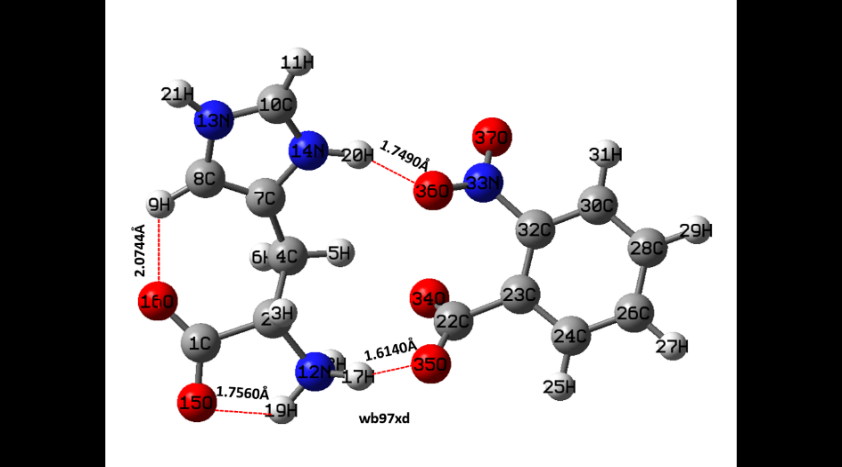
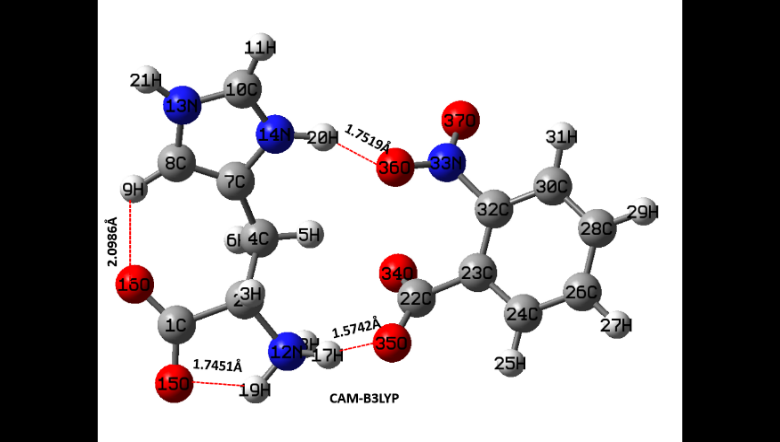
***Supplementary information***

**Investigation on the key features of L-Histidinium 2-nitrobenzoate (LH2NB) for optoelectronic applications: a comparative study**

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In the article we are focused on B3LYP mainly and some other levels of theory like CAM-B3LYP and wb97xd

