Regulating vibrational mode to improve quantum efficiency, insights from theoretical calculations on irid- ium(III) complexes bearing tridentate NCN and NNC chelates

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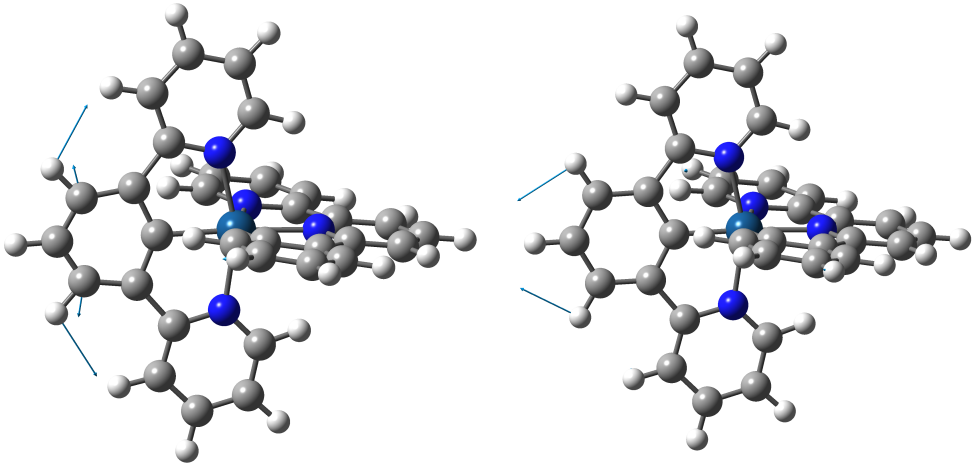
Supplementary Information



(a) mode 94 **(b)** mode 101

Figure ESI-1 The swing vibration modes of hydrogen atoms at the 3,5 position of benzene on NCN ligand.

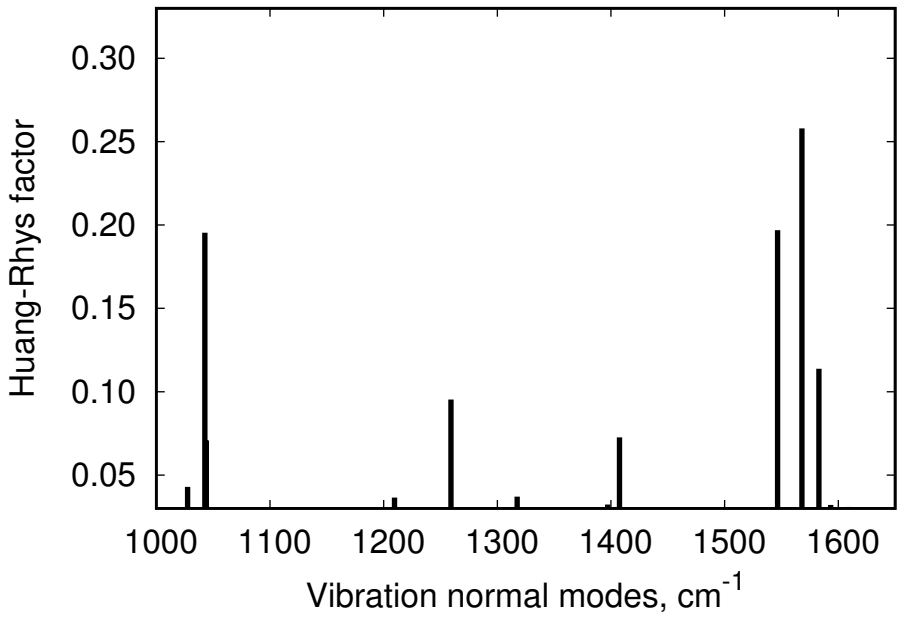


Figure ESI-2 Huang-Rhys factor vs vibration normal modes, for **Ir-0**.

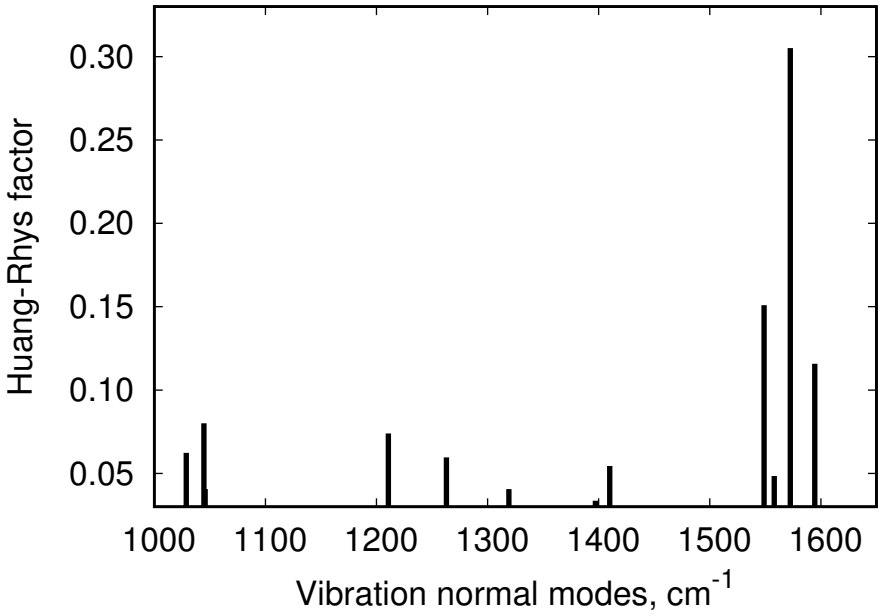


Figure ESI-3 Huang-Rhys factor vs vibration normal modes, for **Ir-1**.

