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Supplementary material

SUPPLEMENTARY MATERIAL TO

Structural study of Pt(II) and Pd(II) complexes with quinoline-2-carboxaldehyde thiosemicarbazone

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*Quinoline-2-carboxaldehyde thiosemicarbazone (**HL**)*

Yield: 0.647 g (51 %); IR (ATR, cm^{-1}): 3393*s*, 3265*m*, 3146*s*, 3062*m*, 3004*m*, 2979*m*, 1605*s*, 1527*vs*, 1501*s*, 1451*s*, 1359*w*, 1321*s*; 1281*s*, 1208*w*, 1111*s*, 1060*m*, 948*vw*, 925*w*, 901*vw*, 867*vw*, 840*m*, 773*w*, 750*m*; ^{1}H-NMR (500 MHz, DMSO-d_6, δ / ppm): 7.58 (1H, *m*), 7.72 (1H, *m*), 7.95 (2H, *m*), 8.20 (1H, *s*), 8.31 (2H, *m*), 8.41(1H, *s*), 8.43 (1H, *s*), 11.77 (1H, *s*). ^{13}C-NMR (126 MHz, DMSO-d_6, δ / ppm): 118.54, 127.55, 128.25, 128.33, 129.20, 130.33, 136.69, 142.96, 147.75, 154.33, 178.91.

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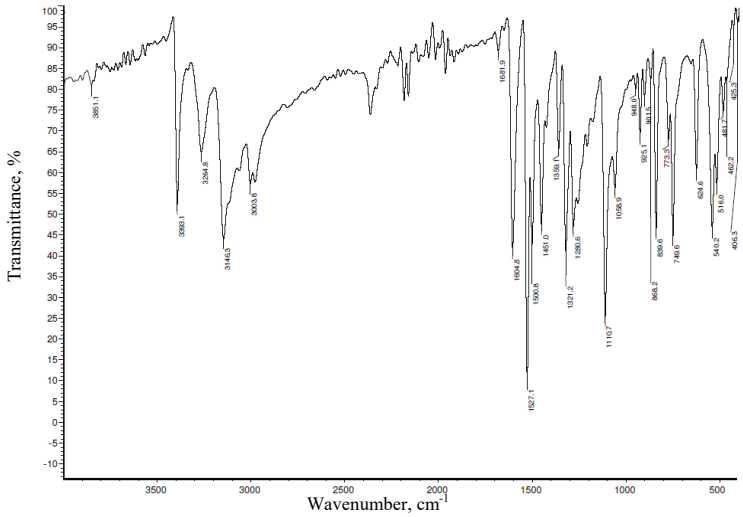

Fig. S-1. IR spectrum of **HL**.

