Supporting Information

Insertion of terminal alkynes into Pt-N bonds of square planar [$PtI_2(Me_2phen)$] complex

Michele Benedetti,[a]* Federica De Castro,[a] Vincenza Lamacchia,[b,c] Concetta Pacifico,[b] Giovanni Natile,[b] and Francesco P. Fanizzi.[a]*

[a.] Dipartimento di Scienze e Tecnologie Biologiche ed Ambientali, Università del Salento, Via Monteroni, I-73100 Lecce, Italy. E-mail: fp.fanizzi@unisalento.it or michele.benedetti@unisalento.it; Fax: +39 0832 298626; Tel: +39 0832 298867.
[b.] Dipartimento di Chimica, Università degli Studi di Bari, Via E. Orabona 4, I-70125 Bari, Italy.
[c.] Present Address: IPSIA Archimede - Via Madonna della Croce, 223, I-76121 Barletta (BT), Italy.

NMR characterization of complexes [PtI_2{κ^2-*N*,*C*-(*Z*)-N1—N10-C=C(H)(Ph)}], 7a, and [PtI_2{κ^2-*N*,*C*-(*Z*)-N1—N10-C=C(H)(*n*-Bu)}], 7b, (N1—N10 = 2,9-dimethyl-1,10-phenanthroline).

(7a). NMR (CD_2Cl_2, 25 °C): $\delta(^1H)$ = 3.29 (*s*, 3H, C9-C*H*$_3$), 3.47 (s, 3H, C2-C*H*$_3$), 6.27 (s, $^3J_{H\text{-}Pt}$ = 80.4 Hz, 1H, β-C=C(*H*)(Ph)), 7.33 (t, $^3J_{H\text{-}H}$ = 7.4 Hz, 1H, *p*-C*H*), 7.43 (t, $^3J_{H\text{-}H}$ = 7.4 Hz, 2H, *m*-C*H*), 7.73 (d, $^3J_{H\text{-}H}$ = 8.1 Hz, 1H, C*H*3), 7.97 (d, $^3J_{H\text{-}H}$ = 8.1 Hz, 1H, C*H*8), 8.04 (m, 2H, C*H*5 and C*H*6), 8.43 (d, $^3J_{H\text{-}H}$ = 8.8 Hz, 1H, C*H*4), 8.72 (d, $^3J_{H\text{-}H}$ = 7.4 Hz, 2H, *o*-C*H*) and 8.76 ppm (d, $^3J_{H\text{-}H}$ = 8.8 Hz, 1H, C*H*7); $\delta(^{13}C)$ = 25.7 (1C, C9-*C*H$_3$), 33.7 (1C, C2-*C*H$_3$), 128.1 (1C, *p*-*C*H), 128.3 (2C, *m*-*C*H), 128.6 (1C, *C*H8), 128.8 (2C, *o*-*C*H), 129.0 (1C, *C*H3), 129.3 (2C, *C*H5-6), 132.6 (1C, β-C=*C*(H)(Ph)), 133.7 (1C, α-*C*=C(H)(Ph)), 135.8 (1C, γ-*C*), 137.1 (1C, *C*7'), 138.1 (1C, *C*4'), 138.2 (1C, *C*H4), 141.1 (1C, *C*H7), 153.6 (1C, *C*9) and 166.7 ppm (1C, *C*2); $\delta(^{15}N)$ = −188 (1N, *N*1) and −172 ppm (1N, *N*10); $\delta(^{195}Pt)$ = −3642 ppm

