Supporting Information

Pseudopolymorph and Infinite Hydrogen Bonding Network of Cyclic Oligomers of *m*-Aminobenzenesulfonic Acid

Kosuke Katagiri, Takako Kato, Hyuma Masu, Masahide Tominaga and Isao Azumaya*

Contents

X-ray Crystallographic Analysis.

Crystal data for 1 (Type I). $C_{18}H_{15}N_3O_6S_3 \cdot 5H_2O$; M = 555.59 g mol^{-1}, colorless prism measuring 0.20 × 0.10 × 0.05 mm, triclinic, P-1, a = 8.434(5), b = 12.342(6), c = 12.702(7) Å, α = 109.453(6), β = 97.697(7), γ = 102.720(7) °, V = 1184.8(11) Å^3, Z = 2, D_c = 1.557 Mg m^{-3}, T = 150 K, μ (MoKα) = 0.377 mm^{-1}, $2\theta_{max}$ = 23.82°, 4717 reflections, 3506 unique reflections (R_{int} = 0.0706) which were used in all calculations. R_1 = 0.1439, wR_2 = 0.2193 (all data) R_1 = 0.0805, wR_2 = 0.1886 ($I > 2\sigma(I)$) for 309 parameters. The positions of hydrogen atoms included in the water molecules were not calculated.

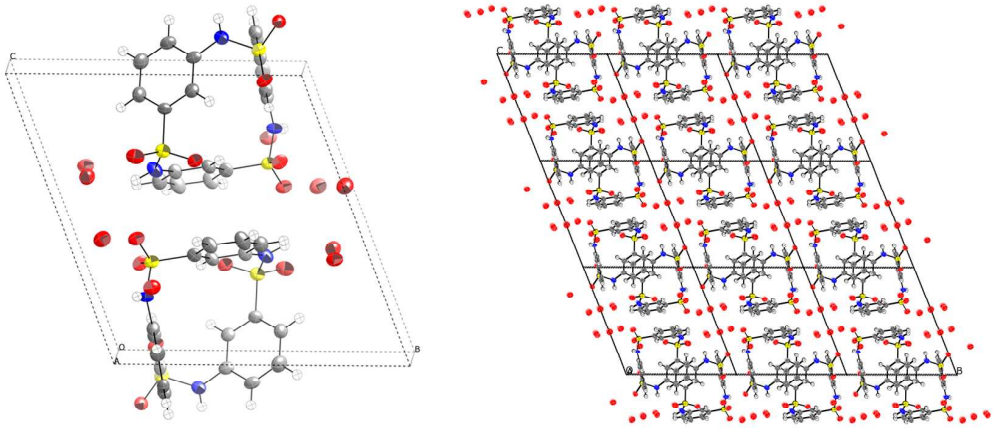

Figure S1. ORTEP diagram of unit cell (left) and packing structure (right) in a crystal of **1** (type I).

Crystal data for 1 (Type II). $C_{18}H_{15}N_3O_6S_3 \cdot CH_4O$; M = 497.55 g mol^{-1}, colorless prism measuring 0.50 × 0.30 × 0.30 mm, monoclinic, $P2_1/n$, a = 8.430(1), b = 8.9689(1), c = 28.364(4) Å, β = 91.132(2) °, V = 2144.2(6) Å^3, Z = 4, D_c = 1.541 Mg m^{-3}, T = 291 K, μ(MoKα) = 0.394 mm^{-1}, $2\theta_{max}$ = 27.47°, 12454 reflections, 4851 unique reflections (R_{int} = 0.0290) which were used in all calculations. R_1 = 0.0557, wR_2 = 0.1327 (all data) R_1 = 0.0403, wR_2 = 0.11170 ($I > 2\sigma(I)$) for 303 parameters.

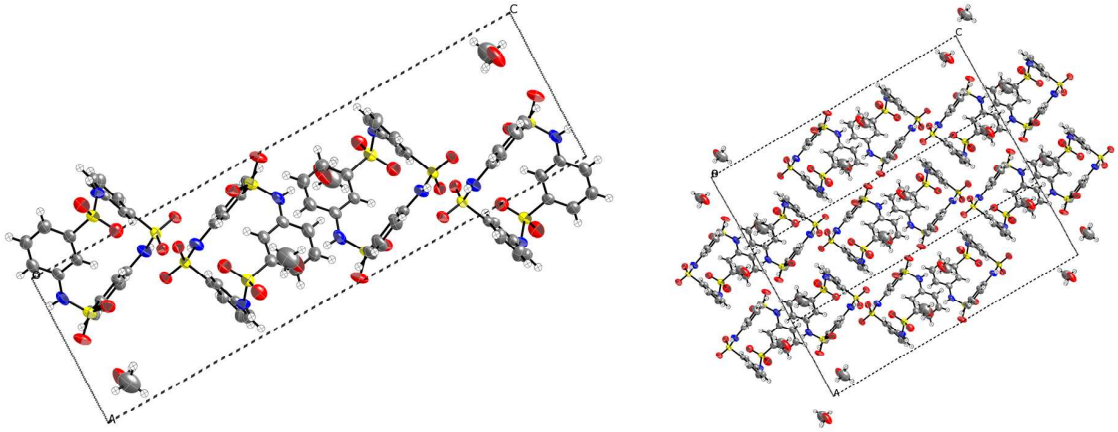

Figure S2. ORTEP diagram of unit cell (left) and packing structure (right) in a crystal of **1** (type II).

