

# Synthesis, Covalency Sequence and Crystal features of Pentagonal Uranyl Acylpyrazolone complexes along with DFT calculation and Hirshfeld analysis

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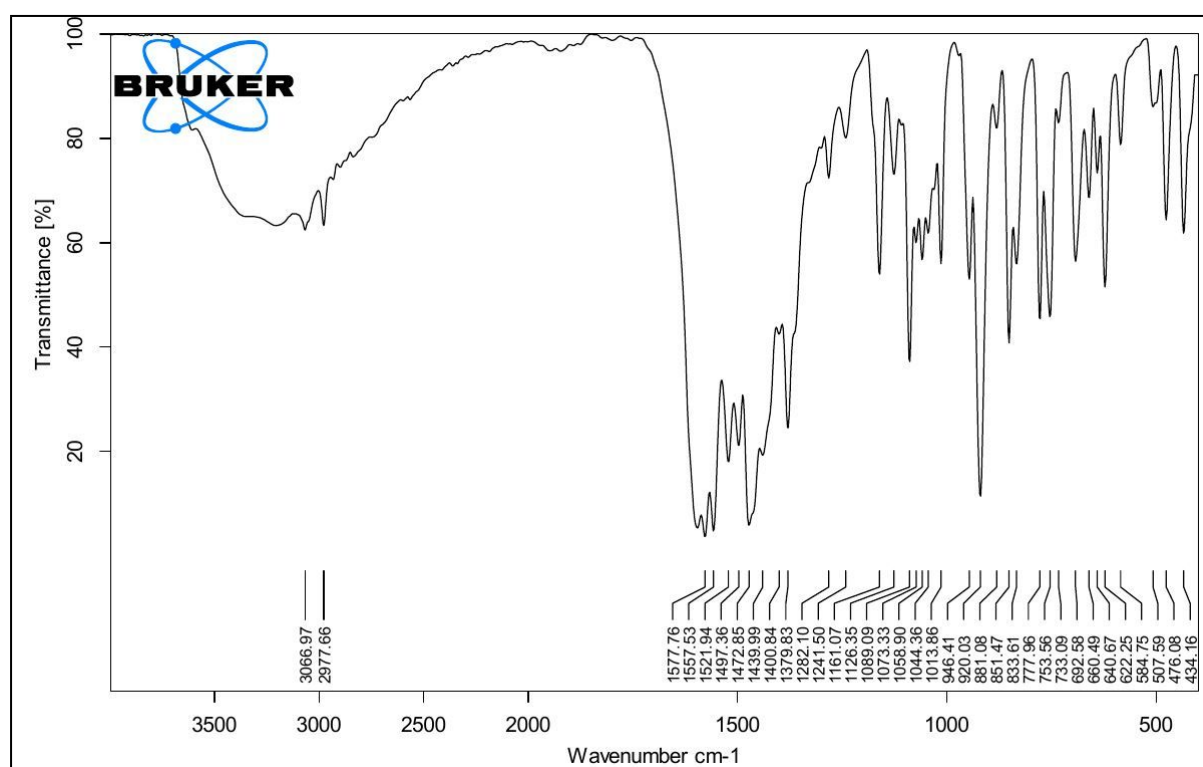
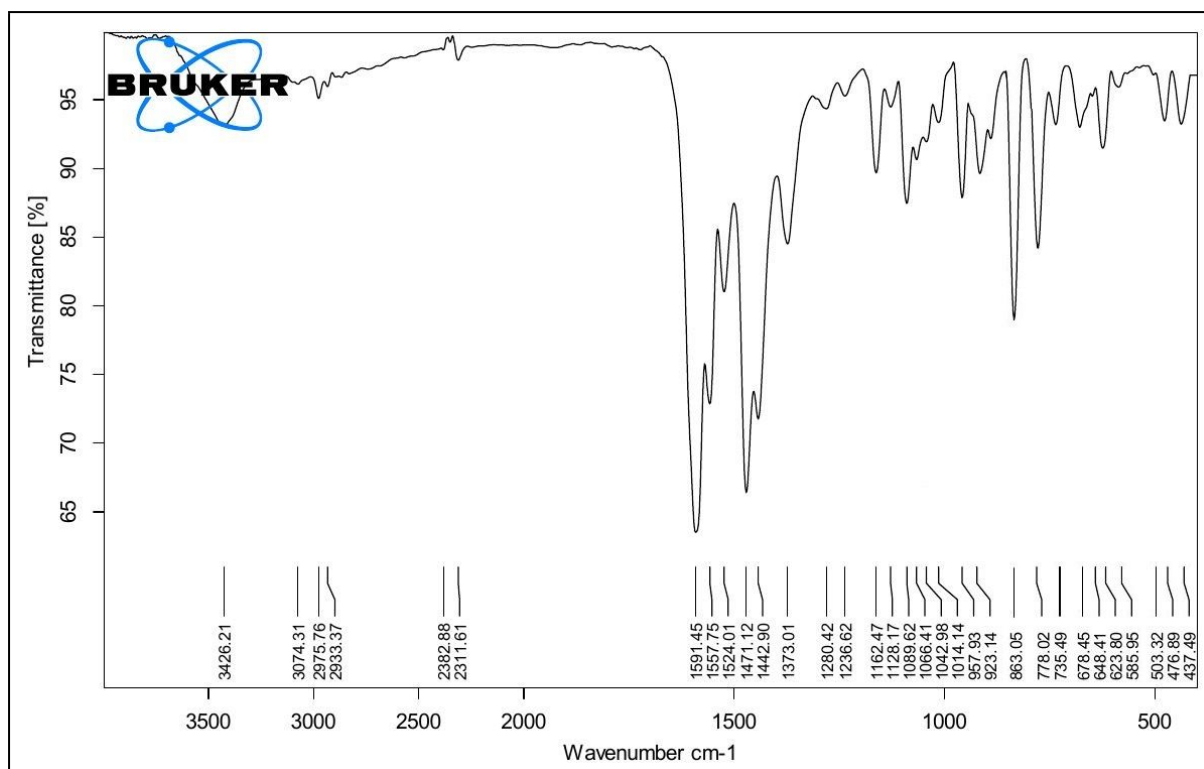
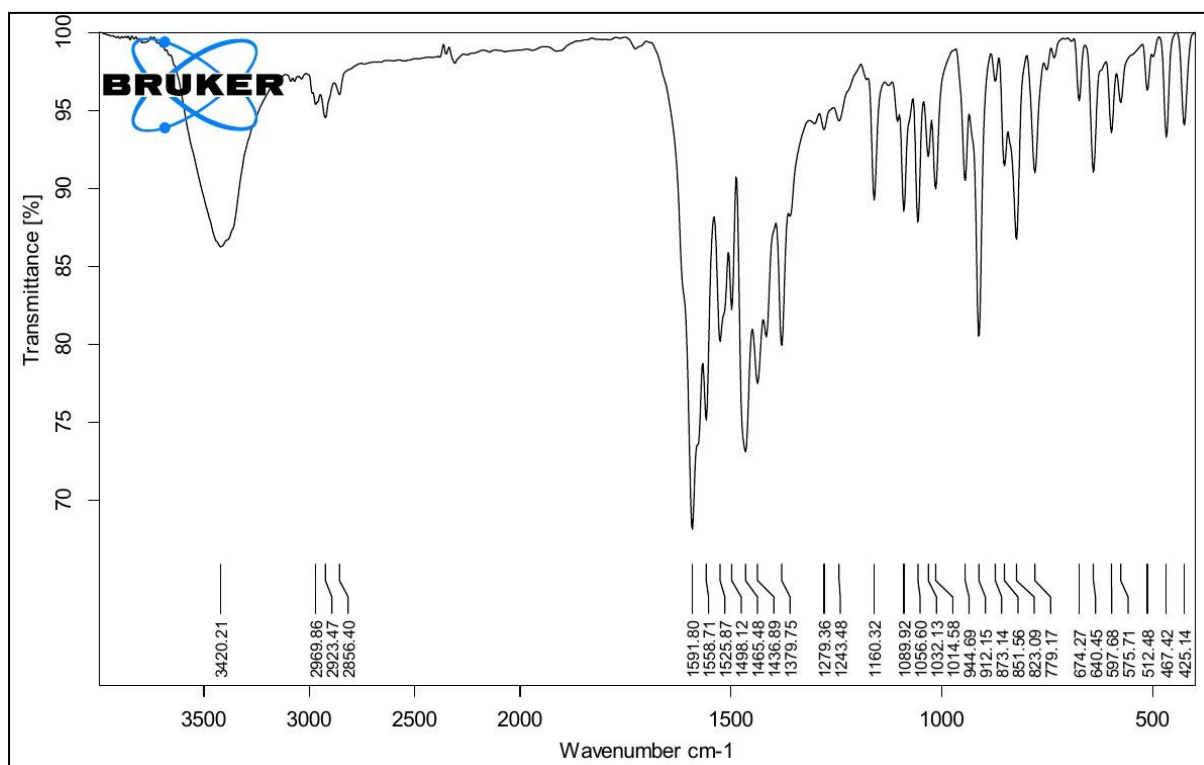


