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Synthesis and Characterization in Solution and in the Solid State of the Palladium Aryl Bromide complexes Pd(Ar)Br{(S)-BINAP}. Formation Of Cyclopalladated Complexes and Direct Observation of a C-N Reductive Elimination To Form Heterocycles

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Inversion Transfer Experiment

The complex **1** (40 mg) was dissolved in benzene-d_6 (1 mL), and the solution was placed in a 10 mm NMR tube under argon. The tube was introduced in a 500 MHz NMR Varian Spectrometer. Then, the program containing the following pulse was applied: RD-π_{sel}-τ_{mix}-p/2-acquisition. The selective pulse was applied to one of the doublets. The mixing time was changed during the program according to a variable delay list file. Sixteen scans were accumulated for each value of the τ_{mix} from the list.

Table 1. Inversion transfer experiment: relative intensities obtained as a function of the evolution time for the inversion of the doublet at 11.4 ppm

Delay (ms)	27.4 ppm	26.0 ppm	12.9 ppm	11.4 ppm
2	1.07	1.00	1.03	-0.86
4	1.05	0.99	1.01	-0.89
8	1.08	1.03	1.02	-0.88
16	1.07	1.01	1.00	-0.84
32	1.09	1.01	0.95	-0.82
64	1.06	1.02	0.88	-0.70
128	1.05	1.04	0.75	-0.45
256	1.07	1.02	0.60	-0.20
512	1.06	1.02	0.46	0.12
1024	1.05	1.03	0.49	0.47
2048	1.05	1.02	0.71	0.75

Table 2. Inversion transfer experiment: relative intensities obtained as a function of the evolution time for the inversion of the doublet at 27.4 ppm

Delay (ms)	27.4 ppm	26.0 ppm	12.9 ppm	11.4 ppm
2	-0.84	0.92	1.00	1.06
4	-0.82	0.96	1.02	1.09
8	-0.80	0.95	1.02	1.06
16	-0.75	0.94	1.01	1.07
32	-0.68	0.87	1.02	1.06
64	-0.55	0.82	1.01	1.10
128	-0.32	0.71	1.00	1.08
256	-0.04	0.58	1.03	1.09
512	0.35	0.55	1.02	1.08
1024	0.70	0.68	1.04	1.10
2048	0.93	0.86	1.05	1.10

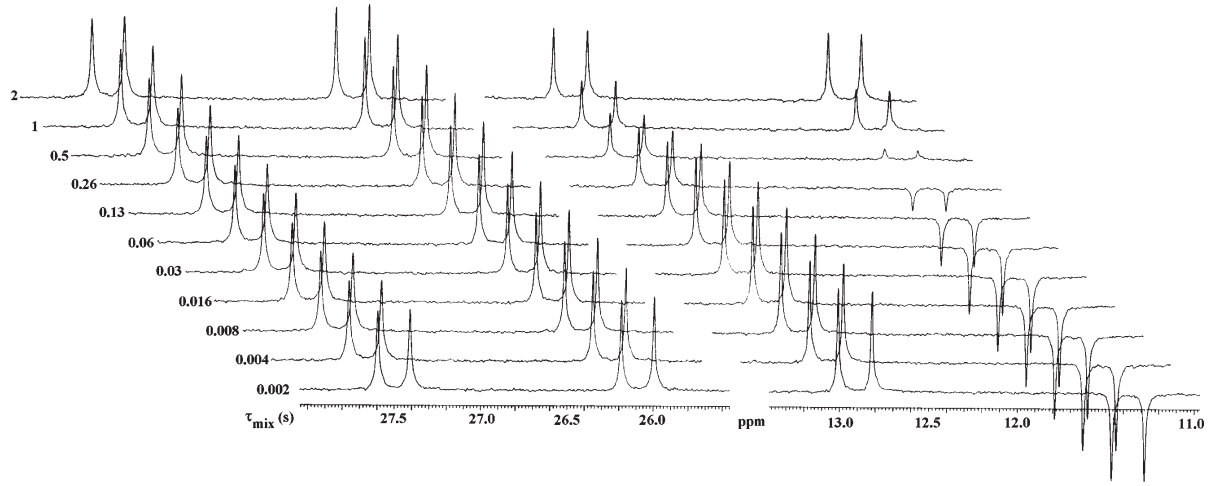

Figura 1. Inversion transfer experiment for **1** in C_6D_6 at room temperature (evolution time for the inversion of the doublet at 11.4 ppm).

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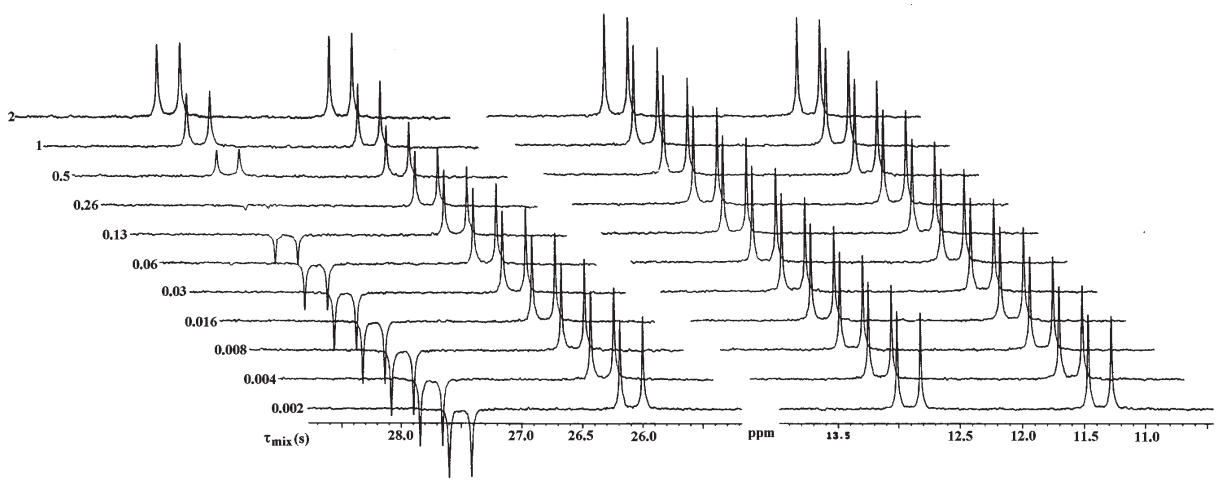

Figura 2. Inversion transfer experiment for **1** in C_6D_6 at room temperature (evolution time for the inversion of the doublet at 27.4 ppm).