

Figure Captions for the Electronic Supplementary Information Section.

Figure S1. Contour plots for the HOMO and LUMO orbitals of the GS of Fe-C₆H₆.

Figure S2. Contour plots for the HOMO and LUMO orbitals of Fe₆-(C₆H₆)₂.

Figure S3a. Contour plots for the HOMO and LUMO orbitals of the M = 5 parallel state of Fe₂-C₆H₆.

Figure S3b. Contour plots for the HOMO and LUMO orbitals of the GS of Fe₂-C₆H₆.

Figure S4. Contour plots for the HOMO and LUMO orbitals of the GS of Fe₂-(C₆H₆)₂

Figure S5. Estimated IR spectra for Fe-C₆H₆, [Fe-C₆H₆]⁺ and [Fe-C₆H₆]⁻.

Figure S6. Calculated IR spectra for Fe-(C₆H₆)₂, [Fe-(C₆H₆)₂]⁺ and [Fe-(C₆H₆)₂]⁻.

Figure S7. Estimated IR spectra for Fe₂-C₆H₆, [Fe₂-C₆H₆]⁺ and [Fe₂-C₆H₆]⁻.

Figure S8. Calculated IR spectra for Fe₂-(C₆H₆)₂, [Fe₂-(C₆H₆)₂]⁺ and [Fe₂-(C₆H₆)₂]⁻.

