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

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## Supporting Information

Date: March 29, 2015

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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).

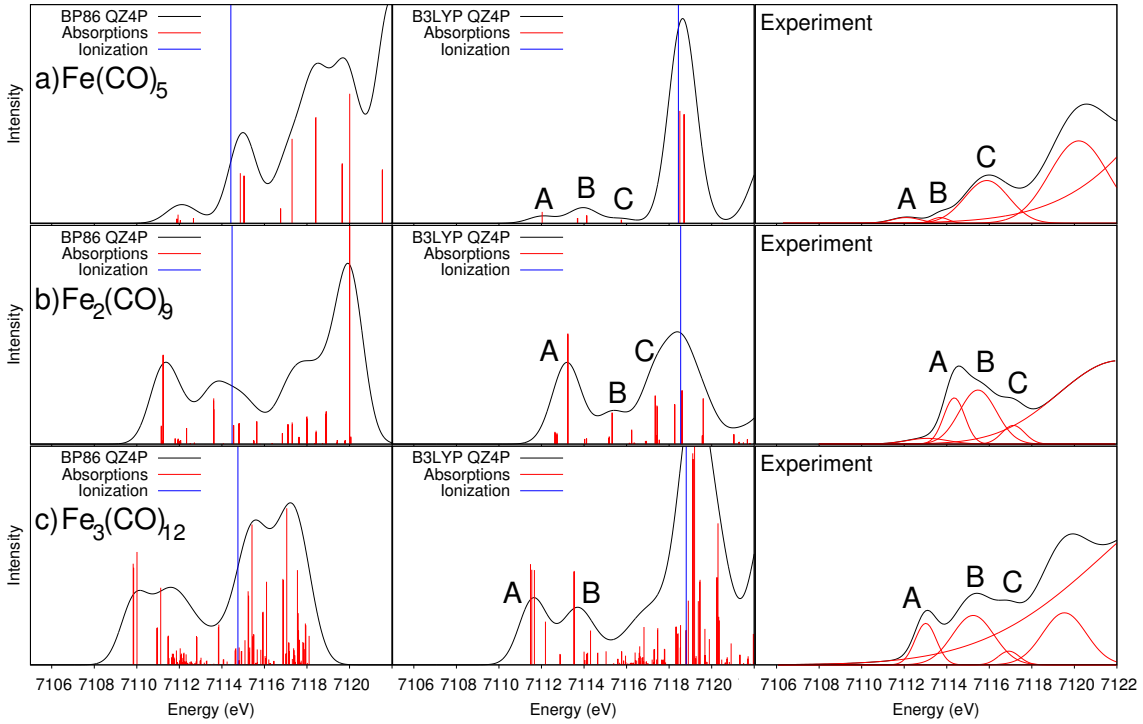

Figure 2: X-ray absorption spectra for $Fe(CO)_5$ and $Fe(CO)_3C_8H_{12}$. Top: experimental spectra; middle: BP86 calculated spectra; bottom: B3LYP calculated spectra.

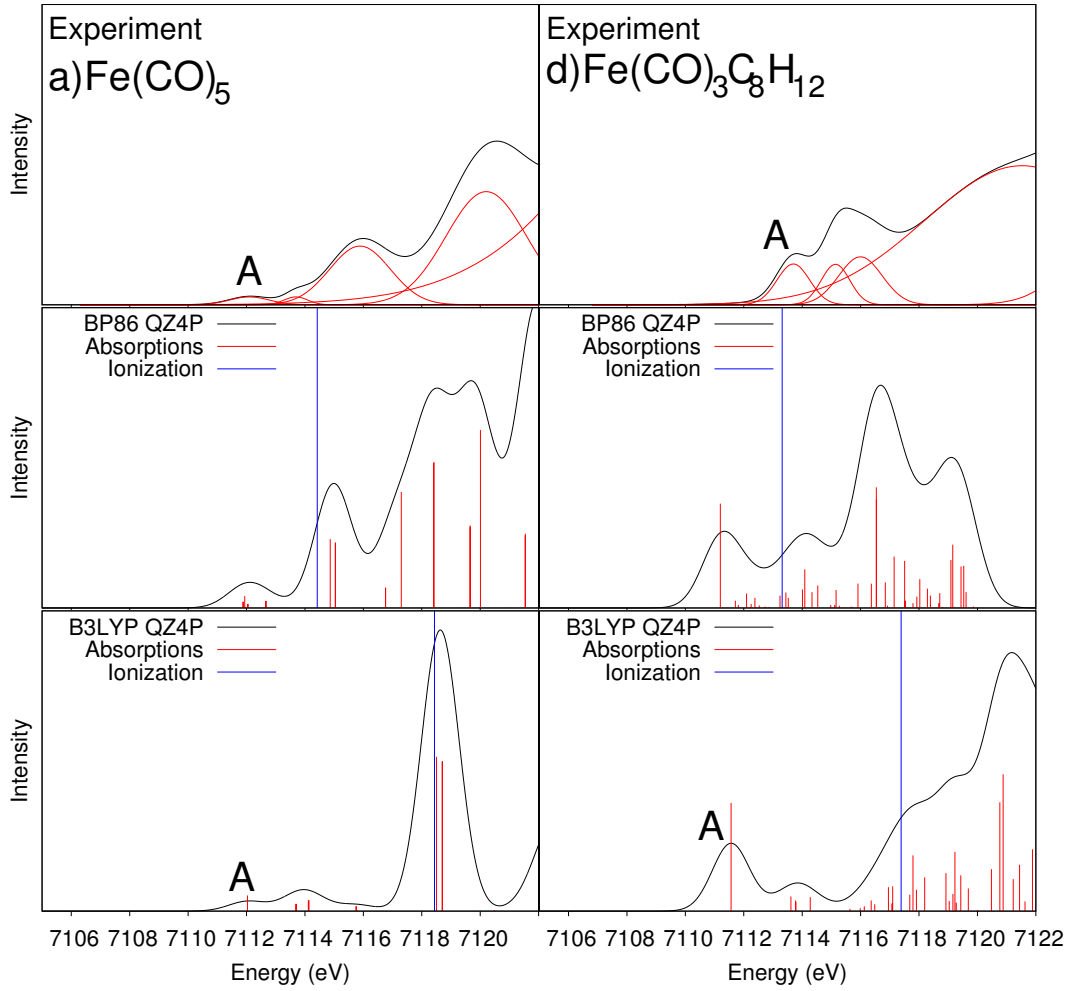

Figure 3: X-ray absorption spectra for $Fe_2(CO)_9$ and $Fe_2(CO)_4Cp_2$. Top: experimental spectra; middle: BP86 calculated spectra; bottom: B3LYP calculated spectra.