

## Supporting Information

# Separation of Carbon Dioxide and Nitrogen Gases through Modified Boron Nitride Nanosheets as a Membrane: Insights from Molecular Dynamics Simulations

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**Table S1.** Parameters for the 12–6 Lennard–Jones potential used in the simulations.

molecule	site	$\epsilon$ (kcal/mol)	$R_{\min}/2$ (Å)	bond length (Å)
CO <sub>2</sub>	C	0.054	1.571	$l_{\text{C-O}} = 1.16$
	O	0.157	1.711	
N <sub>2</sub>	N	0.072	1.857	$l_{\text{N-N}} = 1.10$
	COM*	0	0	
BNNS	B	0.950	2.840	$l_{\text{B-N}} = 1.44$
	N	0.077	0.468	$l_{\text{B-H}} = 1.20$
	O	0.152	1.768	$l_{\text{N-F}} = 1.39$
	F	0.135	1.630	$l_{\text{N-O}} = 1.47$
	H	0.028	1.280	$l_{\text{O-H}} = 0.99$

\*COM: center of mass site

**Cartesian coordinates (Å) for all geometries and together with their corresponding DFT energies.**

**Pore 1.** (The final potential energy from DFT calculations: -14089.10 Hartree)

B	-15.314000000	-15.528000000	0.000000000
N	-16.535000000	-16.233000000	0.000000000
N	-15.314000000	-14.118000000	0.000000000
B	-16.535000000	-13.413000000	0.000000000
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B	-16.535000000	-9.183000000	0.000000000
B	-15.314000000	-7.068000000	0.000000000
N	-16.535000000	-7.773000000	0.000000000
N	-15.314000000	-5.658000000	0.000000000
B	-16.535000000	-4.953000000	0.000000000
B	-15.314000000	-2.838000000	0.000000000
N	-16.535000000	-3.543000000	0.000000000
N	-15.314000000	-1.428000000	0.000000000
B	-16.535000000	-0.723000000	0.000000000
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B	13.9920000000	9.8520000000	0.0000000000
N	12.7710000000	9.1470000000	0.0000000000
N	13.9920000000	11.2620000000	0.0000000000
B	12.7710000000	11.9670000000	0.0000000000
B	13.9920000000	14.0820000000	0.0000000000
N	12.7710000000	13.3770000000	0.0000000000
N	13.9920000000	15.4920000000	0.0000000000
B	12.7710000000	16.1970000000	0.0000000000
B	16.4350000000	-15.5280000000	0.0000000000
N	15.2130000000	-16.2330000000	0.0000000000
N	16.4350000000	-14.1180000000	0.0000000000
B	15.2130000000	-13.4130000000	0.0000000000
B	16.4350000000	-11.2980000000	0.0000000000
N	15.2130000000	-12.0030000000	0.0000000000
N	16.4350000000	-9.8880000000	0.0000000000
B	15.2130000000	-9.1830000000	0.0000000000
B	16.4350000000	-7.0680000000	0.0000000000
N	15.2130000000	-7.7730000000	0.0000000000
N	16.4350000000	-5.6580000000	0.0000000000
B	15.2130000000	-4.9530000000	0.0000000000
B	16.4350000000	-2.8380000000	0.0000000000
N	15.2130000000	-3.5430000000	0.0000000000
N	16.4350000000	-1.4280000000	0.0000000000
B	15.2130000000	-0.7230000000	0.0000000000
B	16.4350000000	1.3920000000	0.0000000000
N	15.2130000000	0.6870000000	0.0000000000
N	16.4350000000	2.8020000000	0.0000000000
B	15.2130000000	3.5070000000	0.0000000000
B	16.4350000000	5.6220000000	0.0000000000
N	15.2130000000	4.9170000000	0.0000000000
N	16.4350000000	7.0320000000	0.0000000000
B	15.2130000000	7.7370000000	0.0000000000
B	16.4350000000	9.8520000000	0.0000000000
N	15.2130000000	9.1470000000	0.0000000000
N	16.4350000000	11.2620000000	0.0000000000
B	15.2130000000	11.9670000000	0.0000000000
B	16.4350000000	14.0820000000	0.0000000000
N	15.2130000000	13.3770000000	0.0000000000
N	16.4350000000	15.4920000000	0.0000000000
B	15.2130000000	16.1970000000	0.0000000000

