Study of duo functional behaviour of 1,2-bis (4-bromobenzamide) benzene by synchronous fluorescence spectroscopy

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SUPPLEMENTARY MATERIAL

Characterization of the 1,2-bis (4-phenylbenzamide) benzene compound (bisamide 1b)

Figure 1: Infrared spectrum of 1,2-bis (4-phenylbenzamide) benzene

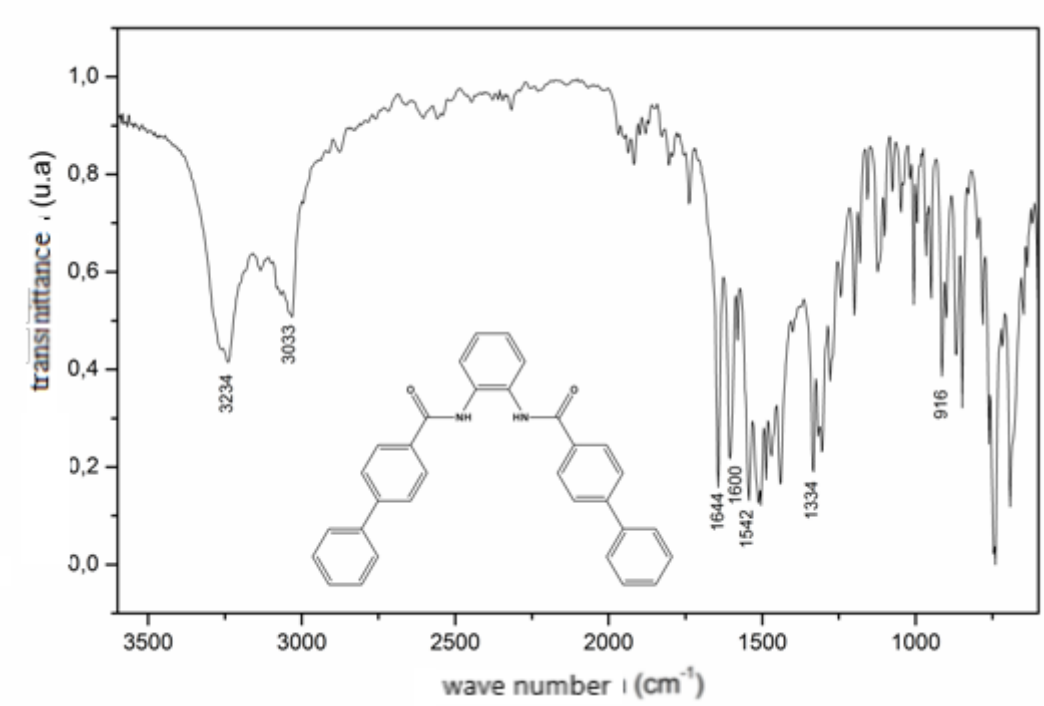
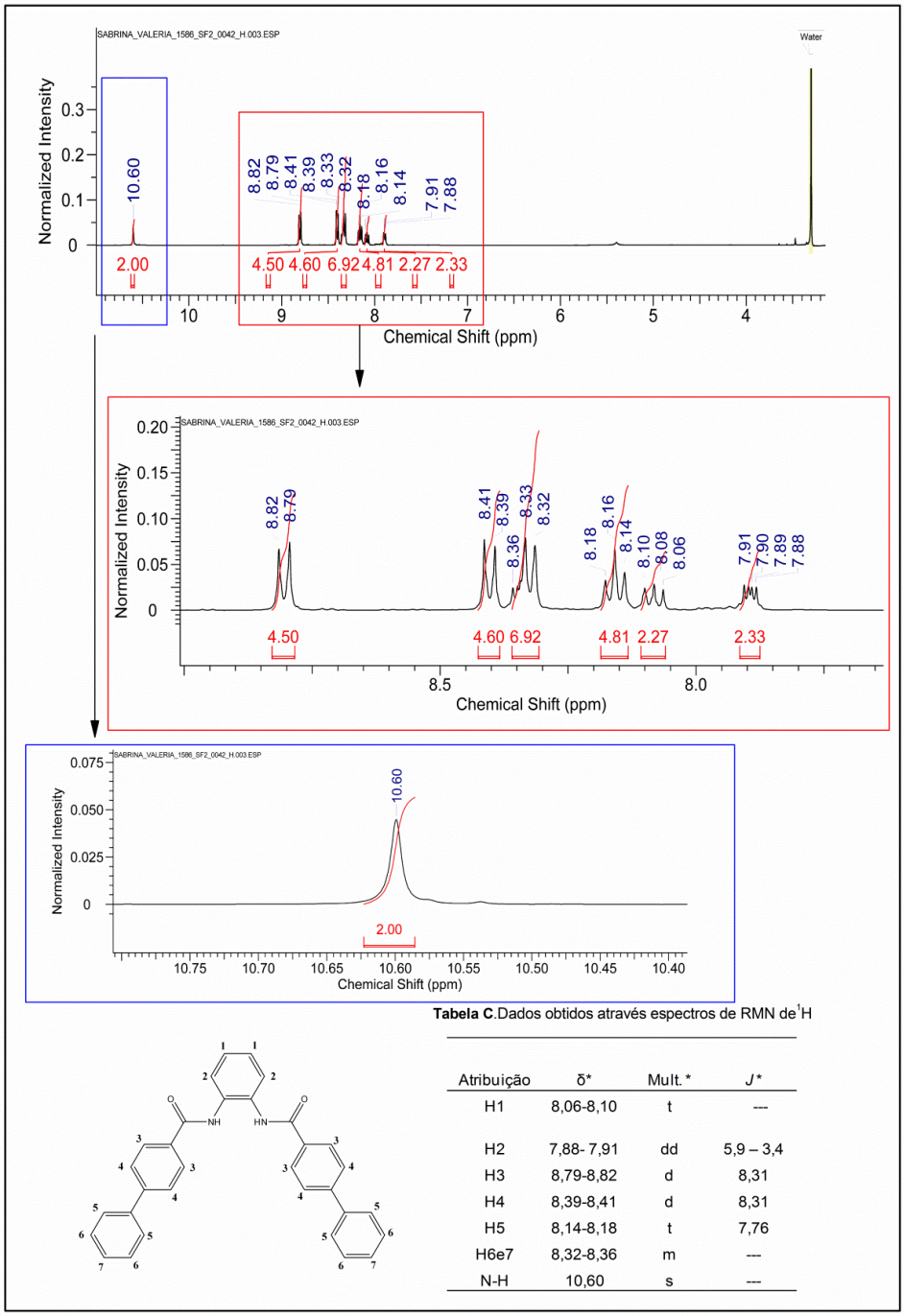


