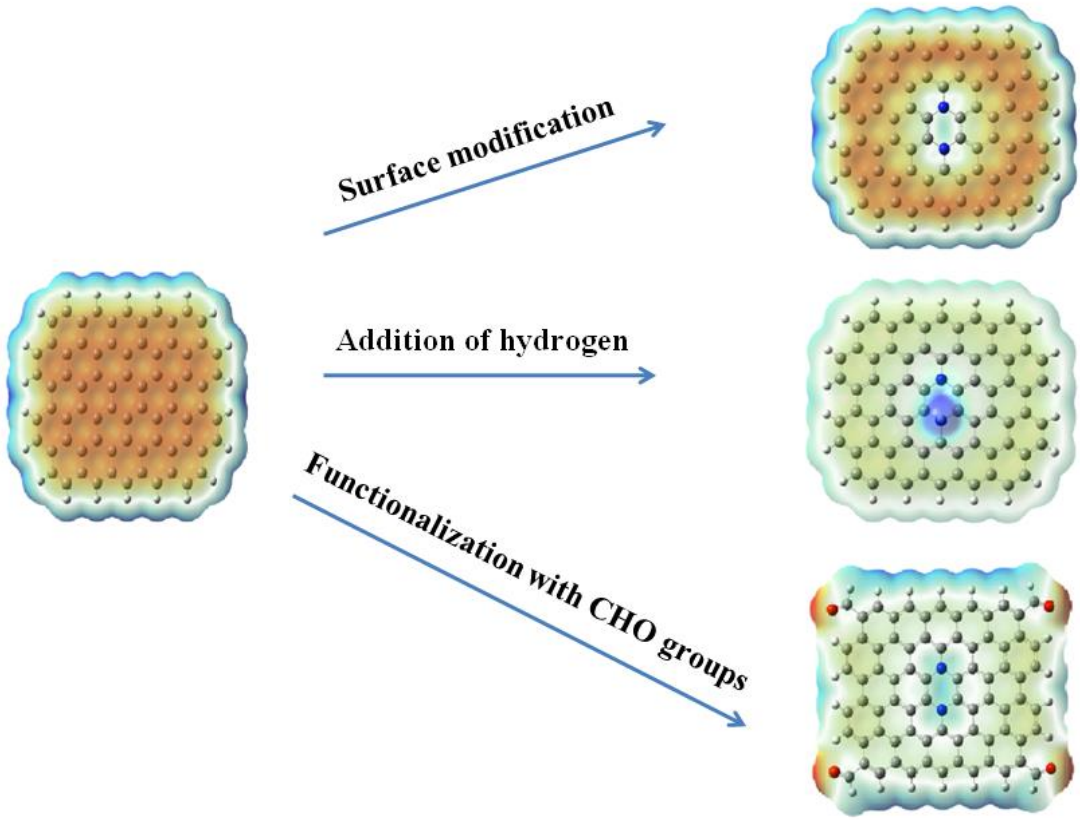
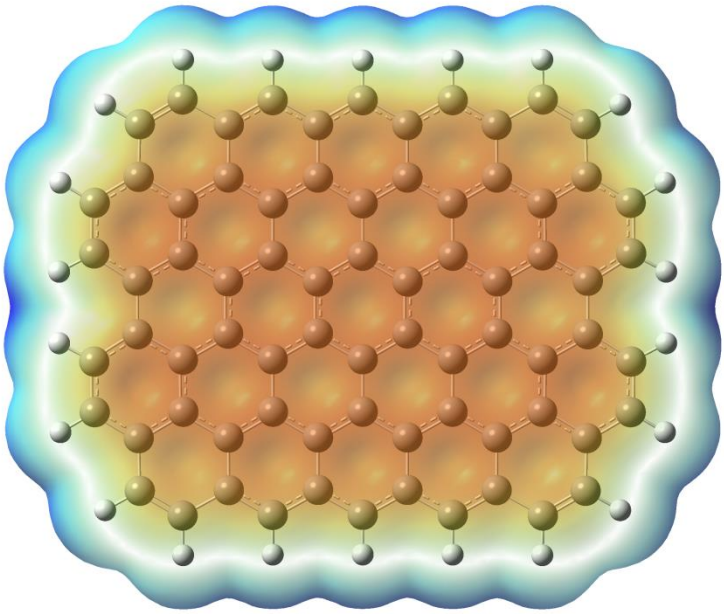
Graphical Abstract

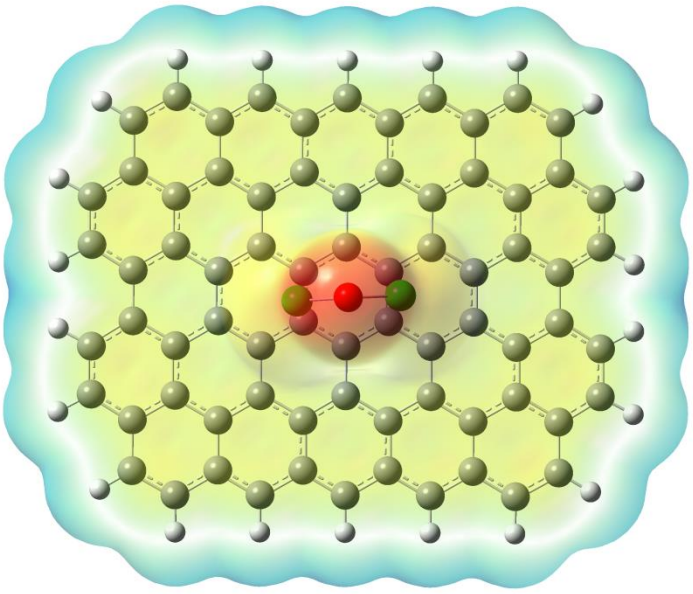


Surface modification of the graphene sheet with heteroatoms, addition of hydrogen atom, and functionalization with CHO groups at edges alter charge distribution and assist to better adsorption of phosgene on it.

