

Supporting Information

Microwave role in the thermal induced S_{RN1} reaction for α -Arylation of Ketones

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Benzyne mechanism evaluation

GC-MS for reaction of 1-phenyl-2-(*para*-tolyl)ethanone

A benzyne mechanism will afford equal amounts of *meta* and *para* 1-phenyl-2-(tolyl)ethanone (**3f**). A CG-MS analysis of the organic extract of the reaction crude showed two signals with m/z 210.10 with a relative integration of 99% (*t*_r= 10.4 min) and 1% (*t*_r= 10.3 min). In this case, the unreacted 4-methyl iodobenzene (**1f**) and the acetophenone in excess are also shown.

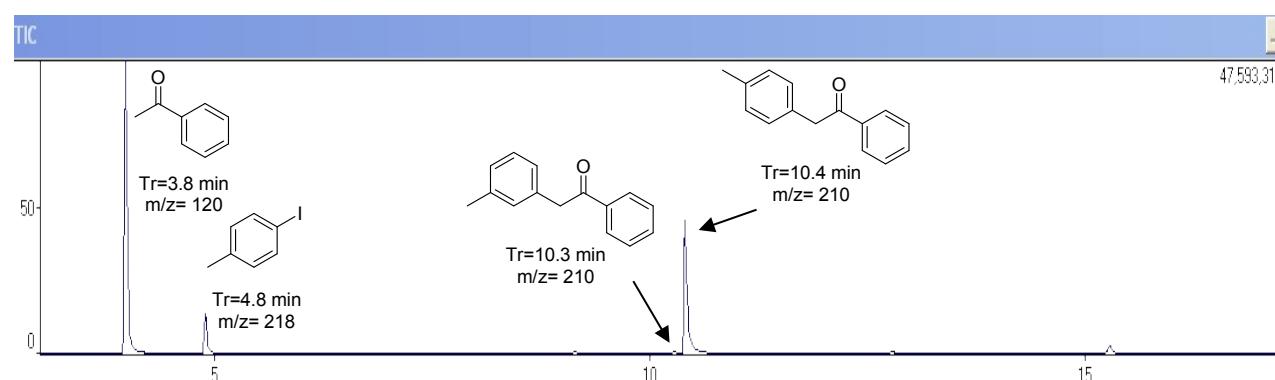
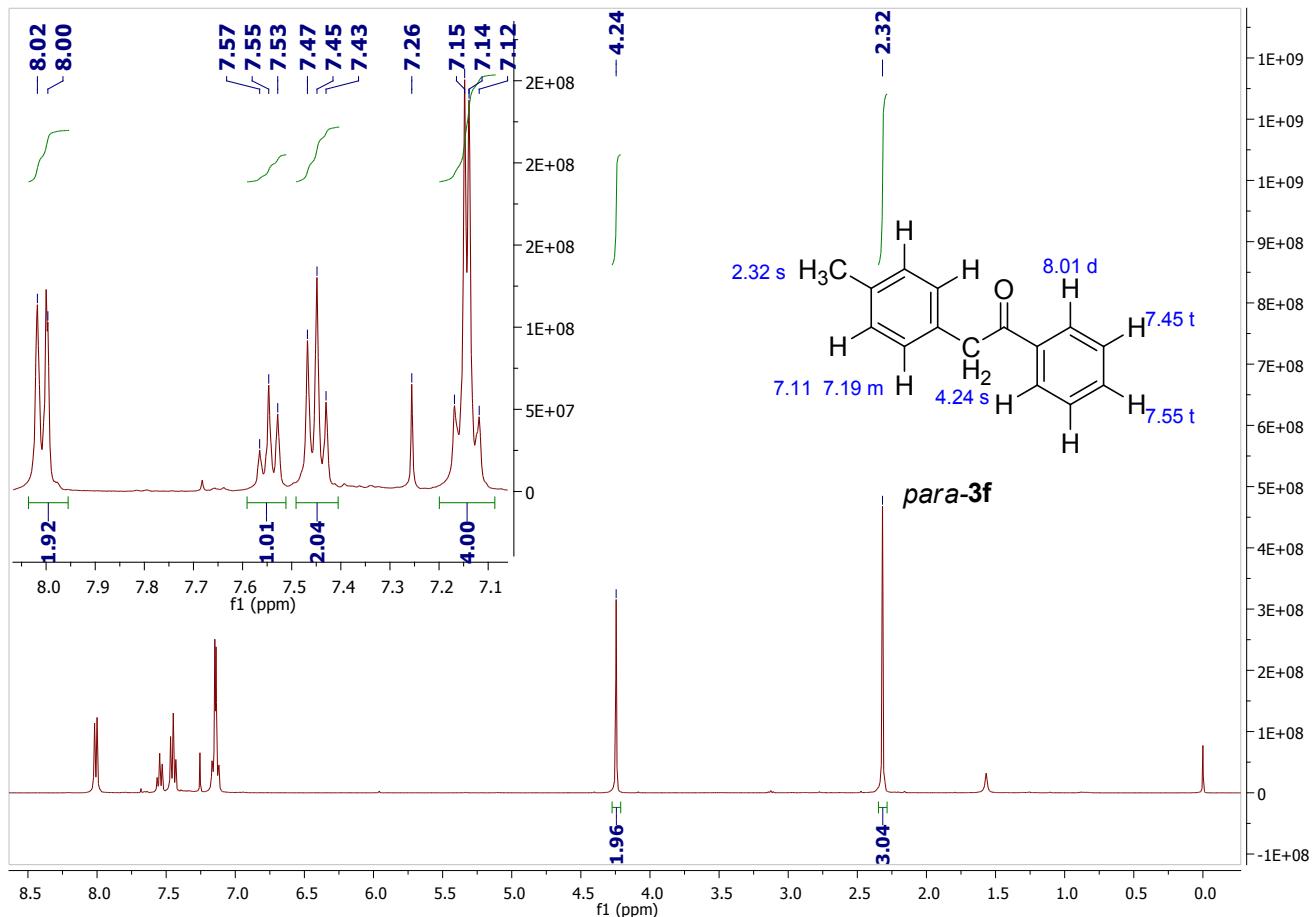