Figure S1 FTIR spectrum of complex I

## Supporting Information



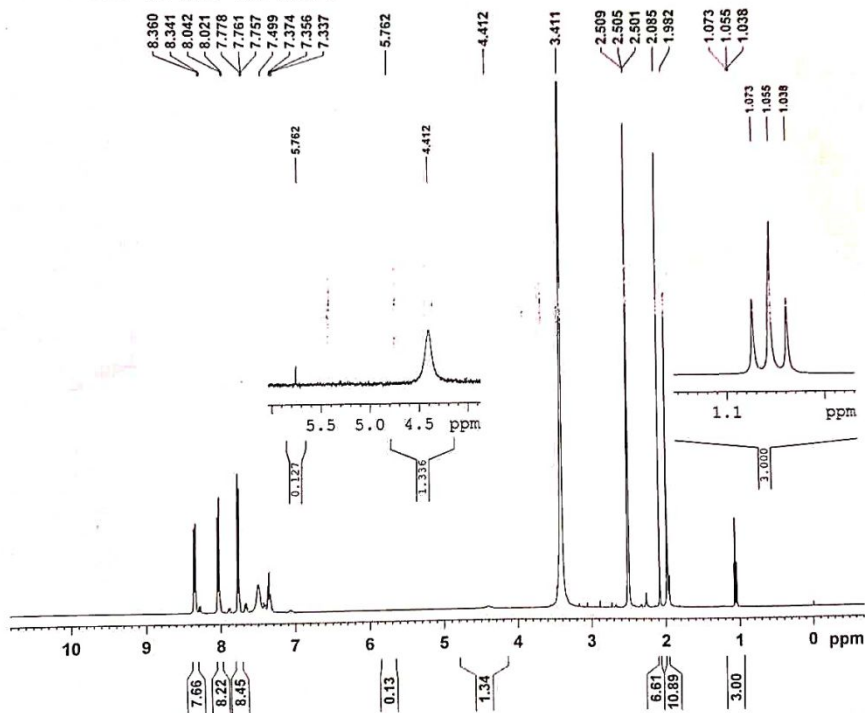
**Figure S2** FTIR spectrum of complex II



