	0.2968(13)	0.23852(8)	0.0857(16)
C20	0.3763(3)	0.0711(14)	0.57377(10)	0.0336(13)
C17	0.2104(3)	0.9955(14)	0.57968(10)	0.0362(13)
C23	0.4631(3)	0.1295(15)	0.57283(11)	0.0430(14)
C1	0.7249(3)	0.0040(14)	0.34498(10)	0.0390(13)
C5	0.6849(3)	0.2118(14)	0.29813(11)	0.0419(13)
C19	0.3439(3)	0.9123(14)	0.59822(10)	0.0420(14)
C4	0.7588(3)	0.1036(14)	0.28702(10)	0.0420(13)
C3	0.8156(3)	0.9461(14)	0.30488(11)	0.0438(14)
C11	0.3818(3)	0.1110(14)	0.40541(10)	0.0407(14)
C18	0.2612(3)	0.8744(14)	0.60116(10)	0.0409(13)
C16	0.5101(3)	0.6198(14)	0.49535(10)	0.0454(15)
C29	0.0699(3)	0.2693(13)	0.70280(10)	0.0420(14)
C24	0.2133(3)	0.3877(15)	0.50792(10)	0.0487(15)
C27	0.9304(3)	0.0869(15)	0.70142(11)	0.0496(15)
C28	0.9950(3)	0.2323(14)	0.71629(10)	0.0430(14)
C32	0.2210(3)	0.2982(17)	0.67292(11)	0.0569(17)
C26	0.9402(3)	0.9763(15)	0.67288(11)	0.0492(15)
C31	0.9825(4)	0.3454(17)	0.74622(13)	0.0638(19)
C7	0.7797(4)	0.1570(17)	0.25623(12)	0.0589(17)
C8	0.5348(3)	0.4141(16)	0.32385(11)	0.0584(17)

Table S9: Bond lengths (Å)

O9-C22	1.362(5)	**O9-C24**	1.431(6)
O12-C30	1.382(5)	**O12-C32**	1.427(5)
O3-C6	1.363(6)	**O3-C8**	1.430(5)
O5-C15	1.203(6)	**O6-C14**	1.365(5)
O6-C16	1.420(5)	**O8-C23**	1.214(6)
O7-C17	1.357(5)	**O7-H7**	0.82
O10-C25	1.358(5)	**O10-H10**	0.82
O1-C1	1.358(5)	**O1-H1**	0.82
O4-C9	1.357(5)	**O4-H4**	0.82
O11-C31	1.198(7)	**C22-C21**	1.355(6)
C22-C17	1.401(7)	**C9-C10**	1.364(6)
C9-C14	1.381(6)	**C13-C14**	1.373(6)
C13-C12	1.395(6)	**C13-H13**	0.93
C21-C20	1.390(6)	**C21-H21**	0.93
C12-C11	1.370(6)	**C12-C15**	1.464(7)
C10-C11	1.375(7)	**C10-H10A**	0.93
C30-C29	1.371(6)	**C30-C25**	1.382(6)
C15-H15	0.93	**C25-C26**	1.362(6)
C2-C1	1.362(6)	**C2-C3**	1.383(6)
C2-H2	0.93	**C6-C5**	1.376(6)

C6-C1	1.395(7)	**O2-C7**	1.206(6)
C20-C19	1.386(6)	**C20-C23**	1.445(7)
C17-C18	1.374(6)	**C23-H23**	0.93
C5-C4	1.382(7)	**C5-H5**	0.93
C19-C18	1.374(6)	**C19-H19**	0.93
C4-C3	1.384(7)	**C4-C7**	1.468(7)
C3-H3	0.93	**C11-H11**	0.93
C18-H18	0.93	**C16-H16A**	0.96
C16-H16B	0.96	**C16-H16C**	0.96
C29-C28	1.386(6)	**C29-H29**	0.93
C24-H24A	0.96	**C24-H24B**	0.96
C24-H24C	0.96	**C27-C28**	1.382(7)
C27-C26	1.386(7)	**C27-H27**	0.93
C28-C31	1.455(7)	**C32-H32A**	0.96
C32-H32B	0.96	**C32-H32C**	0.96
C26-H26	0.93	**C31-H31**	0.93
C7-H7A	0.93	**C8-H8A**	0.96
C8-H8B	0.96	**C8-H8C**	0.96

