

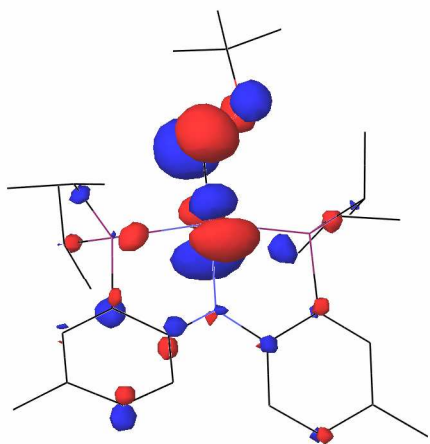
Supporting Information for

Elucidation of Heterocumulene Activation by a Nucleophilic-at-Metal Iridium(I) Carbene

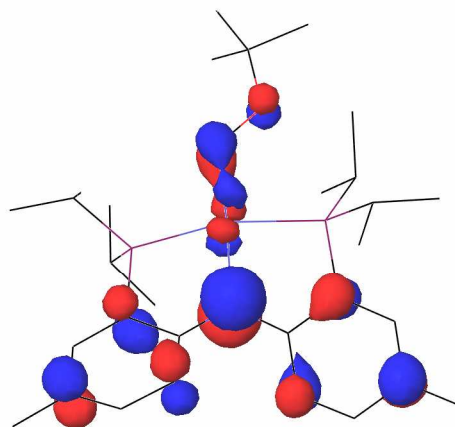
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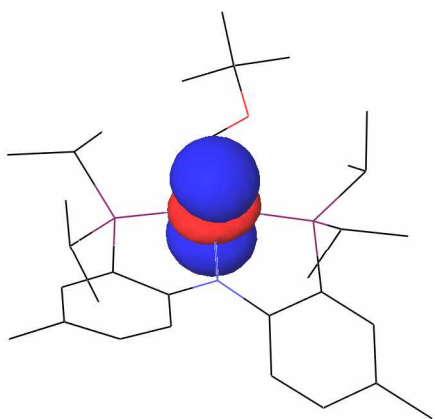
Figure S1. Frontier molecular orbitals for (PNP)Ir=C(H)O ^t Bu (1)	S2
Figure S2. Frontier molecular orbitals for (PNP)Ir-CO (2).....	S3
Figure S3. Frontier molecular orbitals for (PNP)Ir-CS (4)	S4
Figure S4. Frontier molecular orbitals for (PNP)Ir-CNPh (5)	S5



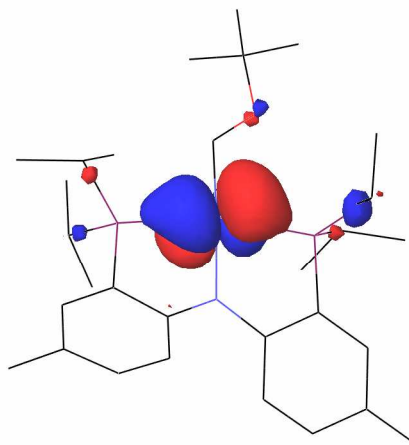
LUMO: -0.983 eV



HOMO: -4.100 eV



HOMO-1: -4.621 eV



HOMO-2: -5.307 eV

Figure S1. Frontier molecular orbitals for (PNP)Ir=C(H)O'Bu (**1**)

