Contribution ID: **339** Type: **Poster Presentation**

Photo-induced isomerisation reactions in mercury dithizonates

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Abstract content
   (Max 300 words)

Most of the natural processes involving photo-active molecules undergo cis-trans isomerisations when they absorb light energy. In this study, we investigate the photo-induced isomerisation reactions in mercury dithizonates through density functional calculations (DFT) in comparison to their corresponding UV-VIS spectroscopy analysis. These molecules isomerise around C=N double bond chromophore, from orange-cis to blue-trans, and these results in bond breaking conformations. From the structural optimisations of these molecules, the ground state energies, electron densities, excitation energy spectra and the ground state potential energy curves are obtained. Gas and solvent phase approximations are carried out; with the gas phase being the better as compared to the experimental data. Within the approximation error associated with DFT, the overall results obtained from calculations agreed with those from the experiments.

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Level for award
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PhD

Main supervisor (name and email)
and his / her institution

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