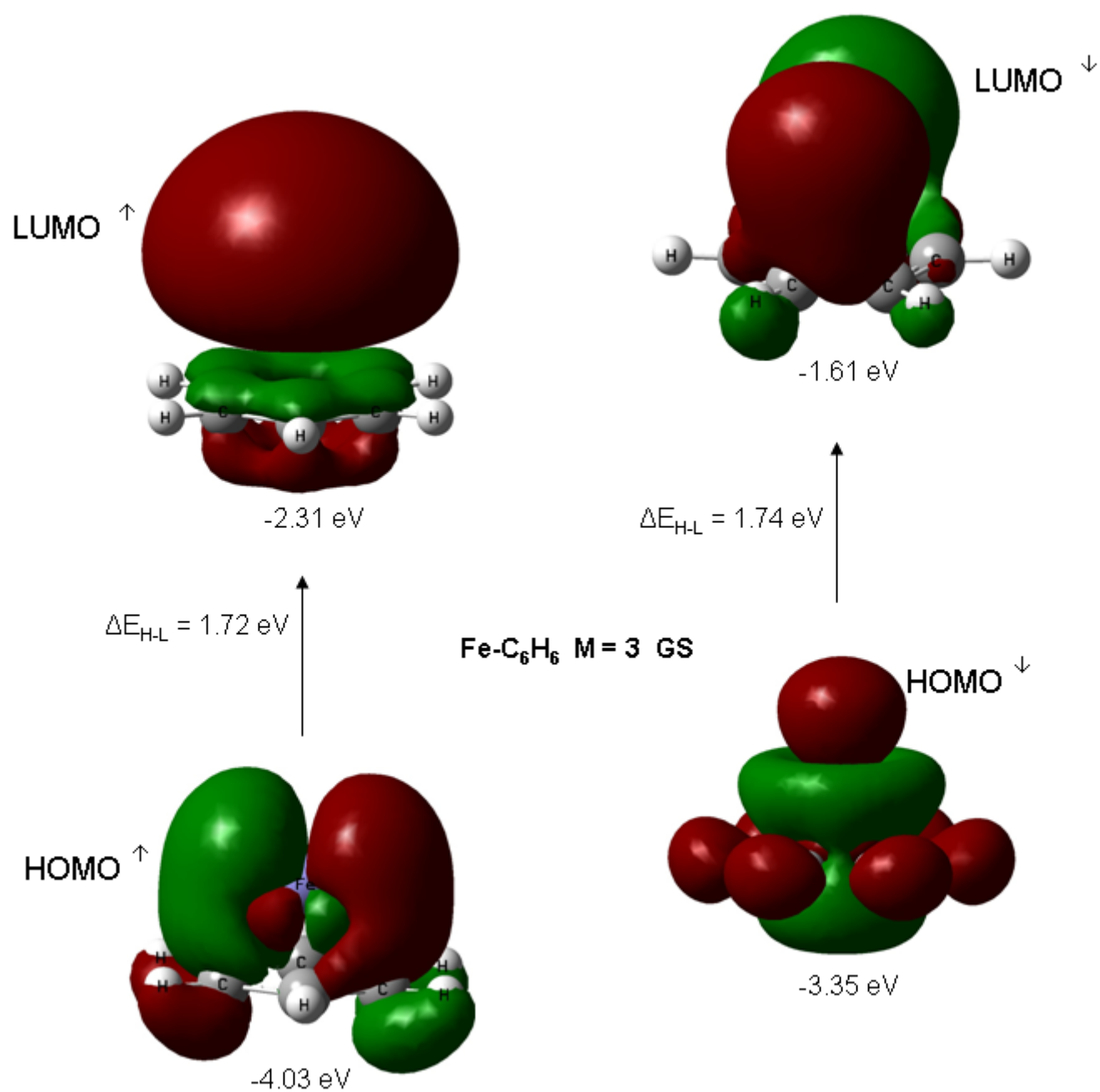


Figure S1