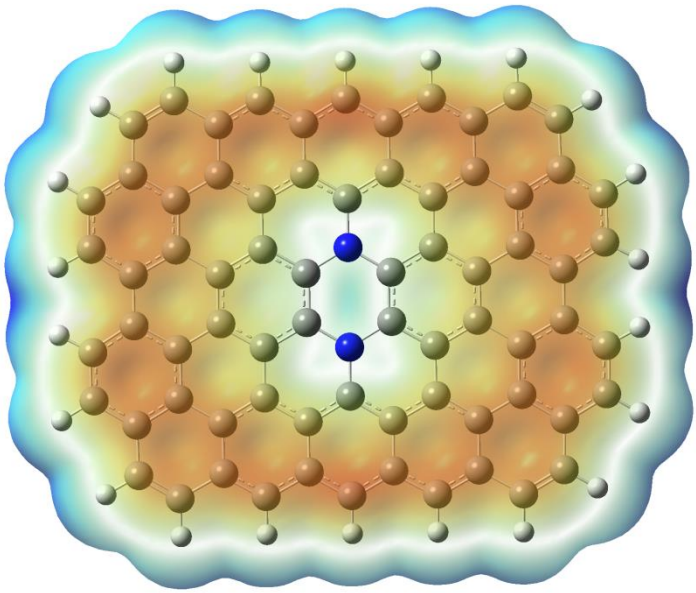
Supplementary Information



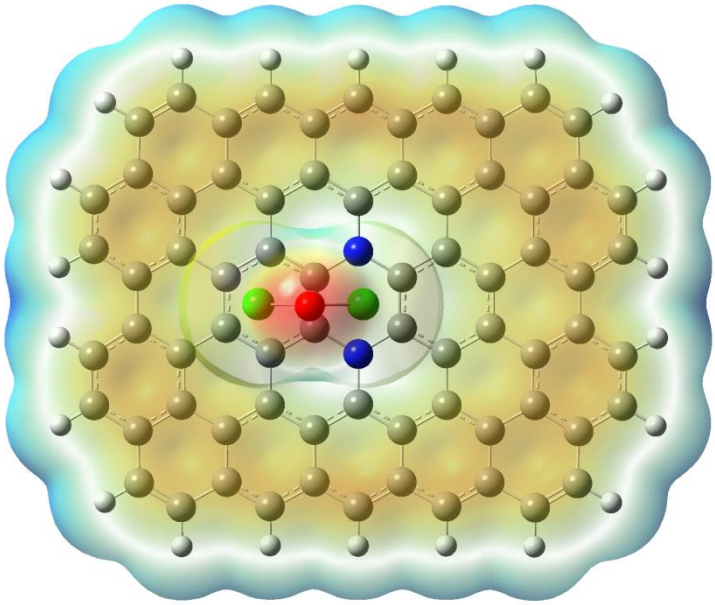
Graphene



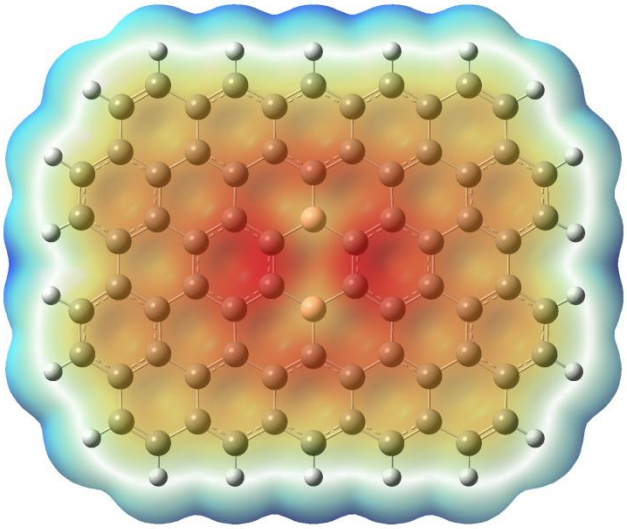
Complex G_1



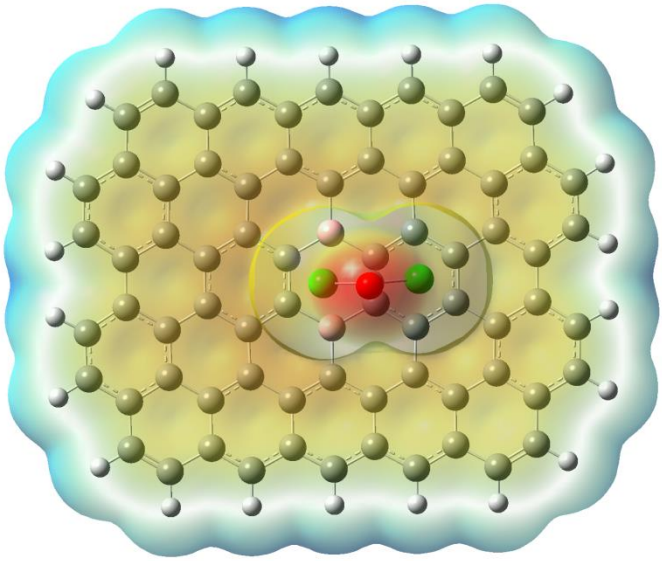
Graphene 2N



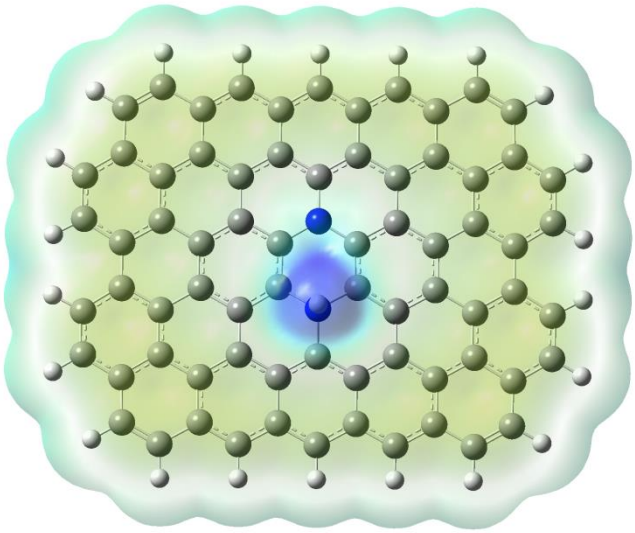
Complex G_2



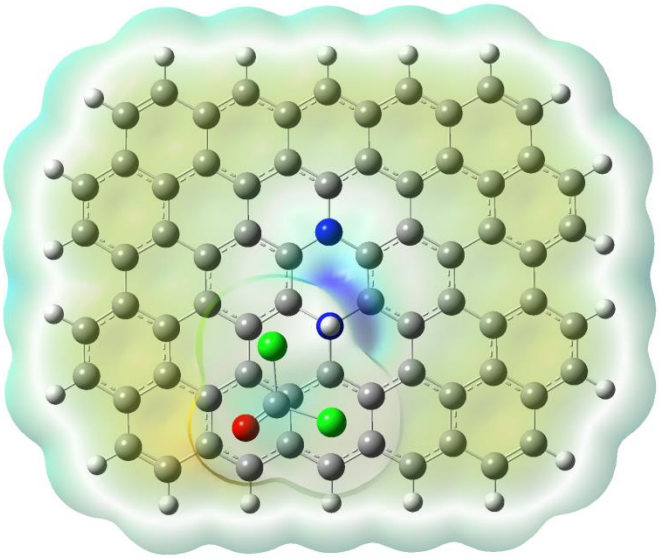
Graphene 2B



