

Supporting information

Stabilization of Cu(0)-nanoparticles into the nanopores of modified montmorillonite: An implication on catalytic approach for “Click” reaction between azides and terminal alkynes

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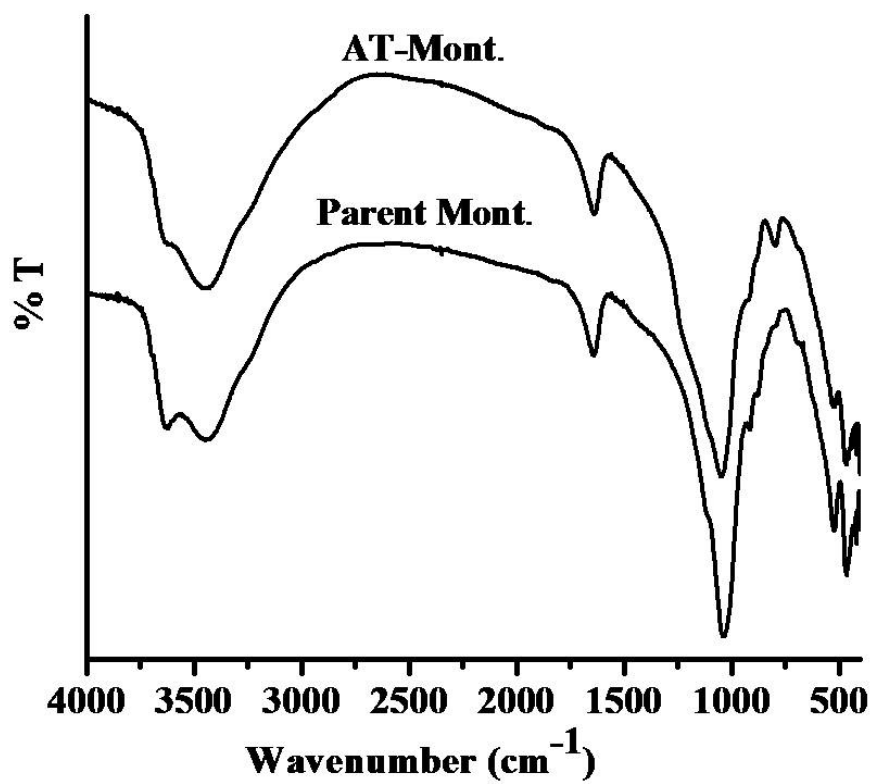


Fig. 1: FTIR spectra of different montmorillonite.

