

**An experimental and theoretical  
study of the Fe L<sub>2,3</sub>-edges and of the  
C and O K-edge XAS  
in *cis*-[( $\eta^5$ -C<sub>5</sub>H<sub>5</sub>)Fe( $\eta^1$ -CO)( $\mu$ -CO)]<sub>2</sub>.  
A curiosity driven unsuccessful  
study!**

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Conference Room – Alfa Building

and at <https://zoom.us/j/83118890920> Passcode: seminar1

**Abstract:**

The relative stability of *trans*-[( $\eta^5$ -C<sub>5</sub>H<sub>5</sub>)Fe( $\eta^1$ -CO)( $\mu$ -CO)]<sub>2</sub> (*trans*-I) and *cis*-I tautomers in *vacuum* and in solvents with different dielectric constants ( $\epsilon$ ) has been investigated by exploiting the density functional theory (DFT). In agreement with the experimental evidence, *trans*-I is found more stable than *cis*-I in *vacuum* (~1.5 kcal/mol;  $\epsilon = 1$ ), while the opposite is true in media with  $\epsilon > 7$ . DFT thermodynamic outcomes clearly indicate that, at the temperatures at which the gas-phase Fe L<sub>2,3</sub>-edges and the C and O K-edge X-ray absorption spectroscopy (XAS) data of I have been collected (365 – 368 K), the predominant species is *trans*-I (~93%). Compositions, oscillator strengths ( $f$ ) and excitation energy ( $EE$ ) values of *cis*-I XAS transitions substantially mirror those of *trans*-I; nevertheless, the negligible contribution of the weighted *cis*-I  $f(EE)$  distributions to the diverse simulated XA spectra of I makes their detailed assignment useless.

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