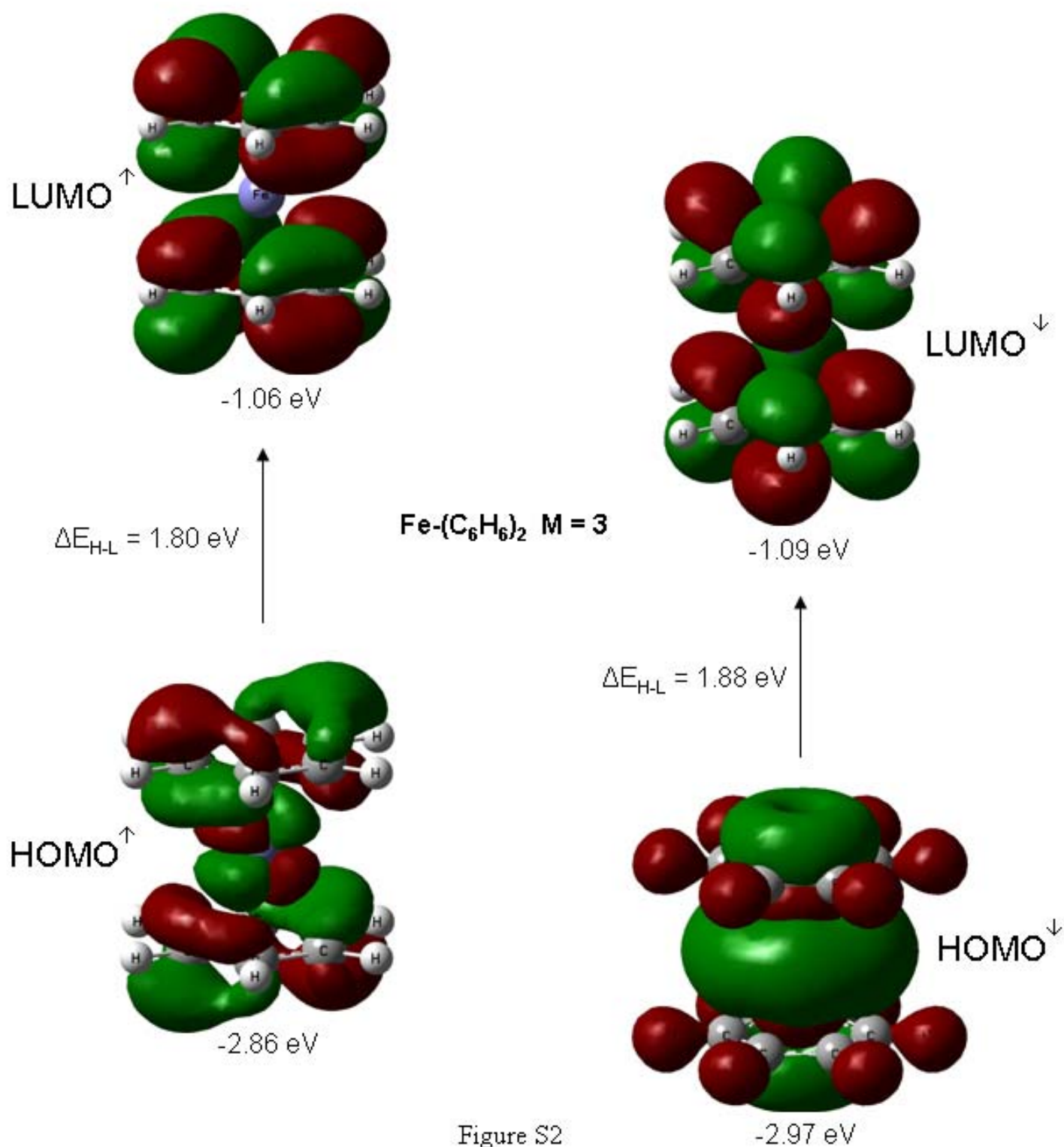


Figure S2

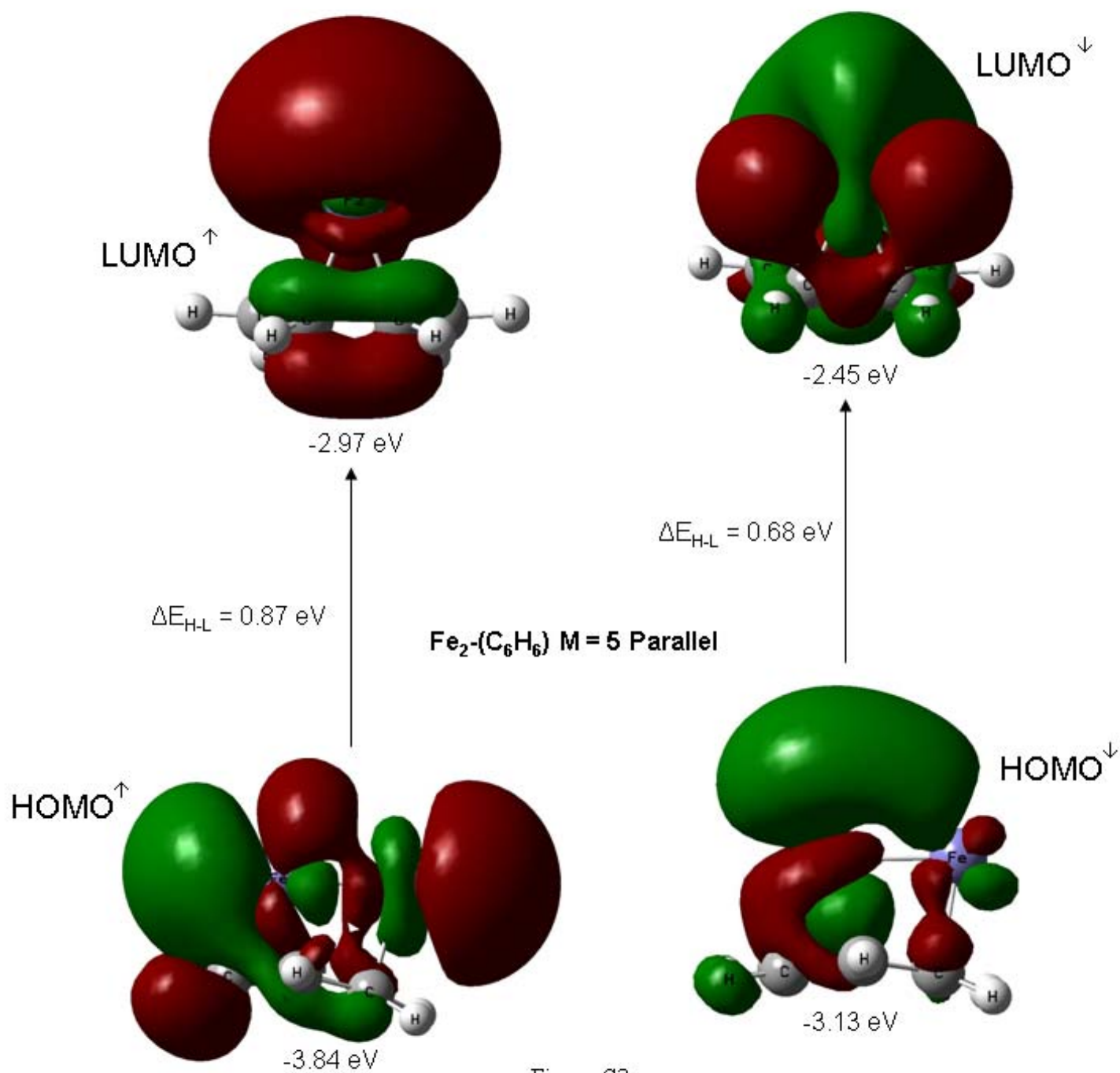


