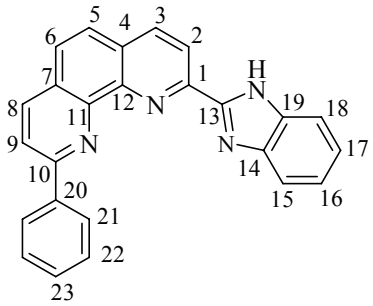
Supplementary Material (ESI) for Dalton Transactions

Chromium(III) complexes bearing 2-benzazole-1,10-phenanthrolines: Synthesis, molecular structures and ethylene oligomerization and polymerization

Min Zhang, Kefeng Wang and Wen-Hua Sun

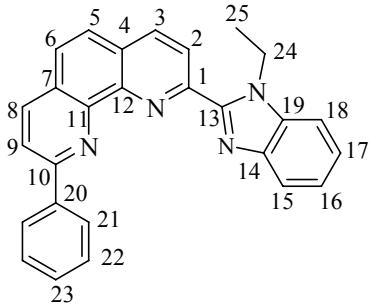
Detail assignments of NMR signals for all new organic compounds:

2-(*1H*-Benzoimidazol-2-yl)-9-phenyl-1,10-phenanthroline (L3)



^{1}H NMR (400 MHz, $CDCl_3$): δ = 13.16 (s, 1 H, N*H*), 8.79 (d, 1 H, J = 8.4 Hz, 3-H), 8.40 (d, 1 H, J = 8.4 Hz, 8-H), 8.34 (d, 1 H, J = 8.4 Hz, 6-H), 8.11–8.09 (m, 2 H, 5-H, 9-H), 7.97 (d, 1 H, J = 8.3 Hz, 2-H), 7.87–7.84 (m, 3 H, 18-H, 2 × 21-H), 7.37–7.34 (m, 4 H, 15-H, 16-H, 2 × 22-H), 7.33–7.31 (m, 1 H, 17-H), 7.27–7.19 (m, 1 H, 23-H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 157.9 (C13), 151.2 (C1), 148.7 (C10), 145.5 (C14), 145.4 (C19), 144.2 (C11), 138.8(C12), 138.0 (C20), 137.0 (C8), 136.9 (C3), 134.7 (C6), 129.2 (C5), 128.9 (C4), 128.0 (2 × C22), 127.9 (2 × C21), 126.8 (C7), 126.2 (C2), 123.5 (C9), 122.0 (C23), 121.5 (C16), 121.4 (C17), 119.7 (C15), 111.3 (C18) ppm.

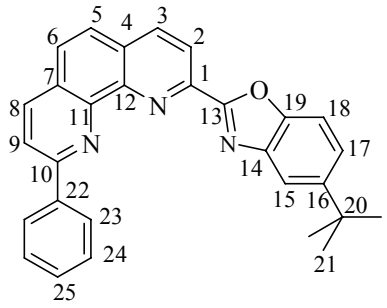
2-(1-Ethyl-benzoimidazol-2-yl)-9-phenyl-1,10-phenanthroline (L4)



^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.83 (d, 1 H, J = 8.4 Hz, 3-H), 8.37–8.35 (m, 2 H, 8-H, 18-H), 8.32 (d, 1 H, J = 8.4 Hz, 6-H), 8.25 (d, 1 H, J = 8.3 Hz, 5-H), 8.08 (d, 1 H, J = 8.4 Hz, 9-H), 7.91 (d, 1 H, J = 8.4 Hz, 2-H), 7.77–7.76 (m, 2 H, 2 × 21-H), 7.56–7.52 (m , 4 H, 15-H, 16-H, 2 × 22-H), 7.37–7.35 (m , 2 H, 17-H, 23-H), 5.57 (dd, 2 H, J_1 = 7.0 Hz, J_2 = 14.0 Hz, 2 × 24-H), 1.70 (t, 3 H, J = 7.0 Hz, 3 × 25-H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 157.1 (C13), 150.3 (C1), 149.6 (C10), 146.4 (C14), 145.7 (C19), 143.1 (C11), 139.8 (C12), 136.9 (C20), 136.8 (C8), 136.6 (C3), 129.6 (C6), 128.8 (C5), 128.7 (C4), 128.0 (2 × C22), 127.8 (2 × C21), 127.1 (C7), 126.1 (C2), 123.7 (C9), 123.5 (C23), 122.7 (C16), 120.4 (C17), 120.3 (C15), 110.4 (C18), 41.2 (C24),