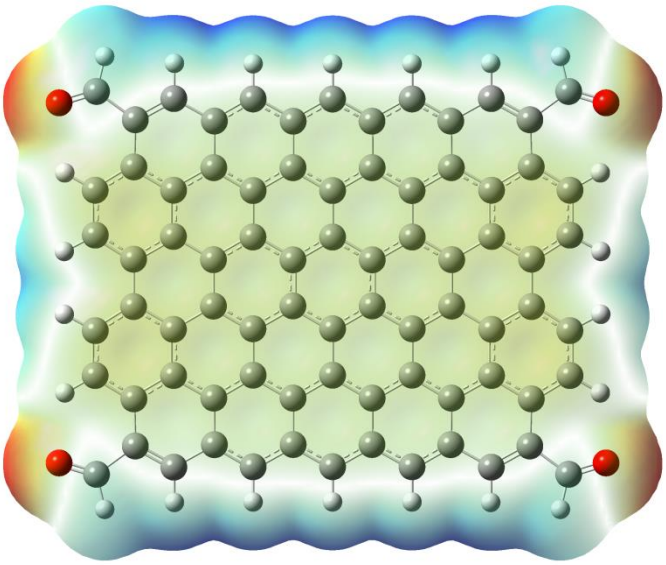
Complex G_3



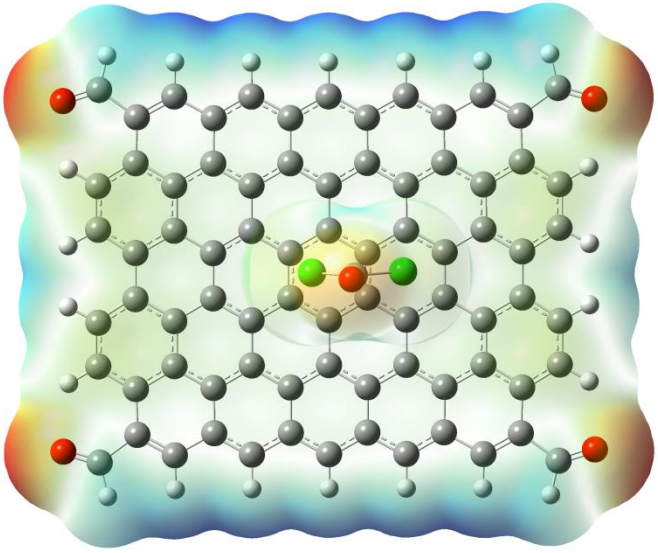
Graphene 2NH



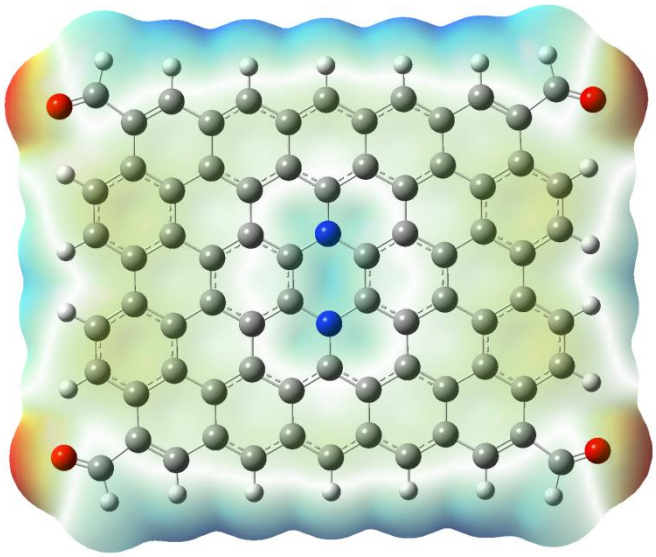
Complex G_4



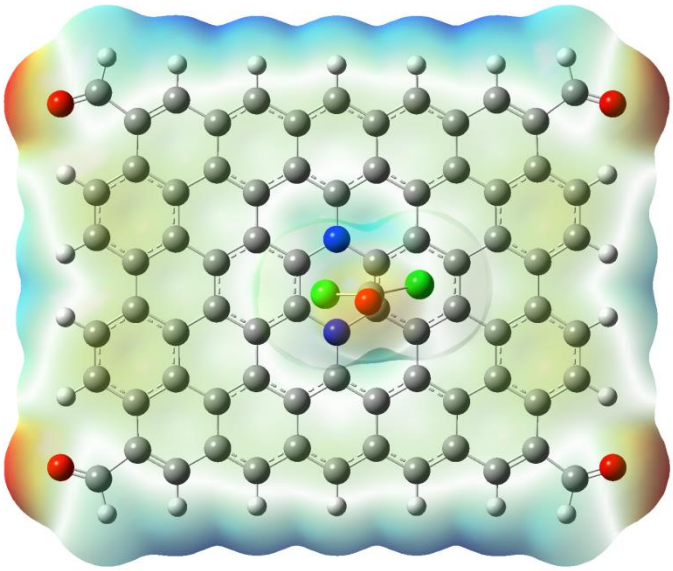
Graphene 4CHO



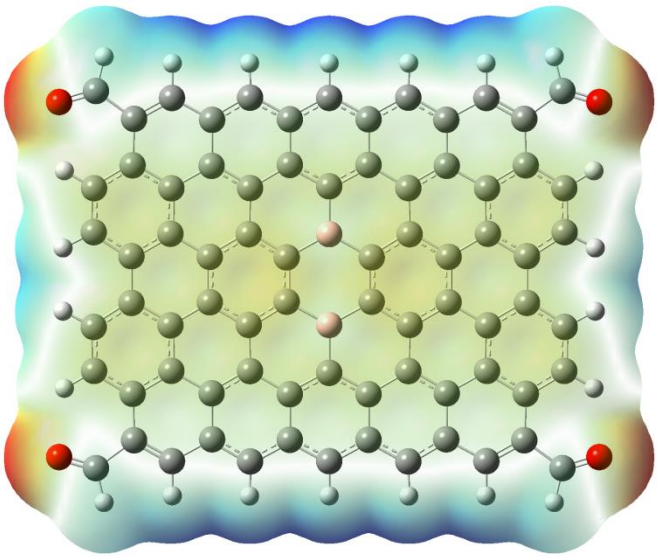
Complex G_5



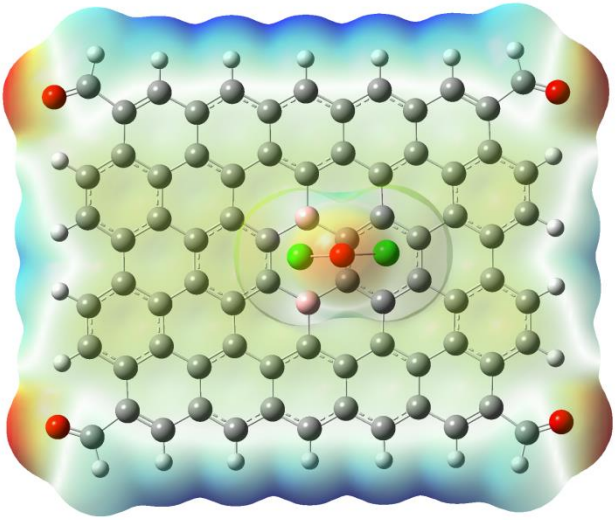
Graphene 2N 4CHO



Complex G_6

