

# Probing Cyanocuprates by Electrospray Ionization Mass Spectrometry

## Addition/Correction

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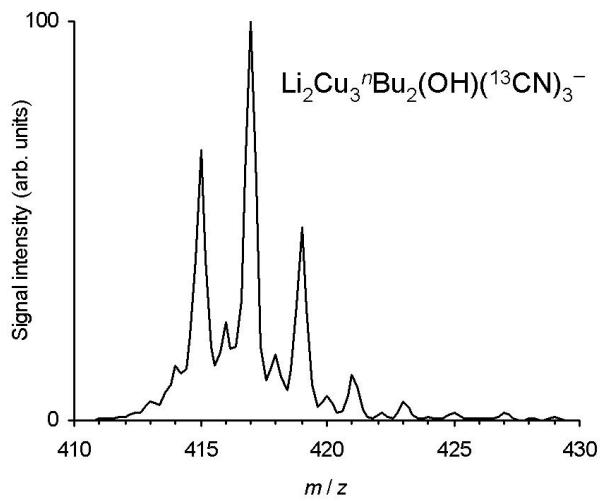
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## Supporting Information

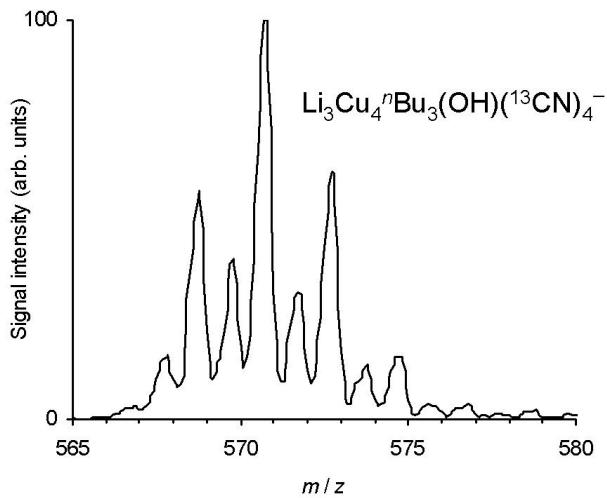
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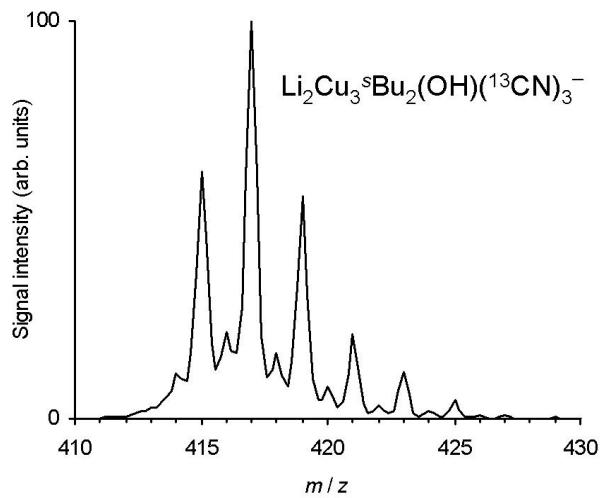
### 1.) Anion-mode ESI mass spectra of $\text{Li}_{0.8}\text{Cu}^n\text{Bu}_{0.8}(^{13}\text{CN})$ solutions



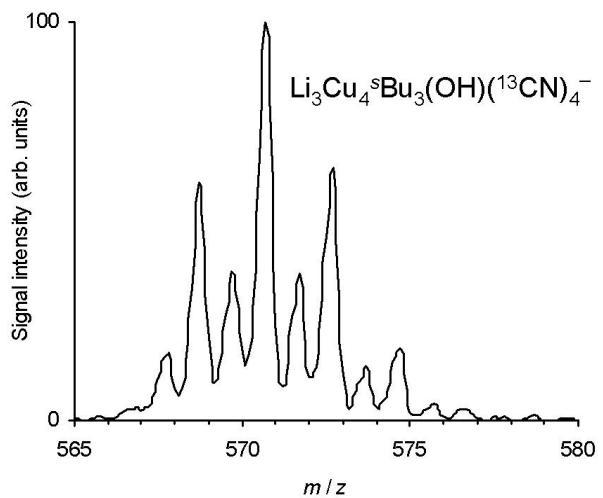
**Figure S1.** Section from the anion-mode ESI mass spectrum of a 25 mM solution of  $\text{Li}_{0.8}\text{Cu}^n\text{Bu}_{0.8}(^{13}\text{CN})$  in THF, showing the isotopic pattern of  $\text{Li}_2\text{Cu}_3^n\text{Bu}_2(\text{OH})(^{13}\text{CN})_3^-$ . The ion at  $m/z = 417$  corresponds to a mixture of  $\text{Li}_2^{63}\text{Cu}_2^{65}\text{Cu}^n\text{Bu}_2(\text{OH})(^{13}\text{CN})_3^-$  and  $^{63}\text{Cu}_3^n\text{Bu}_4^-$ , that at  $m/z = 421$  to  $\text{Li}^{63}\text{Cu}_3^n\text{Bu}_3(^{13}\text{CN})_2^-$ .



