

Electronic supplementary information for

Imidazole-graphyne: A new 2D carbon nitride with a direct bandgap and strong IR refraction

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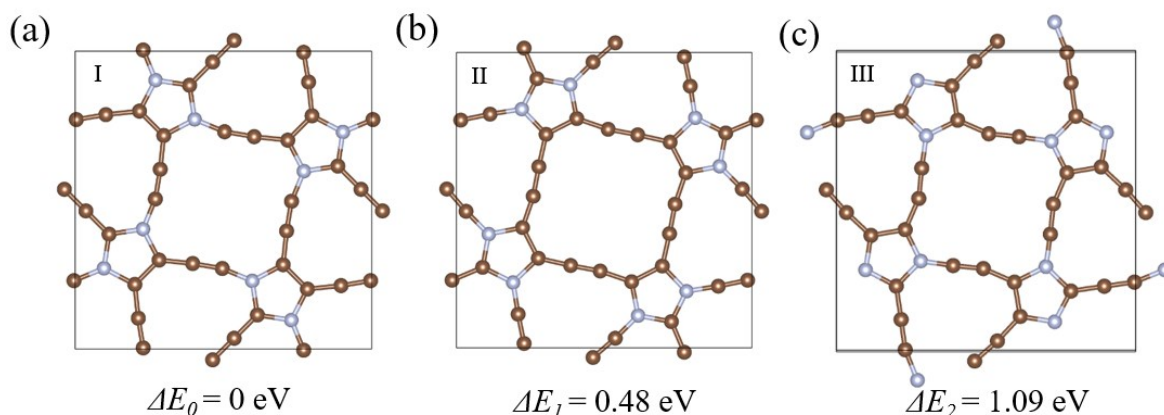


Fig. S1 Three configurations of ID-GY with the relative energy ΔE respective to configuration I. Brown and blue spheres represent C and N atoms, respectively.

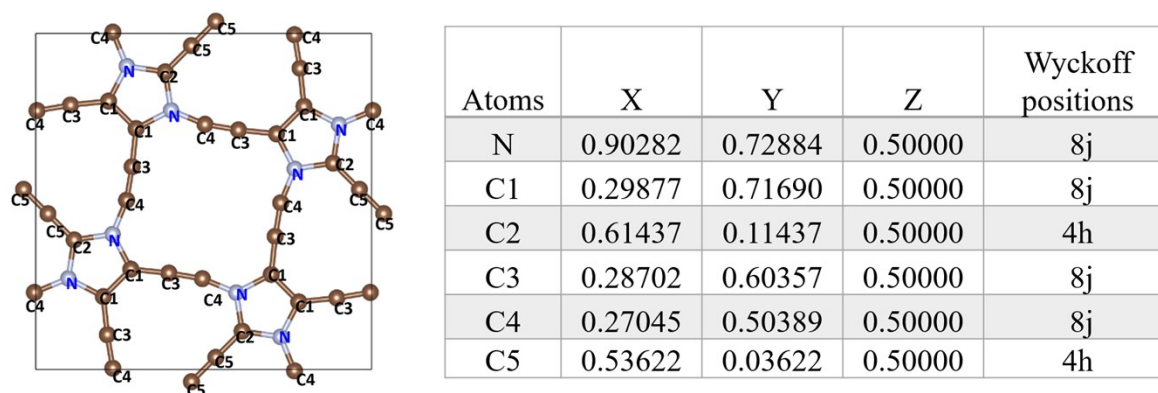


Fig. S2 Inequivalent C atoms and N atom with Wyckoff positions in ID-GY. Brown and blue spheres represent C and N atoms, respectively.

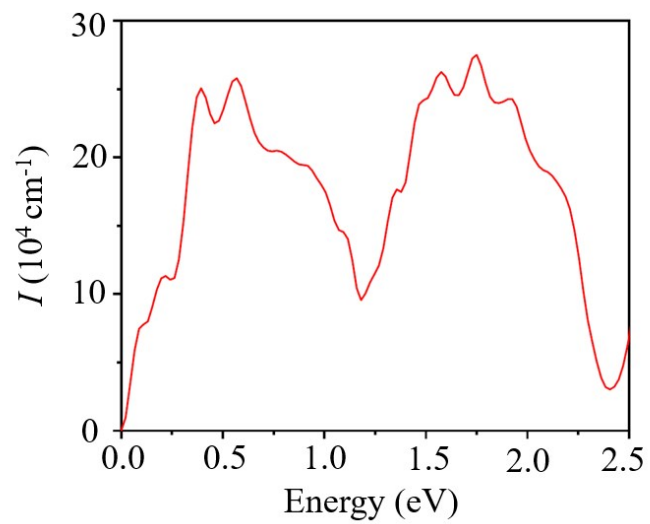


Fig. S3 Absorption coefficient of cp-graphyne.