**Figure S3** FTIR spectrum of complex III

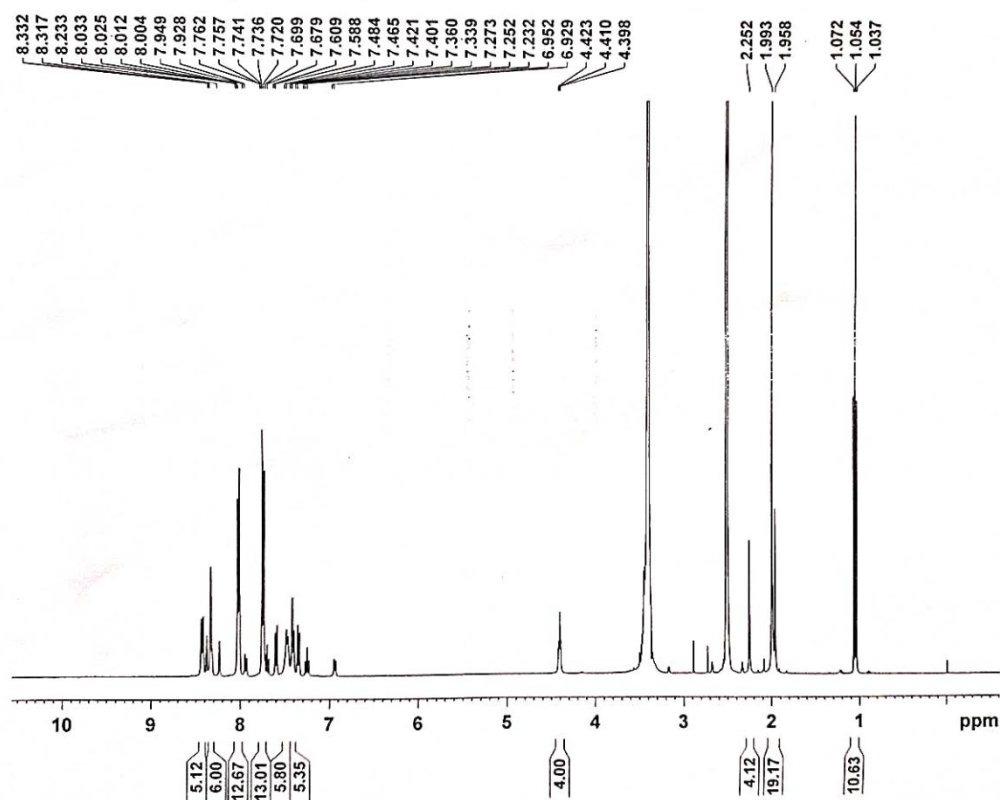
# Supporting Information

UL1 MAITREY 1H 26-08-2021  
 PROTON DMSO {D:\SRC} MSU-Chem 1



**Figure S4**  $^1\text{H-NMR}$  spectrum of complex I

UL2 MAITREY DMSO 1H 08-09-2021  
 PROTON DMSO {D:\ASD} MSU-Chem 1



**Figure S5**  $^1\text{H-NMR}$  spectrum of complex II

# Supporting Information

UL3 MAITREY 9-12-2021  
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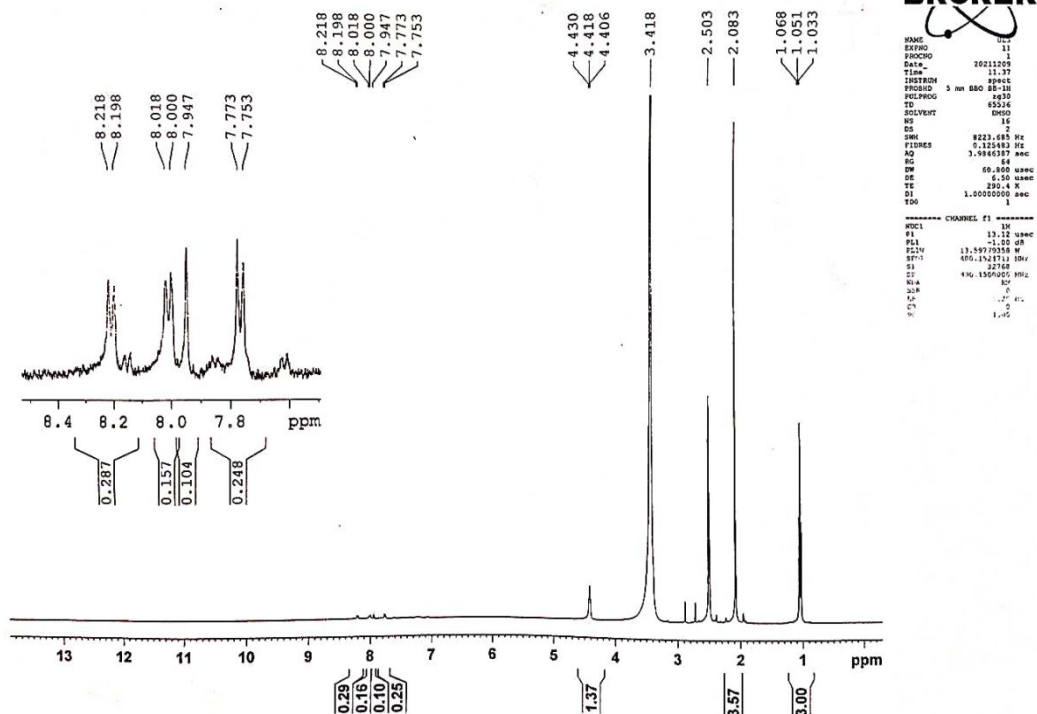


