Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

Supporting Information for

Electron deficient dicyanovinylene-ladder-type pentaphenylene derivative for n-type Organic Field Effect Transistors

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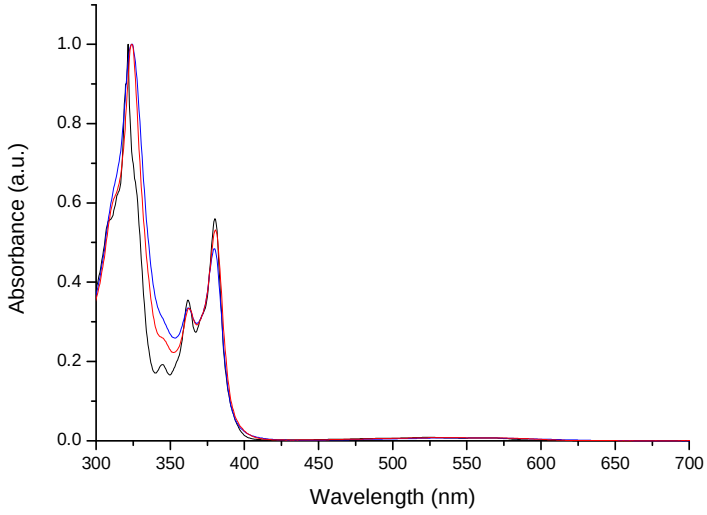


Figure S1. Absorption spectra of **LPP(=O)$_2$** (300/700 nm) in cyclohexane (black line), in THF (red line) and in ethanol (blue line

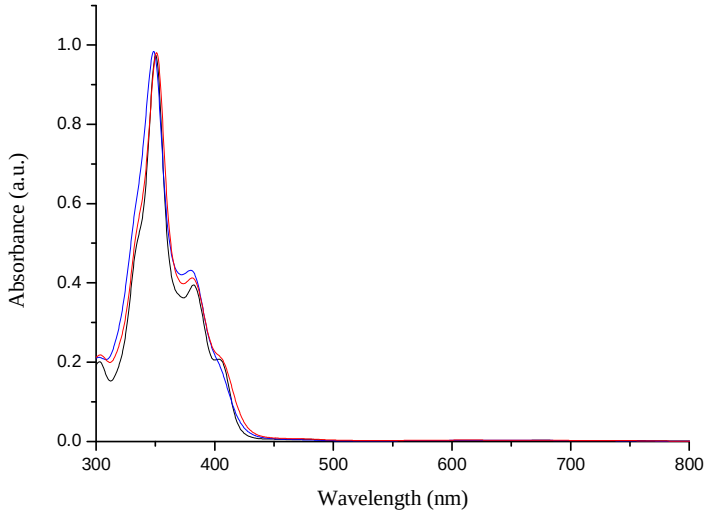


Figure S2. Absorption spectra of **LPP(=C(CN)$_2$)$_2$** (300/850 nm range) in cyclohexane (black line), in THF (red line) and in ethanol (blue line)

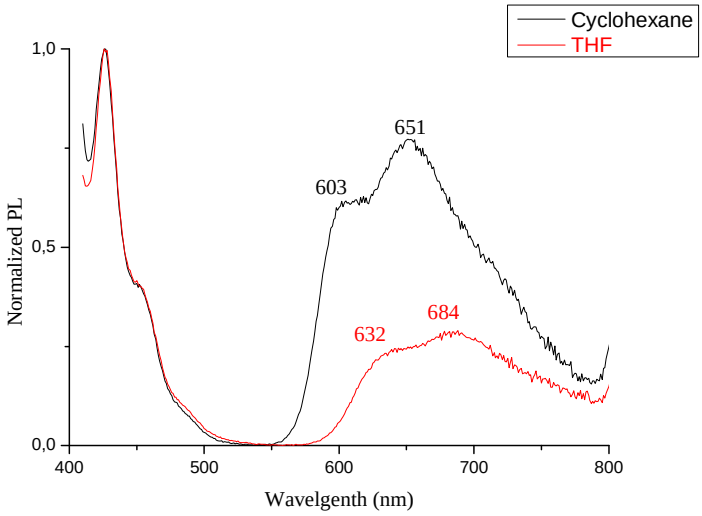


Figure S3. Fluorescence spectra of **4** in cyclohexane and in THF (λexc = 400 nm)