Table S10: Bond angles (°)

C22-O9-C24	117.2(4)	**C30-O12-C32**	117.6(4)
C6-O3-C8	117.7(4)	**C14-O6-C16**	118.2(4)
C17-O7-H7	109.5	**C25-O10-H10**	109.5
C1-O1-H1	109.5	**C9-O4-H4**	109.5
C21-C22-O9	126.6(4)	**C21-C22-C17**	120.1(4)
O9-C22-C17	113.2(4)	**O4-C9-C10**	118.1(4)
O4-C9-C14	120.9(4)	**C10-C9-C14**	121.0(4)
C14-C13-C12	119.2(4)	**C14-C13-H13**	120.4
C12-C13-H13	120.4	**C22-C21-C20**	120.1(4)
C22-C21-H21	119.9	**C20-C21-H21**	119.9
C11-C12-C13	119.9(4)	**C11-C12-C15**	119.9(4)
C13-C12-C15	120.1(4)	**C9-C10-C11**	119.2(5)
C9-C10-H10A	120.4	**C11-C10-H10A**	120.4
C29-C30-O12	125.3(4)	**C29-C30-C25**	120.7(4)
O12-C30-C25	114.0(4)	**O6-C14-C13**	125.5(4)
O6-C14-C9	114.6(4)	**C13-C14-C9**	119.9(4)
O5-C15-C12	125.7(5)	**O5-C15-H15**	117.2
C12-C15-H15	117.2	**O10-C25-C26**	117.8(5)
O10-C25-C30	121.4(4)	**C26-C25-C30**	120.8(5)
C1-C2-C3	120.0(5)	**C1-C2-H2**	120.0
C3-C2-H2	120.0	**O3-C6-C5**	126.2(5)
O3-C6-C1	114.9(4)	**C5-C6-C1**	119.0(5)
C19-C20-C21	119.6(4)	**C19-C20-C23**	118.2(4)
C21-C20-C23	122.1(4)	**O7-C17-C18**	118.4(4)
O7-C17-C22	121.6(4)	**C18-C17-C22**	120.0(4)
O8-C23-C20	124.7(5)	**O8-C23-H23**	117.6

C20-C23-H23	117.6	**O1-C1-C2**	118.5(5)
O1-C1-C6	120.4(4)	**C2-C1-C6**	121.1(5)
C6-C5-C4	120.0(5)	**C6-C5-H5**	120.0
C4-C5-H5	120.0	**C18-C19-C20**	120.5(4)
C18-C19-H19	119.8	**C20-C19-H19**	119.8
C5-C4-C3	120.6(5)	**C5-C4-C7**	121.1(5)
C3-C4-C7	118.3(5)	**C2-C3-C4**	119.3(5)
C2-C3-H3	120.3	**C4-C3-H3**	120.3
C12-C11-C10	120.8(4)	**C12-C11-H11**	119.6
C10-C11-H11	119.6	**C17-C18-C19**	119.6(4)
C17-C18-H18	120.2	**C19-C18-H18**	120.2
O6-C16-H16A	109.5	**O6-C16-H16B**	109.5
H16A-C16-H16B	109.5	**O6-C16-H16C**	109.5
H16A-C16-H16C	109.5	**H16B-C16-H16C**	109.5
C30-C29-C28	118.9(5)	**C30-C29-H29**	120.6
C28-C29-H29	120.6	**O9-C24-H24A**	109.5
O9-C24-H24B	109.5	**H24A-C24-H24B**	109.5
O9-C24-H24C	109.5	**H24A-C24-H24C**	109.5
H24B-C24-H24C	109.5	**C28-C27-C26**	120.2(5)
C28-C27-H27	119.9	**C26-C27-H27**	119.9
C27-C28-C29	120.3(4)	**C27-C28-C31**	118.7(5)
C29-C28-C31	121.0(5)	**O12-C32-H32A**	109.5
O12-C32-H32B	109.5	**H32A-C32-H32B**	109.5
O12-C32-H32C	109.5	**H32A-C32-H32C**	109.5
H32B-C32-H32C	109.5	**C25-C26-C27**	119.1(5)
C25-C26-H26	120.4	**C27-C26-H26**	120.4
O11-C31-C28	126.1(6)	**O11-C31-H31**	117.0
C28-C31-H31	117.0	**O2-C7-C4**	125.0(6)
O2-C7-H7A	117.5	**C4-C7-H7A**	117.5
O3-C8-H8A	109.5	**O3-C8-H8B**	109.5
H8A-C8-H8B	109.5	**O3-C8-H8C**	109.5
H8A-C8-H8C	109.5	**H8B-C8-H8C**	109.5