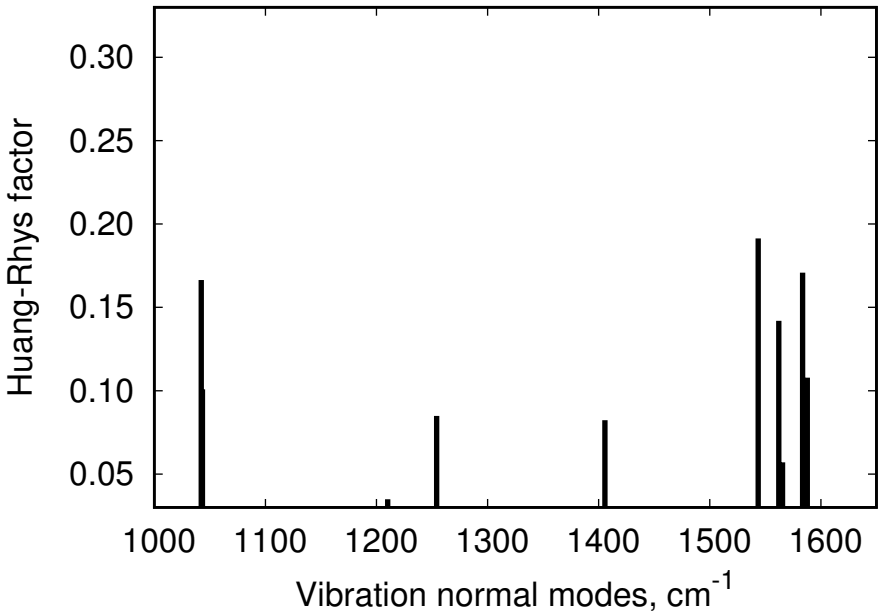


Figure ESI-4 Huang-Rhys factor vs vibration normal modes, for **Ir-2**.

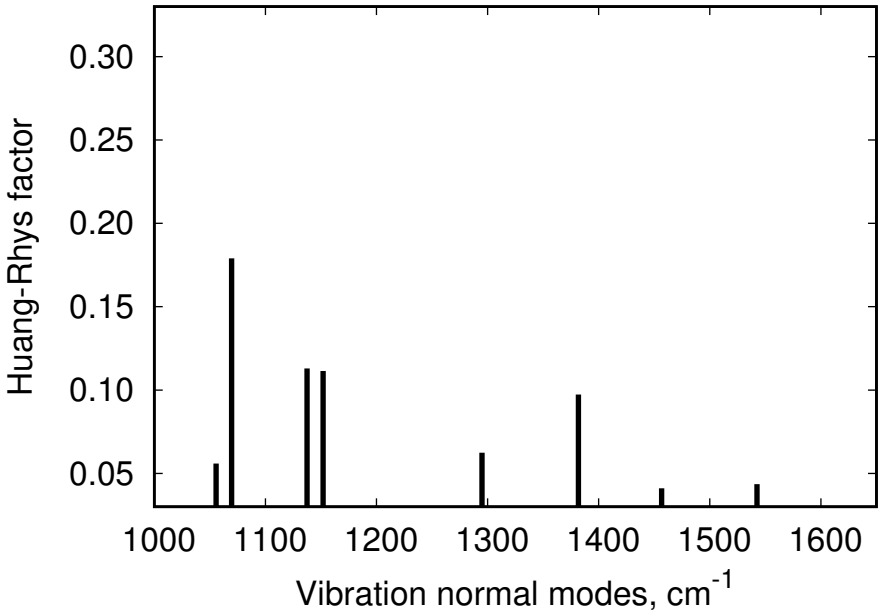


Figure ESI-5 Huang-Rhys factor vs vibration normal modes, for **Ir-3**.

