Supporting Information

Solvent-controlled stereoselective supramolecular synthesis: a case of diastereomeric dimers of 16-*S*-dihydrosteviol

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Table S1. Crystallographic data and X-ray structural experiment parameters for the single crystals of compound **1**.

Compound	**1×$C_4H_8O_2$**	**1×CCl_4**	**1a**	**1×t-BuOH**	**1b**
Empirical formula	$C_{20}H_{32}O_3$, $0.5(C_4H_8O_2)$	$C_{20}H_{32}O_3$, $0.5CCl_4$	$C_{20}H_{32}O_3$	$C_{20}H_{32}O_3$, $1.5((CH_3)_3COH)$	$C_{20}H_{32}O_3$
Formula weight	364.51	397.36	320.45	431.63	320.45
Radiation, wavelength	Cu *K*α, 1.54178 Å	Mo *K*α, 0.71073 Å	Mo *K*α, 0.71073 Å	Mo *K*α, 0.71073 Å	Mo *K*α, 0.71073 Å
Temperature, K	296(2)	100(2)	100(2)	100(2)	101(2)
Crystal system	orthorhombic	orthorhombic	orthorhombic	monoclinic	monoclinic
Space group	$P2_12_12_1$ (No. 19)	$P2_12_12_1$ (No. 19)	$P2_12_12_1$ (No. 19)	$P2_1$ (No. 4)	$I2$ (No. 5)
Unit cell dimensions: *a*, *b*, *c*, Å; α, β, γ, °	12.3232(3), 15.3362(4), 21.8680(6); 90, 90, 90	12.2364(10), 15.9167(13), 21.4647(16); 90, 90, 90	12.0811(7), 14.7248(8), 20.1145(11); 90, 90, 90	14.5023(7), 7.7274(4), 22.8287(11); 90, 92.427(2), 90	21.580(4), 7.2369(13), 22.829(4); 90, 98.164(14), 90
Volume, Å^3	4132.86(19)	4180.5(6)	3578.2(3)	2556.0(2)	3529.1(12)
Z and *Z*′	8 and 2	8 and 2	8 and 2	4 and 2	8 and 2
Calculated density, g cm^{-3}	1.172	1.263	1.190	1.122	1.206
Absorption coefficient, mm^{-1}	0.623	0.327	0.078	0.074	0.079
F(000)	1600	1704	1408	956	1408
Crystal size, mm^3	0.500 × 0.200 × 0.100	0.345 × 0.209 × 0.102	0.484 × 0.322 × 0.091	0.857 × 0.283 × 0.082	0.565 × 0.183 × 0.031
θ range for data collection, °	4.04 to 69.96	2.289 to 26.990	1.966 to 26.999	1.633 to 27.000	1.402 to 24.862
Index ranges	$-11 \le h \le 14$, $-18 \le k \le 18$, $-26 \le l \le 26$	$-15 \le h \le 15$, $-20 \le k \le 20$, $-24 \le l \le 27$	$-15 \le h \le 15$, $-17 \le k \le 18$, $-25 \le l \le 25$	$-18 \le h \le 18$, $-9 \le k \le 9$, $-29 \le l \le 29$	$-25 \le h \le 25$, $-8 \le k \le 8$, $-27 \le l \le 26$
Reflections collected	27780	54626	39180	36255	33546
Independent reflections	7130	9112	7818	11120	6092
R_{int}	0.0269	0.0376	0.0641	0.0354	0.3413
R_σ	0.0247	0.0237	0.0603	0.0339	0.2829
Observed Data [$I > 2\sigma(I)$]	6919	8880	6467	10768	3163
Completeness to θ = 25.242°, %	94.1	99.5	99.9	99.8	99.5
Max. and min. transmission	0.9403 and 0.7459	0.7460 and 0.7098	0.7463 and 0.5785	0.7360 and 0.6872	0.7451 and 0.4325
Data / restraints / parameters	7130 / 4 / 493	9112 / 4 / 482	7818 / 0 / 437	11120 / 1 / 623	6092 / 1233 / 419
Goodness-of-fit on F^2	1.064	1.099	1.047	1.069	1.153
Final *R* indices [$I > 2\sigma(I)$]	*R*1 = 0.0434, *wR*2 = 0.1275	*R*1 = 0.0504, *wR*2 = 0.1317	*R*1 = 0.0521, *wR*2 = 0.1148	*R*1 = 0.0354, *wR*2 = 0.0864	*R*1 = 0.2315, *wR*2 = 0.4662
R indices (all data)	*R*1 = 0.0446, *wR*2 = 0.1291	*R*1 = 0.0514, *wR*2 = 0.1326	*R*1 = 0.0693, *wR*2 = 0.1214	*R*1 = 0.0369, *wR*2 = 0.0873	*R*1 = 0.3270, *wR*2 = 0.5163
Flack parameter	–0.04(17)	0.025(11)	–1.0(5)	–0.2(2)	–4.5(10)
Largest diff. peak and hole, *e* Å^{-3}	0.362 and –0.278	0.824 and –0.680	0.324 and –0.229	0.256 and –0.158	0.701 and –0.629
CCDC number (refcode)	685577(RUKDOR)*	2483694	2483695	2483696	2483697

*X-Ray data from compound **1×$C_4H_8O_2$** was published by us earlier [O. A. Lodochnikova, R. N. Khaibullin, R. Z. Musin, A. T. Gubaidullin and V. E. Kataev, *J. Struct. Chem*., 2009, **50**, 657–662]. In this publication, we present them again for the possibility of direct comparison with the X-ray data of the **1a** crystal formed during spontaneous destruction of **1×$C_4H_8O_2$**.