Electronic Supplementary Material (ESI) for RSC Advances.

Electronic structure and second-order nonlinear optical properties of lemniscular [16]cycloparaphenylene compounds

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Table S1. The computed most intense absorption band (λ, nm) using the B3LYP functional at the different basis sets level for compound **1** along with the experimental value.

Basis set	6-31G(d)	6-31G(d,p)	6-31+G(d)	6-31+G(d,p)	exp
λ	378.38	378.7	387.16	387.76	357

Table S2. The computed most intense absorption band (λ, nm) using the different functionals at 6-31G(d) basis set level for compound **1** along with the experimental value.

Functional	B3LYP	PBE0	CAM-B3LYP	BH&HLYP	PBE0/CH_2Cl_2	Exp
λ	378.38	362.67	319.03	323.26	368.49	357