**Pore 2.** (The final potential energy from DFT calculations: -14101.21 Hartree)



B	-15.2640000000	-15.5100000000	0.0000000000
N	-16.4850000000	-16.2150000000	0.0000000000
N	-15.2640000000	-14.1000000000	0.0000000000
B	-16.4850000000	-13.3950000000	0.0000000000
B	-15.2640000000	-11.2800000000	0.0000000000
N	-16.4850000000	-11.9850000000	0.0000000000
N	-15.2640000000	-9.8700000000	0.0000000000
B	-16.4850000000	-9.1650000000	0.0000000000
B	-15.2640000000	-7.0500000000	0.0000000000
N	-16.4850000000	-7.7550000000	0.0000000000
N	-15.2640000000	-5.6400000000	0.0000000000
B	-16.4850000000	-4.9350000000	0.0000000000
B	-15.2640000000	-2.8200000000	0.0000000000
N	-16.4850000000	-3.5250000000	0.0000000000
N	-15.2640000000	-1.4100000000	0.0000000000
B	-16.4850000000	-0.7050000000	0.0000000000
B	-15.2640000000	1.4100000000	0.0000000000
N	-16.4850000000	0.7050000000	0.0000000000
N	-15.2640000000	2.8200000000	0.0000000000
B	-16.4850000000	3.5250000000	0.0000000000
B	-15.2640000000	5.6400000000	0.0000000000
N	-16.4850000000	4.9350000000	0.0000000000
N	-15.2640000000	7.0500000000	0.0000000000
B	-16.4850000000	7.7550000000	0.0000000000
B	-15.2640000000	9.8700000000	0.0000000000
N	-16.4850000000	9.1650000000	0.0000000000
N	-15.2640000000	11.2800000000	0.0000000000
B	-16.4850000000	11.9850000000	0.0000000000
B	-15.2640000000	14.1000000000	0.0000000000
N	-16.4850000000	13.3950000000	0.0000000000
N	-15.2640000000	15.5100000000	0.0000000000
B	-16.4850000000	16.2150000000	0.0000000000
B	-12.8220000000	-15.5100000000	0.0000000000
N	-14.0430000000	-16.2150000000	0.0000000000
N	-12.8220000000	-14.1000000000	0.0000000000
B	-14.0430000000	-13.3950000000	0.0000000000
B	-12.8220000000	-11.2800000000	0.0000000000
N	-14.0430000000	-11.9850000000	0.0000000000
N	-12.8220000000	-9.8700000000	0.0000000000
B	-14.0430000000	-9.1650000000	0.0000000000
B	-12.8220000000	-7.0500000000	0.0000000000
N	-14.0430000000	-7.7550000000	0.0000000000
N	-12.8220000000	-5.6400000000	0.0000000000
B	-14.0430000000	-4.9350000000	0.0000000000
B	-12.8220000000	-2.8200000000	0.0000000000
N	-14.0430000000	-3.5250000000	0.0000000000
N	-12.8220000000	-1.4100000000	0.0000000000
B	-14.0430000000	-0.7050000000	0.0000000000
B	-12.8220000000	1.4100000000	0.0000000000
N	-14.0430000000	0.7050000000	0.0000000000
N	-12.8220000000	2.8200000000	0.0000000000
B	-14.0430000000	3.5250000000	0.0000000000
B	-12.8220000000	5.6400000000	0.0000000000
N	-14.0430000000	4.9350000000	0.0000000000
N	-12.8220000000	7.0500000000	0.0000000000
B	-14.0430000000	7.7550000000	0.0000000000
B	-12.8220000000	9.8700000000	0.0000000000
N	-14.0430000000	9.1650000000	0.0000000000
N	-12.8220000000	11.2800000000	0.0000000000
B	-14.0430000000	11.9850000000	0.0000000000
B	-12.8220000000	14.1000000000	0.0000000000
N	-14.0430000000	13.3950000000	0.0000000000
N	-12.8220000000	15.5100000000	0.0000000000
B	-14.0430000000	16.2150000000	0.0000000000
B	-10.3800000000	-15.5100000000	0.0000000000
N	-11.6010000000	-16.2150000000	0.0000000000
N	-10.3800000000	-14.1000000000	0.0000000000
B	-11.6010000000	-13.3950000000	0.0000000000
B	-10.3800000000	-11.2800000000	0.0000000000
N	-11.6010000000	-11.9850000000	0.0000000000
N	-10.3800000000	-9.8700000000	0.0000000000
B	-11.6010000000	-9.1650000000	0.0000000000
B	-10.3800000000	-7.0500000000	0.0000000000
N	-11.6010000000	-7.7550000000	0.0000000000
N	-10.3800000000	-5.6400000000	0.0000000000

