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Accessory Publication

Synthesis and characterisation of new palladium(II) complexes containing *N*-alkylamino-3,5-diphenylpyrazole ligands. Crystal structure of [PdCl(L2)](BF₄) {L2 = bis[2-(3,5-diphenyl-1-pyrazolyl)ethyl]ethylamine}

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Table S1. ^1H NMR results: chemical shifts (ppm) and ^1H , ^1H coupling constants (Hz) for **1** and **2** in CDCl_3

Compound	1	2
δ H(16a)	4.50	5.10
δ H(16b)	4.63	5.66
δ H(17 ^a)	3.13	3.15
δ H(17b)	3.44	4.66
δ H _{amino}	5.25	-
$^2J(16\text{a}, 16\text{b})$	13.00	15.86
$^2J(17\text{a}, 17\text{b})$	12.94	14.60
$^3J(17\text{b}, 16\text{b})$	5.93	2.09
$^3J(17\text{b}, 16\text{a})$	6.34	1.73
$^3J(17\text{a}, 16\text{b})$	6.37	11.09
$^3J(17\text{a}, 16\text{a})$	6.82	4.33
$^3J(17\text{a}, \text{H}_{\text{amino}})$	4.33	-
$^3J(17\text{b}, \text{H}_{\text{amino}})$	8.99	-

Table S2. ^1H NMR results: chemical shifts (ppm) and ^1H , ^1H coupling constants (Hz) for **3** and **4** in CD_3CN

Compound	3	4
δ H (16a)	4.83	4.69
δ H (16b)	5.28	5.56
δ H (17a)	3.02	3.16
δ H (17b)	3.25	3.23
δ H _{amino}	5.68	-
$^2J(16a,16b)$	15.57	15.80
$^2J(17a,17b)$	13.28	14.61
$^3J(17b,16b)$	2.24	1.27
$^3J(17b,16a)$	6.54	3.70
$^3J(17a,16b)$	8.61	11.40
$^3J(17a,16a)$	3.00	1.74
$^3J(17a, \text{H}_{\text{amino}})$	5.62	-
$^3J(17b, \text{H}_{\text{amino}})$	8.56	-

