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SUPPORTING INFORMATION

Exploringthe photophysical properties ofunusual π-conjugated porphyrin nanohoops

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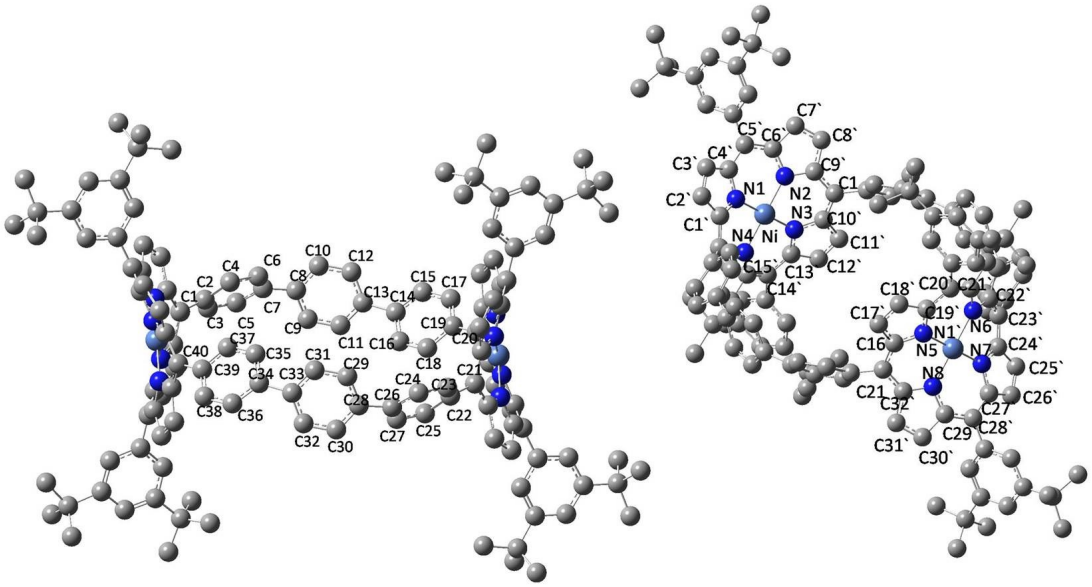
Table S1 The main concerned bond length (Å) for compound **1** between experiment and calculation.



	Calc.	Exp.		Calc.	Exp.		Calc.	Exp.
C1-C2	1.489	1.468	C30-C32	1.392	1.407	C13`-N3	1.377	1.411
C2-C3	1.408	1.360	C31-C33	1.406	1.417	C13`-C14`	1.401	1.367
C2-C4	1.409	1.390	C32-C33	1.406	1.384	C14`-C15`	1.401	1.372
C3-C5	1.396	1.425	C33-C34	1.485	1.468	C15`-N4	1.373	1.355
C4-C6	1.388	1.388	C34-C36	1.406	1.405	Ni`-N5	1.922	1.870
C5-C7	1.406	1.384	C35-C37	1.388	1.379	Ni`-N6	1.918	1.880
C6-C7	1.405	1.348	C36-C38	1.396	1.388	Ni`-N7	1.908	1.845
C7-C8	1.485	1.487	C37-C39	1.409	1.360	Ni`-N8	1.912	1.876
C8-C9	1.406	1.411	C38-C39	1.408	1.360	N5-C16`	1.377	1.403
C8-C10	1.406	1.379	C39-C40	1.489	1.465	C16`-C17`	1.443	1.480
C9-C11	1.392	1.407	Ni-N1	1.908	1.845	C17`-C18`	1.362	1.364
C10-C12	1.392	1.392	Ni-N2	1.912	1.876	C18`-C19`	1.442	1.442
C11-C13	1.406	1.384	Ni-N3	1.922	1.870	C19`-N5	1.377	1.411
C12-C13	1.406	1.417	Ni-N4	1.918	1.880	C19`-C20`	1.401	1.367
C13-C14	1.485	1.468	N1-C1`	1.372	1.384	C20`-C21`	1.403	1.371
C14-C15	1.406	1.405	C1`-C2`	1.440	1.393	C21`-N6	1.373	1.355
C15-C17	1.396	1.388	C2`-C3`	1.365	1.376	C22`-C23`	1.408	1.360
C16-C18	1.388	1.379	C3`-C4`	1.443	1.499	C23`-C24`	1.408	1.399
C17-C19	1.408	1.360	C4`-N1	1.375	1.361	C24`-C25`	1.440	1.393
C18-C19	1.409	1.360	C4`-C5`	1.405	1.405	C24`-N7	1.372	1.384
C19-C20	1.489	1.465	C5`-C6`	1.403	1.440	C25`-C26`	1.365	1.376
C21-C22	1.489	1.468	C6`-N2	1.379	1.319	C26`-C27`	1.443	1.498
C22-C23	1.408	1.360	C6`-C7`	1.443	1.478	C27`-N7	1.375	1.361
C23-C24	1.396	1.425	C7`-C8`	1.364	1.358	C27`-C28`	1.405	1.405
C22-C25	1.409	1.389	C8`-C9`	1.441	1.457	C28`-C29`	1.403	1.440