B	-11.601000000	-4.935000000	0.000000000
B	-10.380000000	-2.820000000	0.000000000
N	-11.601000000	-3.525000000	0.000000000
N	-10.380000000	-1.410000000	0.000000000
B	-11.601000000	-0.705000000	0.000000000
B	-10.380000000	1.410000000	0.000000000
N	-11.601000000	0.705000000	0.000000000
N	-10.380000000	2.820000000	0.000000000
B	-11.601000000	3.525000000	0.000000000
B	-10.380000000	5.640000000	0.000000000
N	-11.601000000	4.935000000	0.000000000
N	-10.380000000	7.050000000	0.000000000
B	-11.601000000	7.755000000	0.000000000
B	-10.380000000	9.870000000	0.000000000
N	-11.601000000	9.165000000	0.000000000
N	-10.380000000	11.280000000	0.000000000
B	-11.601000000	11.985000000	0.000000000
B	-10.380000000	14.100000000	0.000000000
N	-11.601000000	13.395000000	0.000000000
N	-10.380000000	15.510000000	0.000000000
B	-11.601000000	16.215000000	0.000000000
B	-7.937000000	-15.510000000	0.000000000
N	-9.158000000	-16.215000000	0.000000000
N	-7.937000000	-14.100000000	0.000000000
B	-9.158000000	-13.395000000	0.000000000
B	-7.937000000	-11.280000000	0.000000000
N	-9.158000000	-11.985000000	0.000000000
N	-7.937000000	-9.870000000	0.000000000
B	-9.158000000	-9.165000000	0.000000000
B	-7.937000000	-7.050000000	0.000000000
N	-9.158000000	-7.755000000	0.000000000
N	-7.937000000	-5.640000000	0.000000000
B	-9.158000000	-4.935000000	0.000000000
B	-7.937000000	-2.820000000	0.000000000
N	-9.158000000	-3.525000000	0.000000000
N	-7.937000000	-1.410000000	0.000000000
B	-9.158000000	-0.705000000	0.000000000
B	-7.937000000	1.410000000	0.000000000
N	-9.158000000	0.705000000	0.000000000
N	-7.937000000	2.820000000	0.000000000
B	-9.158000000	3.525000000	0.000000000
B	-7.937000000	5.640000000	0.000000000
N	-9.158000000	4.935000000	0.000000000
N	-7.937000000	7.050000000	0.000000000
B	-9.158000000	7.755000000	0.000000000
B	-7.937000000	9.870000000	0.000000000
N	-9.158000000	9.165000000	0.000000000
N	-7.937000000	11.280000000	0.000000000
B	-9.158000000	11.985000000	0.000000000
B	-7.937000000	14.100000000	0.000000000
N	-9.158000000	13.395000000	0.000000000
N	-7.937000000	15.510000000	0.000000000
B	-9.158000000	16.215000000	0.000000000
B	-5.495000000	-15.510000000	0.000000000
N	-6.716000000	-16.215000000	0.000000000
N	-5.495000000	-14.100000000	0.000000000
B	-6.716000000	-13.395000000	0.000000000
B	-5.495000000	-11.280000000	0.000000000
N	-6.716000000	-11.985000000	0.000000000
N	-5.495000000	-9.870000000	0.000000000
B	-6.716000000	-9.165000000	0.000000000
B	-5.495000000	-7.050000000	0.000000000
N	-6.716000000	-7.755000000	0.000000000
N	-5.495000000	-5.640000000	0.000000000
B	-6.716000000	-4.935000000	0.000000000
B	-5.495000000	-2.820000000	0.000000000
N	-6.716000000	-3.525000000	0.000000000
N	-5.495000000	-1.410000000	0.000000000
B	-6.716000000	-0.705000000	0.000000000
B	-5.495000000	1.410000000	0.000000000
N	-6.716000000	0.705000000	0.000000000
N	-5.495000000	2.820000000	0.000000000
B	-6.716000000	3.525000000	0.000000000
B	-5.495000000	5.640000000	0.000000000
N	-6.716000000	4.935000000	0.000000000

