

Supporting Information

Synthesis of Multifunctional Metal-Organic Frameworks and Tuning the Functionalities by Organic Pendant of Ligand

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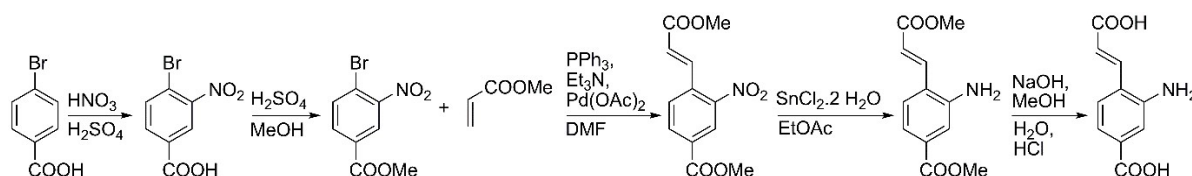
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Experimental Section

A. Synthesis of ligands

Synthesis of 3-amino-4-(2-carboxyvinyl)benzoic acid (H₂CVB-NH₂)



Scheme S1. Preparation of 3-amino-4-(2-carboxyvinyl)benzoic acid.

(a) *4-bromo-3-nitrobenzoic acid*: 4-Bromobenzoic acid (10.00 g, 49.75 mmol) was slowly added in small portions (in about 1 h) to a mixture of fuming HNO₃ (3.4 mL, 93 %) and concentrated H₂SO₄ (120 mL) at 0 °C. The resulting mixture was further stirred at RT for 2 h. The clear solution was then poured over ice; the precipitate formed was filtered and washed with a copious amount of water. The product was dried under vacuum at 80 °C and used without further purification. Yield: 11.80 g (96 %). ¹H NMR (300 MHz, d₆-DMSO, 25 °C): δ=8.43 (s, 1H; Ar-H), 8.05 ppm (m, 2H; Ar-H).

(b) *methyl 4-bromo-3-nitrobenzoate*: 4-bromo-3-nitrobenzoic acid (11.80 g, 47.96 mmol) was suspended in methanol (200 mL), to which concentrated H₂SO₄ (20 mL) was added. The mixture was refluxed overnight, and then methanol was removed by evaporation. When the reaction mixture was cooled to RT, solid resulted, which was extracted with CH₂Cl₂ (150 mL x 3). The collected organic phase was washed with saturated NaHCO₃ solution and dried over MgSO₄. The solvent was evaporated under reduced pressure to yield a crystalline pale yellow solid, which was dried under vacuum at RT and used without further purification. Yield: 11.70 g (94 %). ¹H NMR (300 MHz, CDCl₃, 25 °C): δ=8.47 (s, 1H; Ar-H), 8.08 (d, J = 8.29, 1H; Ar-H), 7.86 (d, J = 8.29 Hz, 1H; Ar-H), 3.99 ppm (s, 3H; -Me).

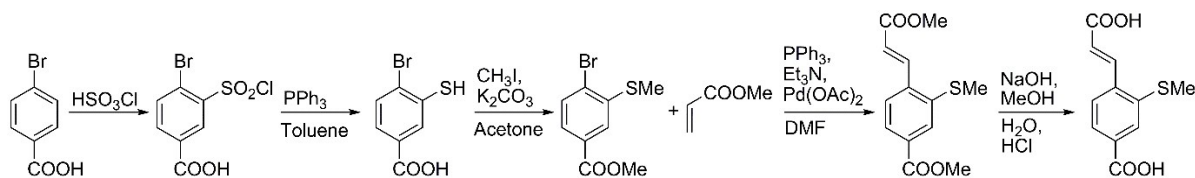
(c) *methyl 4-(3-methoxy-3-oxoprop-1-enyl)-3-nitrobenzoate*: methyl 4-bromo-3-nitrobenzoate (5.30 g, 20 mmol), palladium acetate (0.052 g, 0.23 mmol), and triphenylphosphine (0.120 g, 0.46 mmol) were added to a Schlenk flask and outgassed for 2 h. To this, were added anhydrous N,N-dimethylformamide (8 mL), anhydrous triethylamine (4.0 mL, 30 mmol), and methyl acrylate (10 mL, 110 mmol) under N₂. The clear solution was heated at 110 °C and stirred for 20 h. The black-colored solution was cooled to RT, added to ice water, and acidified with concentrated HCl until the solution became strongly acidic. The brown precipitate formed was extracted with CH₂Cl₂ (200 mL x 5). The combined organic layer was washed with water, dried over MgSO₄, and evaporated under reduced pressure to yield brown solid. The resulting product was purified by silica gel column chromatography by eluting CH₂Cl₂, which gave rise to a pale yellow solid. Yield: 2.70 g (51 %). ¹H

NMR (300 MHz, CDCl₃, 25 °C): δ =8.68 (s, 1H; Ar-H), 8.29 (m, 1H; Ar-H), 8.13 (d, J = 15.82 Hz, 1H; =C-H), 7.74 (d, J = 8.10, 1H; Ar-H), 6.45 (d, J = 15.82 Hz, 1H; =C-H), 4.00 (s, 3H; -Me), 3.86 ppm (s, 3H; -Me).

(d) *methyl 3-amino-4-(3-methoxy-3-oxoprop-1-enyl)benzoate*: methyl 4-(3-methoxy-3-oxoprop-1-enyl)-3-nitrobenzoate (2.65 g, 10 mmol) and SnCl₂·2H₂O (11.28 g, 50 mmol) were dissolved in ethyl acetate (200 mL). The solution was refluxed for 2 h, cooled to RT, and then saturated NaHCO₃ solution was added to make the solution basic. The sticky precipitate formed was filtered through a CELITE pad and washed with ethyl acetate. The filtrate was put into a separating funnel and the organic layer was separated, the aqueous layer was washed with ethyl acetate (100 mL x 2). The combined organic layer was dried over MgSO₄ and evaporated under reduced pressure. The product was purified by silica gel column chromatography by eluting a 1:1 mixture of ethyl acetate and hexane to yield a pale yellow crystalline solid. Yield: 2.10 g (89 %). ¹H NMR (300 MHz, CDCl₃, 25 °C): δ =7.81 (d, J = 16.00 Hz, 1H; =C-H), 7.41 (m, 3H; Ar-H), 6.44 (d, J = 15.80 Hz, 1H; =C-H), 4.10 (br. s, 2H; -NH₂), 3.91 (s, 3H; -Me), 3.83 ppm (s, 3H; -Me).

(e) *3-amino-4-(2-carboxyvinyl)benzoic acid (H₂CVB-NH₂)*: methyl 3-amino-4-(3-methoxy-3-oxoprop-1-enyl)benzoate (2.10 g, 8.92 mmol) and NaOH (5.00 g, 125 mmol) were suspended in methanol (200 mL), stirred and refluxed overnight. The methanol was evaporated and the solid was dissolved in water (~100 mL) and carefully acidified with 3 N HCl until pH became 4 - 5. The precipitate formed was filtered, washed with water and dried under vacuum to yield yellow solid. Yield: 1.55 g, (84%). ¹H NMR (300 MHz, [D₆]DMSO, 25 °C): δ =7.81 (d, J = 15.8, 1H; =C-H), 7.52 (d, J = 8.30, 1H; Ar-H), 7.33 (s, 1H; Ar-H), 7.07 (d, J = 8.20 Hz, 1H; Ar-H), 6.38 (d, J = 15.6, 1H; =C-H), 5.79 ppm (br. s, 2H; -NH₂). Elemental analysis calcd (%) for C₁₀H₉NO₄: C 57.97, H 4.38, N 6.76; found: C 57.48, H 4.45, N 7.01. FTIR (KBr pellet): $\tilde{\nu}$ = 2824 (amino), 1683 (carboxylate), 1617 cm⁻¹ (alkene).

Synthesis of 4-(2-carboxyvinyl)-3-(methylthio)benzoic acid (H₂CVB-SMe)



Scheme S2. Preparation of 4-(2-carboxyvinyl)-3-(methylthio)benzoic acid.

(a) *4-bromo-3-(chlorosulfonyl)benzoic acid*: 4-bromobenzoic acid (10.0 g, 49.7 mmol) was added in small portions to chlorosulfonic acid (25 mL) at 0 °C, and the clear solution was heated overnight at 130 - 140 °C. The solution was cooled to RT and added dropwise to an ice/water mixture (500 mL). The precipitate formed was filtered, washed with water, and dried in air. The solid was then

dissolved in diethyl ether (150 mL) and dried over Na₂SO₄ and evaporated until the dull white powder was formed, which was used without further purification. Yield = 10.9 g, 73 %. ¹H NMR (300 MHz, [D₆]DMSO, 25 °C): δ=8.46 (d, J = 1.9 Hz, 1H; Ar-H), 7.73 ppm (m, 2H; Ar-H).

(b) *4-bromo-3-mercaptopbenzoic acid*: 4-bromo-3-(chlorosulfonyl)benzoic acid (12.0 g, 40.0 mmol) was suspended in anhydrous toluene (200 mL), and purged with N₂ gas. To this suspension, PPh₃ (31.5 g, 120.0 mmol) was added by small portions. On complete addition, the starting material was dissolved. The solution was stirred for about 20 min at RT under N₂ purging. To this, aqueous NaOH (200 mL, 15 %) was added, and then the aqueous layer was separated, washed with toluene, and acidified with conc. HCl. The precipitate formed was extracted with EtOAc (300 mL), dried over MgSO₄, and evaporated under reduced pressure to yield white colored solid, which was used without further purification. Yield: 5.9 g, 63 %. ¹H NMR (300 MHz, [D₆]DMSO, 25 °C): δ=8.14 (br., 1H; Ar-H), 7.62 ppm (br., 2H; Ar-H).

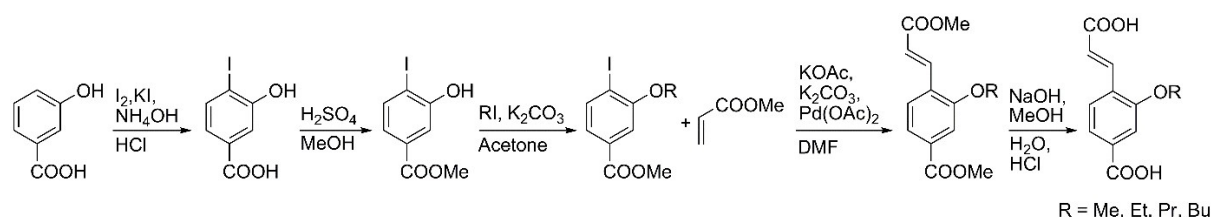
(c) *methyl 4-bromo-3-(methylthio)benzoate*: 4-bromo-3-mercaptopbenzoic acid (5.9 g, 25.3 mmol) was dissolved in dry acetone (200 mL) and K₂CO₃ (6.0 g, 43.4 mmol), and CH₃I (20 mL, excess) was added and refluxed overnight. The mixture was evaporated under reduced pressure and extracted with CH₂Cl₂ and washed with H₂O. The CH₂Cl₂ layer was dried over MgSO₄ and evaporated under reduced pressure to yield pale yellow liquid, which was used without further purification. Yield: 6.3 g, 95 %. ¹H NMR (300 MHz, CDCl₃, 25 °C): δ=7.78 (s, 1H; Ar-H), 7.63 (m, 2H; Ar-H), 3.96 (s, 3H; OMe), 2.55 ppm (s, 3H; SMe).

(d) *Methyl 4-(3-methoxy-3-oxoprop-1-enyl)-3-(methylthio)benzoate*: palladium acetate (0.052 g, 0.23 mmol), and triphenylphosphine (0.120 g, 0.46 mmol) were put in a Schlenk tube and outgassed for 2 h. To this, were added a solution of methyl 4-bromo-3-(methylthio)benzoate (2.61 g, 10 mmol) in anhydrous N,N-dimethylformamide (5 mL), anhydrous triethylamine (2.0 mL, 15 mmol), and methyl acrylate (5 mL, 55 mmol) under N₂. The mixture was stirred at 110 °C for 48 h. The solution was cooled to RT, added to ice water, and acidified with concentrated HCl. The precipitate formed was extracted with CH₂Cl₂ (100 mL x 3). The combined organic layer was washed with water, dried over MgSO₄, and evaporated under reduced pressure to yield brown material, which was purified by silica gel column chromatography by eluting CH₂Cl₂ to result in a yellow solid. Yield: 1.65 g (62 %). ¹H NMR (300 MHz, CDCl₃, 25 °C): δ=8.13 (d, J = 16.0 Hz, 1H; =C-H), 7.96 (s, 1H; Ar-H), 7.82 (d, J = 7.9 Hz, 1H; Ar-H), 7.57 (d, J = 8.10, 1H; Ar-H), 6.45 (d, J = 15.8 Hz, 1H; =C-H), 3.95 (s, 3H; -OMe), 3.84 (s, 3H; -OMe), 2.55 ppm (s, 3H; -SMe).

(e) *4-(2-carboxyvinyl)-3-(methylthio)benzoic acid (H₂CVB-SMe)*: methyl 4-(3-methoxy-3-oxoprop-1-enyl)-3-(methylthio)benzoate (1.60 g, 6.00 mmol) and NaOH (1.0 g, 25 mmol) were dissolved in methanol (150 mL) and refluxed overnight. The methanol was removed by evaporation. The solid formed was dissolved in water (~100 mL) and acidified with HCl to yield yellow

precipitate, which was filtered, washed with water, and dried under vacuum. Yield: 1.40 g, (98%). ¹H NMR (300 MHz, [D₆]DMSO, 25 °C): δ=12.93 (br. s, 2H; -COOH), 7.93 (d, J = 15.8, 1H; =C-H), 7.85 (br. m, 2H; Ar-H), 7.74 (br. s, 1H; Ar-H), 6.60 (d, J = 15.6, 1H; =C-H), 2.58 ppm (br. s, 3H; SMe). Elemental analysis calcd (%) for C₁₁H₁₀O₄S: C 55.45, H 4.23; found: C 53.45, H 4.49. FTIR (KBr pellet): $\tilde{\nu}$ = 1689 (carboxylate), 1629 cm⁻¹ (alkene).

Synthesis of 3-alkoxy-4-(2-carboxyvinyl)benzoic acid (H₂CVB-OR)



Scheme S3. Preparation of 3-alkoxy-4-(2-carboxyvinyl)benzoic acids.

(a) *3-hydroxy-4-iodobenzoic acid*: The compound was synthesized by the reported method.^{S1} The product was used in the next step without further purification. ¹H NMR (300 MHz, [D₆]DMSO, 25 °C): δ=10.68 (br. s, 1H; =O-H), 7.81 (m, 1H; Ar-H), 7.44 (m, 1H; Ar-H), 7.14 ppm (m, 1H; Ar-H).

(b) *methyl 3-hydroxy-4-iodobenzoate*: The mixture of 3-hydroxy-4-iodobenzoic acid (10.6 g, 40.0 mmol), conc.H₂SO₄ (30 mL), and methanol (300 mL) were refluxed overnight with stirring. The clear solution was evaporated under reduced pressure, extracted with CH₂Cl₂, washed with water, dried over MgSO₄. The solvent was removed by evaporation under reduced pressure to yield dull-white crystalline precipitate, which was used in the next step without further purification. Yield: 9.70 g (87 %). ¹H NMR (300 MHz, CDCl₃, 25 °C): δ=7.78 (m, 1H; Ar-H), 7.66 (m, 1H; Ar-H), 7.35 (m, 1H; Ar-H), 3.94 ppm (s, 3H; -CH₃).

(c) *methyl 4-iodo-3-methoxybenzoate*: methyl 3-hydroxy-4-iodobenzoate (5.56 g, 20 mmol), K₂CO₃ (2.40 g, 60 mmol) and iodomethane (4.0 mL, 64 mmol) were mixed with dry acetone (50 mL), and then refluxed overnight. The solvent was evaporated to dryness under reduced pressure, and then water (100 mL) was added and extracted with CH₂Cl₂ (100 mL x 3). The combined CH₂Cl₂ layer was washed with water, dried over MgSO₄, and then evaporated under reduced pressure, which gave rise to pale yellow liquid, which was used in the next step without further purification. Yield = 5.70 g (97 %). ¹H NMR (300 MHz, CDCl₃, 25 °C): δ=7.87 (d, J = 8.1 Hz, 1H; Ar-H), 7.46 (s, 1H; Ar-H), 7.38 (d, J = 7.0 Hz, 1H; Ar-H), 3.96 (s, 3H; Me), 3.94 ppm (s, 3H; Me).

(d) *methyl 3-ethoxy-4-iodobenzoate*: The compound was synthesized by a similar method to that used for the synthesis of *methyl 4-iodo-3-methoxybenzoate*, using iodoethane (5.0 mL, 62.5 mmol). Yield = 5.80 g (95 %). ¹H NMR (300 MHz, CDCl₃, 25 °C): δ=7.86 (m, 1H; Ar-H), 7.43 (m, 1H; Ar-

H), 7.36 (m, 1H; Ar-H), 4.17 (q, J = 7 Hz, 2H; CH₂), 3.92 (s, 3H; CH₃), 1.53 ppm (t, J = 7 Hz, 3H; CH₃).

(e) *methyl 4-iodo-3-propoxybenzoate*: The compound was synthesized by a similar method to that used for *methyl 4-iodo-3-methoxybenzoate*, using iodopropane (6.0 mL, 61.8 mmol). Yield = 6.15 g (96 %). ¹H NMR (300 MHz, CDCl₃, 25 °C): δ=7.86 (d, J = 8.1 Hz, 1H; Ar-H), 7.43 (d, J = 1.9 Hz, 1H; Ar-H), 7.36 (dd, J = 8.1, 1.9 Hz, 1H; Ar-H), 4.17 (t, J = 6.4 Hz, 2H; CH₂), 3.93 (s, 3H; CH₃), 1.90 (m, 2H; CH₂), 1.12 ppm (t, J = 7.3 Hz, 3H; CH₃).

(f) *methyl 3-butoxy-4-iodobenzoate*: The compound was synthesized by a similar method as that used for *methyl 4-iodo-3-methoxybenzoate*, using iodobutane (7.0 mL, 61.5 mmol). Yield = 6.41 g (96 %). ¹H NMR (300 MHz, CDCl₃, 25 °C): δ=7.86 (d, J = 8.1 Hz, 1H; Ar-H), 7.43 (d, J = 1.7 Hz, 1H; Ar-H), 7.36 (dd, J = 8.0, 1.9 Hz, 1H; Ar-H), 4.10 (t, J = 6.3 Hz, 2H; CH₂), 3.93 (s, 3H; CH₃), 1.85 (m, 2H; CH₂), 1.59 (m, 2H; CH₂), 1.02 ppm (t, J = 7.3 Hz, 3H; CH₃).

(g) *methyl 3-methoxy-4-(3-methoxy-3-oxoprop-1-enyl)benzoate*: methyl 4-iodo-3-methoxybenzoate (5.70 g, 19.50 mmol), palladium acetate (0.11 g, 0.50 mmol), potassium acetate (1.96 g, 19.97 mmol) and K₂CO₃ (3.50 g, 25.36 mmol) were added to a Schlenk flask and outgassed for 2 h. To this, were added anhydrous N,N-dimethylformamide (10 mL), and methyl acrylate (6 mL, 66.21 mmol) under N₂. The mixture was stirred at 90 °C for 48 h. The solution was cooled to RT, added to ice water, and acidified with concentrated HCl. The brown precipitate formed was extracted with CH₂Cl₂ (150 mL x 3). The combined CH₂Cl₂ layer was washed with water, dried over MgSO₄. The solvent was removed by evaporation under reduced pressure until brown material resulted. The product was purified by silica gel column chromatography by eluting CH₂Cl₂, which gave rise to white solid. Yield: 3.70 g (76 %). ¹H NMR (300 MHz, CDCl₃, 25 °C): δ=8.00 (d, J = 16.2 Hz, 1H; =C-H), 7.62 (m, 3H; Ar-H), 6.61 (d, J = 16.2 Hz, 1H; =C-H), 3.97 (s, 3H; CH₃), 3.95 (s, 3H; CH₃), 3.83 ppm (s, 3H; -CH₃).

(h) *4-(2-carboxyvinyl)-3-methoxybenzoic acid (H₂CVB-OMe)*: methyl 3-methoxy-4-(3-methoxy-3-oxoprop-1-enyl)benzoate (3.7 g, 14.8 mmol) and NaOH (2.4 g, 60.0 mmol) were added in methanol (200 mL), and the mixture refluxed overnight. Methanol was evaporated under reduced pressure, the precipitate formed was dissolved in water and acidified with conc. HCl. The precipitate formed was filtered by suction, washed with water, and dried under vacuum at 100 °C to yield a white powder. Yield = 2.80 g (85 %). ¹H NMR (300 MHz, [D₆]DMSO, 25 °C): δ=7.82 (m, 2H; =C-H, Ar-H), 7.56 (m, 2H; Ar-H), 6.62 (d, J = 16.2, 1H; =C-H), 3.93 ppm (s, 3H; -CH₃). Elemental analysis calcd (%) for C₁₁H₁₀O₅: C 59.46, H 4.54; found: C 58.42, H 4.35. FTIR (KBr pellet): $\tilde{\nu}$ = 1690 (carboxylate), 1628 cm⁻¹ (alkene).

(i) *methyl 3-ethoxy-4-(3-methoxy-3-oxoprop-1-enyl)benzoate*: The compound was synthesized by a similar method to that used for *methyl 3-methoxy-4-(3-methoxy-3-oxoprop-1-enyl)benzoate*, using methyl 3-ethoxy-4-iodobenzoate (5.75 g, 18.78 mmol). Yield: 4.20 g (85 %). ¹H NMR (300 MHz, CDCl₃, 25 °C): δ=8.00 (d, J = 16.2 Hz, 1H; =C-H), 7.60 (m, 3H; Ar-H), 6.63 (d, J = 16.2 Hz, 1H; =C-H), 4.19 (q, J = 7.0 Hz, 2H; CH₂), 3.95 (s, 3H; CH₃), 3.83 (s, 3H; -CH₃), 1.51 ppm (t, J = 7.0 Hz, 3H; -CH₃).

(j) *4-(2-carboxyvinyl)-3-ethoxybenzoic acid (H₂CVB-OEt)*: The compound was synthesised by a similar method to that used for *4-(2-carboxyvinyl)-3-methoxybenzoic acid*, using methyl 3-ethoxy-4-(3-methoxy-3-oxoprop-1-enyl)benzoate (4.20 g, 15.90 mmol). Yield = 3.52 g (94 %). ¹H NMR (300 MHz, [D₆]DMSO, 25 °C): δ=7.82 (m, 2H; =C-H, Ar-H), 7.53 (m, 2H; Ar-H), 6.64 (d, J = 16.2, 1H; =C-H), 4.18 (q, J = 6.8 Hz, 2H; CH₂), 1.41 ppm (t, J = 6.9 Hz, 3H; -CH₃). Elemental analysis calcd (%) for C₁₂H₁₂O₅: C 61.01, H 5.12; found: C 59.93, H 5.79. FTIR (KBr pellet): $\tilde{\nu}$ = 1690 (carboxylate), 1627 cm⁻¹ (alkene).

(k) *methyl 4-(3-methoxy-3-oxoprop-1-enyl)-3-propoxybenzoate*: The compound was synthesised by a similar method to that used for *methyl 3-methoxy-4-(3-methoxy-3-oxoprop-1-enyl)benzoate*, using methyl 4-iodo-3-propoxybenzoate (6.10 g, 19.05 mmol). Yield: 4.70 g (89 %). ¹H NMR (300 MHz, CDCl₃, 25 °C): δ=8.00 (d, J = 16.2 Hz, 1H; =C-H), 7.59 (m, 3H; Ar-H), 6.64 (d, J = 16.2 Hz, 1H; =C-H), 4.07 (t, J = 6.5 Hz, 2H; CH₂), 3.94 (s, 3H; CH₃), 3.82 (s, 3H; CH₃), 1.93 (m, 2H; CH₂), 1.10 ppm (t, J = 7.4 Hz, 3H; -CH₃).

(l) *4-(2-carboxyvinyl)-3-propoxybenzoic acid (H₂CVB-OPr)*: The compound was synthesised by a similar method to that used for *4-(2-carboxyvinyl)-3-methoxybenzoic acid*, using methyl 4-(3-methoxy-3-oxoprop-1-enyl)-3-propoxybenzoate (4.70 g, 16.88 mmol). Yield = 3.90 g (92 %). ¹H NMR (300 MHz, [D₆]DMSO, 25 °C): δ=7.82 (m, 2H; =C-H, Ar-H), 7.53 (m, 2H; Ar-H), 7.56 (m, 2H; Ar-H), 6.65 (d, J = 16.2, 1H; =C-H), 4.08 (t, J = 6.3 Hz, 2H; CH₂), 1.80 (m, 2H; CH₂), 1.02 ppm (m, 3H; -CH₃). Elemental analysis calcd (%) for C₁₃H₁₄O₅: C 62.39, H 5.64; found: C 61.68, H 6.12. FTIR (KBr pellet): $\tilde{\nu}$ = 1690 (carboxylate), 1627 cm⁻¹ (alkene).

(m) *methyl 3-butoxy-4-(3-methoxy-3-oxoprop-1-enyl)benzoate*: The compound was synthesised by a similar method to that used for *methyl 3-methoxy-4-(3-methoxy-3-oxoprop-1-enyl)benzoate*, using methyl 3-butoxy-4-iodobenzoate (6.40 g, 19.15 mmol). Yield: 4.00 g (68 %). ¹H NMR (300 MHz, CDCl₃, 25 °C): δ=8.00 (d, J = 16.2 Hz, 1H; =C-H), 7.59 (m, 3H; Ar-H), 6.64 (d, J = 16.2 Hz, 1H; =C-H), 4.12 (m, 2H; CH₂), 3.95 (s, 3H; CH₃), 3.83 (s, 3H; CH₃), 1.88 (m, 2H; CH₂), 1.55 (m, 2H; CH₂), 1.03 ppm (m, 3H; -CH₃).

(n) *3-butoxy-4-(2-carboxyvinyl)benzoic acid (H₂CVB-OBu)*: The compound was synthesised by a similar method to that used for *4-(2-carboxyvinyl)-3-methoxybenzoic acid*, using methyl 3-butoxy-4-

(3-methoxy-3-oxoprop-1-enyl)benzoate (4.00 g, 13.68 mmol). Yield = 3.50 g (96 %). ¹H NMR (300 MHz, [D₆]DMSO, 25 °C): δ=7.83 (m, 2H; =C-H, Ar-H), 7.53 (m, 2H; Ar-H), 6.65 (m, 1H; =C-H), 4.11 (m, 2H; CH₂), 1.77 (m, 2H; CH₂), 1.47 (m, 2H; CH₂), 0.97 ppm (m, 3H; -CH₃). Elemental analysis calcd (%) for C₁₄H₁₆O₅: C 63.62, H 6.10; found: C 62.85, H 5.86. FTIR (KBr pellet): $\tilde{\nu}$ = 1689 (carboxylate), 1627 cm⁻¹ (alkene).

B. Synthesis of MOFs

All MOFs were synthesized by using H₂CVB-XR by a similar method to the synthesis of [Zn₄O(CVB-NH₂)₃]•18DMF•H₂O (SNU-170) described in the main text.

Synthesis of [Zn₄O(CVB-SMe)₃]•7DMF•3H₂O (SNU-171). The compound was synthesised by a similar method to that for SNU-170, using H₂CVB-SMe (0.024 g, 0.101 mmol). Yield: 0.025 g (48 %). Anal. Calcd for C₅₄H₇₉N₇O₂₃S₃Zn₄: C, 41.79; H, 5.13; N, 6.32. Found: C, 41.80; H, 5.22; N, 6.23. FTIR (KBr pellet): $\tilde{\nu}$ = 1671 (DMF), 1610 cm⁻¹ (carboxylate).

Synthesis of [Zn₄O(CVB-OMe)₃]•7DMF•3H₂O (SNU-172). The compound was synthesized by a similar method to that for SNU-170, using H₂CVB-OMe (0.023 g, 0.104 mmol). Yield: 0.030 g (60 %). Anal. Calcd for C₅₄H₇₉N₇O₂₆Zn₄: C, 43.13; H, 5.29; N, 6.52. Found: C, 43.46; H, 5.24; N, 6.70. FTIR (KBr pellet): $\tilde{\nu}$ = 1671 (DMF), 1610 cm⁻¹ (carboxylate).

