**Optoelectronic and photovoltaic properties in a P3HT/PCBM complex:**

**A TD-DFT study**

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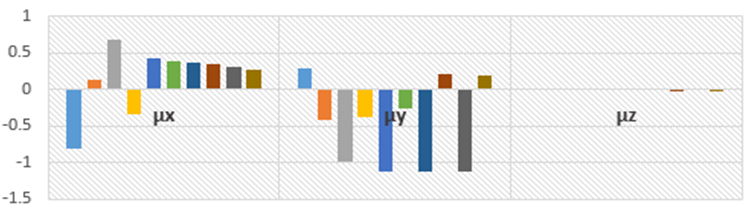
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**M(n=1)**

**M(n=6)**

**M(n=2)**

**M(n=7)**

**M(n=3)**

**M(n=4)**

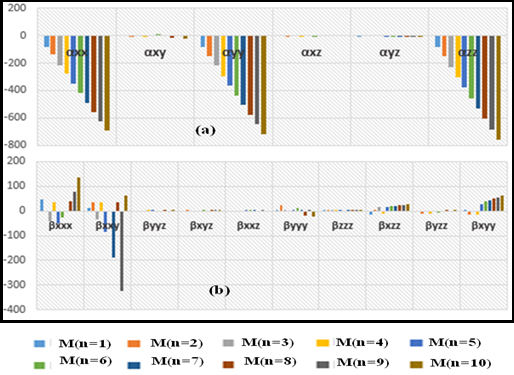
**M(n=5)**

**M(n=8)**

**M(n=9)**

**M(n=10)**

**Fig. 1S.** Electrical dipole moment (DM) of all compounds at TD-DFT B3LYP/6-31 G(d,p).



**Fig. 2S.**  Plots (a) polarizability (α): (b): hyperpolarizability (β) of all compounds at the TD-DFT level B3LYP/6-31 G(d,p).