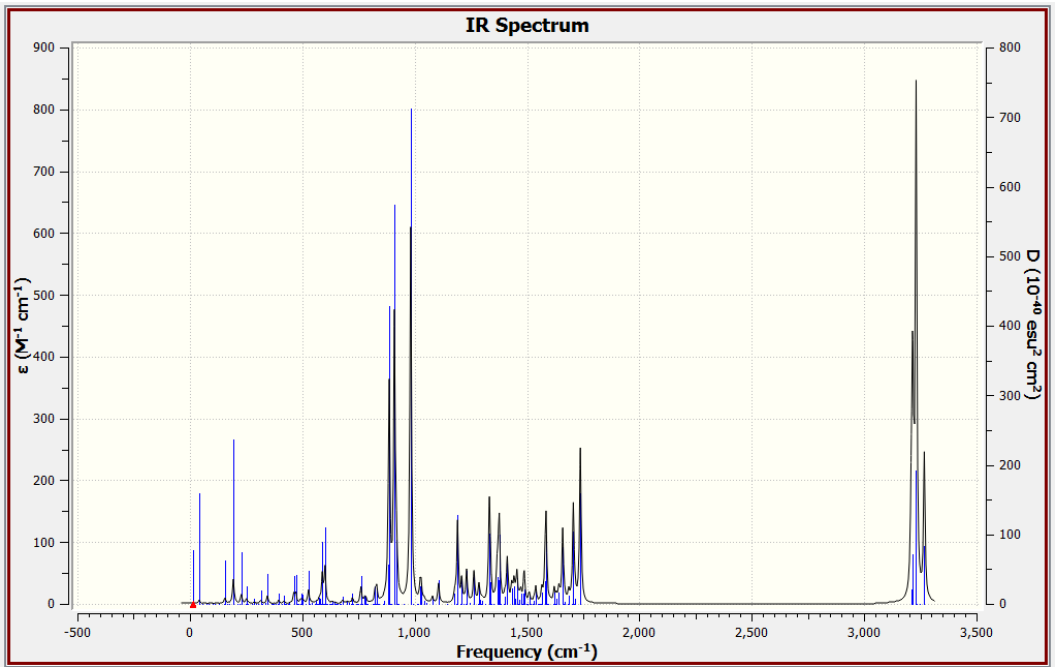


Graphene 2B 4CHO

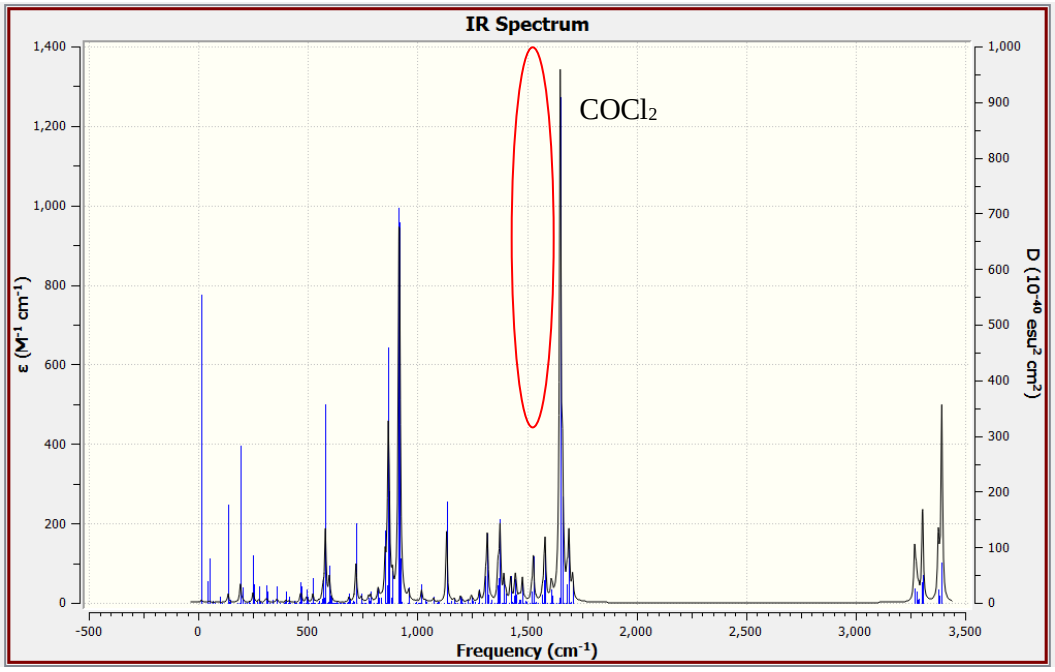


Complex G_7

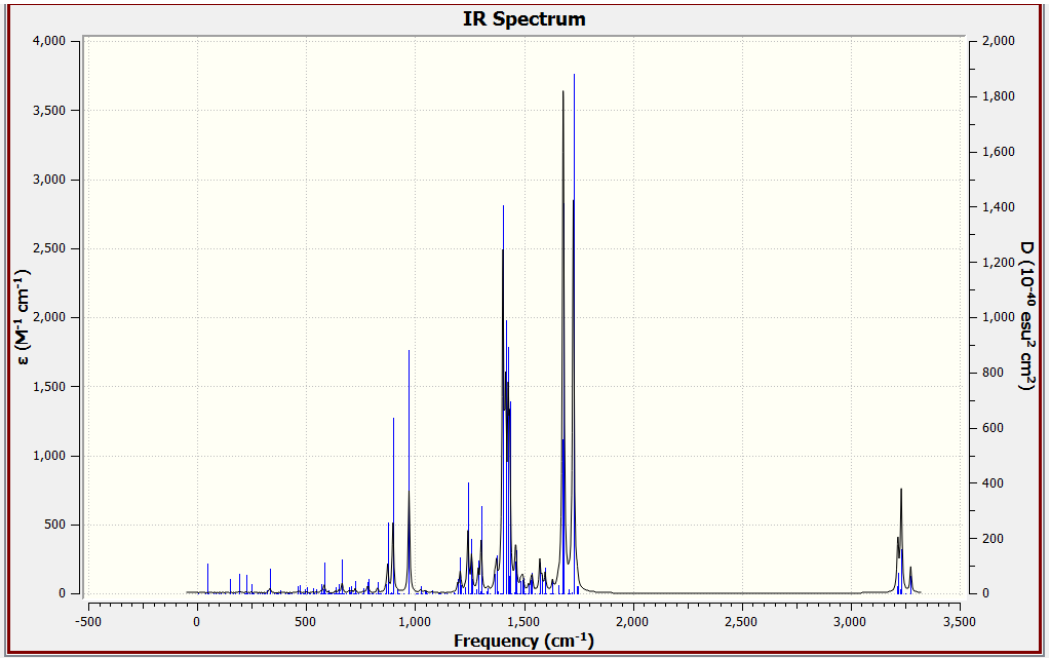
Fig S1: MEP maps of the graphene sheets and binary complexes that formed vial interaction of phosgene with graphene sheet, modified graphene sheets, and functionalized graphene sheets



