Supporting Information for

Stereoselective Cyclotetramerization of a 3-(Hydroxymethyl)salicylaldehyde

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Table 1. Crystal data and structure refinement for **2**.

Empirical formula	$C_{36}H_{32}O_8$
Formula weight	592.62
Temperature	293(2) K
Crystal system	Tetragonal
Space group	$I\bar{4}$
Unit cell dimensions	*a* = 15.7903(9) Å α = 90 deg. *b* = 15.7903(9) Å β = 90 deg. *c* = 5.8038(6) Å γ = 90 deg.
Volume	1447.1(2) $Å^3$
Z	2
Density (calculated)	1.360 g/cm^3
Absorption coefficient	0.096 mm^{-1}
Absorption correction	Semi-empirical from psi-scans
Transmission	0.2425 to 0.2606
F(000)	624
Diffractometer	Enraf-Nonius CAD4
Radiation	Graphite-monochromated MoKα (0.71073 A)
Scan type	ω-2θ
Decay	negligible, based on 3 standards measured every 7200 s exposure (150 reflections)
Crystal size	0.40 × 0.08 × 0.05 mm
Crystal habit	Rod
Crystal color	Colorless
Theta range for data collection	1.82 to 24.99 deg.
Limiting indices	0<=h<=18, 0<=k<=18, -6<=l<=6
Reflections collected	1365
Independent reflections	1269 [R(int) = 0.0232]
Structure solution method	Direct
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	1269 / 0 / 100
Goodness-of-fit on F^2	1.040
Final R indices [I > 4σ(I)]	R1 = 0.0377, wR2 = 0.0841
R indices (all data)	R1 = 0.0513, wR2 = 0.0913
Absolute structure parameter	-2(2)
Largest diff. peak and hole	0.111 and -0.119 e·Å^{-3}

Table 2. Atomic coordinates and equivalent isotropic displacement parameters for **2**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O1	0.40737(10)	0.11306(10)	0.2419(3)	0.0395(4)
O2	0.27815(10)	0.13321(10)	0.0552(3)	0.0415(4)
C1	0.44259(14)	0.17704(13)	0.1124(4)	0.0332(6)
C2	0.52193(14)	0.20731(14)	0.1745(4)	0.0330(6)
C3	0.5558(2)	0.27495(13)	0.0525(4)	0.0365(6)
C4	0.5146(2)	0.3109(2)	-0.1366(4)	0.0375(6)
C5	0.4367(2)	0.27754(14)	-0.1968(4)	0.0392(6)
C6	0.39967(14)	0.21211(14)	-0.0736(4)	0.0344(6)
C7	0.33470(14)	0.0726(2)	0.1375(4)	0.0355(6)
C8	0.3135(2)	0.1787(2)	-0.1346(5)	0.0458(7)
C41	0.5533(2)	0.3834(2)	-0.2679(5)	0.0501(7)

Table 3. Bond lengths [Å] and angles [deg] for **2**.

O1-C1	1.376(3)
O1-C7	1.446(3)
O2-C7	1.393(3)
O2-C8	1.428(3)
C1-C2	1.388(3)
C1-C6	1.390(3)
C2-C3	1.389(3)
C2-C7#1	1.507(3)
C3-C4	1.396(3)
C4-C5	1.384(3)
C4-C41	1.505(3)
C5-C6	1.386(3)
C6-C8	1.501(3)
C1-O1-C7	114.6(2)
C7-O2-C8	111.0(2)
O1-C1-C2	118.4(2)
O1-C1-C6	121.3(2)
C2-C1-C6	120.3(2)
C1-C2-C3	118.7(2)
C1-C2-C7#1	121.0(2)
C3-C2-C7#1	120.2(2)
C2-C3-C4	122.3(2)
C5-C4-C3	117.2(2)
C5-C4-C41	121.6(2)
C3-C4-C41	121.2(2)
C4-C5-C6	121.9(2)
C5-C6-C1	119.5(2)
C5-C6-C8	121.5(2)
C1-C6-C8	119.0(2)
O2-C7-O1	110.4(2)
O2-C7-C2#2	109.3(2)
O1-C7-C2#2	106.3(2)
O2-C8-C6	110.5(2)

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

Table 4. Anisotropic displacement parameters for **2**.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
O1	0.0347(9)	0.0377(9)	0.0459(9)	0.0130(8)	-0.0073(8)	-0.0087(7)
O2	0.0351(9)	0.0395(9)	0.0498(10)	0.0095(9)	-0.0069(8)	-0.0015(7)
C1	0.0349(12)	0.0252(11)	0.0396(14)	0.0020(11)	0.0014(11)	0.0005(9)
C2	0.0304(12)	0.0304(12)	0.0380(13)	0.0001(10)	0.0033(10)	0.0031(10)
C3	0.0309(12)	0.0285(12)	0.0500(14)	-0.0016(11)	0.0018(12)	0.0002(9)
C4	0.0418(14)	0.0282(12)	0.0425(14)	0.0003(11)	0.0055(12)	0.0028(10)
C5	0.0445(14)	0.0324(13)	0.0406(14)	0.0040(10)	-0.0022(12)	0.0068(11)
C6	0.0354(12)	0.0307(12)	0.0371(13)	0.0029(11)	-0.0022(12)	0.0023(10)
C7	0.0336(13)	0.0289(12)	0.0440(14)	0.0018(11)	-0.0040(11)	-0.0003(10)
C8	0.048(2)	0.0425(14)	0.047(2)	0.0102(13)	-0.0130(12)	-0.0054(12)
C41	0.054(2)	0.0357(13)	0.061(2)	0.0111(13)	0.0046(14)	-0.0010(12)

Table 5. Hydrogen coordinates and isotropic displacement parameters for **2**.

	x	y	z	U(eq)
H3	0.6077(2)	0.29706(13)	0.0983(4)	0.036
H5	0.4083(2)	0.29967(14)	-0.3236(4)	0.039
H7	0.35280(14)	0.0352(2)	0.0120(4)	0.035
H8A	0.2766(2)	0.2254(2)	-0.1752(5)	0.046
H8B	0.3179(2)	0.1415(2)	-0.2670(5)	0.046
H41A	0.6071(2)	0.3977(2)	-0.2012(5)	0.050
H41B	0.5164(2)	0.4316(2)	-0.2605(5)	0.050
H41C	0.5612(2)	0.3672(2)	-0.4259(5)	0.050
H41D	0.5160(2)	0.4000(2)	-0.3905(5)	0.050
H41E	0.6067(2)	0.3661(2)	-0.3312(5)	0.050
H41F	0.5619(2)	0.4305(2)	-0.1658(5)	0.050