**Figure S2.** Section from the anion-mode ESI mass spectrum of a 25 mM solution of  $\text{Li}_{0.8}\text{Cu}^n\text{Bu}_{0.8}(^{13}\text{CN})$  in THF, showing the isotopic pattern of  $\text{Li}_3\text{Cu}_4^n\text{Bu}_3(\text{OH})(^{13}\text{CN})_4^-$ .

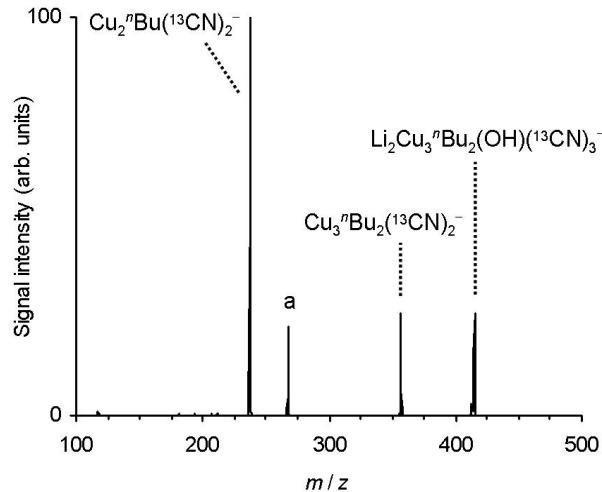


**Figure S3.** Section from the anion-mode ESI mass spectrum of a 25 mM solution of  $\text{Li}_{0.8}\text{Cu}^s\text{Bu}_{0.8}(^{13}\text{CN})$  in THF, showing the isotopic pattern of  $\text{Li}_2\text{Cu}_3^s\text{Bu}_2(\text{OH})(^{13}\text{CN})_3^-$ . The ion at  $m/z = 417$  corresponds to a mixture of  $\text{Li}_2^{63}\text{Cu}_2^{65}\text{Cu}^s\text{Bu}_2(\text{OH})(^{13}\text{CN})_3^-$  and  $^{63}\text{Cu}_3^s\text{Bu}_4^-$ , that at  $m/z = 421$  to  $\text{Li}^{63}\text{Cu}_3^s\text{Bu}_3(^{13}\text{CN})_2^-$ .

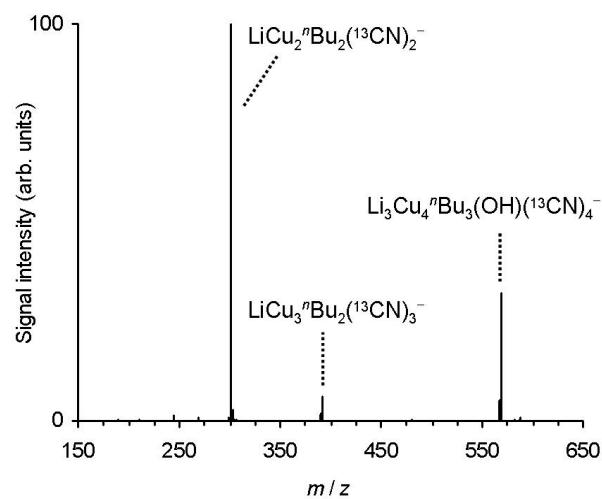


**Figure S4.** Section from the anion-mode ESI mass spectrum of a 25 mM solution of  $\text{Li}_{0.8}\text{Cu}^s\text{Bu}_{0.8}(^{13}\text{CN})$  in THF, showing the isotopic pattern of  $\text{Li}_3\text{Cu}_4^s\text{Bu}_3(\text{OH})(^{13}\text{CN})_4^-$ .