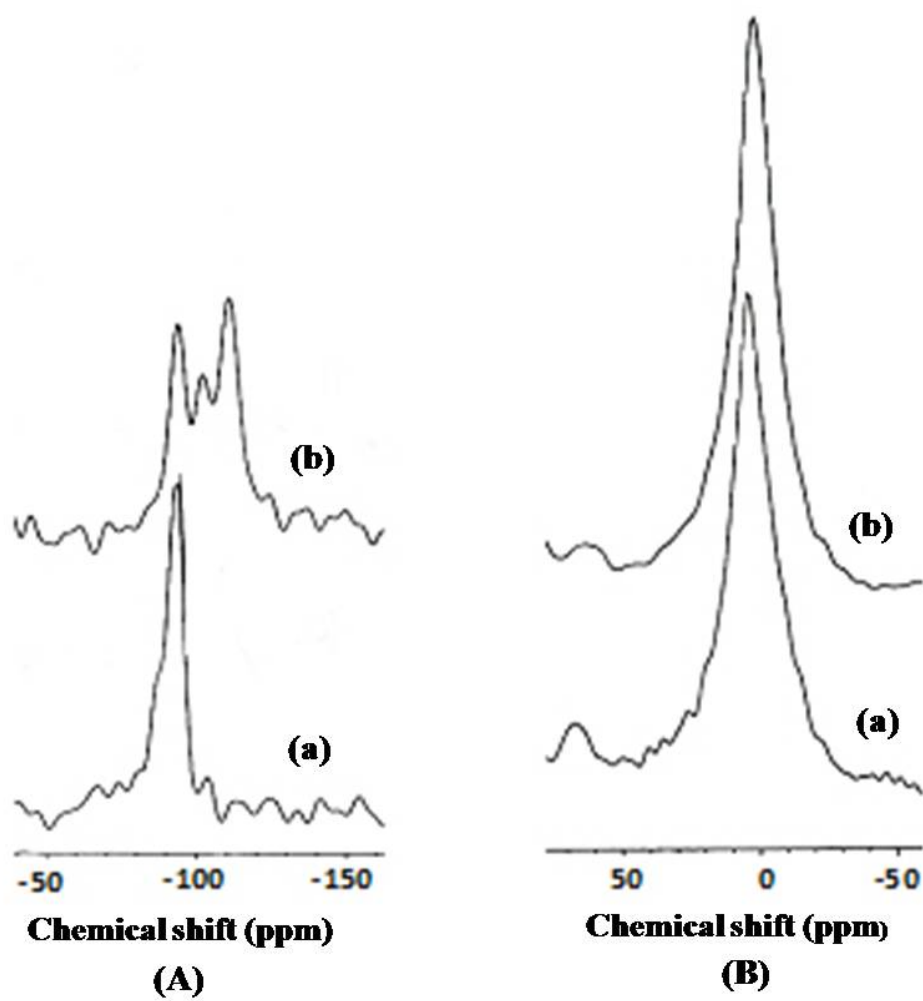
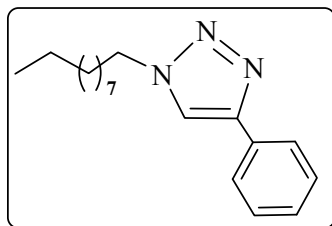
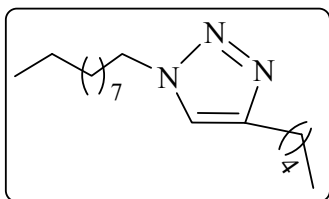


Fig. 2: (A) ^{29}Si and (B) ^{27}Al MAS-NMR spectra of (a) Parent Mont. (b) AT-Mont.

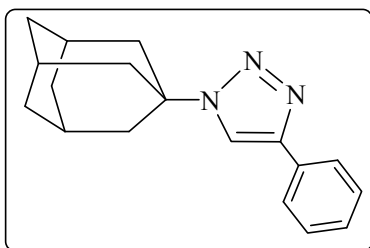
Characterization data of products:



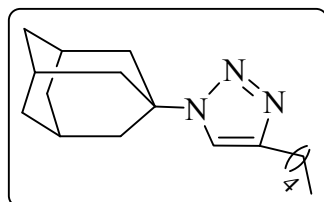
1-Decyl-4-phenyl-1H-[1,2,3]triazole: White solid; Yield: 95%; m.p. 83.6-84.5°C; R_f 0.54 (Ethyl acetate/Hexane = 1:5); ^1H NMR (300 MHz; CDCl_3): δ = 7.85-7.82 (dd, J = 3, 12 Hz, 2H, arom.), 7.74 (s, 1H, triazole), 7.45-7.30 (m, 3H, arom.), 4.40 (t, J = 9 Hz, 2H, CH_2), 1.97-1.92 (m, 2H, CH_2), 1.61 (br s, 6H, CH_2), 1.34-1.33 (m, 2H, CH_2), 1.25 (br s, 6H, CH_2), 0.87 (t, J = 6 Hz, 3H, CH_3); ^{13}C NMR (75 MHz; CDCl_3): δ = 148.0, 130.2, 129.6, 127.5, 124.1, 120.6, 50.3, 31.8, 30.3, 29.7, 26.7, 25.1, 22.4, 14.0; HRMS (ESI): m/z calc. for $\text{C}_{18}\text{H}_{27}\text{N}_3$ 285.435; found 285.2; Elemental analyses: Found: C, 75.65; H, 9.32; N, 14.52%. Calc. for $\text{C}_{18}\text{H}_{27}\text{N}_3$: C, 75.78; H, 9.47; N, 14.73%; FTIR (NaCl thin flim, cm^{-1}): ν 3119, 3090, 1464, 1259, 1215, 1076, 912.