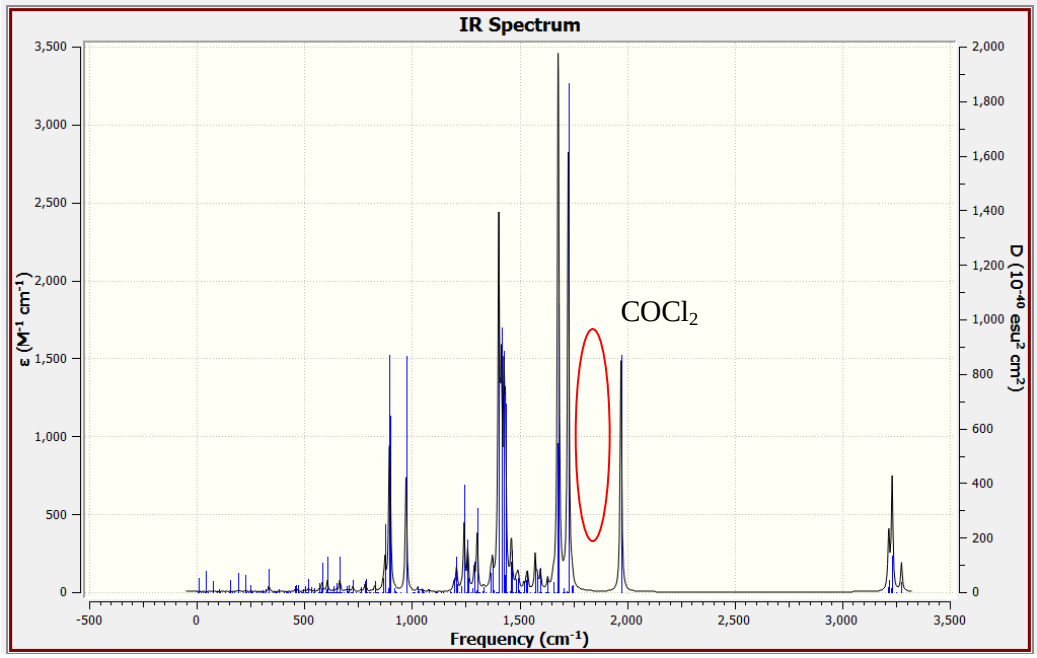
Graphene



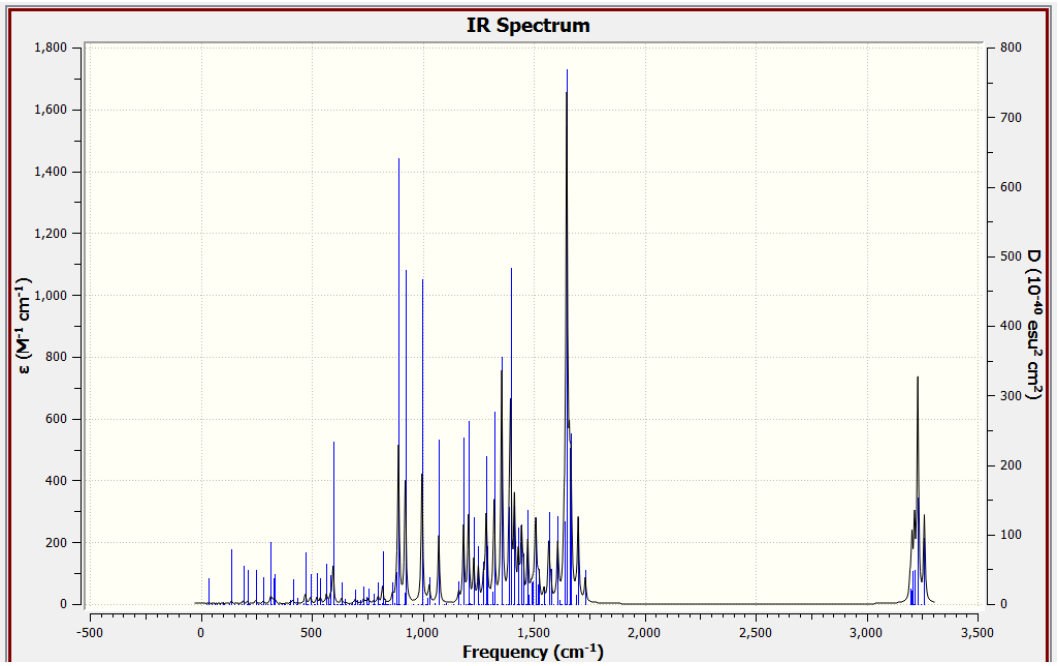
Complex G_1



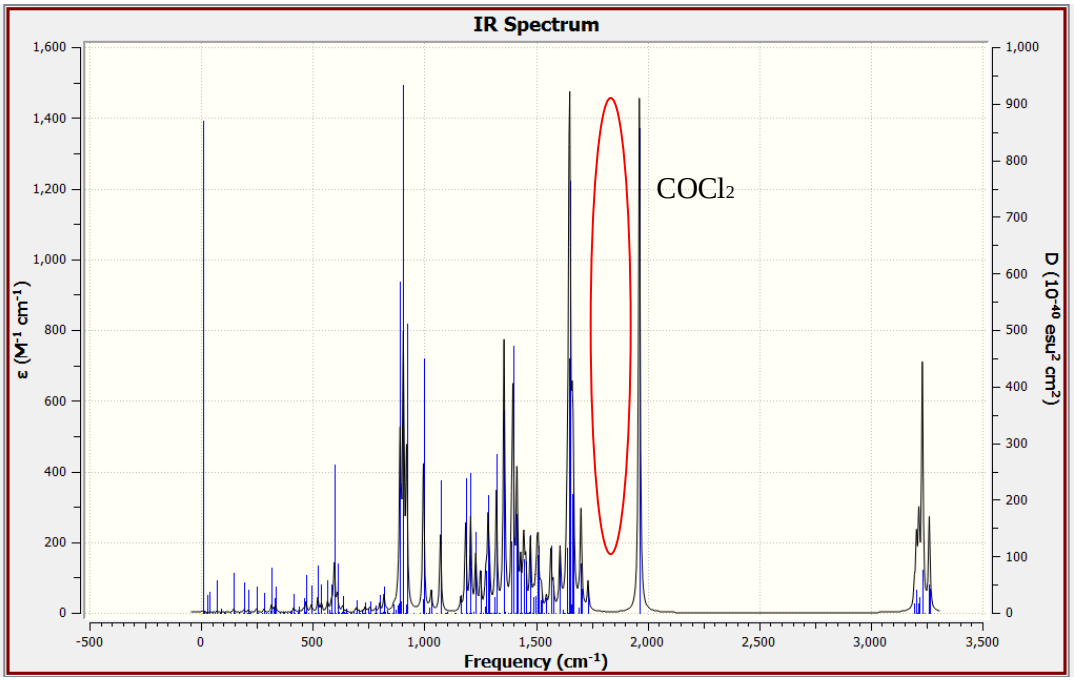
Graphene 2N