(7b). NMR (CD_2Cl_2, 25 °C): $\delta(^1H)$ = 0.905 (m, 3H, ω-C*H*$_3$), 1.37 (m, 3H, ε-C*H*$_2$ + δ-C*H*H), 1.48 (m, 1H, δ-CH*H*), 2.78 (m, 2H, γ-C*H*$_2$), 3.18 (s, 3H, C9-C*H*$_3$), 3.51 (s, 3H, C2-C*H*$_3$), 5.37 (t, $^3J_{H\text{-}H}$ = 7.33 Hz, $^3J_{H\text{-}Pt}$ = 65 Hz, 1H, β-C=C(*H*)(*n*-Bu)), 7.78 (d, $^3J_{H\text{-}H}$ = 8.3 Hz, 1H, C*H*3), 7.85 (d, $^3J_{H\text{-}H}$ = 8.4 Hz, 1H, C*H*8), 8.02 (m, 2H, C*H*5 and C*H*6), 8.45 (d, $^3J_{H\text{-}H}$ = 8.3 Hz, 1H, C*H*4) and 8.77 ppm (d, $^3J_{H\text{-}H}$ = 8.3 Hz, 1H, C*H*7); $\delta(^{13}C)$ = 0.91 (1C, ω-*C*H$_3$), 22.8 (1C, ε-*C*H$_2$), 25.51 (1C, C9-*C*H$_3$), 31.6 (1C, γ-*C*H$_2$), 31.7 (1C, δ-*C*H$_2$), 33.3 (1C, C2-*C*H$_3$), 126.4 (1C, *C*H6), 128.1 ($^1J_{C\text{-}Pt}$ ≈ 1220 Hz, 1C, α-*C*=C(H)(*n*-Bu)), 128.3 (1C, *C*H8), 128.8 (1C, *C*H3), 129.0 (1C, *C*H5), 133.4 (1C, β-C=*C*(H)(*n*-Bu)), 136.5 (1C, *C*7'), 137.9 (1C, *C*H4), 138 (1C, C4'), 141.1 (1C, *C*H7), 152.8 (1C, *C*9) and 166.2 ppm (1C, *C*2); $\delta(^{15}N)$ = −187 (s, $^1J_{N\text{-}Pt}$ = 355 Hz, 1N, *N*1) and −176 ppm (s, $^2J_{N\text{-}Pt}$ = 215 Hz, 1N, *N*10); $\delta(^{195}Pt)$ = −3674 ppm

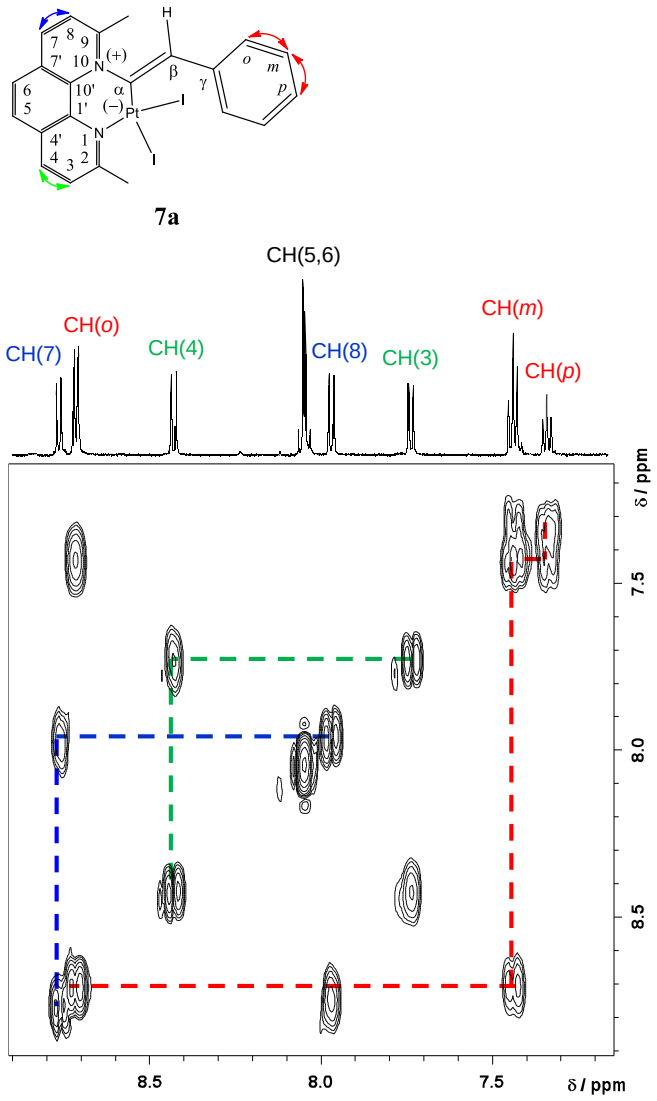

Figure S1. [^{1}H,^{1}H]-COSY NMR spectrum of complex **7a** in CD_2Cl_2. The cross peaks between aromatic CH protons are evidenced with dashed green and blue lines, whereas those between protons of the vinyl and Phenyl systems are evidenced with dashed red lines.