Figure 2. [1]H-NMR (400 MHz, DMSO-d6) of 1,2-bis (4-phenylbenzamide) benzene.



Atribuição	δ*	Mult.*	*J**
H1	8,06-8,10	t	---
H2	7,88- 7,91	dd	5,9 – 3,4
H3	8,79-8,82	d	8,31
H4	8,39-8,41	d	8,31
H5	8,14-8,18	t	7,76
H6e7	8,32-8,36	m	---
N-H	10,60	s	---

Figure 3 .[13]C NMR Spectrum of 1,2-bis (4-phenylbenzamide) benzene.

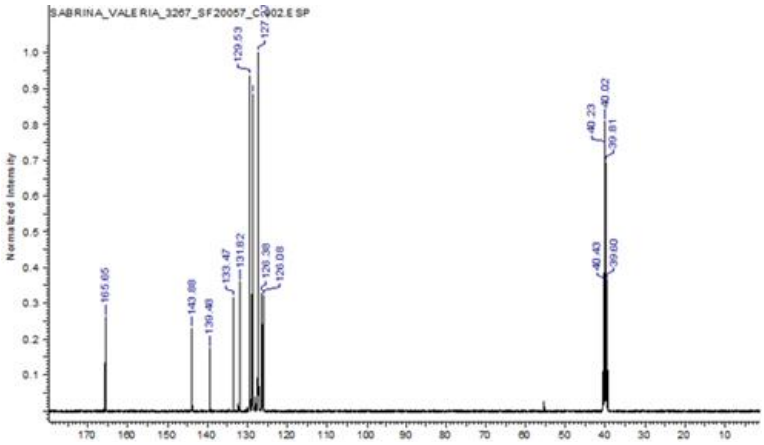
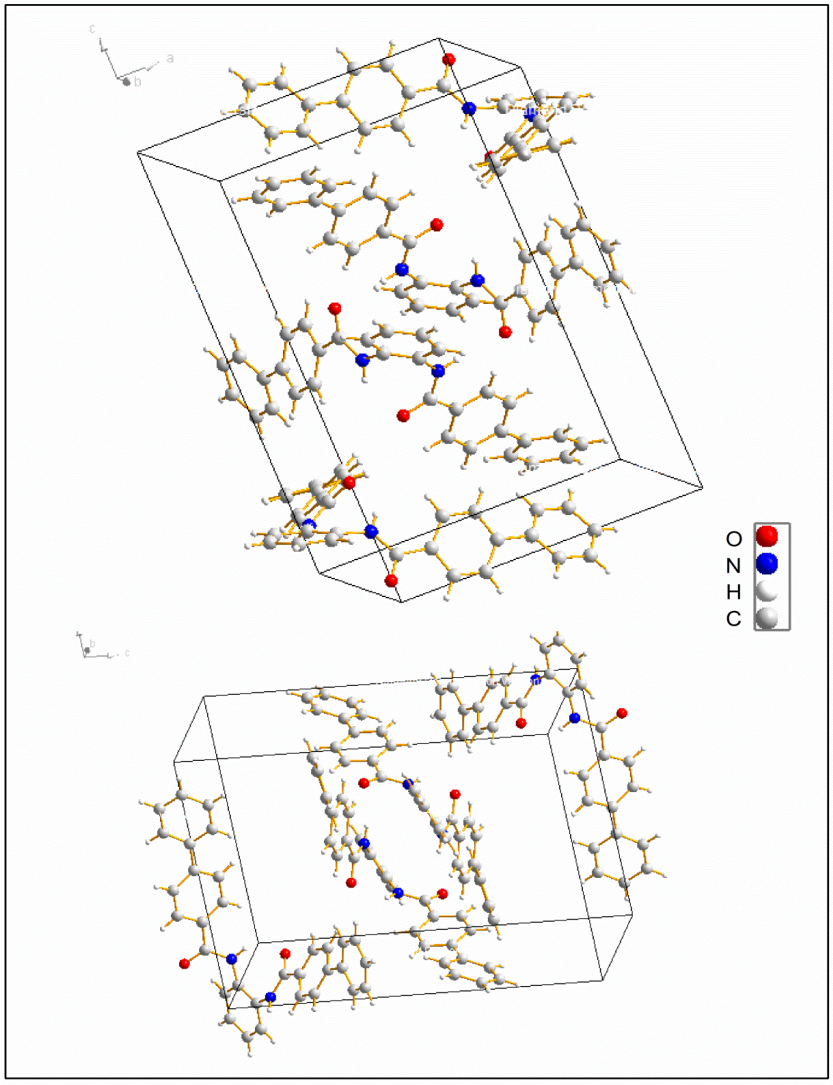


Figure 4. Projection of the structure of 1,2-bis (4-phenylbenzamide) benzene, in the elemental cell