THEORETICAL MODELING

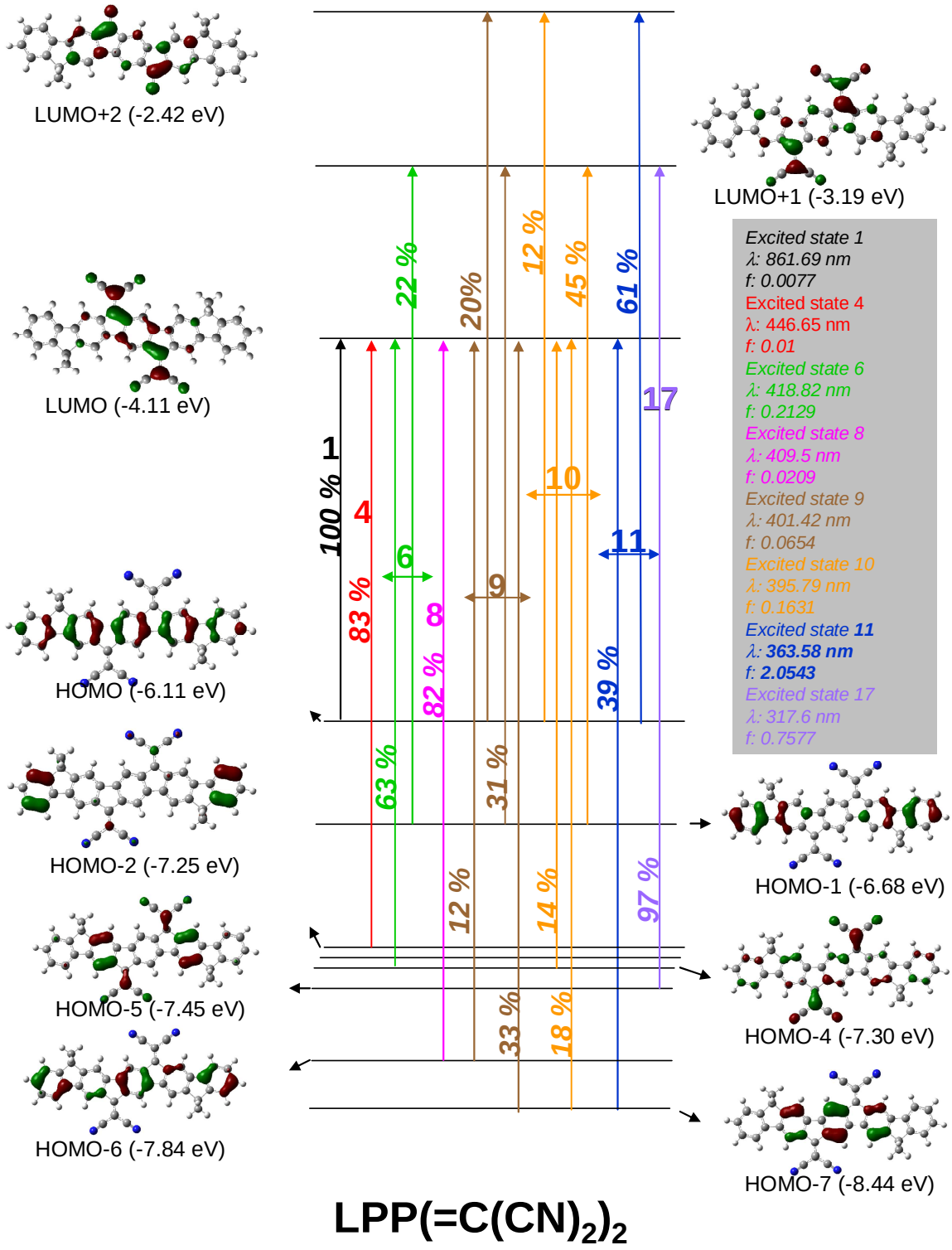


Figure S4. Calculated frontier molecular orbitals by DFT and the 6th first calculated electronic transitions by TD-DFT of **LPP(C=(CN)$_2$)$_2$**, after geometry optimization with DFT B3LYP/6-311G+(d,p), shown with a cut-off 0.04 [e bohr^{-3}]$^{1/2}$