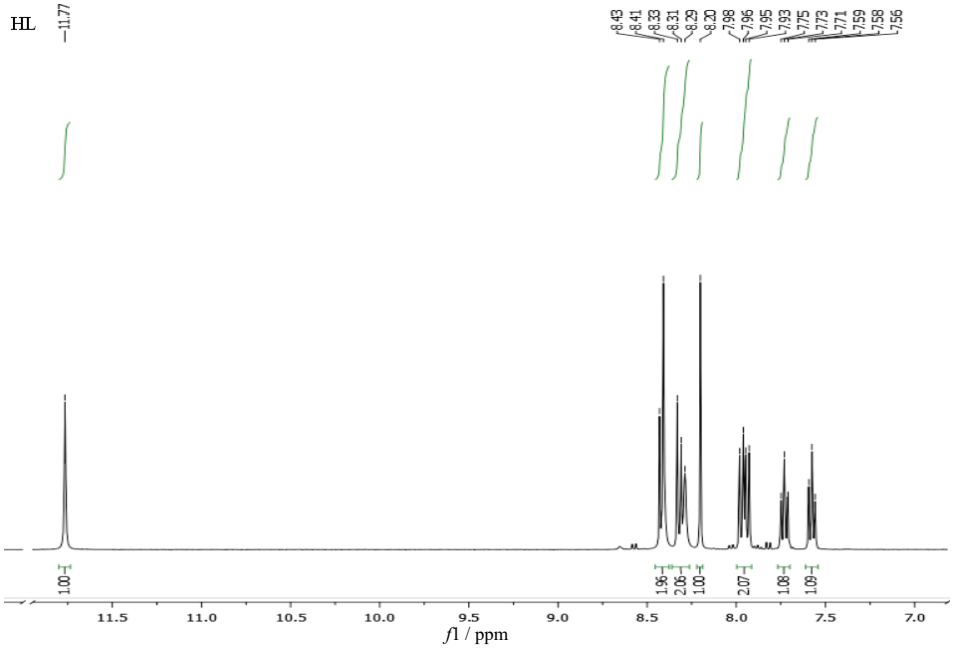

Fig. S-2. ^{1}H-NMR spectrum of **HL**.

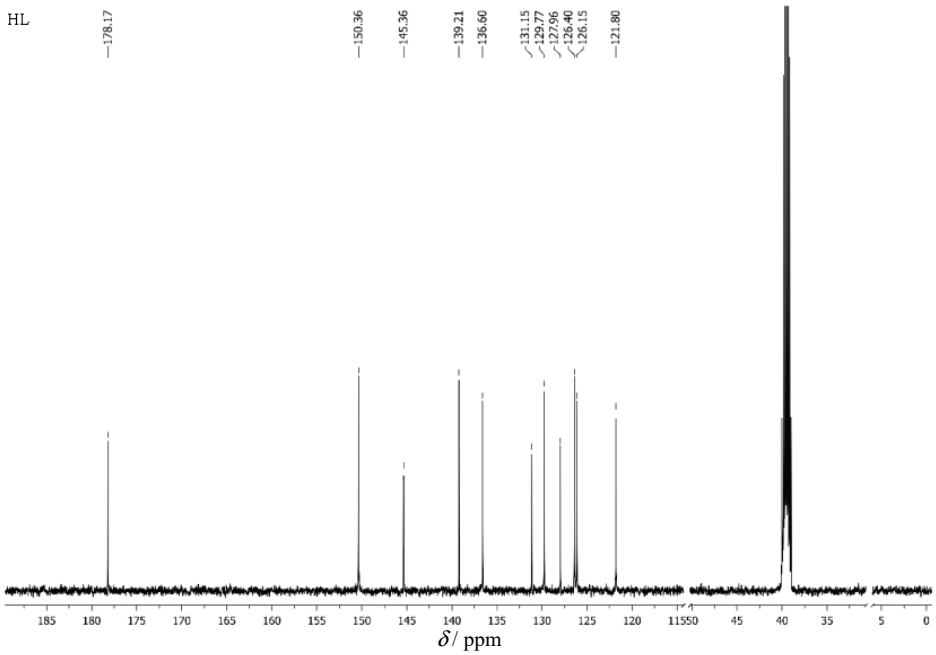

Fig. S-3. ^{13}C-NMR spectrum of **HL**.

Quinoline-2-carboxaldehyde thiosemicarbazonato-N,N,S-*chloridoplatinum(II), [PtLCl] (**1**)*

Yield: 0.04 g (42 %); Anal. calcd. for $C_{11}H_9ClN_4PtS$ (*FW*: 459.82): C, 28.73; H, 1.97; N, 12.18; S, 6.97 %. Found: C, 28.39; H, 1.59; N, 11.89; S, 7.23 %; IR (ATR, cm^{-1}): 3395*m*, 3287*m*, 3224*w*, 3104*m*, 1632*s*, 1576*m*, 1544*m*, 1516*w*, 1471*vs*, 1442*vs*, 1399*s*, 1317*m*, 1290*m*, 1237*w*, 1206*vw*, 1143*m*, 986*w*, 944*vw*, 868*w*, 816*w*, 774*vw*, 745*vw*, 707*w*; ^{1}H-NMR (500 MHz, DMSO-d_6, δ / ppm): 7.70 (1H, *t*), 7.84 (1H, *d*), 7.86 (1H, *m*), 8.05 (1H, *d*), 8.25 (2H, *s*), 8.61 (1H, *s*), 8.74 (1H, *d*), 9.69 (1H, *d*); ^{13}C-NMR (126 MHz, DMSO-d_6, δ / ppm): 121.24, 126.36, 128.08, 128.69, 129.61, 132.54, 141.73, 147.86, 148.24, 161.82, 185.09; Λ_M (1×10^{-3} M, DMSO, Ω^{-1} cm^2 mol^{-1}): 2.76.

