

Supporting information

The Structure-NLO Property relationships of Mobius helical carbon nanohoop under External Electric Field

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Table S1. The atomic coordinates of studied Mobius helicene carbon nanohoop calculated at the M062X/6–31G**.

C	-0.12494600	3.60440800	1.00256600
C	-0.34099800	3.19797900	2.32619300
C	-1.37193000	2.32949000	2.65025900
C	-2.22294800	1.82255300	1.66168200
C	-2.08282400	2.31363200	0.35870300
C	-1.05638100	3.19513000	0.03804200
C	1.17595400	4.22684800	0.64484100
C	1.93581300	4.95534700	1.57269000
C	3.29677800	5.16179200	1.38184500
C	3.94543400	4.66128400	0.24549800
C	3.14902700	4.10148200	-0.76139700
C	1.79287700	3.88322200	-0.56348800
H	0.36067800	3.49427800	3.09917300
H	-1.48791300	1.99798000	3.67800200
H	-2.73567900	1.93931700	-0.42561300
H	-0.94604800	3.52144600	-0.99219400
H	1.46932100	5.31037500	2.48688200
H	3.87677000	5.65899300	2.15453500
H	3.62442000	3.69887900	-1.65054900
H	1.24029400	3.31655400	-1.30600900
C	-2.22636400	-1.92231500	-1.60120300
C	-2.12295300	-2.34212000	-0.27041900
C	-1.36692600	-2.49836600	-2.54369800
C	-1.10905200	-3.20722600	0.12360200
H	-2.78789600	-1.91545000	0.47510300
C	-0.35378300	-3.36034500	-2.14878600
H	-1.45678100	-2.22066300	-3.59003500
C	-0.16311800	-3.67692900	-0.79735900
H	-1.01276900	-3.46638700	1.17442700
H	0.36126100	-3.71420500	-2.88526700
C	1.13980900	-4.24725000	-0.37089900
C	1.76624800	-3.70337000	0.75556900
C	1.89356400	-5.11704900	-1.17177300
C	3.12361900	-3.87985300	0.97282800
H	1.21657600	-3.01879700	1.39374900
C	3.25402900	-5.30067400	-0.94875300
H	1.42108400	-5.61140500	-2.01598900
C	3.91583000	-4.61395200	0.07948300

H	3.59558000	-3.31968700	1.77250200
H	3.82006200	-5.93614100	-1.62393100
C	5.37983400	-4.35596700	0.07970900
C	6.03465000	-3.88438600	1.22535800
C	6.06557600	-4.23388300	-1.13711000
C	7.15653700	-3.07425600	1.11880900
H	5.59084900	-4.04159600	2.20369300
C	7.21060200	-3.45478400	-1.23853600
H	5.62389200	-4.63137200	-2.04577600
C	7.68823500	-2.73495600	-0.13377700
H	7.52653400	-2.58143700	2.01222500
H	7.65304800	-3.29979800	-2.21783300
C	8.35466700	-1.41382000	-0.29467400
C	8.93083200	-0.71266900	0.77685400
C	8.04423400	-0.66932100	-1.44007200
C	8.93115300	0.67741000	0.80181400
H	9.28477900	-1.25385300	1.64965700
C	8.04588200	0.71638300	-1.41588800
H	7.61502200	-1.16281200	-2.30486500
C	8.35691600	1.41697300	-0.24434700
H	9.28320500	1.18810800	1.69369000
H	7.61823100	1.24459500	-2.26131500
C	5.40246700	4.37470700	0.20222200
C	5.98425400	3.78892700	1.33216800
C	6.12864500	4.32554700	-0.99616800
C	7.10315700	2.97534000	1.21410000
H	5.45708500	3.82394100	2.28079700
C	7.25870000	3.52582000	-1.10938200
H	5.74996600	4.84317300	-1.87324700
C	7.68615500	2.72872200	-0.03527900
H	7.41201300	2.39074000	2.07460800
H	7.74882800	3.43712700	-2.07461600
C	-9.18890800	1.14574700	-0.73609300
C	-8.48854200	0.08255900	-0.10090300
C	-7.06629900	0.04910100	-0.07600800
C	-6.38617600	0.89657300	-1.05099100
C	-7.10820900	1.98939900	-1.58852700
C	-8.50673100	2.13085800	-1.36880300
C	-6.46200800	-0.82931700	0.92103800
C	-5.06692100	0.63772600	-1.62663700
C	-4.36246100	0.52985900	1.36237500
C	-5.15368000	-0.63226000	1.54388600
C	-3.11968600	0.67907400	1.95544600
C	-2.51932700	0.22872500	-2.80083800

C	-6.47972800	2.95308900	-2.43917500
H	-7.06482200	3.81234900	-2.75314400
H	-10.27244000	1.16271500	-0.66694100
H	-9.01800400	2.98533700	-1.80142300
H	-1.52161000	0.08485600	-3.20256300
H	-2.80663000	2.12962900	-3.73438200
C	-9.25987500	-0.94626800	0.50814400
C	-8.64746800	-1.96303000	1.16197500
C	-7.25225800	-1.88805800	1.43005700
H	-10.33994700	-0.91209800	0.40134600
H	-9.21332900	-2.79272300	1.57441100
C	-6.69830400	-2.88208500	2.29734100
C	-5.43183900	-2.77673500	2.75787300
C	-4.65619700	-1.62225800	2.43872700
H	-7.33289600	-3.71407800	2.58774800
H	-5.00451600	-3.52800900	3.41530100
C	-2.63433500	-0.34126700	2.80835100
H	-1.64587700	-0.24519200	3.24545200
C	-3.39529300	-1.45273400	3.05264000
H	-3.03565300	-2.23328400	3.71754100
C	-3.22211500	1.37047100	-3.07728400
C	-5.20500700	2.78671800	-2.85689500
C	-4.49436500	1.59957100	-2.50751000
C	-3.07704200	-0.76098900	-1.95696400
C	-4.33322600	-0.55582500	-1.41091800
H	-4.74046100	1.34155100	0.75285500
H	-4.72181800	3.51406900	-3.50248100
H	-4.76393200	-1.34590800	-0.80833600

Table S2 The NICS value of each loop of the studied system and the two electrons gained and lost M062X/6–31G**.

Ring sequence number	2cation	0	2anion
1	-4.2017	-8.9266	2.6520
2	0.6975	-6.2491	3.7199
3	-1.3036	-6.9386	9.5500
4	-1.3035	-6.8487	9.5534
5	0.6971	-6.2984	3.7219
6	-4.9737	-8.9975	2.6318
7	-8.8486	-9.0091	-8.5436
8	-6.3995	-8.5023	-8.0918
9	-5.8006	-8.3141	-5.6466
10	-5.1179	-8.4233	-5.0575
11	-5.8000	-8.6199	-5.6480
12	-6.3983	-8.5842	-6.6238
13	-8.8463	-8.7859	-8.5460

Figure S1. Ring currents of AICD plots of π -conjugation region of the studied system at M062X/6–31G**.