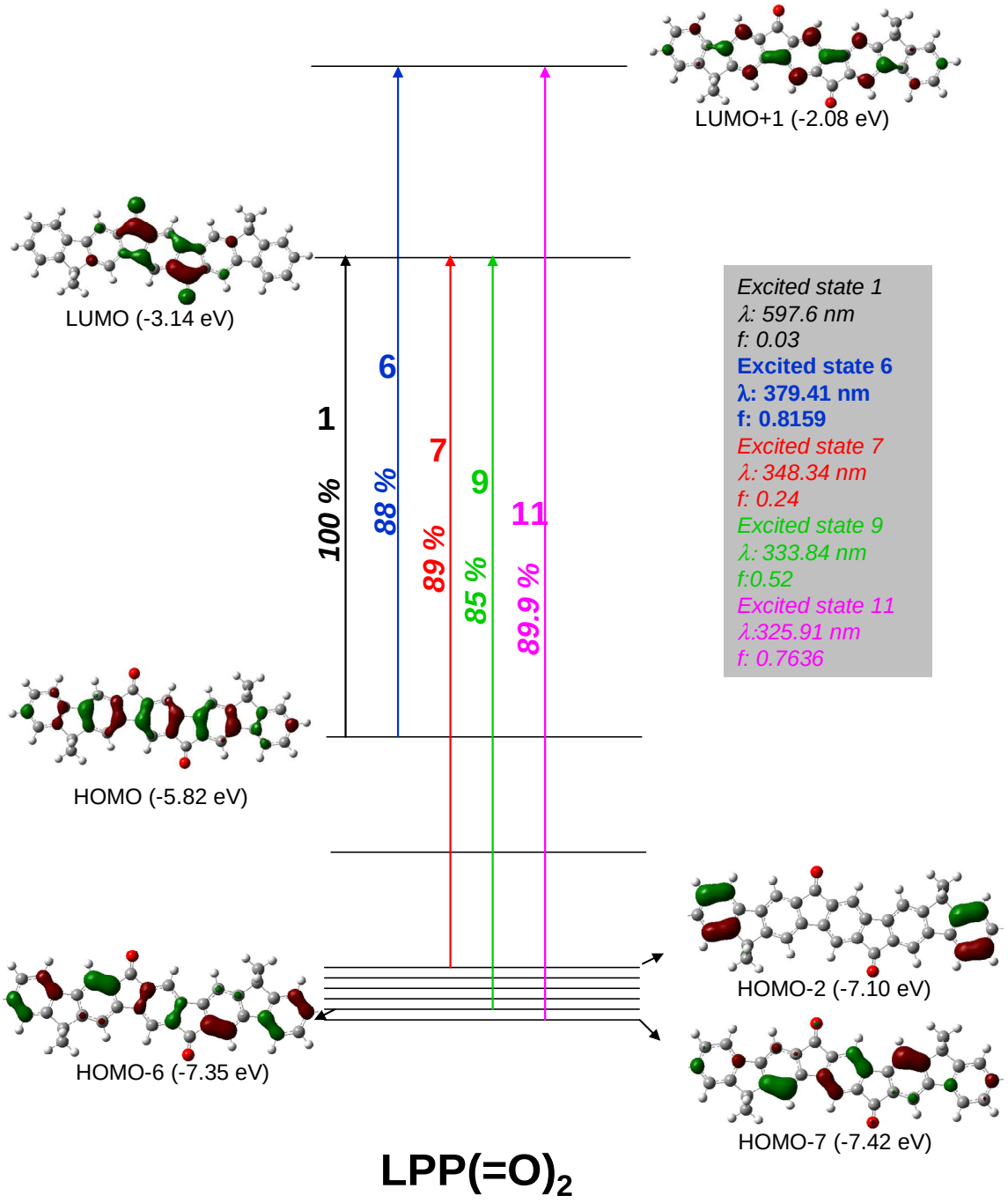


Figure S5: Calculated frontier molecular orbitals by DFT and the 6th first calculated electronic transitions by TD-DFT of **LPP(=O)$_2$**, after geometry optimization with DFT B3LYP/6-311G+(d,p), shown with a cut-off 0.04 [e bohr^{-3}]$^{1/2}$

