

Supporting Information

Triazine functionalized porous organic polymer: Excellent CO₂ storage material and efficient catalyst for Sonogashira C-C cross-coupling reactions

Arindam Modak,¹ Malay Pramanik,¹ Shinji Inagaki,² and Asim Bhaumik*,¹

¹*Department of Materials Science, Indian Association for the Cultivation of Science, Jadavpur,*

Kolkata-700 032, India

²*Toyota Central R&D Laboratories, Inc. Nagakute, Aichi 480-1192, Japan*

Table of Contents

Figure S1	PXRD pattern of TPOP (black) and palladium grafted material Pd-TPOP-1 (red).	Page 2
Figure S2	UV-Visible absorption spectrum of TPOP-1.	Page 3
Figure S3	TG-DTA profile of TPOP-1.	Page 4
Figure S4	(a) N ₂ adsorption-desorption isotherm of Pd-TPOP-1 at 77 K where triangles represents for adsorption and empty circles denote desorption process. (b) NLDT pore size distribution considering N ₂ at 77K on carbon slit pore. Pore Volume = 0.34 cc/g.	Page 5
Figure S5	TG-DTA profile of Pd-TPOP-1.	Page 6
Figure S6	Raman shift of TPOP-1 (black) and Pd-TPOP-1 (blue).	Page 7
Figure S7	CO ₂ adsorption isotherms over three triazine functionalized porous polymeric materials by variation of pyrrole and 4,4',4''-(1,3,5-triazine-2,4,6-triyl)tris(oxy)tribenzaldehyde: 4:3 (TPOP-1-2, a: 273 K, b: 298 K) and 1:1 (TPOP-1-3, c: 273 K, d: 298 K).	Page 8
Figure S8	Recycling efficiency of Pd-TPOP-1 for four successive cross-coupling reactions of iodo benzene with phenyl acetylene	Page 9
NMR data	Spectroscopic data for the reaction products in Sonogashira cross-coupling reaction over Pd-TPOP-1	Pages 10-11

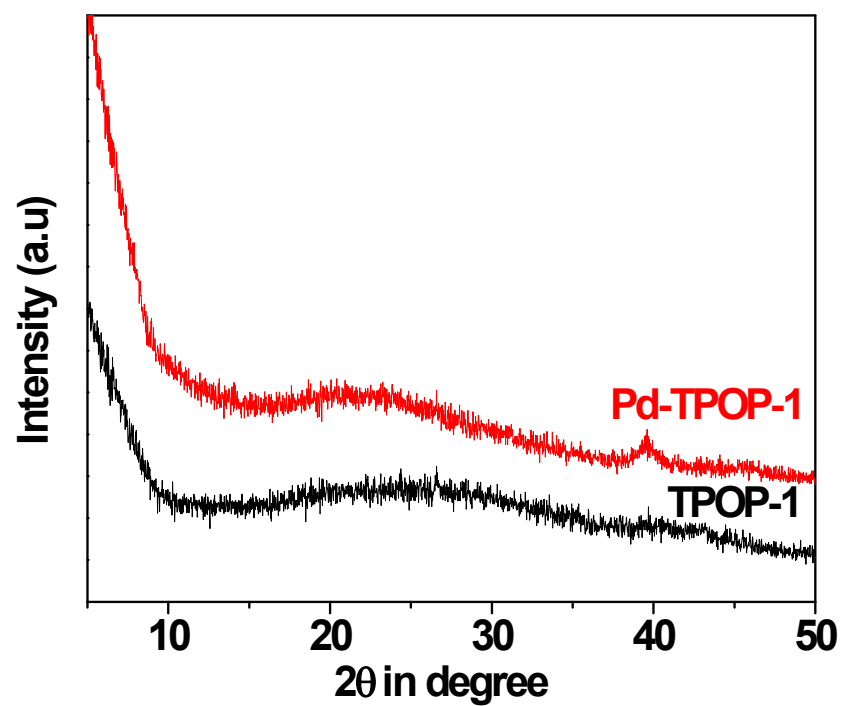


Figure S1. PXRD pattern of TPOP (black) and palladium grafted material Pd-TPOP-1 (red).