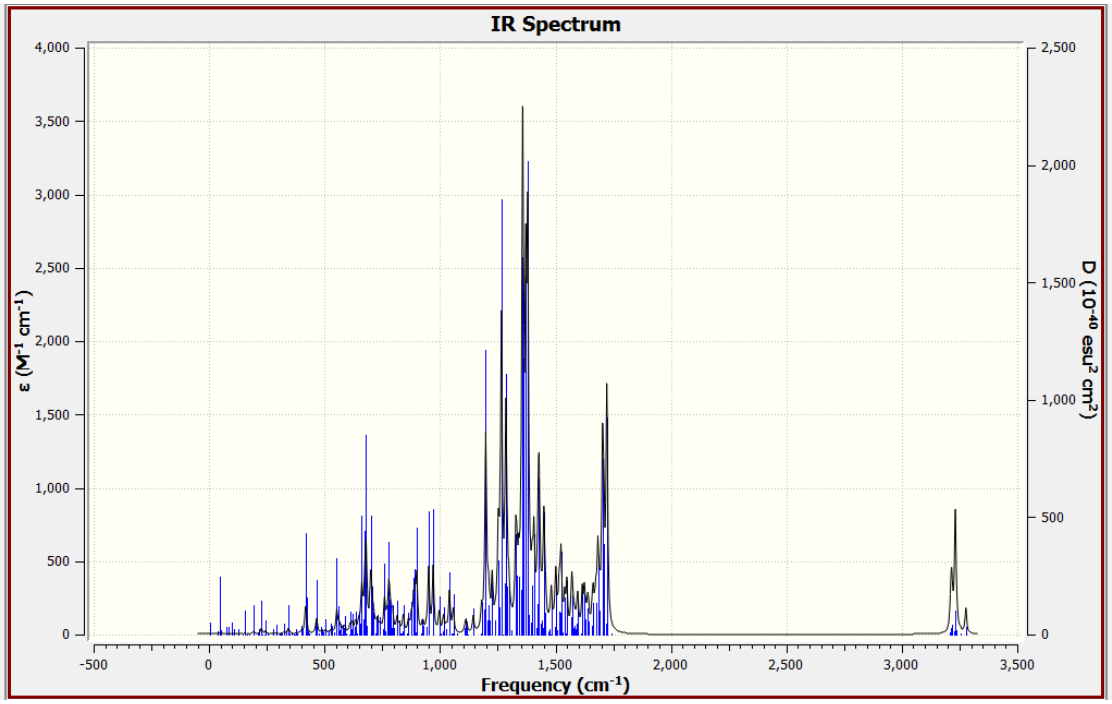
Complex G_2



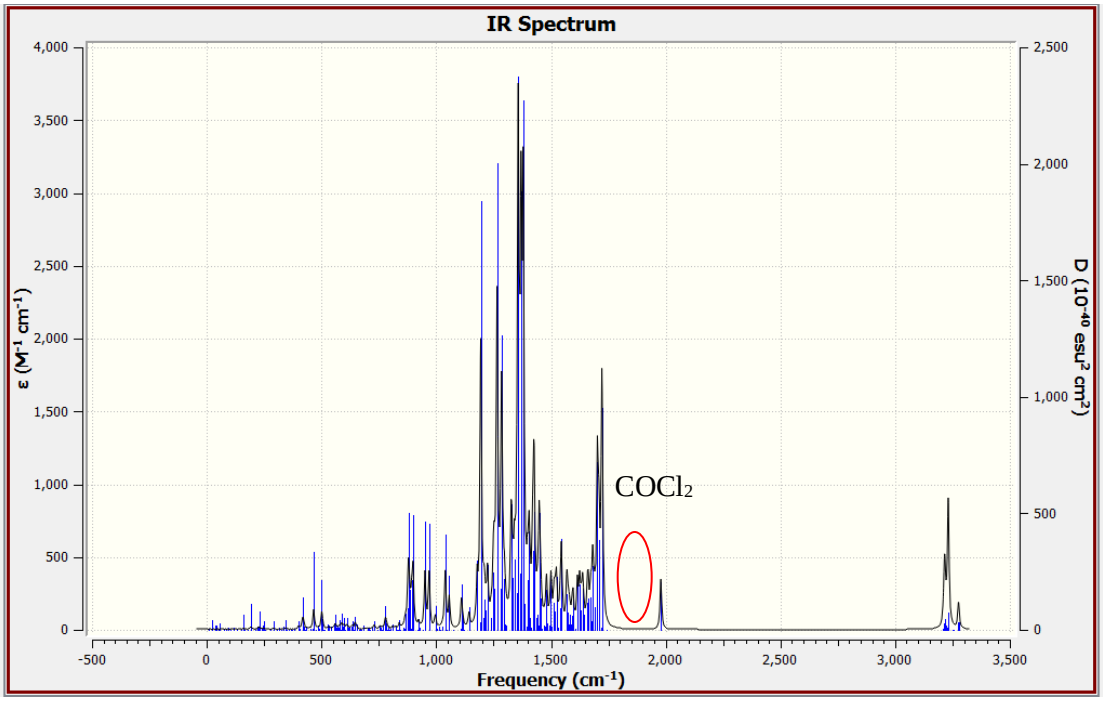
Graphene 2B



Complex G_3



Graphene 2NH