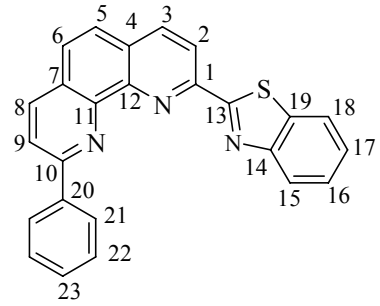
16.0 (C25) ppm.

2-(5-tert-Butylbenzoxazol-2-yl)-9-phenyl-1,10-phenanthroline (L8)



^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.74 (d, J = 8.4 Hz, 1 H, 3-H), 8.50–8.44 (m, 3 H, 2 × 22-H, 8-H), 8.37 (d, J = 8.4 Hz, 1 H, 6-H), 8.21 (d, J = 8.4 Hz, 1 H, 5-H), 7.93 (d, J = 8.7 Hz, 1 H, 9-H), 7.90 (s, 1 H, 15-H), 7.86 (d, J = 8.7 Hz, 1 H, 2-H), 7.71 (d, J = 8.6 Hz, 1 H, 17-H), 7.62 (t, J = 7.4 Hz, 2 H, 2 × 23-H), 7.55–7.52 (m, 2 H, 24-H, 18-H), 1.44 (s, 9 H, 9 × 20-H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 161.5 (C13), 156.6 (C1), 148.8 (C10), 147.8 (C19), 145.6 (C16), 145.3 (C14), 145.1 (C11), 141.3 (C12), 138.7 (C22), 136.4 (C8), 136.3 (C3), 129.3 (C6), 128.8 (C5), 128.3 (2 × C24), 127.5 (2 × C23), 127.3 (C4), 127.0 (C7), 125.2 (C2), 123.4 (C9), 121.6 (C25), 120.0 (C17), 116.3 (C15), 110.0 (C18), 34.2 (C20), 30.8 (3 × C21) ppm.

2-(Benzothiazol-2-yl)-9-phenyl-1,10-phenanthroline (L10)



^{1}H NMR (400 MHz, $CDCl_3$): 8.71 (t, J = 8.0 Hz, 1 H, 15-H), 8.54 (d, 2 H, J = 7.7 Hz, 3-H, 18-H), 8.41–8.28 (m, 2 H, 6-H, 8-H), 8.21–8.14 (m, 2 H, 2 × 21-H), 8.09–8.07 (m, 1 H, 2-H), 7.87–7.77 (m, 2 H, 16-H, 17-H), 7.64 (t, J = 7.6 Hz, 2 H, 5-H, 9-H), 7.55–7.52 (m, 2 H, 2 × 22-H), 7.45 (t, 1 H, J = 7.2 Hz, 23-H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 170.3 (C13), 156.9 (C1), 154.4 (C10), 146.0 (C14), 145.5 (C11), 139.1 (C12), 137.1 (C20), 136.9 (C8), 136.8 (C3), 130.0 (C6), 129.6 (C5), 128.9 (C4), 127.9 (2 × C22), 127.5 (2 × C21), 127.4 (C7), 126.2 (C2) , 125.8 (C9), 125.7 (C23), 123.7 (C16), 122.1 (C17), 120.1 (C15), 119.8 (C18) ppm.

The ^{1}H and ^{13}C NMR data of other ligands were not assigned because they have been appeared in three literatures:

(1) **L1**, **L2** (M. Zhang, S. Zhang, P. Hao, S. Jie, W.-H. Sun, P. Li and X. Lu. *Euro. J. Inorg. Chem.*, 2007, 3816);

(2) **L5**, **L6**, **L7** (M. Zhang, P. Hao, W. Zuo, S. Jie and W.-H. Sun, *J. Organomet. Chem.*, 2008, **693**, 483);

(3) **L9** (H. A. Goodwin, D. W. Mather and F. E. Smith, *Aust. J. Chem.*, 1975, **28**, 33).