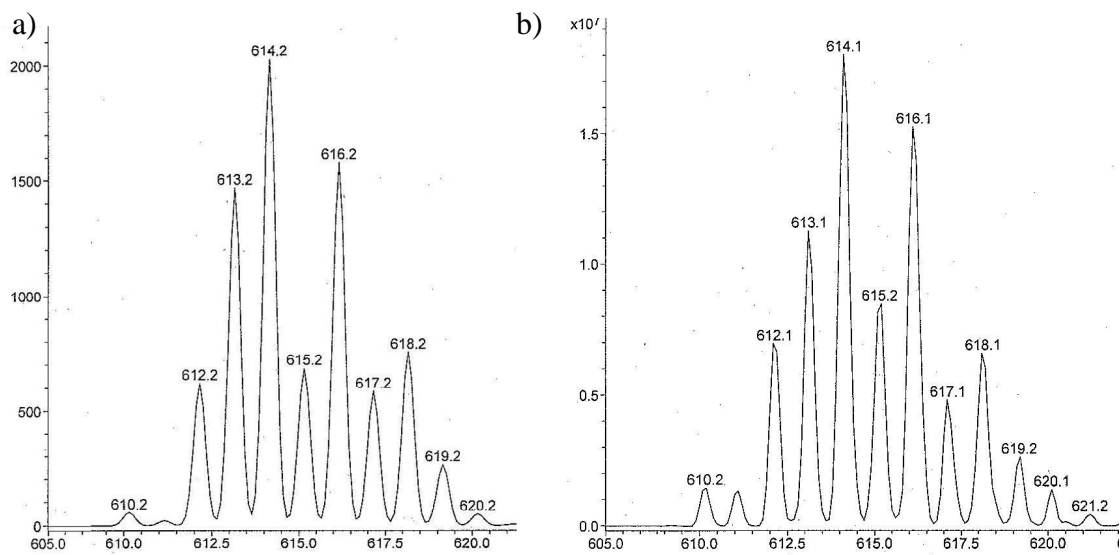
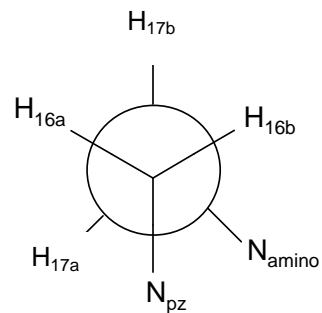
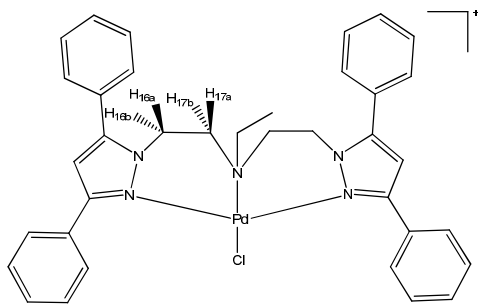
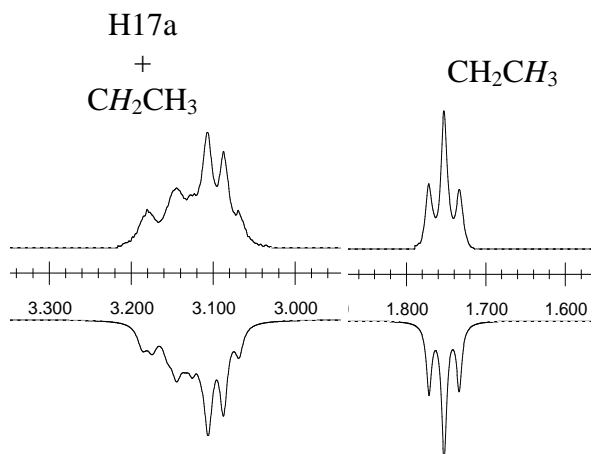
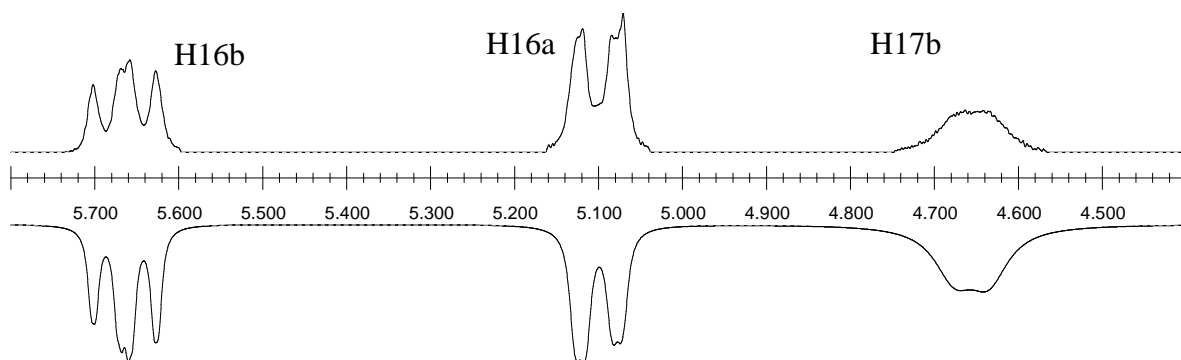


Figure S1 (a) ESI⁺-MS spectra in methanol of fragments [PdCl₂(L1)-HCl-Cl]⁺ for complex **1** and (b) theoretical isotopic distribution of **1**.