N	-5.495000000	7.050000000	0.000000000
B	-6.716000000	7.755000000	0.000000000
B	-5.495000000	9.870000000	0.000000000
N	-6.716000000	9.165000000	0.000000000
N	-5.495000000	11.280000000	0.000000000
B	-6.716000000	11.985000000	0.000000000
B	-5.495000000	14.100000000	0.000000000
N	-6.716000000	13.395000000	0.000000000
N	-5.495000000	15.510000000	0.000000000
B	-6.716000000	16.215000000	0.000000000
B	-3.053000000	-15.510000000	0.000000000
N	-4.274000000	-16.215000000	0.000000000
N	-3.053000000	-14.100000000	0.000000000
B	-4.274000000	-13.395000000	0.000000000
B	-3.053000000	-11.280000000	0.000000000
N	-4.274000000	-11.985000000	0.000000000
N	-3.053000000	-9.870000000	0.000000000
B	-4.274000000	-9.165000000	0.000000000
B	-3.053000000	-7.050000000	0.000000000
N	-4.274000000	-7.755000000	0.000000000
N	-3.053000000	-5.640000000	0.000000000
B	-4.274000000	-4.935000000	0.000000000
N	-4.274000000	-3.525000000	0.000000000
N	-3.053000000	2.820000000	0.000000000
B	-4.274000000	3.525000000	0.000000000
B	-3.053000000	5.640000000	0.000000000
N	-4.274000000	4.935000000	0.000000000
N	-3.053000000	7.050000000	0.000000000
B	-4.274000000	7.755000000	0.000000000
B	-3.053000000	9.870000000	0.000000000
N	-4.274000000	9.165000000	0.000000000
N	-3.053000000	11.280000000	0.000000000
B	-4.274000000	11.985000000	0.000000000
B	-3.053000000	14.100000000	0.000000000
N	-4.274000000	13.395000000	0.000000000
N	-3.053000000	15.510000000	0.000000000
B	-4.274000000	16.215000000	0.000000000
B	-0.611000000	-15.510000000	0.000000000
N	-1.832000000	-16.215000000	0.000000000
N	-0.611000000	-14.100000000	0.000000000
B	-1.832000000	-13.395000000	0.000000000
B	-0.611000000	-11.280000000	0.000000000
N	-1.832000000	-11.985000000	0.000000000
N	-0.611000000	-9.870000000	0.000000000
B	-1.832000000	-9.165000000	0.000000000
B	-0.611000000	-7.050000000	0.000000000
N	-1.832000000	-7.755000000	0.000000000
N	-0.611000000	-5.640000000	0.000000000
B	-1.832000000	-4.935000000	0.000000000
N	-0.611000000	2.820000000	0.000000000
B	-1.832000000	3.525000000	0.000000000
B	-0.611000000	5.640000000	0.000000000
N	-1.832000000	4.935000000	0.000000000
N	-0.611000000	7.050000000	0.000000000
B	-1.832000000	7.755000000	0.000000000
B	-0.611000000	9.870000000	0.000000000
N	-1.832000000	9.165000000	0.000000000
N	-0.611000000	11.280000000	0.000000000
B	-1.832000000	11.985000000	0.000000000
B	-0.611000000	14.100000000	0.000000000
N	-1.832000000	13.395000000	0.000000000
N	-0.611000000	15.510000000	0.000000000
B	-1.832000000	16.215000000	0.000000000
B	1.831000000	-15.510000000	0.000000000
N	0.610000000	-16.215000000	0.000000000
N	1.831000000	-14.100000000	0.000000000
B	0.610000000	-13.395000000	0.000000000
B	1.831000000	-11.280000000	0.000000000
N	0.610000000	-11.985000000	0.000000000
N	1.831000000	-9.870000000	0.000000000
B	0.610000000	-9.165000000	0.000000000
B	1.831000000	-7.050000000	0.000000000
N	0.610000000	-7.755000000	0.000000000
N	1.831000000	-5.640000000	0.000000000
B	0.610000000	-4.935000000	0.000000000

