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**Table S5**: Relative formation energies for all possible sites of Si in B<sub>11</sub>C<sup>p</sup>-CBC.

1 .	
chain	center

	-4.89			
chain end				
	13	near C	-3.63	
	14	far from C	-3.37	
equatorial				
	7	nearest C	-3.87	
	10,12	neighbors of 7	-4.30	
	9,11	neighbors of 10,12	-3.81	
	8	opposite C	-3.90	
polar				
	1	C	-7.22	
	3,5	neighbors of 1	-5.00	
	4,6	under C	-4.79	
	2	other pole opposite C	-4.95	