**Table 1S.** Mulliken charges obtained by B3LYP/6-31G (d,P).

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **M (n1)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 = 0.006** | | | **C2 =0.010** | | | | **C3 =0.004** | | | **C4= 0.002** | | | | | | **S1= 0.487** | | | | | | | **C5= 0.024** | | | | | | **C6=0.041** | | | | | | **C7=0.102** |
| **C8=-0.391** | | | **C9=0.059** | | | | **C10=-0.333** | | | **-------** | | | | | | **-------** | | | | | | | **-------** | | | | | | **-------** | | | | | | **-------** |
| **M (n2)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 = -0.012** | | **C2 =0.007** | | | | **C3 =0.009** | | **C4=0.004** | | | | | | **S1= 0.549** | | | | | | | **C5= 0.008** | | | | | | **C6=-0.006** | | | | | | **C7=0.122** | | |
| **C8= -0.397** | | **C9=0.084** | | | | **C10=-0.384** | | **C11=-0.408** | | | | | | **C12=0.140** | | | | | | | **S2= 0.521** | | | | | | **C13=0.016** | | | | | | **C14=0.003** | | |
| **C15=0.006** | | **C16=0.009** | | | | **C17 =0.007** | | **C18=-0.013** | | | | | | **C19=0.077** | | | | | | | **C20=-0.349** | | | | | | **-------** | | | | | | **-------** | | |
| **M (n3)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 =-0.012** | | | **C2 =0.007** | | | | **C3 =0.009** | | **C4= 0.004** | | | | | | **S1= 0.550** | | | | | | | **C5=0.008** | | | | | | **C6=-0.007** | | | | | | **S2= 0.519** | |
| **C7=0.123** | | | **C8=-0.490** | | | | **C9=0.082** | | **C10=-0.398** | | | | | | **S3=0.523** | | | | | | | **C11=-0.413** | | | | | | **C12=0.113** | | | | | | **C13=0.014** | |
| **C14= 0.007** | | | **C15=0.005** | | | | **C16=0.010** | | **C17 = 0.007** | | | | | | **C18=-0.013** | | | | | | | **C19=0.061** | | | | | | **C20=-0.369** | | | | | | **C21=0.421** | |
| **C22=0.143** | | | **C23=0.016** | | | | **C24=0.004** | | **C25=0.006** | | | | | | **C26=0.009** | | | | | | | **C27=0.007** | | | | | | **C28=-0.012** | | | | | | **C29=0.077** | |
| **C30=-0.348** | | | **-------** | | | | **-------** | | **-------** | | | | | |
| **M (n4)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 = -0.012** | | **C2 =0.007** | | | | **C3 =0.009** | | **C4= 0.004** | | | | | **S1= 0.550** | | | | | | | **C5= -0.465** | | | | | | **C6=-0.465** | | | | | | **S2= 0.519** | | | |
| **C7=0.123** | | **C8=-0.396** | | | | **C9=0.082** | | **C10= -0.253** | | | | | **S3=0.600** | | | | | | | **C11=-0.254** | | | | | | **C12=-0.041** | | | | | | **C13=-0.482** | | | |
| **C14= -0.459** | | **S4=0.524** | | | | **C15=0.006** | | **C16=-0.457** | | | | | **C17 = 0.007** | | | | | | | **C18=-0.013** | | | | | | **C19=0.059** | | | | | | **C20=-0.382** | | | |
| **C21=-0.426** | | **C22=0.115** | | | | **C23=0.013** | | **C24=0.007** | | | | | **C25=0.005** | | | | | | | **C26=0.011** | | | | | | **C27=0.006** | | | | | | **C28= -0.012** | | | |
| **C29=0.060** | | **C30=-0.367** | | | | **C31=-0.421** | | **C32=0.143** | | | | | **C33=0.016** | | | | | | | **C34=0.004** | | | | | | **C35=0.006** | | | | | | **C36=0.009** | | | |
| **C37=0.007** | | **C38=-0.012** | | | | **C39=0.077** | | **C40=-0.347** | | | | | **-------** | | | | | | | **-------** | | | | | | **-------** | | | | | | **-------** | | | |
| **M (n5)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 =-0.012** | | **C2 =0.007** | | | | **C3 =0.009** | | **C4= 0.004** | | | | | **S1= 0.550** | | | | | | | **C5= 0.008** | | | | | | **C6=-0.007** | | | | | | **S2= 0.598** | | | |
| **C7=0.123** | | **C8=-0.490** | | | | **C9=0.082** | | **C10=-0.253** | | | | | **S3= 0.601** | | | | | | | **C11=-0.411** | | | | | | **C12=0.112** | | | | | | **C13=0.014** | | | |
| **C14= 0.006** | | **S4= 0.600** | | | | **C15=0.006** | | **C16=0.009** | | | | | **C17 = 0.007** | | | | | | | **C18=-0.013** | | | | | | **C19= 0.060** | | | | | | **S5=0.524** | | | |
| **C20= -0.383** | | **C21=-0.425** | | | | **C22= 0.115** | | **C23=0.013** | | | | | **C24=0.007** | | | | | | | **C25= 0.005** | | | | | | **C26= 0.010** | | | | | | **C27= 0.007** | | | |
| **C28= -0.012** | | **C29= 0.058** | | | | **C30= -0.381** | | **C31=-0.427** | | | | | **C32= 0.115** | | | | | | | **C33= 0.013** | | | | | | **C34= 0.008** | | | | | | **C35=0.005** | | | |
| **C36=0.011** | | **C37=0.007** | | | | **C38=-0.012** | | **C39=0.060** | | | | | **C40=-0.367** | | | | | | | **C41=-0.421** | | | | | | **C42=0.143** | | | | | | **C43=0.016** | | | |
| **C44=0.004** | | **C45=0.006** | | | | **C46= 0.009** | | **C47=0.007** | | | | | **C48=-0.012** | | | | | | | **C49=0.077** | | | | | | **C50=-0.347** | | | | | | **-------** | | | |
| **M (n=6)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 = -0.012** | **C2 =0.007** | | | **C3 =0.009** | | | | **C4= 0.004** | | | **S1= 0.549** | | | | | | **C5= 0.008** | | | | | | | **C6= -0.006** | | | | | | **S2= 0.598** | | | | | |
| **C7=0.123** | **C8=-0.396** | | | **C9= 0.082** | | | | **C10=-0.398** | | | **S3=0.600** | | | | | | **C11=-0.411** | | | | | | | **C12=0.112** | | | | | | **C13=0.014** | | | | | |
| **C14=0.006** | **S4=0.601** | | | **C15=0.006** | | | | **C16=0.009** | | | **C17=0.007** | | | | | | **C18=-0.013** | | | | | | | **S5=0.600** | | | | | | **C19=0.059** | | | | | |