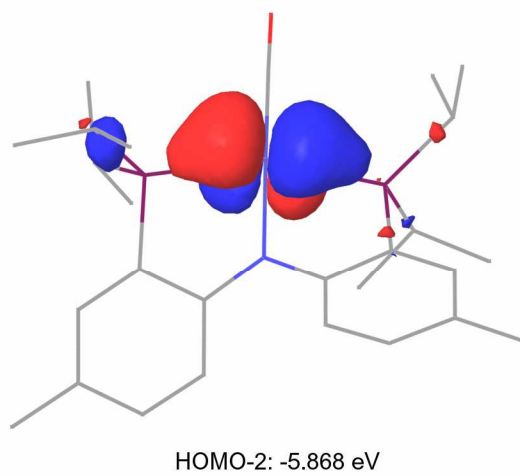
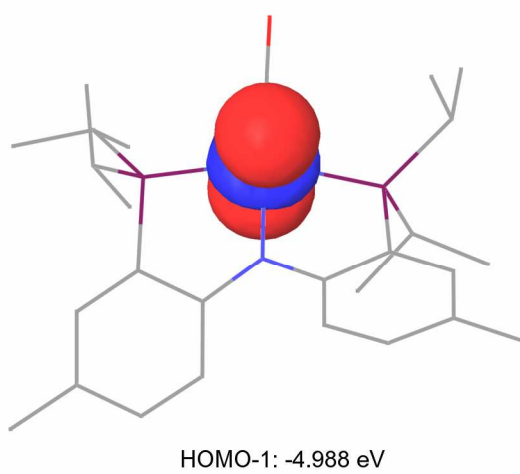
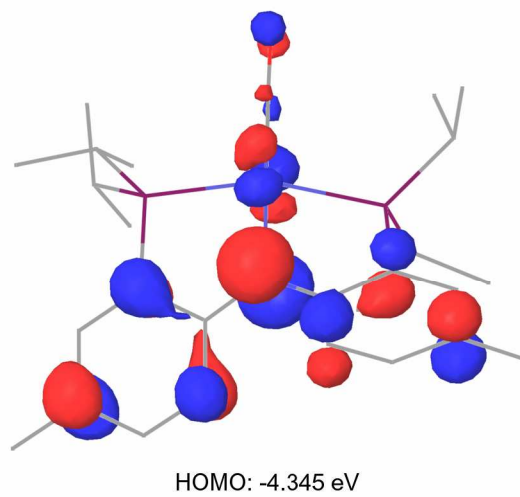
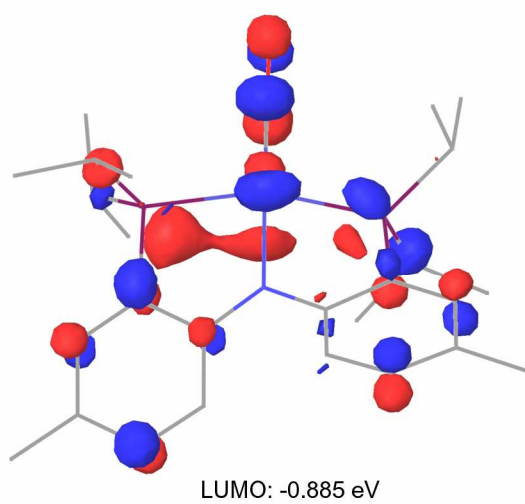
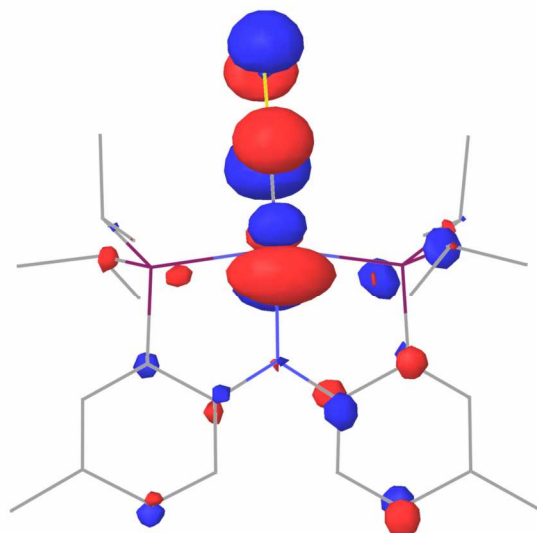
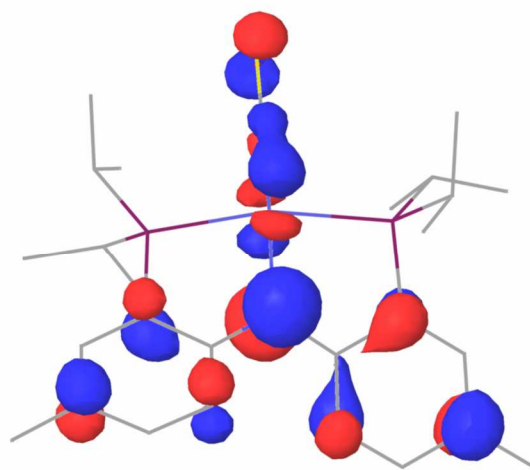


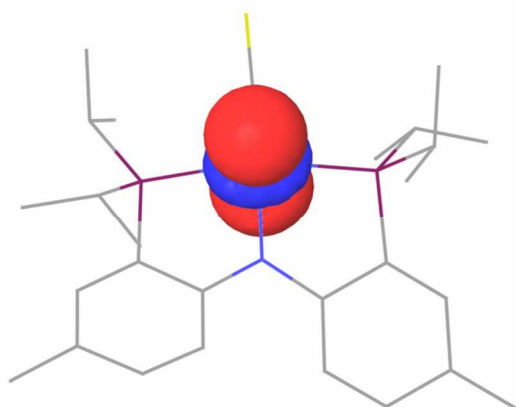
Figure S2. Frontier molecular orbitals for (PNP)Ir-CO (**3**)