Synthesis of [Zn₄O(CVB-OEt)₃]•7DMF•2H₂O (SNU-173). The compound was synthesized by a method similar to the synthesis of SNU-170, using H₂CVB-OEt (0.024 g, 0.102 mmol). Yield: 0.025 g (49 %). Anal. Calcd for C₅₇H₈₃N₇O₂₅Zn₄: C, 44.81; H, 5.48; N, 6.42. Found: C, 45.02; H, 5.67; N, 6.10. FTIR (KBr pellet): $\tilde{\nu}$ = 1671 (DMF), 1608 cm⁻¹ (carboxylate).

Synthesis of [Zn₄O(CVB-OPr)₃]•16DMF•3H₂O (SNU-174). The compound was synthesized by a method similar to the synthesis of SNU-170, using H₂CVB-OPr (0.025 g, 0.100 mmol). Yield: 0.040 g (53 %). Anal. Calcd for C₈₇H₁₅₄N₁₆O₃₅Zn₄: C, 46.53; H, 6.91; N, 9.98. Found: C, 45.45; H, 7.44; N, 9.73. FTIR (KBr pellet): $\tilde{\nu}$ = 1671 (DMF), 1602 cm⁻¹ (carboxylate).

Synthesis of [Zn₄O(CVB-OBu)₃]•15DMF•3H₂O (SNU-175). The compound was synthesized by a method similar to the synthesis of SNU-170, using H₂CVB-OBu (0.027 g, 0.102 mmol). Yield: 0.040 g (54 %). Anal. Calcd for C₈₇H₁₅₃N₁₅O₃₄Zn₄: C, 47.18; H, 6.96; N, 9.48. Found: C, 45.80; H, 7.00; N, 9.48. FTIR (KBr pellet): $\tilde{\nu}$ = 1671 (DMF), 1601 cm⁻¹ (carboxylate).

Synthesis of [Zn₄O(CVB-SMe)₁(CVB-OMe)₂]•7DMF•3H₂O (SNU-176). The compound was synthesized by a method similar to the synthesis of SNU-170, using H₂CVB-SMe (0.012 g, 0.050 mmol) and H₂CVB-OMe (0.011 g, 0.050 mmol). Yield: 0.030 g (40 %). Anal. Calcd for

$C_{54}H_{79}N_7O_{25}SZn_4$: C, 42.67; H, 5.24; N, 6.45. Found: C, 42.97; H, 5.28; N, 6.87. FTIR (KBr pellet): $\tilde{\nu}$ = 1671 (DMF), 1605 cm^{-1} (carboxylate). The ratio between CVB-SMe²⁻ and CVB-OMe²⁻ were confirmed by the NMR analysis of the activated sample, digested in DCI/D₂O (35%), and dissolved in DMSO (Fig. S10).

C. References

S1 G. S. Cockerill, P. C. Levett, D. A. Whiting, *J. Chem. Soc., Perkin Trans. 1*, **1995**, 1103-1113.

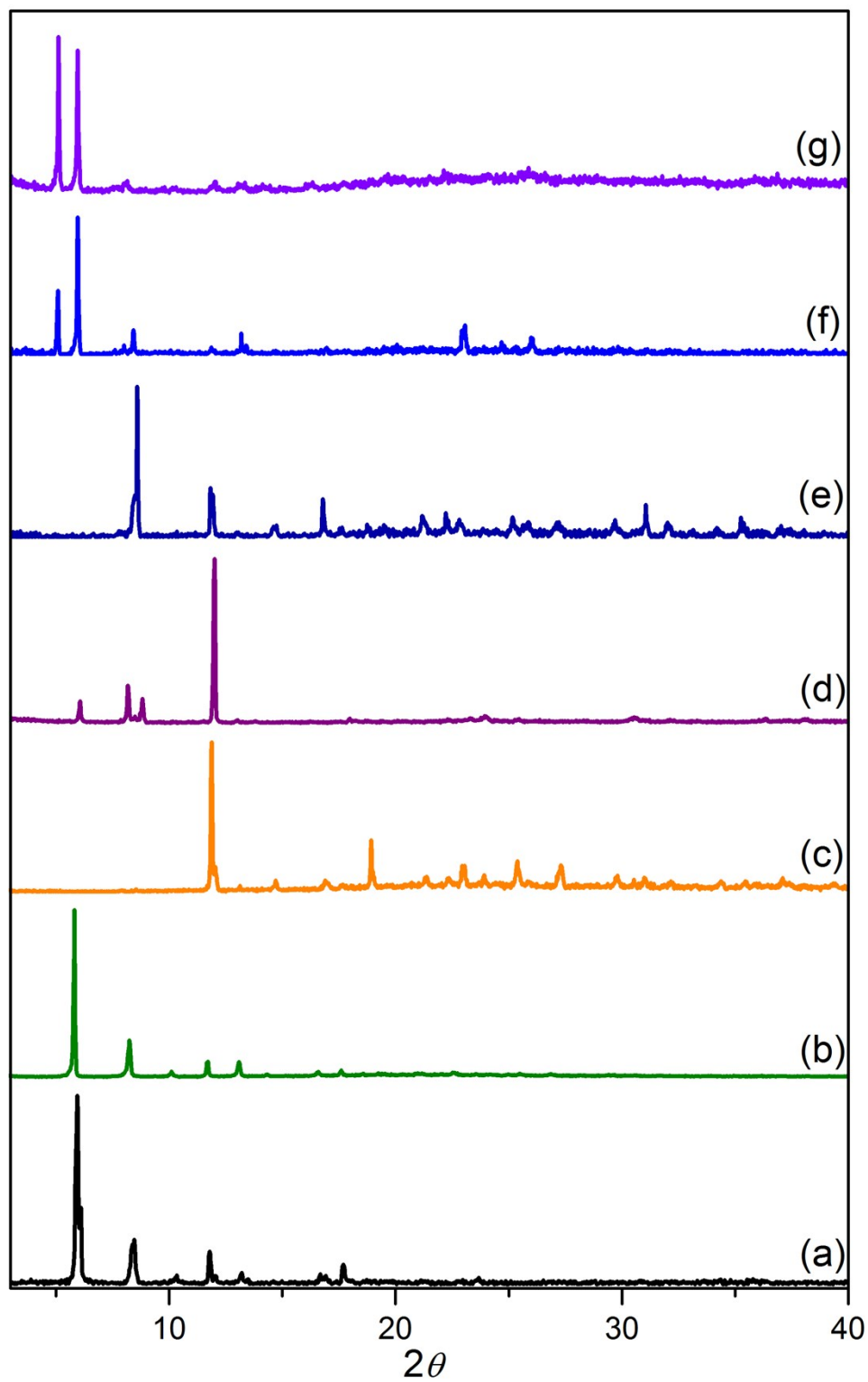


Fig. S1 The PXRD patterns of as-synthesized samples: (a) SNU-70, (b) SNU-170, (c) SNU-171, (d) SNU-172, (e) SNU-173, (f) SNU-174, and (g) SNU-175.

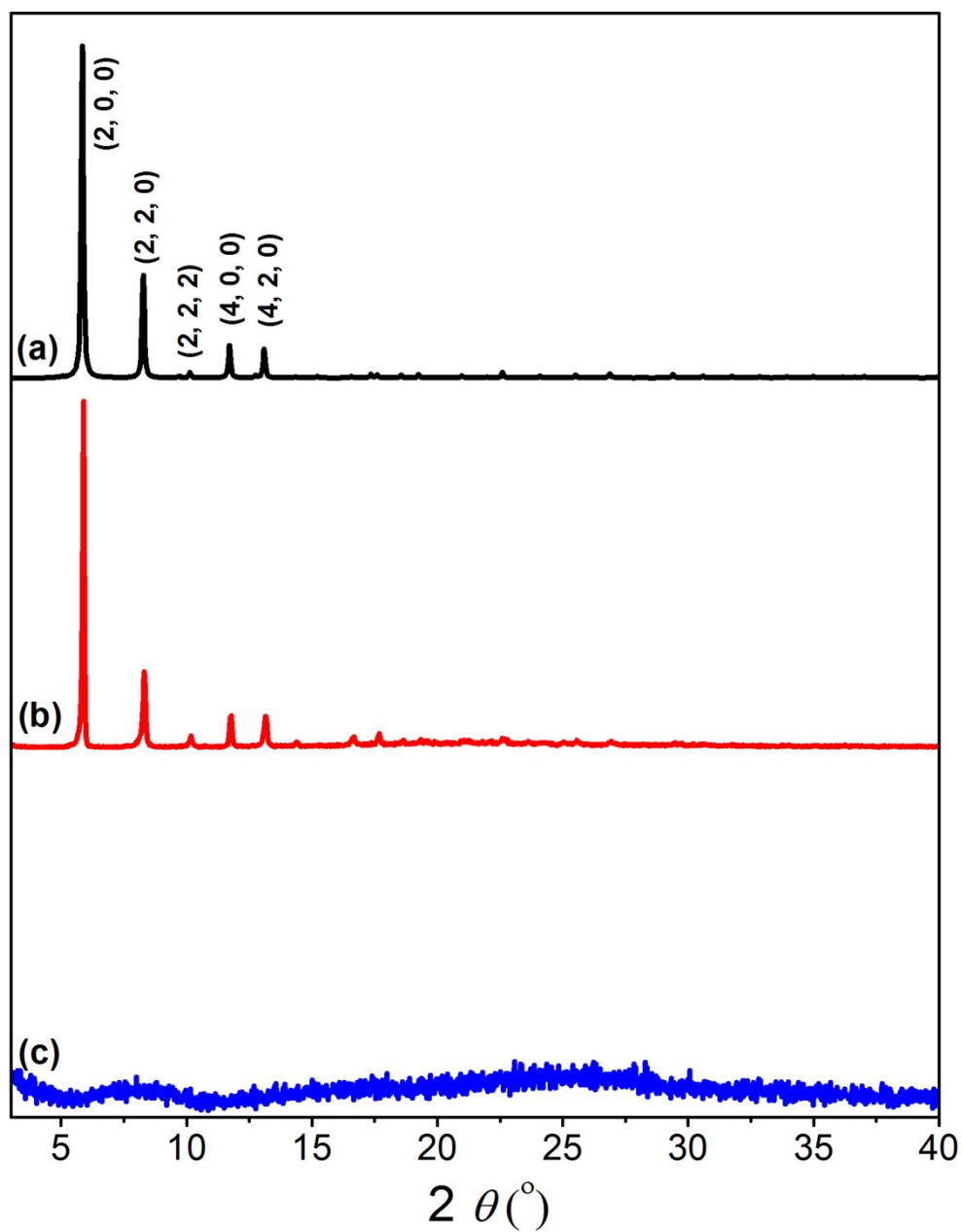


Fig. S2 The PXRd patterns of SNU-170: (a) simulated from the X-ray crystallographic data, (b) measured for as-synthesized sample, and (c) measured after activation with supercritical CO_2 .

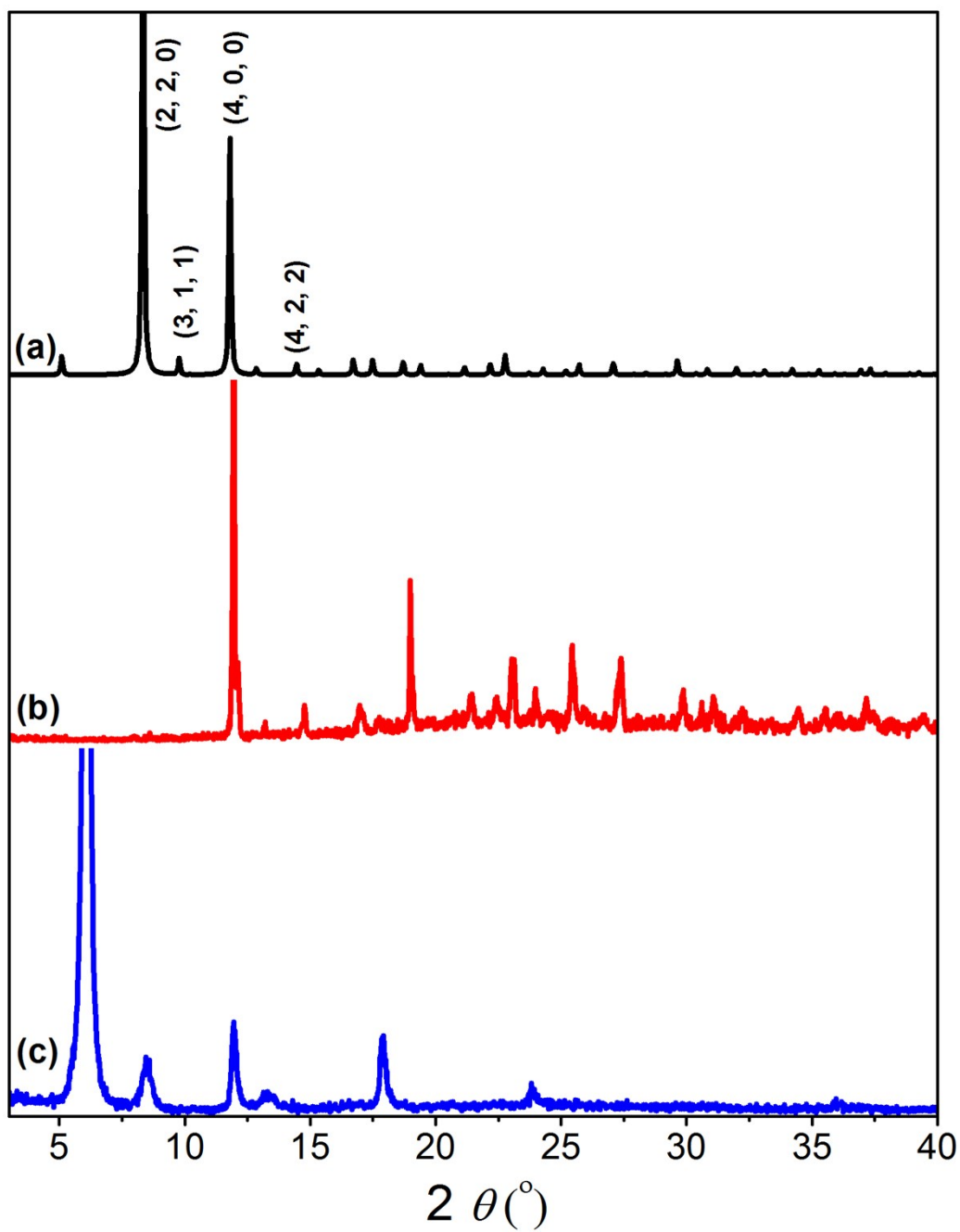


Fig. S3 The PXR D patterns of SNU-171: (a) simulated from the X-ray crystallographic data, (b) measured for as-synthesized sample, and (c) measured after activation with supercritical CO_2 .

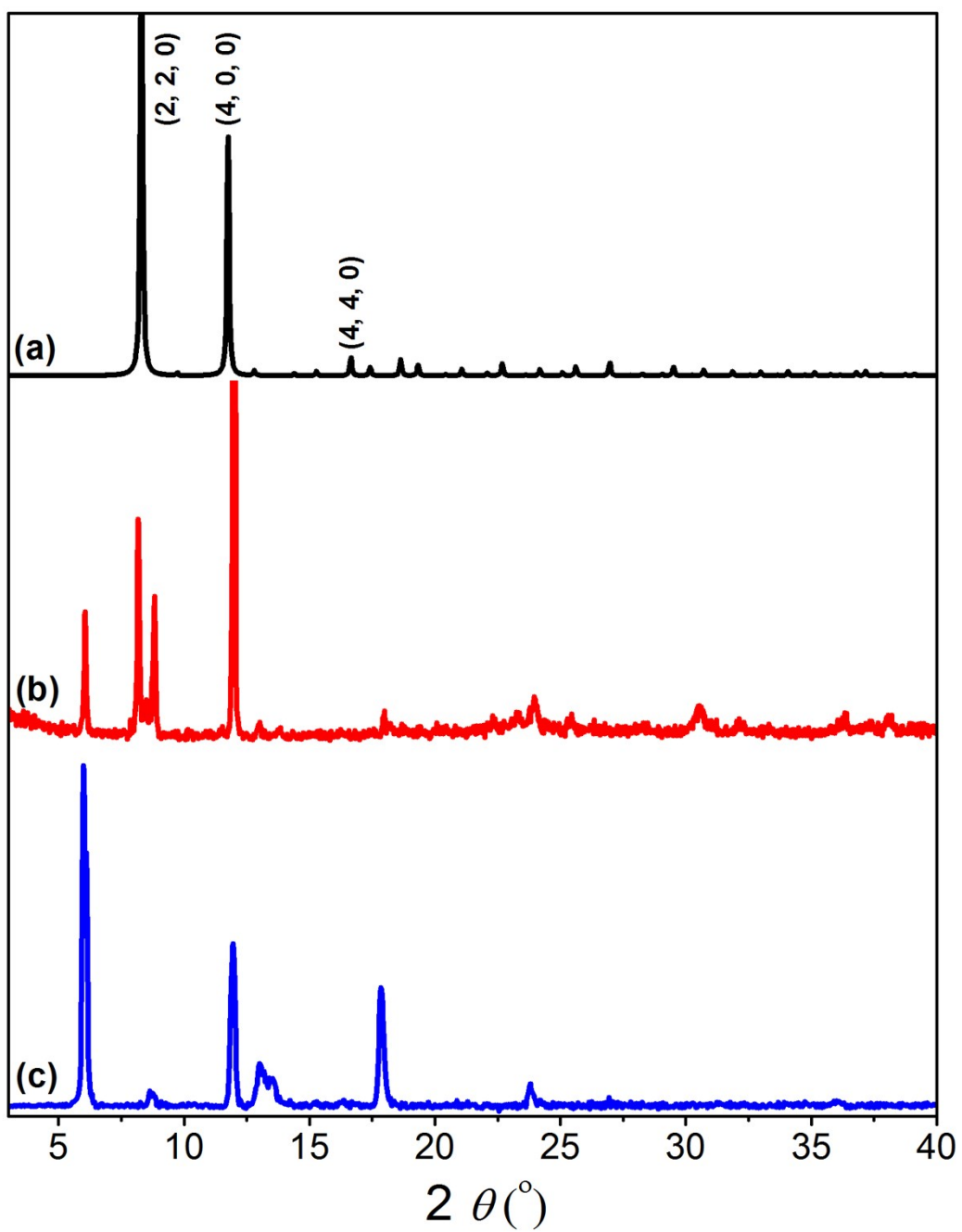


Fig. S4 The PXRD patterns of SNU-172: (a) simulated from the X-ray crystallographic data, (b) measured for as-synthesized sample, and (c) measured after activation with supercritical CO_2 .

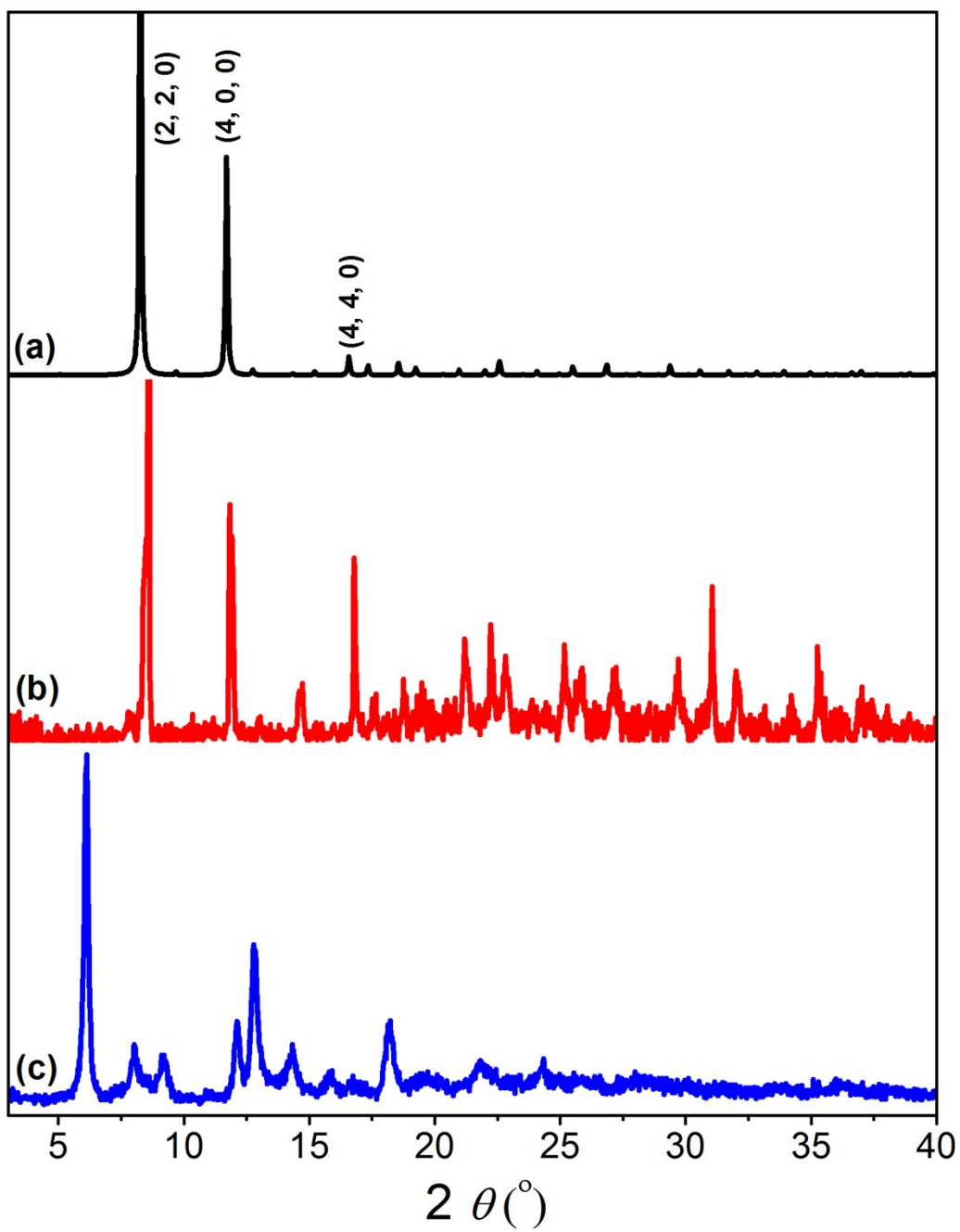


Fig. S5 The PXRD patterns of SNU-173: (a) simulated from the X-ray crystallographic data, (b) measured for as-synthesized sample, and (c) measured after activation with supercritical CO₂.

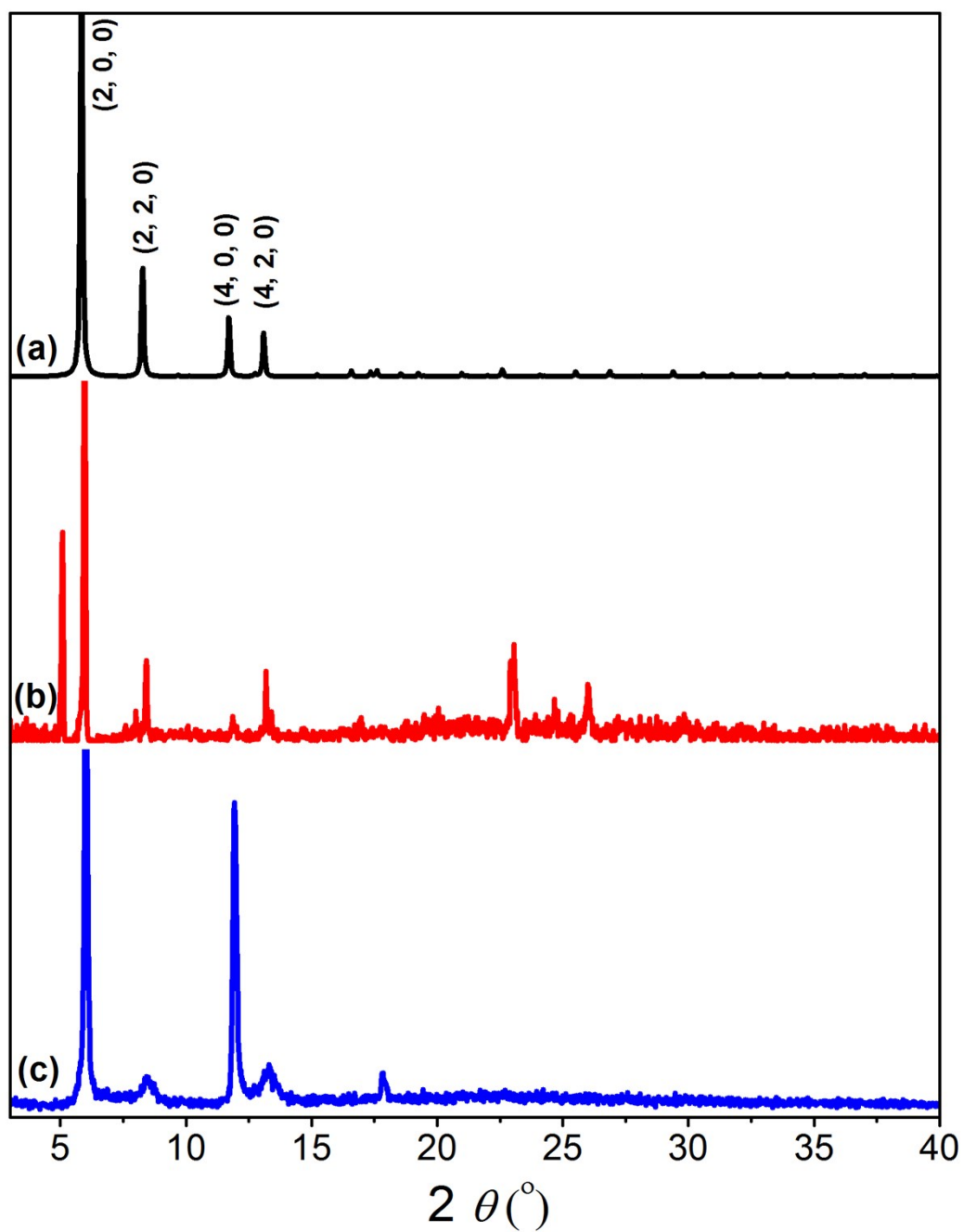


Fig. S6 The PXRD patterns of SNU-174: (a) simulated from the X-ray crystallographic data, (b) measured for as-synthesized sample, and (c) measured after activation with supercritical CO_2 .

