Supporting Information

New Boron Nitride B₂₄N₂₄ Nanotube

Hai-Shun Wu^{a}, Xiao-Hong Xu^a, Fu-Qiang Zhang^a and Haijun Jiao^{b*}*

(a) Department of Chemistry, Shanxi Normal University, Linfen, 041004, China. (b) Leibniz-Institut für Organische Katalyse an der Universität Rostock e.V., Buchbinderstrasse 5-6, 18055 Rostock, Germany

E-mail. hjiao@ifok.uni-rostock.de

Table S1. Total electronic energies (E_{tot} , au), zero-point energies (ZPE, eV) of $\text{B}_{12}\text{N}_{12}$ monomers

Isomer	$E_{\text{tot}}/\text{Fopt}^{\text{a}}$	ZPE (NImag) ^a	$E_{\text{tot}}/\text{sp (HF)}^{\text{b}}$	$E_{\text{tot}}/\text{sp (MP2(fc))}^{\text{b}}$	$E_{\text{tot}}/\text{sp}^{\text{c}}$
$\text{F}_{46}\text{-1 (}T_{\text{h}}\text{)}$	−956.14499	3.5 (0)	−950.56051	−953.37585	−956.34846
$\text{F}_{46}\text{-2 (}C_{2\text{v}}\text{)}$	−955.74171	3.4 (0)	−950.10276	−952.93997	−955.94753
$\text{F}_{46}\text{-3 (}C_1\text{)}$	−955.73064	3.4 (0)	−950.08912	−952.92834	−955.93679
$\text{F}_{46}\text{-4 (}C_1\text{)}$	−955.72345	3.4 (0)	−950.08251	−952.92429	−955.92827
$\text{F}_{46}\text{-5 (}C_{2\text{h}}\text{)}$	−955.55113	3.3 (0)	−949.89442	−952.74703	−955.75649
$\text{F}_{56}\text{-1 (}C_1\text{)}$	−955.80748	3.5 (0)	−950.17703	−953.01232	−956.01358
$\text{F}_{56}\text{-2 (}C_3\text{)}$	−955.80268	3.5 (0)	−950.17131	−953.00648	−956.00909
$\text{F}_{56}\text{-3 (}C_{2\text{v}}\text{)}$	−955.75313	3.5 (0)	−950.10815	−952.95184	−955.95943
$\text{F}_{56}\text{-4 (}C_1\text{)}$	−955.66978	3.4 (0)	−950.01939	−952.86533	−955.87646
$\text{F}_{56}\text{-5 (}C_{2\text{v}}\text{)}$	−955.65227	3.4 (0)	−949.99375	−952.85122	−955.85889
$\text{F}_{456}\text{ (}C_1\text{)}$	−956.01916	3.5 (0)	−950.41639	−953.24171	−956.22369

a) At B3LYP/6-31G*. b) Single-point energies using the B3LYP/6-31G* geometries.

c) Single-point energies at B3LYP/6-311+G* with the B3LYP/6-31G* geometries.

Table 2. Total electronic energies (E_{tot} , au), zero-point energies (ZPE, eV) of $\text{B}_{24}\text{N}_{24}$ isomers

Isomer	$E_{\text{tot}}/\text{Fopt}^{\text{a}}$	ZPE (NImag) ^a
1 (C_{2h})	−1912.35055	7.0 (0)
2 (C_{2h})	−1912.35021	7.0 (0)
3 (C_1)	−1912.36999	7.7 (0) ^b
4 (C_i)	−1912.37588	7.0 (0)
5 (C_1)	−1912.39785	7.7 (0) ^b
6 (D_{2d})	−1912.34963	7.0 (0)
7 (S_6)	−1912.67802	7.2 (0)
8 (S_4)	−1912.74226	7.3 (0)
9 (C_3)	−1912.51021	7.8 (0) ^b

a) At B3LYP/6-31G*. b) At HF/6-31G*