C24-C26	1.406	1.384	C9`-N2	1.369	1.364	C29`-N8	1.379	1.319
C25-C27	1.388	1.388	C9`-C1	1.409	1.362	C29`-C30`	1.443	1.478
C26-C27	1.405	1.348	C1-C10`	1.408	1.373	C30`-C31`	1.364	1.358
C26-C28	1.486	1.487	C10`-N3	1.377	1.404	C31`-C32`	1.441	1.457
C28-C29	1.406	1.379	C10`-C11`	1.443	1.480	C32`-N8	1.369	1.364
C28-C30	1.406	1.411	C11`-C12`	1.362	1.364	C32`-C21	1.409	1.362
C29-C31	1.392	1.391	C12`-C13`	1.442	1.443	C21-C16`	1.408	1.373

Table S2 Calculated the absorption wavelengths (nm), excitation energies (eV) and oscillator strength (*f*) values for the spectra in Fig.1

Funcationals	λ	E	*f*
B3LYP	427	2.90	1.9487
PBE0	418	2.97	2.1329
Cam-B3LYP	400	3.10	2.5005
M052X	396	3.13	2.6633
BHandHLYP	393	3.15	2.8079
Exp.[a]	446		

[a]Experimental data from ref. 31.

Table S3 Calculated the absorption wavelengths (λ in nm), excitation energies (eV), oscillator strength (*f*) values and major contributions for compounds**1**-**8**

Compounds	λ	E	*f*	Major contributions
1	427	2.90	1.9487	H-3->L+2 (41%)
				H-2->L+3 (27%)
2	419	2.96	1.7423	H-3->L+2 (51%)
				H-2->L+3 (13%)
3	423	2.93	2.3237	H-3->L+2 (35%)
				H-2->L+3 (28%)
4	422	2.94	1.1330	H-4->L+3 (22%)
				HOMO->L+6 (28%)
5	427	2.90	1.2592	H-4->L+3 (25%)
				H-3->L+4 (26%)
6	449	2.76	1.4107	H-3->L+1 (40%)
				H-1->L+3 (12%)
7	421	2.94	1.4689	H-3->L+6 (26%)
				H-2->L+7 (33%)
8	421	2.95	0.9946	H-5->L+2 (21%)
				H-3->L+4(20%)

Table S4 Calculated the wavelengths (λ in nm), excitation energies (eV), and rotatory strengths (R) values for the CD spectra in Fig.6

Compounds	λ	E	R
1	379	3.27	0.1264
	427	2.90	-0.8494
2	437	2.84	0.6755
3	388	3.20	-0.0113
	446	2.78	-0.0488
	605	2.05	0.0368
4	391	3.17	-0.2041
5	450	2.75	0.4801
	596	2.08	-00758
6	415	2.99	-28.785
	468	2.65	18.446
7	421	2.94	-0.5182
	523	2.37	0.3809
	607	2.04	-12.7141
8	409	3.03	-19.591
	484	2.56	10.358
	541	2.29	-1.201