| **C20=-0.383** | **C21=-0.425** | | | **C22=0.114** | | | | **C23=0.013** | | | **C24=0.007** | | | | | | **C25=0.005** | | | | | | | **C26=0.010** | | | | | | **C27=0.007** | | | | | |
| **C28=-0.012** | **C29=0.058** | | | **C30=-0.382** | | | | **C31=-0.425** | | | **C32=0.115** | | | | | | **C33=0.013** | | | | | | | **C34=0.007** | | | | | | **C35=0.005** | | | | | |
| **C36=0.010** | **C37=0.007** | | | **C38=-0.012** | | | | **C39=0.058** | | | **C40=-0.381** | | | | | | **C41=-0.427** | | | | | | | **C42=0.115** | | | | | | **C43=0.013** | | | | | |
| **C44=0.008** | **C45=0.005** | | | **C46=0.011** | | | | **C47=0.007** | | | **C48=-0.012** | | | | | | **C49=0.060** | | | | | | | **C50=-0.367** | | | | | | **C51=-0.421** | | | | | |
| **C52=0.143** | **S6=0.524** | | | **C53=0.016** | | | | **C54=0.004** | | | **C55=0.006** | | | | | | **C56=0.009** | | | | | | | **C57= 0.007** | | | | | | **C58=-0.012** | | | | | |
| **C59=0.077** | **C60=-0.347** | | | **-------** | | | | **-------** | | | **-------** | | | | | | **-------** | | | | | | | **-------** | | | | | | **-------** | | | | | |
| **M (n=7)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 = -0.012** | | **C2 =0.007** | | | **C3 =0.009** | | | **C4= 0.004** | | | | **S1=0.550** | | | | | | | **C5=0.008** | | | | | | **C6=-0.007** | | | | | | **S2=0.598** | | | | |
| **C7=0.123** | | **C8=-0.396** | | | **C9=0.082** | | | **C10= -0.398** | | | | **S3=0.600** | | | | | | | **C11=-0.411** | | | | | | **C12=0.112** | | | | | | **C13=0.014** | | | | |
| **C14=0.006** | | **S4=0.600** | | | **C15=0.006** | | | **C16=0.009** | | | | **C17=0.007** | | | | | | | **C18= -0.013** | | | | | | **S5=0.601** | | | | | | **C19=0.059** | | | | |
| **C20=-0.383** | | **C21=-0.425** | | | **C22=0.114** | | | **C23=0.013** | | | | **C24=0.007** | | | | | | | **C25=0.005** | | | | | | **C26= 0.010** | | | | | | **C27=0.007** | | | | |
| **C28=-0.012** | | **C29=0.058** | | | **C30 =-0.382** | | | **C31 =-0.425** | | | | **C32 =0.115** | | | | | | | **C33 =0.013** | | | | | | **C34=0.007** | | | | | | **C35 =0.005** | | | | |
| **C36=0.010** | | **C37=0.007** | | | **C38=-0.012** | | | **C39=0.059** | | | | **C40=-0.382** | | | | | | | **C41=-0.425** | | | | | | **C42=0.115** | | | | | | **C43=0.013** | | | | |
| **C44=0.007** | | **C45=0.005** | | | **C46=0.010** | | | **C47=0.007** | | | | **C48=-0.012** | | | | | | | **C49=0.058** | | | | | | **C50=0.058** | | | | | | **C51=-0.427** | | | | |
| **C52=0.115** | | **S6=0.600** | | | **C53=0.013** | | | **C54=0.008** | | | | **C55=0.005** | | | | | | | **C56=0.011** | | | | | | **S7=0.524** | | | | | | **C57=0.007** | | | | |
| **C58=-0.012** | | **C59=0.060** | | | **C60=-0.367** | | | **C61=-0.421** | | | | **C62=0.143** | | | | | | | **C63=0.016** | | | | | | **C64=0.004** | | | | | | **C65=0.006** | | | | |
| **C66=0.009** | | **C67=0.007** | | | **C68=-0.012** | | | **C69=0.077** | | | | **C70=-0.347** | | | | | | | **-------** | | | | | | **-------** | | | | | | **-------** | | | | |
| **M (n=8)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 = -0.012** | | **C2 =0.007** | | | **C3 =0.009** | | | **C4= 0.004** | | | | **S1=0.550** | | | | | | | **C5=0.008** | | | | | | **C6=-0.007** | | | | | | **S2=0.598** | | | | |
| **C7=0.123** | | **C8=-0.396** | | | **C9=0.082** | | | **C10= -0.398** | | | | **S3=0.600** | | | | | | | **C11=-0.411** | | | | | | **C12=0.112** | | | | | | **C13=0.014** | | | | |
| **C14=0.006** | | **S4=0.600** | | | **C15=0.006** | | | **C16=0.009** | | | | **C17=0.007** | | | | | | | **C18= -0.013** | | | | | | **S5=0.600** | | | | | | **C19=0.060** | | | | |
| **C20=-0.383** | | **C21=-0.425** | | | **C22=0.115** | | | **S6=0.601** | | | | **C23=0.013** | | | | | | | **C24=0.007** | | | | | | **C25= 0.005** | | | | | | **C26=0.010** | | | | |
| **S7=0.600** | | **C27=0.007** | | | **C28=-0.012** | | | **C29=0.058** | | | | **C30 =-0.382** | | | | | | | **S8=0.524** | | | | | | **C31 =-0.425** | | | | | | **C32 =0.115** | | | | |
| **C33=0.013** | | **C34=0.007** | | | **C35 =0.005** | | | **C36=0.010** | | | | **C37=0.007** | | | | | | | **C38=-0.012** | | | | | | **C39=0.058** | | | | | | **C40= -0.382** | | | | |
| **C41=-0.425** | | **C42=0.115** | | | **C43=0.013** | | | **C44=0.007** | | | | **C45=0.005** | | | | | | | **C46=0.010** | | | | | | **C47=0.007** | | | | | | **C48=-0.012** | | | | |
| **C49=0.058** | | **C50=-0.381** | | | **C51=-0.425** | | | **C52=0.115** | | | | **C53=0.013** | | | | | | | **C54=0.007** | | | | | | **C55=0.005** | | | | | | **C56=0.010** | | | | |
| **C57=0.007** | | **C58=-0.012** | | | **C59=0.058** | | | **C60=-0.381** | | | | **C61=-0.427** | | | | | | | **C62=0.115** | | | | | | **C63=0.013** | | | | | | **C64=0.008** | | | | |
| **C65=0.005** | | **C66=0.011** | | | **C67=0.007** | | | **C68=-0.012** | | | | **C69=0.060** | | | | | | | **C70=-0.367** | | | | | | **C71=-0.421** | | | | | | **C72=0.143** | | | | |
| **C73=0.016** | | **C74=0.004** | | | **C75=0.006** | | | **C76=0.009** | | | | **C77=0.007** | | | | | | | **C78=-0.012** | | | | | | **C79= 0.077** | | | | | | **C80=-0.347** | | | | |