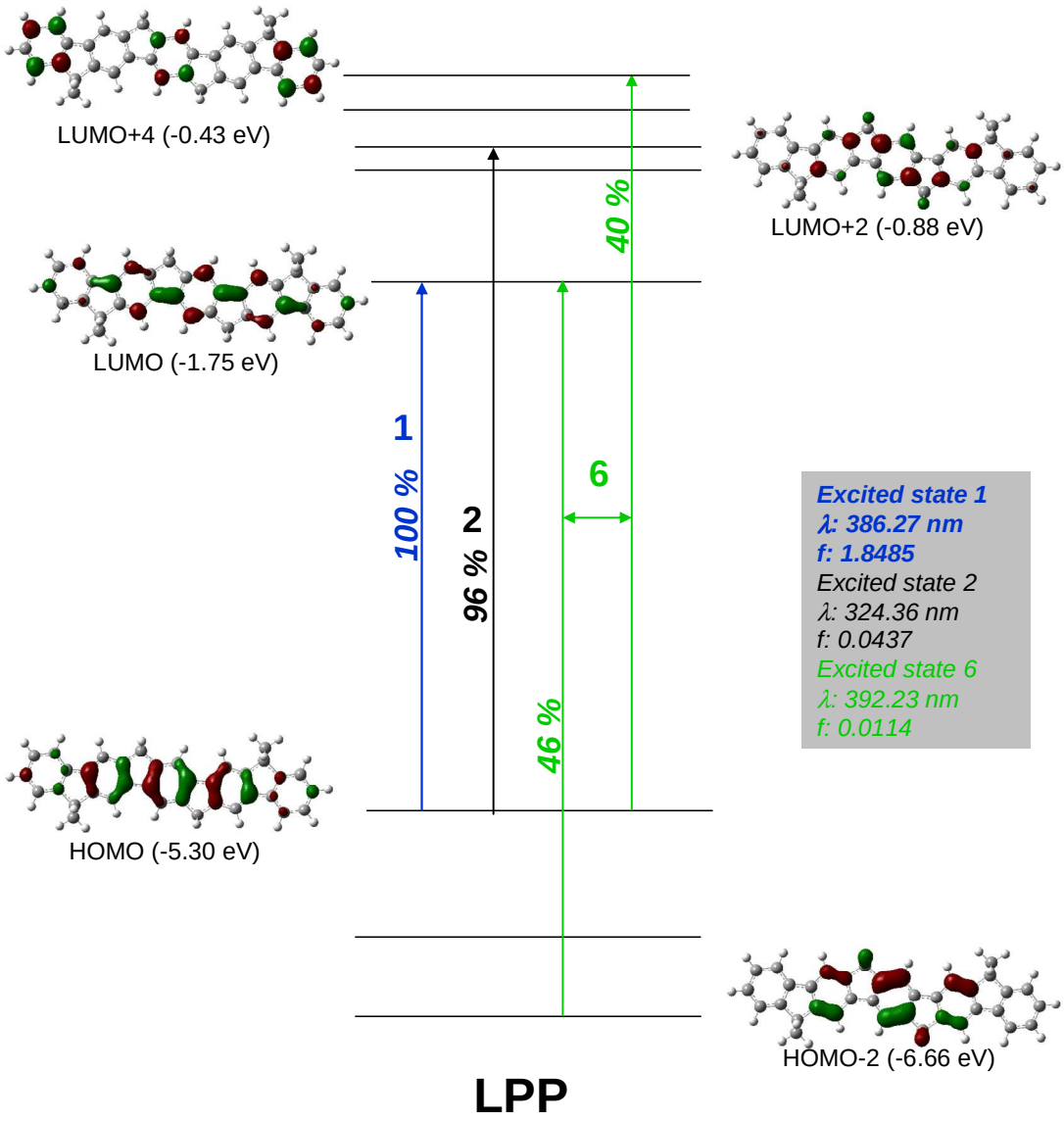