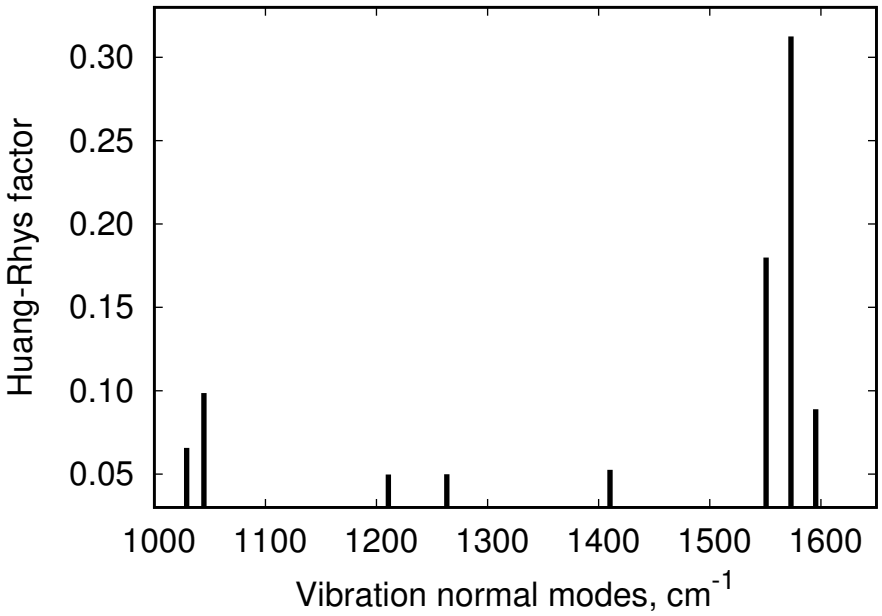
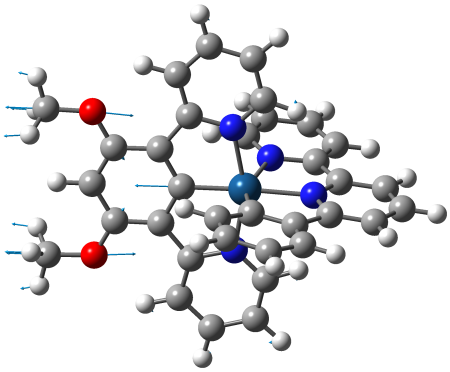
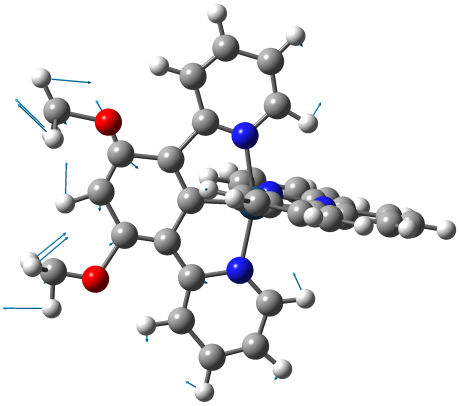


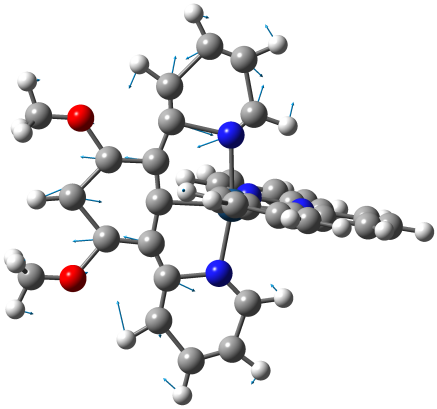
Figure ESI-6 Huang-Rhys factor vs vibration normal modes, for **Ir-4**.



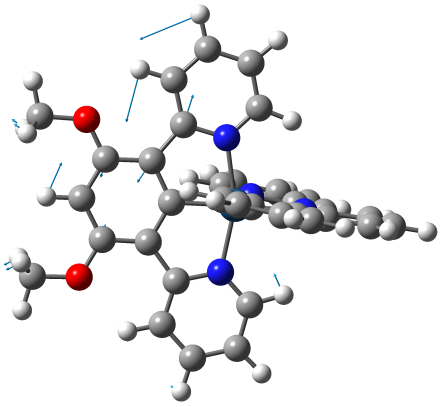
(a) mode 104



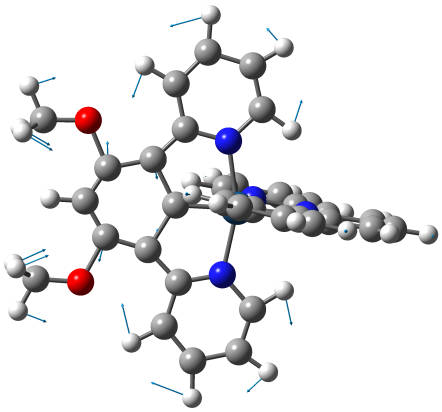
(b) mode 124



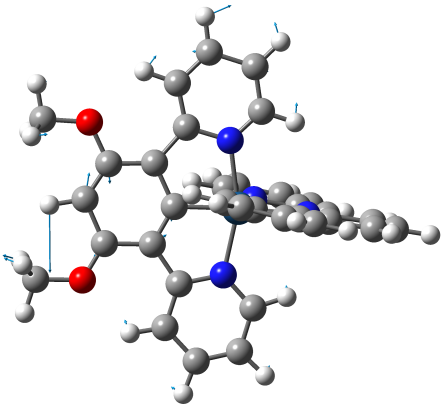
(c) mode 130



(d) mode 136



(e) mode 141



(f) mode 163

Figure ESI-7 Extra stretching vibration mode introduced by CH_3O group, in **Ir-2**.