| **M (n=9)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 =-0.012** | **C2 =0.007** | | | **C3 =0.009** | | | | **C4=0.004** | | | | **S1=0.550** | | | | | | **C5=0.008** | | | | | | | **C6=-0.0071** | | | | | | **S2=0.598** | | | | |
| **C7=0.123** | **C8=-0.396** | | | **C9=0.082** | | | | **C10=-0.398** | | | | **S3=0.600** | | | | | | **C11=-0.411** | | | | | | | **C12=0.112** | | | | | | **C13=0.014** | | | | |
| **C14=0.006** | **S4=0.600** | | | **C15=0.006** | | | | **C16=0.009** | | | | **C17=0.007** | | | | | | **C18=-0.013** | | | | | | | **S5=0.601** | | | | | | **C19=0.059** | | | | |
| **C20=-0.383** | **C21=-0.425** | | | **C22=0.114** | | | | **C23=0.013** | | | | **C24=0.007** | | | | | | **C25=0.005** | | | | | | | **C26=0.010** | | | | | | **C27=0.007** | | | | |
| **C28=0.007** | **C29=0.058** | | | **C30=-0.382** | | | | **C31=-0.425** | | | | **C32=0.115** | | | | | | **C33=0.013** | | | | | | | **C34=0.007** | | | | | | **C35=0.005** | | | | |
| **C36=0.010** | **C37=0.007** | | | **C38=-0.012** | | | | **C39=0.058** | | | | **C40=-0.382** | | | | | | **C41=-0.425** | | | | | | | **C42=0.115** | | | | | | **C43=0.013** | | | | |
| **C44=0.007** | **C45=0.005** | | | **C46=0.010** | | | | **C47=0.007** | | | | **C48=-0.012** | | | | | | **C49=0.058** | | | | | | | **C50=-0.382** | | | | | | **C51=-0.425** | | | | |
| **C52=0.115** | **S6=0.115** | | | **C53=0.013** | | | | **C54=0.007** | | | | **C55=0.005** | | | | | | | **C56=0.010** | | | | | | **S7=0.010** | | | | | | **C57=0.007** | | | | |
| **C58=-0.012** | **C59=0.059** | | | **C60=-0.381** | | | | **C61=-0.425** | | | | **C62=0.115** | | | | | | | **C63=0.013** | | | | | | **C64=0.007** | | | | | | **C65=0.005** | | | | |
| **C66=0.010** | **C67=0.007** | | | **C68=-0.012** | | | | **C69=0.058** | | | | **C70=-0.381** | | | | | | | **C71=-0.427** | | | | | | **C72=0.115** | | | | | | **S8=0.601** | | | | |
| **C73=0.013** | **C74=0.008** | | | **C75=0.005** | | | | **C76=0.011** | | | | **S9=0.524** | | | | | | | **C77=0.007** | | | | | | **C78= -0.012** | | | | | | **C79=0.061** | | | | |
| **C80=-0.367** | **C81=-0.421** | | | **C82=0.143** | | | | **C83=0.016** | | | | **C84=0.004** | | | | | | | **C85=0.006** | | | | | | **C86=0.009** | | | | | | **C87=0.007** | | | | |
| **C88=-0.012** | **C89=0.077** | | | **C90=-0.347** | | | | **-------** | | | | **-------** | | | | | | | **-------** | | | | | | **-------** | | | | | | **-------** | | | | |
| **M (n=10)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 = -0.012** | **C2 =0.007** | | | **C3 =0.009** | | | | **C4=0.004** | | | | **S1=0.550** | | | | | | **C5=0.008** | | | | | | | **C6=-0.007** | | | | | | **S2=0.598** | | | | |
| **C7=0.123** | **C8=-0.396** | | | **C9=0.082** | | | | **C10=-0.398** | | | | **S3=0.600** | | | | | | **C11=-0.411** | | | | | | | **C12=0.112** | | | | | | **C13=0.014** | | | | |
| **C14=0.006** | **S4=0.600** | | | **C15=0.006** | | | | **C16=0.009** | | | | **C17=0.007** | | | | | | **C18=-0.013** | | | | | | | **S5=0.600** | | | | | | **C19=0.060** | | | | |
| **C20=-0.383** | **C21=-0.425** | | | **C22=0.115** | | | | **S6=0.601** | | | | **C23=0.013** | | | | | | **C24=0.007** | | | | | | | **C25=0.005** | | | | | | **C26=0.010** | | | | |
| **S7=0.600** | **C27=0.007** | | | **C28=-0.012** | | | | **C29=0.058** | | | | **C30=-0.382** | | | | | | **S8=0.601** | | | | | | | **C31=-0.425** | | | | | | **C32=0.115** | | | | |
| **C33=0.013** | **C34=0.007** | | | **S9=0.601** | | | | **C35=0.005** | | | | **C36=0.010** | | | | | | **C37=0.007** | | | | | | | **C38= -0.012** | | | | | | **S10=0.524** | | | | |
| **C39=0.058** | **C40=-0.382** | | | **C41=-0.425** | | | | **C42=0.115** | | | | **C43=0.013** | | | | | | **C44=0.007** | | | | | | | **C45=0.005** | | | | | | **C46=0.010** | | | | |
| **C47=0.007** | **C48=-0.012** | | | **C49=0.058** | | | | **C50=-0.381** | | | | **C51=-0.425** | | | | | | | **C52=0.115** | | | | | | **C53=0.013** | | | | | | **C54=0.007** | | | | |
| **C55=0.005** | **C56=0.010** | | | **C57=0.007** | | | | **C58=-0.012** | | | | **C59=0.059** | | | | | | | **C60=-0.382** | | | | | | **C61=-0.425** | | | | | | **C62=0.115** | | | | |
| **C63=0.013** | **C64=0.007** | | | **C65=0.005** | | | | **C66=0.010** | | | | **C67=0.007** | | | | | | | **C68=-0.012** | | | | | | **C69=0.059** | | | | | | **C70=-0.381** | | | | |
| **C71=-0.425** | **C72=0.115** | | | **C73=0.013** | | | | **C74=0.007** | | | | **C75=0.005** | | | | | | | **C76=0.010** | | | | | | **C77=0.007** | | | | | | **C78=-0.012** | | | | |
| **C79=0.059** | **C80=-0.381** | | | **C81=-0.427** | | | | **C82=0.115** | | | | **C83=0.013** | | | | | | | **C84=0.008** | | | | | | **C85=0.005** | | | | | | **C86=0.011** | | | | |
| **C87=0.007** | **C88=-0.012** | | | **C89=0.060** | | | | **C90=-0.367** | | | | **C91=-0.421** | | | | | | | **C92=0.143** | | | | | | **C93=0.016** | | | | | | **C94=0.004** | | | | |
| **C95=0.006** | **C96=0.009** | | | **C97=0.007** | | | | **C98=-0.012** | | | | **C99=0.077** | | | | | | | **C100 = -0.347** | | | | | | **-------** | | | | | | **-------** | | | | |