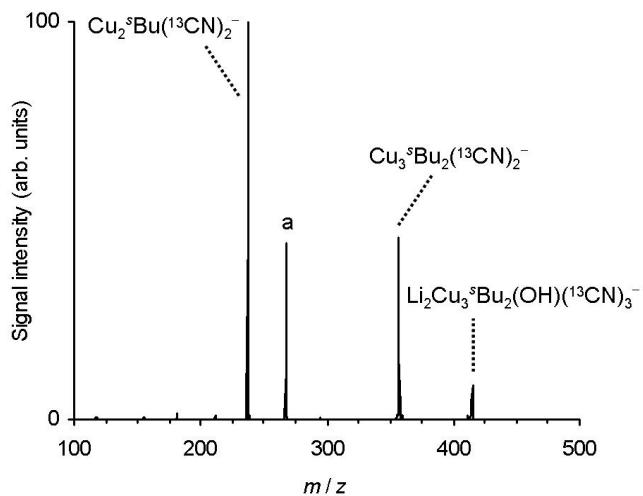
**2.) Mass spectra of mass-selected  $\text{Li}_2\text{Cu}_3{}^{n,s}\text{Bu}_2(\text{OH})(^{13}\text{CN})_3^-$  and  $\text{Li}_3\text{Cu}_4{}^{n,s}\text{Bu}_3(\text{OH})(^{13}\text{CN})_4^-$  anions and their fragment ions**



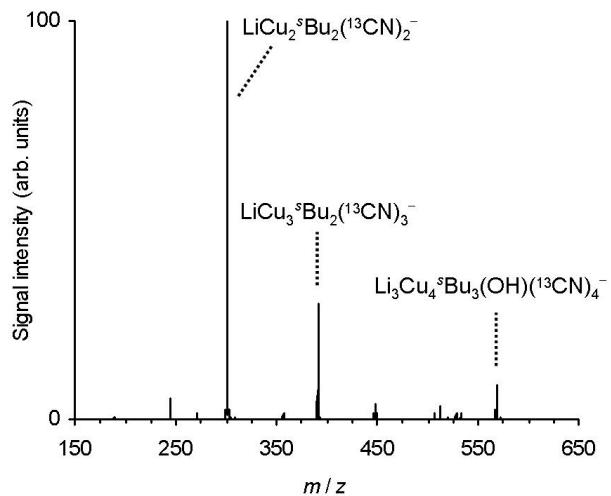
**Figure S5.** Mass spectrum of mass-selected  $\text{Li}_2\text{Cu}_3{}^{n,s}\text{Bu}_2(\text{OH})(^{13}\text{CN})_3^-$  ( $m/z = 415$ ) and its fragment ions produced upon collision-induced dissociation ( $V_{\text{exc}} = 0.18$  V), a =  $\text{Cu}_2{}^{n,s}\text{Bu}(\text{CN})^-$ .



**Figure S6.** Mass spectrum of mass-selected  $\text{Li}_3\text{Cu}_4{}^{n,s}\text{Bu}_3(\text{OH})(^{13}\text{CN})_4^-$  ( $m/z = 569$ ) and its fragment ions produced upon collision-induced dissociation ( $V_{\text{exc}} = 0.19$  V).



**Figure S7.** Mass spectrum of mass-selected  $\text{Li}_2\text{Cu}_3^{\text{s}}\text{Bu}_2(\text{OH})(\text{13CN})_3^-$  ( $m/z = 415$ ) and its fragment ions produced upon collision-induced dissociation ( $V_{\text{exc}} = 0.19$  V), a =  $\text{Cu}_2^{\text{s}}\text{Bu}_2^{(\text{13CN})}\text{--}$ .



**Figure S8.** Mass spectrum of mass-selected  $\text{Li}_3\text{Cu}_4^{\text{s}}\text{Bu}_3(\text{OH})(\text{13CN})_4^-$  ( $m/z = 569$ ) and its fragment ions produced upon collision-induced dissociation ( $V_{\text{exc}} = 0.21$  V).