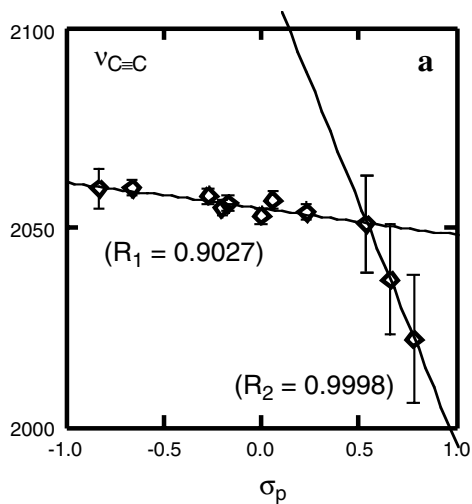
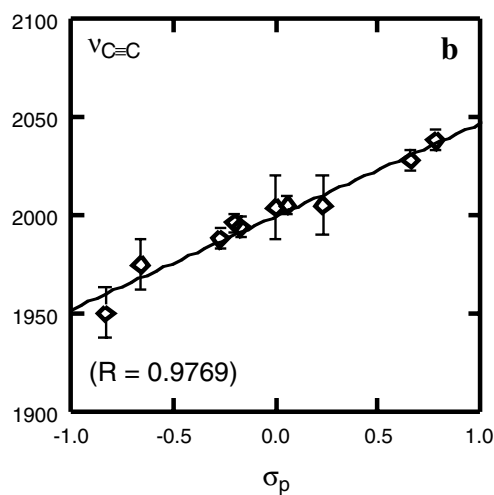


## Paul, Mevellec and Lapinte; Figures S1a-b



$$\nu_{\text{C}\equiv\text{C}} (\text{cm}^{-1}) = -6.589 \sigma_p + 2055$$

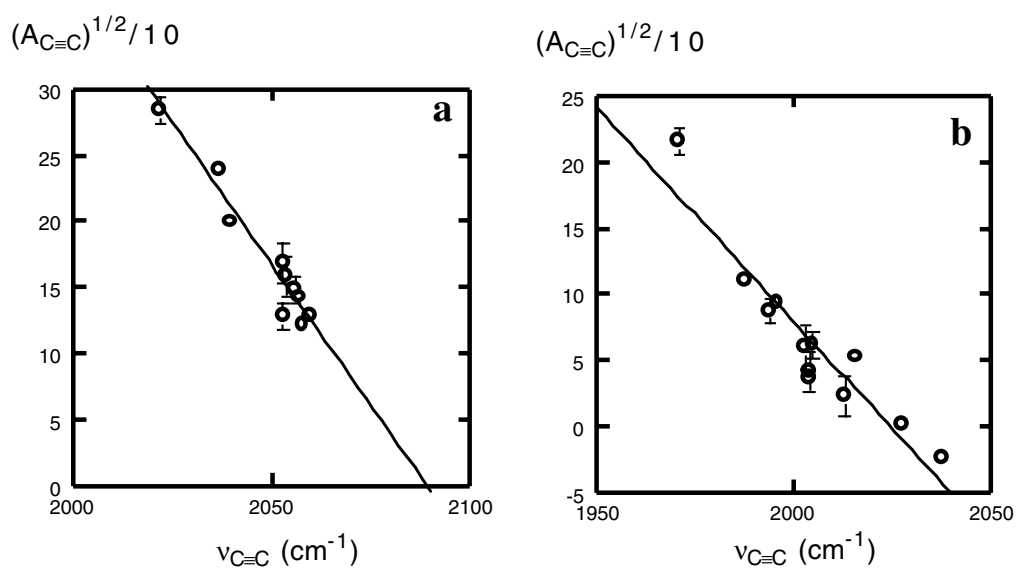
$$\nu_{\text{C}\equiv\text{C}} (\text{cm}^{-1}) = -120.8 \sigma_p + 2116$$