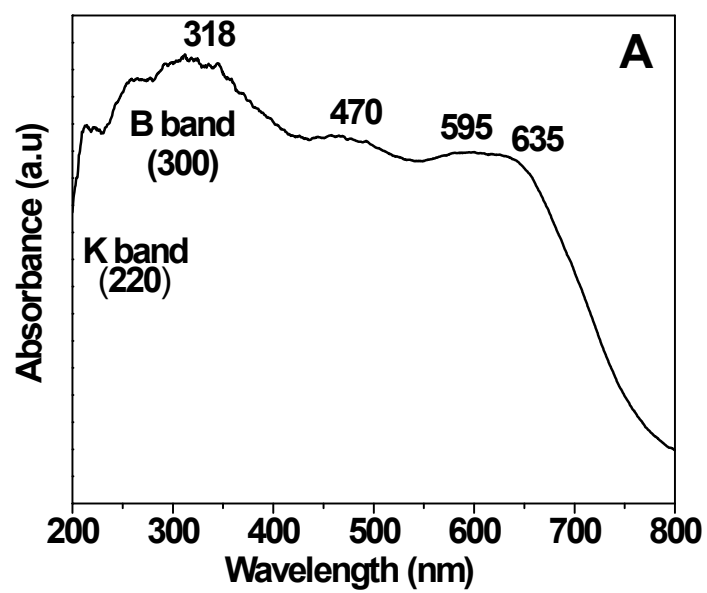


Figure S2. UV-Visible absorption spectrum of TPOP-1.

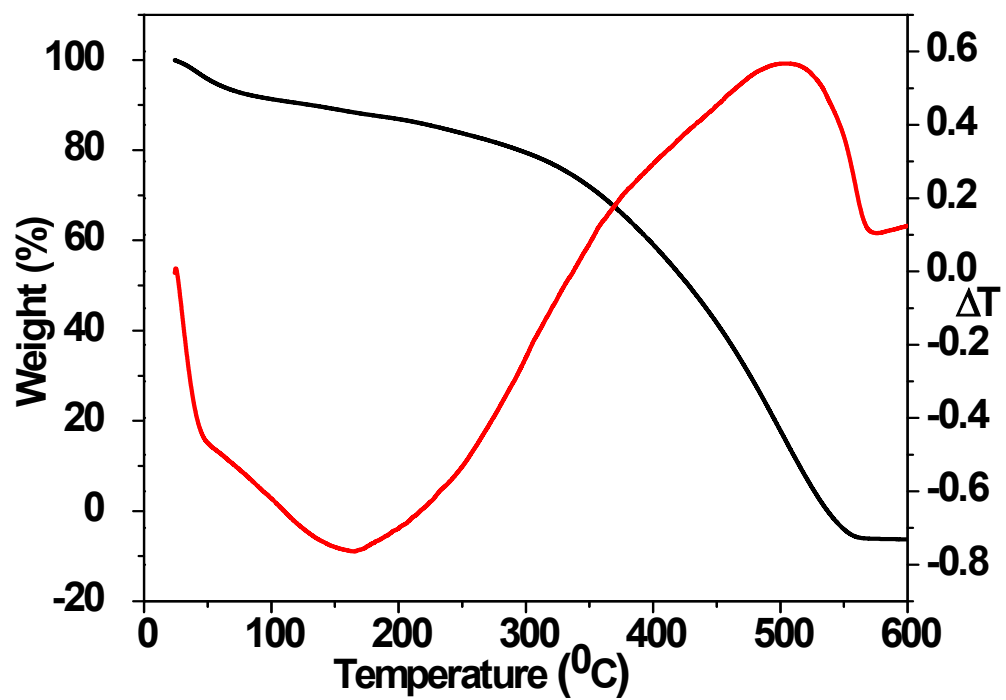


Figure S3. TG-DTA profile of TPOP-1.