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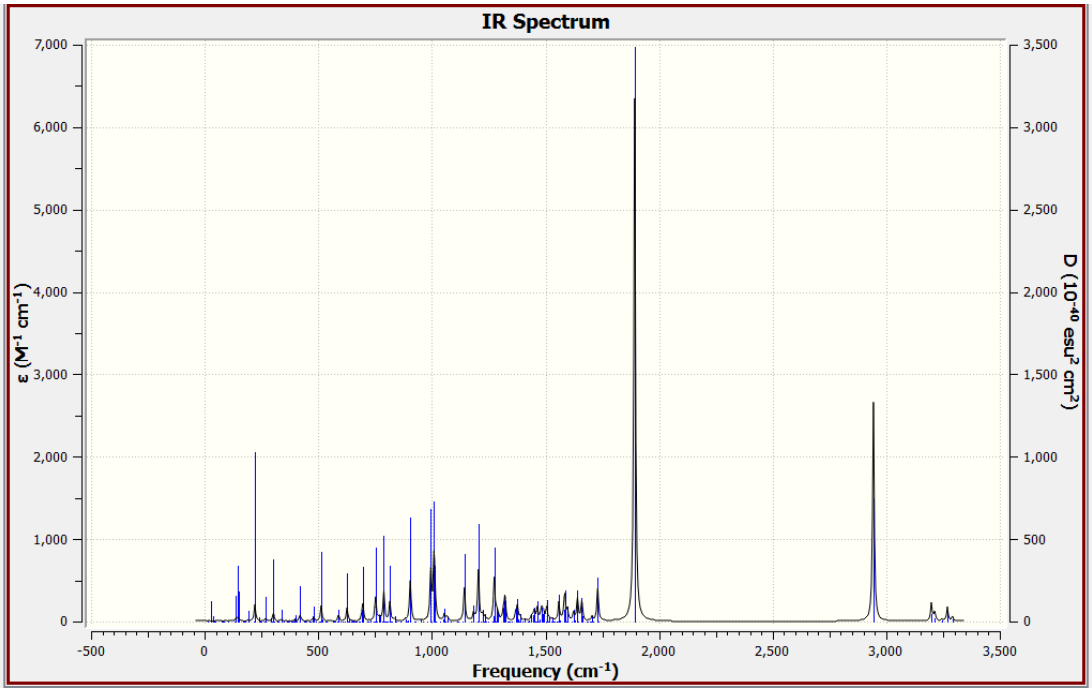
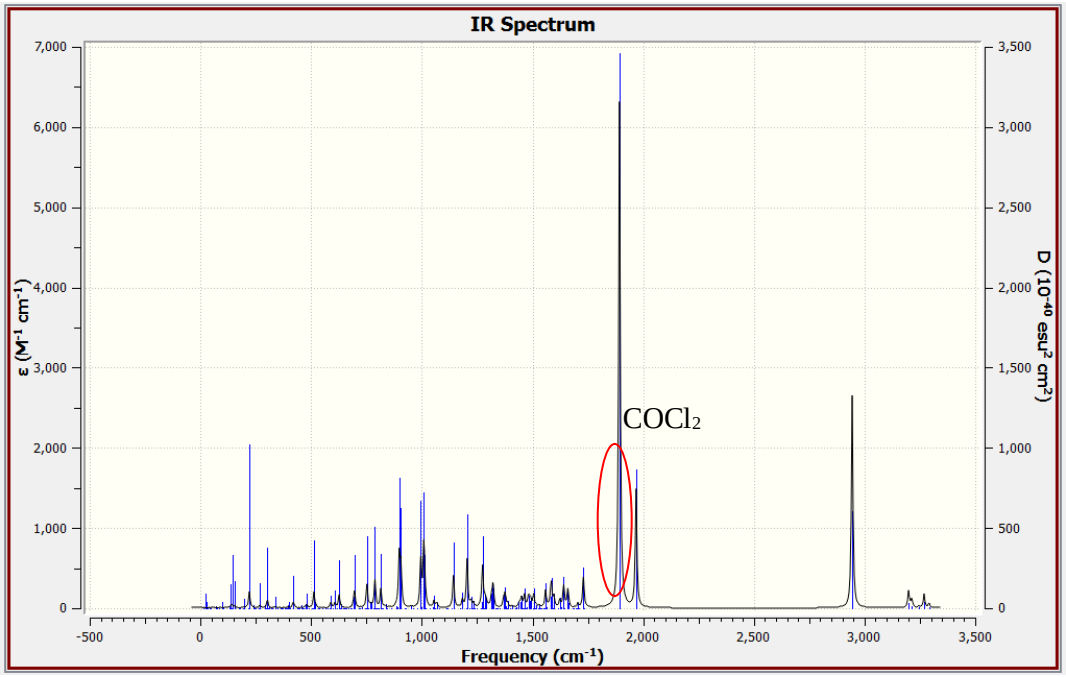
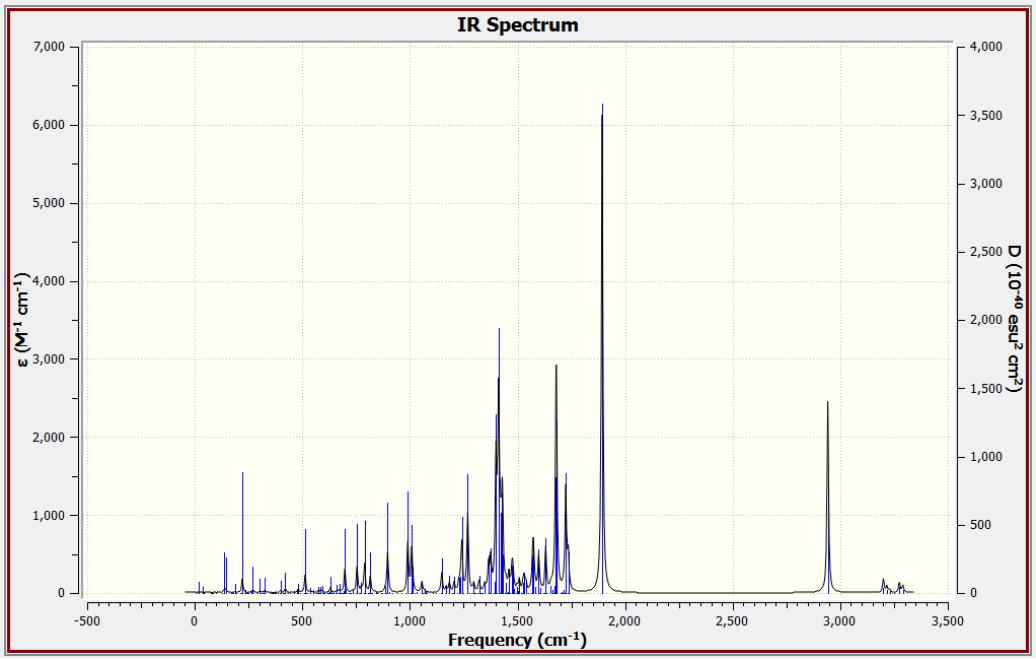


