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SUPPORTING INFORMATION

The photophysical properties of cycloparaphenylene-based compounds with figure-eight configuration

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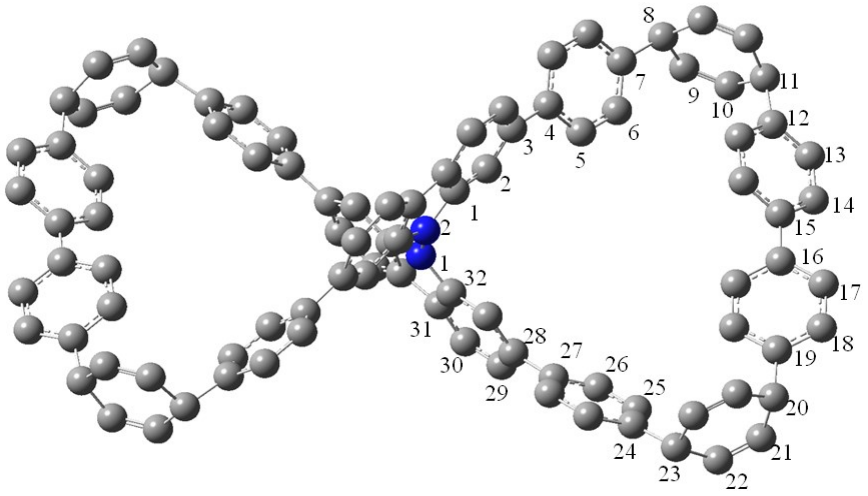
Table S1 The main concerned bond length (Å) for compound **1** between experiment and calculation.



	B3LYP	Experiment	Difference		B3LYP	Experiment	Difference
N1-N2	1.367	1.365	0.002	C16-C17	1.403	1.384	0.019
N2-C1	1.400	1.397	0.003	C17-C18	1.398	1.389	0.009
C1-C2	1.391	1.382	0.009	C18-C19	1.399	1.382	0.017
C2-C3	1.403	1.397	0.006	C19-C20	1.537	1.522	0.015
C3-C4	1.485	1.493	-0.008	C20-C21	1.515	1.510	0.005
C4-C5	1.403	1.390	0.004	C21-C22	1.334	1.317	0.017
C5-C6	1.394	1.387	0.007	C22-C23	1.511	1.500	0.011
C6-C7	1.399	1.388	0.011	C23-C24	1.538	1.526	0.012
C7-C8	1.540	1.527	0.013	C24-C25	1.399	1.388	0.011
C8-C9	1.510	1.505	0.005	C25-C26	1.394	1.375	0.019
C9-C10	1.335	1.320	0.015	C26-C27	1.402	1.399	0.003
C10-C11	1.517	1.510	0.007	C27-C28	1.486	1.481	0.005
C11-C12	1.537	1.527	0.010	C28-C29	1.415	1.409	0.006
C12-C13	1.400	1.382	0.018	C29-C30	1.386	1.368	0.018
C13-C14	1.395	1.379	0.016	C30-C31	1.399	1.399	0.000
C14-C15	1.403	1.384	0.019	C31-C32	1.416	1.405	0.011
C15-C16	1.484	1.484	0.000	C32-N1	1.403	1.401	0.002

Note: the difference is equal to calculation value minus experimental value.

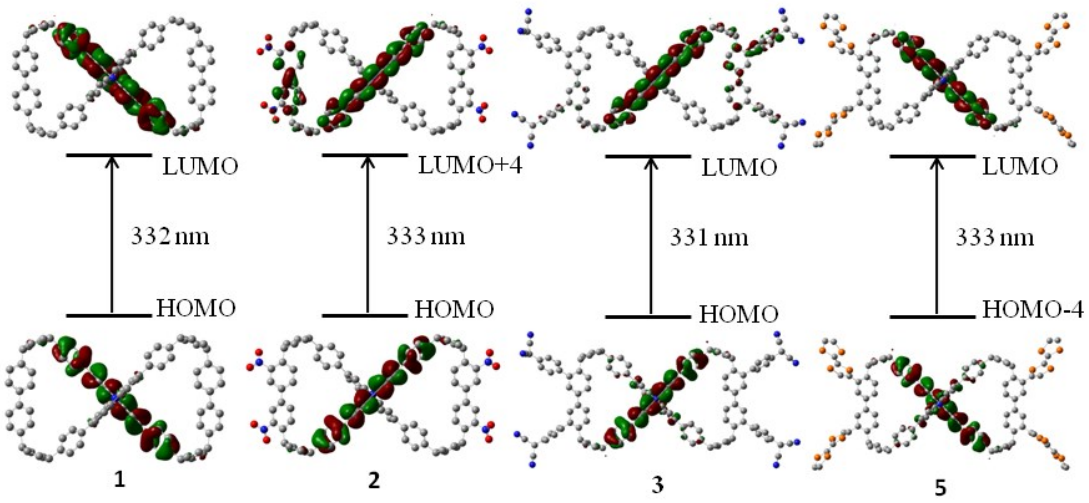


Figure S1. Molecular orbital isosurfaces involved in the main electron transitions of compounds **1**, **2**, **3** and **5**.

