

Supporting Information for:

Unexpected Isomerism in "[Pd(2,9-dimethylphenanthroline)X₂]" (X = Cl, Br, I) Complexes: a Neutral and a Ionic Forms Exist

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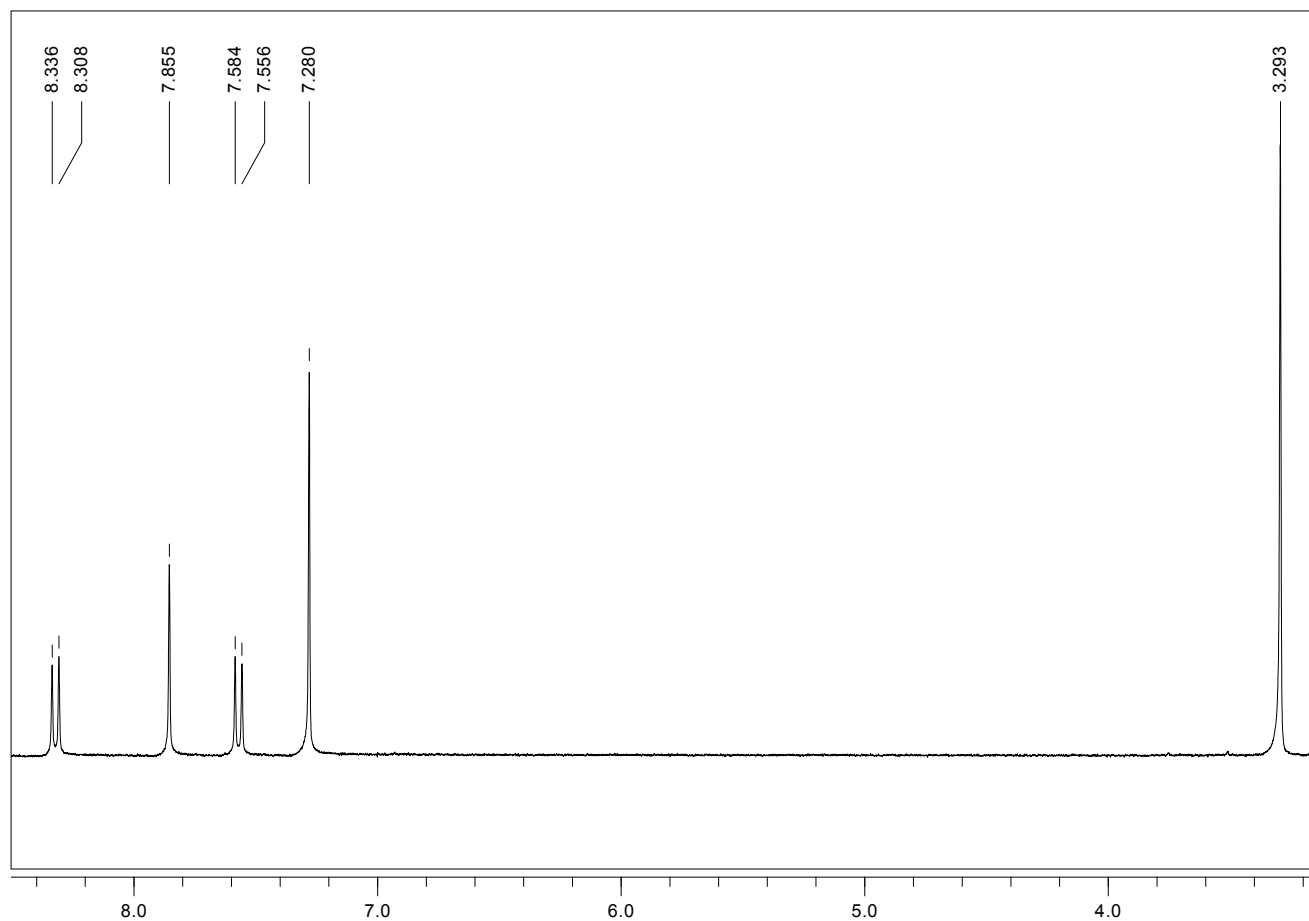
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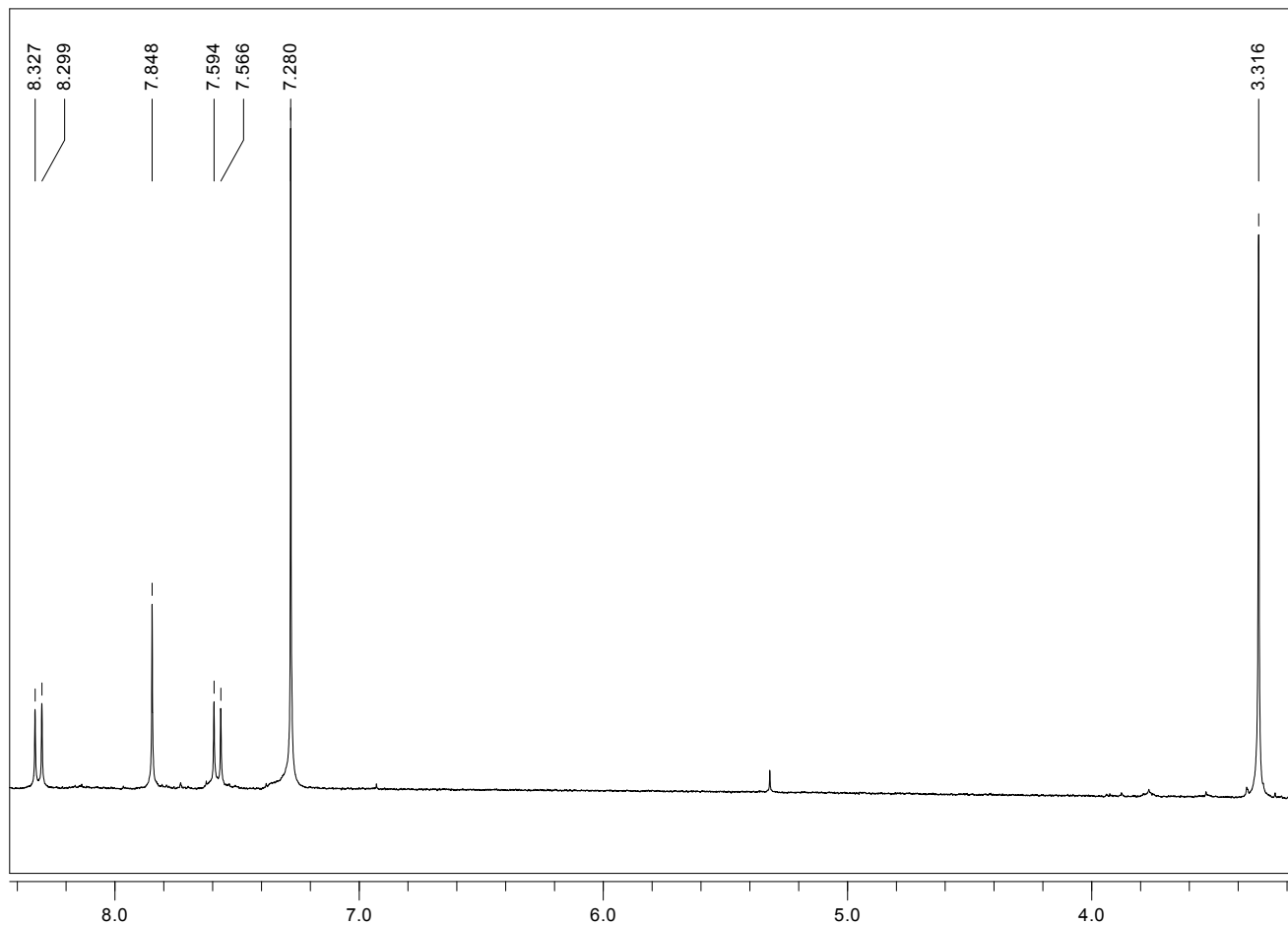
[Pd(Neoc)Cl₂] (**1a**)

¹H NMR (CDCl₃, RT): δ 8.32 (d, 2H, H⁴, H⁷ or H³, H⁸, *J* = 8.4 Hz); 7.86 (s, 2H, H⁵ and H⁶); 7.57 (d, 2H, H³, H⁸ or H⁴, H⁷, *J* = 8.4 Hz); 3.29 (s, 6H, neocuproine CH₃).



[Pd(Neoc)Br₂] (**2a**)

¹H NMR (CDCl₃, RT): δ 8.31 (d, 2H, H⁴, H⁷ or H³, H⁸, *J* = 8.4 Hz); 7.85 (s, 2H, H⁵ and H⁶); 7.58 (d, 2H, H³, H⁸ or H⁴, H⁷, *J* = 8.4 Hz); 3.32 (s, 6H, neocuproine CH₃).



[Pd(Neoc)I₂] (**3a**)

¹H NMR (CDCl₃, RT): δ 8.32 (d, 2H, H⁴, H⁷ or H³, H⁸, *J* = 8.4 Hz); 7.85 (s, 2H, H⁵ and H⁶); 7.58 (d, 2H, H³, H⁸ or H⁴, H⁷, *J* = 8.4 Hz); 3.30 (s, 6H, neocuproine CH₃).

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