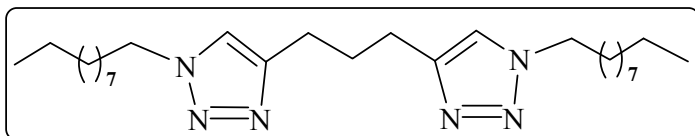
1-Decyl-4-pentyl-1H-[1,2,3]triazole: White solid; Yield: 89%; m.p. 80.6-81.5°C; R_f 0.50 (Ethyl acetate/Hexane = 1:5); ^1H NMR (300 MHz, CDCl_3): δ = 7.24 (s, 1H, triazole), 4.30 (t, J = 9 Hz, 2H, CH_2), 2.70 (t, J = 9 Hz, 2H, CH_2), 1.90-1.85 (m, 2H, CH_2), 1.69-1.64 (m, 2H, CH_2), 1.33 (br s, 6H, CH_2), 1.25 (br s, 12H, CH_2), 0.91 (t, J = 6 Hz, 6H, CH_3); ^{13}C NMR (75 MHz, CDCl_3): δ = 148.4, 120.3, 50.1, 31.8, 31.4, 30.3, 29.4, 29.2, 29.0, 26.5, 25.6, 22.6, 22.4, 14.1, 14.0; HRMS (ESI): m/z calcd. for $\text{C}_{17}\text{H}_{33}\text{N}_3$ 279.472; found 279.3; Elemental analyses: Found: C, 73.01; H, 11.42; N, 14.92%. Calc. for $\text{C}_{17}\text{H}_{33}\text{N}_3$: C, 73.11; H, 11.82; N, 15.05%; FTIR (NaCl thin flim, cm^{-1}): ν 3120, 3087, 1424, 1264, 1202, 996, 917.



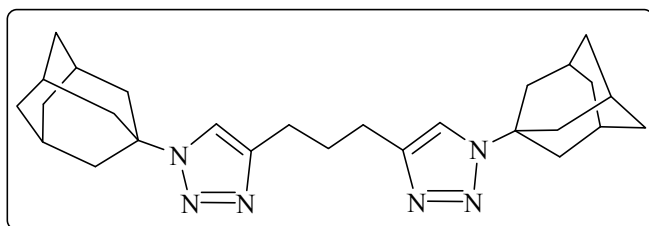
1-Adamantan-1-yl-4-phenyl-1H-[1,2,3]triazole: White solid; Yield: 92%; m.p. 93.6-94.3°C; R_f 0.61 (Ethyl acetate/Hexane = 1:5); ^1H NMR (300 MHz, CDCl_3): δ = 7.85-7.82 (dd, J = 3Hz, 9Hz, 2H, arom.), 7.44 (s, 1H, triazole), 7.42-7.29 (m, 3H, arom.), 2.30 (br s, 3H, CH), 1.81 (br s, 6H, CH_2), 1.58 (br s, 6H, CH_2); ^{13}C NMR (75 MHz, CDCl_3): δ = 147.4, 129.8, 127.6, 125.1, 123.1, 120.6, 50.4, 32.0, 31.7, 30.3, 29.4, 26.5, 25.0, 22.4, 22.4, 17.8; HRMS (ESI): m/z calcd. for $\text{C}_{18}\text{H}_{21}\text{N}_3$ 279.387; found 279.3; Elemental analyses: Found: C, 77.25; H, 7.12; N, 14.92%. Calc. for $\text{C}_{18}\text{H}_{21}\text{N}_3$: C, 77.42; H, 7.52; N, 15.05%; FTIR (NaCl thin flim, cm^{-1}): ν 3118, 3084, 1464, 1243, 1210, 1050, 914.