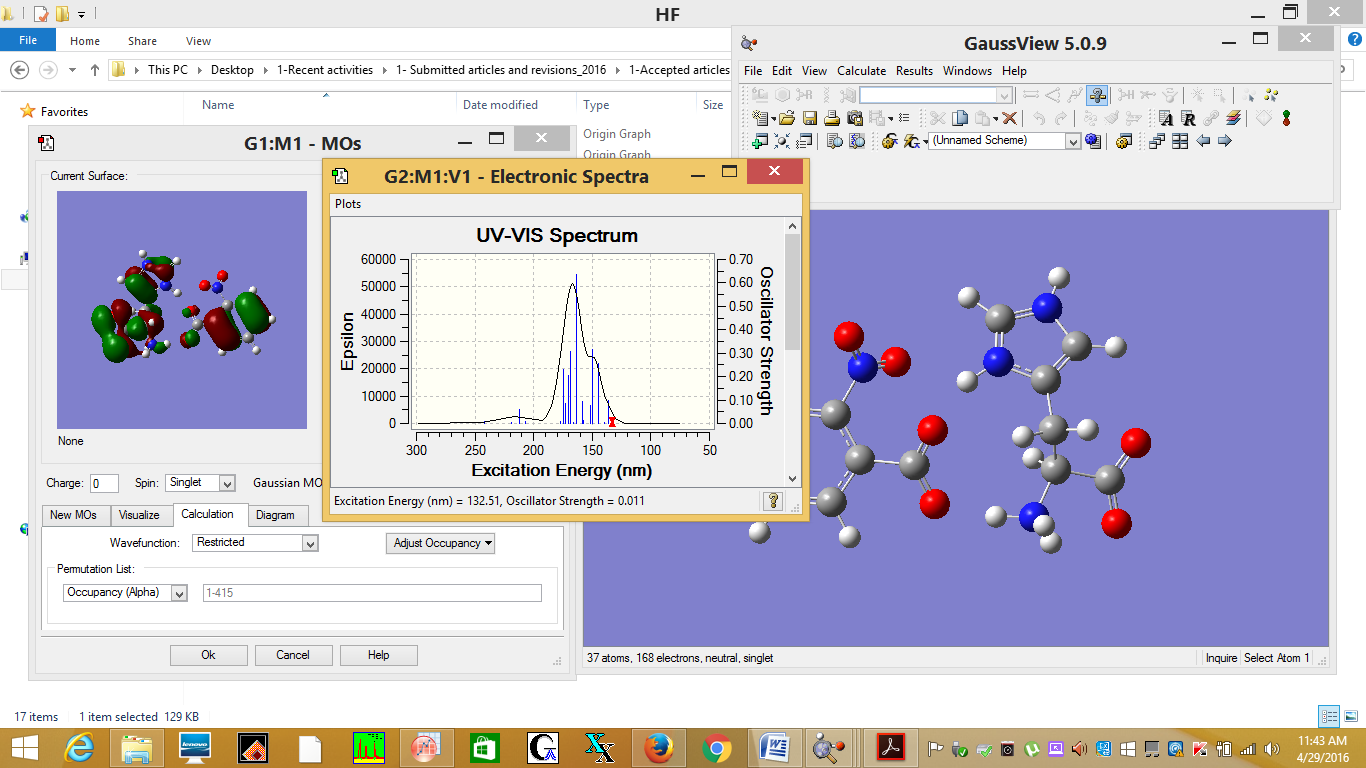


**Figure 1S** Optimized stable geometry of LH2NB by CAM-B3LYP and wb97xd levels of theory using 6-31G\*\* basis set.

***Few results obtained from HF calculation are as follows and the results calculated from other level of theory like CAM/B3LYP and wb97xd are similar to B3LYP which is already explained in the article:***

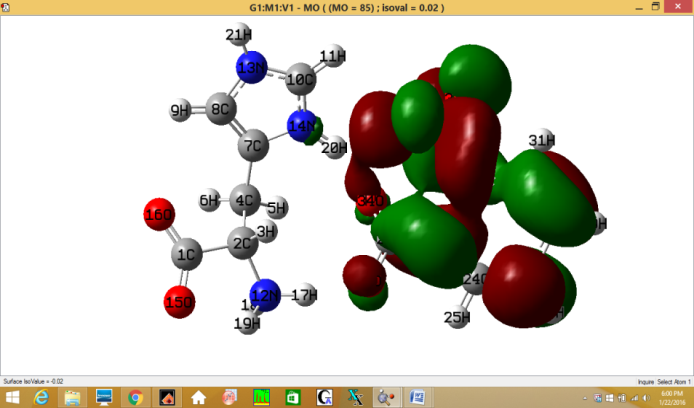
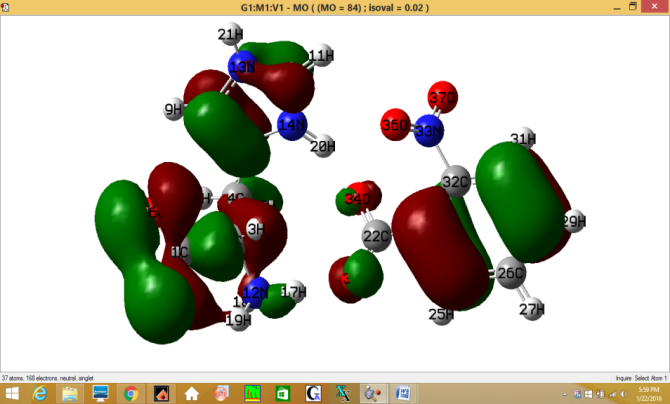
***The explanation on all these results can be made accordingly as explained in the article paper for other level of theory***