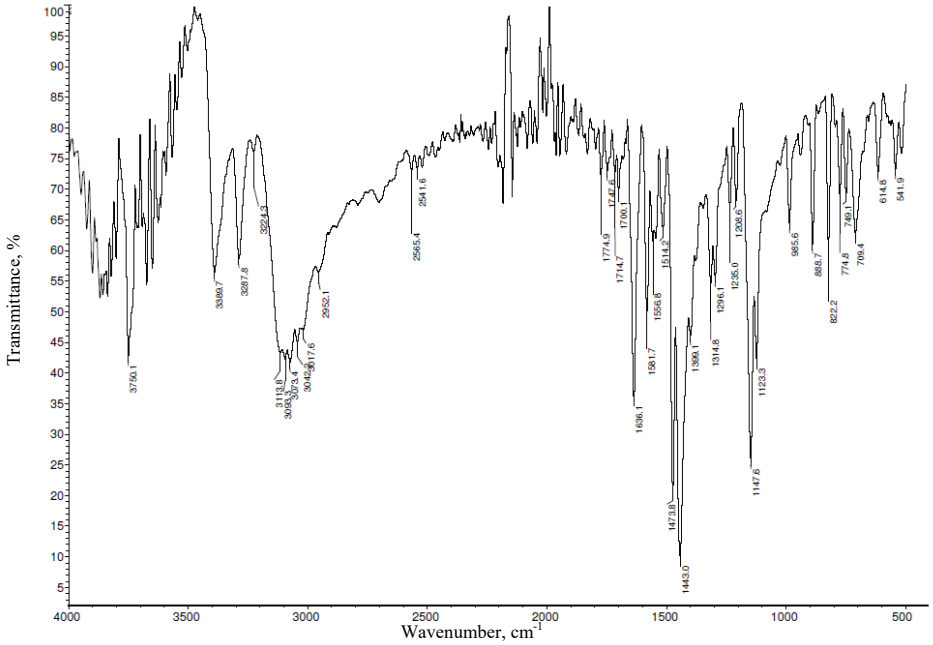

Fig. S-4. IR spectrum of **1**.

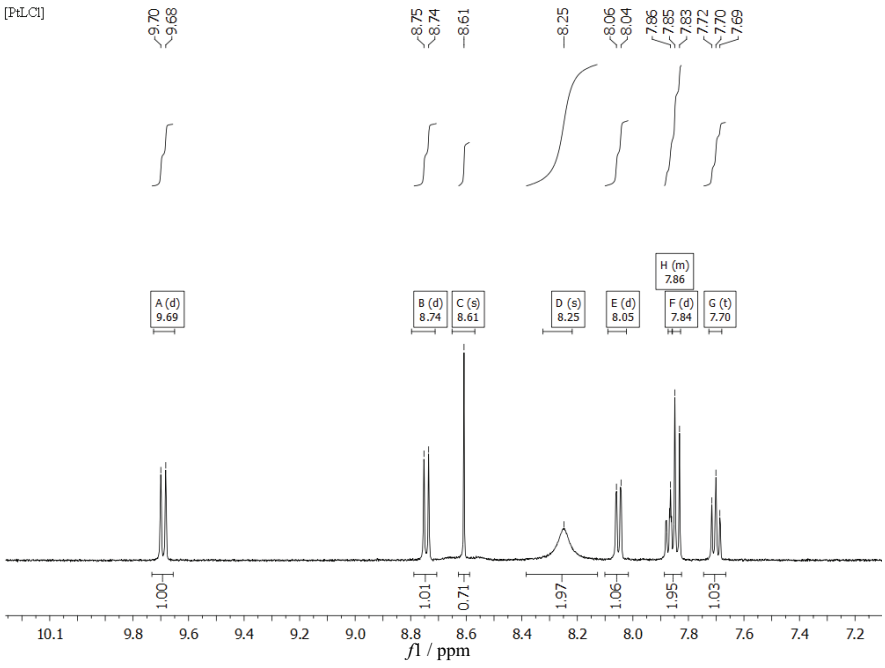

Fig. S-5. ^{1}H-NMR spectrum of **1**.