**Table 2S.** Accumulation of the electron population of atoms in the core, valence and Rydberg orbitals obtained by B3LYP/6-31G (d,P).

|  |  |  |  |
| --- | --- | --- | --- |
| **Compounds** | **Core** | **Valence** | **Rydberg** |
| **M(n=1)** | 31.98920 (99.9663% de 32) | 67.85709 (99.7898% de 68) | 0.15370 (0.1537% de 100) |
| **M(n=2)** | 59.97946 (99.9658% de 60) | 121.74049 (99.787% de 122) | 0.28005 (0.1539% de 182) |
| **M(n=3)** | 89.96896 ( 99.9655% de 90) | 181.61129 (99.786% de 182) | 0.41975 (0.1543% de 272) |
| **M(n=4)** | 119.9584 (99.9654% de 120) | 241.4820 (99.7859% de 242) | 0.55954 (0.1546% de 362) |
| **M(n=5)** | 149.94796 (99.965% de 150) | 301.35279 (99.785% de 302) | 0.69925 (0.1547% de 452) |
| **M(n=6)** | 179.93746 (99.965% de 180) | 361.22350 (99.785% de 362) | 0.83904 (0.1548% de 542) |
| **M(n=7)** | 209.92696 (99.965% de 210) | 421.09427 (99.785% de 422) | 0.97878 (0.1549% de 632) |
| **M(n=8)** | 239.91645 (99.965% de 240) | 480.96490 (99.785% de 482) | 1.11865 (0.1549% de 722) |
| **M(n=9)** | 269.90595 (99.965% de 270) | 540.83575 (99.785% de 542) | 1.25830 (0.1550% de 812) |
| **M(n=10)** | 299.89545 (99.965% de 300) | 600.70643 (99.785% de 602) | 1.39812 (0.1550% de 902) |

