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## Influence of the R-substituents on the Properties of [Ni(R<sub>2</sub>pipdt)(dmit)] Complexes and Crystal Structure where R = CH<sub>2</sub>C<sub>6</sub>H<sub>5</sub>

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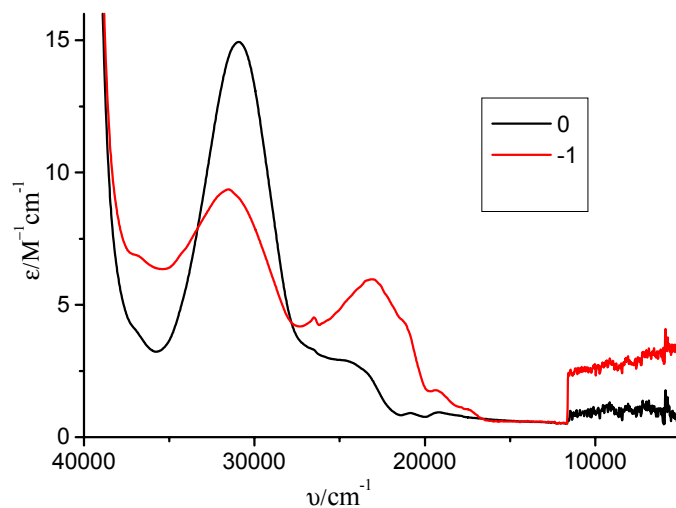
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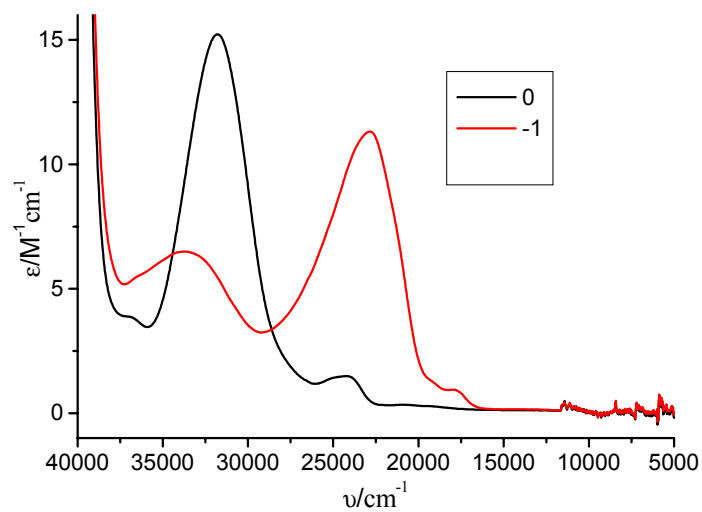
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### Supplementary Information



**Fig. S1** UV/visible spectra of **1a**<sup>0/1-</sup> in 0.1 M TBABF<sub>4</sub>/DMF at 213 K. E<sub>gen</sub> = 0.00 V(0), -1.70 V(-1)



**Fig. S2** UV/visible spectra of  $2a^{0/1-}$  in 0.1 M TBABF<sub>4</sub>/DMF at 213 K.  $E_{\text{gen}} = 0.00 \text{ V}(0)$ , -  
1.70 V(-1)

**Table S1** Peaks observed in the UV/visible spectra for **1a** and **2a** in their neutral and monoanion states at 213 K.  $\epsilon/M^{-1}\text{cm}^{-1}$  are given in brackets.

Compound	neutral, $\nu/\text{cm}^{-1}$ ( $\epsilon/M^{-1}\text{cm}^{-1}$ )	monoanion, $\nu/\text{cm}^{-1}$ ( $\epsilon/M^{-1}\text{cm}^{-1}$ )
<b>1a</b>	30,900 ( $14.9 \times 10^3$ ) 24,100 ( $2.8 \times 10^3$ )	31,500 ( $9.4 \times 10^3$ ) 23,200 ( $6.0 \times 10^3$ )
<b>2a</b>	31,800 ( $15.2 \times 10^3$ ) 24,300 ( $1.5 \times 10^3$ )	33,800 ( $6.5 \times 10^3$ ) 22,800 ( $11.3 \times 10^3$ )

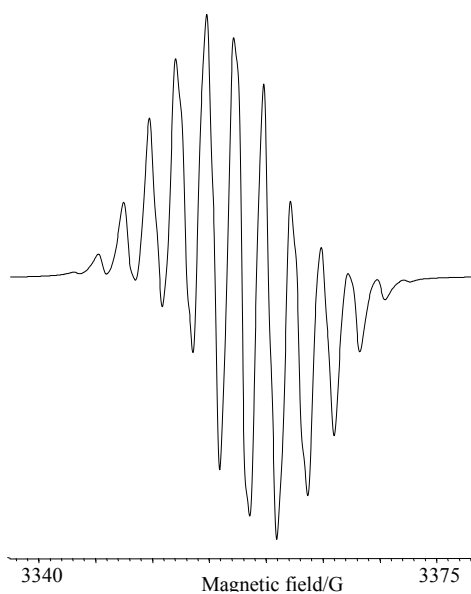


Fig. S3: Simulated EPR spectrum of  $1a^{1-}$  using the parameters given in table 3.