Figure S3a

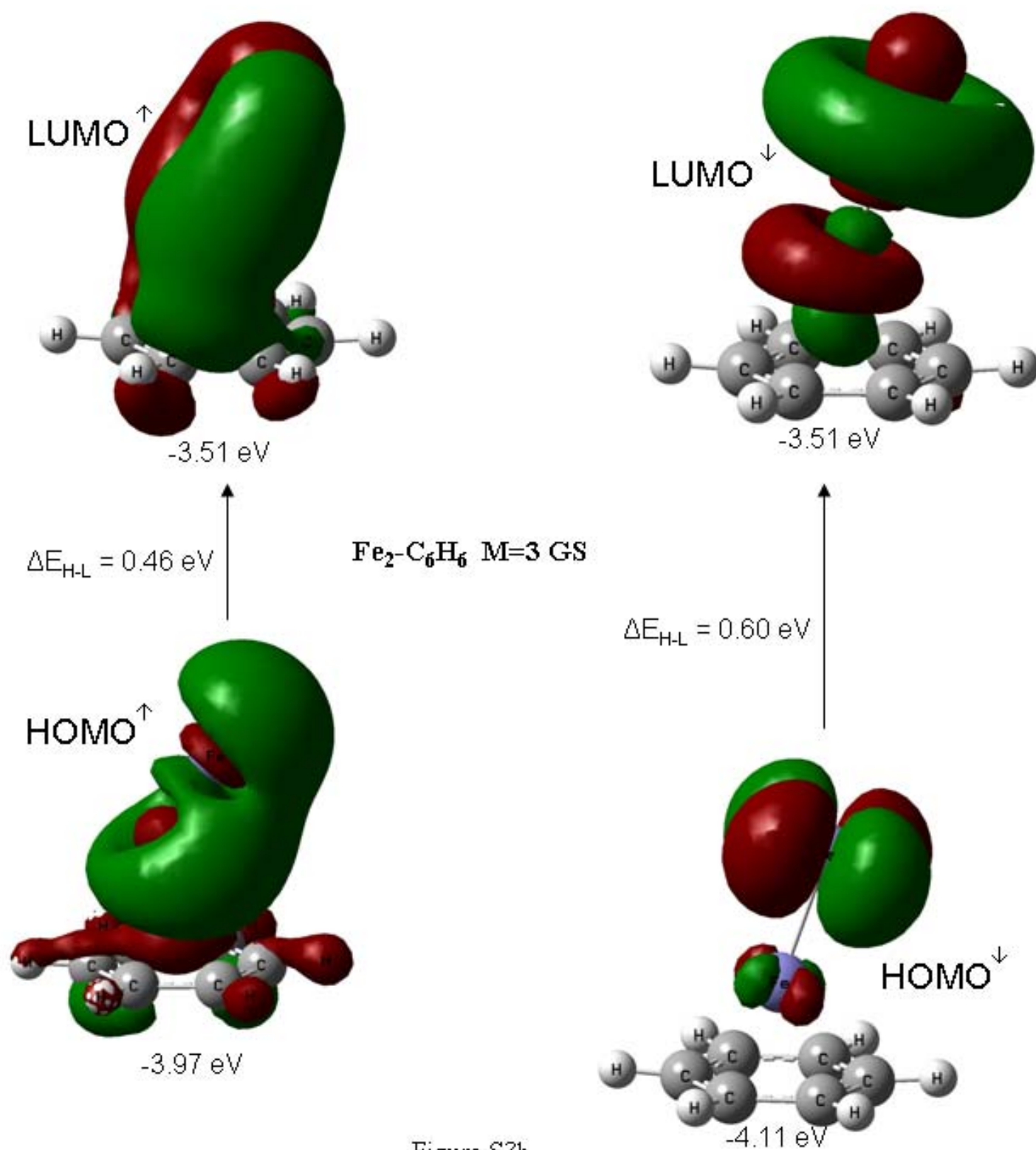


