Supporting Information: Computational determination of the dominant triplet population mechanism in photoexcited benzophenone

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Table S1: Geometrical parameters of S_0, S_1 and T_1, computed at various levels of theory.

Parameter	Method	S_0	S_1	T_1
Bond length (Å)[a]				
C_2O	PBE0	1.21	1.30[b]	1.32[c]
C_2O	CASSCF(12/11)	1.21	1.37	1.35
C_1C_2	PBE0	1.49	1.44[b]	1.44[c]
C_1C_2	CASSCF(12/11)	1.50	1.44	1.44
C_2C_3	PBE0	1.49	1.44[b]	1.44[c]
C_2C_3	CASSCF(12/11)	1.50	1.44	1.44
Angle (degree)[a]				
$C_1C_2C_3$	PBE0	120	127[b]	129[c]
$C_1C_2C_3$	CASSCF(12/11)	120	131	130
Ph-Ph[d]	PBE0	54	40[b]	44[c]
Ph-Ph	CASSCF(12/11)	58	40	44

[a] C_2 blongs to the carbonyl group, and C_1 and C_3 are the carbon atoms direclty bound to it.

[b] TD-DFT calculations, S_0 taken as reference, were performed.

[c] Spin-unrestricted DFT (UDFT) calculations were performed.

[d] Defined as the angle between the two phenyl planes.