FLUORESCENCE STUDY

Figure 5 - Fluorescence spectrum of reactants and solvente

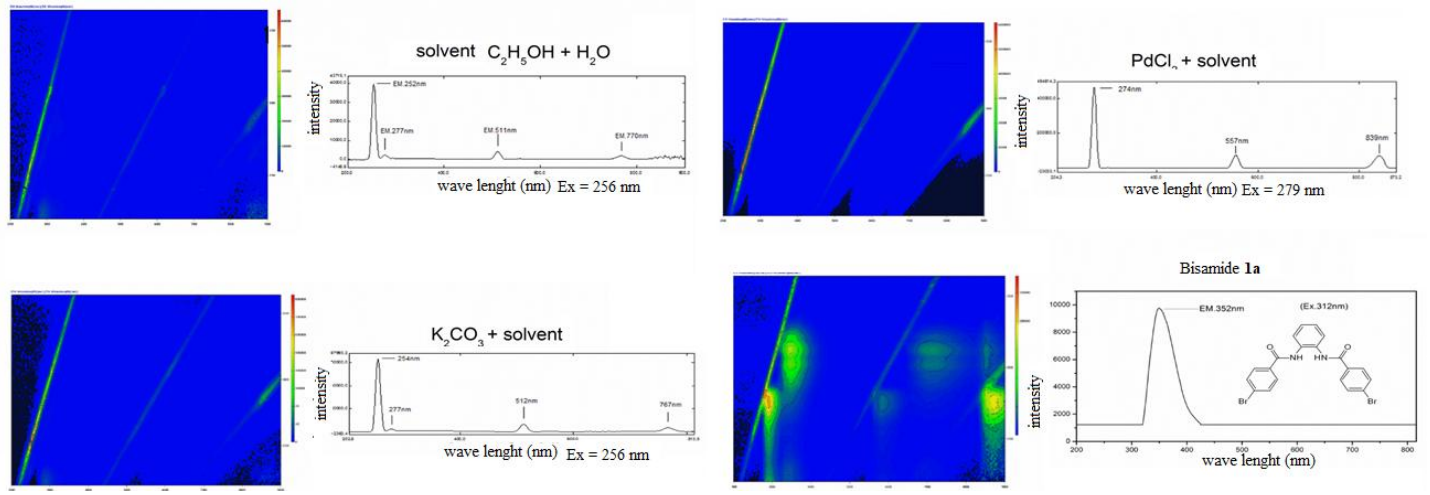


Figure 6 - Fluorescence spectrum of products

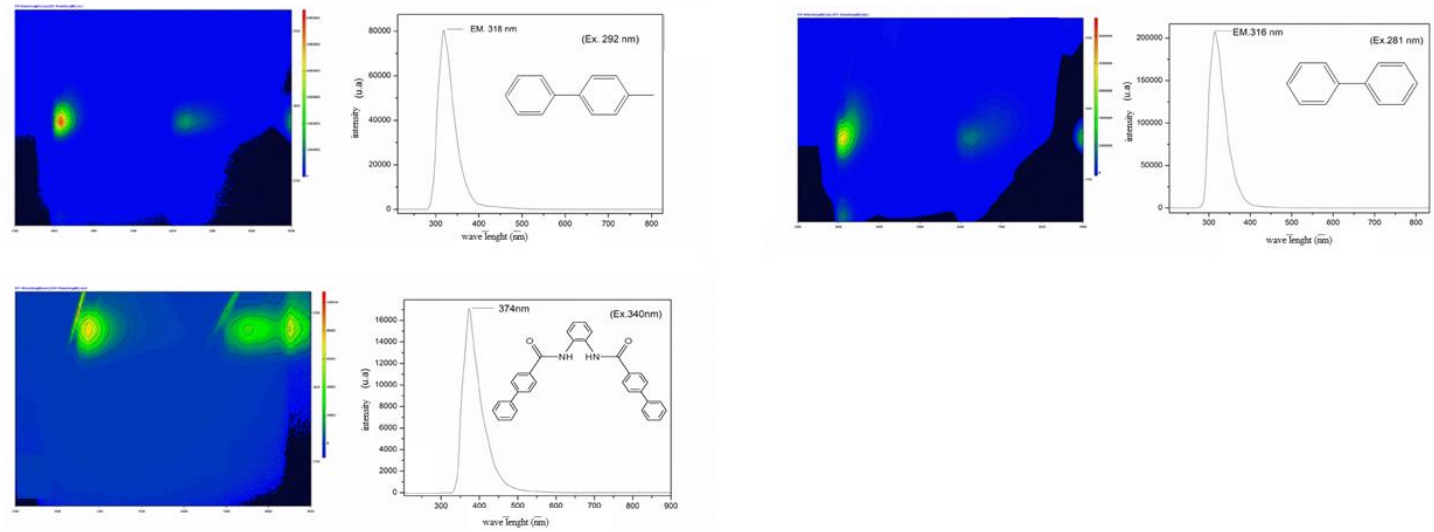