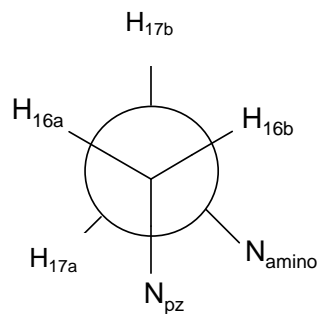
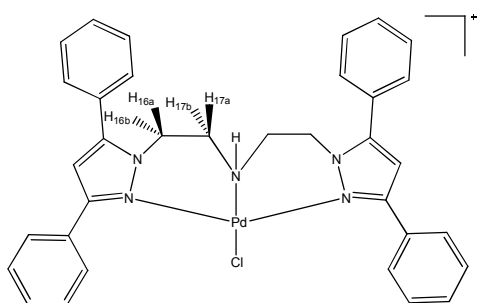


Experimental

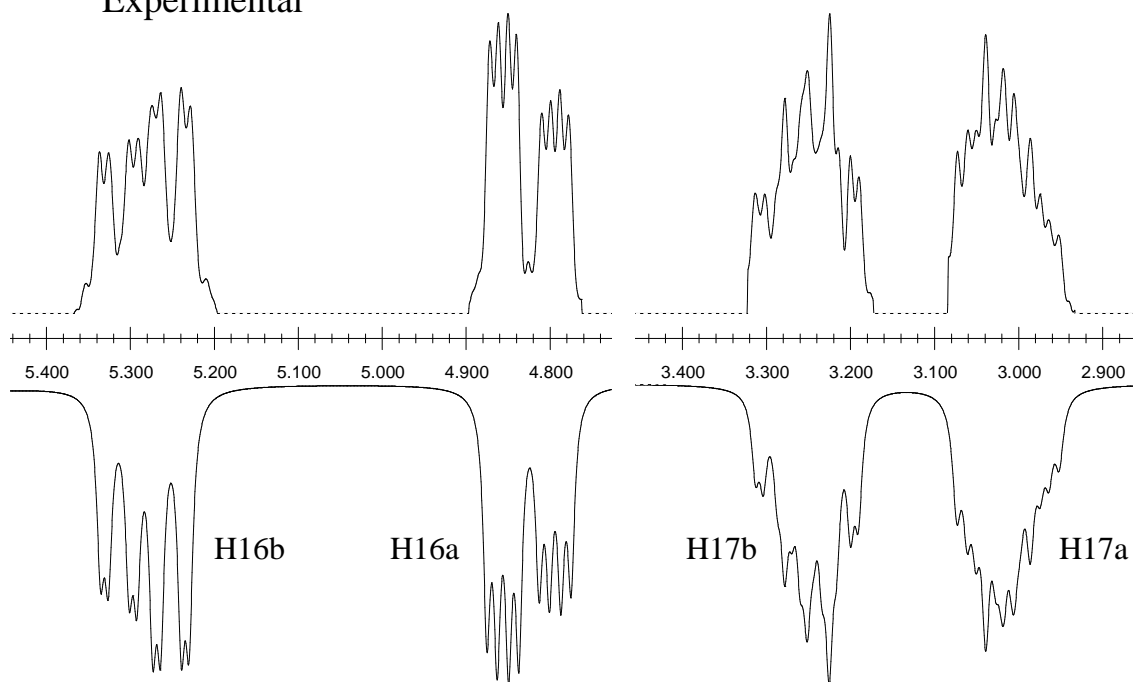


Simulated

Figure S2 The experimental (250 MHz, CDCl_3 , 298 K) and simulated (*g* NMR) ^1H NMR spectra for H-16 and H-17 protons of the $\text{N}_{\text{pz}}\text{CH}_2\text{CH}_2\text{N}_{\text{amino}}$ fragment of $[\text{PdCl}(\text{L}2)]\text{Cl}$ (**2**)

