

Supporting Information for:

**Palladacycles Bearing Tridentate CNS-type Benzamidinate Ligands as
Catalysts for Cross-Coupling Reactions**

Wei-Chi Wang, Kuo-Fu Peng, Ming-Tsz Chen, and Chi-Tien Chen*

Department of Chemistry, National Chung Hsing University, Taichung 402, Taiwan

Spectroscopic data of coupling products

4-Acetyl biphenyl¹ (Table 1, entry 11): ¹H NMR (400 MHz, CDCl₃) δ 2.65 (s, CH₃, 3H), 7.41 (m, Ar-H, 1H), 7.48 (m, Ar-H, 2H), 7.64 (m, Ar-H, 2H), 7.70 (d, J = 6.8 Hz, Ar-H, 2H), 8.05 (m, Ar-H, 2H).

4-Methyl biphenyl¹ (Table 1, entry 12): ¹H NMR (400 MHz, CDCl₃) δ 2.40 (s, CH₃, 3H), 7.26 (m, Ar-H, 2H), 7.34 (t, J = 4.0 Hz, Ar-H, 1H), 7.43 (t, J = 7.4 Hz, Ar-H, 2H), 7.50 (d, J = 7.2 Hz, Ar-H, 2H), 7.59 (m, Ar-H, 2H).

4-tert-butyl biphenyl¹ (Table 1, entry 13): ¹H NMR (400 MHz, CDCl₃) δ 1.36 (s, C(CH₃), 9H), 7.34 (m, Ar-H, 1H), 7.40-7.48 (overlap, Ar-H, 4H), 7.53-7.60 (overlap, Ar-H, 4H).

4-Methoxy biphenyl¹ (Table 1, entry 14): ¹H NMR (400 MHz, CDCl₃) δ 3.851 (s, OCH₃, 3H), 6.980 (dd, J = 8.8 & 1.2 Hz, Ar-H, 2H), 7.318 (m, Ar-H, 1H), 7.414 (m, Ar-H, 2H), 7.521-7.562 (overlap, Ar-H, 4H).

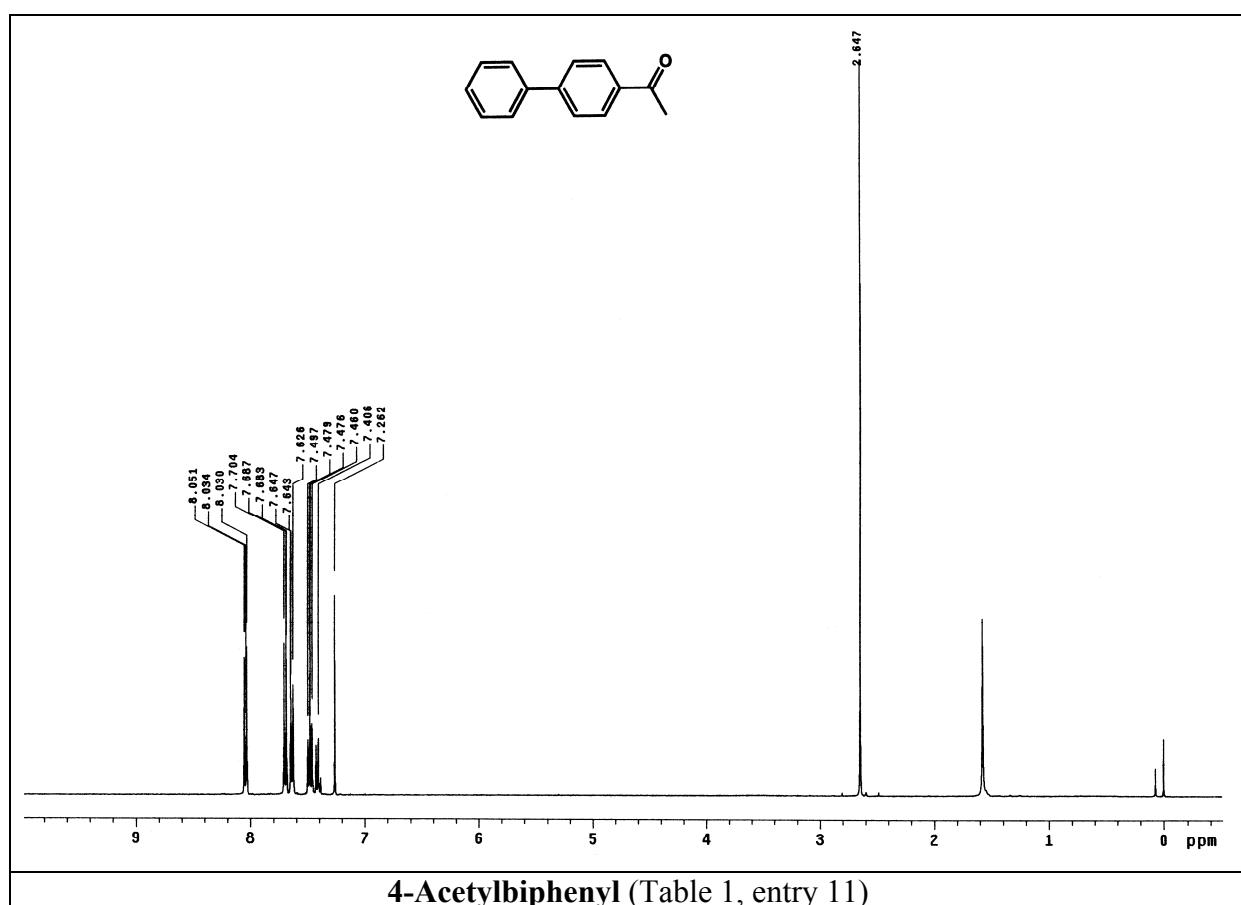
trans-4-Acetyl stilbene² (Table 2, entry 10): ¹H NMR (400 MHz, CDCl₃) δ 2.62 (s, CH₃, 3H), 7.14 (d, J = 16.0 Hz, Ar-H, 1H), 7.28 (d, J = 16.0 Hz, Ar-H, 1H), 7.31 (m, Ar-H, 1H), 7.39 (m, Ar-H, 2H), 7.56 (m, Ar-H, 2H), 7.60 (d, J = 8.4 Hz, Ar-H, 2H), 7.97 (m, Ar-H, 1H).