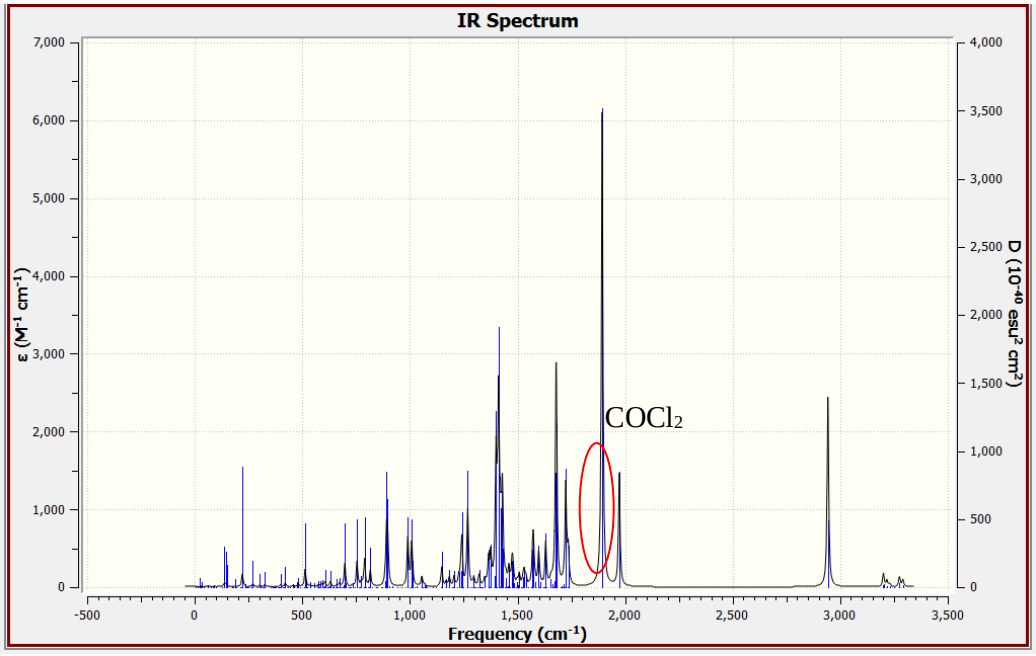
Graphene 4CHO



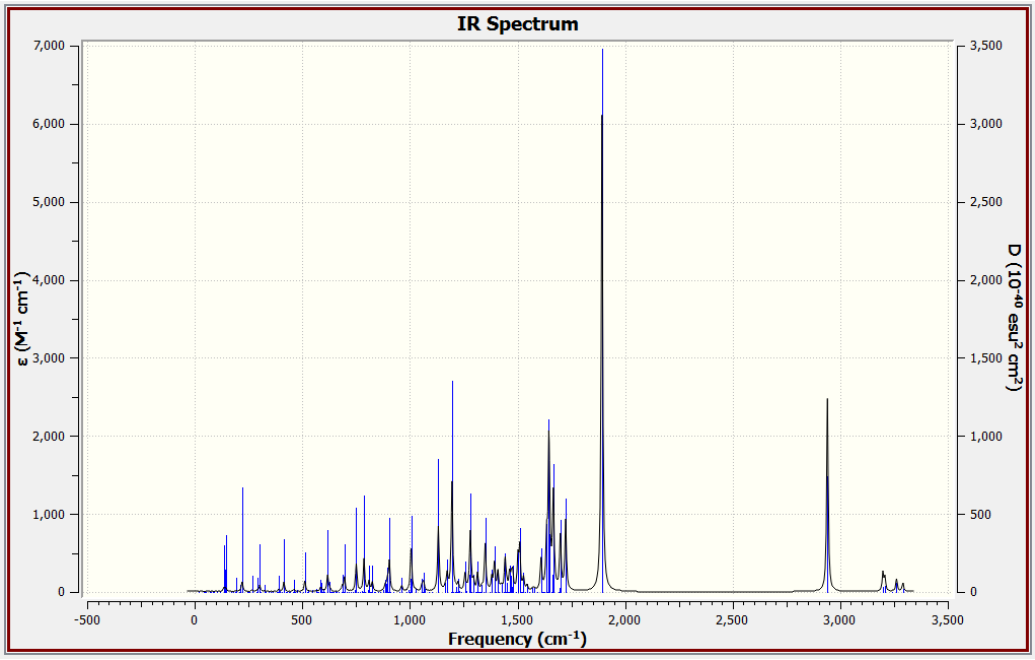
Complex G_5



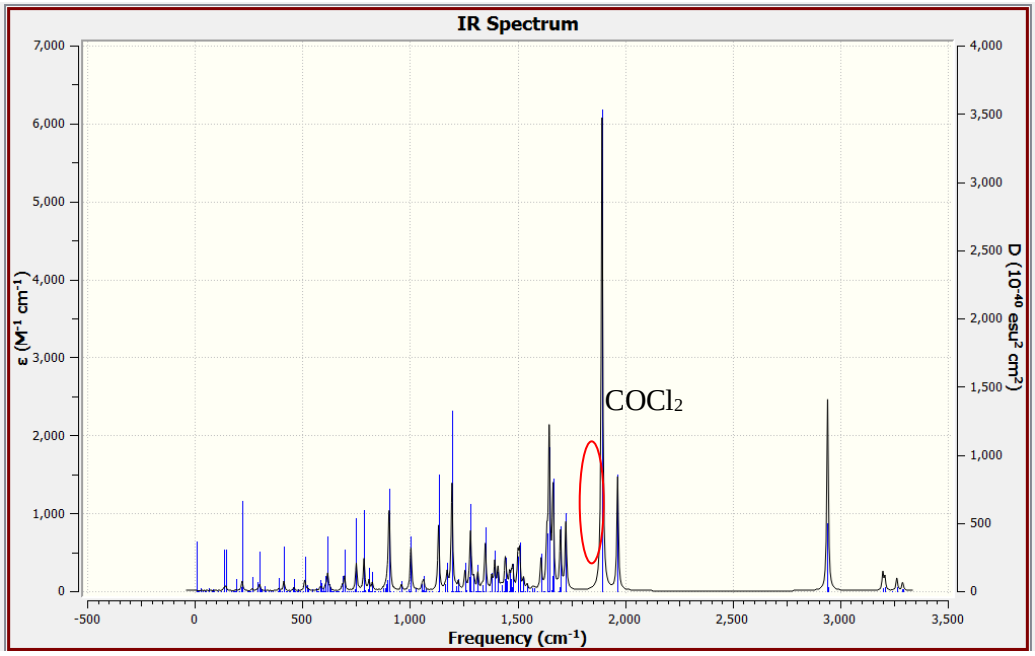
Graphene 2N 4CHO



Complex G_6



Graphene 2B 4CHO



Complex G_7

Fig S2: IR spectra of the proposed materials (graphene sheet, modified graphene sheets, and functionalized graphene sheets) and all complexes