N	1.8310000000	2.8200000000	0.0000000000
B	0.6100000000	3.5250000000	0.0000000000
B	1.8310000000	5.6400000000	0.0000000000
N	0.6100000000	4.9350000000	0.0000000000
N	1.8310000000	7.0500000000	0.0000000000
B	0.6100000000	7.7550000000	0.0000000000
B	1.8310000000	9.8700000000	0.0000000000
N	0.6100000000	9.1650000000	0.0000000000
N	1.8310000000	11.2800000000	0.0000000000
B	0.6100000000	11.9850000000	0.0000000000
B	1.8310000000	14.1000000000	0.0000000000
N	0.6100000000	13.3950000000	0.0000000000
N	1.8310000000	15.5100000000	0.0000000000
B	0.6100000000	16.2150000000	0.0000000000
B	4.2740000000	-15.5100000000	0.0000000000
N	3.0530000000	-16.2150000000	0.0000000000
N	4.2740000000	-14.1000000000	0.0000000000
B	3.0530000000	-13.3950000000	0.0000000000
B	4.2740000000	-11.2800000000	0.0000000000
N	3.0530000000	-11.9850000000	0.0000000000
N	4.2740000000	-9.8700000000	0.0000000000
B	3.0530000000	-9.1650000000	0.0000000000
B	4.2740000000	-7.0500000000	0.0000000000
N	3.0530000000	-7.7550000000	0.0000000000
N	4.2740000000	-5.6400000000	0.0000000000
B	3.0530000000	-4.9350000000	0.0000000000
B	4.2740000000	-2.8200000000	0.0000000000
N	3.0530000000	-3.5250000000	0.0000000000
N	4.2740000000	-1.4100000000	0.0000000000
B	4.2740000000	1.4100000000	0.0000000000
N	4.2740000000	2.8200000000	0.0000000000
B	3.0530000000	3.5250000000	0.0000000000
B	4.2740000000	5.6400000000	0.0000000000
N	3.0530000000	4.9350000000	0.0000000000
N	4.2740000000	7.0500000000	0.0000000000
B	3.0530000000	7.7550000000	0.0000000000
B	4.2740000000	9.8700000000	0.0000000000
N	3.0530000000	9.1650000000	0.0000000000
N	4.2740000000	11.2800000000	0.0000000000
B	3.0530000000	11.9850000000	0.0000000000
B	4.2740000000	14.1000000000	0.0000000000
N	3.0530000000	13.3950000000	0.0000000000
N	4.2740000000	15.5100000000	0.0000000000
B	3.0530000000	16.2150000000	0.0000000000
B	6.7160000000	-15.5100000000	0.0000000000
N	5.4950000000	-16.2150000000	0.0000000000
N	6.7160000000	-14.1000000000	0.0000000000
B	5.4950000000	-13.3950000000	0.0000000000
B	6.7160000000	-11.2800000000	0.0000000000
N	5.4950000000	-11.9850000000	0.0000000000
N	6.7160000000	-9.8700000000	0.0000000000
B	5.4950000000	-9.1650000000	0.0000000000
B	6.7160000000	-7.0500000000	0.0000000000
N	5.4950000000	-7.7550000000	0.0000000000
N	6.7160000000	-5.6400000000	0.0000000000
B	5.4950000000	-4.9350000000	0.0000000000
B	6.7160000000	-2.8200000000	0.0000000000
N	5.4950000000	-3.5250000000	0.0000000000
N	6.7160000000	-1.4100000000	0.0000000000
B	5.4950000000	-0.7050000000	0.0000000000
B	6.7160000000	1.4100000000	0.0000000000
N	5.4950000000	0.7050000000	0.0000000000
N	6.7160000000	2.8200000000	0.0000000000
B	5.4950000000	3.5250000000	0.0000000000
B	6.7160000000	5.6400000000	0.0000000000
N	5.4950000000	4.9350000000	0.0000000000
N	6.7160000000	7.0500000000	0.0000000000
B	5.4950000000	7.7550000000	0.0000000000
B	6.7160000000	9.8700000000	0.0000000000
N	5.4950000000	9.1650000000	0.0000000000
N	6.7160000000	11.2800000000	0.0000000000
B	5.4950000000	11.9850000000	0.0000000000
B	6.7160000000	14.1000000000	0.0000000000
N	5.4950000000	13.3950000000	0.0000000000
N	6.7160000000	15.5100000000	0.0000000000