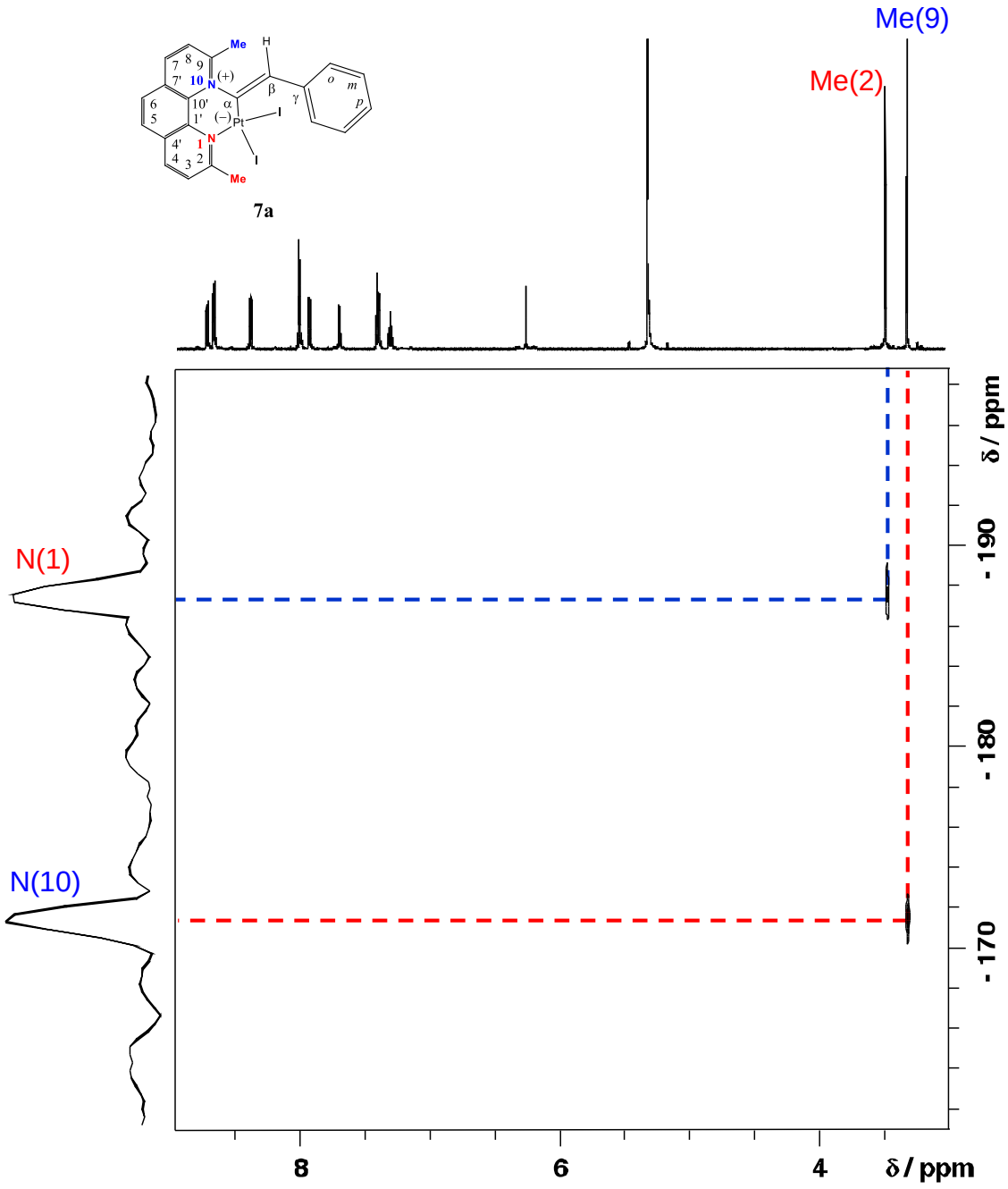

Figure S2. [^{1}H,^{15}N]-HETCOR NMR spectrum of complex **7a** in CD_2Cl_2. The cross peaks between N1 and Me_2phen Me2 protons, are evidenced with dashed red lines, while those of N10 with Me_2phen Me9 protons, are evidenced with dashed blue lines.

