

Electronic Supplemental Information

Title: A novel crownophane trapping CO₂ as carbonic acid at room temperature

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Content

¹H NMR, IR, ESI-MS and elemental analysis data for compounds, **2** ~ **4**.

IR charts of the solid of compound **4** before (a) and after (b) bubbling carbon dioxide in aqueous MeCN.

DTA and TGA thermograms of the complex of **4** with carbonic acid

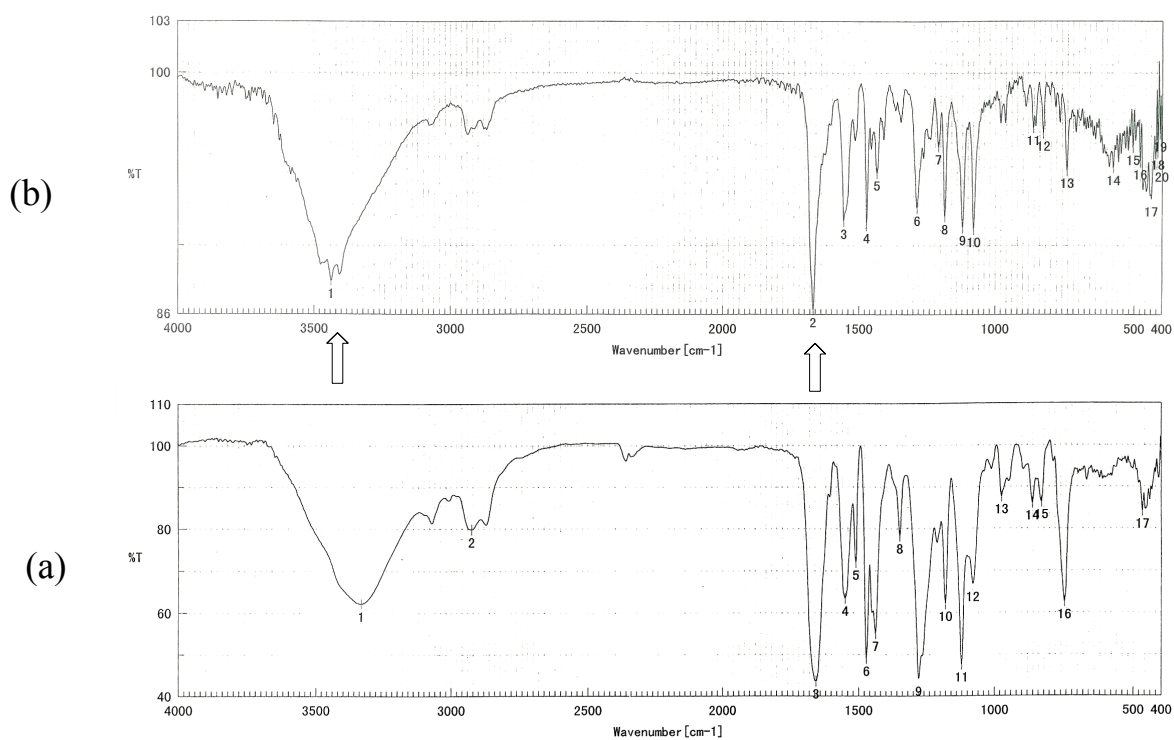
2-bis(2-chloromethylcarbonylethoxy)ethane (**2**): The reaction of bis(2-aminoethoxy)ethane with chloroacetyl chloride gave **2** in 55% yield. mp. 85~88°C; ¹H NMR (300 MHz, CDCl₃, ppm) 3.53 (m, 4H, O-CH₂CH₂-N), 3.61 (m, O-CH₂-CH₂-N), 3.65 (s, 4H, C(=O)-CH₂), 4.07 (s, O-CH₂-CH₂-O), 7.00 (broad, 2H, C-NH); IR (KBr, cm⁻¹) 3310 (amide-NH), 1643 (amide-C=O); ESI mass, calcd for C₁₀H₁₈Cl₂N₂O₄ 300.06, found 323.1 (+ Na⁺).

Compound **3**: mp. 205~206°C; ¹H NMR (300 MHz, CDCl₃, ppm) 3.51 (m, 12H, O-CH₂CH₂-OCH₂-CH₂-N), 4.67 (s, 4H, OCH₂C=CH₂), 4.90 (s, 4H, C(=O)-CH₂), 5.61 (s, 2H, H₂C=C), 7.17 (s, 2H, Ar-H), 7.22 (s, 2H, Ar-H), 7.38 (m, 4H, Ar-H), 7.45 (broad, 2H, C-NH), 7.65 (m, 2H, Ar-H), 7.69 (m, 2H, Ar-H); IR (KBr, cm⁻¹) 3435 (amide-NH), 1676 (amide-C=O); ESI mass, calcd for C₃₄H₃₆N₂O₈ 600.25, found 623.3 (+ Na⁺); Elemental analysis: calcd for C₃₄H₃₆N₂O₈ + 2H₂O C: 64.14, H: 6.33, N: 4.40, Found C: 64.02, H: 6.24, N: 4.27.

Compound **4**: mp. 212~212.5°C; ¹H NMR (300 MHz, CDCl₃, ppm) 3.29 (s, 4H, O-CH₂CH₂-O), 3.50 (m, 8H, O-CH₂-CH₂-N), 3.94 (s, 4H, ArCH₂C=CH₂), 4.72 (s, 2H, H₂C=C), 4.75 (s, 4H, C(=O)-CH₂), 6.78 (s, 2H, OH), 7.33 (broad, 2H, C-NH), 7.10 (s, 2H, Ar-H), 7.35 (t, J=3.9Hz, 4H, Ar-H), 7.69 (d, J=8.7Hz, 2H, Ar-H), 7.85 (d, J=8.7Hz, 2H, Ar-H); IR (KBr, cm⁻¹) 3334 (amide-NH, OH), 1656 (amide-C=O); ESI mass, calcd for C₃₄H₃₆N₂O₈ 600.25, found 623.3(+ Na⁺); Elemental analysis: calcd for C₃₄H₃₆N₂O₈ + 1/2H₂O C: 66.98, H: 6.12, N: 4.59, Found C: 66.97, H: 5.97, N: 4.53.

IR charts

IR spectra of the solid of compound **4** before (a) and after (b) bubbling carbon dioxide in aqueous MeCN.



DTA and TGA thermograms of the complex of **4** with carbonic acid

