

Supplementary Information

Second-order nonlinear optical properties of [60]fullerene-fused dihydrocarboline derivatives: a theoretical study on switch effect

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Contents

Table S1 The calculated β_{tot} values ($\times 10^{-30}$ esu) of **I**, **II-2**, **III**, **IV**, **V** and **VI** by ω B97XD functionals with 6-31+G(d) and 6-31+G(d,p) basis sets.

Table S2 The calculated β_{tot} values ($\times 10^{-30}$ esu) of **II-2**, **III**, **V** and their reduced states at ω B97XD/6-31+G(d) level.

Table S1 The calculated β_{tot} values ($\times 10^{-30}$ esu) of **I**, **II-2**, **III**, **IV**, **V** and **VI** by ω B97XD functionals with 6-31+G(d) and 6-31+G(d,p) basis sets.

System	ω B97XD/6-31+G(d)	ω B97XD/6-31+G(d,p)
I	17.6	17.5
II-2	26.0	25.9
III	40.2	40.0
IV	50.7	50.3
V	9.3	9.6
VI	0.6	0.67

Table S2 The calculated β_{tot} values ($\times 10^{-30}$ esu) of **II-2**, **III**, **V** and their reduced states at ω B97XD/6-31+G(d) level.

System	β_{tot}	System	β_{tot}	System	β_{tot}
II	26.0	III	40.2	V	9.3
II⁻	42	III⁻	53	V⁻	280
II²⁻	1506	III²⁻	4662	V²⁻	4442
II³⁻	1131	III³⁻	992	V³⁻	927