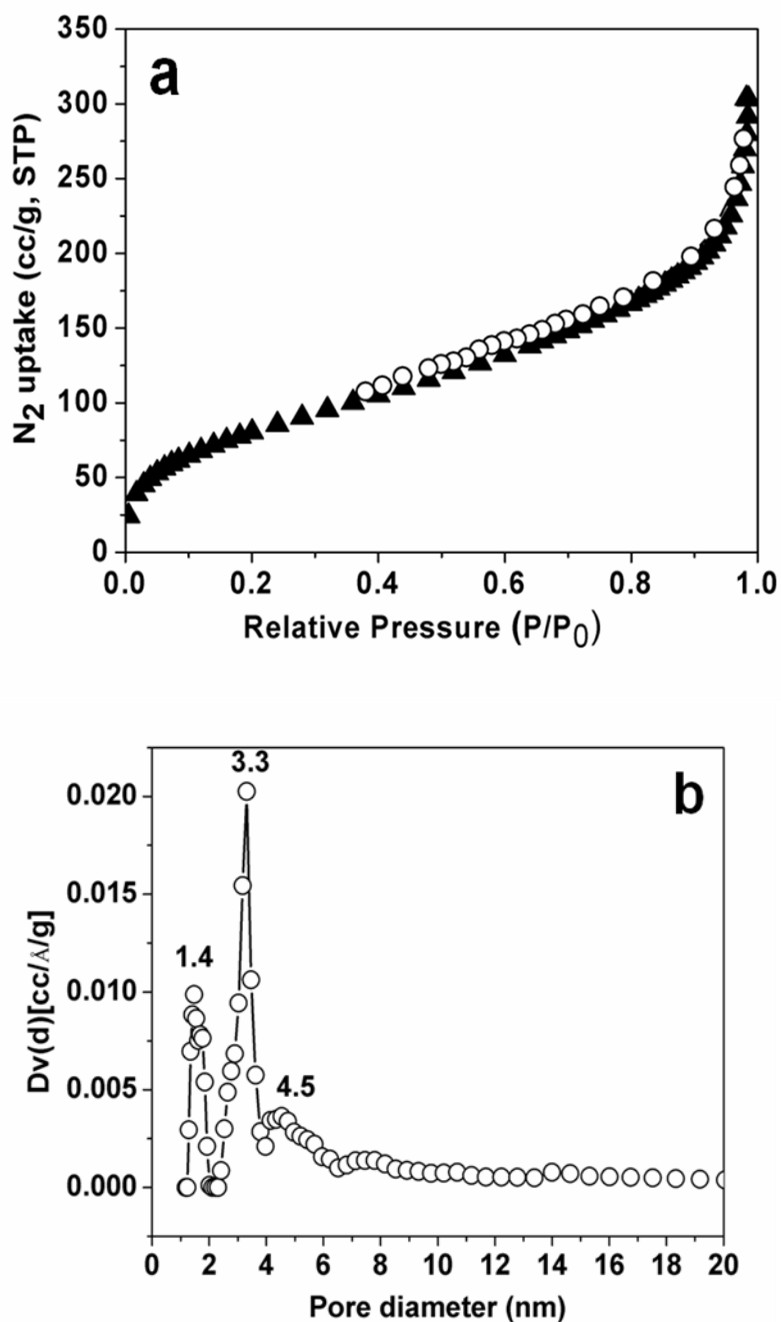


Figure S4. (a) N₂ adsorption-desorption isotherm of Pd-TPOP-1 at 77 K, where filled triangles represents for adsorption and empty circles denote desorption process. (b) NLDFT pore size distribution considering N₂ at 77 K on carbon slit pore. Pore Volume = 0.34 cc/g.