Figure S3b

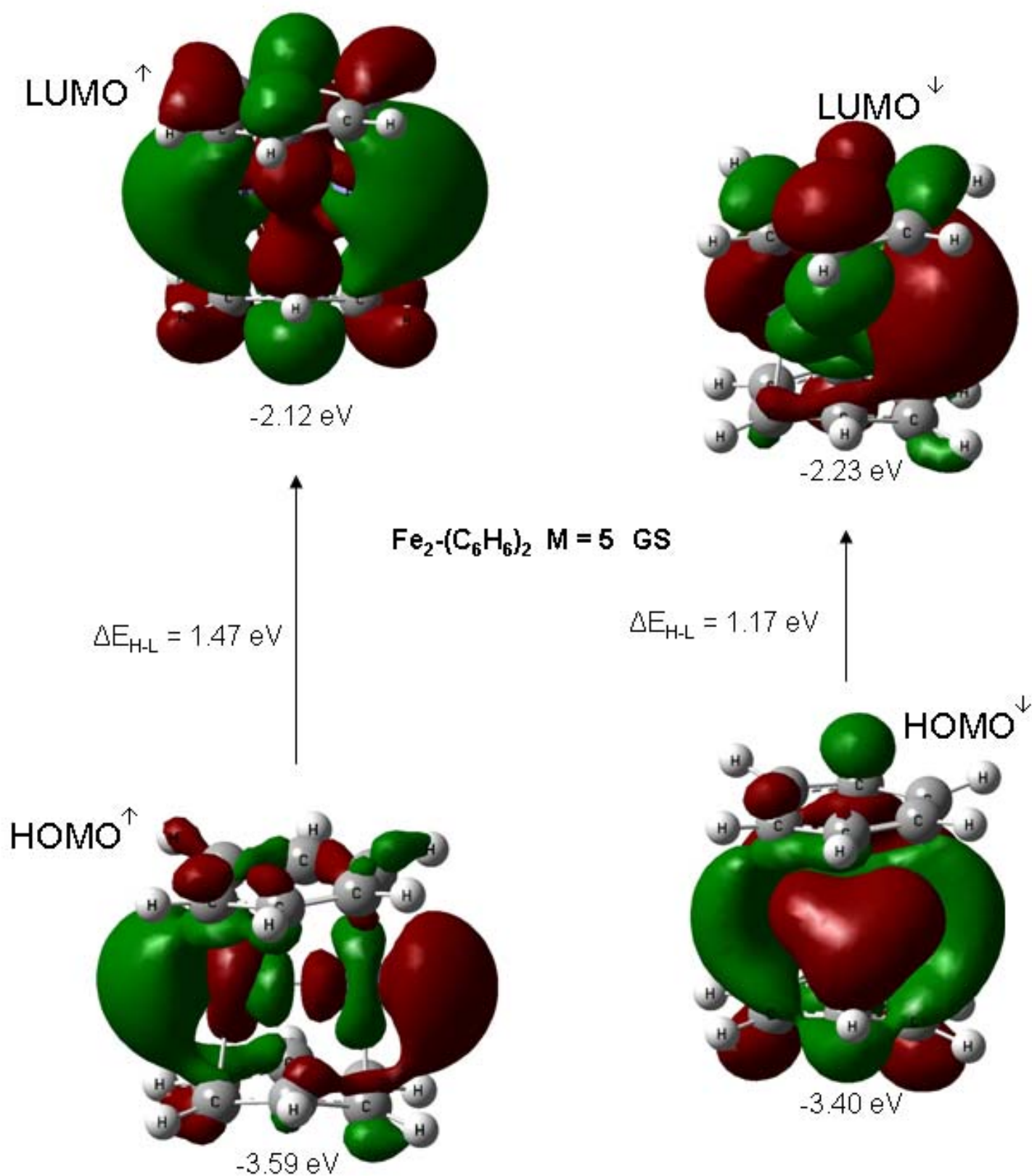


Figure S4