Figure S6 <sup>1</sup>H-NMR spectrum of complex III

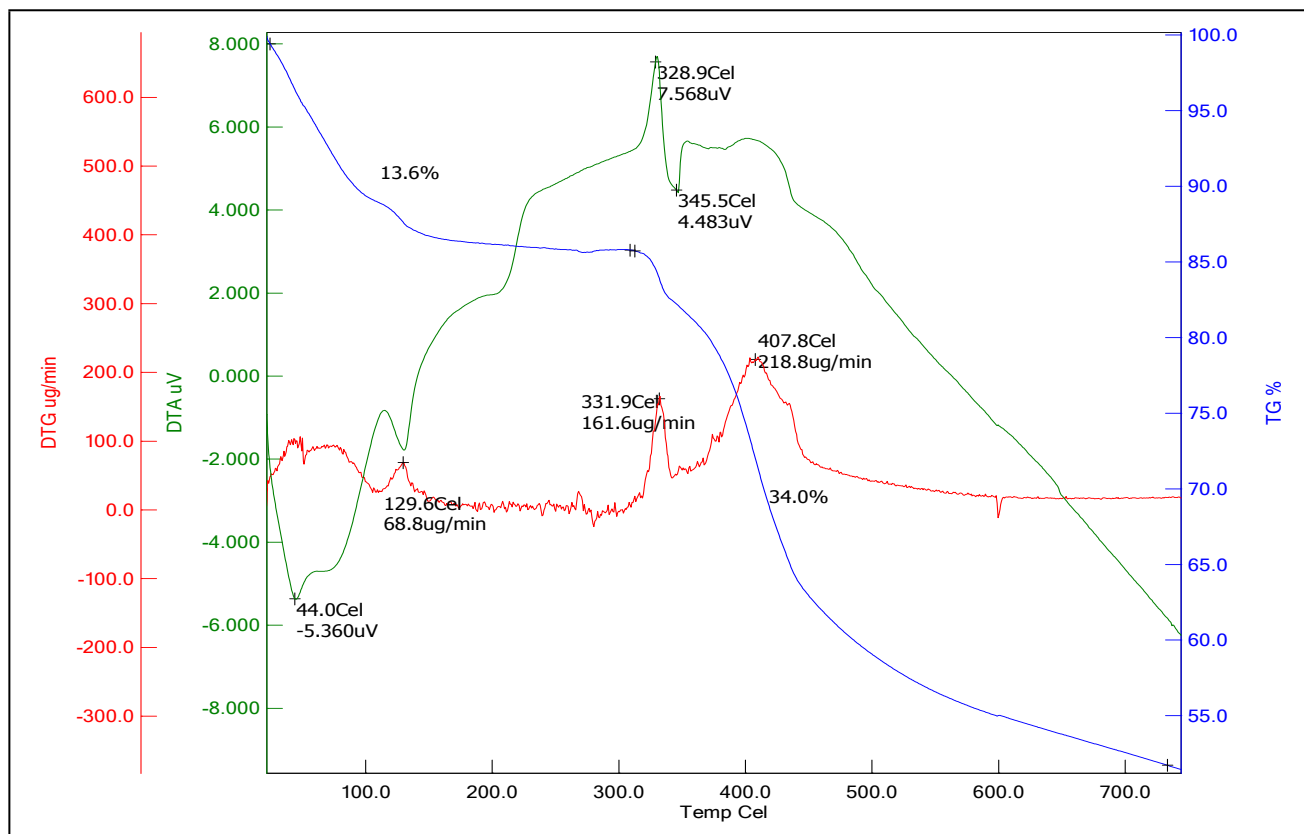


Figure S7 TG-DTA plot of complex I

## Supporting Information