Table S11: Torsion angles (°)

C24-O9-C22-C21	1.7(7)	**C24-O9-C22-C17**	-178.6(5)
O9-C22-C21-C20	-179.1(5)	**C17-C22-C21-C20**	1.3(8)
C14-C13-C12-C11	-0.5(7)	**C14-C13-C12-C15**	175.7(4)
O4-C9-C10-C11	179.0(5)	**C14-C9-C10-C11**	-1.1(8)
C32-O12-C30-C29	2.9(8)	**C32-O12-C30-C25**	-175.6(5)
C16-O6-C14-C13	-3.4(7)	**C16-O6-C14-C9**	177.9(5)
C12-C13-C14-O6	179.6(4)	**C12-C13-C14-C9**	-1.8(8)
O4-C9-C14-O6	1.3(7)	**C10-C9-C14-O6**	-178.7(5)
O4-C9-C14-C13	-177.5(5)	**C10-C9-C14-C13**	2.6(8)
C11-C12-C15-O5	170.5(5)	**C13-C12-C15-O5**	-5.6(8)
C29-C30-C25-O10	-179.5(5)	**O12-C30-C25-O10**	-0.9(7)
C29-C30-C25-C26	-0.4(8)	**O12-C30-C25-C26**	178.2(5)

C8-O3-C6-C5	2.0(7)	**C8-O3-C6-C1**	-178.9(5)
C22-C21-C20-C19	1.0(8)	**C22-C21-C20-C23**	-175.5(5)
C21-C22-C17-O7	177.9(5)	**O9-C22-C17-O7**	-1.9(7)
C21-C22-C17-C18	-2.9(8)	**O9-C22-C17-C18**	177.4(5)
C19-C20-C23-O8	-173.1(6)	**C21-C20-C23-O8**	3.4(9)
C3-C2-C1-O1	179.6(5)	**C3-C2-C1-C6**	0.1(8)
O3-C6-C1-O1	0.9(7)	**C5-C6-C1-O1**	-179.9(5)
O3-C6-C1-C2	-179.7(5)	**C5-C6-C1-C2**	-0.5(8)
O3-C6-C5-C4	179.7(5)	**C1-C6-C5-C4**	0.5(7)
C21-C20-C19-C18	-1.6(8)	**C23-C20-C19-C18**	175.1(5)
C6-C5-C4-C3	-0.3(8)	**C6-C5-C4-C7**	-179.4(5)
C1-C2-C3-C4	0.1(8)	**C5-C4-C3-C2**	0.0(8)
C7-C4-C3-C2	179.1(5)	**C13-C12-C11-C10**	2.0(8)
C15-C12-C11-C10	-174.1(5)	**C9-C10-C11-C12**	-1.2(8)
O7-C17-C18-C19	-178.4(5)	**C22-C17-C18-C19**	2.3(8)
C20-C19-C18-C17	-0.1(8)	**O12-C30-C29-C28**	-178.6(5)
C25-C30-C29-C28	-0.2(8)	**C26-C27-C28-C29**	0.1(9)
C26-C27-C28-C31	-180.0(5)	**C30-C29-C28-C27**	0.4(8)
C30-C29-C28-C31	-179.5(5)	**O10-C25-C26-C27**	180.0(5)
C30-C25-C26-C27	0.9(8)	**C28-C27-C26-C25**	-0.7(9)
C27-C28-C31-O11	177.4(6)	**C29-C28-C31-O11**	-2.7(10)
C5-C4-C7-O2	0.7(10)	**C3-C4-C7-O2**	-178.4(6)