**Table 3S.** NBO charges obtained by B3LYP/6-31G (d,P).

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **M (n1)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 = -0.453** | | | **C2 =-0.457** | | | | **C3 =-0.454** | | **C4 = -0.453** | | | | | **S1 = 0.496** | | | | | | | **C5= -0.458** | | | | | | | **C6=-0.470** | | | | | **C7 = -0.302** | | |
| **C8=-0.247** | | | **C9 = -0.280** | | | | **C10 = -0.486** | | **-------** | | | | | **-------** | | | | | | | **-------** | | | | | | | **-------** | | | | | **-------** | | |
| **M (n2)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 = -0.685** | | **C2 =-0.452** | | | | **C3 =-0.457** | | | **C4 = -0.453** | | | | | | **S1 = 0.505** | | | | | | | **C5=0.461** | | | | | | **C6=-0.465** | | | | | | **C7 = -0.056** | |
| **C8=-0.490** | | **C9 = -0.277** | | | | **C10 = -0.253** | | | **C11 = -0.257** | | | | | | **C12 = -0.054** | | | | | | | **S2 =0.506** | | | | | | **C13 = -0.482** | | | | | | **C14= -0.459** | |
| **C15= -0.452** | | **C16=-0.457** | | | | **C17 = -0.452** | | | **C18 = -0.685** | | | | | | **C19 = -0.285** | | | | | | | **C20 = -0.470** | | | | | | **-------** | | | | | | **-------** | |
| **M (n3)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 = -0.685** | | | **C2 =-0.452** | | | | **C3 =-0.457** | | **C4 = -0.453** | | | | **S1 = 0.505** | | | | | | | **C5= -0.461** | | | | | | | **C6=-0.465** | | | | | | | **S2 = 0.518** | |
| **C7 = -0.056** | | | **C8=-0.490** | | | | **C9 = -0.279** | | **C10 = -0.253** | | | | **S3=0.507** | | | | | | | **C11 = -0.253** | | | | | | | **C12 = -0.041** | | | | | | | **C13 = -0.482** | |
| **C14= -0.459** | | | **C15= -0.452** | | | | **C16=-0.457** | | **C17 = -0.452** | | | | **C18 = -0.685** | | | | | | | **C19 = -0.279** | | | | | | | **C20 = -0.246** | | | | | | | **C21 = -0.257** | |
| **C22 = -0.054** | | | **C23 = -0.482** | | | | **C24 = -0.459** | | **C25=-0.452** | | | | **C26=-0.457** | | | | | | | **C27 = -0.452** | | | | | | | **C28 = -0.685** | | | | | | | **C29 = -0.285** | |
| **C30 = -0.470** | | | **-------** | | | | **-------** | |
| **M (n4)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 = -0.685** | | **C2 =0.007** | | | | **C3 =0.009** | | | **C4 = 0.004** | | | | | | **S1 = 0.504** | | | | | | | **C5= -0.461** | | | | **C6=-0.465** | | | | | | **S2 = 0.518** | | | |
| **C7 = -0.056** | | **C8=-0.490** | | | | **C9 = -0.279** | | | **C10 = -0.398** | | | | | | **S3= 0.519** | | | | | | | **C11 =-0.254** | | | | **C12 = -0.041** | | | | | | **C13 = -0.482** | | | |
| **C14= -0.459** | | **S4 = 0.507** | | | | **C15= -0.452** | | | **C16=-0.457** | | | | | | **C17 = -0.452** | | | | | | | **C18 = -0.685** | | | | **C19 = -0.281** | | | | | | **C20 = -0.245** | | | |
| **C21 = -0.253** | | **C22 = -0.042** | | | | **C23 = -0.482** | | | **C24 = -0.459** | | | | | | **C25=-0.452** | | | | | | | **C26=-0.457** | | | | **C27 = -0.452** | | | | | | **C28 = -0.685** | | | |
| **C29=-0.279** | | **C30=-0.245** | | | | **C31=-0.257** | | | **C32=-0.054** | | | | | | **C33=-0.482** | | | | | | | **C34= -0.459** | | | | **C35=-0.452** | | | | | | **C36=-0.457** | | | |
| **C37 = -0.452** | | **C38 = -0.685** | | | | **C39 = -0.285** | | | **C40 = -0.469** | | | | | | **-------** | | | | | | | **-------** | | | | **-------** | | | | | | **-------** | | | |
| **M (n5)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 = -0.685** | | **C2 =-0.453** | | | | **C3 =-0.457** | | | **C4 = -0.453** | | | | | | **S1 = 0.504** | | | | | | | **C5= -0.461** | | | | **C6=-0.465** | | | | | | **S2 = 0.518** | | | |
| **C7 = -0.056** | | **C8=-0.396** | | | | **C9 = -0.279** | | | **C10 = -0.398** | | | | | | **S3= 0.519** | | | | | | | **C11 = -0.254** | | | | **C12 = -0.041** | | | | | | **C13 = -0.482** | | | |
| **C14= -0.459** | | **S4 = 0.519** | | | | **C15= -0.452** | | | **C16=-0.457** | | | | | | **C17 = -0.452** | | | | | | | **C18 = -0.685** | | | | **C19 = -0.281** | | | | | | **S5=0.507** | | | |
| **C20 = -0.245** | | **C21 = -0.253** | | | | **C22 = -0.041** | | | **C23 = -0.482** | | | | | | **C24 = -0.459** | | | | | | | **C25= -0.452** | | | | **C26= -0.457** | | | | | | **C27 = -0.452** | | | |
| **C28 = -0.685** | | **C29 = -0.281** | | | | **C30 = -0.244** | | | **C31 = -0.253** | | | | | | **C32 = -0.041** | | | | | | | **C33 = -0.482** | | | | **C34 = -0.459** | | | | | | **C35 = -0.452** | | | |
| **C36 = -0.459** | | **C37 = -0.452** | | | | **C38 = -0.685** | | | **C39 = -0.279** | | | | | | **C40 = -0.245** | | | | | | | **C41 = -0.257** | | | | **C42 = -0.054** | | | | | | **C43 = -0.482** | | | |
| **C44 = -0.459** | | **C45 = -0.4527** | | | | **C46 = -0.457** | | | **C47 = -0.452** | | | | | | **C48 = -0.6855** | | | | | | | **C49 = -0.285** | | | | **C50 = -0.469** | | | | | | **-------** | | | |
| **M (n=6)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 = -0.685** | **C2 =-0.452** | | | | **C3 =-0.457** | | | | **C4 = -0.453** | **S1 = 0.504** | | | | | | **C5=-0.461** | | | | | | | **C6= -0.465** | | | | | | **S2 = 0.518** | | | | | | |
| **C7 = -0.056** | **C8 = -0.490** | | | | **C9 = -0.279** | | | | **C10 = -0.253** | **S3 = 0.518** | | | | | | **C11 = -0.254** | | | | | | | **C12 = -0.041** | | | | | | **C13 = -0.482** | | | | | | |
| **C14 = -0.459** | **S4 = 0.519** | | | | **C15=-0.452** | | | | **C16=-0.457** | **C17 = -0.452** | | | | | | **C18 = -0.685** | | | | | | | **S5 = 0.519** | | | | | | **C19 = -0.281** | | | | | | |