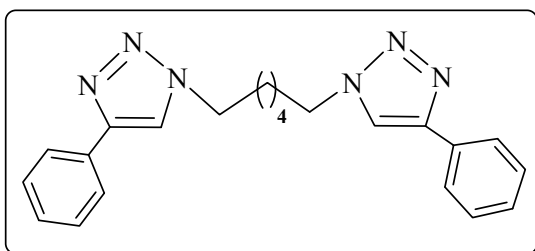
1-Adamantan-1-yl-4-pentyl-1H-[1,2,3]triazole: White solid; Yield: 87%; m.p. 101.3-102.3°C; R_f 0.48 (Ethyl acetate/Hexane = 1:5); ^1H NMR (300 MHz, CDCl_3): δ = 7.32 (s, 1H, triazole), 2.70 (t, J = 9Hz, 2H, CH_2), 2.23 (br s, 3H, CH), 2.00 (br s, 6H, CH_2), 1.78 (br s, 6H, CH_2), 1.73-1.31 (m, 6H, CH_2), 0.898 (t, J = 6Hz, 3H, CH_3); ^{13}C NMR (75 MHz, CDCl_3): δ = 148.1, 120.5, 50.3, 31.7, 31.4, 30.3, 29.7, 29.0, 27.9, 27.0, 26.2, 25.6, 22.6, 22.4, 14.1; HRMS (ESI): m/z calcd. for $\text{C}_{17}\text{H}_{27}\text{N}_3$ 273.424; found 273.2; Elemental analyses: Found: C, 74.15; H, 9.78; N, 15.20%. Calc. for $\text{C}_{17}\text{H}_{27}\text{N}_3$: C, 74.72; H, 9.89; N, 15.38%; FTIR (NaCl thin flim, cm^{-1}): ν 3119, 3074, 1550, 1219, 1147.6, 1101.



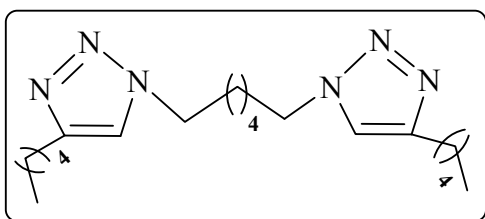
1,3-Bis(1-decyl-1H-1,2,3-triazol-4-yl)propane: White solid; Yield: 92%; m.p. 98-98.5°C; R_f 0.64 (Ethyl acetate/Hexane = 1:1); ^1H NMR (300 MHz, CDCl_3): δ = 7.31 (s, 2H, triazole), 4.30 (t, J = 9 Hz, 4H, CH_2), 2.77 (t, J = 6 Hz, 4H, CH_2), 2.11-2.03 (m, 2H, CH_2), 1.87-1.85 (m, 4H, CH_2), 1.30 (br s, 10H, CH_2), 1.25 (br s, 18H, CH_2), 0.875 (t, J = 6 Hz, 6H, CH_3); ^{13}C NMR (75 MHz, CDCl_3): δ = 148.1, 120.7, 50.6, 31.1, 31.4, 30.3, 29.9, 29.4, 29.1, 26.5, 25.6, 23.6, 22.4, 14.0; HRMS (ESI): m/z calcd. for $\text{C}_{27}\text{H}_{50}\text{N}_6(\text{M}+\text{H})$ 459.48; found 460.3; Elemental analyses: Found: C, 70.74; H, 10.02; N, 18.16%. Calc. for $\text{C}_{27}\text{H}_{50}\text{N}_6$: C, 70.36; H, 10.91; N, 18.34%; FTIR (NaCl thin flim, cm^{-1}): ν 3130, 3074, 1462, 1369, 1261, 1209, 1149, 1058.