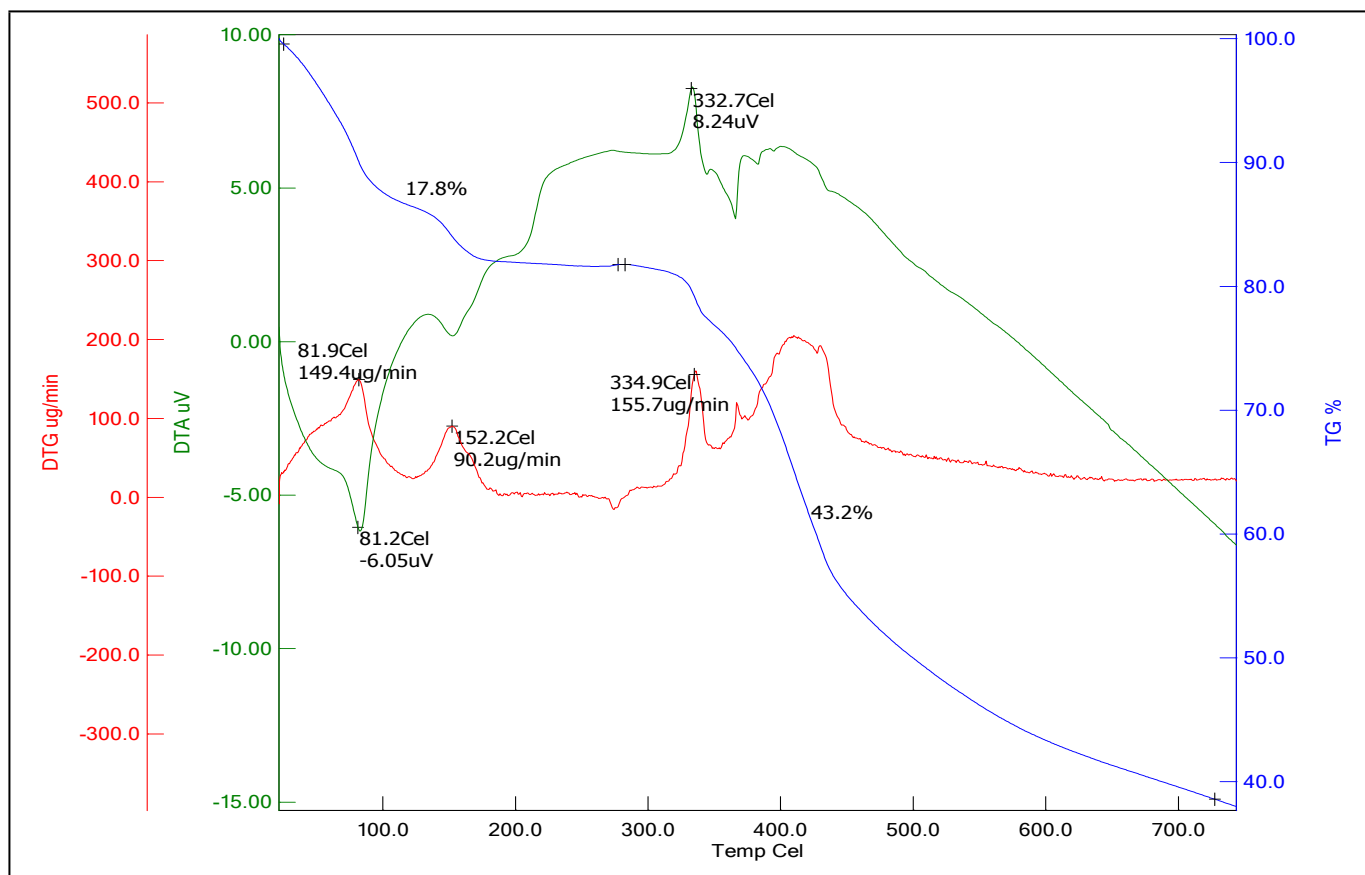


Figure S8 TG-DTA plot of complex II

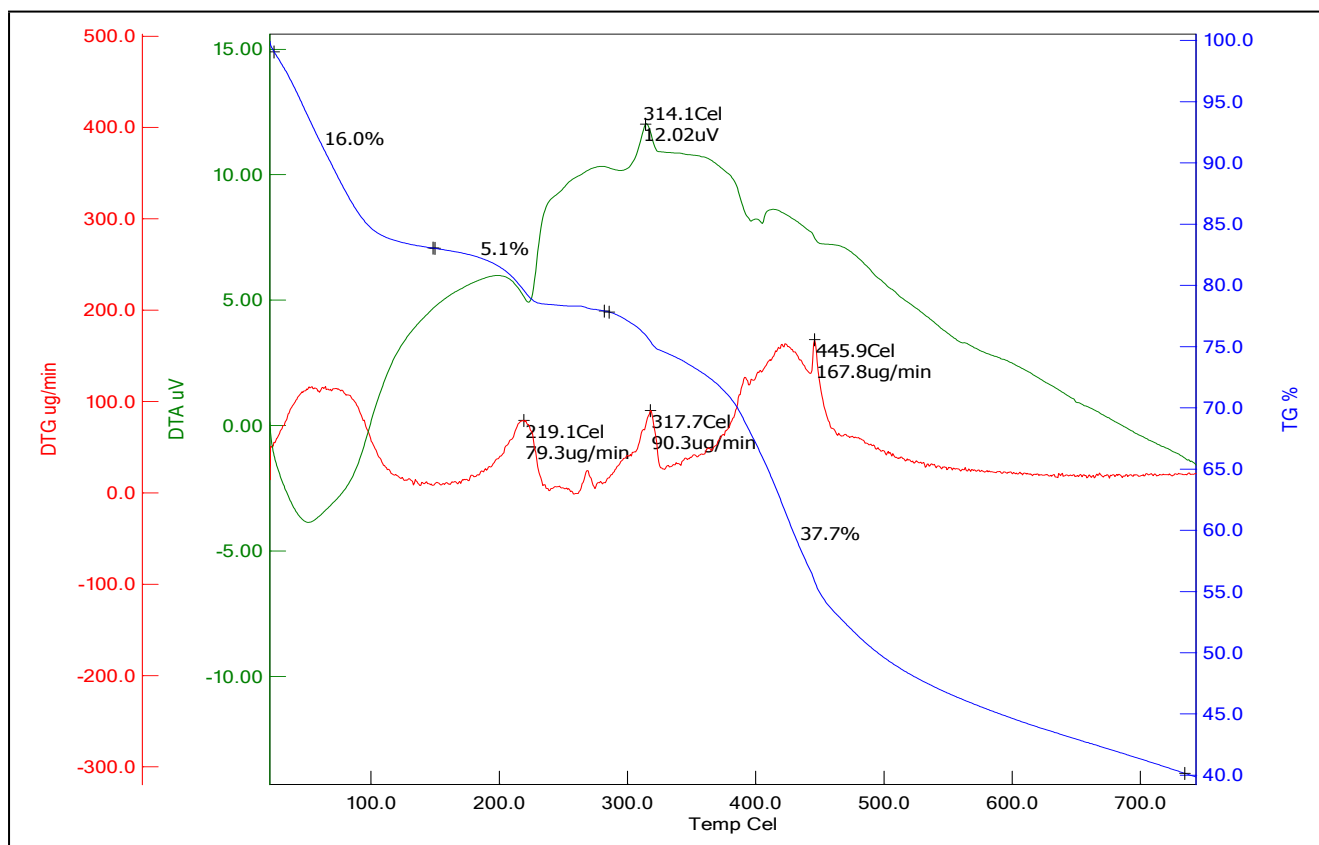


Figure S9 TG-DTA plot of complex III