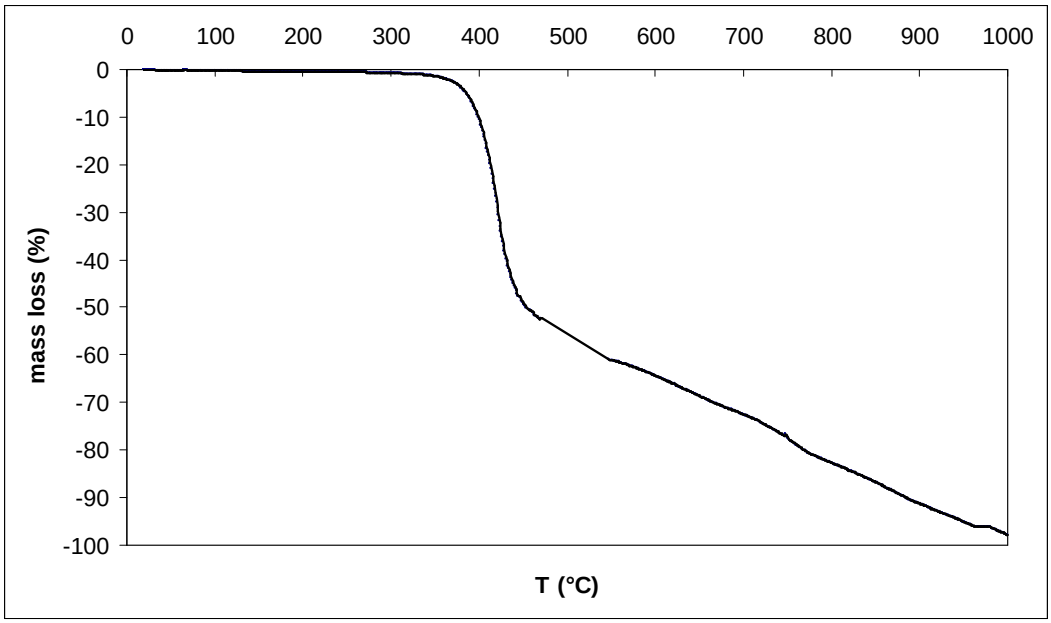