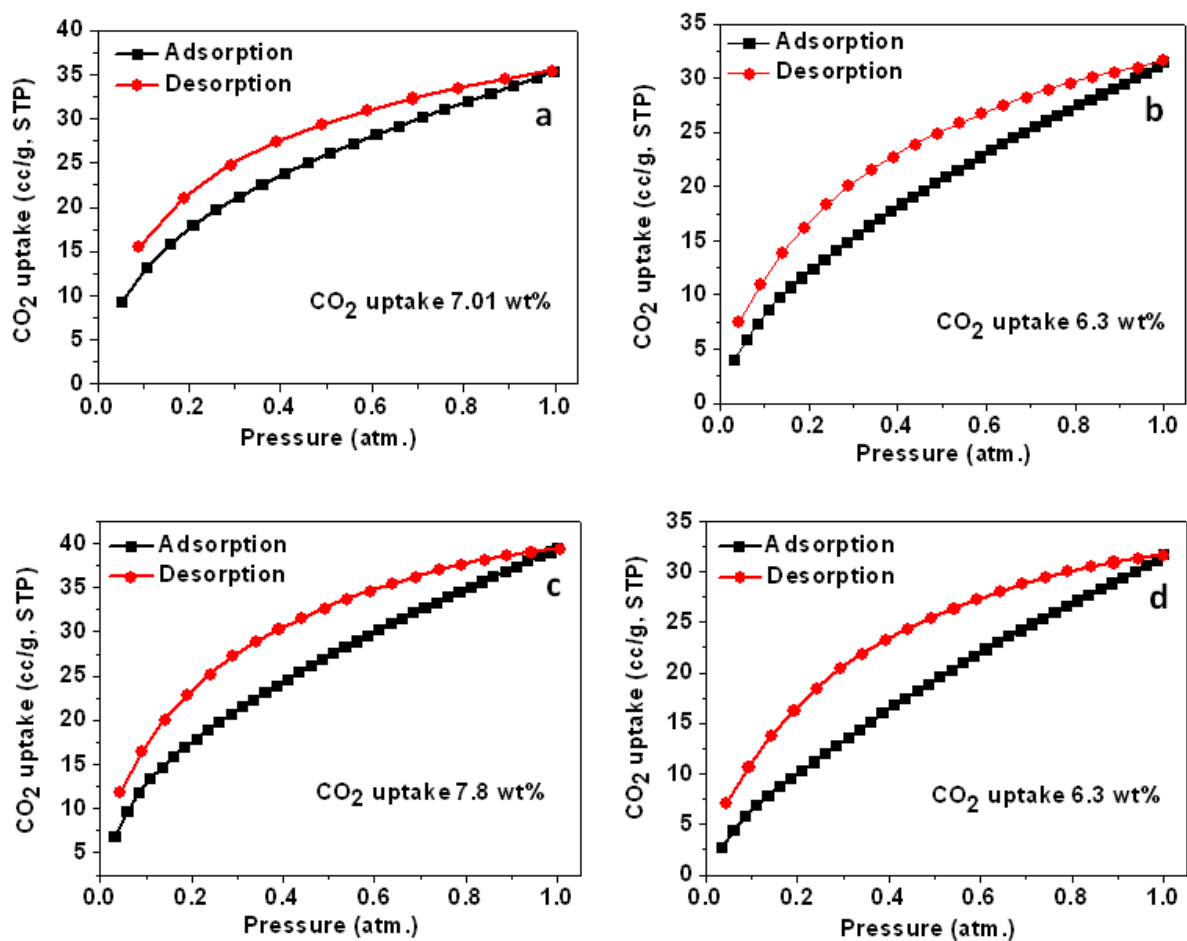


Figure S5. CO₂ adsorption isotherms over three triazine functionalized porous polymeric materials by variation of pyrrole and 4,4',4''-(1,3,5-triazine-2,4,6-triyl)tris(oxy)tribenzaldehyde: 4:3 (TPOP-1-2, a: 273 K, b: 298 K) and 1:1 (TPOP-1-3, c: 273 K, d: 298 K).