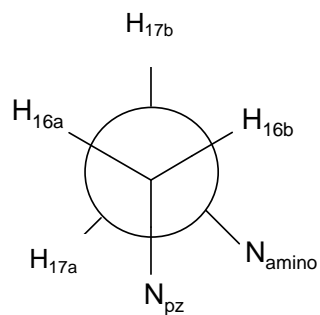
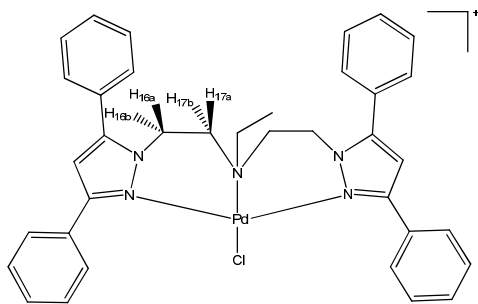


Experimental

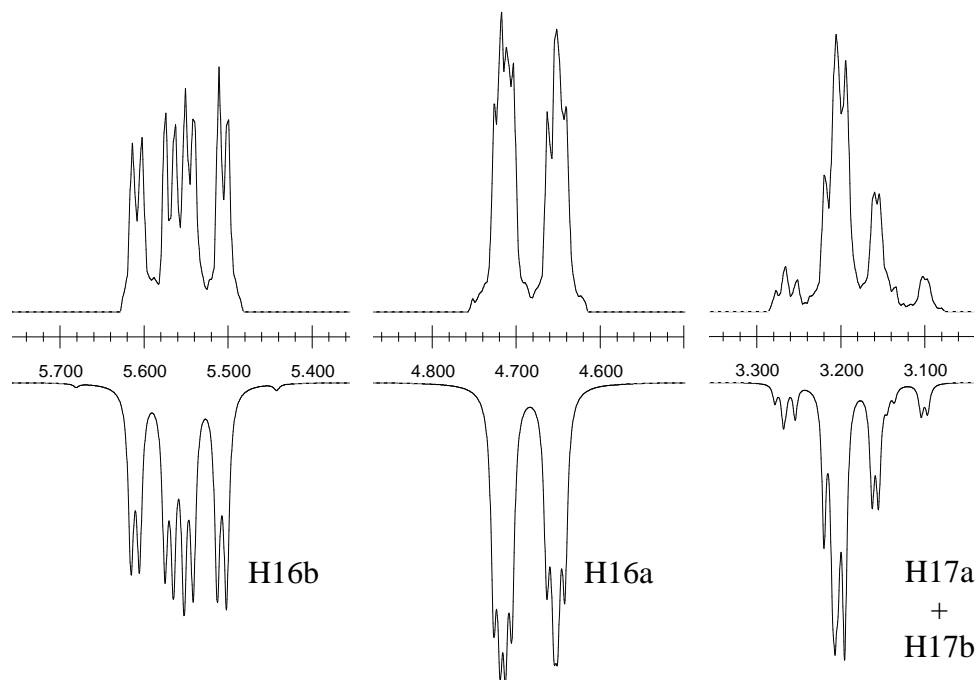


Simulated

Figure S3 The experimental (250 MHz, CD_3CN , 338 K) and simulated (*g* NMR) ^1H NMR spectra for H-16 and H-17 protons of the $\text{N}_{\text{pz}}\text{CH}_2\text{CH}_2\text{N}_{\text{amino}}$ fragment of $[\text{PdCl}(\text{L1})](\text{BF}_4)$ (**3**)



Experimental



Simulated

Figure S4 The experimental (250 MHz, CD₃CN, 298 K) and simulated (g NMR) ¹H NMR spectra for H-16 and H-17 protons of the N_{pz}CH₂CH₂N_{amino} fragment of [PdCl(L2)](BF₄) (**4**)