Figure S6: Calculated frontier molecular orbitals by DFT and the 6th first calculated electronic transitions by TD-DFT of **LPP**, after geometry optimization with DFT B3LYP/6-311G+(d,p), shown with a cut-off 0.04 [e bohr^{-3}]$^{1/2}$

THERMAL ANALYSES

LPP(=O)$_2$



***Td*=385°C**

Fig S7: ATG curve of **LPP(=C(CN)$_2$)$_2$**

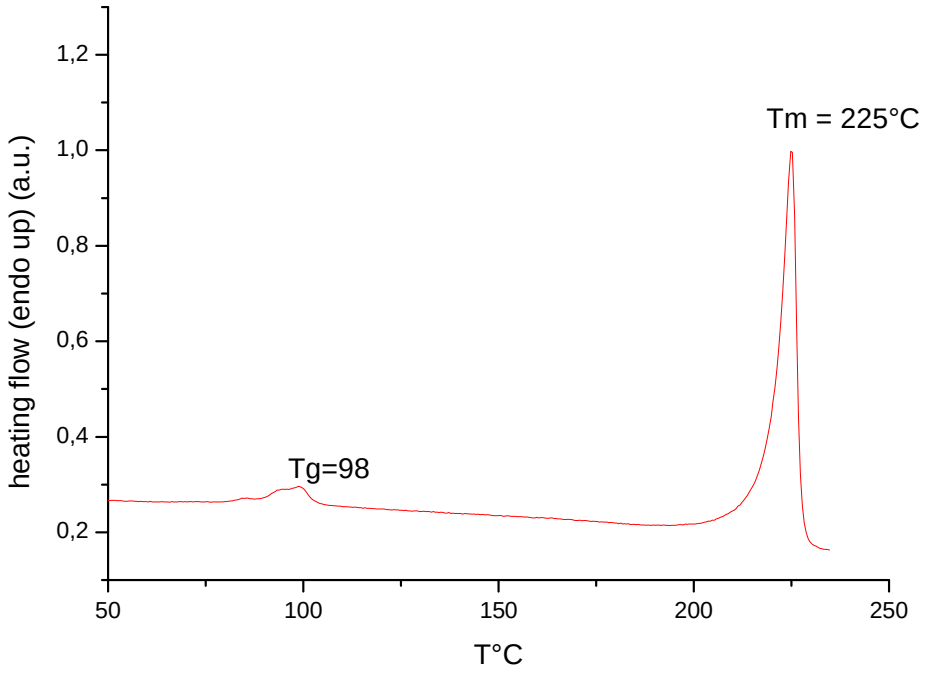


Fig S8: DSC curve (second heating cycle) of **LPP(=O)$_2$**

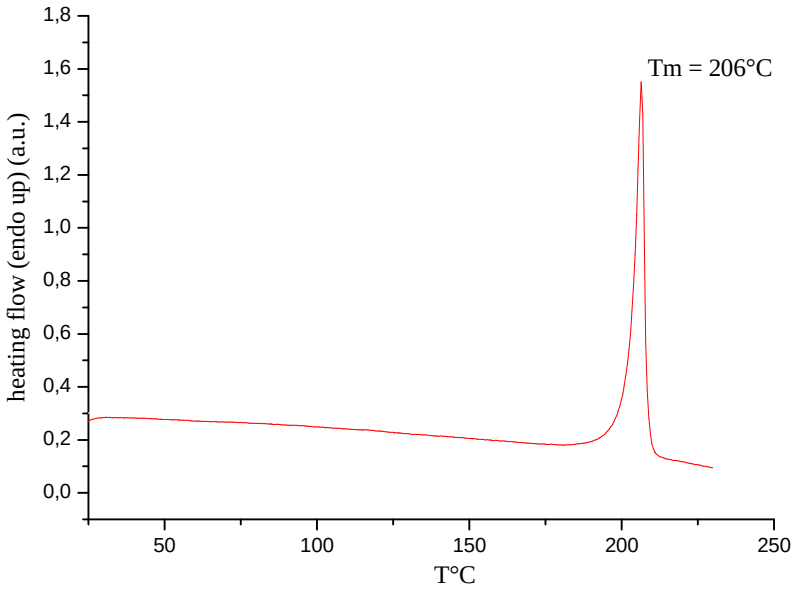
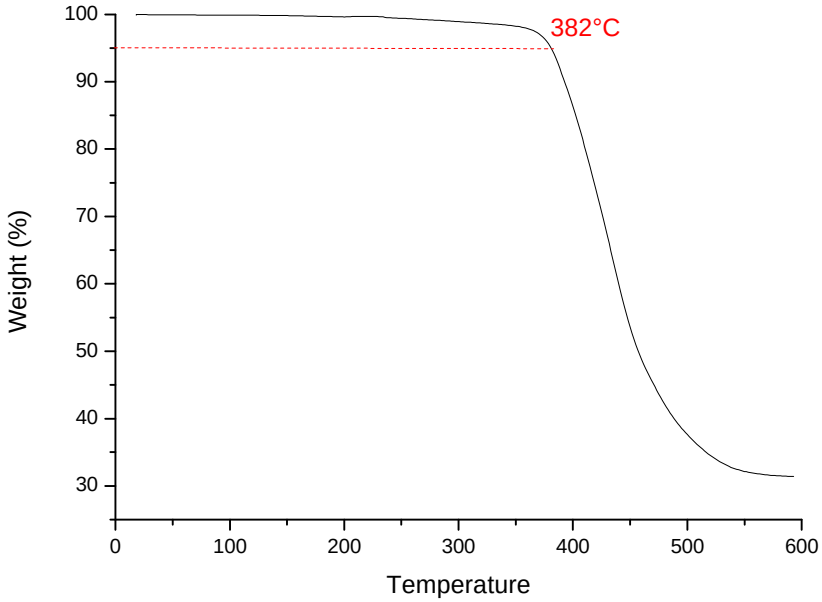