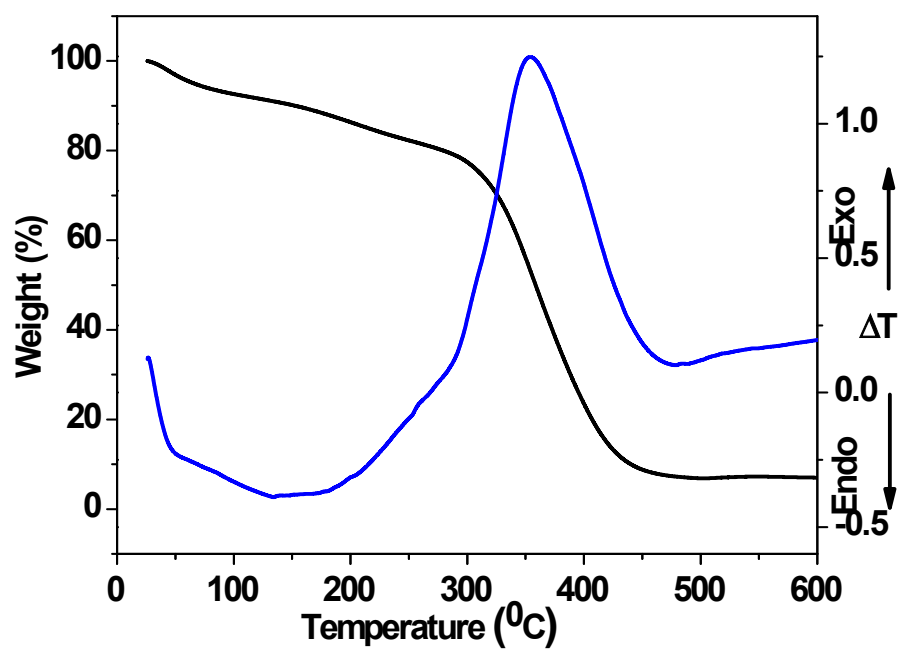


Figure S6. TG-DTA profile of Pd-TPOP-1

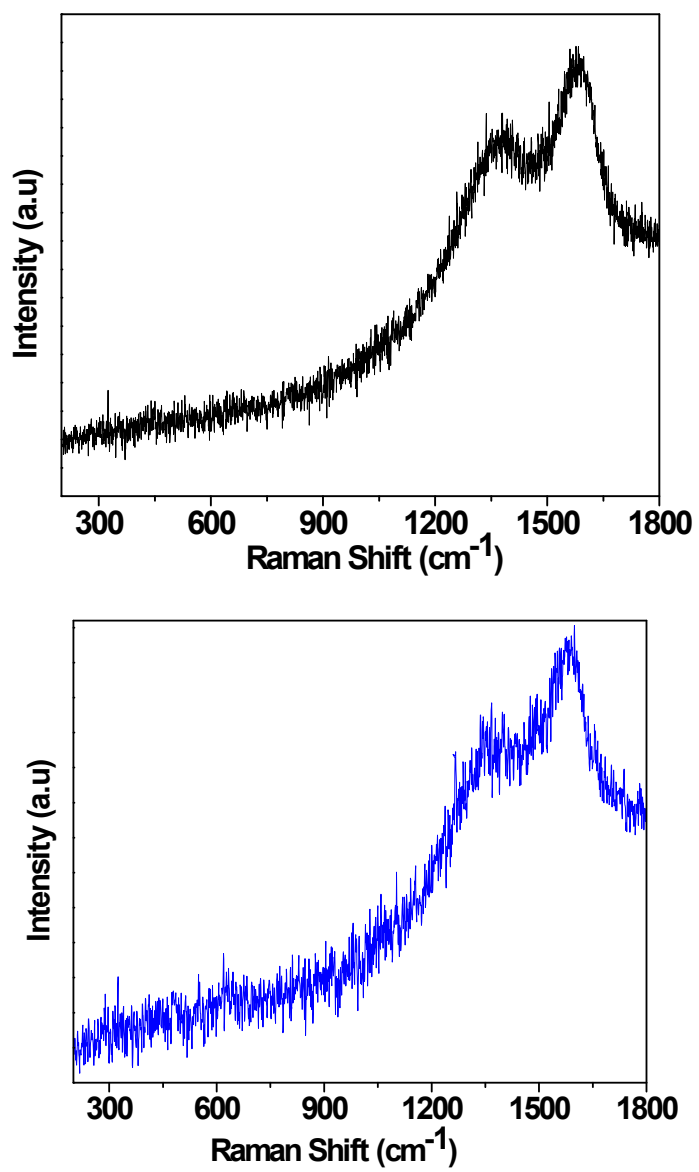


Figure S7. Raman shift of TPOP-1 (black) and Pd-TPOP-1 (blue).