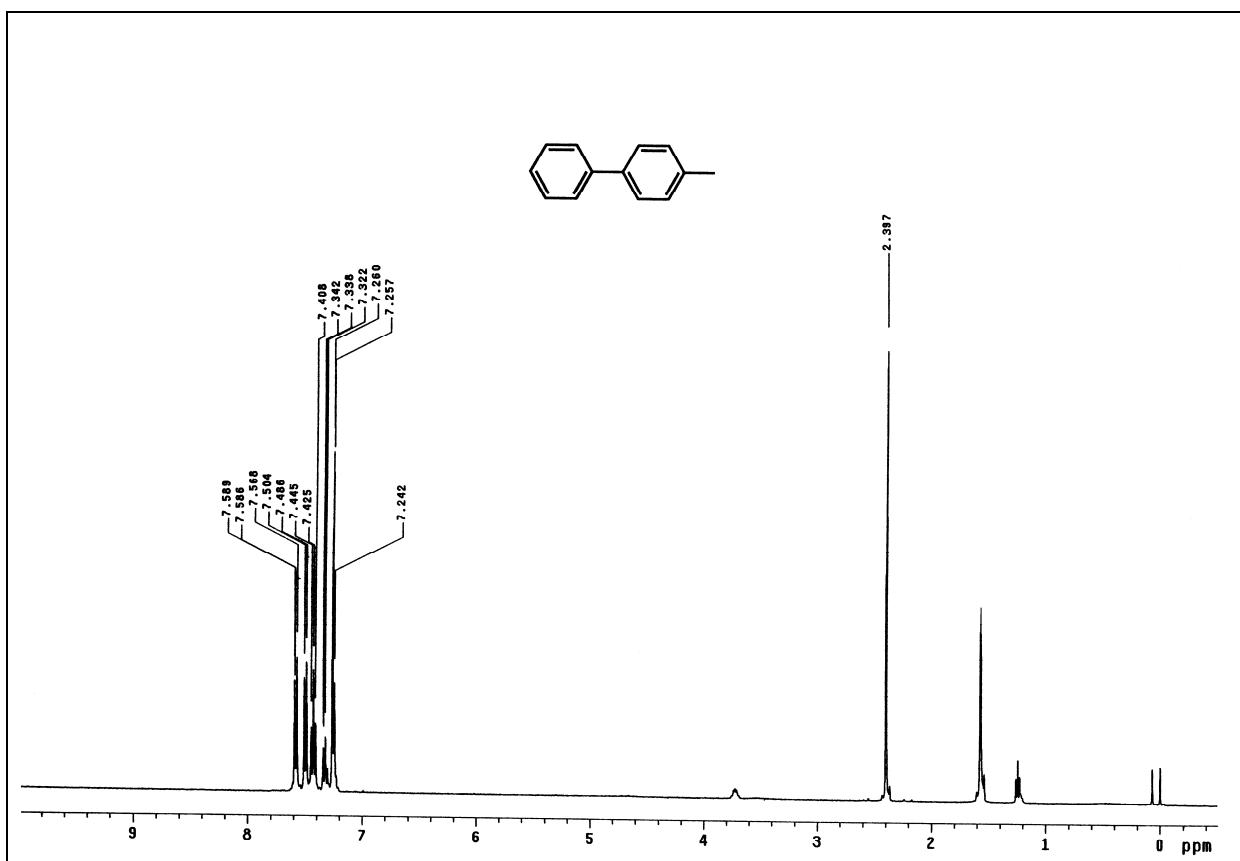
trans-4-methyl stilbene³ (Table 2, entry 20): ¹H NMR (400 MHz, CDCl₃) δ 2.36 (s, CH₃, 3H), 7.07 (d, J = 2.4 Hz, Ar-H, 2H), 7.17 (d, J = 8.0 Hz, Ar-H, 2H), 7.25 (m, Ar-H, 1H), 7.36 (m, Ar-H, 2H), 7.42 (m, Ar-H, 2H), 7.51 (m, Ar-H, 2H).