Fig S9: DSC curve (second heating cycle) of **LPP(=C(CN)$_2$)$_2$**



***Td*=382°C**

Fig S10: ATG curve of **LPP(=C(CN)$_2$)$_2$**

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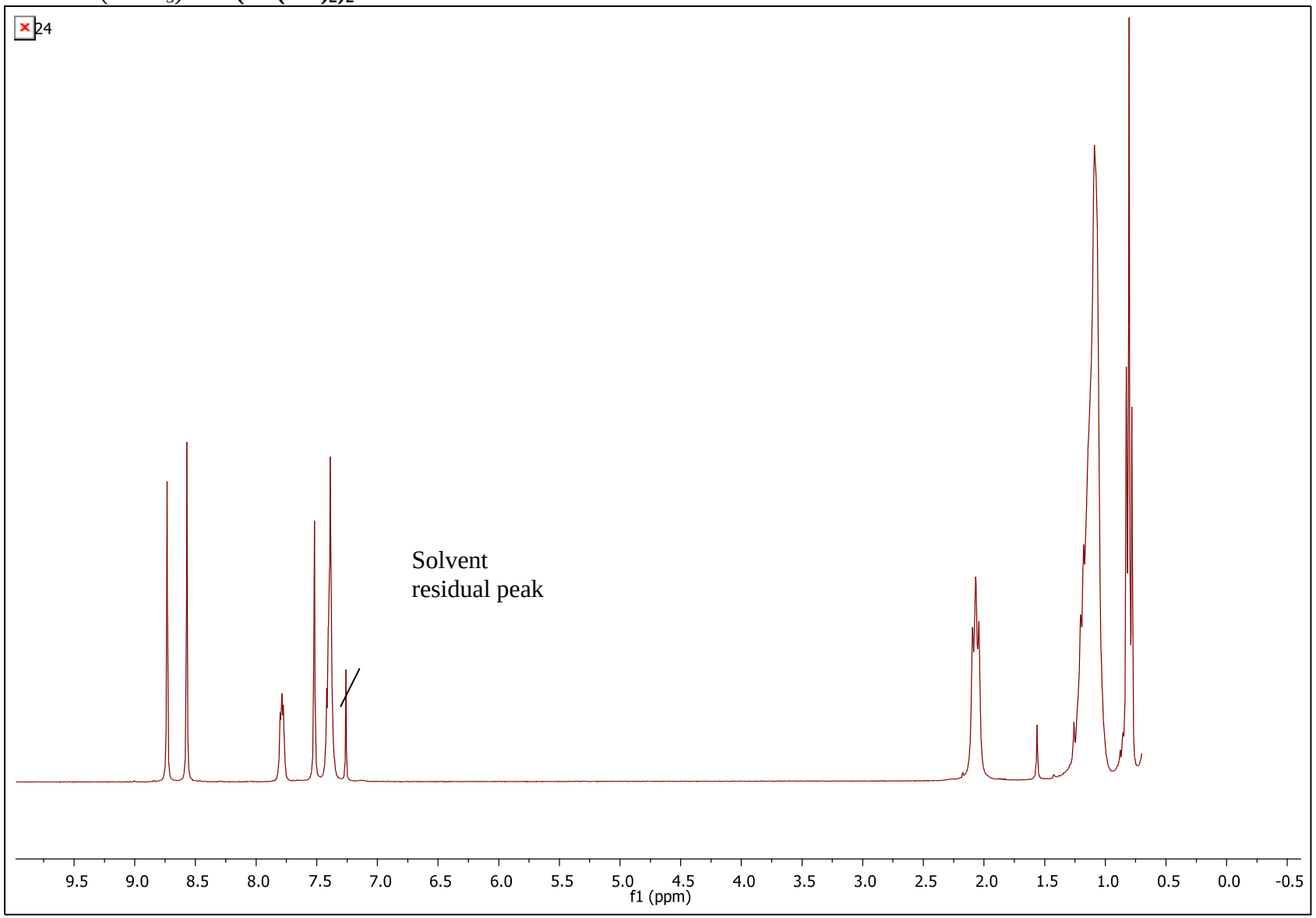