Table S12: Anisotropic atomic displacement parameters (Å²)

The anisotropic atomic 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}
O9	0.0278(18)	0.075(3)	0.041(2)	0.015(2)	-0.0055(16)	-0.001(2)
O12	0.035(2)	0.083(3)	0.044(2)	-0.009(2)	-0.0012(17)	-0.012(2)
O3	0.038(2)	0.070(3)	0.041(2)	-0.003(2)	0.0001(17)	0.010(2)
O5	0.029(2)	0.084(3)	0.049(2)	0.013(2)	0.0050(18)	-0.005(2)
O6	0.0303(18)	0.076(3)	0.035(2)	0.0135(19)	-0.0026(16)	0.008(2)
O8	0.030(2)	0.095(3)	0.050(2)	0.014(3)	0.0019(18)	-0.009(2)
O7	0.029(2)	0.084(3)	0.047(3)	0.012(2)	0.0040(17)	-0.003(2)
O10	0.039(2)	0.096(3)	0.038(2)	-0.019(2)	0.0012(17)	-0.015(2)
O1	0.044(2)	0.090(3)	0.036(2)	0.008(2)	-0.0033(17)	0.008(2)
O4	0.026(2)	0.094(4)	0.046(2)	0.015(2)	0.0063(18)	-0.002(2)
O11	0.090(3)	0.100(4)	0.043(2)	-0.019(2)	0.003(2)	0.004(3)
C22	0.034(3)	0.039(3)	0.027(3)	0.005(3)	-0.004(2)	0.004(3)
C9	0.025(3)	0.047(4)	0.034(3)	-0.002(3)	0.000(2)	0.000(3)
C13	0.033(3)	0.042(4)	0.034(3)	0.002(3)	0.003(2)	0.000(3)
C21	0.026(3)	0.041(3)	0.033(3)	0.005(3)	0.003(2)	-0.002(3)
C12	0.027(3)	0.036(3)	0.034(3)	-0.004(3)	-0.001(2)	-0.001(2)
C10	0.033(3)	0.057(4)	0.036(3)	0.013(3)	0.005(2)	0.001(3)
C30	0.038(3)	0.045(4)	0.035(3)	0.004(3)	0.002(2)	0.000(3)
C14	0.023(3)	0.042(3)	0.031(3)	-0.002(3)	-0.002(2)	0.002(2)
C15	0.027(3)	0.052(4)	0.041(3)	-0.011(3)	-0.006(3)	0.003(3)
C25	0.039(3)	0.050(4)	0.035(3)	-0.001(3)	-0.009(3)	0.002(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C2	0.037(3)	0.055(4)	0.036(3)	0.004(3)	-0.003(2)	-0.001(3)
C6	0.036(3)	0.043(4)	0.037(3)	-0.004(3)	0.000(2)	-0.002(3)
O2	0.086(3)	0.121(5)	0.050(3)	0.022(3)	0.009(2)	0.022(3)
C20	0.025(3)	0.041(4)	0.035(3)	0.003(2)	-0.001(2)	0.002(2)
C17	0.024(3)	0.048(4)	0.036(3)	-0.003(3)	0.002(2)	0.000(3)
C23	0.036(3)	0.054(4)	0.039(3)	0.001(3)	-0.006(3)	0.010(3)
C1	0.037(3)	0.051(4)	0.029(3)	-0.004(3)	-0.001(2)	-0.007(3)
C5	0.041(3)	0.048(4)	0.036(3)	0.000(3)	-0.005(3)	-0.002(3)
C19	0.037(3)	0.056(4)	0.032(3)	0.010(3)	-0.007(2)	0.004(3)
C4	0.045(3)	0.045(4)	0.037(3)	-0.001(3)	-0.001(3)	-0.005(3)
C3	0.035(3)	0.050(4)	0.046(3)	-0.004(3)	0.002(3)	-0.002(3)
C11	0.037(3)	0.053(4)	0.032(3)	0.001(3)	-0.006(2)	0.004(3)
C18	0.040(3)	0.058(4)	0.025(3)	0.011(3)	0.000(2)	-0.001(3)
C16	0.047(3)	0.056(4)	0.032(3)	0.011(3)	-0.004(2)	0.004(3)
C29	0.046(3)	0.049(4)	0.031(3)	-0.001(3)	-0.009(2)	0.001(3)
C24	0.047(3)	0.063(4)	0.037(3)	0.008(3)	-0.013(3)	-0.004(3)
C27	0.036(3)	0.063(4)	0.050(4)	0.002(3)	0.013(3)	0.009(3)
C28	0.046(3)	0.049(4)	0.034(3)	0.000(3)	0.003(3)	0.011(3)
C32	0.041(3)	0.071(5)	0.059(3)	-0.014(3)	0.001(3)	-0.019(3)
C26	0.033(3)	0.072(4)	0.043(3)	-0.009(3)	-0.003(3)	-0.004(3)
C31	0.071(4)	0.075(5)	0.046(4)	-0.005(4)	0.007(3)	0.015(4)
C7	0.058(4)	0.072(5)	0.047(4)	0.008(3)	0.010(3)	0.001(4)
C8	0.047(4)	0.072(5)	0.056(4)	0.004(3)	-0.001(3)	0.022(3)

