

Electric field-induced bond length and bandgap tunability for enhanced reactivity of nitride nanorings

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Supplementary information:

Table S1: The HOMO and LUMO energy values of Al₉N₉ and B₉N₉ nanorings with different external electric field values, respectively.

System/electric field (EF) (a.u.)	Al ₉ N ₉ nanoring		B ₉ N ₉ nanoring	
	HOMO (eV)	LUMO (eV)	HOMO (eV)	LUMO (eV)
0.00	-8.72	-1.16	-9.75	0.30
0.01	-8.68	-1.18	-9.74	-0.13
0.02	-8.60	-1.34	-9.73	-0.95
0.03	-8.52	-1.60	-9.72	-1.88
0.04	-8.47	-2.59	-9.82	-4.73
0.05	-8.51	-3.60	-11.30	-7.91

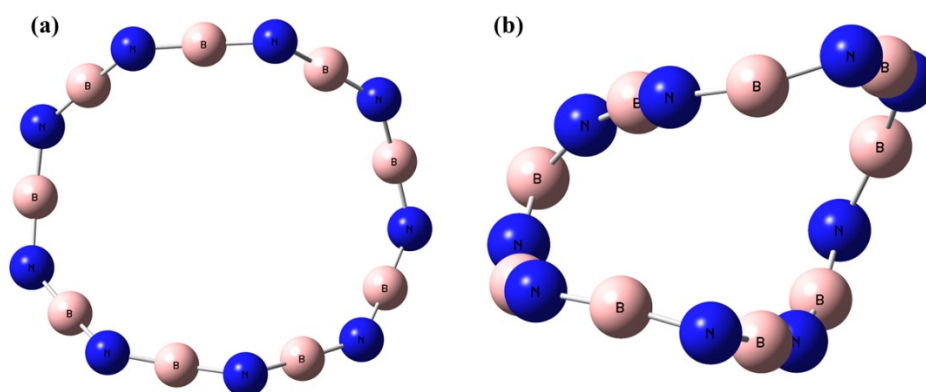


Figure S1: The geometrical structure of B₉N₉ nanoring at 0.04 a.u. (a) and 0.05 a.u. (b) value of the external electric field, respectively (Boron is shown as a pink sphere and nitrogen is indicated as a blue sphere, respectively).