| **C20 = -0.245** | **C21 = -0.253** | | | | **C22 = -0.041** | | | | **C23 = -0.482** | **C24 = -0.459** | | | | | | **C25=-0.452** | | | | | | | **C26=-0.457** | | | | | | **C27 =-0.452** | | | | | | |
| **C28 =-0.685** | **C29 =-0.281** | | | | **C30 = -0.244** | | | | **C31 = -0.254** | **C32 = -0.041** | | | | | | **C33 = -0.482** | | | | | | | **C34 =-0.459** | | | | | | **C35=-0.452** | | | | | | |
| **C36=-0.457** | **C37 =-0.452** | | | | **C38 =-0.685** | | | | **C39 =-0.281** | **C40 =-0.244** | | | | | | **C41 =-0.254** | | | | | | | **C42 =-0.041** | | | | | | **C43 =-0.482** | | | | | | |
| **C44 =-0.459** | **C45=-0.452** | | | | **C46=-0.457** | | | | **C47 =-0.452** | **C48 =-0.685** | | | | | | **C49 = -0.279** | | | | | | | **C50 =-0.245** | | | | | | **C51 =-0.257** | | | | | | |
| **C52 =-0.054** | **S6 = 0.507** | | | | **C53 =-0.482** | | | | **C54 =-0.459** | **C55=-0.452** | | | | | | **C56=-0.457** | | | | | | | **C57 =-0.452** | | | | | | **C58 =-0.685** | | | | | | |
| **C59 =-0.285** | **C60 =-0.469** | | | | **-------** | | | | **-------** | **-------** | | | | | | **-------** | | | | | | | **-------** | | | | | | **-------** | | | | | | |
| **M (n=7)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 = -0.685** | **C2 =-0.453** | | | | **C3 =-0.457** | | | | **C4 = -0.453** | | | **S1 = 0.504** | | | | | | | **C5=-0.461** | | | | | | **C6=-0.465** | | | | | | **S2 = 0.518** | | | | |
| **C7 = -0.056** | **C8 = -0.490** | | | | **C9 = -0.279** | | | | **C10 = -0.253** | | | **S3 = 0.518** | | | | | | | **C11 = -0.254** | | | | | | **C12 = -0.041** | | | | | | **C13 = -0.482** | | | | |
| **C14 = -0.459** | **S4 = 0.518** | | | | **C15=-0.452** | | | | **C16=-0.457** | | | **C17 =-0.452** | | | | | | | **C18 =-0.685** | | | | | | **S5 = 0.519** | | | | | | **C19 =-0.281** | | | | |
| **C20 =-0.245** | **C21 =-0.253** | | | | **C22 =-0.041** | | | | **C23 =-0.482** | | | **C24 =-0.459** | | | | | | | **C25=-0.452** | | | | | | **C26=-0.457** | | | | | | **C27 =-0.452** | | | | |
| **C28 =-0.685** | **C29 =-0.281** | | | | **C30 =-0.244** | | | | **C31 =-0.254** | | | **C32 =-0.041** | | | | | | | **C33 =-0.482** | | | | | | **C34 =-0.459** | | | | | | **C35 =-0.452** | | | | |
| **C36= -0.457** | **C37 =-0.452** | | | | **C38 =-0.685** | | | | **C39 =-0.281** | | | **C40 = -0.244** | | | | | | | **C41 = -0.254** | | | | | | **C42 = -0.041** | | | | | | **C43 = -0.482** | | | | |
| **C44 = -0.459** | **C45 = -0.452** | | | | **C46 = -0.457** | | | | **C47 = -0.452** | | | **C48 = -0.685** | | | | | | | **C49 = -0.281** | | | | | | **C50 =-0.244** | | | | | | **C51 =-0.254** | | | | |
| **C52 =-0.041** | **S6 = 0.519** | | | | **C53 =-0.483** | | | | **C54 =-0.459** | | | | | | **C55=-0.452** | | | | **C56=-0.457** | | | | | | **S7 = 0.507** | | | | | | **C57 =-0.452** | | | | |
| **C58 =-0.685** | **C59 =-0.279** | | | | **C60 =-0.244** | | | | **C61 =-0.257** | | | | | | **C62 =-0.054** | | | | **C63 =-0.482** | | | | | | **C64 =-0.459** | | | | | | **C65=-0.452** | | | | |
| **C66=-0.457** | **C67 =-0.452** | | | | **C68 =-0.685** | | | | **C69 =-0.285** | | | | | | **C70 =-0.469** | | | | **-------** | | | | | | **-------** | | | | | | **-------** | | | | |
| **M (n=8)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 =-0.685** | | | **C2 =-0.452** | | **C3 =-0.457** | | | | **C4 = -0.453** | | | **S1 = 0.50468** | | | | | | | **C5=-0.461** | | | | | | **C6=-0.465** | | | | | | **S2 = 0.518** | | | | |
| **C7 = -0.056** | | | **C8 = -0.490** | | **C9 = -0.279** | | | | **C10 = -0.253** | | | **S3 = 0.518** | | | | | | | **C11 = -0.254** | | | | | | **C12 = -0.041** | | | | | | **C13 = -0.482** | | | | |
| **C14 = -0.482** | | | **S4 = 0.518** | | **C15=-0.452** | | | | **C16=-0.457** | | | **C17 =-0.452** | | | | | | | **C18 = -0.685** | | | | | | **S5 = 0.518** | | | | | | **C19 =-0.281** | | | | |
| **C20 =-0.245** | | | **C21 =-0.253** | | **C22 =-0.041** | | | | **S6 = 0.519** | | | **C23 =-0.482** | | | | | | | **C24 =-0.459** | | | | | | **C25= -0.452** | | | | | | **C26=-0.457** | | | | |
| **S7 = 0.519** | | | **C27 =-0.452** | | **C28 =-0.685** | | | | **C29 =-0.281** | | | **C30 =-0.244** | | | | | | | **S8 = 0.507** | | | | | | **C31 =-0.254** | | | | | | **C32 =-0.041** | | | | |
| **C33= -0.482** | | | **C34 =-0.459** | | **C35 =-0.457** | | | | **C36=-0.457** | | | **C37 =-0.452** | | | | | | | **C38 =-0.685** | | | | | | **C39 =-0.281** | | | | | | **C40 = -0.281** | | | | |
| **C41 = -0.254** | | | **C42 = -0.041** | | **C43 = -0.482** | | | | **C44 = -0.459** | | | **C45 = -0.452** | | | | | | | **C46 = -0.457** | | | | | | **C47 = -0.452** | | | | | | **C48 = -0.685** | | | | |
| **C49 = -0.281** | | | **C50 =-0.244** | | **C51 =-0.254** | | | | **C52 =-0.041** | | | | | | **C53 =-0.482** | | | | **C54 =-0.459** | | | | | | **C55=-0.452** | | | | | | **C56=-0.457** | | | | |
| **C57 =-0.452** | | | **C58 =-0.685** | | **C59 = -0.281** | | | | **C60 =-0.244** | | | | | | **C61 =-0.254** | | | | **C62 =-0.041** | | | | | | **C63 =-0.483** | | | | | | **C64 =-0.459** | | | | |
| **C65=-0.452** | | | **C66=-0.457** | | **C67 =-0.452** | | | | **C68 =-0.685** | | | | | | **C69 =-0.279** | | | | **C70 =-0.244** | | | | | | **C71 =-0.257** | | | | | | **C72 =-0.053** | | | | |
| **C73 =-0.482** | | | **C74 =-0.459** | | **C75=-0.452** | | | | **C76=-0.457** | | | | | | **C77 =-0.452** | | | | **C78 =-0.685** | | | | | | **C79 =-0.285** | | | | | | **C80 =-0.469** | | | | |
| **M (n=9)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 = -0.685** | | | **C2 =-0.453** | | **C3 =-0.457** | | | | **C4 =-0.453** | | | **S1 = 0.504** | | | | | | **C5 = -0.461** | | | | | | | **C6 = -0.465** | | | | | | **S2 = 0.518** | | | | |