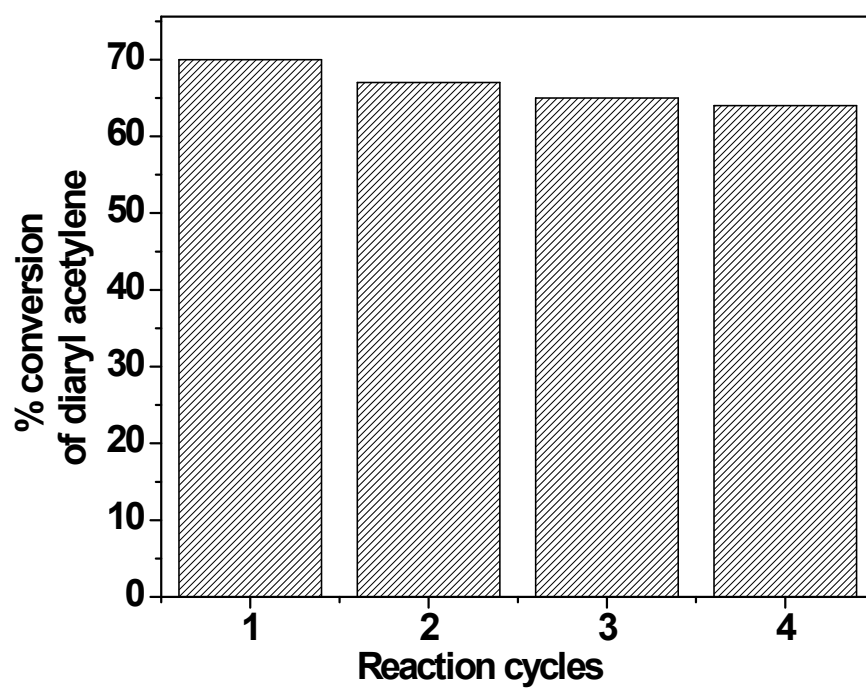
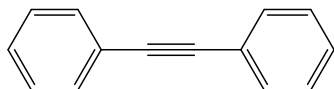


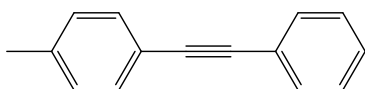
Figure S8. Recycling efficiency of Pd-TPOP-1 for four successive cross-coupling reactions of iodo benzene with phenyl acetylene.

Spectroscopic data for the reaction products in Sonogashira cross-coupling reaction with Pd-TPOP-1



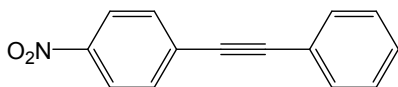
Diphenyl acetylene: ^1H NMR (300 MHz, CDCl_3) $\delta = 7.62$ (d, 4H, $J = 6.4$ Hz, ArH), $\delta = 7.48$ (m, 6H, ArH) ppm

^{13}C (75 MHz, CDCl_3): $\delta = 132.8, 129.6, 128.58, 121.96, 81.9$ ppm.



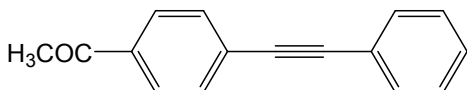
4-methyl diphenyl acetylene: ^1H NMR (500 MHz, CDCl_3) $\delta = 2.81$ (s, 3H, $-\text{CH}_3$), $\delta = 7.6$ (m, 4H, ArH), $\delta = 7.86$ (d, 2H, $J = 9$ Hz, ArH), $\delta = 7.65$ (d, 2H, $J = 8.5$ Hz, ArH), $\delta = 7.58$ (m, 1H, ArH) ppm.

^{13}C (125 MHz, CDCl_3): $\delta = 129, 140.5, 132, 119, 94, 125.8, 132.1, 129.3, 128.2$, ppm .