$$\nu_{\text{C}\equiv\text{C}} (\text{cm}^{-1}) = 47.62 \sigma_p + 2000$$

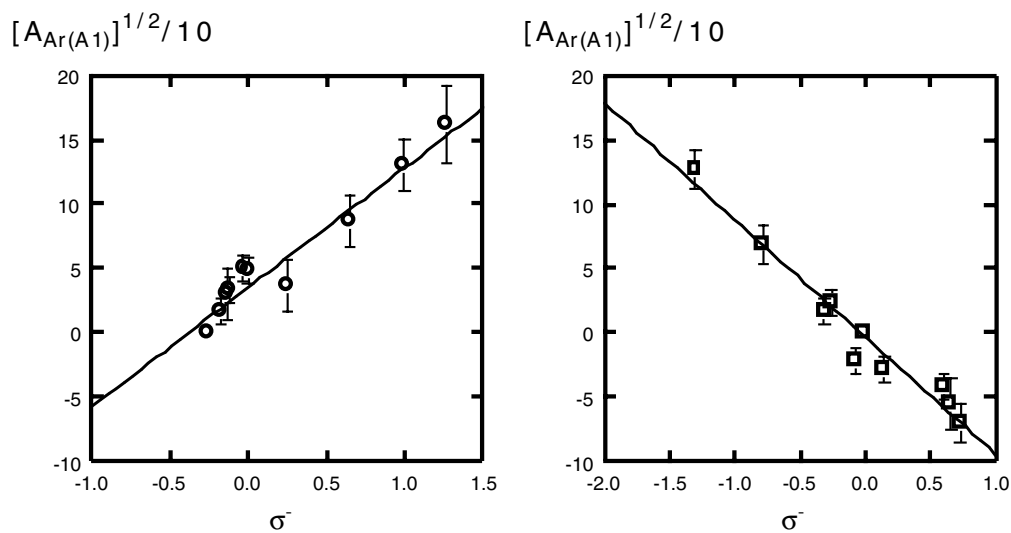
Solution infrared  $\nu_{\text{C}\equiv\text{C}}$  vs.  $\sigma_p$  correlations for  $[(\eta^2\text{-dppe})(\eta^5\text{-C}_5\text{H}_5)\text{FeC}\equiv\text{C}(\text{C}_6\text{H}_4)\text{X}]^{n+}$ ,  $n[\text{PF}_6]^-$  complexes for  $n = 0$  (a) and  $n = 1$  (b) with  $X = \text{NO}_2, \text{CN}, \text{CF}_3, \text{Br}, \text{F}, \text{H}, \text{Me}, \text{tBu}, \text{OMe}, \text{NH}_2$ .

## Paul, Mevellec and Lapinte; Figures S2a-b



Solution infrared  $[A_{C\equiv C}]^{1/2}/10$  vs.  $\nu_{C\equiv C}$  correlations for  $[(\eta^2\text{-dppe})(\eta^5\text{-C}_5\text{H}_5)\text{FeC}\equiv\text{C}(\text{C}_6\text{H}_4)\text{X}^{n+}]$ ,  $n[\text{PF}_6^-]$  complexes for  $n = 0$  (a) and  $n = 1$  (b).

## Paul, Mevellec and Lapinte; Figures S3a-b



Solution infrared  $[A_{Ar(A1)}]^{1/2}/10$  vs. ESP correlations for  $[(\eta^2\text{-dppe})(\eta^5\text{-C}_5\text{H}_5)\text{FeC}\equiv\text{C}(\text{C}_6\text{H}_4)\text{X}]^{n+}$ ,  $n[\text{PF}_6]^-$  complexes for  $n = 0$  (left graph) and  $n = 1$  (right graph) with  $X = \text{NO}_2, \text{CN}, \text{CF}_3, \text{Br}, \text{F}, \text{H}, \text{Me}, \text{}^t\text{Bu}, \text{OMe}, \text{NH}_2$ .