Table S13: Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2)

	x/a	y/b	z/c	U(eq)
H7	0.1050	0.0561	0.5699	0.08
H10	0.0650	-0.0275	0.6251	0.086
H1	0.6648	0.0333	0.3778	0.085
H4	0.6191	0.9499	0.4340	0.083
H13	0.3768	0.7332	0.4682	0.043
H21	0.3461	0.2886	0.5352	0.04
H10A	0.4871	1.2344	0.3856	0.051
H15	0.2287	1.0103	0.4170	0.048
H2	0.8355	-0.2074	0.3463	0.051
H23	0.4945	0.0358	0.5877	0.052
H5	0.6473	0.3183	0.2860	0.05
H19	0.3784	-0.1691	0.6127	0.05
H3	0.8652	-0.1264	0.2973	0.053
H11	0.3479	1.1993	0.3910	0.049
H18	0.2398	-0.2326	0.6176	0.049
H16A	0.4778	0.7878	0.5054	0.068
H16B	0.5559	0.5571	0.5072	0.068
H16C	0.4777	0.4195	0.4915	0.068
H29	0.1136	0.3658	0.7128	0.05

	x/a	y/b	z/c	U(eq)
H24A	0.2457	0.5873	0.5121	0.073
H24B	0.1674	0.4527	0.4962	0.073
H24C	0.2456	0.2224	0.4975	0.073
H27	-0.1197	0.0632	0.7106	0.06
H32A	0.2116	0.5275	0.6799	0.085
H32B	0.2658	0.2996	0.6595	0.085
H32C	0.2336	0.1503	0.6891	0.085
H26	-0.1029	-0.1240	0.6629	0.059
H31	-0.0697	0.3230	0.7538	0.077
H7A	0.8299	0.0768	0.2499	0.071
H8A	0.5552	0.6229	0.3154	0.088
H8B	0.4889	0.4656	0.3360	0.088
H8C	0.5184	0.2598	0.3086	0.088