Figure 7 - Study of the Suzuki coupling mechanism - Transmetalation step

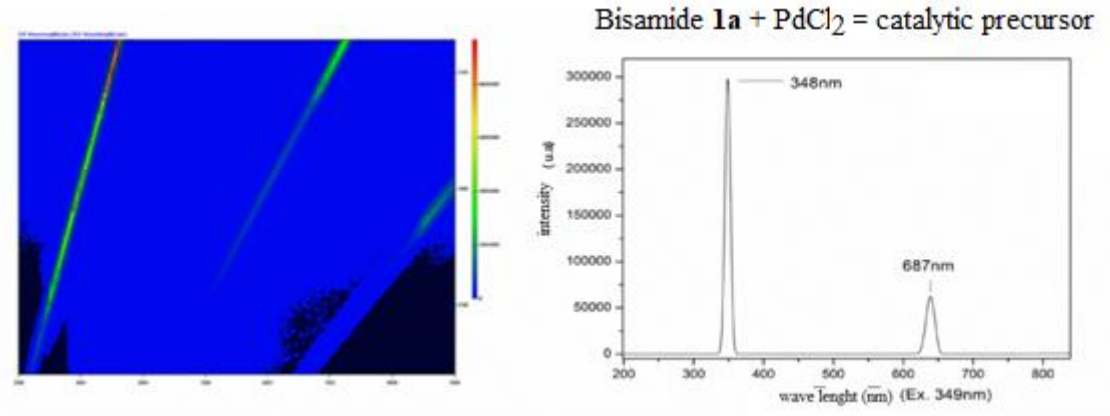
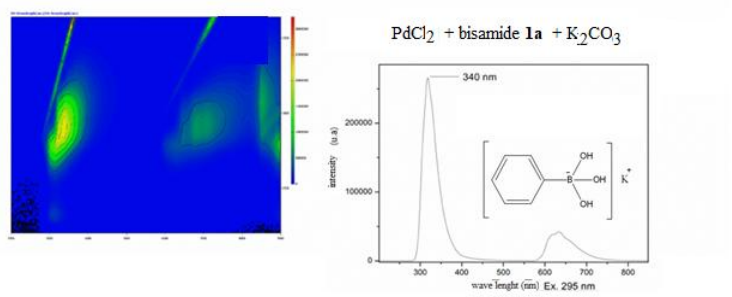
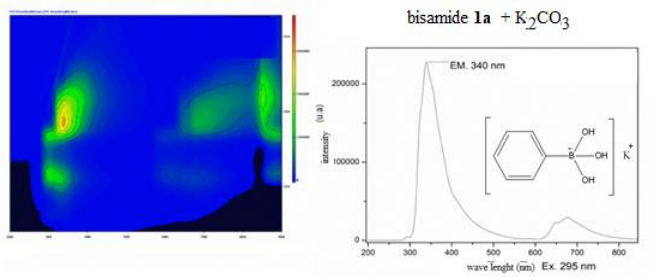


