Supplementary Information

Magic Electron Counts and Bonding in Tubular Boranes

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Total Energy and Cartesian Coordinates of borane nanotubes optimized at
B3LYP/6-31G* level of theory

B22H22(2-)

HF = -560.24597

Cartesian Coordinates

H	0.000000	2.882304	0.785385
H	2.741234	0.890681	0.785385
B	-1.421523	0.461881	-2.317213
B	0.000000	1.494678	-2.317213
B	-0.878550	-1.209220	-2.317213
B	0.878550	-1.209220	-2.317213
B	1.421523	0.461881	-2.317213
B	1.605575	-0.521683	-0.816533
B	0.000000	-1.688201	-0.816533
B	-0.992300	1.365783	-0.816533
B	-1.605575	-0.521683	-0.816533
B	0.992300	1.365783	-0.816533
H	-1.694176	-2.331833	0.785385
H	1.694176	2.331833	-0.785385
B	0.000000	1.688201	0.816533
B	0.992300	-1.365783	0.816533
B	-1.605575	0.521683	0.816533
B	-0.992300	-1.365783	0.816533
B	1.605575	0.521683	0.816533
H	-2.741234	0.890681	0.785385
H	1.694176	-2.331833	0.785385
H	-2.448649	0.795614	-2.835738
H	0.000000	2.574662	-2.835738
H	2.448649	0.795614	-2.835738
H	1.513348	-2.082945	-2.835738
H	-1.513348	-2.082945	-2.835738
H	2.741234	-0.890681	-0.785385
H	0.000000	-2.882304	-0.785385
H	-2.741234	-0.890681	-0.785385
H	-1.694176	2.331833	-0.785385
H	0.000000	-2.574662	2.835738
B	0.000000	0.000000	3.236736
B	-0.878550	1.209220	2.317213
B	0.000000	0.000000	-3.236736
H	-2.448649	-0.795614	2.835738
H	0.000000	0.000000	4.435565
H	0.000000	0.000000	-4.435565
B	1.421523	-0.461881	2.317213
B	-1.421523	-0.461881	2.317213
H	-1.513348	2.082945	2.835738
B	0.000000	-1.494678	2.317213
B	0.878550	1.209220	2.317213
H	2.448649	-0.795614	2.835738
H	1.513348	2.082945	2.835738

B27H27(2-)

HF = -687.50763

Cartesian Coordinates

H	0.000000	2.567583	-3.611234
H	-1.509187	-2.077218	-3.611234
B	-0.881511	-1.213296	-3.070695
H	-2.441916	0.793427	-3.611234
H	1.509187	-2.077218	3.611234
H	0.000000	0.000000	-5.185174
B	0.000000	1.499717	-3.070695
H	2.441916	0.793427	-3.611234
H	1.509187	-2.077218	-3.611234
B	0.881511	-1.213296	-3.070695
B	1.426315	0.463438	-3.070695
B	-1.426315	0.463438	-3.070695
B	-1.019606	1.403367	-1.598561
B	0.000000	-1.734657	-1.598561
B	1.019606	1.403367	-1.598561
B	-1.649757	-0.536039	-1.598561
B	1.649757	-0.536039	-1.598561
H	-1.720904	2.368621	-1.542875
H	-2.784481	-0.904733	-1.542875
H	0.000000	-2.927776	-1.542875
H	2.784481	-0.904733	-1.542875
H	1.720904	2.368621	-1.542875
H	-1.509187	-2.077218	3.611234
B	0.000000	0.000000	-3.987973
B	0.000000	1.577343	0.000000
B	-0.927139	-1.276097	0.000000
B	1.500142	0.487426	0.000000
B	-1.500142	0.487426	0.000000
B	0.927139	-1.276097	0.000000
H	0.000000	2.766413	0.000000
H	2.631015	0.854869	0.000000
H	-2.631015	0.854869	0.000000
H	-1.626057	-2.238075	0.000000
H	1.626057	-2.238075	0.000000
B	0.000000	0.000000	3.987973
H	-2.441916	0.793427	3.611234
B	1.019606	1.403367	1.598561
B	0.000000	-1.734657	1.598561
B	-1.019606	1.403367	1.598561
B	-1.649757	-0.536039	1.598561
B	1.649757	-0.536039	1.598561
H	1.720904	2.368621	1.542875
H	-1.720904	2.368621	1.542875
H	-2.784481	-0.904733	1.542875
H	0.000000	-2.927776	1.542875
H	2.784481	-0.904733	1.542875
H	0.000000	0.000000	5.185174
H	0.000000	2.567583	3.611234
B	0.000000	1.499717	3.070695
B	-0.881511	-1.213296	3.070695
B	1.426315	0.463438	3.070695
B	-1.426315	0.463438	3.070695
B	0.881511	-1.213296	3.070695
H	2.441916	0.793427	3.611234