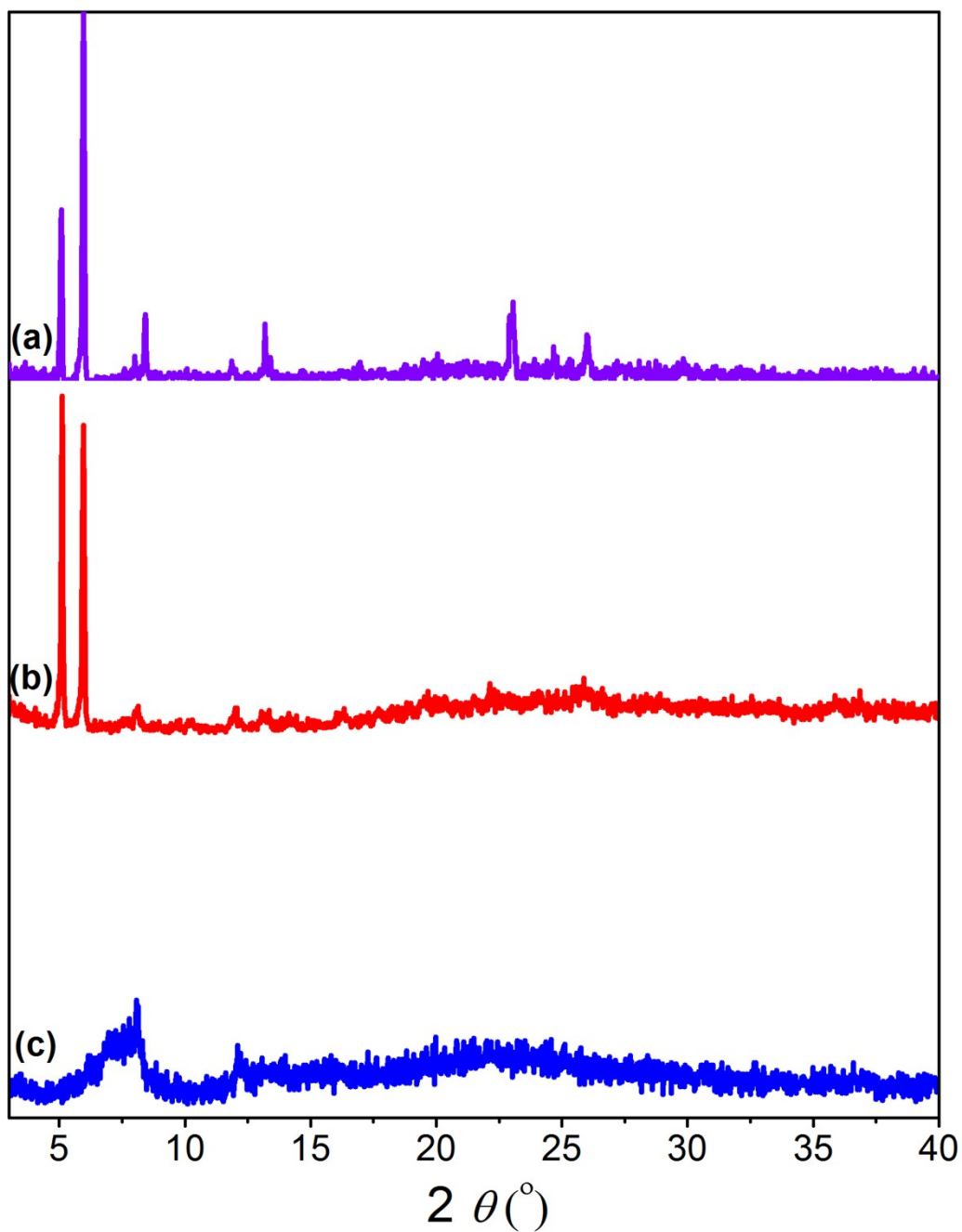


Fig. S7 The PXRD patterns of SNU-175: (a) measured for an as-synthesized sample of SNU-174, (b) measured for an as-synthesized sample of SNU-175, and (c) measured for SNU-175 after activation with supercritical CO₂₂.

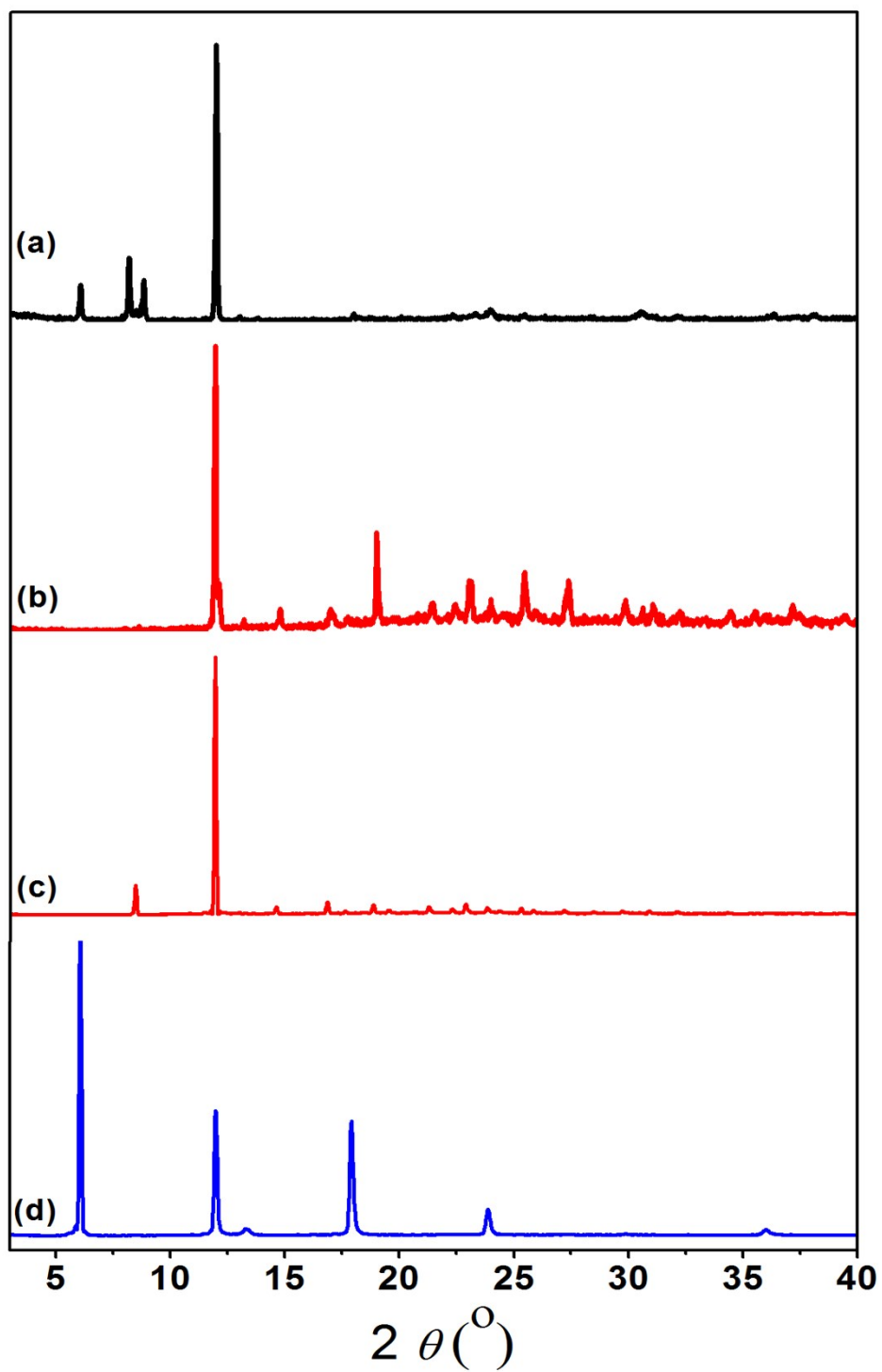


Fig. S8 The PXRD patterns of SNU-176: (a) as-synthesized sample of SNU-172, (b) as-synthesized sample of SNU-171, (c) as-synthesized sample of SNU-176, and (d) after activation of SNU-176 by using supercritical CO_2 .

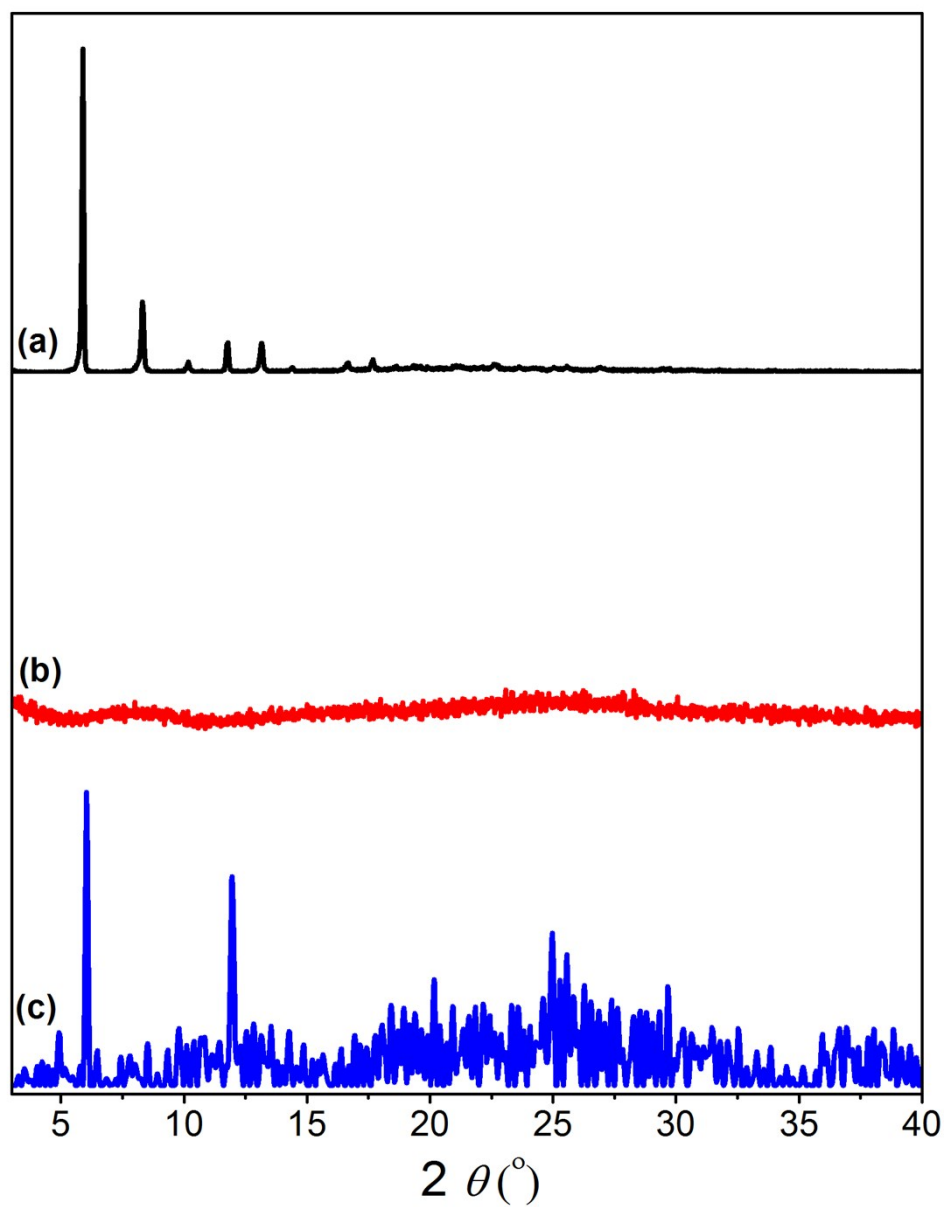


Fig. S9 The PXR D patterns of SNU-170: (a) as-synthesized sample, (b) SNU-170' resulted from the treatment with supercritical CO_2 , and (c) SNU-170' after immersed in DMF for 1 hour.

| | | | | | |
|------------------------|----------------------|-------------------|--|------------------------|----------------------|
| Acquisition Time (sec) | 5.3084 | Comment | Zn_CVB_SMe_OMe_SCD/DMSO/DCI_lock_DMSO | Date | 20 Jan 2014 18:36:00 |
| Date Stamp | 20 Jan 2014 18:36:00 | File Name | D:\SkyDrive\DATA\NMR\140120TKP\11\PDATA\111r | Origin | spect |
| Frequency (MHz) | 300.13 | Nucleus | 1H | Number of Transients | 16 |
| Original Points Count | 32768 | Owner | root | Points Count | 32768 |
| Receiver Gain | 256.00 | SW(cyclical) (Hz) | 6172.84 | Solvent | DMSO-d6 |
| Spectrum Type | STANDARD | Sweep Width (Hz) | 6172.65 | Temperature (degree C) | 23.600 |
| | | | | Pulse Sequence | zg30 |
| | | | | Spectrum Offset (Hz) | 1853.4263 |

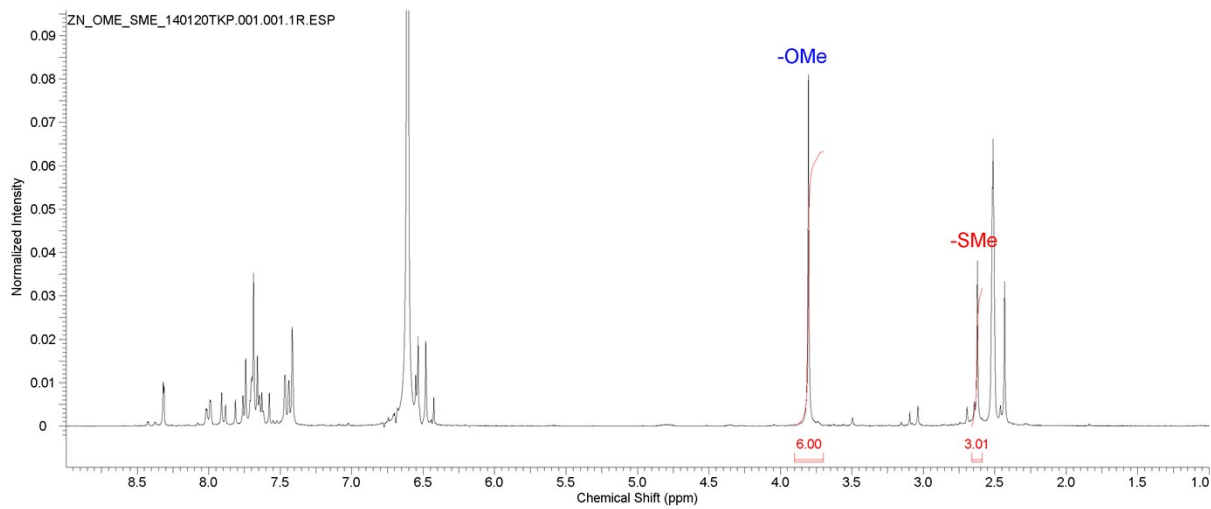


Fig. S10 ¹H NMR spectrum of [Zn₄O(CVB-SMe)₁(CVB-OMe)₂] (SNU-176') digested in DMSO-d₆/DCI.

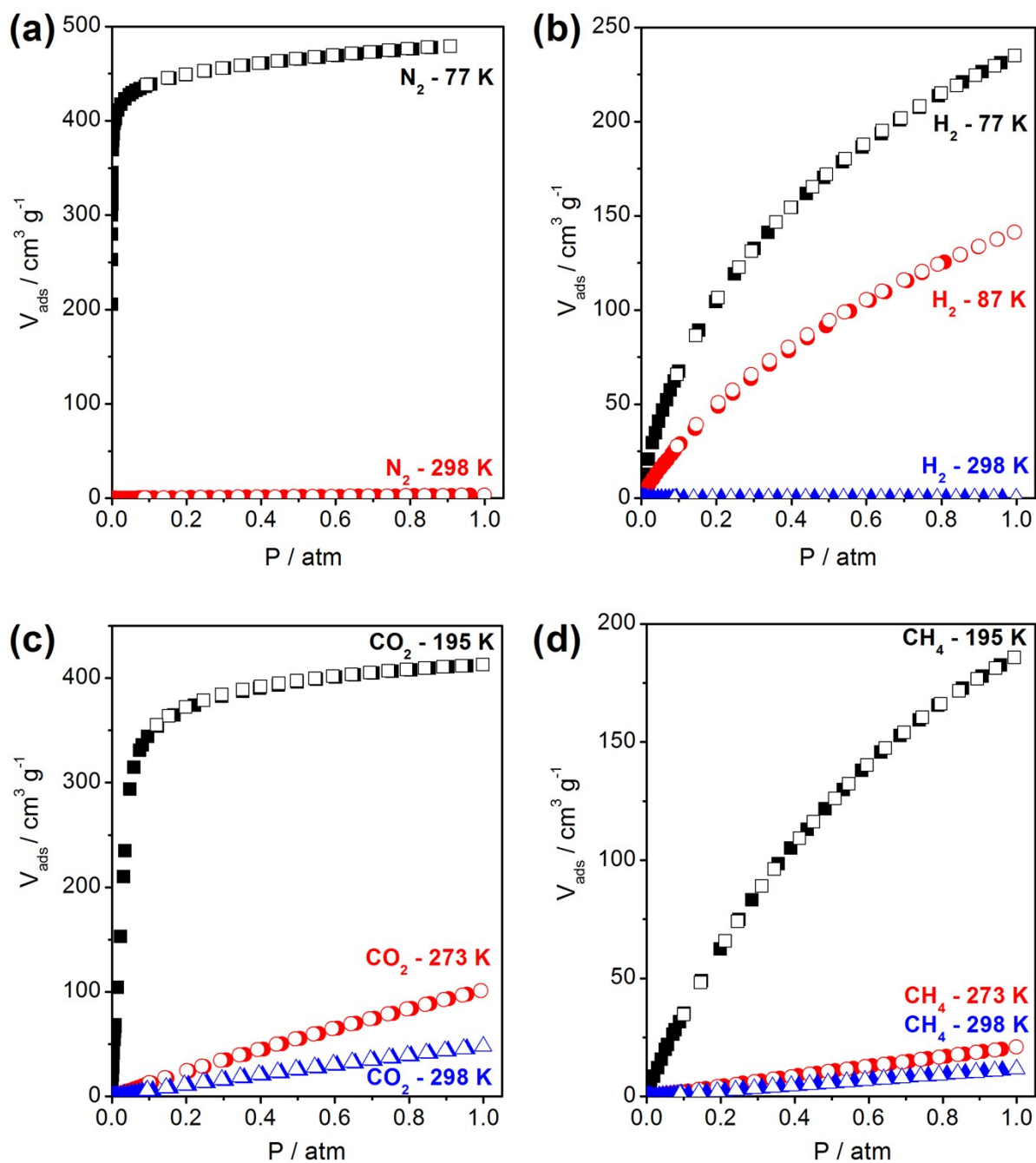


Fig. S11 Gas adsorption isotherms of SNU-176': a) N_2 at 77 K (black) and 298 K (red), b) H_2 at 77 K (black), 87 K (red) and 298 K (blue), c) CO_2 at 195 K (black), 273 K (red) and 298 K (blue), and d) CH_4 at 195 K (black), 273 K (red), and 298 K (blue). Filled shapes: adsorption; open shapes: desorption

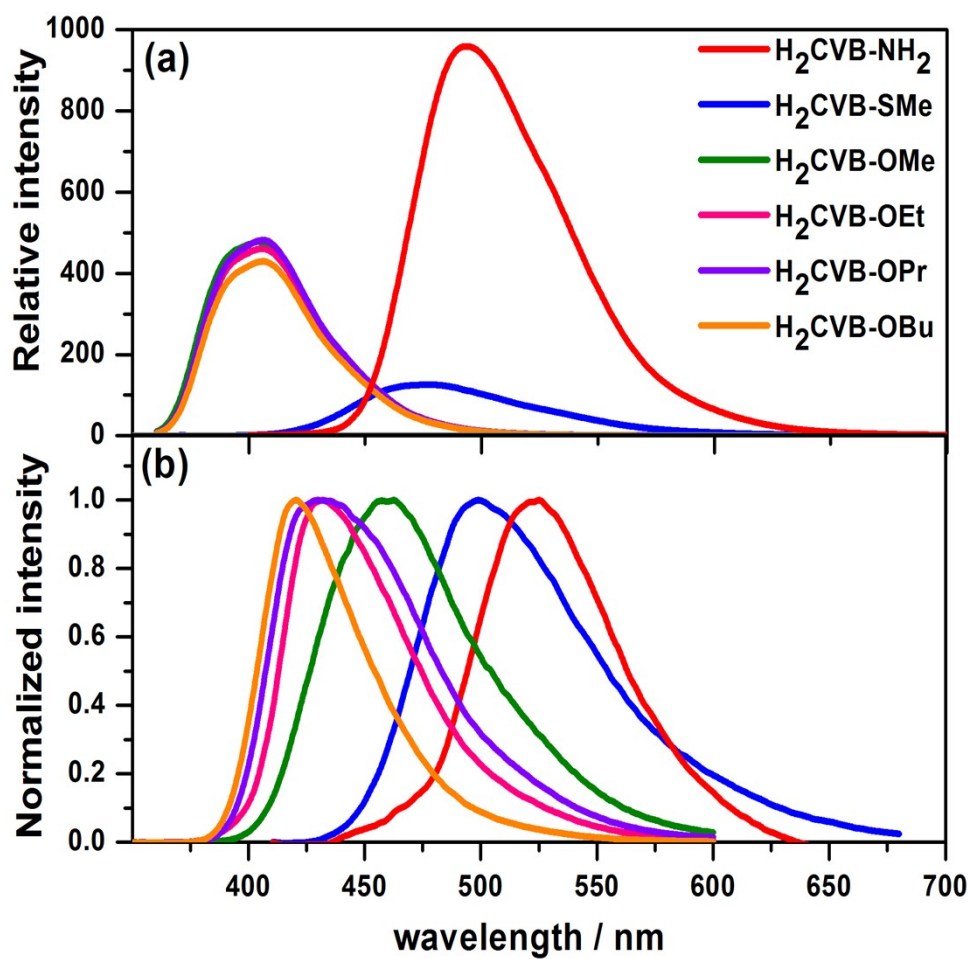


Fig. S12 Photoluminescence spectra of various ligands: (a) In the DMF solution (1×10^{-4} M), excitation at 395 nm for H₂CVB-NH₂, 362 nm for H₂CVB-SMe, and 350 nm for the rest of the samples. (b) Pure solid, excitation at 360 nm for H₂CVB-NH₂ and H₂CVB-SMe, and 320 nm for the rest of the samples.

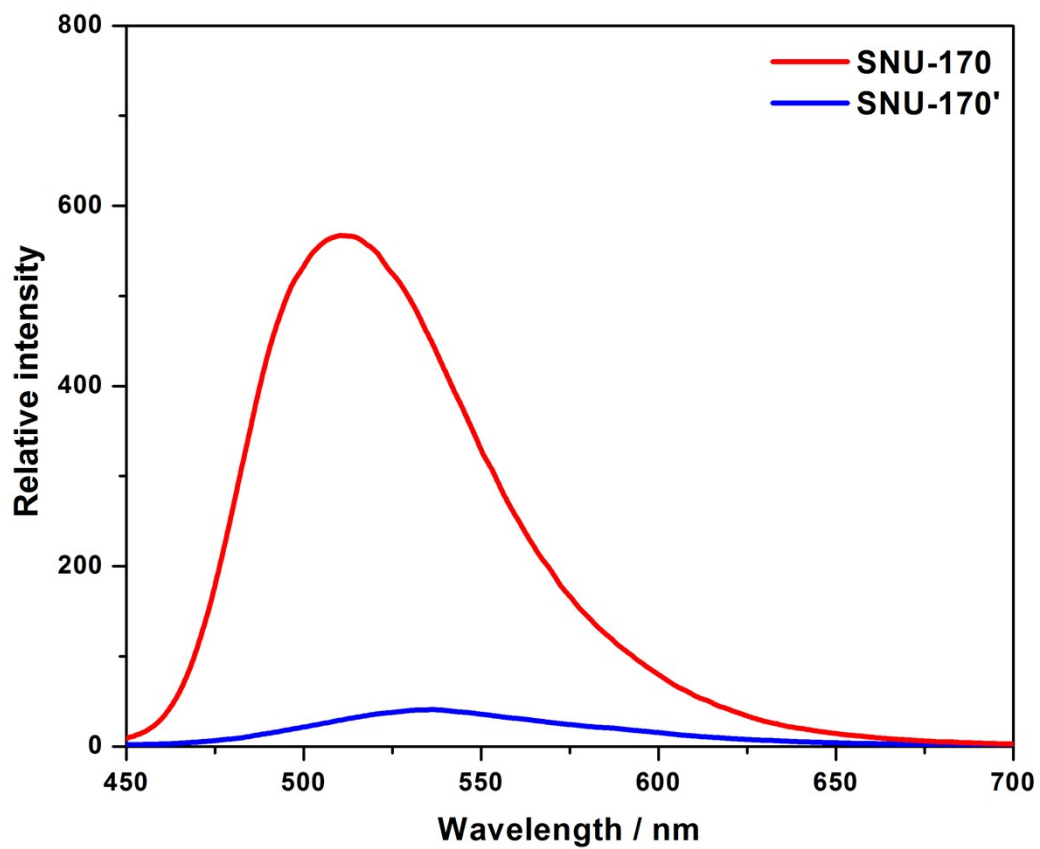


Fig. S13 Comparison of the photoluminescence intensities of as-synthesized (SNU-170, red) and activated (SNU-170', blue) MOFs.

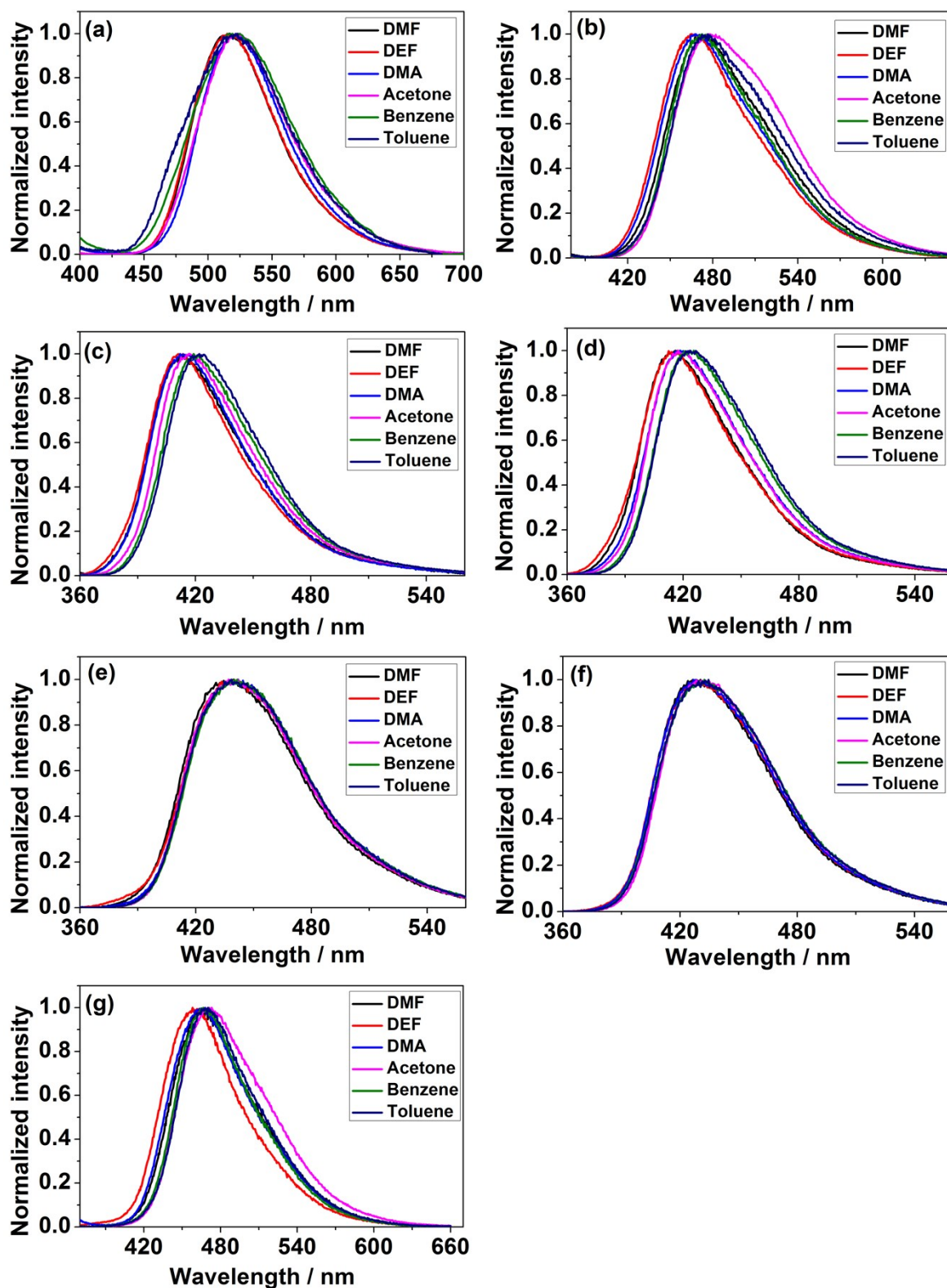


Fig. S14 Photoluminescence spectra changes of the activated MOFs on the addition of various solvents: (a) SNU-170', (b) SNU-171', (c) SNU-172', (d) SNU-173', (e) SNU-174', (f) SNU-175', and (g) SNU-176'.