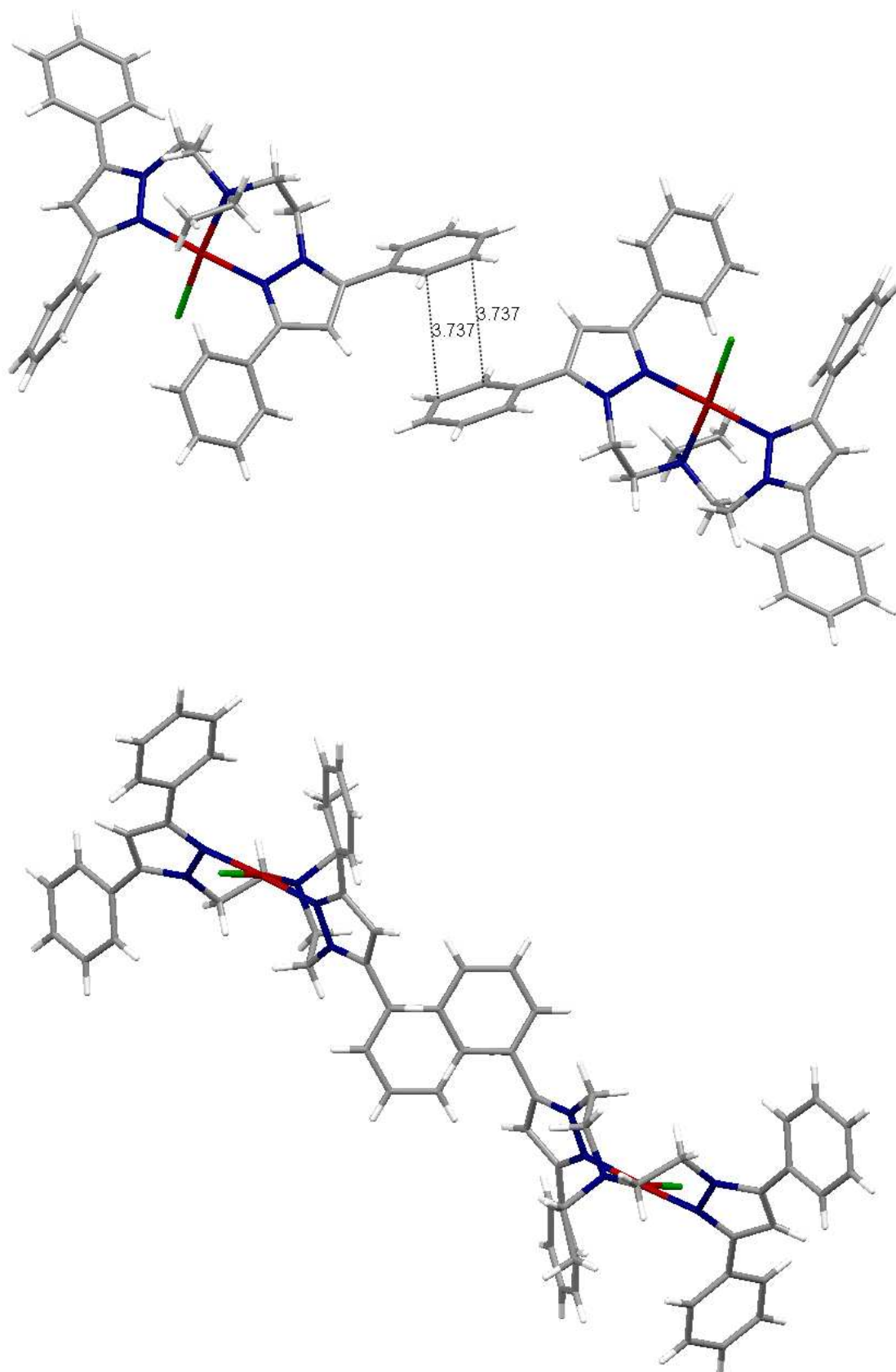


Figure S5 Two different views from the parallel displaced π - π stacking interactions of $[\text{PdCl}(\text{L}2)]^+$ cation