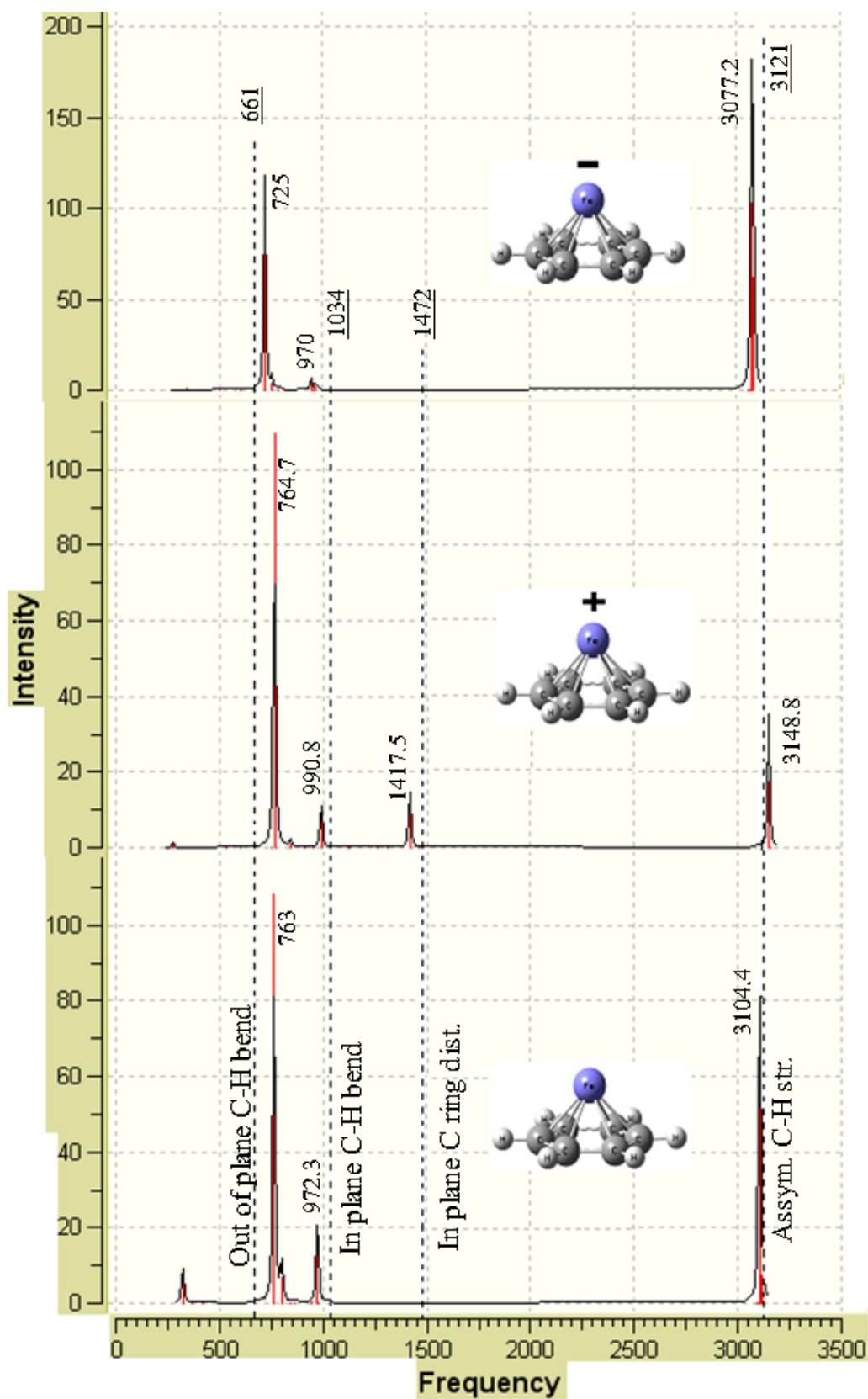


Figure S5

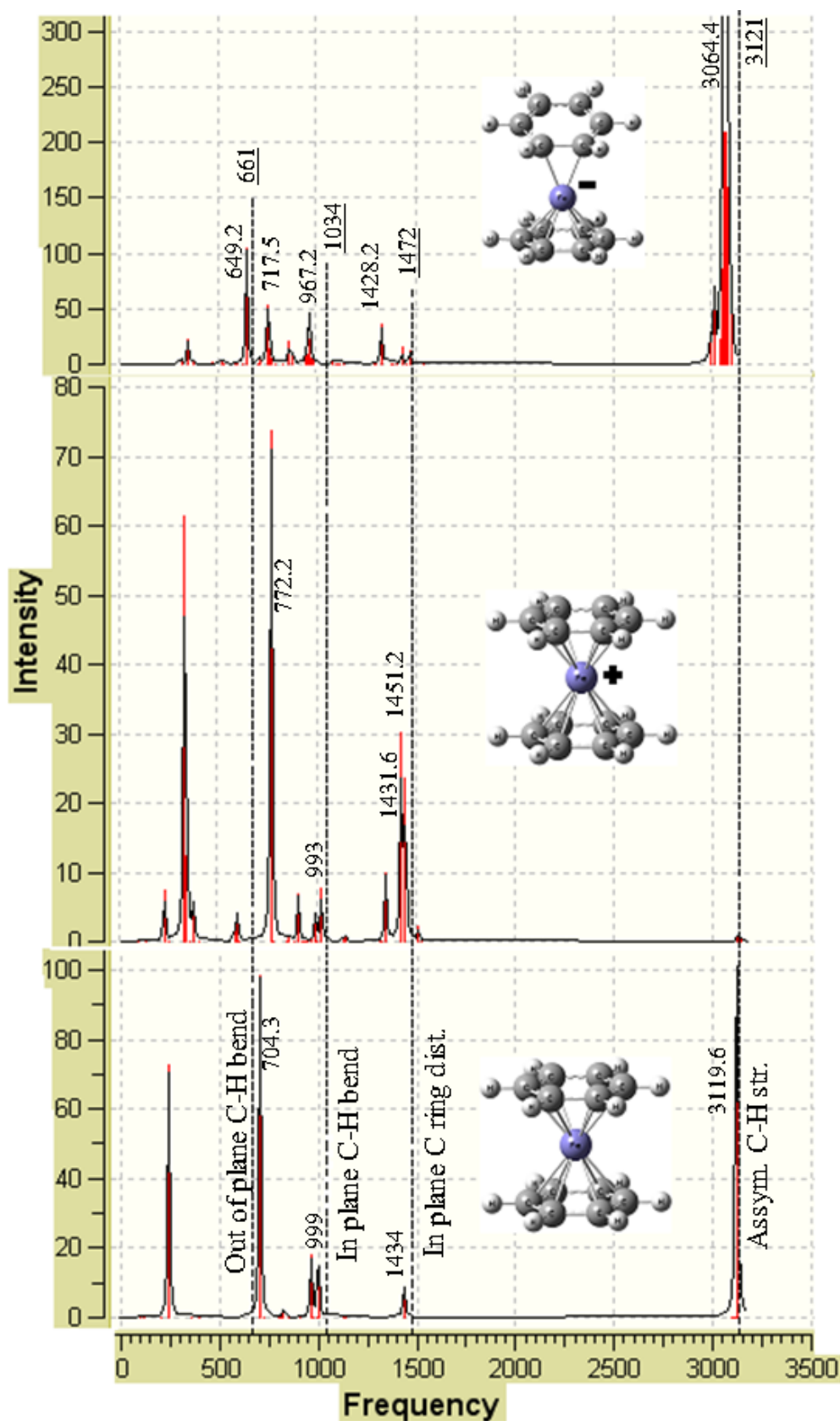