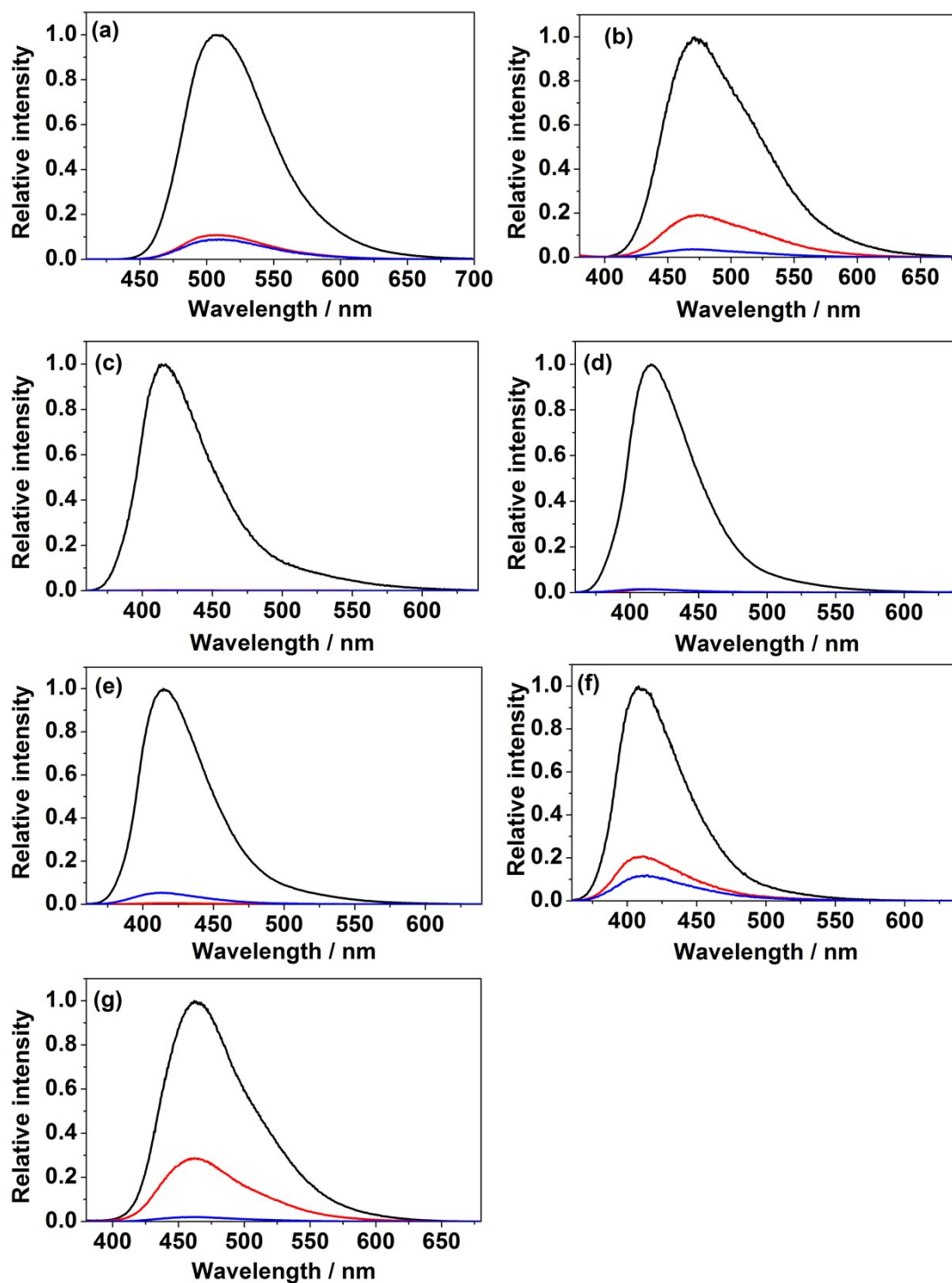


Fig. S15 Changes of photoluminescence spectra of as-synthesized MOFs on the addition of a drop of 0.5 M DMF solution of nitrobenzene (NB) and 2,4-dinitrotoluene (DNT). Black, MOF; Red, MOF + NB; Blue, MOF + DNT: (a) SNU-170, (b) SNU-171, (c) SNU-172, (d) SNU-173, (e) SNU-174, (f) SNU-175, and (g) SNU-176.

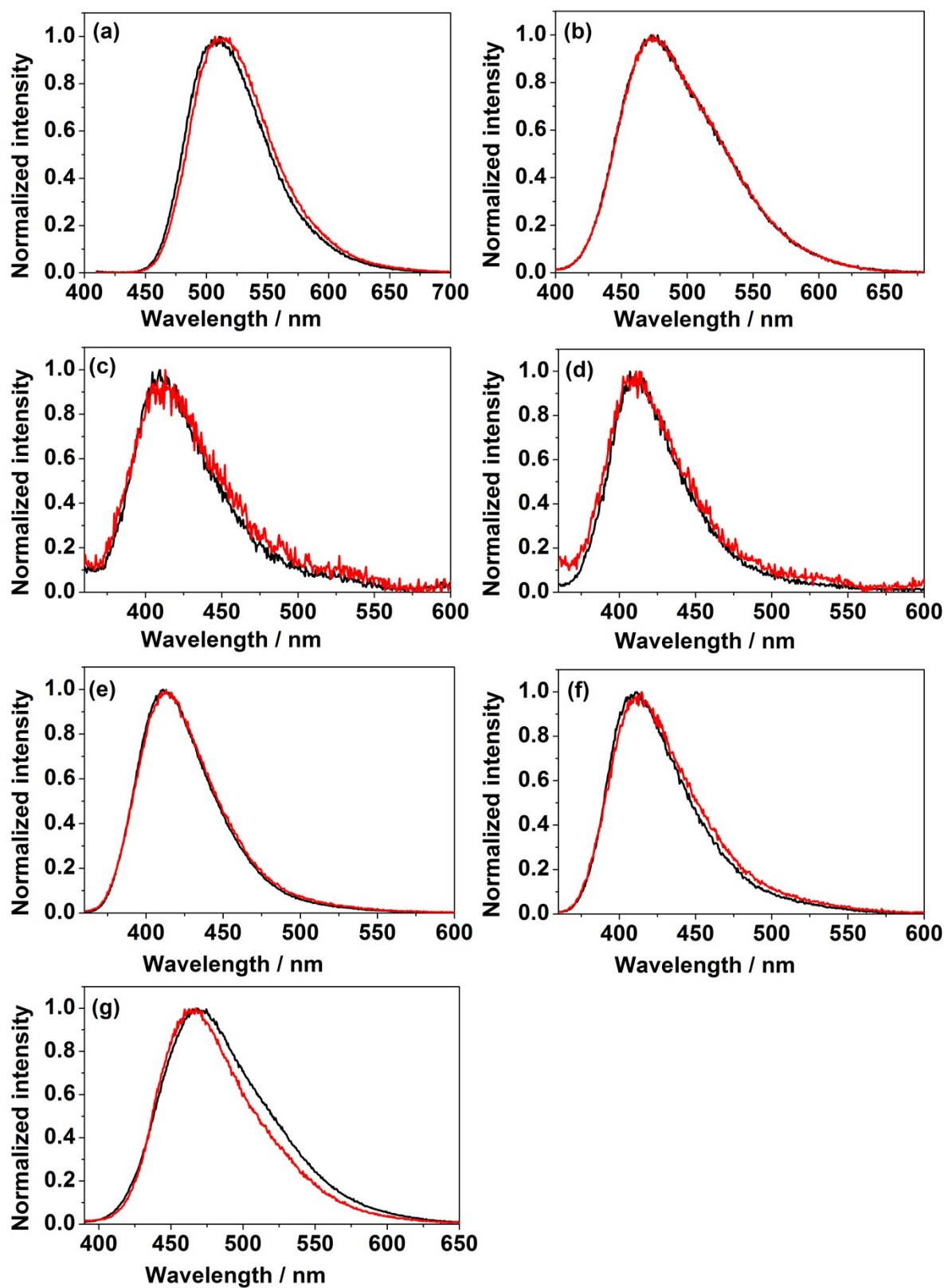


Fig. S16 Normalized luminescence spectra of as-synthesized MOFs after the addition of a drop of 0.5 M DMF solution of nitrobenzene (NB) and 2,4-dinitrotoluene (DNT). Black: MOF + NB, Red: MOF + DNT. (a) SNU-170, (b) SNU-171, (c) SNU-172, (d) SNU-173, (e) SNU-174, (f) SNU-175, and (g) SNU-176.

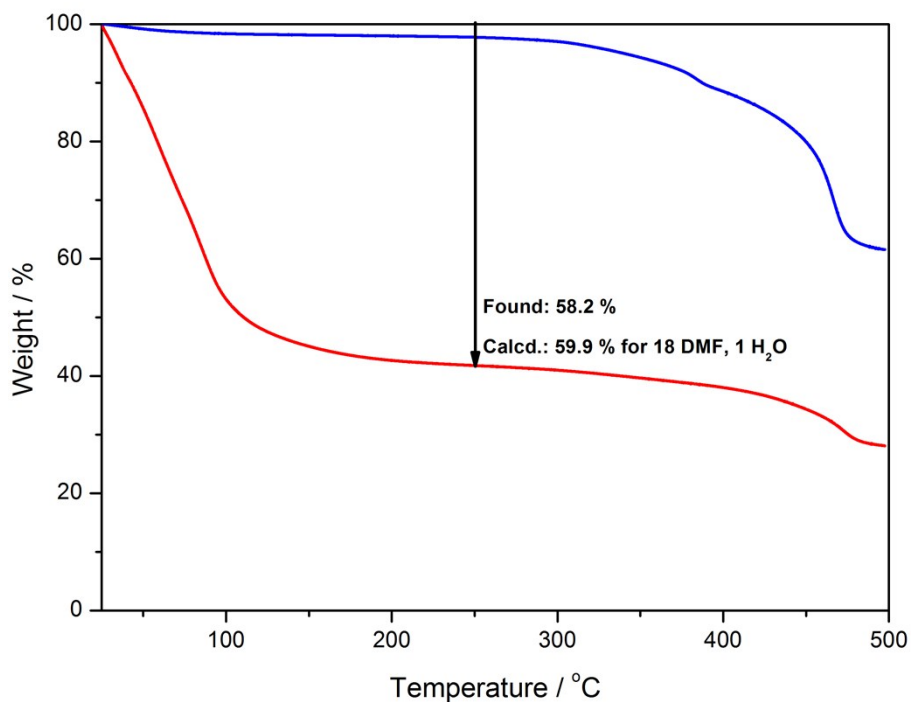


Fig. S17 TGA curves of $[\text{Zn}_4\text{O}(\text{CVB-NH}_2)_3] \cdot 18\text{DMF} \cdot \text{H}_2\text{O}$ (SNU-170, red) and its dried sample $[\text{Zn}_4\text{O}(\text{CVB-NH}_2)_3]$ (SNU-171', blue) obtained by treatment with supercritical CO_2 .

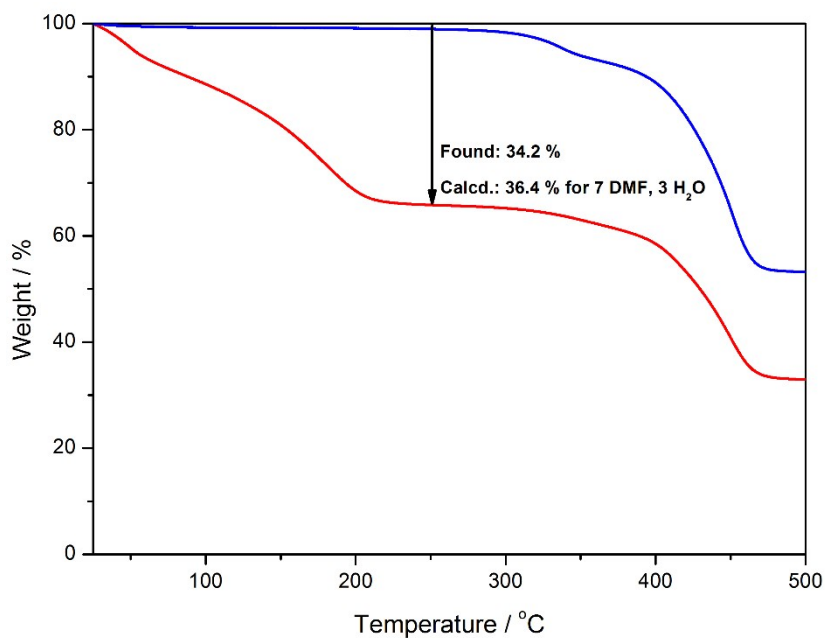


Fig. S18 TGA curves of $[\text{Zn}_4\text{O}(\text{CVB-SMe})_3] \cdot 7\text{DMF} \cdot 3\text{H}_2\text{O}$ (SNU-171, red) and its dried sample $[\text{Zn}_4\text{O}(\text{CVB-SMe})_3]$ (SNU-171', blue) obtained by treatment with supercritical CO_2 .

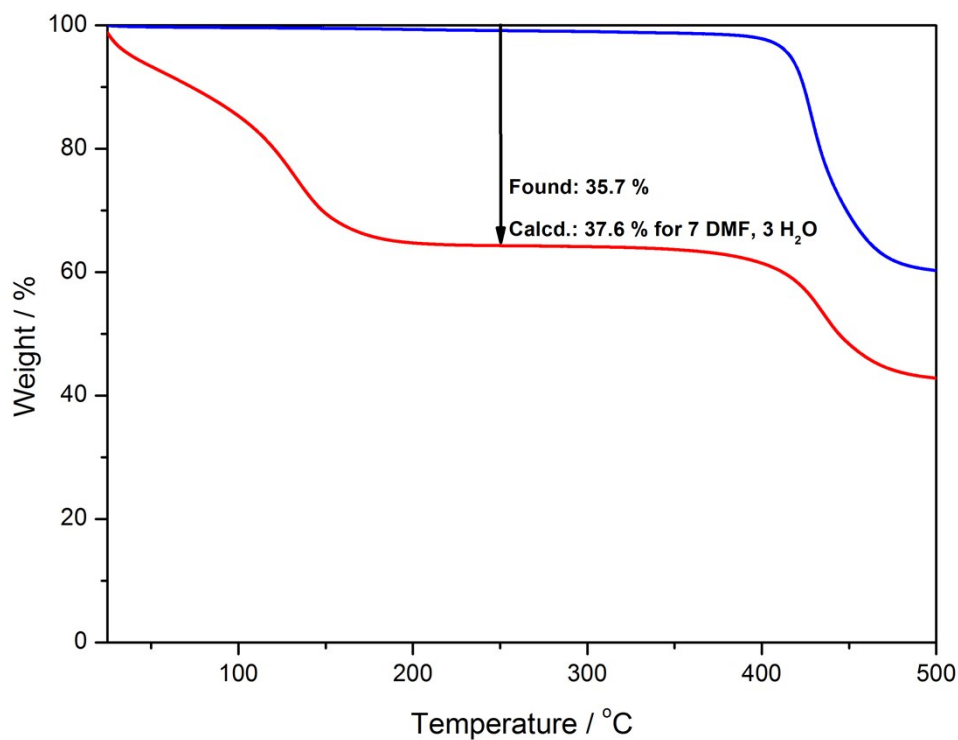


Fig. S19 TGA curves of $[\text{Zn}_4\text{O}(\text{CVB-OMe})_3] \cdot 7\text{DMF} \cdot 3 \text{H}_2\text{O}$ (SNU-172, red) and its dried sample $[\text{Zn}_4\text{O}(\text{CVB-OMe})_3]$ (SNU-172', blue) obtained by treatment with supercritical CO_2 .

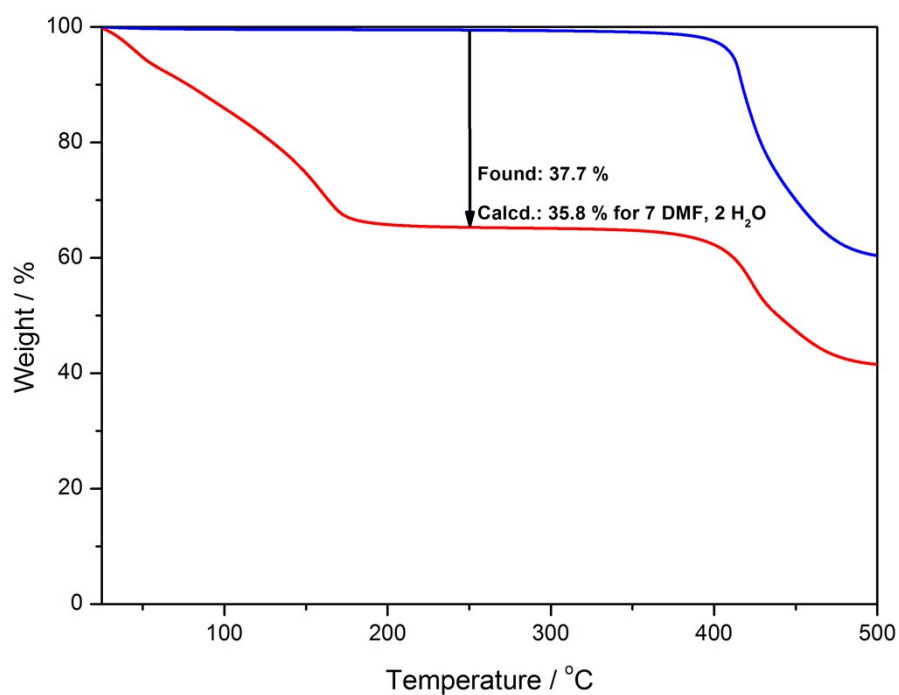


Fig. S20 TGA curves of $[\text{Zn}_4\text{O}(\text{CVB-OEt})_3] \cdot 7\text{DMF} \cdot 2\text{H}_2\text{O}$ (SNU-173, red) and its dried sample $[\text{Zn}_4\text{O}(\text{CVB-OEt})_3]$ (SNU-173', blue) obtained by treatment with supercritical CO_2 .

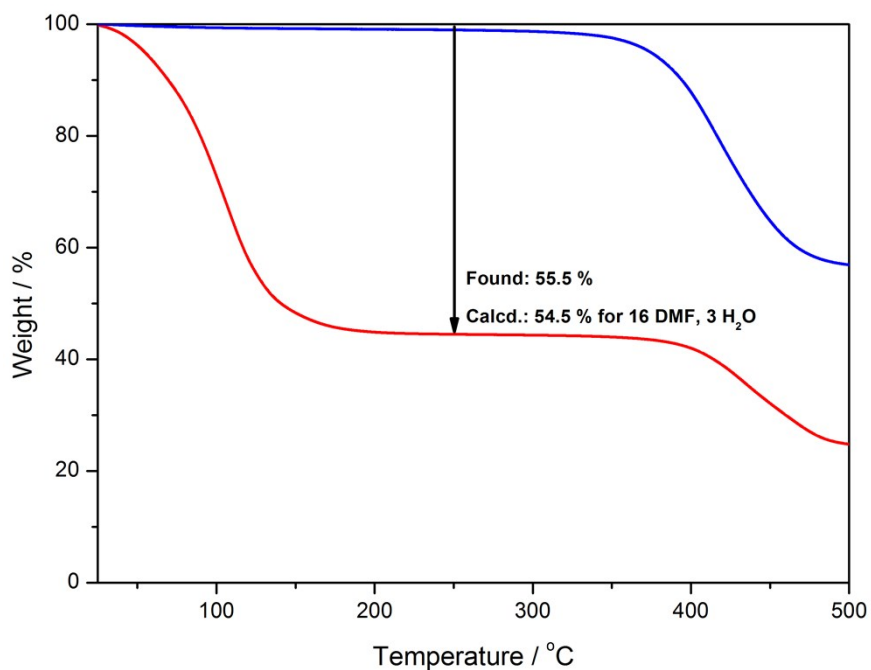


Fig. S21 TGA curves of $[\text{Zn}_4\text{O}(\text{CVB-OPr})_3] \cdot 16\text{DMF} \cdot 3\text{H}_2\text{O}$ (SNU-174, red) and its dried sample $[\text{Zn}_4\text{O}(\text{CVB-OPr})_3]$ (SNU-174', blue) obtained by treatment with supercritical CO_2 .

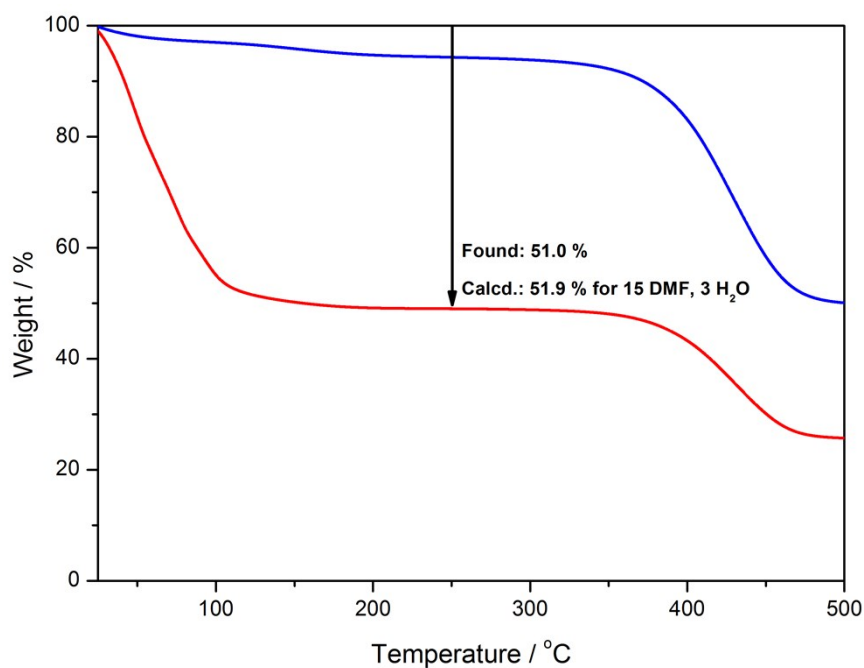


Fig. S22 TGA curves of $[\text{Zn}_4\text{O}(\text{CVB-OBu})_3] \cdot 15\text{DMF} \cdot 3\text{H}_2\text{O}$ (SNU-175, red) and its dried sample $[\text{Zn}_4\text{O}(\text{CVB-OBu})_3]$ (SNU-175', blue) obtained by treatment with supercritical CO_2 .

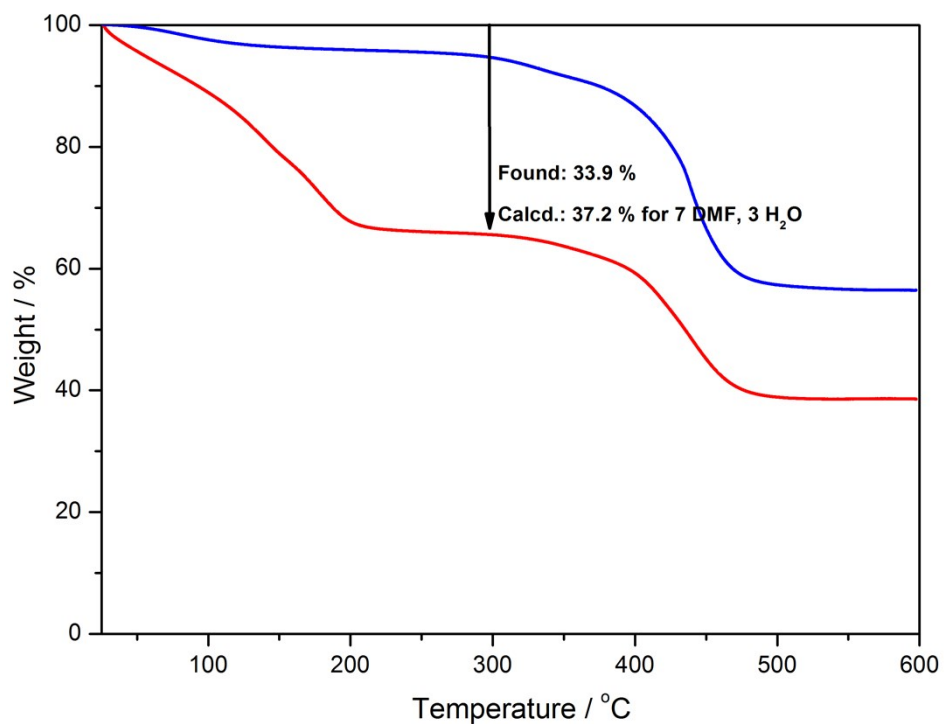


Fig. S23 TGA curves of $[\text{Zn}_4\text{O}(\text{CVB-SMe})_1(\text{CVB-OMe})_2]\cdot 7\text{DMF}\cdot 3\text{H}_2\text{O}$ (SNU-176, red) and its dried sample $[\text{Zn}_4\text{O}(\text{CVB-SMe})_1(\text{CVB-OMe})_2]$ (SNU-176', blue) obtained by treatment with supercritical CO_2 .

Table S1. Crystallographic data for **SNU-170 ~ SNU-174** (squeezed data)

| | SNU-170 | SNU-171 | SNU-172 | SNU-173 | SNU-174 |
|--|---|---|---|---|--|
| formula | C ₁₂₀ H ₈₄ N ₁₂ O ₅₂ Zn ₁₆ | C ₂₆₄ H ₁₉₂ O ₁₀₄ S ₂₄ Zn ₃₂ | C ₂₆₄ H ₁₉₂ O ₁₀₄ Zn ₃₂ | C ₂₈₈ H ₂₄₀ O ₁₀₄ Zn ₃₂ | C ₁₅₆ H ₁₄₄ O ₆₄ Zn ₁₆ |
| F.W. | 3571.91 | 7889.44 | 7120.00 | 7456.63 | 4088.62 |
| crystal system | cubic | cubic | cubic | cubic | cubic |
| space group | <i>Fm-3m</i> | <i>Fd-3m</i> | <i>Fd-3m</i> | <i>Fd-3</i> | <i>Fm-3m</i> |
| λ (Å) | 0.70000 | 0.69998 | 0.69999 | 0.70000 | 0.70000 |
| a (Å) | 30.197(10) | 29.970(10) | 30.089(3) | 30.222(10) | 30.206(10) |
| V (Å ³) | 27535(27) | 26919(27) | 27241(8) | 27604(27) | 27560(27) |
| Z | 2 | 2 | 2 | 2 | 2 |
| D_{calcd} (g cm ⁻³) | 0.431 | 0.973 | 0.868 | 0.897 | 0.493 |
| T (K) | 293 | 293 | 293 | 293 | 293 |
| GOF (F^2) | 1.344 | 1.429 | 1.174 | 1.435 | 1.229 |
| R_I [$I > 2\sigma(I)$] ^a | 0.0988 | 0.1334 | 0.1156 | 0.1054 | 0.0927 |
| wR_2 [$I > 2\sigma(I)$] ^b | 0.3146 | 0.3691 | 0.3886 | 0.3617 | 0.2909 |

^a $R_1 = \sum(|F_o| - |F_c|) / \sum|F_o|$; ^b $wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (AP)^2 + (BP)]$, $P = (F_o^2 + 2F_c^2)/3$; A = 0.2000, B = 0.0000 for **SNU-170**; A = 0.2000, B = 0.0000 for **SNU-171**; A = 0.2000, B = 0.0000 for **SNU-172**; A = 0.2000, B = 0.0000 for **SNU-173**; A = 0.2000, B = 0.0000 for **SNU-174**.

Table S2. CO₂ separation parameters for vacuum swing adsorption (VSA) process ^a

| Sample | Gas mixtures | N_I^{ads} (mol kg ⁻¹) | ΔN_I (mol kg ⁻¹) | R (%) | α_{12}^{ads} | S |
|-----------------|--|-------------------------------------|--------------------------------------|---------|---------------------|------|
| SNU-170' | CO ₂ :CH ₄ (1:1) | 0.465 | 0.427 | 91.8 | 4.00 | 7.00 |
| | CO ₂ :N ₂ (1:9) | 0.082 | 0.075 | 92.2 | 7.73 | 7.06 |
| SNU-171' | CO ₂ :CH ₄ (1:1) | 1.042 | 0.934 | 89.6 | 2.86 | 14.0 |
| | CO ₂ :N ₂ (1:9) | 0.216 | 0.195 | 89.9 | 13.97 | 20.9 |
| SNU-172' | CO ₂ :CH ₄ (1:1) | 1.104 | 0.985 | 89.2 | 4.35 | 16.6 |
| | CO ₂ :N ₂ (1:9) | 0.235 | 0.211 | 89.7 | 14.9 | 22.6 |
| SNU-173' | CO ₂ :CH ₄ (1:1) | 1.271 | 1.133 | 89.1 | 4.69 | 15.0 |
| | CO ₂ :N ₂ (1:9) | 0.274 | 0.248 | 90.1 | 17.09 | 13.2 |
| SNU-174' | CO ₂ :CH ₄ (1:1) | 0.335 | 0.300 | 89.5 | 4.50 | 6.8 |
| | CO ₂ :N ₂ (1:9) | 0.070 | 0.063 | 90.1 | - | - |
| SNU-176' | CO ₂ :CH ₄ (1:1) | 1.102 | 0.989 | 89.8 | 4.32 | 14.8 |
| | CO ₂ :N ₂ (1:9) | 0.225 | 0.205 | 90.1 | 15.34 | 25.0 |

^a Adsorption at 1 bar, Desorption at 0.1 bar.

