

Calculated Triplet Energies (Photosensitizers & Photocatalysts)

B3LYP-D3 / cc-PVTZ(-f) [LACV3P** (metals)] / PCM: Benzene

species	ET (calculated)	ET (measured)
[Ir(ppy) ₂ (dtbpy)]PF ₆	49.0	49.2 ¹
Ir(ppy) ₃	57.6	58.1 ¹
Ir(CF ₃ ppy) ₃	56.6	–
[Ir(dFppy) ₂ (dtbpy)]PF ₆	63.8	–
Ir(dFppy) ₃	63.0	63.5 ¹
[Ir(dF(Me)ppy) ₂ (dtbpy)]PF ₆	64.7	–
[Ir(dF(CF ₃)ppy) ₂ (dtbpy)]PF ₆	60.4	61.7 ²
[Ir(dF(CF ₃)ppy) ₂ (5,5'-dCF ₃ bpy)]PF ₆	58.9	–
[Ir(dF(CF ₃)ppy) ₂ (4,4'-dCF ₃ bpy)]PF ₆	59.2	–
[Ir(dF(Me)ppy) ₂ (4,4'-dCF ₃ bpy)]PF ₆	55.6	–
benzophenone	69.2	69.1 ³
thioxanthone	63.1	63.3 ³
3,3'-F-TX	67.2	69.1 ⁴
3,3'-MeO-TX	68.0	71.2 ⁴
2,2'-MeO-TX	52.8	55.2 ⁴
[Ru(bpy) ₃]Cl ₂	54.2	49.0 ³
[Ru(bpzy) ₃]Cl ₂	45.2	–
[Ru(4,4'-dCF ₃ -bpy) ₃]Cl ₂	53.8	–

¹ Glorius et. al, *Chem. Soc. Rev.* **2018**, 47, 7190–7202

² Wenger et. al, *J. Am. Chem. Soc.* **2022**, 144, 963–976

³ Glorius et. al, *Chem* **2020**, 6, 1888–1903

⁴ Booker-Milburn et. al, *J. Am. Chem. Soc.* **2020**, 142, 14947–14956