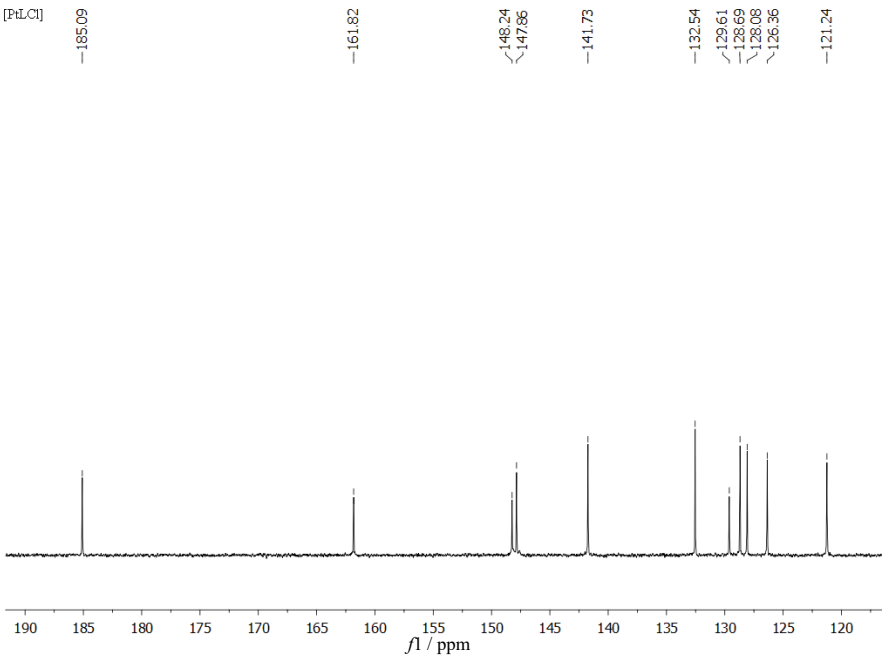

Fig. S-6. ^{13}C-NMR spectrum of **1**.

Quinoline-2-carboxaldehyde thiosemicarbazonato-N,N,S-*chloridopalladium(II), [PdLCl] (**2**)*

Yield: 0.03 g (39 %); Anal. calcd. for $C_{11}H_9ClN_4PdS$ (*FW*: 371.13): C, 35.60; H, 2.44; N, 15.10; S, 8.64 %. Found: C, 35.28; H, 2.52; N, 14.93; S, 8.35 %; IR (ATR, cm^{-1}): 3422*s*, 3362*s*, 3294*s*, 3127*s*, 3041*m*, 2959*m*, 1638*s*, 1598*w*, 1578*w*, 1475*vs*, 1449*vs*, 1398*m*, 1320*w*, 1293*w*, 1233*w*, 1158*s*, 991*w*, 852*w*, 817*w*, 776*w*, 747*w*; ^{1}H-NMR (500 MHz, DMSO-d_6, δ / ppm): 7.69 (1H, *t*), 7.83 (2H, *m*), 8.04 (1H, *d*), 8.06 (1H, *s*), 8.11 (1H, *s*), 8.70 (1H, *d*), 9.48 (1H, *d*); ^{13}C-NMR (126 MHz, DMSO-d_6, δ / ppm): 121.59, 126.9, 128.43, 128.65, 132.27, 141.28, 147.42, 147.55, 159.17, 182.77; Λ_M (1 × 10^{-3} M, DMSO, Ω^{-1} cm^2 mol^{-1}): 1.98.