Table S3. The photoluminescence spectra (λ_{max} , nm) of the activated MOFs on the addition of various solvents ^a

| | none | DMF | DEF | DMA | Acetone | Benzene | Toluene |
|-----------------|------|-----|-----|-----|---------|---------|---------|
| SNU-170' | 536 | 517 | 515 | 523 | 525 | 519 | 522 |
| SNU-171' | 482 | 473 | 468 | 468 | 478 | 473 | 477 |
| SNU-172' | 442 | 414 | 414 | 412 | 417 | 419 | 422 |
| SNU-173' | 440 | 416 | 417 | 419 | 418 | 426 | 424 |
| SNU-174' | 442 | 440 | 442 | 442 | 437 | 440 | 439 |
| SNU-175' | 440 | 427 | 427 | 428 | 433 | 433 | 435 |
| SNU-176' | 470 | 467 | 458 | 468 | 473 | 467 | 470 |

^a A few drops of solvents were added to the activated MOFs. Measured at room temperature.

Table S4. N₂ adsorption data of SNU-170', SNU-171', SNU-172' and SNU-173' at 77 K.

| SNU-170' | | SNU-171' | | SNU-172' | | SNU-173' | |
|----------|---|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 9.91E-05 | 47.0311 | 8.66E-05 | 171.9842 | 1.75E-05 | 82.1943 | 3.66E-05 | 124.9302 |
| 1.99E-04 | 74.7807 | 1.79E-04 | 215.6568 | 1.18E-04 | 211.718 | 1.20E-04 | 197.6302 |
| 3.06E-04 | 94.5341 | 2.80E-04 | 243.2024 | 2.18E-04 | 242.882 | 2.28E-04 | 228.7104 |
| 4.04E-04 | 108.4955 | 3.82E-04 | 261.9872 | 3.23E-04 | 265.2492 | 3.23E-04 | 244.5093 |
| 5.13E-04 | 121.582 | 4.83E-04 | 275.5355 | 4.29E-04 | 278.2017 | 4.24E-04 | 255.7349 |
| 6.01E-04 | 130.5536 | 5.84E-04 | 285.1517 | 6.07E-04 | 292.1352 | 5.98E-04 | 268.1802 |
| 7.04E-04 | 139.8179 | 6.85E-04 | 293.7318 | 7.15E-04 | 298.0606 | 7.15E-04 | 274.2604 |
| 8.12E-04 | 148.5998 | 7.86E-04 | 300.0394 | 8.02E-04 | 302.0418 | 7.94E-04 | 277.6163 |
| 9.15E-04 | 156.3689 | 8.88E-04 | 305.2063 | 9.09E-04 | 306.0811 | 9.42E-04 | 282.8511 |
| 1.03E-03 | 164.0691 | 9.96E-04 | 310.2336 | 1.02E-03 | 309.5943 | 1.02E-03 | 285.3744 |
| 2.03E-03 | 221.7157 | 2.01E-03 | 332.4378 | 2.06E-03 | 328.8336 | 2.08E-03 | 304.2663 |
| 3.05E-03 | 268.8091 | 3.01E-03 | 342.2072 | 3.00E-03 | 337.5705 | 3.00E-03 | 312.7791 |
| 4.03E-03 | 307.9705 | 4.02E-03 | 348.2296 | 4.02E-03 | 343.6697 | 4.02E-03 | 319.1465 |
| 5.04E-03 | 343.2114 | 5.02E-03 | 352.4864 | 5.01E-03 | 347.9435 | 5.05E-03 | 323.843 |
| 7.46E-03 | 412.7773 | 6.04E-03 | 355.8298 | 7.02E-03 | 353.9934 | 6.78E-03 | 329.5965 |
| 7.41E-03 | 412.5682 | 7.04E-03 | 358.5073 | 7.02E-03 | 353.9992 | 7.66E-03 | 331.9256 |
| 8.70E-03 | 442.3341 | 8.10E-03 | 360.8586 | 8.60E-03 | 357.3828 | 8.34E-03 | 333.507 |
| 9.39E-03 | 457.7954 | 9.09E-03 | 362.7078 | 9.24E-03 | 358.5606 | 9.45E-03 | 335.8232 |
| 9.32E-03 | 459.6318 | 1.01E-02 | 364.2915 | 9.73E-03 | 359.3394 | 1.01E-02 | 336.8779 |
| 1.26E-02 | 526.8432 | 2.00E-02 | 374.0215 | 2.06E-02 | 370.6516 | 1.75E-02 | 346.4453 |
| 2.06E-02 | 705.1136 | 2.96E-02 | 379.4614 | 2.77E-02 | 374.768 | 3.18E-02 | 356.0023 |
| 2.90E-02 | 847.9409 | 4.05E-02 | 383.7227 | 3.80E-02 | 379.0311 | 4.04E-02 | 359.7884 |
| 4.10E-02 | 928.0523 | 5.23E-02 | 387.1162 | 4.62E-02 | 381.723 | 5.07E-02 | 363.2395 |
| 5.38E-02 | 957.1841 | 6.09E-02 | 389.1702 | 5.69E-02 | 384.3025 | 5.70E-02 | 365.0163 |
| 6.15E-02 | 967.7363 | 7.10E-02 | 391.209 | 7.04E-02 | 386.8795 | 7.09E-02 | 368.2361 |
| 7.19E-02 | 978.0909 | 8.13E-02 | 392.9915 | 7.71E-02 | 387.9557 | 8.07E-02 | 370.1454 |
| 8.32E-02 | 987.0023 | 8.94E-02 | 394.2643 | 8.62E-02 | 389.2672 | 9.09E-02 | 371.8453 |
| 1.01E-01 | 998.2523 | 1.06E-01 | 396.4699 | 1.02E-01 | 391.2541 | 1.05E-01 | 373.9325 |
| 1.32E-01 | 1012.4454 | 1.49E-01 | 401.0316 | 1.53E-01 | 396.2746 | 1.56E-01 | 379.5744 |
| 1.79E-01 | 1027.4501 | 2.00E-01 | 405.138 | 2.05E-01 | 399.9819 | 1.99E-01 | 383.0686 |
| 2.49E-01 | 1042.3182 | 2.51E-01 | 408.7576 | 2.50E-01 | 402.3574 | 2.50E-01 | 386.3651 |
| 3.04E-01 | 1051.6091 | 3.04E-01 | 411.7248 | 2.99E-01 | 404.8803 | 3.02E-01 | 388.9791 |
| 3.48E-01 | 1057.8068 | 3.55E-01 | 414.3022 | 3.51E-01 | 407.0369 | 3.54E-01 | 391.2709 |
| 3.98E-01 | 1064.175 | 4.06E-01 | 416.6383 | 4.02E-01 | 408.8918 | 4.04E-01 | 393.2186 |
| 4.51E-01 | 1069.3932 | 4.56E-01 | 418.7985 | 4.54E-01 | 410.5016 | 4.56E-01 | 394.8942 |
| 5.01E-01 | 1074.3613 | 5.06E-01 | 420.8374 | 5.04E-01 | 412.1008 | 5.06E-01 | 396.4628 |
| 5.53E-01 | 1078.7318 | 5.57E-01 | 422.7594 | 5.55E-01 | 413.5402 | 5.57E-01 | 397.7907 |
| 6.03E-01 | 1082.8114 | 6.07E-01 | 424.6056 | 6.05E-01 | 414.923 | 6.07E-01 | 399.1116 |
| 6.54E-01 | 1086.5409 | 6.57E-01 | 426.3895 | 6.56E-01 | 416.1024 | 6.58E-01 | 400.2419 |
| 7.05E-01 | 1089.8182 | 7.08E-01 | 428.1083 | 7.06E-01 | 417.2369 | 7.07E-01 | 401.3244 |
| 7.55E-01 | 1092.9319 | 7.58E-01 | 429.8013 | 7.56E-01 | 418.3737 | 7.58E-01 | 402.3791 |
| 8.02E-01 | 1097.0205 | 8.08E-01 | 431.4563 | 8.07E-01 | 419.4828 | 8.08E-01 | 403.2895 |
| 8.55E-01 | 1100.2181 | 8.58E-01 | 433.1068 | 8.56E-01 | 420.5131 | 8.58E-01 | 404.3767 |
| 9.06E-01 | 1102.9773 | 9.04E-01 | 435.4429 | 9.07E-01 | 421.5533 | 9.08E-01 | 404.9837 |

Table S5. N₂ adsorption data of SNU-174', SNU-175' and SNU-176' at 77 K.

| SNU-174' | | SNU-175' | | SNU-176' | |
|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 8.66E-05 | 17.0289 | 9.60E-05 | 1.6617 | 1.00E-04 | 205.3386 |
| 1.86E-04 | 22.8088 | 2.09E-04 | 1.8787 | 1.94E-04 | 252.3943 |
| 2.88E-04 | 26.6626 | 3.27E-04 | 1.9311 | 2.97E-04 | 279.6057 |
| 3.90E-04 | 29.6033 | 4.12E-04 | 1.9453 | 4.11E-04 | 299.94 |
| 4.91E-04 | 32.0953 | 5.27E-04 | 1.9541 | 4.98E-04 | 311.0529 |
| 5.92E-04 | 34.3031 | 6.21E-04 | 1.9588 | 6.06E-04 | 321.6514 |
| 6.92E-04 | 36.2252 | 7.32E-04 | 1.9626 | 7.01E-04 | 328.8214 |
| 7.94E-04 | 37.9542 | 8.29E-04 | 1.9652 | 8.10E-04 | 335.6 |
| 8.94E-04 | 39.7491 | 9.23E-04 | 1.9672 | 9.27E-04 | 341.3828 |
| 9.95E-04 | 41.792 | 1.01E-03 | 1.972 | 1.00E-03 | 344.7314 |
| 2.00E-03 | 54.3438 | 2.12E-03 | 1.9922 | 2.06E-03 | 369.0614 |
| 3.00E-03 | 63.2632 | 3.18E-03 | 2.0129 | 3.00E-03 | 379.0186 |
| 4.00E-03 | 70.1323 | 4.23E-03 | 2.0323 | 4.08E-03 | 386.0043 |
| 5.00E-03 | 75.6538 | 5.28E-03 | 2.0513 | 5.02E-03 | 390.2943 |
| 6.02E-03 | 80.401 | 6.33E-03 | 2.0707 | 7.06E-03 | 396.8128 |
| 7.03E-03 | 84.3986 | 7.37E-03 | 2.0884 | 7.06E-03 | 396.8414 |
| 8.02E-03 | 87.7705 | 8.42E-03 | 2.1181 | 8.61E-03 | 400.37 |
| 9.01E-03 | 90.8667 | 9.47E-03 | 2.1409 | 9.27E-03 | 401.6571 |
| 1.00E-02 | 93.6374 | 1.05E-02 | 2.1648 | 1.02E-02 | 402.6757 |
| 1.91E-02 | 107.4798 | 2.12E-02 | 2.6631 | 1.66E-02 | 410.9485 |
| 2.93E-02 | 118.547 | 3.26E-02 | 2.9256 | 2.48E-02 | 417.2614 |
| 4.23E-02 | 124.5879 | 4.27E-02 | 3.0827 | 3.60E-02 | 422.9214 |
| 5.44E-02 | 127.4609 | 5.28E-02 | 3.1892 | 4.74E-02 | 427.1014 |
| 6.01E-02 | 128.6133 | 6.29E-02 | 3.2801 | 5.55E-02 | 429.4371 |
| 6.95E-02 | 130.019 | 7.29E-02 | 3.3666 | 6.53E-02 | 431.7928 |
| 7.99E-02 | 131.3354 | 8.27E-02 | 3.5438 | 7.61E-02 | 433.9014 |
| 9.03E-02 | 132.4697 | 9.29E-02 | 3.6256 | 9.06E-02 | 436.25 |
| 1.08E-01 | 134.0628 | 1.12E-01 | 3.7938 | 1.05E-01 | 438.4586 |
| 1.55E-01 | 137.1626 | 1.61E-01 | 4.1936 | 1.56E-01 | 444.3986 |
| 2.06E-01 | 139.8839 | 2.12E-01 | 4.6074 | 2.00E-01 | 448.3786 |
| 2.57E-01 | 142.3088 | 2.61E-01 | 5.0818 | 2.51E-01 | 452.05 |
| 3.07E-01 | 144.4787 | 3.11E-01 | 5.5457 | 3.02E-01 | 455.2885 |
| 3.56E-01 | 146.9241 | 3.61E-01 | 6.0552 | 3.54E-01 | 458.1229 |
| 4.08E-01 | 148.9554 | 4.11E-01 | 6.5848 | 4.05E-01 | 460.6386 |
| 4.58E-01 | 150.8744 | 4.61E-01 | 7.1404 | 4.56E-01 | 462.8614 |
| 5.08E-01 | 152.7395 | 5.11E-01 | 7.699 | 5.06E-01 | 465.0128 |
| 5.58E-01 | 154.5748 | 5.62E-01 | 8.2023 | 5.56E-01 | 467.0057 |
| 6.09E-01 | 156.3697 | 6.10E-01 | 9.5607 | 6.06E-01 | 468.9543 |
| 6.59E-01 | 158.1679 | 6.61E-01 | 10.334 | 6.57E-01 | 470.6943 |
| 7.09E-01 | 159.9405 | 7.11E-01 | 11.0033 | 7.07E-01 | 472.3871 |
| 7.59E-01 | 161.7051 | 7.61E-01 | 11.7465 | 7.57E-01 | 474.0114 |
| 8.09E-01 | 163.5327 | 8.11E-01 | 12.5533 | 8.07E-01 | 475.6386 |
| 8.59E-01 | 165.3335 | 8.62E-01 | 13.1973 | 8.57E-01 | 477.1871 |
| 9.09E-01 | 167.2337 | 9.11E-01 | 14.1541 | 9.08E-01 | 478.6314 |

Table S6. N₂ adsorption data of SNU-170', SNU-171', SNU-172' and SNU-173' at 298 K.

| SNU-170' | | SNU-171' | | SNU-172' | | SNU-173' | |
|----------|---|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 3.30E-02 | 0.0011 | 2.28E-02 | 0.0075 | 4.08E-03 | 0.0002 | 7.29E-02 | 0.0052 |
| 4.30E-02 | 0.0255 | 3.29E-02 | 0.0508 | 5.06E-03 | 0.0033 | 8.30E-02 | 0.0432 |
| 5.30E-02 | 0.0513 | 4.27E-02 | 0.0852 | 6.11E-03 | 0.0068 | 9.29E-02 | 0.0789 |
| 6.30E-02 | 0.0809 | 5.29E-02 | 0.1284 | 7.11E-03 | 0.0102 | 1.12E-01 | 0.1424 |
| 7.29E-02 | 0.1152 | 6.28E-02 | 0.1719 | 9.38E-03 | 0.0186 | 1.61E-01 | 0.3178 |
| 8.29E-02 | 0.144 | 7.26E-02 | 0.2304 | 1.00E-02 | 0.0207 | 2.11E-01 | 0.5152 |
| 9.29E-02 | 0.1737 | 8.28E-02 | 0.2641 | 1.33E-02 | 0.0217 | 2.62E-01 | 0.7014 |
| 1.12E-01 | 0.2138 | 9.29E-02 | 0.3134 | 2.24E-02 | 0.0522 | 3.11E-01 | 0.8796 |
| 1.62E-01 | 0.3487 | 1.12E-01 | 0.3848 | 3.30E-02 | 0.0871 | 3.61E-01 | 1.0797 |
| 2.11E-01 | 0.5023 | 1.61E-01 | 0.5786 | 4.29E-02 | 0.1203 | 4.11E-01 | 1.2759 |
| 2.62E-01 | 0.6251 | 2.11E-01 | 0.8171 | 5.29E-02 | 0.1587 | 4.62E-01 | 1.458 |
| 3.12E-01 | 0.7663 | 2.61E-01 | 0.9536 | 6.29E-02 | 0.1952 | 5.11E-01 | 1.6554 |
| 3.62E-01 | 0.8801 | 3.11E-01 | 1.1426 | 7.29E-02 | 0.2361 | 5.61E-01 | 1.8601 |
| 4.11E-01 | 1.0152 | 3.62E-01 | 1.3735 | 8.28E-02 | 0.2759 | 6.11E-01 | 2.0655 |
| 4.62E-01 | 1.1169 | 4.11E-01 | 1.5507 | 9.26E-02 | 0.3169 | 6.61E-01 | 2.252 |
| 5.11E-01 | 1.2403 | 4.61E-01 | 1.6533 | 1.12E-01 | 0.3876 | 7.11E-01 | 2.4535 |
| 5.62E-01 | 1.3437 | 5.11E-01 | 1.8813 | 1.61E-01 | 0.5681 | 7.61E-01 | 2.6652 |
| 6.12E-01 | 1.4722 | 5.61E-01 | 1.9728 | 2.11E-01 | 0.7661 | 8.11E-01 | 2.8787 |
| 6.61E-01 | 1.5697 | 6.11E-01 | 2.1871 | 2.61E-01 | 0.9387 | 8.62E-01 | 3.0583 |
| 7.11E-01 | 1.7132 | 6.61E-01 | 2.3013 | 3.11E-01 | 1.1216 | 9.11E-01 | 3.2815 |
| 7.62E-01 | 1.8175 | 7.11E-01 | 2.5233 | 3.61E-01 | 1.2897 | 9.61E-01 | 3.4979 |
| 8.11E-01 | 1.9016 | 7.61E-01 | 2.6529 | 4.11E-01 | 1.4707 | 9.99E-01 | 3.6719 |
| 8.61E-01 | 2.0094 | 8.11E-01 | 2.8253 | 4.61E-01 | 1.6332 | | |
| 9.11E-01 | 2.139 | 8.62E-01 | 3.0401 | 5.11E-01 | 1.8168 | | |
| 9.61E-01 | 2.2821 | 9.11E-01 | 3.1335 | 5.61E-01 | 1.9835 | | |
| 9.99E-01 | 2.4144 | 9.61E-01 | 3.3689 | 6.11E-01 | 2.1748 | | |
| | | 9.99E-01 | 3.4261 | 6.61E-01 | 2.3394 | | |
| | | | | 7.11E-01 | 2.5237 | | |
| | | | | 7.61E-01 | 2.6968 | | |
| | | | | 8.10E-01 | 2.879 | | |
| | | | | 8.61E-01 | 3.0514 | | |
| | | | | 9.10E-01 | 3.2204 | | |
| | | | | 9.61E-01 | 3.4014 | | |
| | | | | 9.99E-01 | 3.5502 | | |

Table S7. N₂ adsorption data of SNU-174', SNU-175' and SNU-176' at 298 K.

| SNU-174' | | SNU-175' | | SNU-176' | |
|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 5.62E-01 | 0.018 | Nil | Nil | 3.31E-02 | 0.0269 |
| 6.12E-01 | 0.0779 | | | 4.31E-02 | 0.0611 |
| 6.62E-01 | 0.1253 | | | 5.31E-02 | 0.0992 |
| 7.12E-01 | 0.1927 | | | 6.30E-02 | 0.139 |
| 7.62E-01 | 0.2524 | | | 7.29E-02 | 0.1858 |
| 8.12E-01 | 0.3412 | | | 8.27E-02 | 0.2318 |
| 8.62E-01 | 0.4042 | | | 9.28E-02 | 0.2805 |
| 9.12E-01 | 0.4972 | | | 1.12E-01 | 0.358 |
| 9.62E-01 | 0.5784 | | | 1.61E-01 | 0.5371 |
| 9.99E-01 | 0.6359 | | | 2.11E-01 | 0.7449 |
| | | | | 2.61E-01 | 0.9054 |
| | | | | 3.11E-01 | 1.1029 |
| | | | | 3.61E-01 | 1.2479 |
| | | | | 4.11E-01 | 1.4421 |
| | | | | 4.61E-01 | 1.5524 |
| | | | | 5.11E-01 | 1.7099 |
| | | | | 5.61E-01 | 1.8763 |
| | | | | 6.11E-01 | 2.0132 |
| | | | | 6.61E-01 | 2.1408 |
| | | | | 7.11E-01 | 2.3474 |
| | | | | 7.61E-01 | 2.4608 |
| | | | | 8.11E-01 | 2.6712 |
| | | | | 8.61E-01 | 2.8492 |
| | | | | 9.11E-01 | 2.9597 |
| | | | | 9.61E-01 | 3.1163 |
| | | | | 9.99E-01 | 3.3782 |

Table S8. H₂ adsorption data of SNU-170', SNU-171', SNU-172' and SNU-173' at 77 K.

| SNU-170' | | SNU-171' | | SNU-172' | | SNU-173' | |
|----------|---|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 2.27E-04 | 0.8189 | 9.68E-05 | 0.1239 | 2.03E-04 | 0.2844 | 2.23E-04 | 0.8111 |
| 2.27E-04 | 0.8181 | 3.34E-04 | 0.5259 | 2.05E-04 | 0.288 | 2.23E-04 | 0.812 |
| 2.93E-04 | 0.8382 | 3.34E-04 | 0.5259 | 4.43E-04 | 0.6709 | 4.40E-04 | 1.6452 |
| 4.39E-04 | 0.8792 | 4.03E-04 | 0.6332 | 4.41E-04 | 0.6693 | 4.38E-04 | 1.6421 |
| 5.06E-04 | 0.8971 | 4.95E-04 | 0.7782 | 6.71E-04 | 1.0245 | 6.66E-04 | 2.4423 |
| 6.38E-04 | 0.931 | 5.94E-04 | 0.9328 | 6.67E-04 | 1.0199 | 6.63E-04 | 2.4334 |
| 7.07E-04 | 0.9485 | 6.95E-04 | 1.0861 | 8.80E-04 | 1.3412 | 8.93E-04 | 3.1731 |
| 8.38E-04 | 0.9816 | 7.96E-04 | 1.2383 | 8.76E-04 | 1.3359 | 8.88E-04 | 3.1583 |
| 8.99E-04 | 0.9963 | 8.98E-04 | 1.388 | 8.95E-04 | 1.3627 | 8.97E-04 | 3.1829 |
| 1.05E-03 | 1.0342 | 1.00E-03 | 1.5357 | 1.15E-03 | 1.7446 | 1.18E-03 | 4.0228 |
| 2.07E-03 | 1.3183 | 2.49E-03 | 3.4764 | 2.21E-03 | 3.2145 | 2.16E-03 | 6.5159 |
| 3.11E-03 | 1.6012 | 3.58E-03 | 4.7468 | 3.07E-03 | 4.3368 | 3.26E-03 | 8.7473 |
| 4.00E-03 | 1.8437 | 4.57E-03 | 5.8439 | 4.04E-03 | 5.5274 | 4.08E-03 | 10.2032 |
| 5.03E-03 | 2.1207 | 5.56E-03 | 6.8947 | 5.08E-03 | 6.7481 | 5.14E-03 | 11.8501 |
| 6.18E-03 | 2.4276 | 6.54E-03 | 7.8765 | 6.38E-03 | 8.1815 | 6.22E-03 | 13.3686 |
| 7.11E-03 | 2.6831 | 7.62E-03 | 8.9263 | 7.24E-03 | 9.0892 | 7.22E-03 | 14.637 |
| 8.49E-03 | 3.051 | 8.24E-03 | 9.5107 | 8.24E-03 | 10.1189 | 8.50E-03 | 16.164 |
| 9.29E-03 | 3.2609 | 9.35E-03 | 10.5337 | 9.11E-03 | 10.9741 | 9.16E-03 | 16.9081 |
| 1.18E-02 | 3.9268 | 1.09E-02 | 11.5063 | 1.01E-02 | 11.4315 | 1.06E-02 | 17.7563 |
| 1.96E-02 | 6.049 | 2.05E-02 | 19.0228 | 2.00E-02 | 19.6837 | 2.03E-02 | 26.3666 |
| 2.93E-02 | 8.5553 | 3.06E-02 | 25.8887 | 3.05E-02 | 27.0426 | 2.97E-02 | 33.049 |
| 3.94E-02 | 11.0952 | 4.11E-02 | 32.3642 | 4.00E-02 | 32.8789 | 4.00E-02 | 39.5051 |
| 4.87E-02 | 13.4683 | 4.94E-02 | 37.1214 | 5.01E-02 | 38.5556 | 5.04E-02 | 45.4145 |
| 5.92E-02 | 15.9383 | 6.10E-02 | 43.2506 | 5.87E-02 | 43.061 | 6.07E-02 | 50.6488 |
| 6.95E-02 | 18.1563 | 7.00E-02 | 47.5989 | 7.02E-02 | 48.736 | 7.09E-02 | 55.5457 |
| 8.02E-02 | 20.339 | 7.97E-02 | 52.106 | 8.11E-02 | 53.7 | 7.93E-02 | 59.3538 |
| 9.00E-02 | 22.4207 | 8.99E-02 | 56.5636 | 8.83E-02 | 56.8487 | 9.08E-02 | 64.2187 |
| 1.07E-01 | 26.1536 | 1.02E-01 | 61.3236 | 9.48E-02 | 59.5658 | 1.01E-01 | 68.2592 |
| 1.49E-01 | 34.9584 | 1.50E-01 | 78.4766 | 1.51E-01 | 80.2933 | 1.54E-01 | 86.774 |
| 1.98E-01 | 44.2659 | 2.01E-01 | 93.6876 | 1.93E-01 | 93.1083 | 1.99E-01 | 99.7663 |
| 2.49E-01 | 53.4523 | 2.39E-01 | 103.2198 | 2.43E-01 | 106.2896 | 2.51E-01 | 111.8743 |
| 2.99E-01 | 62.3282 | 3.02E-01 | 117.3054 | 2.94E-01 | 118.3518 | 2.99E-01 | 122.9232 |
| 3.49E-01 | 70.7093 | 3.42E-01 | 125.0696 | 3.53E-01 | 130.3067 | 3.38E-01 | 130.2407 |
| 4.00E-01 | 78.5927 | 3.90E-01 | 133.5771 | 3.91E-01 | 137.4731 | 4.02E-01 | 141.0151 |
| 4.51E-01 | 85.9241 | 4.40E-01 | 141.6493 | 4.39E-01 | 145.4772 | 4.42E-01 | 146.9895 |
| 5.00E-01 | 93.1732 | 4.92E-01 | 149.1323 | 4.89E-01 | 153.3036 | 4.90E-01 | 153.6314 |
| 5.51E-01 | 100.19 | 5.43E-01 | 155.9906 | 5.41E-01 | 160.6471 | 5.38E-01 | 160.4221 |
| 6.02E-01 | 106.8064 | 6.08E-01 | 163.791 | 5.92E-01 | 167.4223 | 5.92E-01 | 166.3384 |
| 6.50E-01 | 113.7275 | 6.49E-01 | 168.395 | 6.53E-01 | 174.7782 | 6.43E-01 | 171.8012 |
| 7.02E-01 | 120.1645 | 7.08E-01 | 174.6223 | 6.84E-01 | 178.2663 | 7.05E-01 | 178.6128 |
| 7.52E-01 | 126.2461 | 7.50E-01 | 178.7272 | 7.53E-01 | 185.6176 | 7.60E-01 | 183.1709 |
| 8.02E-01 | 132.2011 | 8.09E-01 | 184.1095 | 7.80E-01 | 189.2653 | 8.00E-01 | 186.3965 |
| 8.53E-01 | 137.8811 | 8.52E-01 | 187.767 | 8.54E-01 | 196.2746 | 8.59E-01 | 191.086 |
| 9.02E-01 | 143.2611 | 9.10E-01 | 192.55 | 8.88E-01 | 199.286 | 9.01E-01 | 194.2907 |
| 9.53E-01 | 148.7732 | 9.52E-01 | 195.807 | 9.31E-01 | 202.9969 | 9.59E-01 | 198.4581 |
| 9.99E-01 | 153.5734 | 9.97E-01 | 199.1019 | 9.76E-01 | 206.6715 | 9.97E-01 | 201.0709 |