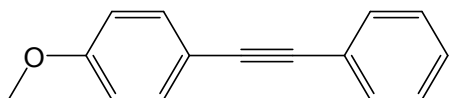
4-nitro diphenyl acetylene: ^1H NMR (300 MHz, CDCl_3) $\delta = 8.3$ (d, 2H, $J = 8.88$ Hz, ArH), $\delta = 7.8$ (d, 2H, $J = 8.88$ Hz, ArH), $\delta = 7.6$ (d, 2H, $J = 6.14$ Hz, ArH), $\delta = 7.42$ (m, 3H, ArH) ppm.

^{13}C (75 MHz, CDCl_3) : $\delta = 147.1, 132.8, 131.9, 130.1, 129.4, 128.68, 128.58, 123.78, 122.25, 95$ ppm.



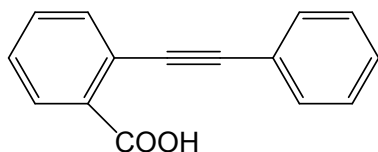
4-acetyl diphenyl acetylene: ^1H NMR (300 MHz, CDCl_3) $\delta = 2.6$ (s, 3H, COCH_3), $\delta = 7.9$ (d, 2H, $J = 8.6$ Hz, ArH), $\delta = 7.5$ (m, 3H, ArH), $\delta = 7.8$ (m, 4H, ArH) ppm.

^{13}C (75 MHz, CDCl_3) : $\delta = 196, 138, 126, 95, 132.2, 122, 125, 128.4, 132.5$ ppm.



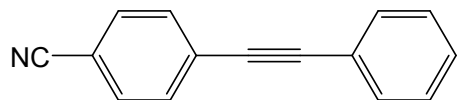
4-methoxy diphenyl acetylene: ^1H NMR (500 MHz, CDCl_3) $\delta = 3.9$ (s, 3H, $-\text{OCH}_3$), $\delta = 7.5$ (m, 3H, ArH), $\delta = 7.8$ (d, $J = 9$ Hz, 2H, ArH), $\delta = 7.5$ (m, 2H, ArH), $\delta = 6.9$ (d, $J = 9$ Hz, ArH, 2H) ppm

^{13}C (125 MHz, CDCl_3): $\delta = 56, 162, 138, 129, 125, 131, 124, 94$ ppm.



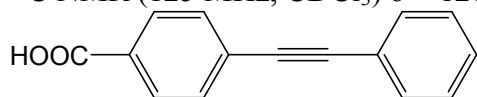
1-carboxy diphenyl acetylene: ^1H NMR (500 MHz, CDCl_3) δ = 8.2 (d, 1H, $J=8$ Hz, ArH), 8.0 (d, 2H, $J=8$ Hz, ArH), 7.20 (1H, t, $J=7.5$ Hz, ArH), 7.64 (4H, m, ArH), 7.48 (1H, d, $J=7.5$, ArH) ppm

^{13}C (125 MHz, CDCl_3): δ = 172, 135, 134, 128, 94, 128, 130, 134, 125 ppm.



4-cyano diphenyl acetylene: ^1H NMR (500 MHz, CDCl_3): δ = 7.8 (d, 2H, $J=8.5$ Hz, ArH), 7.9 (d, 2H, $J=8$ Hz, ArH), 7.5 (d, 2H, $J=8$ Hz, ArH), 7.3 (m, 3H, ArH) ppm.

^{13}C NMR (125 MHz, CDCl_3) δ = 126, 123, 134, 118, 92, 135, 132, 128 ppm.



4-carboxy diphenyl acetylene: ^1H NMR (500 MHz, CDCl_3) δ = 7.98 (d, 2H, $J=8.5$ Hz, ArH), 7.66 (d, 2H, $J=8$ Hz, ArH), 7.4 (d, 2H, $J=8$ Hz, ArH), 7.3 (m, 3H, ArH) ppm.

^{13}C NMR (125 MHz, CDCl_3) δ = 172, 130, 127.5, 129, 132.3, 94 ppm.