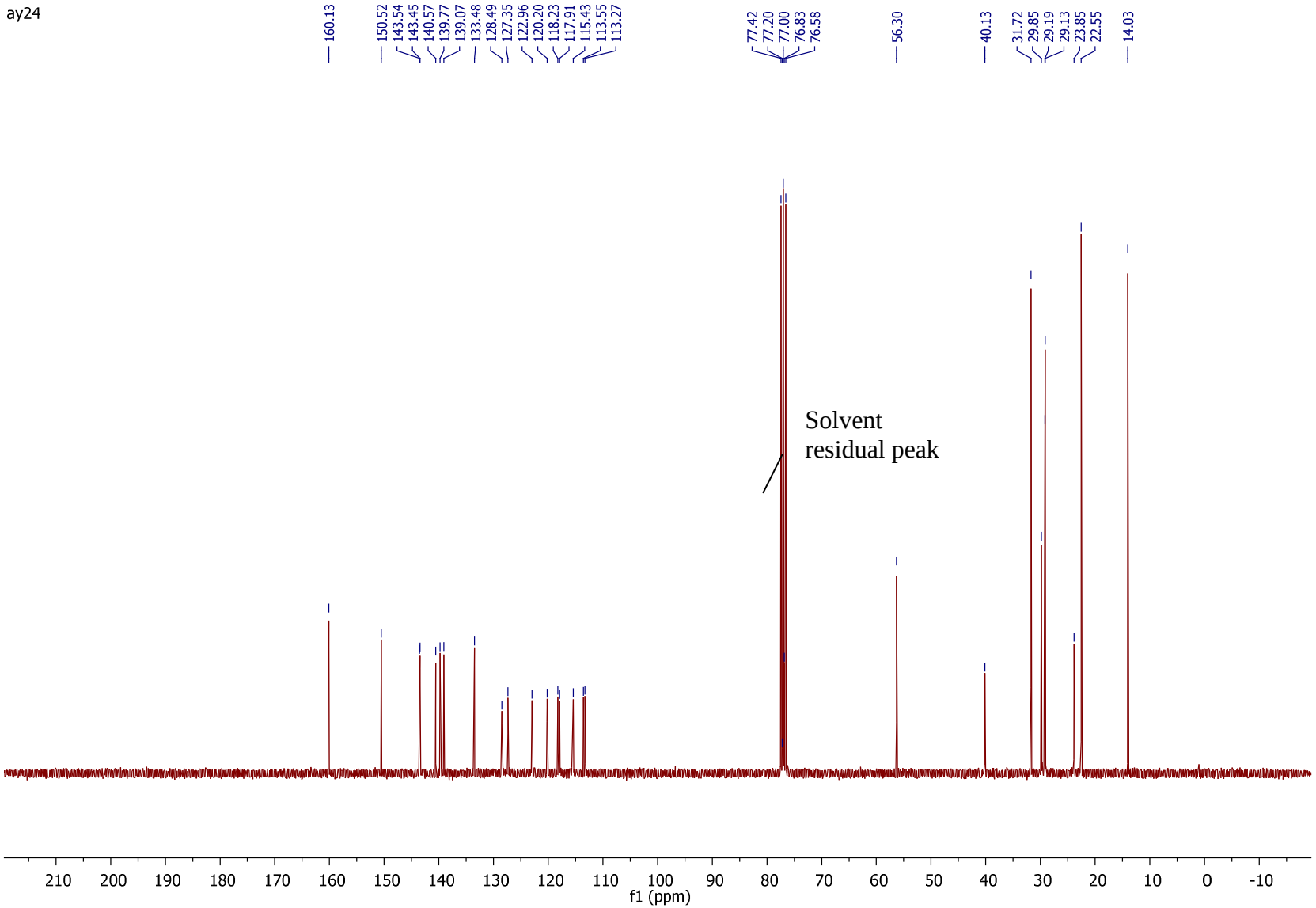
Copy of NMR spectra

^{1}H NMR ($CDCl_3$) **LPP(C=(CN)$_2$)$_2$**



^{13}C NMR ($CDCl_3$) **LPP(C=(CN)$_2$)$_2$**



DEPT ($CDCl_3$) **LPP(C=(CN)$_2$)$_2$**