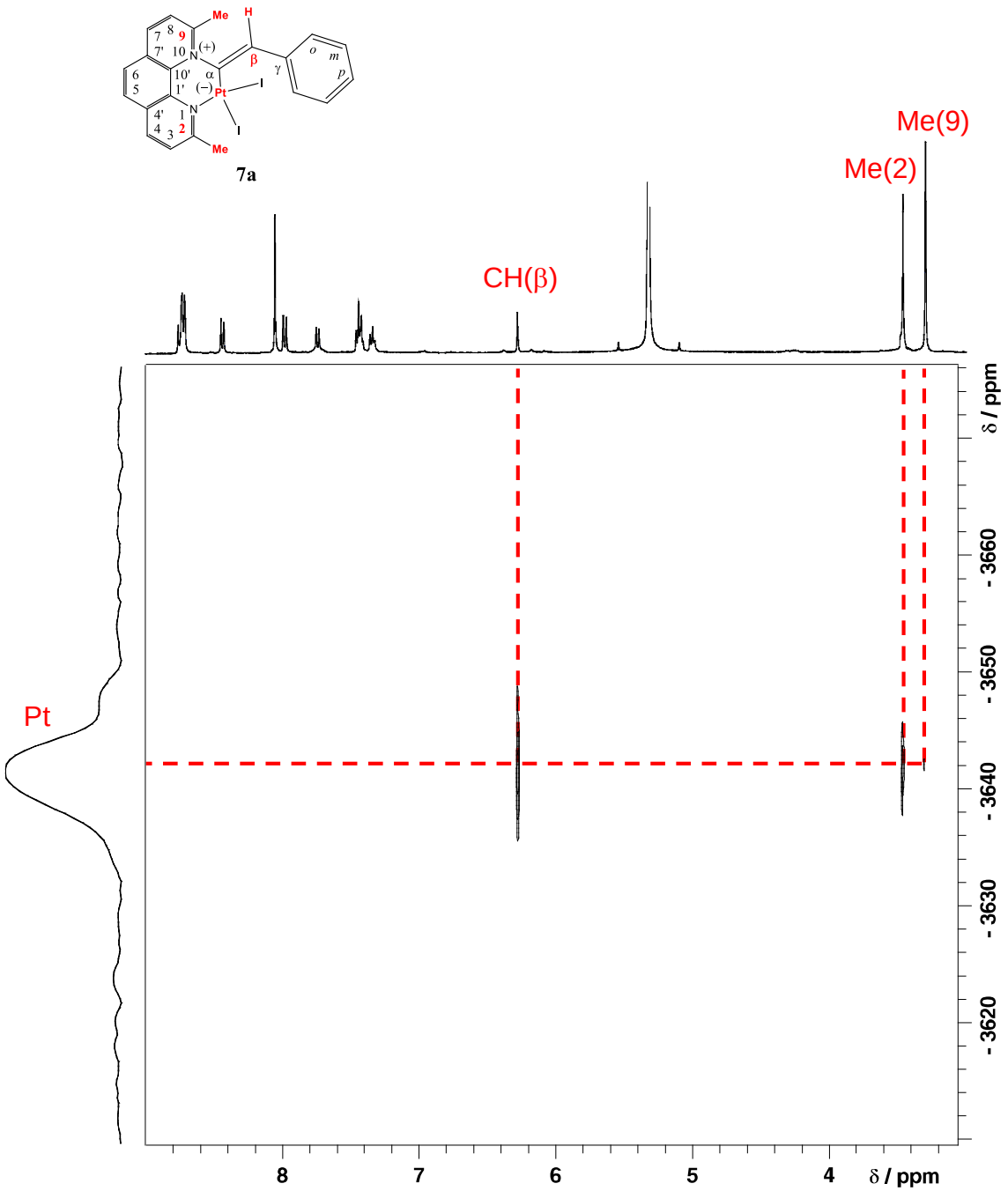

Figure S3. [^{1}H,^{195}Pt]-HETCOR NMR spectrum of complex **7a** in CD_2Cl_2. The cross peaks of the ^{195}Pt with the vinylic CHβ proton and the Me2 and Me9 protons of Me_2phen, are evidenced with dashed red lines.

