Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information: Non-equilibrium steady state conductivity in cyclo[18]carbon and its boron nitride analogue

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Table 1: Geometry for C_{18} from v2RDM/cc-pVDZ in [18,18] active space (Å)

Atom	x	y	z
C	-0.62380942	3.72630650	0.00000000
C	0.62291449	3.72644050	0.00000000
C	1.91872330	3.25535916	0.00000000
C	2.87613180	2.45050631	0.00000000
C	3.55842912	1.27046048	0.00000000
C	-1.91590384	3.25626082	0.00000000
C	-2.87717842	2.44866627	0.00000000
C	-3.55840715	1.26984949	0.00000000
C	-3.77964735	0.03106409	0.00000000
C	-3.53059019	-1.33568054	0.00000000
C	-2.90752173	-2.40348888	0.00000000
C	-1.88440979	-3.27483555	0.00000000
C	-0.67478512	-3.71888232	0.00000000
C	0.67612030	-3.71819133	0.00000000
C	1.88479478	-3.27299239	0.00000000
C	2.90530809	-2.40446204	0.00000000
C	3.52962681	-1.33625313	0.00000000
C	3.78062606	0.03039037	0.00000000

Table 2: Geometry for B_9N_9 from v2RDM/cc-pVDZ in [18,18] active space (Å)

Atom	x	y	z
B	0.00000000	3.61651835	0.00000000
B	-2.32411949	2.77006952	0.00000000
B	-3.56155765	0.62773507	0.00000000
B	-3.13177767	-1.80771364	0.00000000
B	-1.23655144	-3.39829903	0.00000000
B	1.23655144	-3.39829903	0.00000000
B	3.13177767	-1.80771364	0.00000000
B	3.56155765	0.62773507	0.00000000
B	2.32411949	2.77006952	0.00000000
N	1.31643579	3.61850522	0.00000000
N	-1.31643579	3.61850522	0.00000000
N	-3.33518148	1.92494573	0.00000000
N	-3.79190846	-0.66823481	0.00000000
N	-2.47514473	-2.95013688	0.00000000
N	0.00000000	-3.85026071	0.00000000
N	2.47514473	-2.95013688	0.00000000
N	3.79190846	-0.66823481	0.00000000
N	3.33518148	1.92494573	0.00000000