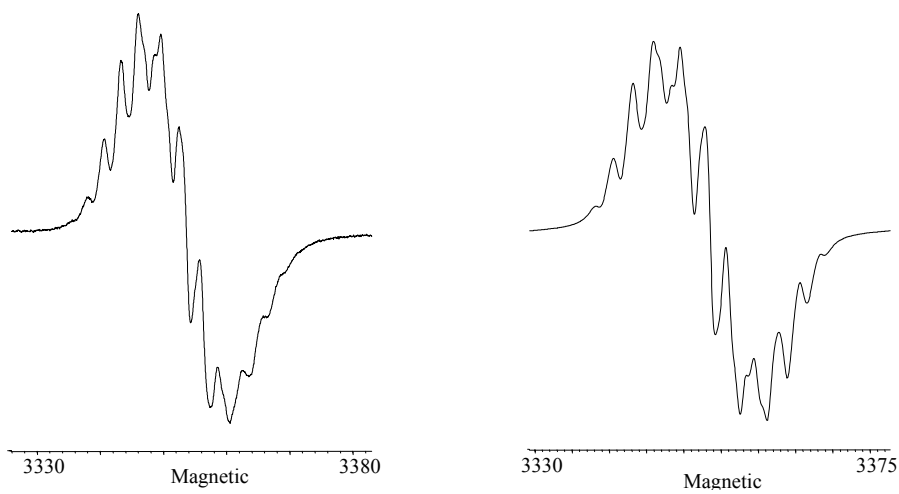


Fig. S4: Left - EPR spectrum of  $1b^-$  in solution of 0.1 M TBABF<sub>4</sub> in DMF at 293 K.  $E_{\text{gen}} = -1.50$  V; Right – Simulated EPR spectrum of  $1b^-$  using the parameters given in table 3

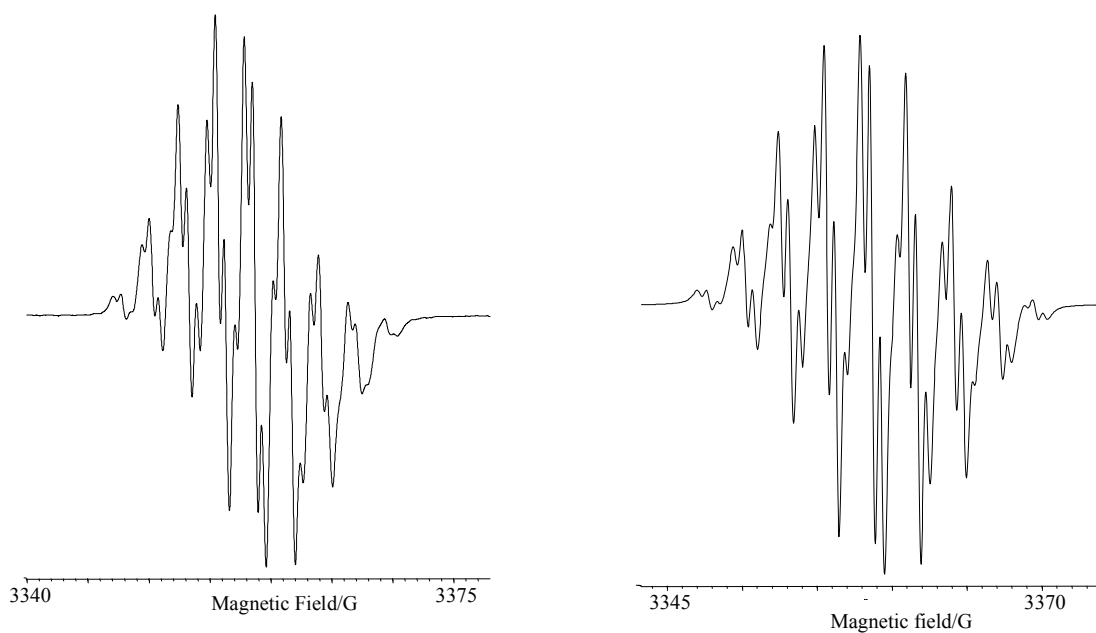


Fig. S5: Left - EPR spectrum of  $2a^-$  in solution of 0.1 M TBABF<sub>4</sub> in DMF at 293 K.  $E_{\text{gen}} = -1.70$  V; Right – Simulated EPR spectrum of  $2a^-$  using the parameters given in table 4

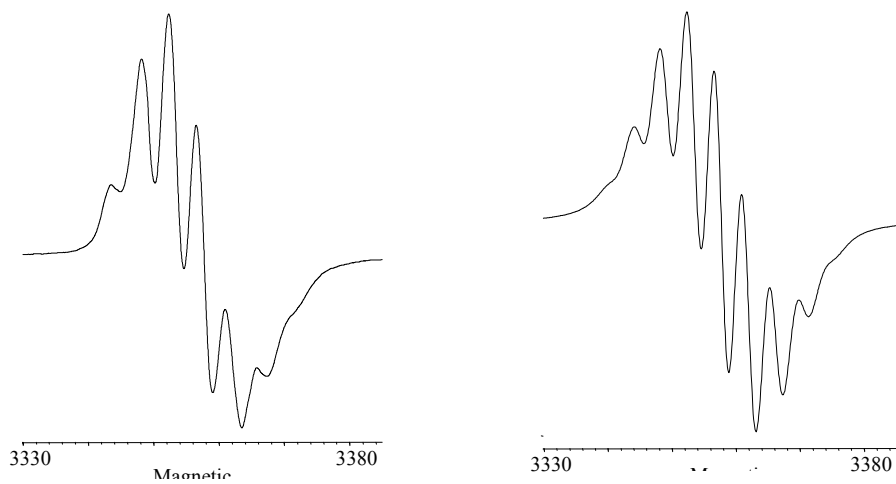


Fig. S6: Left – EPR spectrum of  $2b^-$  in solution of 0.1 M TBABF<sub>4</sub> in DMF at 233 K.  $E_{\text{gen}} = -1.00$  V; Right – Simulated EPR spectrum of  $2b^-$  using the parameters given in table 4