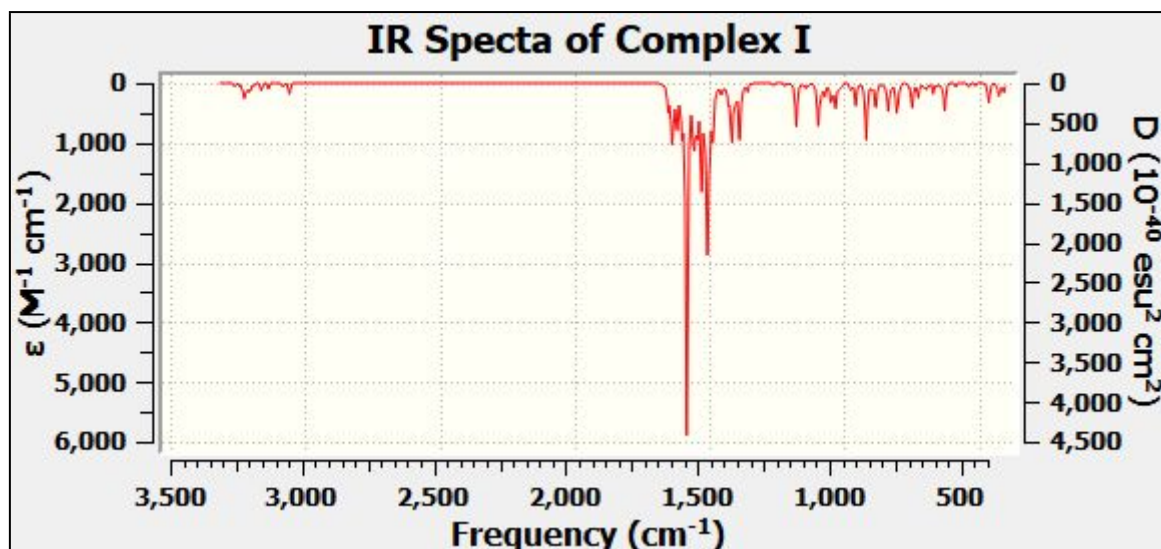


Figure S10 FTIR spectrum of complex I through computational analysis

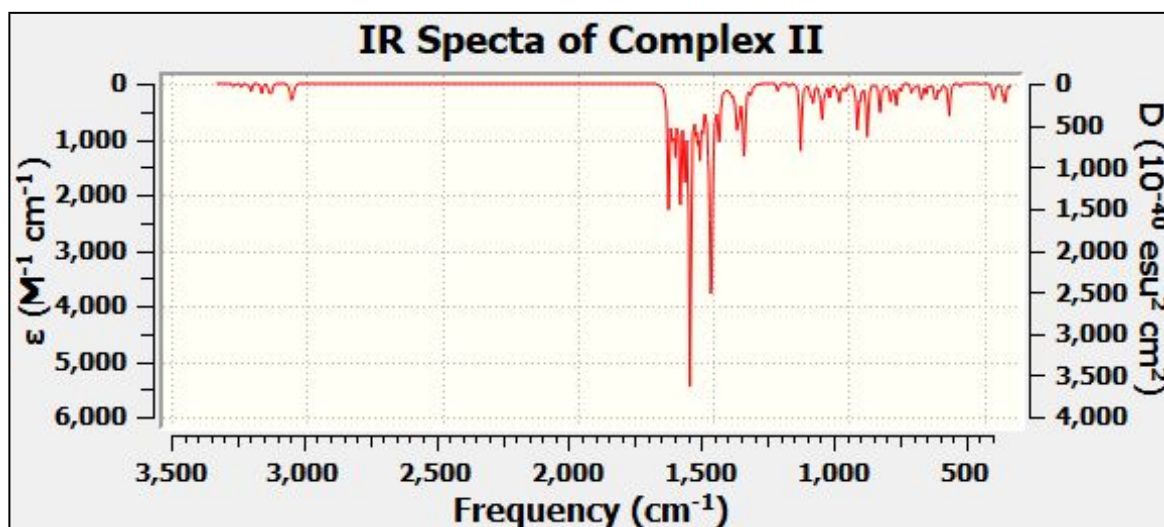


Figure S11 FTIR spectrum of