Figure S1. GC-MS chromatogram of reaction of the reaction of Acetophenone (1.5 mmol), *t*BuOK (1.55 mmol), and 4 methyl-Iodobencene (0.5 mmol) in 2 mL of DMSO heated to 70°C by microwave irradiation (150 W_{max}) under N₂ atmosphere for 10 min. GC-MS analyses were performed employing a 25 m x 0.2 mm x 0.33 μ m with a 5% phenylpolysiloxane phase column.

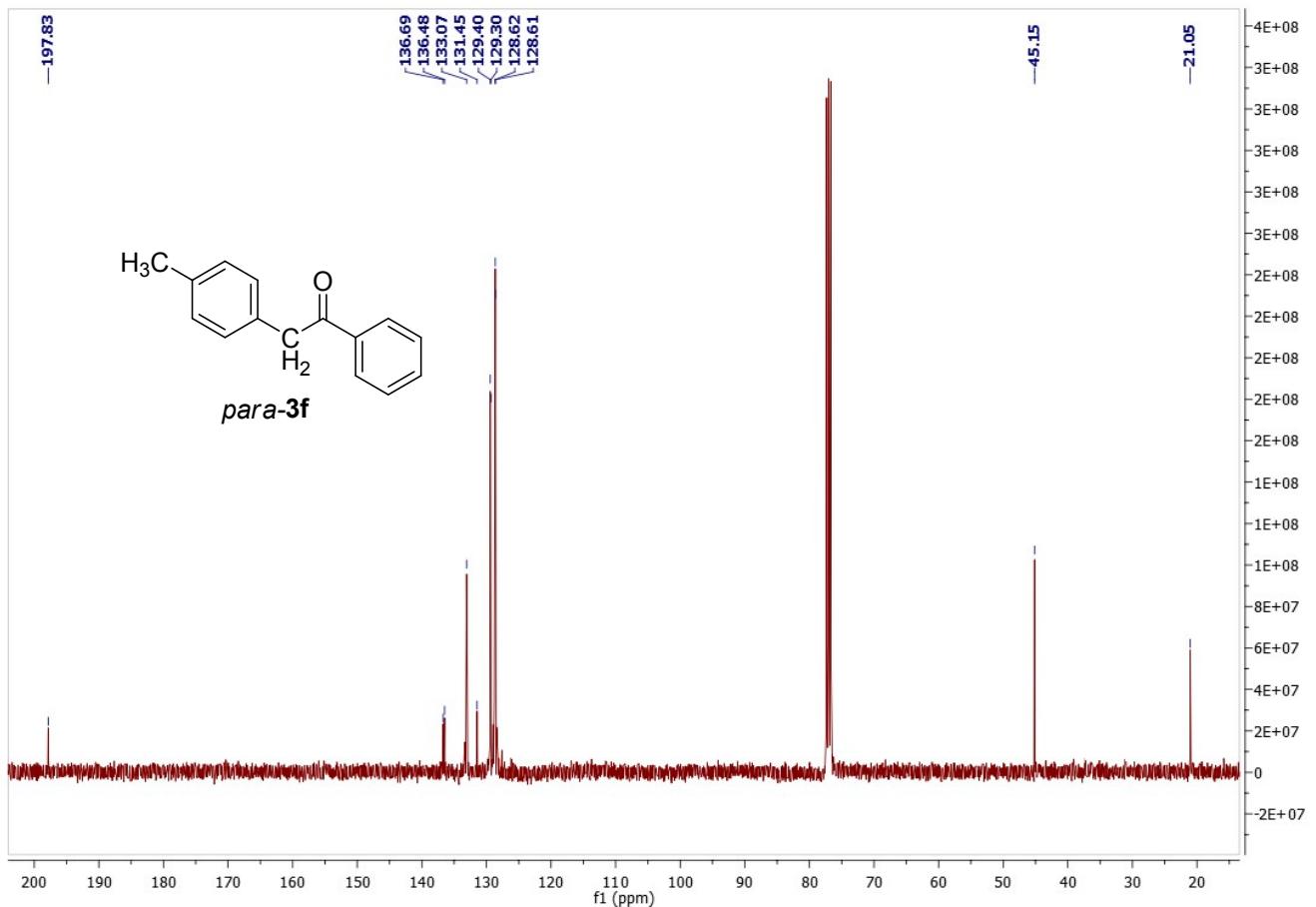
¹H-NMR spectra of 1-phenyl-2-(*para*-tolyl)ethanone

After purification in a short silica gel column and then by identification by RMN, only one product was found, and identified as 1-phenyl-2-(*para*-tolyl)ethanone. This known compound present spectral data as shown in the literature, in agreement with the proposed structure. ¹ [¹H-RMN , δ H (400 MHz, CDCl₃) 8.01 (1 H, d, *J* 8.5), 7.55 (1 H, t, *J* 7.4), 7.45 (1 H, t, *J* 7.6), 7.19 – 7.10 (1 H, m).

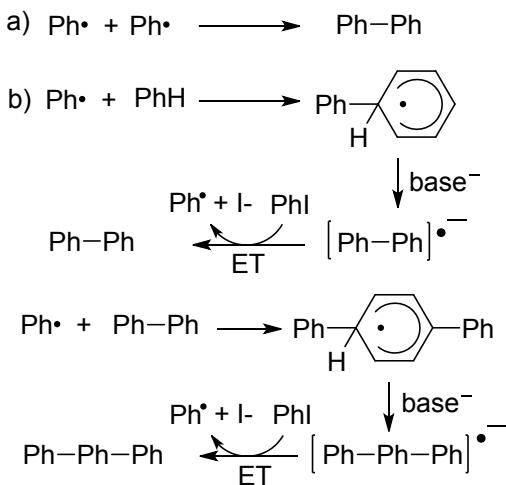


¹³C-NMR spectra of 1-phenyl-2-(*para*-tolyl)ethanone

¹³C NMR (101 MHz, CDCl₃) δ = 197.8, 136.7, 136.5, 133.1, 131.5, 129.4, 129.3, 128.6, 128.6, 45.2, 21.1.