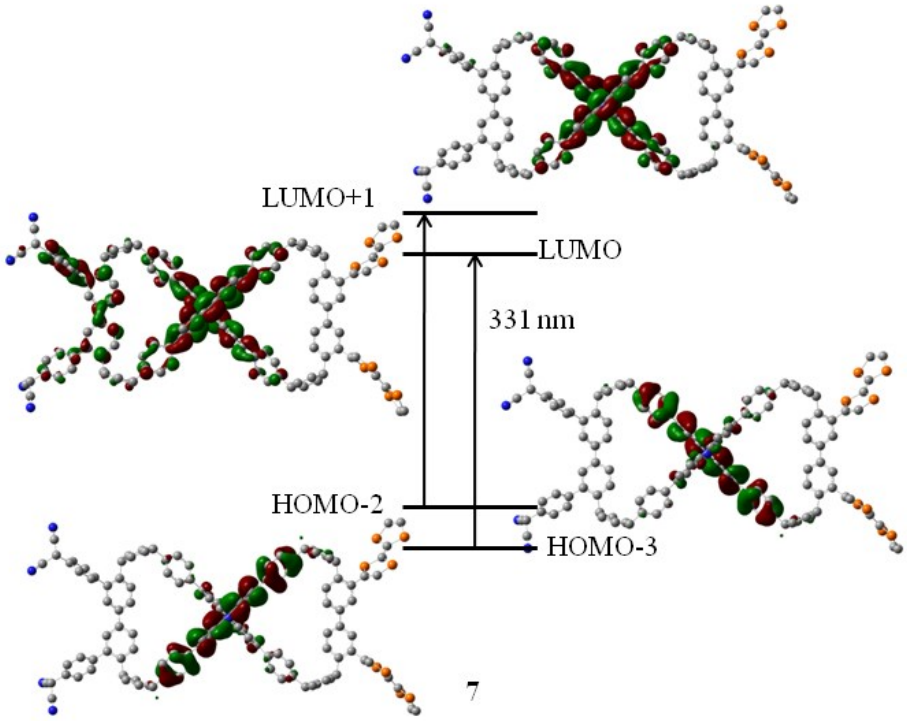


Figure S2. Molecular orbital isosurfaces involved in the main electron transitions of compound **7**.

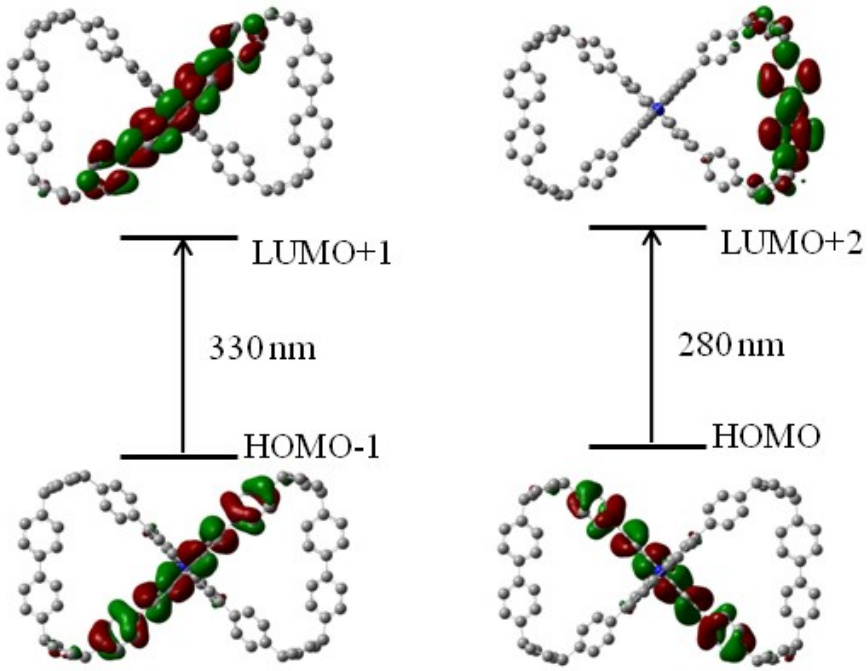


Figure S3. Molecular orbitals involved into the main CD transitions of compound **1**.