Figure 8: Fluorescence study of catalytic precursor formation





CHARACTERIZATION OF BIPHENYLS, OBTAINED IN THE SUZUKI COUPLING

- **4-Cyanobiphenyl:** White solid. PF=85-87 °C (85 – 87 °C) [1]

^{1}H NMR (400 MHz, $CDCl_3$, δ(ppm)): 7,33 – 7,42 (m, 3H, aromatic); 7,50 – 7,53 (m, 2H, aromatic); 7,59 – 7,66 (m, 4H, aromatic).

^{13}C NMR (400 MHz, $CDCl_3$, δ(ppm)): 55,32; 114,17; 126,71; 128,13; 128,70; 133,74; 140,80; 159,11.

GC-MS (IE, 70 eV) m/z (%): M^+ 179 (100); 151 (20); 76 (15); 63 (8); 51 (7); 89 (6); 126 (4); 39 (4); 113 (3); 100 (2); 164 (2)

- **4-Methoxybiphenyl:** White solid. PF = 89 – 91 °C. (89 – 90 °C).[1]

^{1}H NMR (400 MHz, $CDCl_3$, δ(ppm)): 3,88 (s, 3H, OMe); 7,0 – 7,02 (d, 2H, aromáticos); ,28 – 7,33 (m, 1H, aromatic); 7,43 – 7,46 (m, 2H, aromatic); δ 7,55 – 7,59 (m, 4H, aromatic);

^{13}C NMR (400 MHz, $CDCl_3$, δ(ppm)): 55,32; 114,17; 126,71; 128,13; 128,70; 133,74; 140,80; 159,11.

GC-MS (IE, 70 eV) m/z (%): M+ 184 (100); 141 (74); 169 (61); 115 (57);139 (15); 63 (11); 89 (8); 76 (8); 39 (6); 51 (5); 102 (3).

- **4-Methylbiphenyl:** White solid, PF. 50- 51°C.[1]

***^{1}H NMR (400 MHz, $CDCl_3$,* δ ppm):** 2,5 (s, 3 H, Me); 7,25–7,31 (m, 2 H, aromatic); 7,31-7,33 (m, 1 H aromatic); 7,38–7,43 (m, 2 H, aromatic); 7,49- 7,51 (d, *2* H, aromatic); 7,56 – 7,59 (d, *2* H, aromatic).

GC-MS (IE, 70 eV) m/z (%): M+ 168 (100); 167 (70); 152 (27); 115 (11); 83(10); 91 (8); 63 (7); 51 (5); 39 (5); 139 (5); 102 (3).

- **4-Methoxy-4'-methylbiphenyl:** White solid,. PF = 111 – 113 °C (111 – 112 °C)[1]

^{1}H RMN (400 MHz, $CDCl_3$, δ(ppm)): 2,41 (s, 3H, Me); 3,87 (s, 3H, OMe); 6,98–7,00 (d, 2H, aromatic); 7,24–7,28 (m, 2H, aromatic); 7,47–7,49 (d, 2H, aromatic); 7,53–7,55 (d, 2H, aromatic).

^{13}C RMN (400 MHz, $CDCl_3$, δ(ppm)): 21,08; 55,34; 114,15; 126,59; 127,96;129,45; 133,36; 137,95; 158,92.

GC-MS (IE, 70 eV) m/z (%) : 198 (M+100); 183 (65); 155 (49); 128 (17);152 (15); 115 (12); 99 (7); 77 (7); 63 (6); 51 (5); 39 (4). 89 (3); 168 (2).]

REFERENCES

1- M.K. Marchewka, *Acta Chimica Slovenica*, 2003, **50**, 239.