B	5.495000000	16.215000000	0.000000000
B	9.158000000	-15.510000000	0.000000000
N	7.937000000	-16.215000000	0.000000000
N	9.158000000	-14.100000000	0.000000000
B	7.937000000	-13.395000000	0.000000000
B	9.158000000	-11.280000000	0.000000000
N	7.937000000	-11.985000000	0.000000000
N	9.158000000	-9.870000000	0.000000000
B	7.937000000	-9.165000000	0.000000000
B	9.158000000	-7.050000000	0.000000000
N	7.937000000	-7.755000000	0.000000000
N	9.158000000	-5.640000000	0.000000000
B	7.937000000	-4.935000000	0.000000000
B	9.158000000	-2.820000000	0.000000000
N	7.937000000	-3.525000000	0.000000000
N	9.158000000	-1.410000000	0.000000000
B	7.937000000	-0.705000000	0.000000000
B	9.158000000	1.410000000	0.000000000
N	7.937000000	0.705000000	0.000000000
N	9.158000000	2.820000000	0.000000000
B	7.937000000	3.525000000	0.000000000
B	9.158000000	5.640000000	0.000000000
N	7.937000000	4.935000000	0.000000000
N	9.158000000	7.050000000	0.000000000
B	7.937000000	7.755000000	0.000000000
B	9.158000000	9.870000000	0.000000000
N	7.937000000	9.165000000	0.000000000
N	9.158000000	11.280000000	0.000000000
B	7.937000000	11.985000000	0.000000000
B	9.158000000	14.100000000	0.000000000
N	7.937000000	13.395000000	0.000000000
N	9.158000000	15.510000000	0.000000000
B	7.937000000	16.215000000	0.000000000
B	11.600000000	-15.510000000	0.000000000
N	10.379000000	-16.215000000	0.000000000
N	11.600000000	-14.100000000	0.000000000
B	10.379000000	-13.395000000	0.000000000
B	11.600000000	-11.280000000	0.000000000
N	10.379000000	-11.985000000	0.000000000
N	11.600000000	-9.870000000	0.000000000
B	10.379000000	-9.165000000	0.000000000
B	11.600000000	-7.050000000	0.000000000
N	10.379000000	-7.755000000	0.000000000
N	11.600000000	-5.640000000	0.000000000
B	10.379000000	-4.935000000	0.000000000
B	11.600000000	-2.820000000	0.000000000
N	10.379000000	-3.525000000	0.000000000
N	11.600000000	-1.410000000	0.000000000
B	10.379000000	-0.705000000	0.000000000
B	11.600000000	1.410000000	0.000000000
N	10.379000000	0.705000000	0.000000000
N	11.600000000	2.820000000	0.000000000
B	10.379000000	3.525000000	0.000000000
B	11.600000000	5.640000000	0.000000000
N	10.379000000	4.935000000	0.000000000
N	11.600000000	7.050000000	0.000000000
B	10.379000000	7.755000000	0.000000000
B	11.600000000	9.870000000	0.000000000
N	10.379000000	9.165000000	0.000000000
N	11.600000000	11.280000000	0.000000000
B	10.379000000	11.985000000	0.000000000
B	11.600000000	14.100000000	0.000000000
N	10.379000000	13.395000000	0.000000000
N	11.600000000	15.510000000	0.000000000
B	10.379000000	16.215000000	0.000000000
B	14.042000000	-15.510000000	0.000000000
N	12.821000000	-16.215000000	0.000000000
N	14.042000000	-14.100000000	0.000000000
B	12.821000000	-13.395000000	0.000000000
B	14.042000000	-11.280000000	0.000000000
N	12.821000000	-11.985000000	0.000000000
N	14.042000000	-9.870000000	0.000000000
B	12.821000000	-9.165000000	0.000000000
B	14.042000000	-7.050000000	0.000000000
N	12.821000000	-7.755000000	0.000000000

N	14.042000000	-5.640000000	0.000000000
B	12.821000000	-4.935000000	0.000000000
B	14.042000000	-2.820000000	0.000000000
N	12.821000000	-3.525000000	0.000000000
N	14.042000000	-1.410000000	0.000000000
B	12.821000000	-0.705000000	0.000000000
B	14.042000000	1.410000000	0.000000000
N	12.821000000	0.705000000	0.000000000
N	14.042000000	2.820000000	0.000000000
B	12.821000000	3.525000000	0.000000000
B	14.042000000	5.640000000	0.000000000
N	12.821000000	4.935000000	0.000000000
N	14.042000000	7.050000000	0.000000000
B	12.821000000	7.755000000	0.000000000
B	14.042000000	9.870000000	0.000000000
N	12.821000000	9.165000000	0.000000000
N	14.042000000	11.280000000	0.000000000
B	12.821000000	11.985000000	0.000000000
B	14.042000000	14.100000000	0.000000000
N	12.821000000	13.395000000	0.000000000
N	14.042000000	15.510000000	0.000000000
B	12.821000000	16.215000000	0.000000000
B	16.485000000	-15.510000000	0.000000000
N	15.263000000	-16.215000000	0.000000000
N	16.485000000	-14.100000000	0.000000000
B	15.263000000	-13.395000000	0.000000000
B	16.485000000	-11.280000000	0.000000000
N	15.263000000	-11.985000000	0.000000000
N	16.485000000	-9.870000000	0.000000000
B	15.263000000	-9.165000000	0.000000000
B	16.485000000	-7.050000000	0.000000000
N	15.263000000	-7.755000000	0.000000000
N	16.485000000	-5.640000000	0.000000000
B	15.263000000	-4.935000000	0.000000000
B	16.485000000	-2.820000000	0.000000000
N	15.263000000	-3.525000000	0.000000000
N	16.485000000	-1.410000000	0.000000000
B	15.263000000	-0.705000000	0.000000000
B	16.485000000	1.410000000	0.000000000
N	15.263000000	0.705000000	0.000000000
N	16.485000000	2.820000000	0.000000000
B	15.263000000	3.525000000	0.000000000
B	16.485000000	5.640000000	0.000000000
N	15.263000000	4.935000000	0.000000000
N	16.485000000	7.050000000	0.000000000
B	15.263000000	7.755000000	0.000000000
B	16.485000000	9.870000000	0.000000000
N	15.263000000	9.165000000	0.000000000
N	16.485000000	11.280000000	0.000000000
B	15.263000000	11.985000000	0.000000000
B	16.485000000	14.100000000	0.000000000
N	15.263000000	13.395000000	0.000000000
N	16.485000000	15.510000000	0.000000000
B	15.263000000	16.215000000	0.000000000

