High-Resolution X-ray Absorption Spectroscopy of Iron Carbonyl Complexes

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Supporting Information

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Figure 1: X-ray absorption spectra of Fe(CO)$_5$, Fe$_2$(CO)$_9$ and Fe$_3$(CO)$_{12}$ calculated with the BP86 and B3LYP exchange–correlation functionals and the experimental results. For the calculated spectra the blue vertical line indicates the ionisation threshold (i.e. the negative of the energy of the 1s core orbital).
Figure 2: X-ray absorption spectra for Fe(CO)$_5$ and Fe(CO)$_3$C$_8$H$_{12}$. Top: experimental spectra; middle: BP86 calculated spectra; bottom: B3LYP calculated spectra.
Figure 3: X-ray absorption spectra for Fe$_2$(CO)$_9$ and Fe$_2$(CO)$_4$Cp$_2$. Top: experimental spectra; middle: BP86 calculated spectra; bottom: B3LYP calculated spectra.