***Figure 1S. UV-Vis spectrum at TD-HF/6-31G\*\****

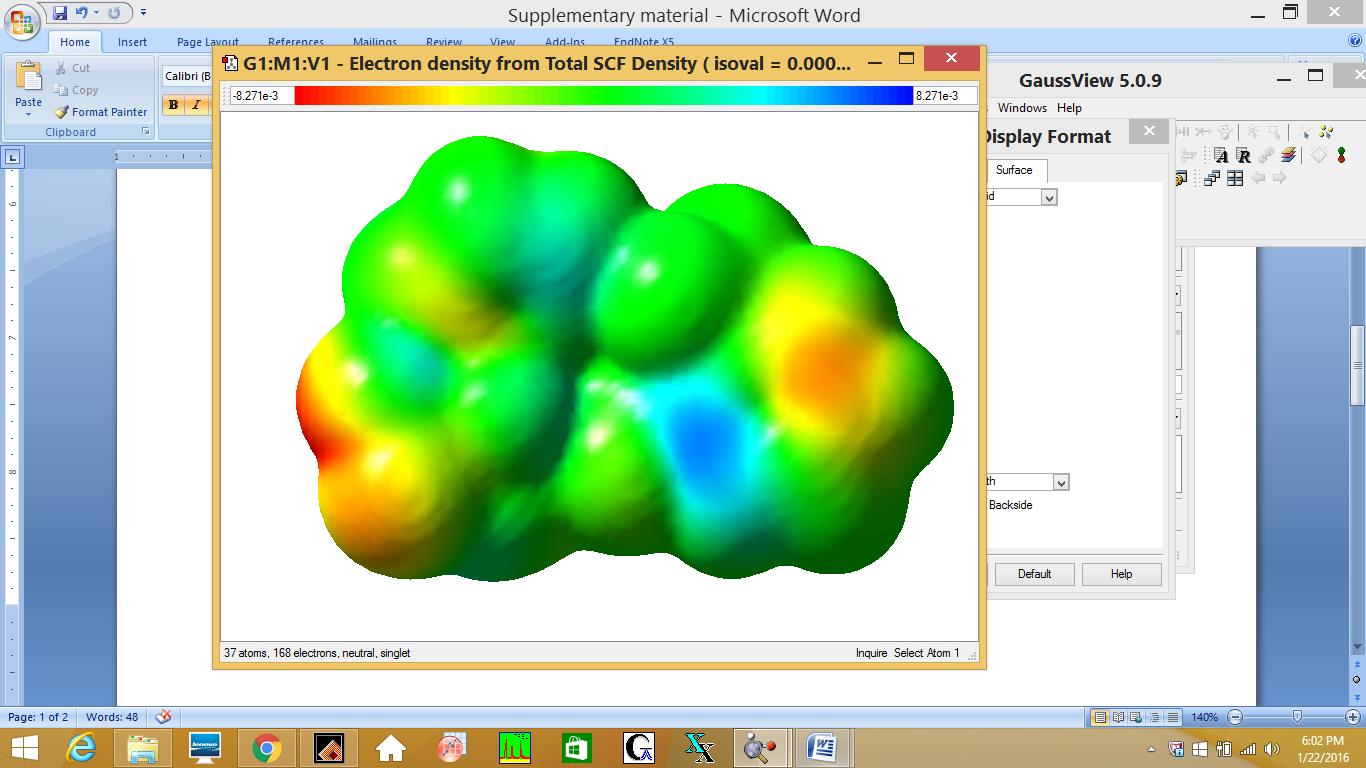
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***Figure 2S. HOMO - LUMO 3-D plots obtained at HF/6-31G\*\*.***

***LUMO= 0.077 a.u. HOMO= - 0.353 a.u.***

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***Figure 3S MEP plot calculated at HF/6-31G\*\* level of theory***

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