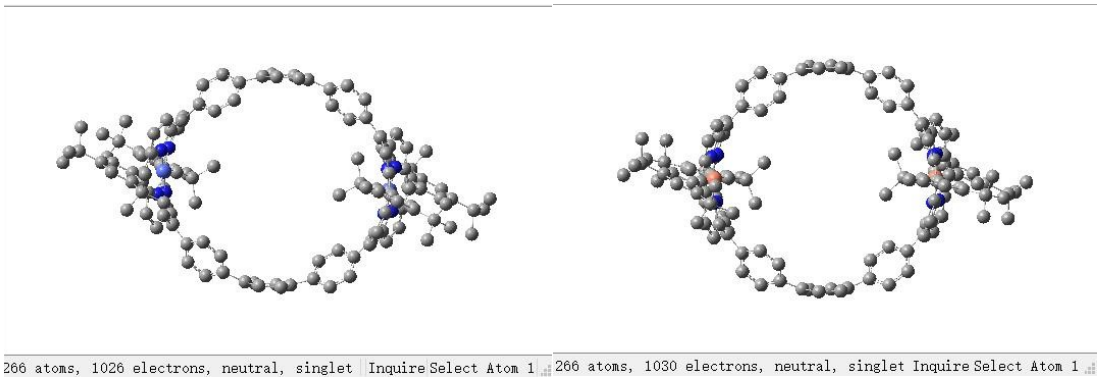


Fig. S1. The atom, electron numbers and charges, multiplicities for compounds **4** (left) and **5** (right) in GaussView.

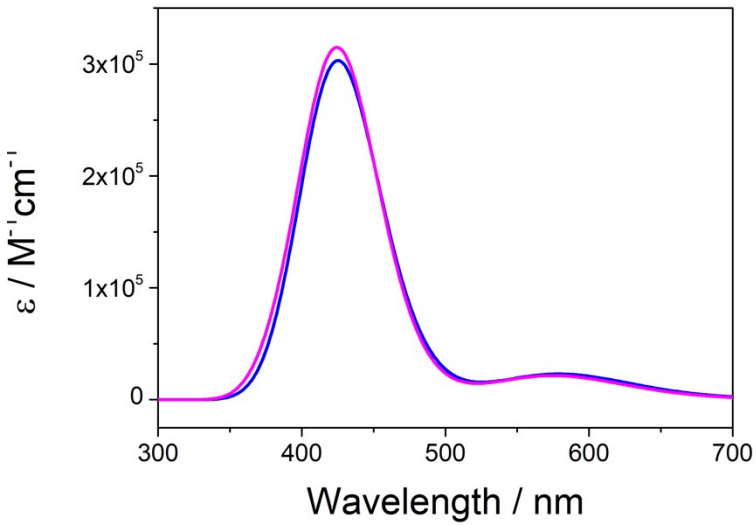


Fig. S2. The simulated UV-visible absorption spectra for compound **4** with two geometries from open-shell singlet and closed-shell singlet optimization, respectively.

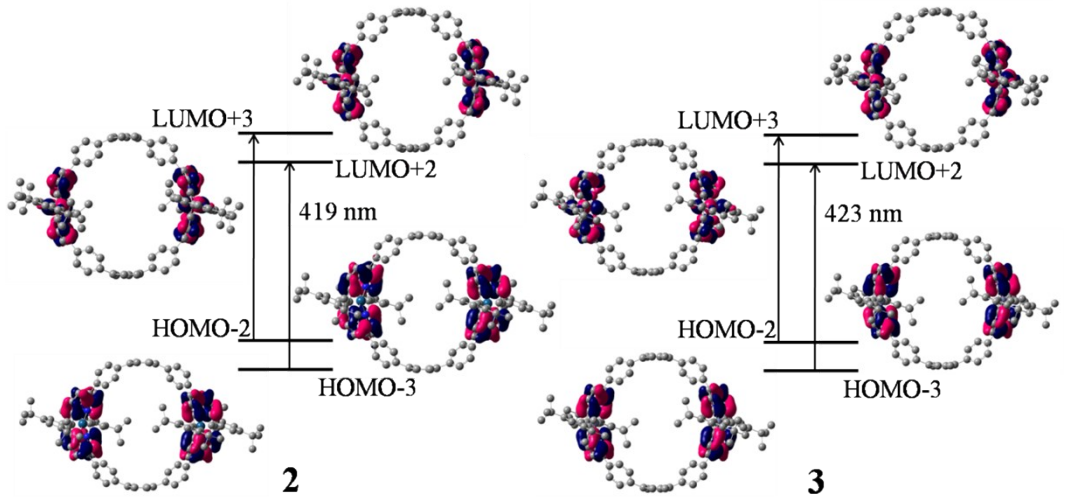


Fig. S3 Molecular orbital isosurfaces involved in the main electron transitions of compounds **2** and **3**.