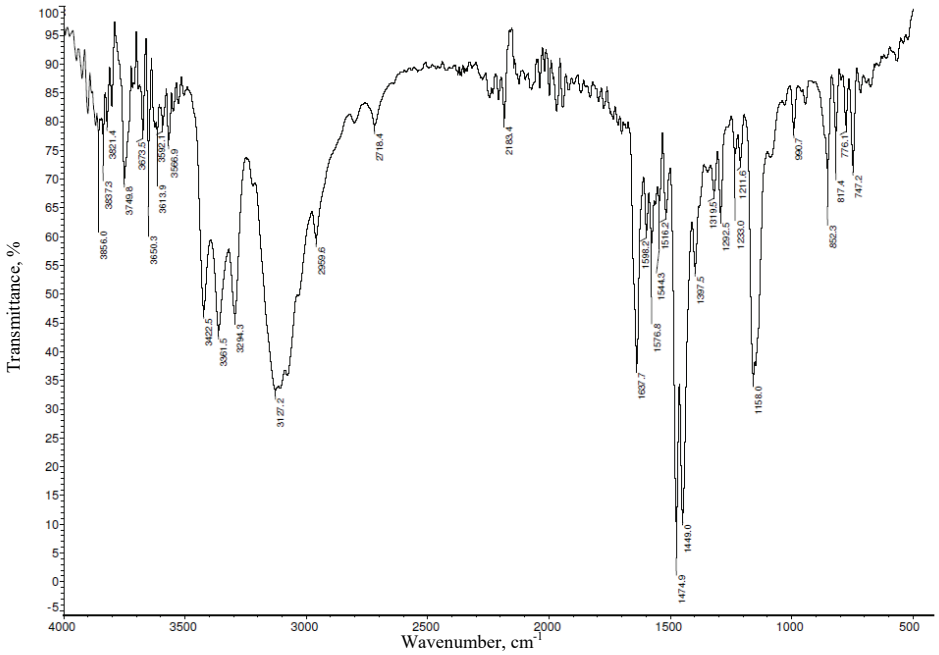

Fig. S-7. IR spectrum of **2**.

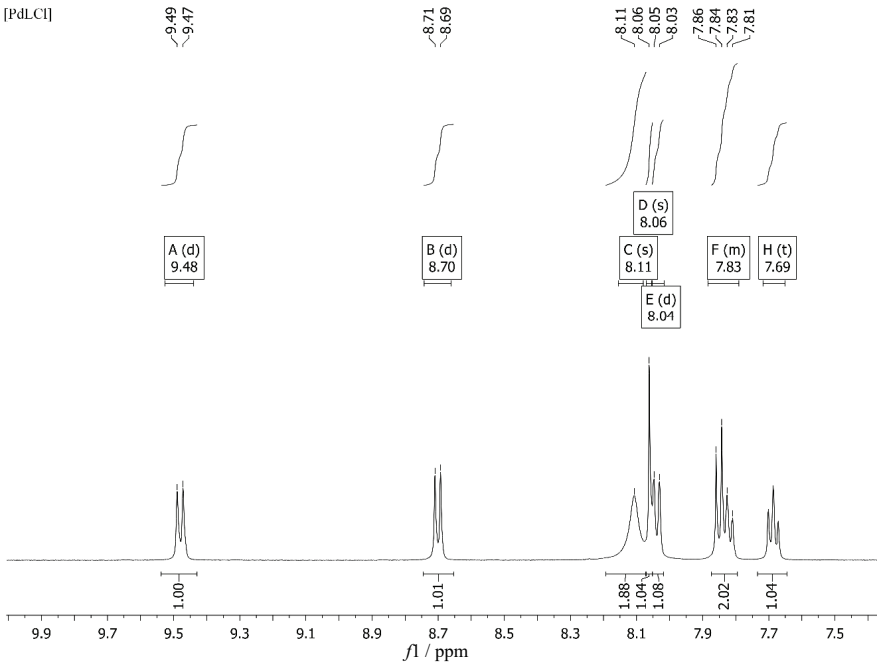

Fig. S-8. ^{1}H-NMR spectrum of **2**.