Table S9. H₂ adsorption data of SNU-174', SNU-175' and SNU-176' at 77 K.

| SNU-174' | | SNU-175' | | SNU-176' | |
|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 1.30E-04 | 0.0421 | 1.31E-04 | 0.1974 | 9.51E-05 | 0.1179 |
| 2.18E-04 | 0.0867 | 2.10E-04 | 0.2142 | 3.26E-04 | 0.5183 |
| 3.19E-04 | 0.1363 | 3.14E-04 | 0.2288 | 3.26E-04 | 0.5182 |
| 4.16E-04 | 0.1843 | 4.16E-04 | 0.2393 | 3.94E-04 | 0.63 |
| 5.15E-04 | 0.2355 | 5.17E-04 | 0.2457 | 9.08E-04 | 1.438 |
| 6.17E-04 | 0.2842 | 6.18E-04 | 0.247 | 8.65E-04 | 1.3755 |
| 7.15E-04 | 0.3348 | 7.46E-04 | 0.2436 | 8.45E-04 | 1.3438 |
| 8.16E-04 | 0.3842 | 7.96E-04 | 0.2383 | 8.42E-04 | 1.3386 |
| 9.16E-04 | 0.4343 | 9.58E-04 | 0.228 | 9.03E-04 | 1.4331 |
| 1.02E-03 | 0.4829 | 1.09E-03 | 0.1687 | 1.41E-03 | 2.1816 |
| 2.14E-03 | 1.0182 | 2.11E-03 | 0.1883 | 2.41E-03 | 3.5852 |
| 3.12E-03 | 1.461 | 3.26E-03 | 0.1357 | 3.40E-03 | 4.8883 |
| 4.18E-03 | 1.9261 | 4.22E-03 | 0.142 | 4.41E-03 | 6.1501 |
| 5.02E-03 | 2.2465 | 5.31E-03 | 0.1306 | 5.45E-03 | 7.3824 |
| 6.09E-03 | 2.67 | 6.37E-03 | 0.0908 | 6.51E-03 | 8.5818 |
| 7.04E-03 | 3.134 | 7.49E-03 | 0.0993 | 7.56E-03 | 9.7192 |
| 8.46E-03 | 3.6112 | 8.42E-03 | 0.0836 | 8.43E-03 | 10.6446 |
| 9.39E-03 | 3.9046 | 9.47E-03 | 0.0805 | 9.22E-03 | 11.4586 |
| 1.18E-02 | 4.4066 | 1.05E-02 | 0.0883 | 1.03E-02 | 12.6947 |
| 2.17E-02 | 6.8831 | 2.32E-02 | 0.1371 | 1.91E-02 | 20.7144 |
| 2.98E-02 | 8.6066 | 3.28E-02 | 0.206 | 3.03E-02 | 29.4123 |
| 3.96E-02 | 10.6685 | 4.29E-02 | 0.2617 | 3.79E-02 | 34.7287 |
| 5.00E-02 | 12.6809 | 5.29E-02 | 0.3091 | 4.72E-02 | 40.7817 |
| 5.98E-02 | 14.5411 | 6.30E-02 | 0.3509 | 5.71E-02 | 46.6816 |
| 6.98E-02 | 16.3417 | 7.29E-02 | 0.4126 | 6.77E-02 | 52.2654 |
| 8.02E-02 | 17.9957 | 8.29E-02 | 0.4693 | 7.82E-02 | 57.3726 |
| 9.00E-02 | 19.629 | 9.30E-02 | 0.5261 | 8.88E-02 | 62.1989 |
| 1.08E-01 | 22.2935 | 1.12E-01 | 0.6137 | 9.98E-02 | 67.2129 |
| 1.52E-01 | 28.1542 | 1.61E-01 | 1.0647 | 1.54E-01 | 89.1253 |
| 2.02E-01 | 33.9605 | 2.11E-01 | 1.3964 | 1.99E-01 | 104.2623 |
| 2.52E-01 | 39.5436 | 2.61E-01 | 1.7632 | 2.49E-01 | 118.9634 |
| 3.03E-01 | 44.4536 | 3.11E-01 | 2.1509 | 3.01E-01 | 132.4956 |
| 3.54E-01 | 49.2959 | 3.61E-01 | 2.4238 | 3.38E-01 | 141.0687 |
| 4.04E-01 | 53.6789 | 4.12E-01 | 2.8063 | 4.01E-01 | 154.2343 |
| 4.55E-01 | 57.5845 | 4.61E-01 | 3.1472 | 4.41E-01 | 161.6686 |
| 5.04E-01 | 61.7313 | 5.12E-01 | 3.5273 | 4.87E-01 | 170.0914 |
| 5.56E-01 | 64.9202 | 5.61E-01 | 3.9422 | 5.38E-01 | 178.4057 |
| 6.05E-01 | 68.6247 | 6.11E-01 | 4.2331 | 5.89E-01 | 186.2029 |
| 6.56E-01 | 71.6793 | 6.61E-01 | 4.6168 | 6.40E-01 | 193.5071 |
| 7.06E-01 | 74.7325 | 7.11E-01 | 4.9977 | 6.90E-01 | 200.8486 |
| 7.56E-01 | 77.9456 | 7.58E-01 | 6.3337 | 7.42E-01 | 207.3829 |
| 8.07E-01 | 80.3785 | 8.11E-01 | 6.8438 | 7.93E-01 | 213.5757 |
| 8.57E-01 | 83.4354 | 8.61E-01 | 7.1981 | 8.57E-01 | 220.8386 |
| 9.07E-01 | 85.6855 | 9.11E-01 | 7.6281 | 9.09E-01 | 226.2257 |
| 9.57E-01 | 88.3446 | 9.61E-01 | 8.0472 | 9.59E-01 | 231.1429 |
| 9.99E-01 | 90.7094 | 9.99E-01 | 8.3126 | 9.96E-01 | 234.8043 |

Table S10. H₂ adsorption data of SNU-170', SNU-171', SNU-172' and SNU-173' at 87 K.

| SNU-170' | | SNU-171' | | SNU-172' | | SNU-173' | |
|----------|---|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 1.12E-04 | 0.0067 | 1.18E-04 | 0.0367 | 9.64E-05 | 0.0286 | 9.88E-05 | 0.0631 |
| 1.97E-04 | 0.0181 | 2.12E-04 | 0.0796 | 2.08E-04 | 0.0776 | 2.09E-04 | 0.1694 |
| 3.42E-04 | 0.0386 | 3.12E-04 | 0.1239 | 3.11E-04 | 0.1216 | 2.94E-04 | 0.248 |
| 4.03E-04 | 0.0468 | 4.11E-04 | 0.1674 | 4.09E-04 | 0.1637 | 4.09E-04 | 0.3531 |
| 5.40E-04 | 0.0663 | 5.12E-04 | 0.2107 | 5.10E-04 | 0.2062 | 4.94E-04 | 0.4286 |
| 6.03E-04 | 0.0747 | 6.13E-04 | 0.2536 | 6.11E-04 | 0.2482 | 6.12E-04 | 0.5335 |
| 7.41E-04 | 0.0944 | 7.13E-04 | 0.2957 | 7.10E-04 | 0.29 | 6.95E-04 | 0.6069 |
| 8.03E-04 | 0.1026 | 8.14E-04 | 0.338 | 8.11E-04 | 0.3317 | 8.14E-04 | 0.7093 |
| 9.41E-04 | 0.1222 | 9.14E-04 | 0.3793 | 9.12E-04 | 0.373 | 8.97E-04 | 0.7808 |
| 1.00E-03 | 0.1304 | 1.01E-03 | 0.4203 | 1.01E-03 | 0.4146 | 1.02E-03 | 0.8811 |
| 2.14E-03 | 0.3013 | 2.14E-03 | 0.8891 | 2.54E-03 | 1.0494 | 2.65E-03 | 2.215 |
| 3.09E-03 | 0.4418 | 3.11E-03 | 1.2827 | 3.56E-03 | 1.4577 | 3.64E-03 | 2.9602 |
| 4.06E-03 | 0.583 | 4.13E-03 | 1.6808 | 4.54E-03 | 1.849 | 4.64E-03 | 3.6739 |
| 5.04E-03 | 0.7254 | 5.04E-03 | 2.0255 | 5.52E-03 | 2.2284 | 5.65E-03 | 4.354 |
| 6.09E-03 | 0.8754 | 6.07E-03 | 2.41 | 6.49E-03 | 2.6008 | 6.68E-03 | 5.0227 |
| 7.10E-03 | 1.0195 | 7.02E-03 | 2.6977 | 7.54E-03 | 2.9944 | 7.79E-03 | 5.7052 |
| 8.47E-03 | 1.2119 | 8.29E-03 | 3.1508 | 8.11E-03 | 3.209 | 8.47E-03 | 6.114 |
| 9.22E-03 | 1.3191 | 9.51E-03 | 3.5876 | 9.28E-03 | 3.6377 | 9.27E-03 | 6.586 |
| 1.24E-02 | 1.6297 | 1.18E-02 | 4.1311 | 1.07E-02 | 4.0128 | 1.10E-02 | 7.2519 |
| 2.05E-02 | 2.7028 | 2.14E-02 | 7.1845 | 1.94E-02 | 7.0239 | 1.94E-02 | 11.3003 |
| 3.03E-02 | 3.9579 | 3.16E-02 | 10.2426 | 3.04E-02 | 10.4952 | 2.93E-02 | 15.2426 |
| 4.01E-02 | 5.1796 | 4.16E-02 | 13.0744 | 3.98E-02 | 13.2484 | 4.00E-02 | 18.8976 |
| 5.01E-02 | 6.405 | 5.15E-02 | 15.7869 | 4.99E-02 | 16.0868 | 5.03E-02 | 22.1251 |
| 6.02E-02 | 7.6105 | 6.19E-02 | 18.4421 | 5.99E-02 | 18.7655 | 6.07E-02 | 25.1046 |
| 6.99E-02 | 8.7498 | 6.92E-02 | 20.2825 | 7.01E-02 | 21.3462 | 7.05E-02 | 27.7721 |
| 8.02E-02 | 9.9284 | 8.13E-02 | 23.2019 | 8.02E-02 | 23.8376 | 8.10E-02 | 30.4167 |
| 9.05E-02 | 11.098 | 8.91E-02 | 25.0197 | 9.03E-02 | 26.2146 | 9.07E-02 | 32.8138 |
| 1.07E-01 | 12.966 | 1.05E-01 | 28.4445 | 9.93E-02 | 28.2315 | 1.04E-01 | 35.7844 |
| 1.50E-01 | 17.4633 | 1.44E-01 | 36.4554 | 1.50E-01 | 38.7144 | 1.54E-01 | 46.0712 |
| 1.99E-01 | 22.3724 | 1.92E-01 | 45.2497 | 1.93E-01 | 46.5503 | 1.91E-01 | 52.9098 |
| 2.49E-01 | 27.0684 | 2.42E-01 | 53.662 | 2.42E-01 | 54.7135 | 2.54E-01 | 63.0516 |
| 3.00E-01 | 31.6129 | 2.93E-01 | 61.4105 | 2.93E-01 | 62.5352 | 2.94E-01 | 68.9134 |
| 3.50E-01 | 35.9328 | 3.44E-01 | 68.5602 | 3.44E-01 | 69.729 | 3.41E-01 | 75.3973 |
| 4.00E-01 | 40.1457 | 4.08E-01 | 76.7705 | 4.04E-01 | 77.5244 | 3.91E-01 | 81.7055 |
| 4.51E-01 | 44.0872 | 4.50E-01 | 81.7456 | 4.49E-01 | 82.9067 | 4.42E-01 | 87.6309 |
| 5.01E-01 | 47.9835 | 5.08E-01 | 88.3786 | 5.05E-01 | 89.4689 | 4.94E-01 | 93.2326 |
| 5.51E-01 | 51.7059 | 5.50E-01 | 92.8222 | 5.37E-01 | 92.8404 | 5.44E-01 | 98.5228 |
| 6.01E-01 | 55.3179 | 5.99E-01 | 97.6952 | 6.05E-01 | 99.9311 | 6.08E-01 | 104.6894 |
| 6.52E-01 | 58.7815 | 6.48E-01 | 102.7656 | 6.37E-01 | 103.0715 | 6.49E-01 | 108.2728 |
| 7.02E-01 | 62.2966 | 6.99E-01 | 107.4519 | 7.04E-01 | 109.5477 | 7.08E-01 | 113.6362 |
| 7.52E-01 | 65.5898 | 7.50E-01 | 111.8791 | 7.39E-01 | 112.5653 | 7.51E-01 | 116.8465 |
| 8.02E-01 | 68.8575 | 8.00E-01 | 116.1503 | 7.99E-01 | 117.7041 | 7.99E-01 | 120.6581 |
| 8.53E-01 | 71.99 | 8.51E-01 | 120.1206 | 8.37E-01 | 120.7912 | 8.48E-01 | 124.4221 |
| 9.03E-01 | 75.0863 | 9.01E-01 | 123.9945 | 8.83E-01 | 124.4311 | 9.09E-01 | 128.7791 |
| 9.53E-01 | 78.0825 | 9.51E-01 | 127.6074 | 9.49E-01 | 129.4176 | 9.52E-01 | 131.6314 |
| 9.98E-01 | 80.7644 | 9.98E-01 | 130.9964 | 9.85E-01 | 132.056 | 9.96E-01 | 134.636 |

Table S11. H₂ adsorption data of SNU-174', SNU-175' and SNU-176' at 87 K.

| SNU-174' | | SNU-175' | | SNU-176' | |
|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 1.22E-04 | 0.0011 | 3.28E-02 | 0.0551 | 1.17E-04 | 0.0356 |
| 2.15E-04 | 0.0107 | 4.35E-02 | 0.141 | 2.11E-04 | 0.0765 |
| 3.04E-04 | 0.021 | 5.30E-02 | 0.2159 | 3.11E-04 | 0.119 |
| 4.06E-04 | 0.033 | 6.31E-02 | 0.3156 | 4.11E-04 | 0.1609 |
| 5.07E-04 | 0.0451 | 7.30E-02 | 0.4311 | 5.11E-04 | 0.2025 |
| 6.06E-04 | 0.0572 | 8.30E-02 | 0.5436 | 6.11E-04 | 0.2439 |
| 7.07E-04 | 0.069 | 9.31E-02 | 0.6561 | 7.12E-04 | 0.2849 |
| 8.06E-04 | 0.0805 | 1.12E-01 | 0.8053 | 8.12E-04 | 0.3256 |
| 9.07E-04 | 0.0924 | 1.62E-01 | 1.1541 | 9.13E-04 | 0.366 |
| 1.01E-03 | 0.1045 | 2.12E-01 | 1.6371 | 1.01E-03 | 0.4065 |
| 2.20E-03 | 0.2779 | 2.62E-01 | 1.985 | 2.12E-03 | 0.8594 |
| 3.17E-03 | 0.4239 | 3.11E-01 | 2.4645 | 3.07E-03 | 1.2383 |
| 4.12E-03 | 0.5668 | 3.62E-01 | 2.8655 | 4.05E-03 | 1.6223 |
| 5.12E-03 | 0.7193 | 4.11E-01 | 3.3241 | 5.05E-03 | 2.0046 |
| 6.13E-03 | 0.8713 | 4.62E-01 | 3.6333 | 6.03E-03 | 2.3744 |
| 7.09E-03 | 1.0306 | 5.11E-01 | 4.1415 | 7.04E-03 | 2.7433 |
| 8.60E-03 | 1.2415 | 5.62E-01 | 4.4024 | 8.18E-03 | 3.1613 |
| 9.81E-03 | 1.5965 | 6.11E-01 | 4.7943 | 9.27E-03 | 3.5477 |
| 1.19E-02 | 1.9682 | 6.61E-01 | 5.1138 | 1.17E-02 | 4.1985 |
| 2.05E-02 | 2.955 | 7.12E-01 | 5.4883 | 2.11E-02 | 7.2865 |
| 3.05E-02 | 4.0793 | 7.61E-01 | 5.72 | 3.11E-02 | 10.3484 |
| 4.08E-02 | 5.2333 | 8.11E-01 | 6.1002 | 4.14E-02 | 13.2672 |
| 5.07E-02 | 6.345 | 8.62E-01 | 6.434 | 5.15E-02 | 16.0294 |
| 6.10E-02 | 7.4136 | 9.12E-01 | 6.715 | 6.13E-02 | 18.6109 |
| 7.06E-02 | 8.4137 | 9.61E-01 | 7.1873 | 6.89E-02 | 20.5083 |
| 8.09E-02 | 9.3938 | 9.99E-01 | 7.724 | 8.12E-02 | 23.556 |
| 9.05E-02 | 10.355 | | | 8.88E-02 | 25.375 |
| 1.09E-01 | 11.836 | | | 1.04E-01 | 28.9041 |
| 1.56E-01 | 15.3844 | | | 1.43E-01 | 37.0089 |
| 2.05E-01 | 19.0698 | | | 2.05E-01 | 48.9237 |
| 2.56E-01 | 22.4339 | | | 2.45E-01 | 55.7483 |
| 3.06E-01 | 25.7072 | | | 2.92E-01 | 63.4679 |
| 3.56E-01 | 28.7802 | | | 3.42E-01 | 71.0351 |
| 4.07E-01 | 31.7409 | | | 3.93E-01 | 78.2221 |
| 4.57E-01 | 34.4851 | | | 4.44E-01 | 85.0003 |
| 5.06E-01 | 37.2008 | | | 4.94E-01 | 91.4756 |
| 5.57E-01 | 39.7685 | | | 5.56E-01 | 99.2117 |
| 6.07E-01 | 42.3053 | | | 6.08E-01 | 105.1063 |
| 6.57E-01 | 44.8049 | | | 6.50E-01 | 109.4483 |
| 7.07E-01 | 47.1679 | | | 7.08E-01 | 115.4219 |
| 7.58E-01 | 49.38 | | | 7.49E-01 | 119.7514 |
| 8.07E-01 | 51.4176 | | | 8.09E-01 | 125.3387 |
| 8.58E-01 | 53.4849 | | | 8.51E-01 | 129.0897 |
| 9.08E-01 | 55.4679 | | | 8.99E-01 | 133.4381 |
| 9.58E-01 | 57.4677 | | | 9.50E-01 | 137.486 |
| 9.99E-01 | 59.1986 | | | 9.95E-01 | 141.1641 |

Table S12. CO₂ adsorption data of SNU-170', SNU-171', SNU-172' and SNU-173' at 195 K.

| SNU-170' | | SNU-171' | | SNU-172' | | SNU-173' | |
|----------|---|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 1.09E-04 | 0.0966 | 5.35E-05 | 0.1376 | 9.87E-05 | 2.639 | 5.04E-05 | 0.1084 |
| 2.14E-04 | 0.2672 | 1.29E-04 | 1.5874 | 2.07E-04 | 5.7771 | 1.31E-04 | 3.2438 |
| 3.01E-04 | 0.3865 | 2.29E-04 | 3.1213 | 2.94E-04 | 7.551 | 2.26E-04 | 6.3174 |
| 4.03E-04 | 0.5346 | 3.40E-04 | 4.5838 | 4.33E-04 | 10.3272 | 3.40E-04 | 9.3148 |
| 5.09E-04 | 0.6774 | 4.59E-04 | 5.98 | 5.21E-04 | 11.7557 | 4.19E-04 | 11.2477 |
| 6.19E-04 | 0.8102 | 5.62E-04 | 7.0922 | 6.26E-04 | 13.2457 | 5.19E-04 | 13.0349 |
| 7.01E-04 | 0.9104 | 6.27E-04 | 7.733 | 7.24E-04 | 14.5084 | 6.23E-04 | 14.7038 |
| 8.18E-04 | 1.0484 | 7.77E-04 | 9.0851 | 7.94E-04 | 15.3662 | 7.20E-04 | 16.0507 |
| 9.01E-04 | 1.1462 | 8.30E-04 | 9.5557 | 9.26E-04 | 16.7884 | 8.23E-04 | 17.3935 |
| 9.96E-04 | 1.2558 | 1.01E-03 | 11.075 | 9.96E-04 | 17.5063 | 1.04E-03 | 20.0063 |
| 2.55E-03 | 3.3793 | 2.02E-03 | 18.8336 | 2.02E-03 | 27.2837 | 2.04E-03 | 29.3909 |
| 3.60E-03 | 4.7697 | 3.01E-03 | 25.4575 | 3.03E-03 | 34.881 | 3.01E-03 | 36.7846 |
| 4.54E-03 | 5.941 | 4.05E-03 | 32.0693 | 4.04E-03 | 41.661 | 4.00E-03 | 43.4552 |
| 5.63E-03 | 7.2807 | 5.09E-03 | 38.2371 | 5.03E-03 | 47.7567 | 5.01E-03 | 49.6934 |
| 7.05E-03 | 8.9342 | 7.05E-03 | 50.1071 | 7.18E-03 | 60.0451 | 6.96E-03 | 60.8855 |
| 7.06E-03 | 8.9358 | 7.05E-03 | 50.1188 | 7.18E-03 | 60.0525 | 7.75E-03 | 65.1982 |
| 8.78E-03 | 10.9201 | 8.51E-03 | 58.5696 | 8.52E-03 | 67.1471 | 8.41E-03 | 68.6209 |
| 9.57E-03 | 11.9384 | 9.32E-03 | 63.4974 | 9.28E-03 | 70.8465 | 9.22E-03 | 73.0048 |
| 1.06E-02 | 13.0259 | 9.64E-03 | 64.7975 | 9.45E-03 | 71.6436 | 9.56E-03 | 74.1501 |
| 1.68E-02 | 20.0866 | 1.61E-02 | 102.1505 | 1.56E-02 | 104.032 | 1.67E-02 | 109.211 |
| 2.69E-02 | 31.5316 | 2.48E-02 | 158.2312 | 2.48E-02 | 150.4451 | 2.54E-02 | 149.2465 |
| 3.69E-02 | 42.007 | 3.36E-02 | 216.3456 | 3.34E-02 | 192.9762 | 3.54E-02 | 193.5174 |
| 4.73E-02 | 51.5364 | 4.37E-02 | 259.5252 | 4.28E-02 | 236.1025 | 4.62E-02 | 235.7814 |
| 5.80E-02 | 60.055 | 5.44E-02 | 277.9187 | 5.09E-02 | 262.6475 | 5.58E-02 | 254.1372 |
| 6.67E-02 | 66.4066 | 6.51E-02 | 289.2369 | 6.28E-02 | 283.3377 | 6.45E-02 | 263.2849 |
| 7.64E-02 | 72.8182 | 7.58E-02 | 296.6217 | 7.36E-02 | 293.4246 | 7.64E-02 | 272.0744 |
| 8.61E-02 | 78.9923 | 8.56E-02 | 301.3622 | 8.99E-02 | 303.1516 | 8.40E-02 | 276.4105 |
| 1.02E-01 | 88.85 | 1.03E-01 | 307.9976 | 9.97E-02 | 307.2664 | 9.89E-02 | 283.25 |
| 1.27E-01 | 103.4266 | 1.31E-01 | 316.5215 | 1.30E-01 | 317.027 | 1.47E-01 | 297.6465 |
| 1.76E-01 | 131.2584 | 1.75E-01 | 326.1241 | 1.80E-01 | 326.6746 | 1.82E-01 | 304.2697 |
| 2.21E-01 | 161.9625 | 2.31E-01 | 334.3113 | 2.22E-01 | 332.3664 | 2.29E-01 | 311.3058 |
| 2.60E-01 | 210.9641 | 3.02E-01 | 341.8795 | 2.74E-01 | 337.5688 | 2.82E-01 | 317.4581 |
| 2.72E-01 | 256.9864 | 3.46E-01 | 345.8055 | 3.30E-01 | 341.8566 | 3.49E-01 | 323.6116 |
| 2.95E-01 | 305.9159 | 3.98E-01 | 349.3886 | 4.00E-01 | 346.0033 | 4.03E-01 | 327.6116 |
| 4.12E-01 | 322.6046 | 4.49E-01 | 352.6927 | 4.58E-01 | 348.7656 | 4.48E-01 | 330.4686 |
| 5.03E-01 | 330.5682 | 5.01E-01 | 355.6614 | 4.99E-01 | 350.4984 | 4.97E-01 | 333.5093 |
| 5.50E-01 | 334.2886 | 5.52E-01 | 358.0977 | 5.47E-01 | 352.3729 | 5.48E-01 | 336.2 |
| 6.01E-01 | 337.7682 | 6.03E-01 | 360.4809 | 5.98E-01 | 354.109 | 6.00E-01 | 338.5895 |
| 6.51E-01 | 341.5295 | 6.55E-01 | 362.3346 | 6.50E-01 | 355.6483 | 6.50E-01 | 340.8442 |
| 7.00E-01 | 345.0318 | 7.03E-01 | 364.4235 | 7.01E-01 | 357.0508 | 7.00E-01 | 343.0407 |
| 7.52E-01 | 348.0136 | 7.56E-01 | 366.1832 | 7.53E-01 | 358.209 | 7.52E-01 | 344.9814 |
| 8.00E-01 | 351.3705 | 8.04E-01 | 367.9672 | 8.02E-01 | 359.4115 | 8.02E-01 | 346.8372 |
| 8.54E-01 | 354.0136 | 8.54E-01 | 369.9712 | 8.53E-01 | 360.468 | 8.52E-01 | 348.5814 |
| 9.04E-01 | 356.3591 | 9.07E-01 | 371.3107 | 9.04E-01 | 361.4631 | 9.03E-01 | 350.3163 |
| 9.53E-01 | 358.8341 | 9.56E-01 | 372.6077 | 9.55E-01 | 362.377 | 9.54E-01 | 351.7663 |
| 9.99E-01 | 361.0182 | 9.99E-01 | 373.7788 | 9.99E-01 | 363.1877 | 9.99E-01 | 353.1581 |

Table S13. CO₂ adsorption data of SNU-174', SNU-175' and SNU-176' at 195 K.