### Pore 3. (The final potential energy from DFT calculations: -14911.04 Hartree)

B	-15.275000000	-15.526000000	0.000000000
N	-16.496000000	-16.231000000	0.000000000
N	-15.275000000	-14.116000000	0.000000000
B	-16.496000000	-13.411000000	0.000000000
B	-15.275000000	-11.296000000	0.000000000
N	-16.496000000	-12.001000000	0.000000000
N	-15.275000000	-9.886000000	0.000000000
B	-16.496000000	-9.181000000	0.000000000
B	-15.275000000	-7.066000000	0.000000000
N	-16.496000000	-7.771000000	0.000000000
N	-15.275000000	-5.656000000	0.000000000
B	-16.496000000	-4.951000000	0.000000000
B	-15.275000000	-2.836000000	0.000000000
N	-16.496000000	-3.541000000	0.000000000

N	-15.2750000000	-1.4260000000	0.0000000000
B	-16.4960000000	-0.7210000000	0.0000000000
B	-15.2750000000	1.3940000000	0.0000000000
N	-16.4960000000	0.6890000000	0.0000000000
N	-15.2750000000	2.8040000000	0.0000000000
B	-16.4960000000	3.5090000000	0.0000000000
B	-15.2750000000	5.6240000000	0.0000000000
N	-16.4960000000	4.9190000000	0.0000000000
N	-15.2750000000	7.0340000000	0.0000000000
B	-16.4960000000	7.7390000000	0.0000000000
B	-15.2750000000	9.8540000000	0.0000000000
N	-16.4960000000	9.1490000000	0.0000000000
N	-15.2750000000	11.2640000000	0.0000000000
B	-16.4960000000	11.9690000000	0.0000000000
B	-15.2750000000	14.0840000000	0.0000000000
N	-16.4960000000	13.3790000000	0.0000000000
N	-15.2750000000	15.4940000000	0.0000000000
B	-16.4960000000	16.1990000000	0.0000000000
B	-12.8330000000	-15.5260000000	0.0000000000
N	-14.0540000000	-16.2310000000	0.0000000000
N	-12.8330000000	-14.1160000000	0.0000000000
B	-14.0540000000	-13.4110000000	0.0000000000
B	-12.8330000000	-11.2960000000	0.0000000000
N	-14.0540000000	-12.0010000000	0.0000000000
N	-12.8330000000	-9.8860000000	0.0000000000
B	-14.0540000000	-9.1810000000	0.0000000000
B	-12.8330000000	-7.0660000000	0.0000000000
N	-14.0540000000	-7.7710000000	0.0000000000
N	-12.8330000000	-5.6560000000	0.0000000000
B	-14.0540000000	-4.9510000000	0.0000000000
B	-12.8330000000	-2.8360000000	0.0000000000
N	-14.0540000000	-3.5410000000	0.0000000000
N	-12.8330000000	-1.4260000000	0.0000000000
B	-14.0540000000	-0.7210000000	0.0000000000
B	-12.8330000000	1.3940000000	0.0000000000
N	-14.0540000000	0.6890000000	0.0000000000
N	-12.8330000000	2.8040000000	0.0000000000
B	-14.0540000000	3.5090000000	0.0000000000
B	-12.8330000000	5.6240000000	0.0000000000
N	-14.0540000000	4.9190000000	0.0000000000
N	-12.8330000000	7.0340000000	0.0000000000
B	-14.0540000000	7.7390000000	0.0000000000
B	-12.8330000000	9.8540000000	0.0000000000
N	-14.0540000000	9.1490000000	0.0000000000
N	-12.8330000000	11.2640000000	0.0000000000
B	-14.0540000000	11.9690000000	0.0000000000
B	-12.8330000000	14.0840000000	0.0000000000
N	-14.0540000000	13.3790000000	0.0000000000
N	-12.8330000000	15.4940000000	0.0000000000
B	-14.0540000000	16.1990000000	0.0000000000
B	-10.3910000000	-15.5260000000	0.0000000000
N	-11.6120000000	-16.2310000000	0.0000000000
N	-10.3910000000	-14.1160000000	0.0000000000
B	-11.6120000000	-13.4110000000	0.0000000000
B	-10.3910000000	-11.2960000000	0.0000000000
N	-11.6120000000	-12.0010000000	0.0000000000
N	-10.3910000000	-9.8860000000	0.0000000000
B	-11.6120000000	-9.1810000000	0.0000000000
B	-10.3910000000	-7.0660000000	0.0000000000
N	-11.6120000000	-7.7710000000	0.0000000000
N	-10.3910000000	-5.6560000000	0.0000000000
B	-11.6120000000	-4.9510000000	0.0000000000
B	-10.3910000000	-2.8360000000	0.0000000000
N	-11.6120000000	-3.5410000000	0.0000000000
N	-10.3910000000	-1.4260000000	0.0000000000
B	-11.6120000000	-0.7210000000	0.0000000000
B	-10.3910000000	1.3940000000	0.0000000000
N	-11.6120000000	0.6890000000	0.0000000000
N	-10.3910000000	2.8040000000	0.0000000000
B	-11.6120000000	3.5090000000	0.0000000000
B	-10.3910000000	5.6240000000	0.0000000000
N	-11.6120000000	4.9190000000	0.0000000000
N	-10.3910000000	7.0340000000	0.0000000000
B	-11.6120000000	7.7390000000	0.0000000000
B	-10.3910000000	9.8540000000	0.0000000000