trans-4-methoxystilbene^{2,3} (Table 2, entry 21): ¹H NMR (400 MHz, CDCl₃) δ 3.83 (s, OCH₃, 3H), 6.90 (d, J = 8.8 Hz, Ar-H, 2H), 6.97 (d, J = 16.0 Hz, Ar-H, 1H), 7.07 (d, J = 16.4 Hz, Ar-H, 1H), 7.23 (m, Ar-H, 1H), 7.34 (t, J = 7.6 Hz, Ar-H, 2H), 7.45-7.50 (overlap, Ar-H, 4H).

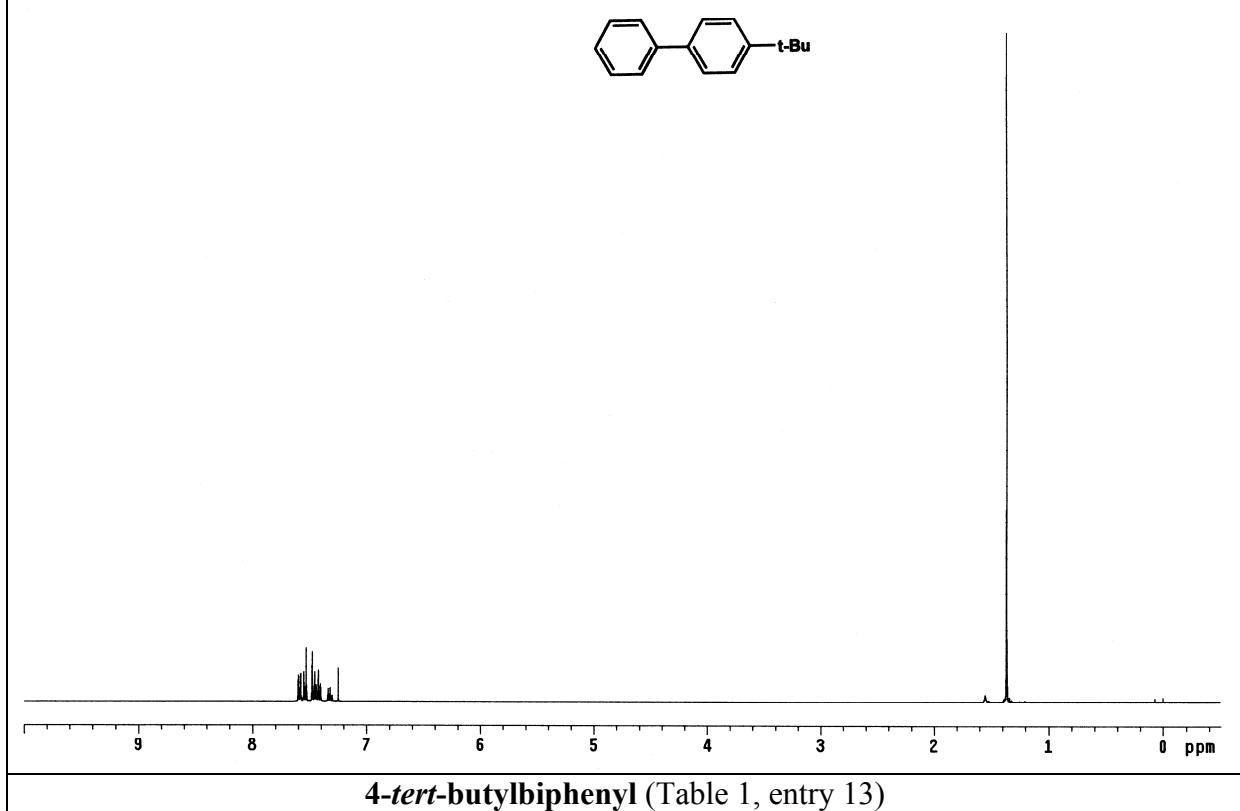
Reference:

1. W. Su, S. Urgaonkar, P. A. McLaughlin and J. G. Verkade, *J. Am. Chem. Soc.*, 2004, **126**, 16433.
2. A. F. Litte and G. C. Fu, *J. Org. Chem.*, 1999, **64**, 10.
3. Q. Yao, E. P. Kinney and C. Zheng, *Org. Lett.*, 2004, **6**, 2997.

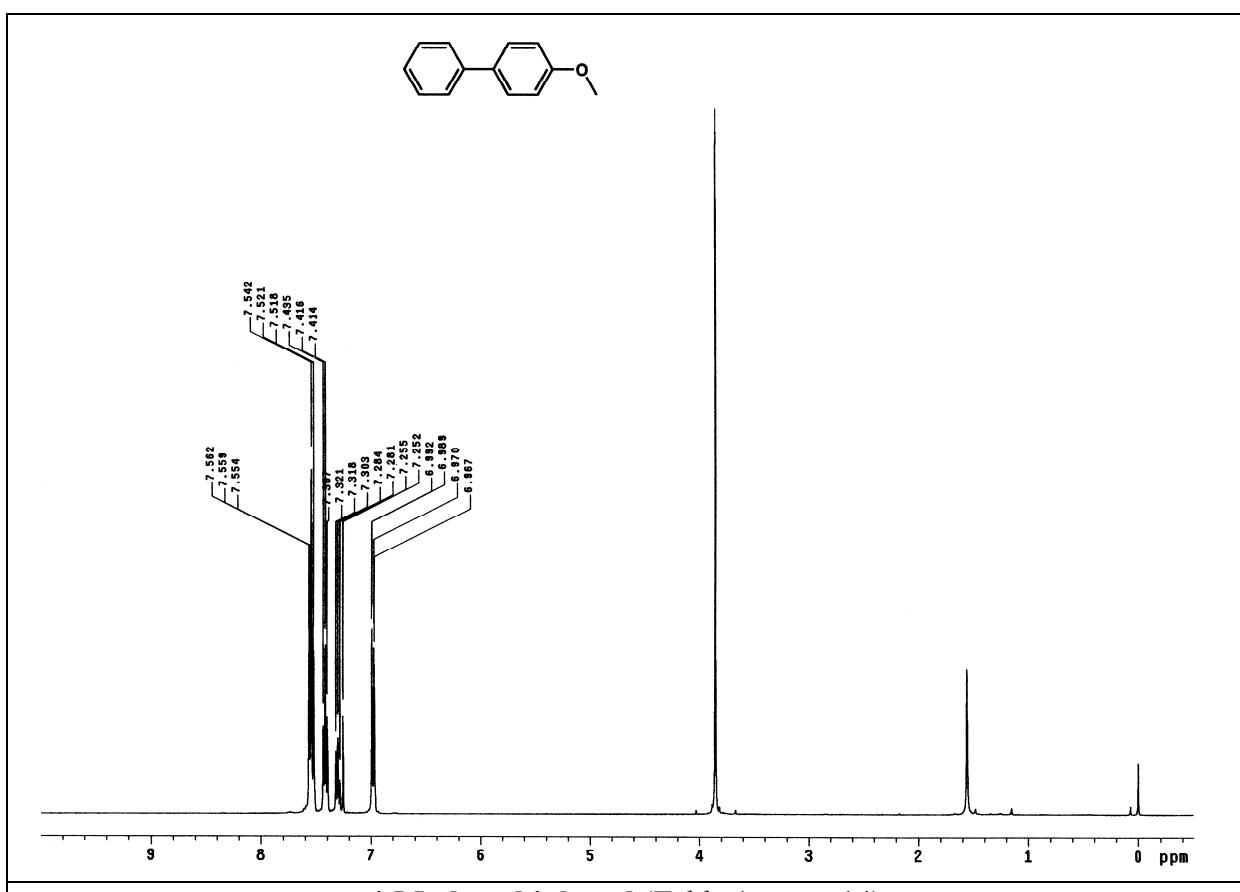




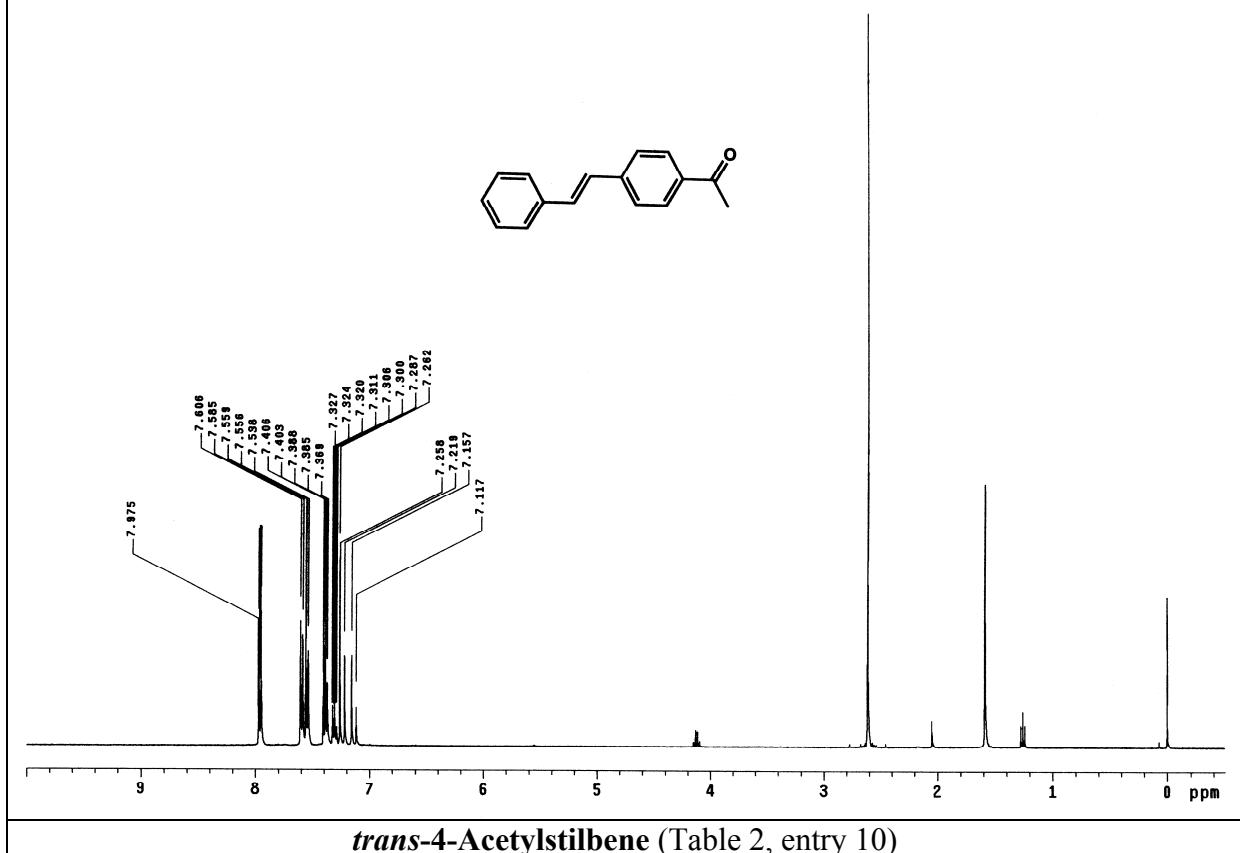
4-Methylbiphenyl (Table 1, entry 12)



4-*tert*-butylbiphenyl (Table 1, entry 13)



4-Methoxybiphenyl (Table 1, entry 14)



trans-4-Acetylstilbene (Table 2, entry 10)