| SNU-174' | | SNU-175' | | SNU-176' | |
|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 9.37E-05 | 0.038 | 1.65E-04 | 1.6686 | 9.29E-05 | 0.9734 |
| 2.06E-04 | 0.0543 | 2.43E-04 | 2.2238 | 2.30E-04 | 3.0867 |
| 3.07E-04 | 0.0697 | 3.74E-04 | 2.7713 | 3.10E-04 | 4.0352 |
| 3.95E-04 | 0.0862 | 4.88E-04 | 3.3093 | 3.97E-04 | 5.1515 |
| 5.04E-04 | 0.1278 | 6.09E-04 | 3.747 | 5.00E-04 | 6.3711 |
| 6.00E-04 | 2.521 | 5.94E-04 | 3.7719 | 5.95E-04 | 7.4774 |
| 7.02E-04 | 3.3357 | 8.11E-04 | 4.3716 | 7.70E-04 | 9.2923 |
| 7.98E-04 | 3.667 | 8.07E-04 | 4.3766 | 8.54E-04 | 10.1346 |
| 9.12E-04 | 3.9843 | 1.05E-03 | 4.9628 | 9.45E-04 | 11.0301 |
| 1.01E-03 | 4.2521 | 1.02E-03 | 4.9696 | 1.04E-03 | 11.9496 |
| 2.01E-03 | 6.242 | 2.04E-03 | 6.9382 | 2.00E-03 | 20.1169 |
| 3.06E-03 | 7.9269 | 3.08E-03 | 8.3343 | 3.01E-03 | 27.6854 |
| 4.01E-03 | 9.2233 | 4.12E-03 | 9.4077 | 4.00E-03 | 34.6406 |
| 5.07E-03 | 10.5634 | 5.14E-03 | 10.5133 | 5.00E-03 | 41.1376 |
| 6.13E-03 | 11.7852 | 6.87E-03 | 11.7364 | 7.14E-03 | 54.1904 |
| 7.04E-03 | 12.7295 | 7.92E-03 | 12.8425 | 7.13E-03 | 54.1791 |
| 8.07E-03 | 13.7416 | 8.50E-03 | 13.1572 | 8.53E-03 | 62.3959 |
| 9.13E-03 | 14.7563 | 9.20E-03 | 13.516 | 9.29E-03 | 66.8683 |
| 1.02E-02 | 15.7506 | 1.02E-02 | 14.0427 | 9.58E-03 | 68.0363 |
| 1.95E-02 | 22.3883 | 1.72E-02 | 16.8665 | 1.57E-02 | 103.9124 |
| 2.92E-02 | 29.1346 | 2.70E-02 | 19.6867 | 2.37E-02 | 152.4814 |
| 4.12E-02 | 37.1775 | 4.02E-02 | 22.5121 | 3.25E-02 | 209.7729 |
| 4.97E-02 | 42.174 | 4.67E-02 | 23.6865 | 3.63E-02 | 234.6643 |
| 5.97E-02 | 47.4575 | 5.58E-02 | 25.0718 | 4.94E-02 | 293.5714 |
| 6.98E-02 | 52.4258 | 6.56E-02 | 26.4807 | 5.94E-02 | 314.6414 |
| 7.99E-02 | 57.1556 | 7.57E-02 | 27.8126 | 7.52E-02 | 330.7443 |
| 9.00E-02 | 61.6372 | 8.62E-02 | 29.0892 | 8.28E-02 | 335.86 |
| 1.00E-01 | 66.0761 | 1.02E-01 | 30.9328 | 9.77E-02 | 343.7186 |
| 1.46E-01 | 86.0611 | 1.51E-01 | 36.1634 | 1.23E-01 | 353.6257 |
| 1.99E-01 | 121.7174 | 2.01E-01 | 40.9484 | 1.67E-01 | 364.5343 |
| 2.49E-01 | 182.7333 | 2.54E-01 | 45.1724 | 2.24E-01 | 373.7257 |
| 3.00E-01 | 191.1525 | 3.01E-01 | 47.0582 | 2.97E-01 | 382.1257 |
| 3.55E-01 | 198.4166 | 3.52E-01 | 48.7141 | 3.53E-01 | 386.9785 |
| 3.97E-01 | 202.9689 | 4.03E-01 | 50.1744 | 3.98E-01 | 390.1814 |
| 4.46E-01 | 207.7055 | 4.54E-01 | 51.4212 | 4.49E-01 | 393.1929 |
| 4.97E-01 | 212.1452 | 5.05E-01 | 52.5306 | 4.99E-01 | 396.0457 |
| 5.48E-01 | 216.2863 | 5.56E-01 | 53.5383 | 5.51E-01 | 398.4785 |
| 5.99E-01 | 220.0593 | 6.07E-01 | 54.461 | 6.02E-01 | 400.6943 |
| 6.50E-01 | 223.4888 | 6.58E-01 | 55.2171 | 6.53E-01 | 402.67 |
| 7.01E-01 | 226.6646 | 7.09E-01 | 55.796 | 7.04E-01 | 404.4914 |
| 7.51E-01 | 229.7035 | 7.61E-01 | 56.1969 | 7.54E-01 | 406.0714 |
| 8.01E-01 | 232.82 | 8.11E-01 | 56.5175 | 8.05E-01 | 407.6671 |
| 8.51E-01 | 235.8875 | 8.51E-01 | 59.516 | 8.55E-01 | 409.0657 |
| 9.02E-01 | 238.5951 | 9.04E-01 | 60.5128 | 9.06E-01 | 410.3557 |
| 9.53E-01 | 241.1656 | 9.57E-01 | 61.2228 | 9.56E-01 | 411.5385 |
| 9.99E-01 | 243.5215 | 9.99E-01 | 61.9569 | 9.99E-01 | 412.6571 |

Table S14. CO₂ adsorption data of SNU-170', SNU-171', SNU-172' and SNU-173' at 273 K.

| SNU-170' | | SNU-171' | | SNU-172' | | SNU-173' | |
|----------|---|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 3.00E-03 | 0.0298 | 1.21E-04 | 0.0021 | 9.77E-05 | 0.004 | 1.37E-04 | 0.0311 |
| 4.34E-03 | 0.0801 | 2.07E-04 | 0.0096 | 2.28E-04 | 0.0148 | 2.15E-04 | 0.0423 |
| 5.02E-03 | 0.1045 | 3.04E-04 | 0.0177 | 3.30E-04 | 0.0228 | 3.10E-04 | 0.0565 |
| 6.31E-03 | 0.1531 | 4.06E-04 | 0.0267 | 4.26E-04 | 0.0308 | 4.09E-04 | 0.0712 |
| 7.00E-03 | 0.1781 | 5.04E-04 | 0.0354 | 5.25E-04 | 0.0393 | 5.08E-04 | 0.0857 |
| 9.14E-03 | 0.2658 | 6.05E-04 | 0.0442 | 6.24E-04 | 0.0481 | 6.11E-04 | 0.101 |
| 9.98E-03 | 0.2998 | 7.05E-04 | 0.0532 | 7.24E-04 | 0.0572 | 7.14E-04 | 0.1161 |
| 1.40E-02 | 0.0399 | 8.06E-04 | 0.0614 | 8.21E-04 | 0.0662 | 8.03E-04 | 0.1291 |
| 2.34E-02 | 0.3733 | 9.06E-04 | 0.0696 | 9.21E-04 | 0.0756 | 9.36E-04 | 0.1489 |
| 3.36E-02 | 0.751 | 1.01E-03 | 0.079 | 1.02E-03 | 0.0852 | 1.09E-03 | 0.1369 |
| 4.35E-02 | 1.1404 | 2.21E-03 | 0.2295 | 2.14E-03 | 0.2315 | 2.02E-03 | 0.2856 |
| 5.36E-02 | 1.5589 | 3.19E-03 | 0.3513 | 3.15E-03 | 0.3626 | 3.06E-03 | 0.4501 |
| 6.32E-02 | 1.9559 | 4.19E-03 | 0.4728 | 4.17E-03 | 0.4948 | 4.12E-03 | 0.6151 |
| 7.34E-02 | 2.3575 | 5.24E-03 | 0.6015 | 5.15E-03 | 0.6225 | 5.17E-03 | 0.7795 |
| 8.39E-02 | 2.7864 | 6.25E-03 | 0.7258 | 6.19E-03 | 0.7577 | 6.24E-03 | 0.9458 |
| 9.34E-02 | 3.1826 | 7.20E-03 | 0.8407 | 7.18E-03 | 0.8864 | 7.05E-03 | 1.0701 |
| 1.12E-01 | 3.9391 | 9.02E-03 | 1.0654 | 8.42E-03 | 1.0476 | 8.02E-03 | 1.222 |
| 1.60E-01 | 5.8242 | 9.74E-03 | 1.1515 | 9.22E-03 | 1.1516 | 9.05E-03 | 1.3821 |
| 2.10E-01 | 7.8305 | 1.32E-02 | 1.3145 | 1.13E-02 | 1.4155 | 1.01E-02 | 1.5454 |
| 2.60E-01 | 9.7821 | 2.12E-02 | 2.2626 | 2.04E-02 | 2.5837 | 2.16E-02 | 3.2901 |
| 3.10E-01 | 11.7554 | 3.07E-02 | 3.3446 | 3.02E-02 | 3.816 | 3.17E-02 | 4.8195 |
| 3.60E-01 | 13.7082 | 4.08E-02 | 4.5522 | 4.01E-02 | 5.0603 | 3.94E-02 | 5.937 |
| 4.10E-01 | 15.7523 | 5.07E-02 | 5.6907 | 5.01E-02 | 6.2969 | 5.47E-02 | 8.1063 |
| 4.60E-01 | 17.7304 | 6.07E-02 | 6.7939 | 6.00E-02 | 7.5123 | 6.04E-02 | 8.901 |
| 5.10E-01 | 19.7118 | 7.07E-02 | 7.9402 | 6.99E-02 | 8.7101 | 7.17E-02 | 10.4536 |
| 5.60E-01 | 21.6042 | 8.07E-02 | 9.0657 | 7.99E-02 | 9.9024 | 7.95E-02 | 11.4933 |
| 6.09E-01 | 23.5443 | 9.06E-02 | 10.1665 | 8.99E-02 | 11.0788 | 9.16E-02 | 13.0905 |
| 6.60E-01 | 25.5805 | 1.08E-01 | 12.0596 | 1.02E-01 | 12.4445 | 1.06E-01 | 14.8871 |
| 7.09E-01 | 27.4723 | 1.50E-01 | 16.5733 | 1.49E-01 | 17.6566 | 1.56E-01 | 21.0676 |
| 7.60E-01 | 29.3341 | 1.99E-01 | 21.581 | 2.05E-01 | 23.6545 | 2.07E-01 | 26.8299 |
| 8.09E-01 | 31.4175 | 2.59E-01 | 27.6537 | 2.48E-01 | 28.103 | 2.57E-01 | 32.4209 |
| 8.59E-01 | 33.3793 | 3.00E-01 | 31.7737 | 3.04E-01 | 33.6468 | 3.06E-01 | 37.9983 |
| 9.09E-01 | 35.2107 | 3.58E-01 | 37.4563 | 3.49E-01 | 37.8994 | 3.57E-01 | 43.2533 |
| 9.59E-01 | 37.0993 | 4.00E-01 | 41.5262 | 4.04E-01 | 43.0959 | 4.07E-01 | 48.1799 |
| 9.99E-01 | 38.9248 | 4.58E-01 | 47.1447 | 4.36E-01 | 45.9774 | 4.57E-01 | 52.9349 |
| | | 4.99E-01 | 51.1185 | 5.03E-01 | 52.0119 | 5.07E-01 | 57.539 |
| | | 5.58E-01 | 56.6044 | 5.35E-01 | 54.8845 | 5.57E-01 | 62.0187 |
| | | 5.99E-01 | 60.4425 | 6.03E-01 | 60.7544 | 5.98E-01 | 65.5543 |
| | | 6.57E-01 | 65.6778 | 6.35E-01 | 63.5088 | 6.56E-01 | 70.588 |
| | | 6.99E-01 | 69.5241 | 7.01E-01 | 68.9933 | 6.97E-01 | 74.026 |
| | | 7.57E-01 | 74.753 | 7.35E-01 | 71.7663 | 7.57E-01 | 78.8616 |
| | | 7.98E-01 | 78.5323 | 8.01E-01 | 77.1202 | 7.98E-01 | 82.1886 |
| | | 8.57E-01 | 83.6421 | 8.35E-01 | 79.7995 | 8.57E-01 | 86.8057 |
| | | 9.07E-01 | 88.0749 | 8.77E-01 | 83.156 | 8.98E-01 | 90.0088 |
| | | 9.49E-01 | 91.6258 | 9.50E-01 | 88.6819 | 9.57E-01 | 94.4428 |
| | | 9.93E-01 | 95.4681 | 9.81E-01 | 91.1098 | 9.95E-01 | 97.2726 |

Table S15. CO₂ adsorption data of SNU-174', SNU-175' and SNU-176' at 273 K.

| SNU-174' | | SNU-175' | | SNU-176' | |
|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 1.21E-04 | 0.0007 | 3.11E-04 | 0.001 | 1.11E-04 | 0.0051 |
| 2.25E-04 | 0.0011 | 4.12E-04 | 0.0045 | 2.10E-04 | 0.0119 |
| 3.23E-04 | 0.0019 | 5.13E-04 | 0.0076 | 3.06E-04 | 0.0199 |
| 4.22E-04 | 0.0037 | 6.12E-04 | 0.0109 | 4.05E-04 | 0.0283 |
| 5.22E-04 | 0.0053 | 7.14E-04 | 0.0135 | 5.04E-04 | 0.037 |
| 6.21E-04 | 0.0074 | 8.16E-04 | 0.016 | 6.04E-04 | 0.0459 |
| 7.21E-04 | 0.0091 | 9.15E-04 | 0.0183 | 7.04E-04 | 0.055 |
| 8.22E-04 | 0.011 | 1.02E-03 | 0.0205 | 8.03E-04 | 0.064 |
| 9.22E-04 | 0.0128 | 2.26E-03 | 0.078 | 9.04E-04 | 0.0731 |
| 1.02E-03 | 0.0143 | 3.22E-03 | 0.1211 | 1.00E-03 | 0.0822 |
| 2.34E-03 | 0.0828 | 4.21E-03 | 0.1644 | 2.20E-03 | 0.233 |
| 3.02E-03 | 0.1166 | 5.23E-03 | 0.208 | 3.18E-03 | 0.3568 |
| 4.03E-03 | 0.169 | 6.19E-03 | 0.2478 | 4.21E-03 | 0.4869 |
| 5.04E-03 | 0.2212 | 7.21E-03 | 0.2896 | 5.20E-03 | 0.6123 |
| 6.05E-03 | 0.2728 | 9.05E-03 | 0.3643 | 6.25E-03 | 0.745 |
| 7.36E-03 | 0.339 | 9.87E-03 | 0.3959 | 7.17E-03 | 0.8611 |
| 9.38E-03 | 0.4413 | 1.22E-02 | 0.5049 | 8.97E-03 | 1.0899 |
| 9.99E-03 | 0.4698 | 2.15E-02 | 0.8502 | 9.72E-03 | 1.1848 |
| 1.29E-02 | 0.595 | 3.11E-02 | 1.1764 | 1.26E-02 | 1.4421 |
| 2.21E-02 | 0.9695 | 4.13E-02 | 1.4897 | 2.05E-02 | 2.4385 |
| 3.20E-02 | 1.3897 | 5.14E-02 | 1.7681 | 3.00E-02 | 3.6196 |
| 4.21E-02 | 1.8136 | 6.17E-02 | 1.9963 | 4.00E-02 | 4.8583 |
| 5.22E-02 | 2.2134 | 7.20E-02 | 2.2371 | 5.00E-02 | 6.0759 |
| 6.24E-02 | 2.6277 | 8.20E-02 | 2.4557 | 6.00E-02 | 7.3001 |
| 7.20E-02 | 2.997 | 9.21E-02 | 2.6637 | 7.00E-02 | 8.5058 |
| 8.23E-02 | 3.3943 | 1.10E-01 | 3.0889 | 8.00E-02 | 9.7031 |
| 9.22E-02 | 3.7808 | 1.57E-01 | 4.021 | 8.99E-02 | 10.8887 |
| 1.11E-01 | 4.4704 | 2.09E-01 | 4.6637 | 1.07E-01 | 12.8482 |
| 1.59E-01 | 6.0386 | 2.59E-01 | 5.4192 | 1.49E-01 | 17.5751 |
| 2.09E-01 | 7.7417 | 3.09E-01 | 6.135 | 2.08E-01 | 24.1421 |
| 2.59E-01 | 9.2604 | 3.59E-01 | 6.7465 | 2.49E-01 | 28.5427 |
| 3.09E-01 | 10.8071 | 4.09E-01 | 7.337 | 3.07E-01 | 34.81 |
| 3.60E-01 | 12.23 | 4.59E-01 | 7.9002 | 3.58E-01 | 40.0637 |
| 4.08E-01 | 13.71 | 5.10E-01 | 8.4638 | 4.08E-01 | 45.2301 |
| 4.59E-01 | 15.1594 | 5.60E-01 | 8.9463 | 4.57E-01 | 50.226 |
| 5.09E-01 | 16.5475 | 6.10E-01 | 9.4747 | 5.07E-01 | 55.2261 |
| 5.58E-01 | 17.9072 | 6.60E-01 | 9.9228 | 5.57E-01 | 60.155 |
| 6.08E-01 | 19.2573 | 7.10E-01 | 10.338 | 6.07E-01 | 65.0307 |
| 6.59E-01 | 20.5566 | 7.60E-01 | 10.7134 | 6.57E-01 | 69.8499 |
| 7.09E-01 | 21.8628 | 8.09E-01 | 11.1731 | 7.06E-01 | 74.6584 |
| 7.59E-01 | 23.1135 | 8.60E-01 | 11.5837 | 7.56E-01 | 79.3431 |
| 8.09E-01 | 24.4264 | 9.10E-01 | 11.9354 | 8.06E-01 | 84.0881 |
| 8.59E-01 | 25.5988 | 9.60E-01 | 12.279 | 8.56E-01 | 88.6701 |
| 9.09E-01 | 26.8857 | 9.99E-01 | 12.6347 | 9.06E-01 | 93.3059 |
| 9.59E-01 | 27.8859 | | | 9.56E-01 | 97.7823 |
| 9.99E-01 | 29.1517 | | | 9.93E-01 | 101.1333 |

Table S16. CO₂ adsorption data of SNU-170', SNU-171', SNU-172' and SNU-173' at 298 K.

| SNU-170' | | SNU-171' | | SNU-172' | | SNU-173' | |
|----------|---|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 1.02E-03 | 0.0028 | 2.33E-03 | 0.0576 | 1.16E-04 | 0.0019 | 1.29E-04 | 0.0107 |
| 2.01E-03 | 0.0177 | 3.00E-03 | 0.0887 | 2.16E-04 | 0.0034 | 2.30E-04 | 0.0143 |
| 3.03E-03 | 0.0317 | 4.34E-03 | 0.1549 | 3.08E-04 | 0.0061 | 3.27E-04 | 0.0177 |
| 4.01E-03 | 0.0464 | 5.02E-03 | 0.1856 | 4.05E-04 | 0.0092 | 4.30E-04 | 0.0213 |
| 5.00E-03 | 0.0617 | 6.04E-03 | 0.2355 | 5.03E-04 | 0.0125 | 5.21E-04 | 0.0255 |
| 6.00E-03 | 0.0771 | 7.37E-03 | 0.3004 | 6.02E-04 | 0.016 | 6.12E-04 | 0.0312 |
| 7.05E-03 | 0.0922 | 9.36E-03 | 0.4005 | 7.01E-04 | 0.0197 | 7.15E-04 | 0.0409 |
| 9.03E-03 | 0.1304 | 1.02E-02 | 0.4415 | 8.01E-04 | 0.0234 | 8.07E-04 | 0.0513 |
| 9.79E-03 | 0.1416 | 1.31E-02 | 0.5405 | 9.01E-04 | 0.0271 | 9.04E-04 | 0.0603 |
| 1.29E-02 | 0.1561 | 2.20E-02 | 0.9719 | 1.00E-03 | 0.0308 | 1.02E-03 | 0.0691 |
| 2.23E-02 | 0.2792 | 3.18E-02 | 1.4693 | 2.16E-03 | 0.0931 | 2.11E-03 | 0.1347 |
| 3.27E-02 | 0.464 | 4.18E-02 | 1.9796 | 3.17E-03 | 0.1483 | 3.04E-03 | 0.1901 |
| 4.28E-02 | 0.6008 | 5.20E-02 | 2.4905 | 4.19E-03 | 0.2037 | 4.08E-03 | 0.2531 |
| 5.24E-02 | 0.7979 | 6.18E-02 | 2.9776 | 5.18E-03 | 0.2551 | 5.13E-03 | 0.3175 |
| 6.29E-02 | 1.076 | 7.19E-02 | 3.4809 | 6.16E-03 | 0.3056 | 6.18E-03 | 0.3833 |
| 7.27E-02 | 1.294 | 8.16E-02 | 4.0073 | 7.20E-03 | 0.3597 | 7.24E-03 | 0.4479 |
| 8.26E-02 | 1.5138 | 9.18E-02 | 4.5374 | 8.89E-03 | 0.4497 | 8.29E-03 | 0.5131 |
| 9.26E-02 | 1.7251 | 1.10E-01 | 5.4062 | 9.76E-03 | 0.4966 | 9.35E-03 | 0.5789 |
| 1.03E-01 | 1.9296 | 1.57E-01 | 7.5946 | 1.24E-02 | 0.6024 | 1.04E-02 | 0.6444 |
| 1.52E-01 | 2.8933 | 2.06E-01 | 9.9531 | 2.01E-02 | 1.0129 | 2.08E-02 | 1.2435 |
| 2.01E-01 | 3.9464 | 2.56E-01 | 12.2852 | 2.97E-02 | 1.5252 | 3.08E-02 | 1.8905 |
| 2.52E-01 | 5.0192 | 3.06E-01 | 14.6191 | 3.95E-02 | 2.0579 | 4.08E-02 | 2.5274 |
| 3.01E-01 | 6.128 | 3.56E-01 | 16.8407 | 4.95E-02 | 2.6027 | 5.83E-02 | 3.6111 |
| 3.51E-01 | 7.2033 | 4.06E-01 | 19.0922 | 5.95E-02 | 3.1509 | 6.22E-02 | 3.8652 |
| 4.01E-01 | 8.3131 | 4.56E-01 | 21.3369 | 6.95E-02 | 3.6955 | 7.11E-02 | 4.4244 |
| 4.51E-01 | 9.4578 | 5.05E-01 | 23.6147 | 7.95E-02 | 4.2344 | 8.10E-02 | 5.024 |
| 5.01E-01 | 10.545 | 5.56E-01 | 25.7667 | 8.94E-02 | 4.7692 | 9.10E-02 | 5.63 |
| 5.51E-01 | 11.4727 | 6.05E-01 | 27.9205 | 1.06E-01 | 5.6279 | 1.09E-01 | 6.6604 |
| 6.01E-01 | 12.497 | 6.55E-01 | 30.0901 | 1.48E-01 | 7.6995 | 1.53E-01 | 9.251 |
| 6.51E-01 | 13.6372 | 7.05E-01 | 32.3158 | 1.94E-01 | 10.0798 | 2.02E-01 | 12.0514 |
| 7.01E-01 | 14.6694 | 7.55E-01 | 34.4798 | 2.44E-01 | 12.5267 | 2.52E-01 | 14.901 |
| 7.51E-01 | 15.7048 | 8.05E-01 | 36.6022 | 2.93E-01 | 14.9777 | 3.01E-01 | 17.9312 |
| 8.01E-01 | 16.8139 | 8.55E-01 | 38.6981 | 3.43E-01 | 17.4001 | 3.51E-01 | 20.8837 |
| 8.51E-01 | 17.894 | 9.05E-01 | 40.7151 | 3.92E-01 | 19.8013 | 4.02E-01 | 23.594 |
| 9.00E-01 | 19.0217 | 9.55E-01 | 42.6749 | 4.43E-01 | 22.149 | 4.52E-01 | 26.1551 |
| 9.51E-01 | 19.968 | 9.99E-01 | 44.6162 | 5.07E-01 | 24.9292 | 5.02E-01 | 28.679 |
| 9.96E-01 | 20.8096 | | | 5.56E-01 | 27.1907 | 5.53E-01 | 31.1297 |
| | | | | 6.06E-01 | 29.5232 | 6.03E-01 | 33.556 |
| | | | | 6.56E-01 | 31.8168 | 6.53E-01 | 35.9434 |
| | | | | 7.06E-01 | 34.0656 | 7.03E-01 | 38.2547 |
| | | | | 7.58E-01 | 36.1585 | 7.53E-01 | 40.5521 |
| | | | | 8.05E-01 | 38.3929 | 8.03E-01 | 42.8241 |
| | | | | 8.56E-01 | 40.5768 | 8.53E-01 | 45.0733 |
| | | | | 9.08E-01 | 42.6193 | 9.03E-01 | 47.2743 |
| | | | | 9.56E-01 | 44.648 | 9.53E-01 | 49.4449 |
| | | | | 9.99E-01 | 46.5286 | 9.99E-01 | 51.4269 |

Table S17. CO₂ adsorption data of SNU-174', SNU-175' and SNU-176' at 298 K.

| SNU-174' | | SNU-175' | | SNU-176' | |
|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 5.11E-03 | 0.0086 | 5.32E-03 | 0.0017 | 7.21E-04 | 0.0016 |
| 6.13E-03 | 0.0255 | 6.38E-03 | 0.0107 | 8.21E-04 | 0.0033 |
| 7.07E-03 | 0.0406 | 7.44E-03 | 0.0198 | 9.20E-04 | 0.0051 |
| 9.38E-03 | 0.0816 | 8.49E-03 | 0.0293 | 1.02E-03 | 0.007 |
| 1.02E-02 | 0.0957 | 9.54E-03 | 0.0389 | 2.31E-03 | 0.0717 |
| 1.35E-02 | 0.0549 | 1.06E-02 | 0.048 | 3.01E-03 | 0.1062 |
| 2.27E-02 | 0.1625 | 2.27E-02 | 0.1632 | 4.35E-03 | 0.1752 |
| 3.25E-02 | 0.3755 | 3.28E-02 | 0.2924 | 5.01E-03 | 0.2087 |
| 4.30E-02 | 0.6162 | 4.26E-02 | 0.4086 | 6.00E-03 | 0.2601 |
| 5.26E-02 | 0.8448 | 5.28E-02 | 0.5271 | 7.34E-03 | 0.3294 |
| 6.28E-02 | 0.99 | 6.28E-02 | 0.6477 | 9.26E-03 | 0.4312 |
| 7.28E-02 | 1.1963 | 7.27E-02 | 0.765 | 1.01E-02 | 0.4752 |
| 8.30E-02 | 1.3909 | 8.27E-02 | 0.8903 | 1.35E-02 | 0.5056 |
| 9.28E-02 | 1.5438 | 9.27E-02 | 1.0208 | 2.20E-02 | 0.9459 |
| 1.12E-01 | 1.8536 | 1.12E-01 | 1.2199 | 3.22E-02 | 1.4791 |
| 1.61E-01 | 2.5616 | 1.61E-01 | 1.7127 | 4.21E-02 | 2.0048 |
| 2.10E-01 | 3.3647 | 2.11E-01 | 2.2445 | 5.21E-02 | 2.535 |
| 2.61E-01 | 4.05 | 2.60E-01 | 3.1095 | 6.22E-02 | 3.0675 |
| 3.10E-01 | 4.7398 | 3.09E-01 | 4.3808 | 7.22E-02 | 3.6019 |
| 3.61E-01 | 5.5537 | 3.61E-01 | 5.2328 | 8.22E-02 | 4.1331 |
| 4.10E-01 | 6.1584 | 4.11E-01 | 5.81 | 9.22E-02 | 4.6672 |
| 4.61E-01 | 6.9578 | 4.61E-01 | 6.3108 | 1.10E-01 | 5.5977 |
| 5.10E-01 | 7.614 | 5.11E-01 | 6.7296 | 1.56E-01 | 7.9272 |
| 5.61E-01 | 8.4004 | 5.61E-01 | 7.157 | 2.06E-01 | 10.4368 |
| 6.10E-01 | 9.0046 | 6.11E-01 | 7.5382 | 2.56E-01 | 12.8987 |
| 6.62E-01 | 9.8251 | 6.61E-01 | 7.9331 | 3.06E-01 | 15.3777 |
| 7.09E-01 | 10.3263 | 7.11E-01 | 8.3336 | 3.55E-01 | 17.7684 |
| 7.62E-01 | 11.1128 | 7.61E-01 | 8.6557 | 4.05E-01 | 20.1999 |
| 8.10E-01 | 11.5992 | 8.11E-01 | 9.0427 | 4.55E-01 | 22.5569 |
| 8.62E-01 | 12.3123 | 8.62E-01 | 9.3019 | 5.05E-01 | 24.9521 |
| 9.09E-01 | 12.7777 | 9.11E-01 | 9.6254 | 5.55E-01 | 27.2931 |
| 9.61E-01 | 13.6608 | 9.61E-01 | 10.0099 | 6.05E-01 | 29.6474 |
| 9.99E-01 | 14.0967 | 9.99E-01 | 10.2924 | 6.55E-01 | 31.925 |
| | | | | 7.05E-01 | 34.265 |
| | | | | 7.55E-01 | 36.5264 |
| | | | | 8.05E-01 | 38.8426 |
| | | | | 8.55E-01 | 41.0917 |
| | | | | 9.04E-01 | 43.3739 |
| | | | | 9.55E-01 | 45.6917 |
| | | | | 9.99E-01 | 47.9284 |

Table S18. CH₄ adsorption data of SNU-170', SNU-171', SNU-172' and SNU-173' at 195 K.