Figure S6

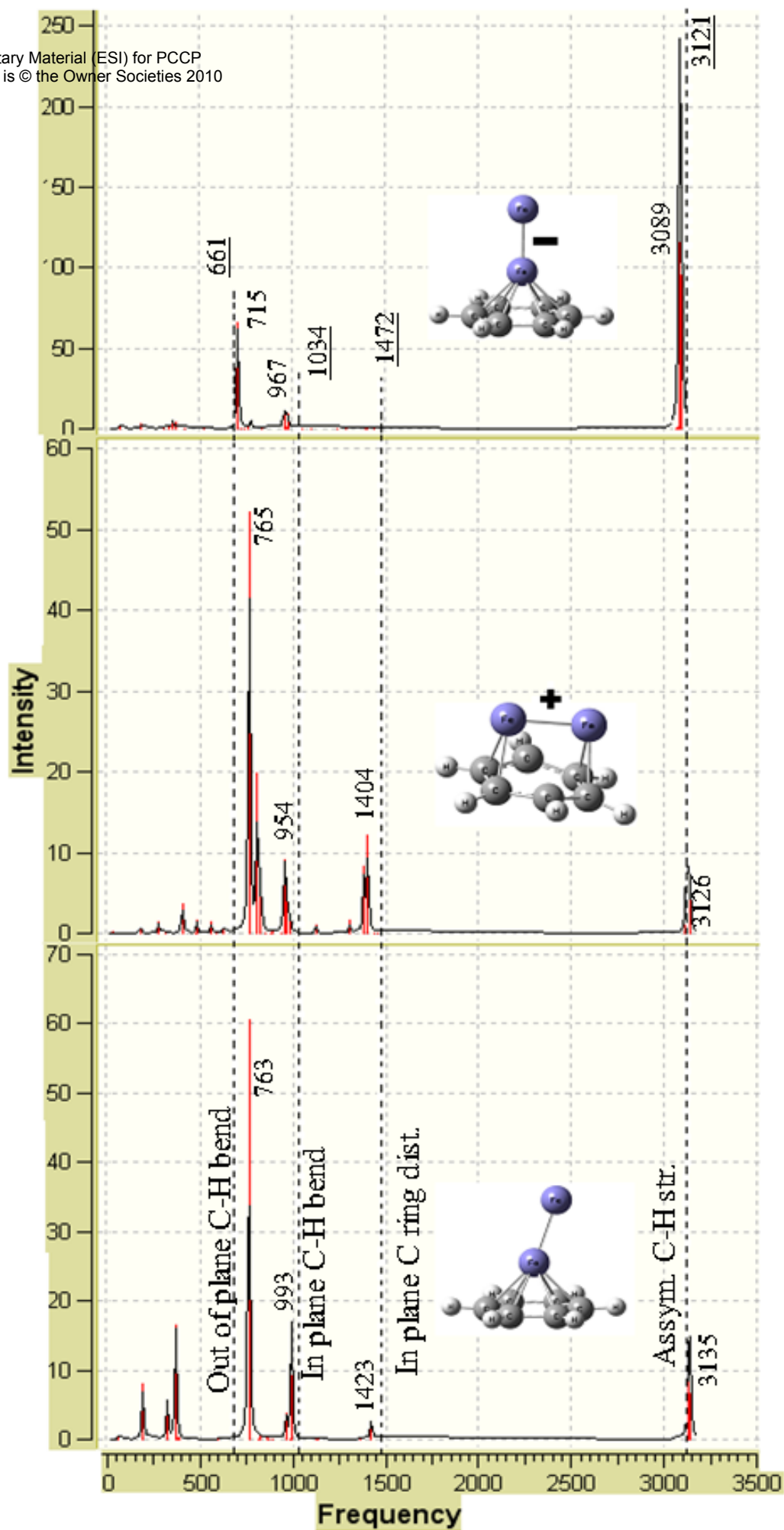


