Supporting Information

Curved Macrocyclic Nanocarbons with Tunable Electronic and Nonlinear Optical Properties: Theoretical Insights

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Table S1 Calculated absorption wavelengths (λ, nm) with the largest oscillator strength (*f*) values and excited-state numbers (Sn) of compounds **1**-**6**.

Compounds	Sn	λ	*f*
1	12	335	3.6388
2	10	327	5.0595
3	20	325	3.1553
4	12	340	3.3698
5	38	308	1.5906
6	25	324	1.3536

Table S2 Calculated λ_e and λ_h values of compounds **1**-**6**.

Compounds	λ_e (eV)	λ_h (eV)
1	0.2242	0.0894
2	0.2690	0.1458
3	0.0599	0.0764
4	0.1557	0.2449
5	0.2287	0.1785
6	0.3061	0.2266

Table S3 Static first hyperpolarizability β_{tot} (x10^2 au) of compounds **1-6** calculated at the functionals M062X, BHandHLYP and CAM-B3LYP and the basis set 6-311G(d).

Compounds	M062X	BHandHLYP	CAM-B3LYP
1	2.39	2.13	1.79
2	0.36	0.24	0.20
3	2.18	1.75	1.60
4	4.22	4.52	4.06
5	29.07	31.53	23.93
6	154.82	160.46	149.85