| SNU-170' | | SNU-171' | | SNU-172' | | SNU-173' | |
|----------|---|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 2.10E-04 | 0.0073 | 1.87E-04 | 0.0756 | 1.07E-04 | 0.0204 | 2.35E-04 | 0.2501 |
| 3.02E-04 | 0.0215 | 2.92E-04 | 0.1484 | 2.09E-04 | 0.0645 | 2.35E-04 | 0.2478 |
| 4.02E-04 | 0.0369 | 3.99E-04 | 0.2178 | 3.14E-04 | 0.1049 | 3.00E-04 | 0.3271 |
| 5.07E-04 | 0.0535 | 5.04E-04 | 0.2848 | 4.08E-04 | 0.1404 | 7.63E-04 | 0.9623 |
| 5.98E-04 | 0.0678 | 6.08E-04 | 0.3501 | 5.05E-04 | 0.177 | 7.25E-04 | 0.9187 |
| 7.49E-04 | 0.0928 | 7.12E-04 | 0.4137 | 6.03E-04 | 0.216 | 7.15E-04 | 0.8982 |
| 8.12E-04 | 0.1014 | 8.14E-04 | 0.4763 | 7.05E-04 | 0.2548 | 7.21E-04 | 0.8993 |
| 9.05E-04 | 0.1135 | 9.16E-04 | 0.5376 | 8.07E-04 | 0.2926 | 1.16E-03 | 1.4573 |
| 9.99E-04 | 0.1295 | 1.02E-03 | 0.5984 | 9.08E-04 | 0.3299 | 1.12E-03 | 1.4141 |
| 2.11E-03 | 0.3345 | 1.02E-03 | 0.5998 | 1.01E-03 | 0.3673 | 1.11E-03 | 1.3944 |
| 3.07E-03 | 0.5091 | 2.12E-03 | 1.2587 | 2.02E-03 | 0.7703 | 2.23E-03 | 2.7496 |
| 4.10E-03 | 0.684 | 3.10E-03 | 1.8298 | 3.03E-03 | 1.1701 | 3.34E-03 | 3.989 |
| 5.09E-03 | 0.8529 | 4.16E-03 | 2.4258 | 4.03E-03 | 1.556 | 4.43E-03 | 5.1052 |
| 6.08E-03 | 1.0007 | 5.02E-03 | 2.8982 | 5.03E-03 | 1.9374 | 5.48E-03 | 6.1106 |
| 7.10E-03 | 1.1622 | 6.19E-03 | 3.5298 | 6.09E-03 | 2.336 | 6.56E-03 | 7.0918 |
| 8.78E-03 | 1.3931 | 7.07E-03 | 3.994 | 7.87E-03 | 2.995 | 7.71E-03 | 8.0815 |
| 9.59E-03 | 1.51 | 8.74E-03 | 4.8649 | 8.53E-03 | 3.2325 | 8.21E-03 | 8.5 |
| 1.18E-02 | 1.8249 | 9.23E-03 | 5.1123 | 9.36E-03 | 3.5349 | 9.19E-03 | 9.2948 |
| 2.07E-02 | 2.7055 | 1.11E-02 | 6.0114 | 1.09E-02 | 4.0909 | 1.02E-02 | 10.2832 |
| 3.23E-02 | 3.8866 | 1.94E-02 | 10.1116 | 1.81E-02 | 6.845 | 1.86E-02 | 16.3065 |
| 4.07E-02 | 4.6434 | 3.08E-02 | 15.3343 | 2.93E-02 | 10.7939 | 3.00E-02 | 23.3049 |
| 5.04E-02 | 5.3626 | 3.94E-02 | 19.0177 | 3.77E-02 | 13.5817 | 3.95E-02 | 28.2314 |
| 6.15E-02 | 6.1645 | 5.05E-02 | 23.6429 | 4.71E-02 | 16.6638 | 5.08E-02 | 33.7564 |
| 7.10E-02 | 6.7007 | 5.96E-02 | 27.1289 | 5.72E-02 | 19.6497 | 5.83E-02 | 36.9708 |
| 8.11E-02 | 7.2165 | 6.96E-02 | 30.667 | 6.74E-02 | 22.5203 | 6.78E-02 | 40.7751 |
| 9.15E-02 | 7.6931 | 7.97E-02 | 34.0282 | 7.78E-02 | 25.3408 | 7.76E-02 | 44.6286 |
| 1.10E-01 | 8.5438 | 8.99E-02 | 37.4804 | 8.84E-02 | 27.9802 | 8.81E-02 | 48.5022 |
| 1.58E-01 | 10.6469 | 1.02E-01 | 41.3862 | 9.92E-02 | 30.6422 | 9.89E-02 | 52.3693 |
| 2.07E-01 | 12.7809 | 1.55E-01 | 58.6722 | 1.41E-01 | 41.9046 | 1.43E-01 | 67.215 |
| 2.58E-01 | 14.5743 | 1.99E-01 | 71.3855 | 1.89E-01 | 53.6654 | 1.93E-01 | 81.6484 |
| 3.08E-01 | 16.4272 | 2.56E-01 | 86.3214 | 2.39E-01 | 65.178 | 2.54E-01 | 96.2455 |
| 3.58E-01 | 18.1504 | 2.87E-01 | 94.1204 | 2.88E-01 | 75.8193 | 2.85E-01 | 103.0737 |
| 4.09E-01 | 19.6756 | 3.55E-01 | 109.2576 | 3.39E-01 | 86.1631 | 3.56E-01 | 115.8551 |
| 4.58E-01 | 21.2011 | 3.90E-01 | 116.1238 | 3.90E-01 | 95.6541 | 3.90E-01 | 121.3605 |
| 5.08E-01 | 22.798 | 4.35E-01 | 124.2092 | 4.51E-01 | 105.8713 | 4.37E-01 | 127.6023 |
| 5.58E-01 | 24.2609 | 4.83E-01 | 132.7052 | 4.83E-01 | 110.7336 | 4.85E-01 | 134.0581 |
| 6.08E-01 | 25.7473 | 5.34E-01 | 140.6456 | 5.51E-01 | 120.5689 | 5.36E-01 | 140.3337 |
| 6.58E-01 | 27.185 | 5.86E-01 | 148.1236 | 5.83E-01 | 125.0467 | 5.88E-01 | 145.7663 |
| 7.08E-01 | 28.5114 | 6.39E-01 | 154.9393 | 6.24E-01 | 130.7631 | 6.40E-01 | 150.9361 |
| 7.58E-01 | 29.8707 | 7.04E-01 | 162.676 | 6.71E-01 | 136.968 | 7.06E-01 | 156.4326 |
| 8.08E-01 | 31.2475 | 7.57E-01 | 168.2797 | 7.54E-01 | 145.7328 | 7.58E-01 | 160.4465 |
| 8.58E-01 | 32.557 | 8.08E-01 | 173.1402 | 8.02E-01 | 150.1959 | 8.00E-01 | 163.3139 |
| 9.09E-01 | 33.7239 | 8.58E-01 | 177.6942 | 8.54E-01 | 154.4262 | 8.58E-01 | 167.1302 |
| 9.59E-01 | 35.0143 | 9.00E-01 | 181.1832 | 9.03E-01 | 158.6328 | 9.01E-01 | 169.8 |
| 9.99E-01 | 36.1823 | 9.58E-01 | 185.7934 | 9.53E-01 | 162.7287 | 9.50E-01 | 172.357 |
| | | 9.97E-01 | 188.5422 | 9.99E-01 | 166.1484 | 9.96E-01 | 175.0581 |

Table S19. CH₄ adsorption data of SNU-174', SNU-175' and SNU-176' at 195 K.

| SNU-174' | | SNU-175' | | SNU-176' | |
|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 9.50E-05 | 0.0363 | 2.62E-01 | 0.0034 | 9.52E-05 | 0.0124 |
| 2.10E-04 | 0.0517 | 3.12E-01 | 0.0629 | 1.96E-04 | 0.0658 |
| 3.08E-04 | 0.0648 | 3.62E-01 | 0.1601 | 3.02E-04 | 0.1146 |
| 4.11E-04 | 0.0787 | 4.12E-01 | 0.2369 | 3.95E-04 | 0.156 |
| 5.11E-04 | 0.0924 | 4.62E-01 | 0.3149 | 4.94E-04 | 0.2001 |
| 6.04E-04 | 0.1051 | 5.12E-01 | 0.4249 | 6.27E-04 | 0.2582 |
| 7.03E-04 | 0.1188 | 5.62E-01 | 0.5073 | 7.08E-04 | 0.2927 |
| 8.23E-04 | 0.1355 | 6.12E-01 | 0.6081 | 7.98E-04 | 0.3313 |
| 9.28E-04 | 0.1501 | 6.61E-01 | 0.7359 | 8.97E-04 | 0.3735 |
| 1.02E-03 | 0.1612 | 7.11E-01 | 0.8425 | 9.97E-04 | 0.4163 |
| 2.05E-03 | 0.3094 | 7.62E-01 | 0.9248 | 2.01E-03 | 0.8897 |
| 3.11E-03 | 0.4642 | 8.11E-01 | 1.1084 | 3.02E-03 | 1.3455 |
| 4.03E-03 | 0.5896 | 8.61E-01 | 1.2543 | 4.08E-03 | 1.8186 |
| 5.06E-03 | 0.7289 | 9.12E-01 | 1.4023 | 5.10E-03 | 2.2629 |
| 6.12E-03 | 0.8677 | 9.61E-01 | 1.7698 | 6.07E-03 | 2.6814 |
| 7.18E-03 | 1.004 | 9.99E-01 | 1.9346 | 7.14E-03 | 3.1296 |
| 8.24E-03 | 1.1372 | | | 8.18E-03 | 3.5685 |
| 9.29E-03 | 1.2672 | | | 9.33E-03 | 4.0433 |
| 1.04E-02 | 1.3951 | | | 1.12E-02 | 4.804 |
| 2.08E-02 | 2.4191 | | | 2.00E-02 | 8.3896 |
| 3.09E-02 | 3.3735 | | | 2.97E-02 | 12.0923 |
| 4.11E-02 | 4.2672 | | | 3.97E-02 | 15.7319 |
| 5.90E-02 | 5.6673 | | | 5.09E-02 | 19.7709 |
| 6.23E-02 | 5.9795 | | | 5.71E-02 | 21.8177 |
| 7.16E-02 | 6.6705 | | | 7.11E-02 | 26.2074 |
| 8.15E-02 | 7.3951 | | | 7.74E-02 | 28.0401 |
| 9.15E-02 | 8.097 | | | 8.97E-02 | 31.5453 |
| 1.10E-01 | 9.2856 | | | 1.02E-01 | 35.1843 |
| 1.56E-01 | 12.1389 | | | 1.49E-01 | 48.9149 |
| 2.06E-01 | 14.9964 | | | 1.99E-01 | 62.3057 |
| 2.56E-01 | 17.8377 | | | 2.49E-01 | 74.7583 |
| 3.06E-01 | 20.5434 | | | 2.85E-01 | 83.132 |
| 3.56E-01 | 23.1614 | | | 3.55E-01 | 98.3539 |
| 4.06E-01 | 25.7495 | | | 3.90E-01 | 105.0183 |
| 4.56E-01 | 28.2859 | | | 4.35E-01 | 113.0346 |
| 5.06E-01 | 30.7575 | | | 4.82E-01 | 121.5954 |
| 5.56E-01 | 33.2086 | | | 5.32E-01 | 129.7184 |
| 6.06E-01 | 35.6256 | | | 5.82E-01 | 137.866 |
| 6.56E-01 | 38.0027 | | | 6.33E-01 | 145.5986 |
| 7.06E-01 | 40.3904 | | | 6.85E-01 | 152.6857 |
| 7.56E-01 | 42.7207 | | | 7.37E-01 | 159.2057 |
| 8.06E-01 | 45.0207 | | | 7.88E-01 | 165.42 |
| 8.56E-01 | 47.3115 | | | 8.54E-01 | 172.5957 |
| 9.06E-01 | 49.6033 | | | 9.07E-01 | 177.7857 |
| 9.56E-01 | 51.8603 | | | 9.57E-01 | 182.4171 |
| 9.99E-01 | 53.971 | | | 9.94E-01 | 185.7257 |

Table S20. CH₄ adsorption data of SNU-170', SNU-171', SNU-172' and SNU-173' at 273 K.

| SNU-170' | | SNU-171' | | SNU-172' | | SNU-173' | |
|----------|---|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 9.19E-03 | 0.0011 | 6.01E-03 | 0.0026 | 2.19E-04 | 0.0002 | 2.24E-02 | 0.1585 |
| 9.87E-03 | 0.0038 | 7.08E-03 | 0.0213 | 3.17E-04 | 0.0012 | 3.21E-02 | 0.4028 |
| 1.30E-02 | 0.0655 | 9.42E-03 | 0.0711 | 4.18E-04 | 0.0023 | 4.23E-02 | 0.6549 |
| 2.27E-02 | 0.1475 | 1.00E-02 | 0.079 | 5.18E-04 | 0.0034 | 6.06E-02 | 1.1015 |
| 3.26E-02 | 0.2045 | 1.31E-02 | 0.0915 | 6.17E-04 | 0.0044 | 6.28E-02 | 1.1582 |
| 4.26E-02 | 0.2879 | 2.28E-02 | 0.2924 | 7.17E-04 | 0.0055 | 7.23E-02 | 1.3835 |
| 5.32E-02 | 0.41 | 3.27E-02 | 0.4977 | 8.18E-04 | 0.0066 | 8.23E-02 | 1.6239 |
| 6.26E-02 | 0.4704 | 4.29E-02 | 0.6793 | 9.17E-04 | 0.0076 | 9.23E-02 | 1.8648 |
| 7.32E-02 | 0.5814 | 5.25E-02 | 0.8819 | 1.02E-03 | 0.0087 | 1.11E-01 | 2.3072 |
| 8.27E-02 | 0.6877 | 6.24E-02 | 1.1405 | 2.29E-03 | 0.0344 | 1.58E-01 | 3.4474 |
| 9.27E-02 | 0.7974 | 7.26E-02 | 1.3442 | 3.20E-03 | 0.0526 | 2.08E-01 | 4.6191 |
| 1.12E-01 | 1.0257 | 8.28E-02 | 1.5984 | 4.20E-03 | 0.0727 | 2.58E-01 | 5.7994 |
| 1.61E-01 | 1.5382 | 9.29E-02 | 1.8214 | 5.30E-03 | 0.0947 | 3.08E-01 | 6.9626 |
| 2.11E-01 | 2.0672 | 1.11E-01 | 2.2021 | 6.18E-03 | 0.1119 | 3.58E-01 | 8.1254 |
| 2.61E-01 | 2.6383 | 1.60E-01 | 3.2651 | 7.17E-03 | 0.1318 | 4.08E-01 | 9.2785 |
| 3.10E-01 | 3.2217 | 2.10E-01 | 4.348 | 9.01E-03 | 0.1697 | 4.58E-01 | 10.4261 |
| 3.61E-01 | 3.8039 | 2.60E-01 | 5.4209 | 9.77E-03 | 0.1852 | 5.08E-01 | 11.5615 |
| 4.10E-01 | 4.4507 | 3.10E-01 | 6.4661 | 1.28E-02 | 0.2285 | 5.58E-01 | 12.6808 |
| 4.61E-01 | 4.8747 | 3.60E-01 | 7.4989 | 2.17E-02 | 0.4105 | 6.08E-01 | 13.8021 |
| 5.11E-01 | 5.442 | 4.09E-01 | 8.5963 | 3.20E-02 | 0.6177 | 6.58E-01 | 14.9023 |
| 5.61E-01 | 5.8676 | 4.59E-01 | 9.5523 | 4.20E-02 | 0.8208 | 7.08E-01 | 15.995 |
| 6.11E-01 | 6.4594 | 5.10E-01 | 10.5785 | 5.14E-02 | 1.0108 | 7.58E-01 | 17.0865 |
| 6.61E-01 | 6.8965 | 5.60E-01 | 11.5608 | 6.16E-02 | 1.2161 | 8.08E-01 | 18.1464 |
| 7.10E-01 | 7.4793 | 6.09E-01 | 12.5576 | 7.19E-02 | 1.4267 | 8.58E-01 | 19.2086 |
| 7.61E-01 | 8.0721 | 6.59E-01 | 13.5271 | 8.17E-02 | 1.627 | 9.08E-01 | 20.2787 |
| 8.11E-01 | 8.5239 | 7.10E-01 | 14.5434 | 9.18E-02 | 1.8329 | 9.58E-01 | 21.3343 |
| 8.61E-01 | 8.9868 | 7.59E-01 | 15.5388 | 1.10E-01 | 2.1949 | 9.99E-01 | 22.2866 |
| 9.11E-01 | 9.555 | 8.09E-01 | 16.5288 | 1.56E-01 | 3.1308 | | |
| 9.61E-01 | 10.0152 | 8.60E-01 | 17.4501 | 2.05E-01 | 4.1413 | | |
| 9.99E-01 | 10.6843 | 9.09E-01 | 18.4093 | 2.55E-01 | 5.142 | | |
| | | 9.60E-01 | 19.3073 | 3.05E-01 | 6.1509 | | |
| | | 9.99E-01 | 20.2397 | 3.55E-01 | 7.1276 | | |
| | | | | 4.05E-01 | 8.1348 | | |
| | | | | 4.55E-01 | 9.1037 | | |
| | | | | 5.05E-01 | 10.0901 | | |
| | | | | 5.55E-01 | 11.0565 | | |
| | | | | 6.05E-01 | 12.0253 | | |
| | | | | 6.55E-01 | 12.9792 | | |
| | | | | 7.05E-01 | 13.9394 | | |
| | | | | 7.55E-01 | 14.8803 | | |
| | | | | 8.05E-01 | 15.8422 | | |
| | | | | 8.55E-01 | 16.7762 | | |
| | | | | 9.05E-01 | 17.682 | | |
| | | | | 9.55E-01 | 18.5909 | | |
| | | | | 9.99E-01 | 19.4387 | | |

Table S21. CH₄ adsorption data of SNU-174', SNU-175' and SNU-176' at 273 K.

| SNU-174' | | SNU-175' | | SNU-176' | |
|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 4.30E-02 | 0.0648 | 3.12E-01 | 0.018 | 2.33E-03 | 0.0217 |
| 5.31E-02 | 0.1325 | 3.62E-01 | 0.1402 | 3.23E-03 | 0.0395 |
| 6.32E-02 | 0.2024 | 4.12E-01 | 0.2529 | 4.04E-03 | 0.0563 |
| 7.27E-02 | 0.2923 | 4.62E-01 | 0.3874 | 5.04E-03 | 0.0777 |
| 8.28E-02 | 0.3156 | 5.12E-01 | 0.5163 | 6.25E-03 | 0.1033 |
| 9.27E-02 | 0.4127 | 5.62E-01 | 0.63 | 7.01E-03 | 0.119 |
| 1.12E-01 | 0.547 | 6.12E-01 | 0.7691 | 9.08E-03 | 0.1657 |
| 1.61E-01 | 0.9367 | 6.62E-01 | 0.8953 | 9.87E-03 | 0.1826 |
| 2.11E-01 | 1.4125 | 7.11E-01 | 1.0672 | 1.29E-02 | 0.2084 |
| 2.61E-01 | 1.7224 | 7.61E-01 | 1.2608 | 2.24E-02 | 0.4048 |
| 3.11E-01 | 2.2126 | 8.11E-01 | 1.4728 | 3.25E-02 | 0.6197 |
| 3.61E-01 | 2.5853 | 8.62E-01 | 1.5747 | 4.27E-02 | 0.8356 |
| 4.11E-01 | 3.0372 | 9.12E-01 | 1.719 | 5.23E-02 | 1.041 |
| 4.61E-01 | 3.4497 | 9.61E-01 | 1.9224 | 6.28E-02 | 1.2661 |
| 5.11E-01 | 3.8493 | 9.99E-01 | 1.9959 | 7.28E-02 | 1.4823 |
| 5.61E-01 | 4.1905 | | | 8.26E-02 | 1.6917 |
| 6.11E-01 | 4.6359 | | | 9.26E-02 | 1.912 |
| 6.62E-01 | 4.9726 | | | 1.11E-01 | 2.3131 |
| 7.10E-01 | 5.4106 | | | 1.60E-01 | 3.3738 |
| 7.61E-01 | 5.6554 | | | 2.09E-01 | 4.48 |
| 8.10E-01 | 6.1475 | | | 2.60E-01 | 5.5552 |
| 8.61E-01 | 6.4504 | | | 3.09E-01 | 6.6581 |
| 9.12E-01 | 6.8434 | | | 3.60E-01 | 7.6925 |
| 9.61E-01 | 7.1984 | | | 4.09E-01 | 8.7715 |
| 9.99E-01 | 7.6518 | | | 4.59E-01 | 9.8133 |
| | | | | 5.09E-01 | 10.8846 |
| | | | | 5.59E-01 | 11.9118 |
| | | | | 6.09E-01 | 12.9254 |
| | | | | 6.59E-01 | 13.9155 |
| | | | | 7.10E-01 | 14.9759 |
| | | | | 7.59E-01 | 15.976 |
| | | | | 8.09E-01 | 16.9911 |
| | | | | 8.59E-01 | 17.9751 |
| | | | | 9.09E-01 | 18.9883 |
| | | | | 9.59E-01 | 19.9531 |
| | | | | 9.99E-01 | 20.9094 |

Table S22. CH₄ adsorption data of SNU-170', SNU-171', SNU-172' and SNU-173' at 298 K.

| SNU-170' | | SNU-171' | | SNU-172' | | SNU-173' | |
|----------|---|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 1.62E-01 | 0.3189 | 1.27E-02 | 0.1442 | 2.00E-03 | 0.0094 | 2.28E-02 | 0.0471 |
| 2.12E-01 | 0.7472 | 2.23E-02 | 0.2577 | 3.36E-03 | 0.0243 | 3.26E-02 | 0.1741 |
| 2.61E-01 | 1.0319 | 3.19E-02 | 0.3755 | 4.01E-03 | 0.0313 | 4.26E-02 | 0.3051 |
| 3.11E-01 | 1.4084 | 4.22E-02 | 0.4958 | 5.31E-03 | 0.0457 | 6.13E-02 | 0.5391 |
| 3.61E-01 | 1.7068 | 5.24E-02 | 0.6544 | 6.21E-03 | 0.0552 | 6.29E-02 | 0.5624 |
| 4.11E-01 | 2.1507 | 6.21E-02 | 0.728 | 7.22E-03 | 0.0661 | 7.27E-02 | 0.6888 |
| 4.61E-01 | 2.452 | 7.18E-02 | 0.8493 | 9.15E-03 | 0.0885 | 8.26E-02 | 0.8165 |
| 5.11E-01 | 2.739 | 8.18E-02 | 0.9864 | 9.89E-03 | 0.0969 | 9.26E-02 | 0.94 |
| 5.61E-01 | 3.0865 | 9.17E-02 | 1.0997 | 1.30E-02 | 0.1145 | 1.11E-01 | 1.1769 |
| 6.12E-01 | 3.3039 | 1.11E-01 | 1.3012 | 2.27E-02 | 0.2259 | 1.60E-01 | 1.7902 |
| 6.62E-01 | 3.5849 | 1.60E-01 | 1.8972 | 3.22E-02 | 0.3287 | 2.10E-01 | 2.4063 |
| 7.11E-01 | 4.1352 | 2.09E-01 | 2.5395 | 4.19E-02 | 0.441 | 2.60E-01 | 3.042 |
| 7.61E-01 | 4.3341 | 2.59E-01 | 3.0927 | 5.25E-02 | 0.563 | 3.10E-01 | 3.6685 |
| 8.11E-01 | 4.7704 | 3.09E-01 | 3.78 | 6.23E-02 | 0.6763 | 3.60E-01 | 4.3075 |
| 8.61E-01 | 4.9761 | 3.59E-01 | 4.3869 | 7.23E-02 | 0.7917 | 4.10E-01 | 4.9397 |
| 9.11E-01 | 5.4322 | 4.09E-01 | 5.0226 | 8.23E-02 | 0.9086 | 4.60E-01 | 5.5691 |
| 9.61E-01 | 5.7731 | 4.59E-01 | 5.5634 | 9.23E-02 | 1.0234 | 5.10E-01 | 6.2114 |
| 9.99E-01 | 6.1636 | 5.09E-01 | 6.1903 | 1.11E-01 | 1.2305 | 5.60E-01 | 6.8372 |
| | | 5.59E-01 | 6.6569 | 1.58E-01 | 1.7712 | 6.10E-01 | 7.4602 |
| | | 6.09E-01 | 7.352 | 2.08E-01 | 2.3589 | 6.60E-01 | 8.0752 |
| | | 6.59E-01 | 7.9488 | 2.58E-01 | 2.9282 | 7.10E-01 | 8.6984 |
| | | 7.09E-01 | 8.6013 | 3.08E-01 | 3.5044 | 7.60E-01 | 9.3256 |
| | | 7.59E-01 | 9.0452 | 3.58E-01 | 4.0667 | 8.10E-01 | 9.917 |
| | | 8.09E-01 | 9.6914 | 4.08E-01 | 4.6577 | 8.60E-01 | 10.5356 |
| | | 8.59E-01 | 10.312 | 4.58E-01 | 5.1961 | 9.10E-01 | 11.1555 |
| | | 9.09E-01 | 10.8992 | 5.08E-01 | 5.7649 | 9.60E-01 | 11.7526 |
| | | 9.59E-01 | 11.3384 | 5.58E-01 | 6.3348 | 9.99E-01 | 12.3071 |
| | | 9.99E-01 | 12.0026 | 6.07E-01 | 6.8907 | | |
| | | | | 6.58E-01 | 7.4465 | | |
| | | | | 7.08E-01 | 8.024 | | |
| | | | | 7.58E-01 | 8.5791 | | |
| | | | | 8.08E-01 | 9.131 | | |
| | | | | 8.58E-01 | 9.6807 | | |
| | | | | 9.08E-01 | 10.2327 | | |
| | | | | 9.58E-01 | 10.7708 | | |
| | | | | 9.99E-01 | 11.2639 | | |

Table S23. CH₄ adsorption data of SNU-174', SNU-175' and SNU-176' at 298 K.

| SNU-174' | | SNU-175' | | SNU-176' | |
|----------|---|----------|---|----------|---|
| P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) | P (atm) | V _{ads} (cm ³ g ⁻¹) |
| 1.12E-01 | 0.0514 | Nil | Nil | 4.31E-03 | 0.0083 |
| 1.61E-01 | 0.2658 | | | 5.04E-03 | 0.0151 |
| 2.11E-01 | 0.525 | | | 6.09E-03 | 0.0263 |
| 2.61E-01 | 0.6984 | | | 7.26E-03 | 0.0377 |
| 3.11E-01 | 0.9429 | | | 9.21E-03 | 0.0613 |
| 3.62E-01 | 1.1115 | | | 9.91E-03 | 0.0688 |
| 4.12E-01 | 1.3638 | | | 1.32E-02 | 0.0354 |
| 4.62E-01 | 1.5356 | | | 2.33E-02 | 0.1454 |
| 5.12E-01 | 1.7467 | | | 3.28E-02 | 0.2454 |
| 5.61E-01 | 1.9055 | | | 4.27E-02 | 0.3522 |
| 6.11E-01 | 2.2143 | | | 5.31E-02 | 0.4672 |
| 6.61E-01 | 2.3531 | | | 6.31E-02 | 0.5765 |
| 7.11E-01 | 2.5944 | | | 7.31E-02 | 0.6878 |
| 7.61E-01 | 2.6735 | | | 8.30E-02 | 0.8096 |
| 8.11E-01 | 2.9558 | | | 9.30E-02 | 0.9252 |
| 8.61E-01 | 3.1678 | | | 1.12E-01 | 1.1372 |
| 9.11E-01 | 3.4642 | | | 1.61E-01 | 1.7119 |
| 9.61E-01 | 3.5986 | | | 2.11E-01 | 2.3352 |
| 9.99E-01 | 3.8696 | | | 2.61E-01 | 2.8965 |
| | | | | 3.11E-01 | 3.5343 |
| | | | | 3.61E-01 | 4.0947 |
| | | | | 4.11E-01 | 4.6821 |
| | | | | 4.61E-01 | 5.293 |
| | | | | 5.10E-01 | 5.8703 |
| | | | | 5.61E-01 | 6.4348 |
| | | | | 6.11E-01 | 7.0155 |
| | | | | 6.61E-01 | 7.5451 |
| | | | | 7.11E-01 | 8.1547 |
| | | | | 7.61E-01 | 8.6802 |
| | | | | 8.11E-01 | 9.2801 |
| | | | | 8.61E-01 | 9.857 |
| | | | | 9.11E-01 | 10.4222 |
| | | | | 9.61E-01 | 11.0046 |
| | | | | 9.99E-01 | 11.5466 |