Scheme S1. Generation of terphenylenes



Yield and temperature profiles in the coupling reaction of PhI, and acetophenone

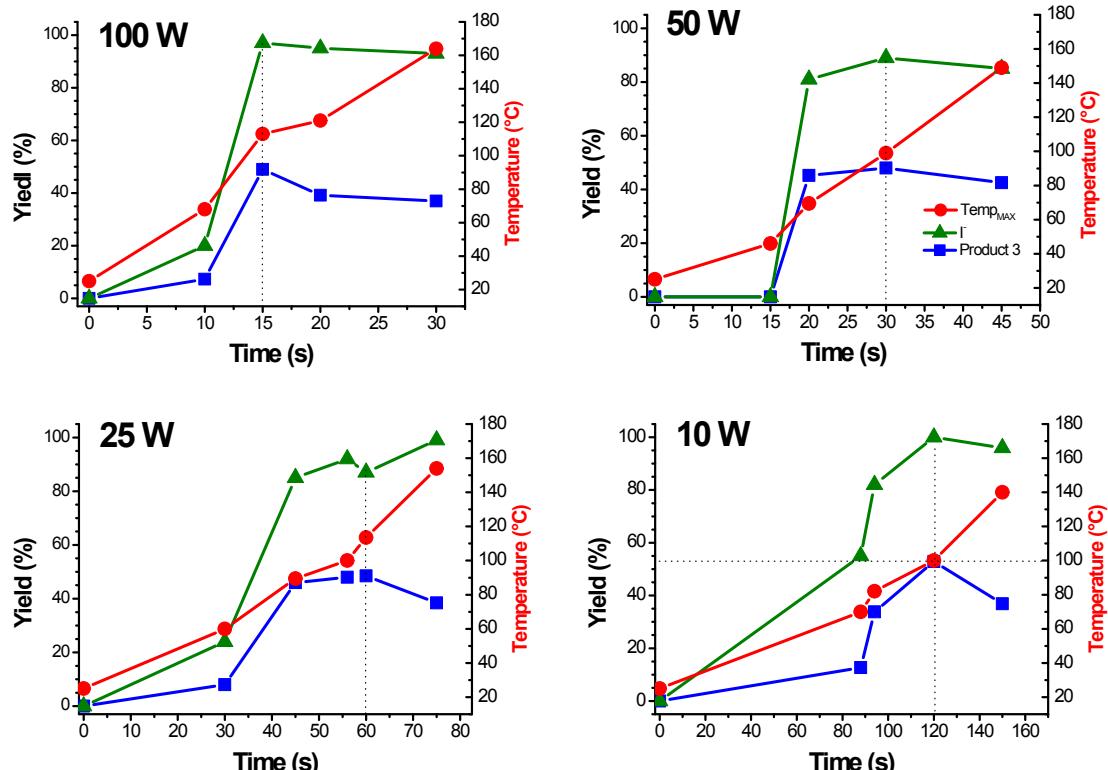


Figure S2. Yield and temperature profiles in the coupling reaction of 0.5 mmol PhI, 1.5mmol acetophenone and 2.5 mmol *t*BuOK heated by microwave with pulses of 100, 50, 25 and 10 W vs time. Blue squares (■), product 3 % yield, quantified by NMR with internal standard, % I⁻ determined potentiometrically with Ag/Ag⁺ in green ▲, and temperature by IR sensor inside the CEM Discover reactor in red ●. Dotted lines indicate 1500 J point.

References

¹ P. Nilsson, M. Larhed, and A. Hallberg *J. Am. Chem. Soc.* **2001**, 123, 8217-8225, b) Anders. E. Gassner, T. *Chem Ber*, **1984**, 117,1034.