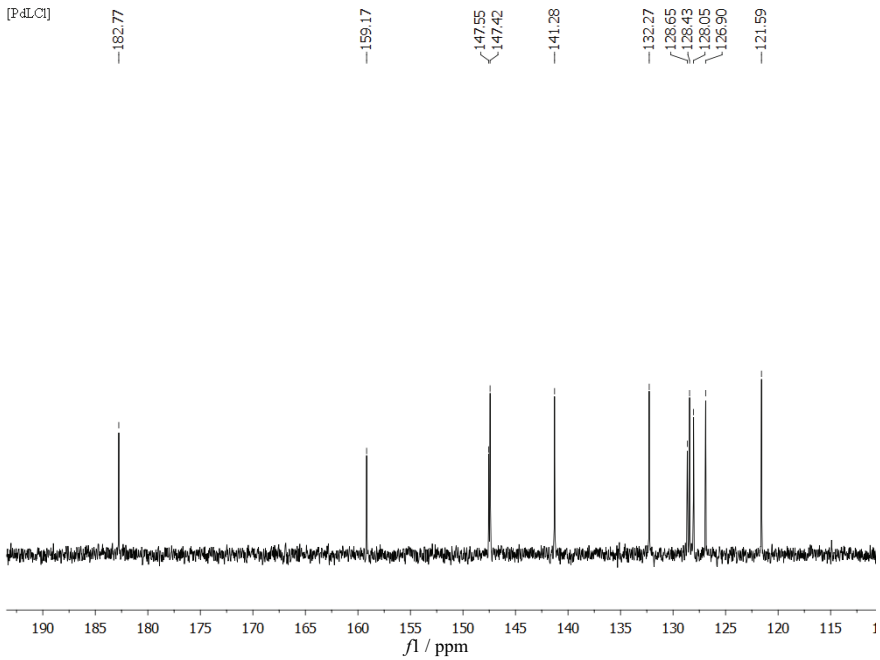

Fig. S-9. ^{13}C-NMR spectrum of **2**.

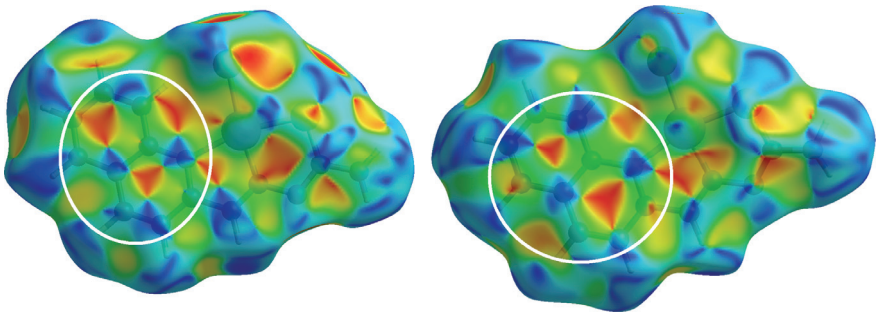

Fig. S-10. Views of the Hirshfeld surface for **1** (left) and **2** (right) mapped over the shape-index property highlighting blue regions about bright-red spots within the quinoline rings, which are highlighted by the white circles.

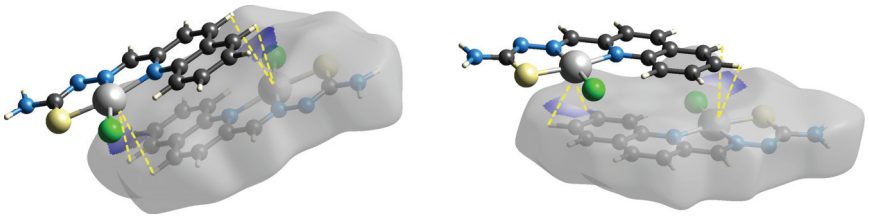

Fig. S-11. Blue patches on the Hirshfeld surfaces for **1** (left) and **2** (right) with highlighted corresponding M···H interactions.