SUPPLEMENTAL MATERIAL

Ultrasonically assisted rate enhancements in trichloroisocyanuric acid/DMF/ NaNO₂ triggered nitration of aromatic compounds and decarboxylative nitration of α , β unsaturated acids

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Spectra of certain β -Nitro Styrenes:

β - Nitro styrene: ¹HNMR (300MHz, CDCl₃): δ 6.40-6.44 (d, 1H, H-8, J=18Hz), 7.62-7.65 (m, 3H, H-3, H-4, H-5), 7.80 (d, 1H, H-7, J=18 Hz), 7.48 (d, 2H, H-2, and H-6, J=7.95 Hz); ¹³C NMR δ 129.1, 129.4, 130.0, 139.0, 132.1, 137.1; m/z = 149.

2-Chloro β - Nitro styrene: ¹HNMR (300MHz, CDCl₃): δ 6.68 (d, 1H, H-8, J = 18.5 Hz), 7.28 (dd, 1H, H-4, J=9.0 Hz, J=7.5 Hz), 7.60 (dd, 1H, H-5, J=10 Hz, J = 8.0 Hz), 7.64 (d, 1H, H-3, J = 8.5 Hz), 7.75 (d, 1H, H-6, J=8.0 Hz), 8.32 (d, 1H, H-7, J = 18.5 Hz); ¹³C NMR δ 127.7, 128.6, 128.7, 130.9, 133.0, 135.2, 136.2, 138.9; m/z = 183.

2- Methyl β - Nitro styrene: ¹HNMR (300MHz, CDCl₃): δ 2.95 (s, 3H, Me), 6.78 (d, 1H, H-8, J=18.5 Hz), 7.18 (dd, 1H, H-4, J=10 Hz, J = 8.5 Hz), 7.35 (dd, 1H, H-5, J = 9.5 Hz, J = 8.5 Hz), 7.54 (d, 1H, H-3, J=8.0 Hz), 7.78 (d, 1H, H-6, J = 9.5Hz), 8.28 (d, 1H, H-7, J=18.5 Hz); ¹³C NMR δ 20.1, 126.9, 127.5, 129.1, 131.6, 132.1, 136.9, 137.8, 139.4; m/z = 163.

4- Chloro β - Nitro styrene ¹HNMR (300MHz, CDCl₃): δ 6.68 (d, 1H, H-8, J=18.0 Hz), 7.24 (d, 2H, H-2 and H-6, J=8.0 Hz), 7.68 (d, 2H, H-3 and H-5, J=8.5Hz) 8.28 (d, 1H, H-7, J=18.0 Hz); ¹³C NMR δ 128.4, 129.6, 130.1, 137.3, 137.5, 138.2; m/z = 184.

4- Nitro β - Nitro styrene: ¹HNMR (300MHz, CDCl₃): δ 6.62 (d, 1H, H-8, J=18 Hz), 7.42 (d, 2H, H-2 and H-6, J=9.0 Hz); δ 7.78 (d, 2H, H-3 and H-5, J=9.5 Hz), 8.18 (d, 1H, H-7, J=18.0 Hz); ¹³C NMR δ 124.2, 129.6, 135.9, 136.0, 139.7, 149.3; m/z = 194.

4- Methyl β - Nitro Styrene: ¹HNMR (300MHz, CDCl₃): δ 3.02 (s, 3H, CH₃), 6.68 (d, 1H, H-8, J=18 Hz); 7.44 (d, 2H, H-2 and H-6, J=8.0 Hz), 7.65 (d, 2H, H-3 and H-5, J=8.0 Hz), 7.85 (H-7, d,1H, J=18.0 Hz); ¹³C NMR δ 21.8, 127.4, 129.4, 130.3, 136.4, 139.4, 143.3; m/z = 163.

4- Methoxy β - Nitro Styrene: ¹HNMR (300MHz, CDCl₃): δ 3.82 (s, 3H, CH₃); 6.45 (d, 1H, H-8, J=18.0 Hz); 7.48 (d, 2H, H-3 and H-5, J=8.5 Hz), 7.75 (d, 2H, H-2 and H-6, J=8.0 Hz), 7.88 (d, 1H, H-7, J=18.0 Hz); ¹³C NMR δ 55.4, 114.8, 122.4, 131.1, 134.8, 138.9, 162.8; m/z = 179.

2- OMe β - Nitro styrene: ¹H NMR δ 3.95(s, 3H, Me), 6.98 (m, 2H), 7.45 (m, 2H), 7.88 (d, 1H, J = 18.5 Hz), 8.12 (d, 1H, J = 18.5 Hz); ¹³C NMR δ 55.8, 111.5, 119.2, 121.3, 132.6, 133.6, 135.7, 138.4, 159.7; m/z = 179

1-Nitro Ethene: ¹HNMR (300MHz, CDCl₃): δ 5.92 (dd, 1H, H_b, J=11.3 Hz, J = 1.5Hz), 6.65 (dd, 1H, H_a, J=15.5 Hz, J=11.3 Hz), 7.25 (dd, 1H, H_c, J=15.5Hz, J=1.5 Hz); m/z = 73.

1-Nitro Propene: ¹HNMR (300MHz, CDCl₃): δ 2.12 (d, 3H, CH₃, J = 6.9 Hz), 7.00 (d, 1H, H_a, J=16.5Hz), 7.18 (m 1H, H_b) m/z = 87.

Supplementary Data - IR Spectra of TCICA, DMF, and (TCICA-DMF) Adduct

Fig-1: Infra Red Spectrum of TCCA

Fig-2: Infra Red Spectrum of DMF

Figure-3: IR Spectrum of TCICA-DMF Adduct

Spectra of some Represented compounds as Supporting Data:

Figure 4: ¹H NMR of β -Nitro Styrene

Figure 5: ¹H NMR of 4-Methoxy β - Nitro Styrene

Figure 6: ¹H NMR of 4-Methyl β - Nitro Styrene

Figure 7: ¹H NMR of 4-Nitro β -Nitro Styrene

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Figure 8: ¹H NMR of 4-Nitro Phenol

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Figure 9: MS spectrum of 4-Nitro Phenol

Figure 10: ¹³C NMR of β-Nitro Styrene

Figure 11: ¹³C NMR of 4- Chloro β-Nitro Styrene

Figure 12: ¹³C NMR of 2- Chloro β-Nitro Styrene

Figure 13: ^{13}C NMR of 4- Methyl β -Nitro Styrene

Figure 14: ^{13}C NMR of 2- Methyl β -Nitro Styrene

Figure 15: ¹³C NMR of 4- Nitro β-nitro Styrene

Figure 16: ¹³C NMR of 4- Methoxy β-Nitro Styrene

Figure 17: ^{13}C NMR of 2- Methoxy β -Nitro Styrene