Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Table S1. Relaxed lattice constants **a** in [0001] plane (in Å) and **c** along (0001) direction (in Å), and unit cell volume V (in $Å^3$).

Structure	Site	a	c	V
B_{12}-CCC	No Si	5.64	12.12	111.4
	Chain Center	5.62	12.62	115.1
	Chain End	6.17	11.77	129.0
	Equatorial	5.78	12.43	120.0
	Polar	5.70	12.70	118.7
B_{12}-CBC	No Si	5.66	12.13	112.0
	Chain Center	5.62	12.62	115.1
	Chain End	5.87	12.32	122.4
	Equatorial	5.79	12.45	120.5
	Polar	5.73	12.70	120.1
$B_{11}C^P$-CBC	No Si	5.60	12.06	109.0
	Chain Center	5.62	12.44	113.0
	Chain End	5.90	12.28	123.0
	Equatorial	5.71	12.59	118.2
	Polar	5.73	12.70	120.1