complex II through computational analysis

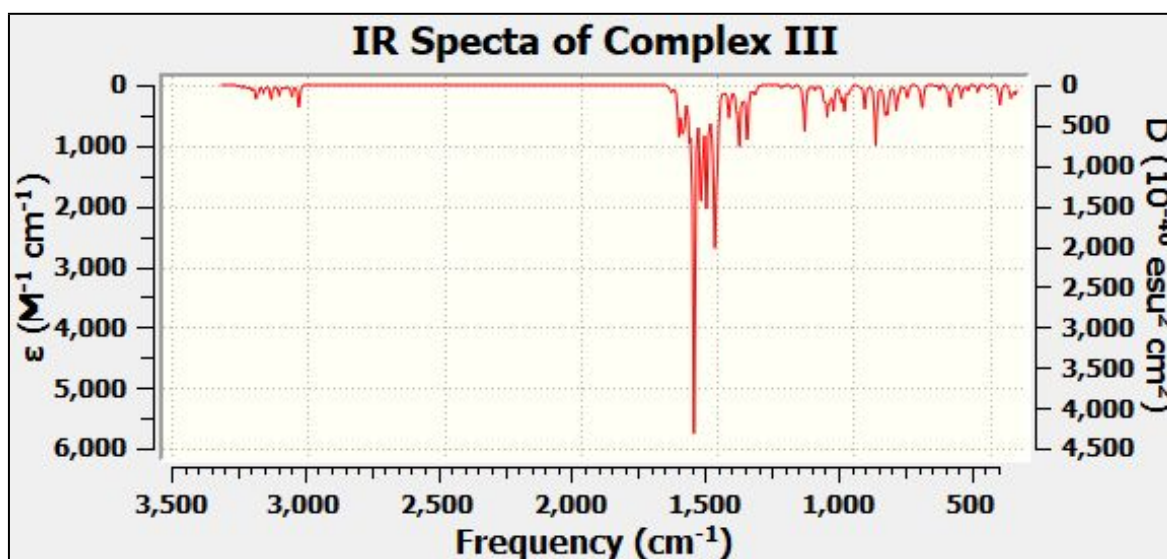
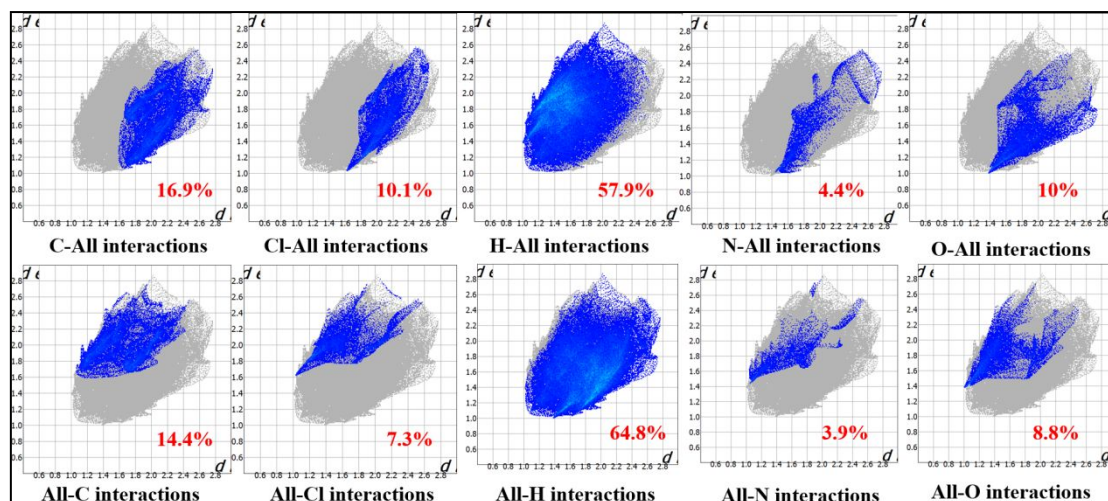
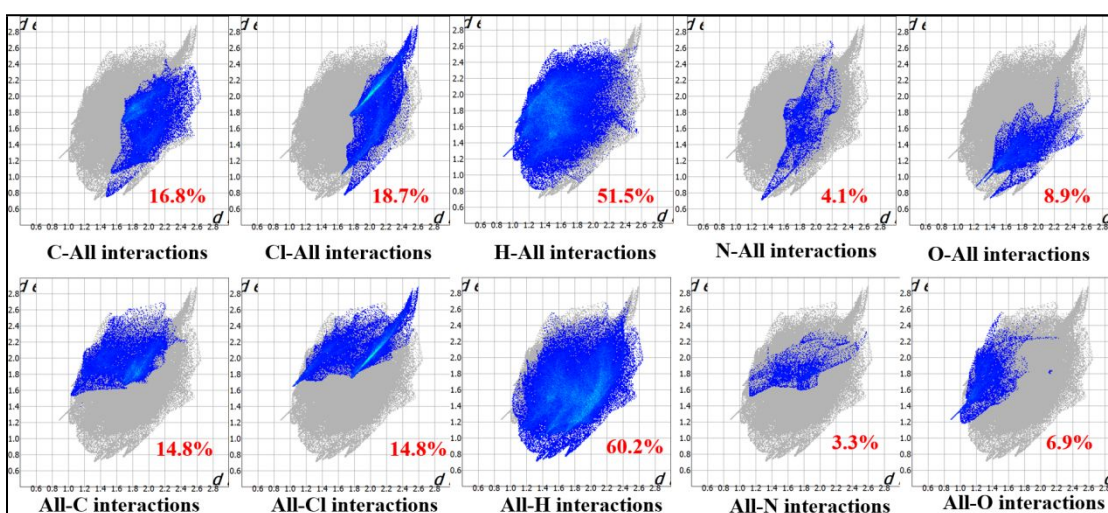