1,3-Bis(1-adamantan-1-yl-1H-1,2,3-triazol-4-yl)propane: Brown solid; Yield: 92%; m.p. 91-93.5°C; R_f 0.60 (Ethyl acetate/Hexane = 2:3); ^1H NMR (300 MHz, CDCl_3): δ = 7.35 (s, 1H, triazole), 7.09 (s, 1H, triazole), 2.77 (t, J = 9 Hz, 4H, CH_2), 2.15 (br s, 6H, CH), 1.97-1.71 (m, 2H, CH_2), 1.53 (br s, 12H, CH_2), 1.18 (br s, 12H, CH_2); ^{13}C NMR (75 MHz, CDCl_3): δ = 148.2, 124.5, 50.3, 44.7, 31.8, 31.2, 30.4, 29.7, 29.4, 29.0, 26.5, 25.6, 24.3, 22.6, 22.4, 18.7; HRMS (ESI): m/z calcd. for $\text{C}_{27}\text{H}_{38}\text{N}_6(\text{M}+\text{H})$ 447.651; found 447.4; Elemental analyses: Found: C, 72.39; H, 8.32; N, 18.40%. Calc. for $\text{C}_{27}\text{H}_{38}\text{N}_6$: C, 72.54; H, 8.50; N, 18.80%; FTIR (NaCl thin flim, cm^{-1}): ν 3010, 2912, 1726, 1548, 1454, 1359, 1261, 1143, 1012.



1,6-Bis(4-phenyl-1H-1,2,3-triazole)hexane: Brown solid; Yield: 85%; m.p. 97-98.5°C; R_f 0.56 (Ethyl acetate/Hexane = 2:3); $^1\text{H NMR}$ (300 MHz, CDCl_3): δ = 7.85-7.82 (dd, J = 3, 12 Hz, 4H, arom.), 7.75 (s, 2H, triazole), 7.46-7.34 (m, 6H, CH_2), 4.42 (t, J = 9 Hz, 4H, CH_2), 3.27 (t, J = 6 Hz, 4H, CH_2), 2.00-1.95 (m, 2H, CH_2), 1.64-1.55 (m, 2H, CH_2); $^{13}\text{C NMR}$ (75 MHz, CDCl_3): δ = 148.1, 132.5, 128.2, 127.0, 125.2, 124.3, 51.2, 31.2, 29.5, 29.0, 26.5, 25.6, 20.6; HRMS (ESI): m/z calcd. for $\text{C}_{22}\text{H}_{24}\text{N}_6$ 372.476; found 372.2; Elemental analyses: Found: C, 70.39; H, 6.28; N, 22.34%. Calc. for $\text{C}_{22}\text{H}_{24}\text{N}_6$: C, 70.94; H, 6.49; N, 22.56%; FTIR (NaCl thin flim, cm^{-1}): ν 3118, 2942, 1552, 1464, 1359, 1266, 1113, 1066.



1,6-Bis(4-pentyl-1H-1,2,3-triazole)hexane: Brown solid; Yield: 88%; m.p. 95-97.5°C; R_f 0.52 (Ethyl acetate/Hexane = 2:3); $^1\text{H NMR}$ (300 MHz, CDCl_3): δ = 7.27 (s, 1H, triazole), 7.25 (s, 1H, triazole), 4.32 (t, J = 9 Hz, 4H, CH_2), 3.26 (t, J = 6 Hz, 4H, CH_2), 2.70 (t, J = 6 Hz, 4H, CH_2), 1.90 (t, J = 6 Hz, 4H, CH_2), 1.70-1.56 (m, 6H, CH_2), 1.34 (br s, 6H, CH_2), 0.897 (t, J = 6 Hz, 6H, CH_3); $^{13}\text{C NMR}$ (75 MHz, CDCl_3): δ = 147.4, 124.5, 50.5, 31.4, 30.5, 29.4, 26.5, 25.4, 22.8, 22.4, 20.1, 14.0; HRMS (ESI): m/z calcd. for $\text{C}_{20}\text{H}_{36}\text{N}_6$ 360.55; found 360.4; Elemental analyses: Found: C, 66.55; H, 10.00; N, 23.11%. Calc. for $\text{C}_{20}\text{H}_{36}\text{N}_6$: C, 66.62; H, 10.06; N, 23.31%; FTIR (NaCl thin flim, cm^{-1}): ν 3110, 3012, 1760, 1548, 1319, 1254, 1133, 1031.