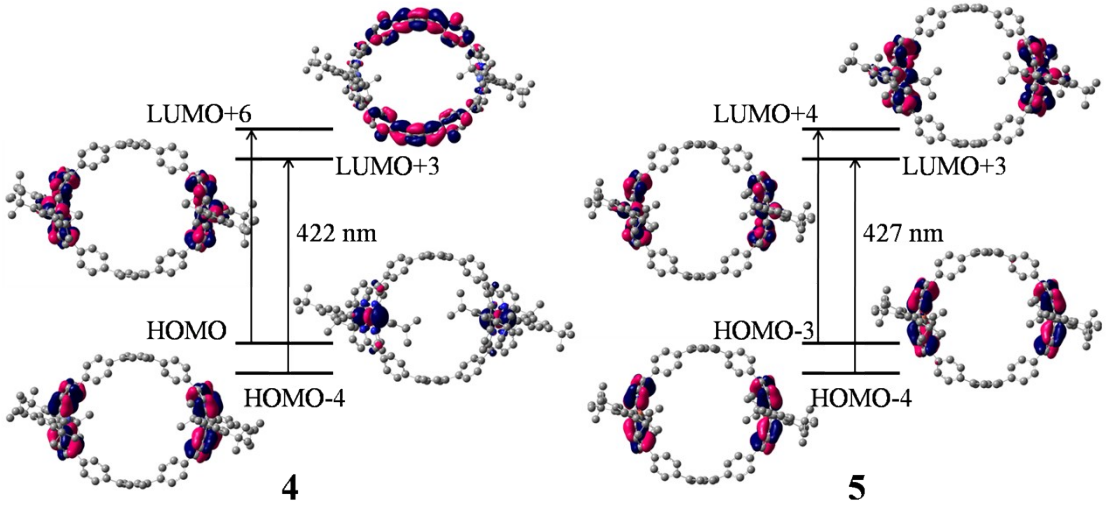


Fig. S4 Molecular orbital isosurfaces involved in the main electron transitions of compounds **4** and **5**.

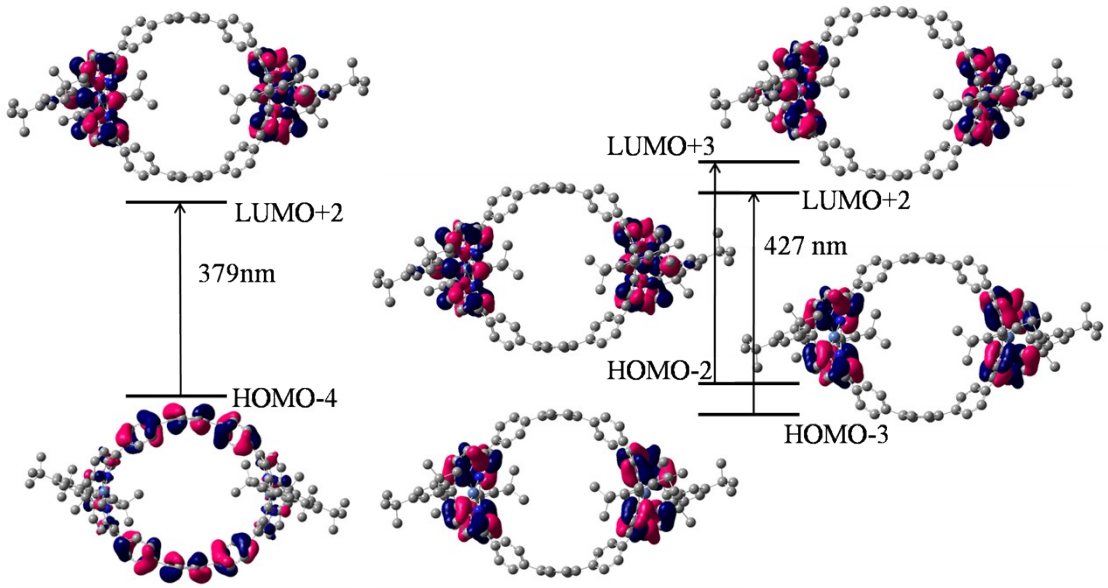


Fig. S5 Molecular orbitals involved into the main CD transitions of compound **1**.