Figure S12 FTIR spectrum of complex III through computational analysis

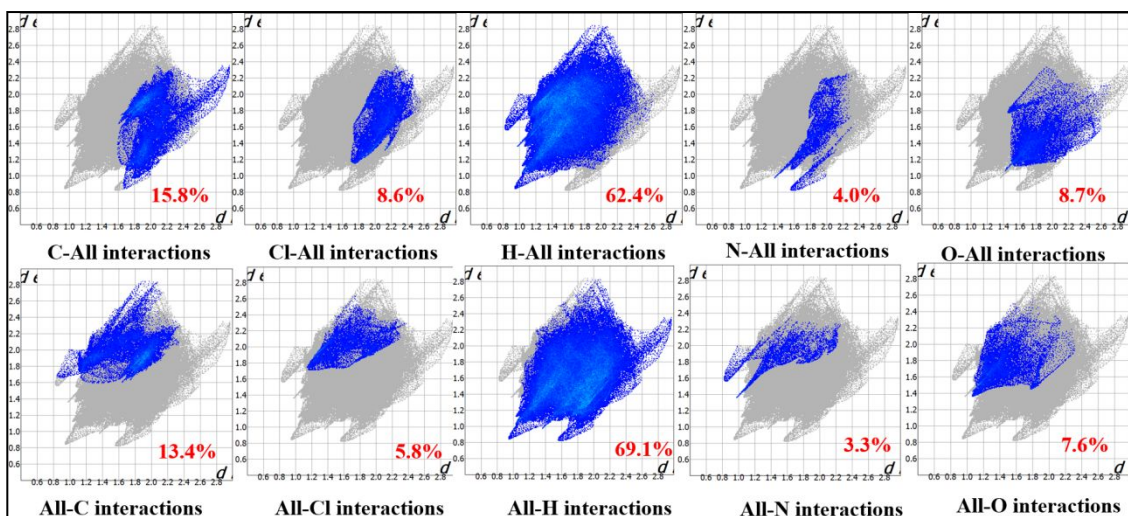
## Supporting Information



**Figure S13** Two dimensional fingerprint plots for atom-all and all-atom interactions in complex I



**Figure S14** Two dimensional fingerprint plots for atom-all and all-atom interactions in complex II



**Figure S15** Two dimensional fingerprint plots for atom-all and all-atom interactions in complex III