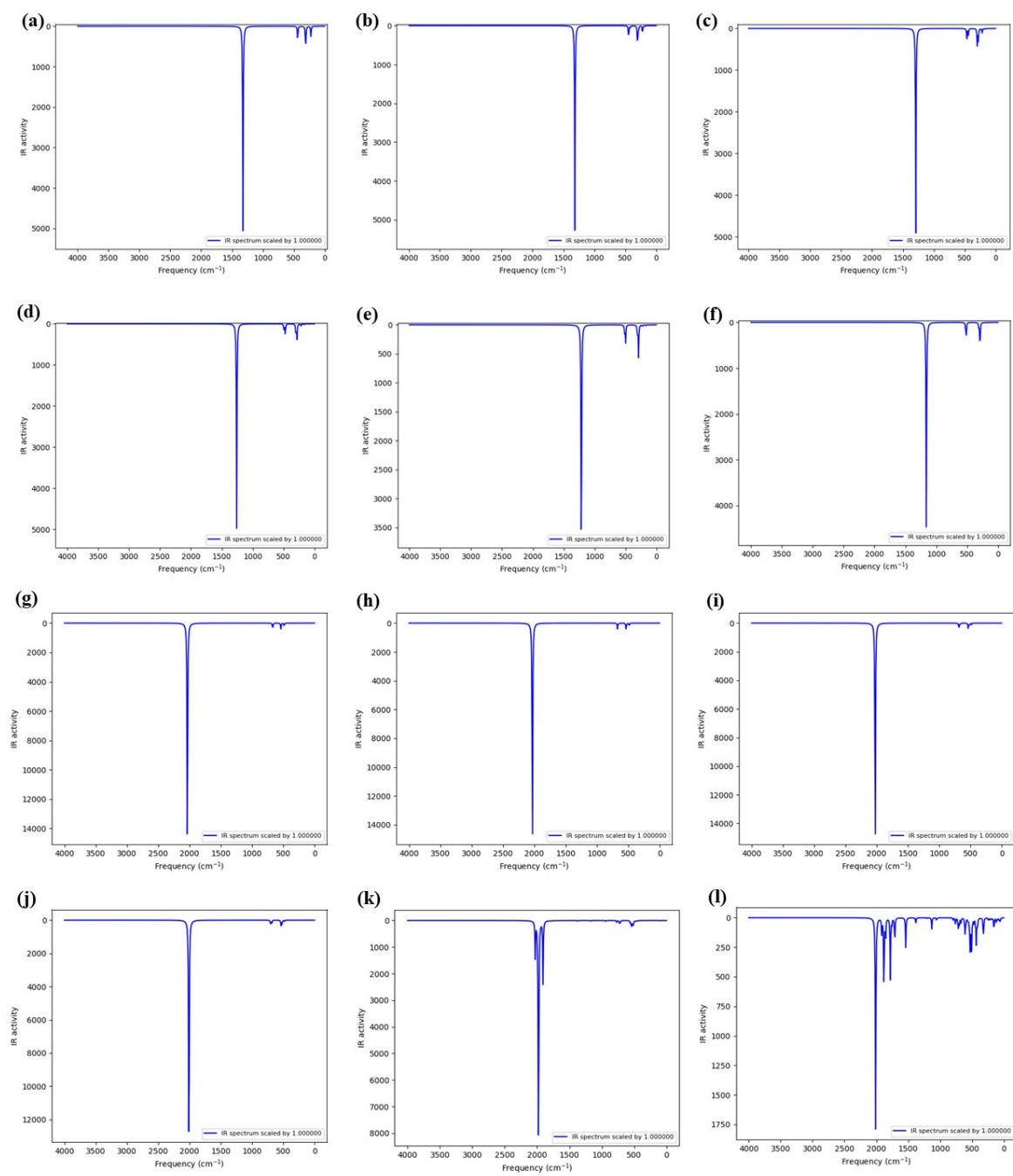


Figure S2: The IR spectra of Al_9N_9 nanoring (a-f), and B_9N_9 nanoring (i-l), at external electric field from 0.00 to 0.05 a.u., respectively.

