

Table S5: Relative formation energies for all possible sites of Si in B₁₁C^p-CBC.

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