Crystal data for 1 (Type III). $C_{18}H_{15}N_3O_6S_3 \cdot C_4H_6N_2$; M = 547.62 g mol^{-1}, colorless prism measuring 0.40 × 0.20 × 0.10 mm, triclinic, P-1, a = 9.949(2), b = 10.949(2), c = 11.940(3) Å, α = 81.215(3), β = 75.704(3), γ = 77.805(7) °, V = 1225.0(5) Å^3, Z = 2, D_c = 1.485 Mg m^{-3}, T = 150 K, μ (MoKα) = 0.352 mm^{-1}, $2\theta_{max}$ = 27.50°, 7386 reflections, 5344 unique reflections (R_{int} = 0.0280) which were used in all calculations. R_1 = 0.0562, wR_2 = 0.1413 (all data) R_1 = 0.0448, wR_2 = 0.1299 ($I > 2\sigma(I)$) for 327 parameters.

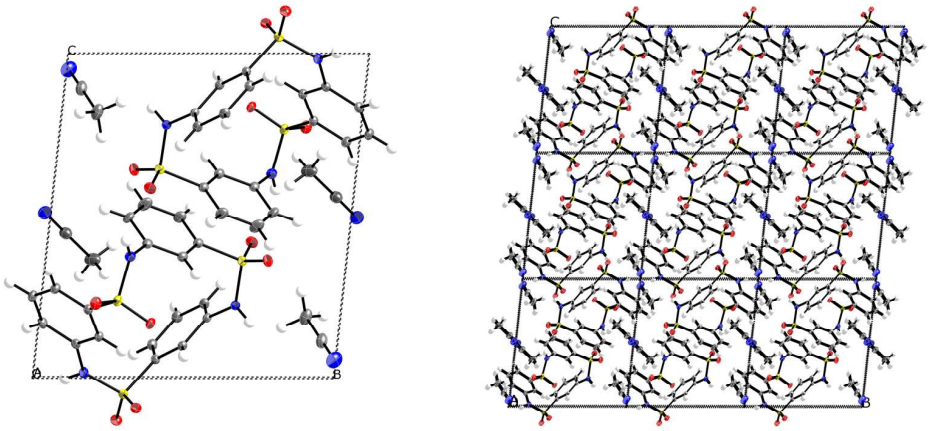

Figure S3. ORTEP diagram of unit cell (left) and packing structure (right) in a crystal of **1** (type III).

Crystal data for 2. $C_{24}H_{20}N_4O_8S_4$; M = 620.68 g mol^{-1}, colorless prism measuring 0.15 × 0.10 × 0.05 mm, tetragonal, $I4_1/a$, a = 15.428(4), b = 15.428(4), c = 21.819(2) Å, V = 5193.3(19) Å^3, Z = 8, D_c = 1.588 Mg m^{-3}, T = 303 K, μ = 0.424 mm^{-1}, $2\theta_{max}$ = 23.93°, 8033 reflections, 1844 unique (R_{int} = 0.0886), R_1 = 0.0901, wR_2 = 0.1159 (all data) R_1 = 0.0394, wR_2 = 0.0925 ($I > 2\sigma(I)$) for 181 parameters.

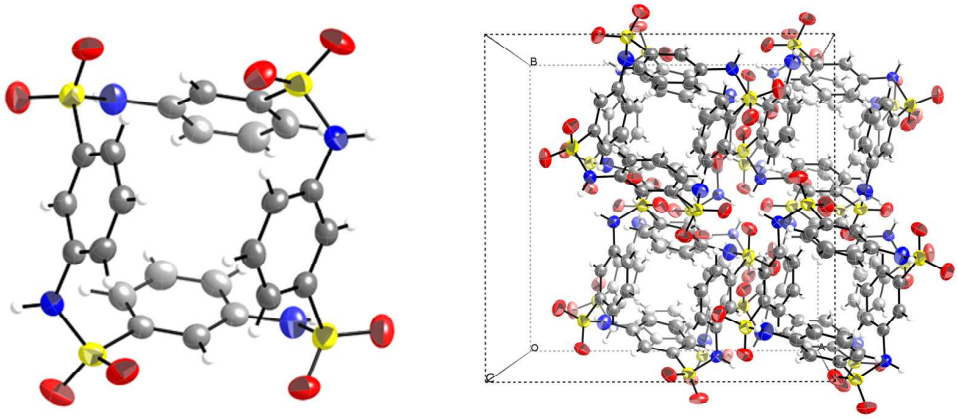

Figure S4. ORTEP diagram of asymmetric unit (left) and packing structure (right) in a crystal of **2**.