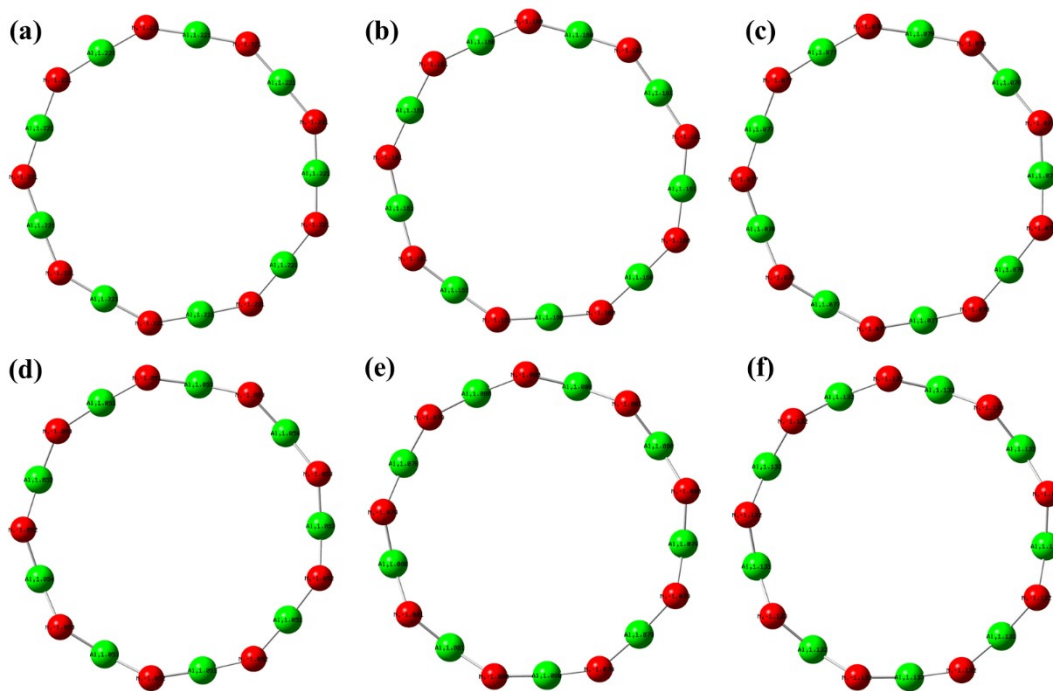


Figure S3: The Mulliken charge distribution of Al_9N_9 nanoring with respect to the external electric field (Red spheres represent negatively charged atoms, while green spheres represent positively charged atoms, respectively).

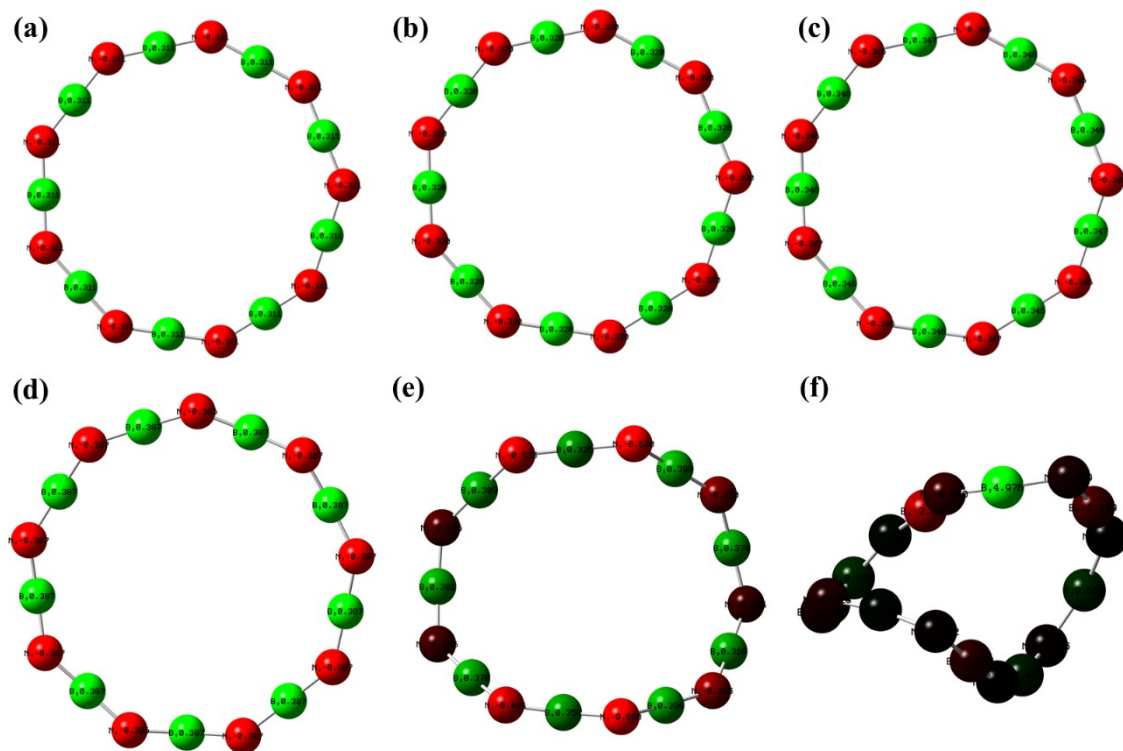


Figure S4: The Mulliken charge distribution of B_9N_9 nanoring with respect to the external electric field (Red spheres represent negatively charged atoms, while green spheres represent positively charged atoms, respectively).