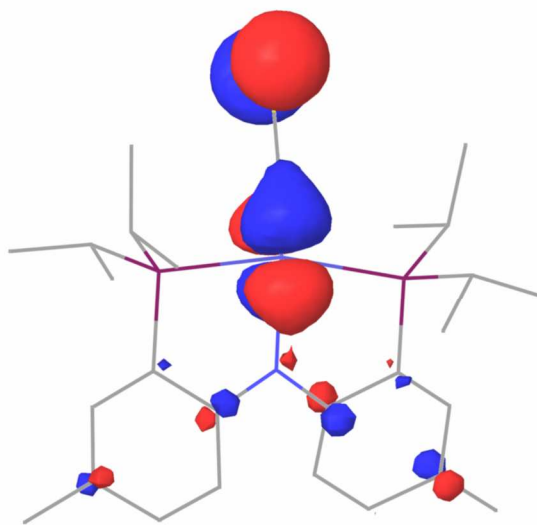
LUMO: -1.200 eV



HOMO: -4.441 eV



HOMO-1: -5.199 eV



HOMO-2: -5.488 eV

Figure S3. Frontier molecular orbitals for (PNP)Ir-CS (**5**)

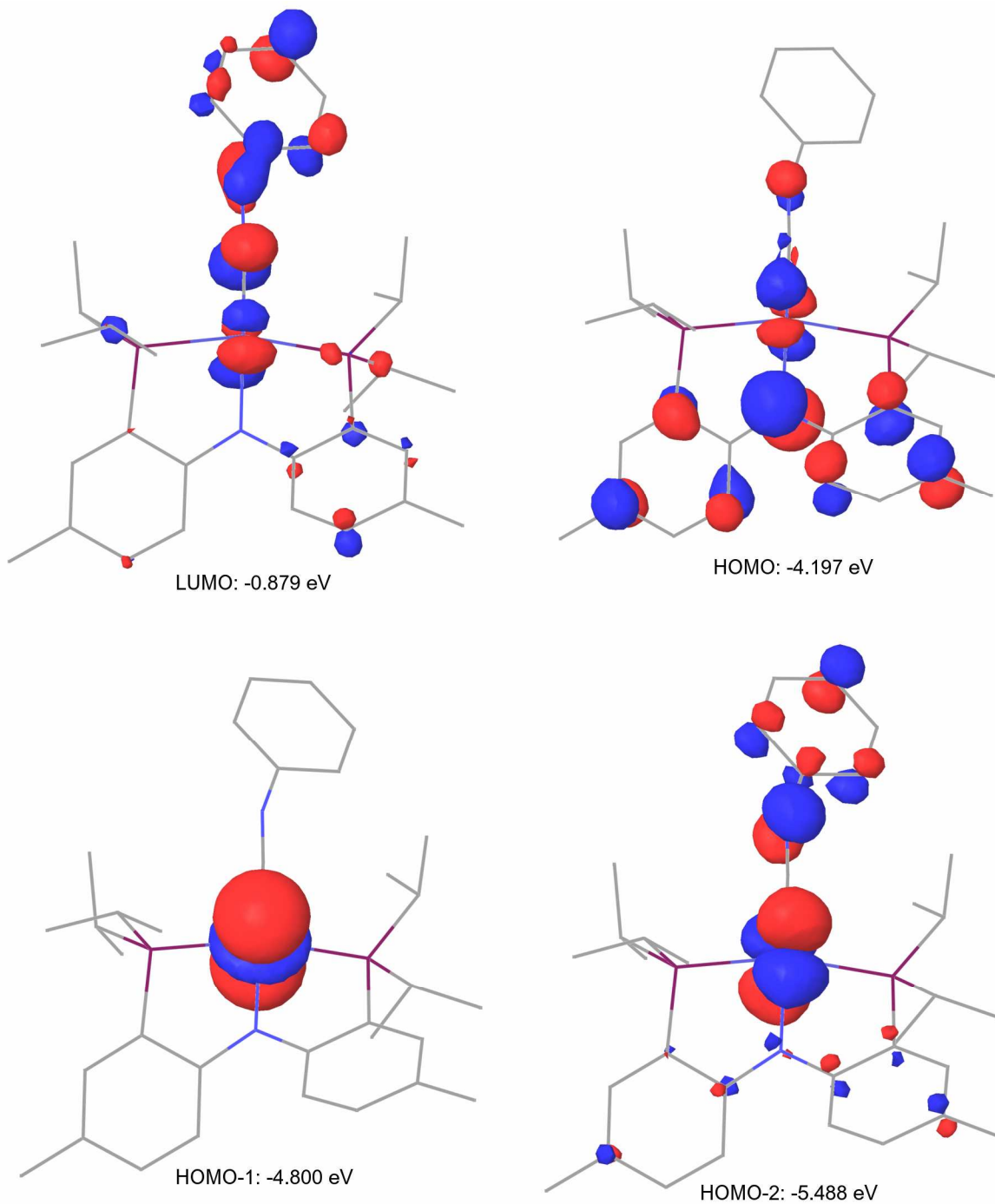


Figure S4. molecular orbitals for (PNP)Ir-CNPh (**6**)