| **C7 = -0.056** | | | **C8 = -0.490** | | **C9 = -0.279** | | | | **C10 = -0.253** | | | **S3 = 0.518** | | | | | | **C11 = -0.254** | | | | | | | **C12 = -0.0417** | | | | | | **C13 = -0.482** | | | | |
| **C14 = -0.459** | | | **S4 = 0.518** | | **C15 = -0.452** | | | | **C16 = -0.457** | | | **C17 = -0.452** | | | | | | **C18 = -0.685** | | | | | | | **S5 = 0.519** | | | | | | **C19 = -0.281** | | | | |
| **C20 = -0.245** | | | **C21 = -0.253** | | **C22 = -0.041** | | | | **C23 = -0.482** | | | **C24 = -0.459** | | | | | | **C25 = -0.452** | | | | | | | **C26 = -0.457** | | | | | | **C27 = -0.452** | | | | |
| **C28 = -0.685** | | | **C29 = -0.281** | | **C30 = -0.244** | | | | **C31 = -0.254** | | | **C32 = -0.041** | | | | | | **C33 = -0.482** | | | | | | | **C34 = -0.459** | | | | | | **C35 = -0.452** | | | | |
| **C36 = -0.457** | | | **C37 = -0.452** | | **C38 = -0.685** | | | | **C39 = -0.281** | | | **C40 = -0.244** | | | | | | **C41 = -0.254** | | | | | | | **C42 = -0.041** | | | | | | **C43 = -0.482** | | | | |
| **C44 = -0.459** | | | **C45 = -0.452** | | **C46 = -0.457** | | | | **C47 = -0.452** | | | **C48 = -0.685** | | | | | | **C49 = -0.281** | | | | | | | **C50 = -0.244** | | | | | | **C51 = -0.254** | | | | |
| **C52 = -0.041** | | | **S6 = 0.518** | | **C53 = -0.482** | | | | **C54 = -0.459** | | | **C55 = -0.452** | | | | | | | **C56 = -0.457** | | | | | | **S7=0.519** | | | | | | **C57 = -0.452** | | | | |
| **C58 = -0.685** | | | **C59 = -0.281** | | **C60 = -0.244** | | | | **C61 = -0.254** | | | **C62 = -0.041** | | | | | | | **C63 = -0.482** | | | | | | **C64 = -0.459** | | | | | | **C65 = -0.452** | | | | |
| **C66 = -0.457** | | | **C67 = -0.452** | | **C68 = -0.685** | | | | **C69 = -0.281** | | | **C70=-0.244** | | | | | | | **C71=-0.254** | | | | | | **C72=-0.041** | | | | | | **S8 = 0.519** | | | | |
| **C73 =-0.483** | | | **C74 =-0.459** | | **C75=-0.452** | | | | **C76 = -0.457** | | | **S9=0.507** | | | | | | | **C77 = -0.452** | | | | | | **C78 = -0.685** | | | | | | **C79 = -0.279** | | | | |
| **C80 = -0.244** | | | **C81 = -0.257** | | **C82 = -0.053** | | | | **C83 = -0.482** | | | **C84 = -0.459** | | | | | | | **C85 = -0.452** | | | | | | **C86 = -0.457** | | | | | | **C87 = -0.452** | | | | |
| **C88 = -0.685** | | | **C89 = -0.285** | | **C90 = -0.469** | | | | **-------** | | | **-------** | | | | | | | **-------** | | | | | | **-------** | | | | | | **-------** | | | | |
| **M (n=10)** | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **C1 = -0.685** | **C2 =-0.452** | | | **C3 =-0.457** | | | | **C4 =-0.453** | | | **S1 = 0.504** | | | | | | **C5 = -0.461** | | | | | | | **C6 = -0.465** | | | | | | **S2 = 0.518** | | | | | |
| **C7 = -0.056** | **C8 = -0.490** | | | **C9 = -0.279** | | | | **C10 = -0.253** | | | **S3 = 0.518** | | | | | | **C11 = -0.254** | | | | | | | **C12 = -0.041** | | | | | | **C13 = -0.482** | | | | | |
| **C14 = -0.459** | **S4 = 0.518** | | | **C15 = -0.452** | | | | **C16 = -0.457** | | | **C17 = -0.452** | | | | | | **C18 = -0.685** | | | | | | | **S5 = 0.519** | | | | | | **C19 = -0.281** | | | | | |
| **C20 = -0.245** | **C21 = -0.253** | | | **C22 = -0.041** | | | | **S6 = 0.519** | | | **C23 = -0.482** | | | | | | **C24 = -0.459** | | | | | | | **C25 = -0.452** | | | | | | **C26 = -0.457** | | | | | |
| **S7=0.519** | **C27 = -0.452** | | | **C28 = -0.685** | | | | **C29 = -0.281** | | | **C30 = -0.244** | | | | | | **S8 = 0.519** | | | | | | | **C31 = -0.254** | | | | | | **C32 = -0.041** | | | | | |
| **C33 = -0.482** | **C34 = -0.459** | | | **S9= 0.519** | | | | **C35 = -0.452** | | | **C36 = -0.457** | | | | | | **C37 = -0.452** | | | | | | | **C38 = -0.685** | | | | | | **S10 = 0.507** | | | | | |
| **C39 = -0.281** | **C40 = -0.244** | | | **C41 = -0.254** | | | | **C42 = -0.041** | | | **C43 = -0.482** | | | | | | **C44 = -0.459** | | | | | | | **C45 = -0.452** | | | | | | **C46 = -0.457** | | | | | |
| **C47 = -0.452** | **C48 = -0.685** | | | **C49 = -0.281** | | | | | **C50 = -0.244** | | **C51 = -0.244** | | | | | | | **C52 = -0.041** | | | | | | **C53 = -0.482** | | | | | | **C54 = -0.459** | | | | | |
| **C55 = -0.452** | **C56 = -0.457** | | | **C57 = -0.452** | | | | | **C58 = -0.685** | | **C59 = -0.281** | | | | | | | **C60 = -0.244** | | | | | | **C61 = -0.254** | | | | | | **C62 = -0.041** | | | | | |
| **C63 = -0.482** | **C64 = -0.459** | | | **C65 = -0.452** | | | | | **C66 = -0.457** | | **C67 = -0.452** | | | | | | | **C68 = -0.685** | | | | | | **C69 = -0.281** | | | | | | **C70=-0.244** | | | | | |
| **C71=-0.254** | **C72=-0.041** | | | **C73 =-0.041** | | | | | **C74 =-0.459** | | **C75=-0.452** | | | | | | | **C76 = -0.457** | | | | | | **C77 = -0.452** | | | | | | **C78 = -0.685** | | | | | |
| **C79= -0.281** | **C80 = -0.244** | | | **C81 = -0.254** | | | | | **C82 = -0.041** | | **C83 = -0.483** | | | | | | | **C84 = -0.459** | | | | | | **C85 = -0.452** | | | | | | **C86 = -0.457** | | | | | |
| **C87 = -0.452** | **C88 = -0.685** | | | **C89 = -0.279** | | | | | **C90 = -0.244** | | **C91 = -0.257** | | | | | | | **C92 = -0.053** | | | | | | **C93 = -0.482** | | | | | | **C94 = -0.459** | | | | | |
| **C95 = -0.452** | **C96 = -0.457** | | | **C97 = -0.452** | | | | | **C98 = -0.685** | | **C99 = -0.285** | | | | | | | **C100 = -0.469** | | | | | | **-------** | | | | | | **-------** | | | | | |

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**Fig. 3S.**  NBO and Mulliken charge curves obtained by B3LYP/6-31G (d,P).