Figure S7

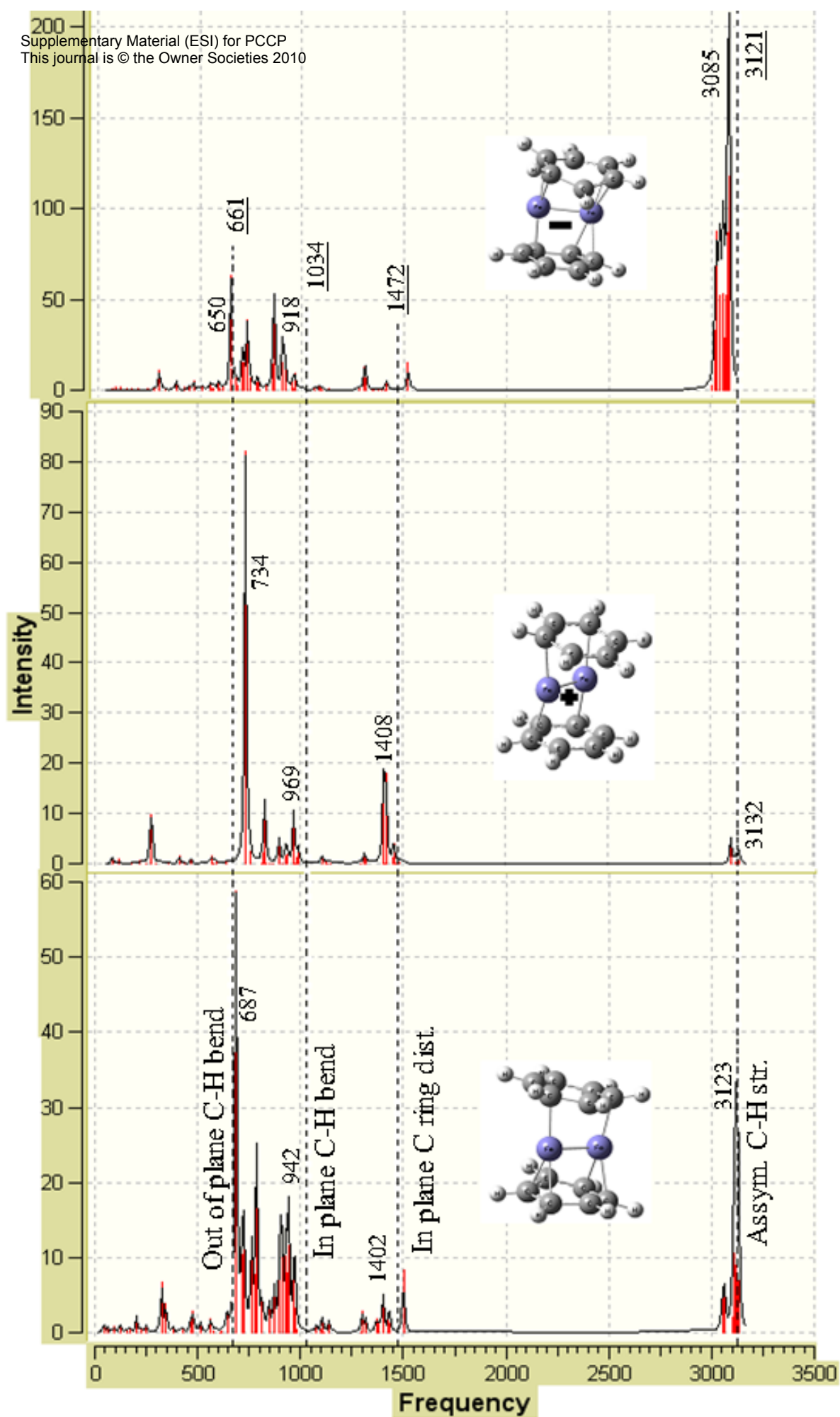


Figure S8