

# SAIP 2011



Contribution ID : 307

## **Density Functional Calculation of Metal Dithizonates**

Wednesday 13 Jul 2011 at 14:45 (00h15')

### **Content :**

Understanding molecular dynamics on potential energy surfaces has been at the heart of ultrafast transient absorption in the recent years [Philipp K, et al., 2005],[Karel G, et al., 2008]. Based on the on-going experiment at our ultrafast laboratory, we ran density functional calculations on metal dithizonates, starting with their kernel molecule, formalimine, to validate what we observe experimentally. This we treated in terms of ground state energy, absorption spectrum, vibrational frequency and potential energy surface using two different softwares: Amsterdam Density Functional (ADF) and Gaussian(09). The overall results show that B3LYP functional combined with CEP-31G basis set gave the closest results to the experimentally observed data.

### **Level (Hons, MSc, PhD, other)? :**

MSc

### **Consider for a student award (Yes / No)? :**

Yes

### **Short Paper :**

Yes

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