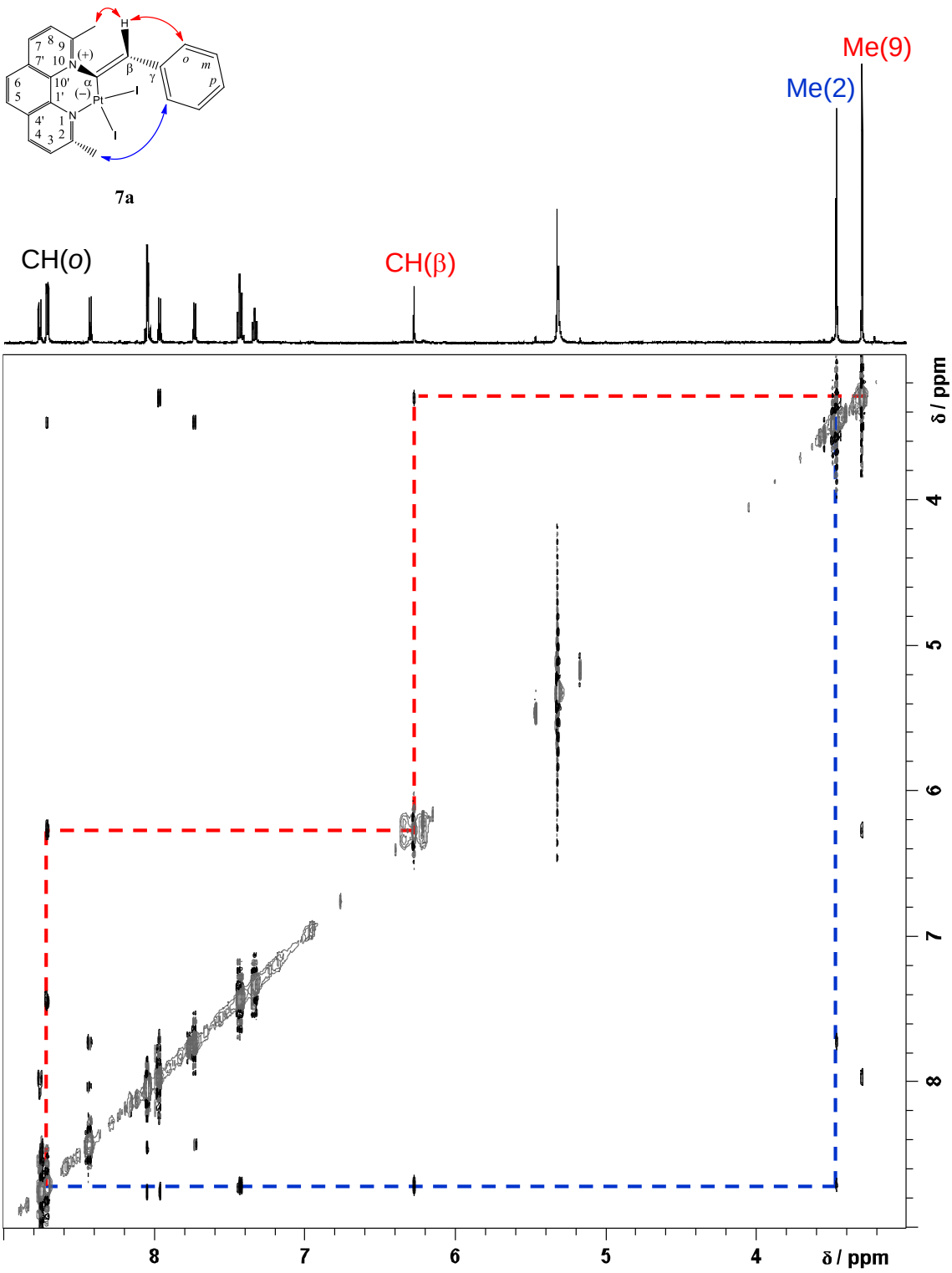

Figure S4. [^{1}H,^{1}H]-NOESY NMR spectrum of complex **7a** in CD_2Cl_2. The cross peak of Me2 protons of Me_2phen with the *o*-CH's of the phenyl system is evidenced with dashed blue lines, whereas the cross peaks of the vinylic proton CH(β) with the Me(9) protons of Me_2phen and and the *o*-CH's of the Phenyl system are evidenced with dashed red lines.