N	-11.612000000	9.149000000	0.000000000
N	-10.391000000	11.264000000	0.000000000
B	-11.612000000	11.969000000	0.000000000
B	-10.391000000	14.084000000	0.000000000
N	-11.612000000	13.379000000	0.000000000
N	-10.391000000	15.494000000	0.000000000
B	-11.612000000	16.199000000	0.000000000
B	-7.948000000	-15.526000000	0.000000000
N	-9.169000000	-16.231000000	0.000000000
N	-7.948000000	-14.116000000	0.000000000
B	-9.169000000	-13.411000000	0.000000000
B	-7.948000000	-11.296000000	0.000000000
N	-9.169000000	-12.001000000	0.000000000
N	-7.948000000	-9.886000000	0.000000000
B	-9.169000000	-9.181000000	0.000000000
B	-7.948000000	-7.066000000	0.000000000
N	-9.169000000	-7.771000000	0.000000000
N	-7.948000000	-5.656000000	0.000000000
B	-9.169000000	-4.951000000	0.000000000
B	-7.948000000	-2.836000000	0.000000000
N	-9.169000000	-3.541000000	0.000000000
N	-7.948000000	-1.426000000	0.000000000
B	-9.169000000	-0.721000000	0.000000000
B	-7.948000000	1.394000000	0.000000000
N	-9.169000000	0.689000000	0.000000000
N	-7.948000000	2.804000000	0.000000000
B	-9.169000000	3.509000000	0.000000000
B	-7.948000000	5.624000000	0.000000000
N	-9.169000000	4.919000000	0.000000000
N	-7.948000000	7.034000000	0.000000000
B	-9.169000000	7.739000000	0.000000000
B	-7.948000000	9.854000000	0.000000000
N	-9.169000000	9.149000000	0.000000000
N	-7.948000000	11.264000000	0.000000000
B	-9.169000000	11.969000000	0.000000000
B	-7.948000000	14.084000000	0.000000000
N	-9.169000000	13.379000000	0.000000000
N	-7.948000000	15.494000000	0.000000000
B	-9.169000000	16.199000000	0.000000000
B	-5.506000000	-15.526000000	0.000000000
N	-6.727000000	-16.231000000	0.000000000
N	-5.506000000	-14.116000000	0.000000000
B	-6.727000000	-13.411000000	0.000000000
B	-5.506000000	-11.296000000	0.000000000
N	-6.727000000	-12.001000000	0.000000000
N	-5.506000000	-9.886000000	0.000000000
B	-6.727000000	-9.181000000	0.000000000
B	-5.506000000	-7.066000000	0.000000000
N	-6.727000000	-7.771000000	0.000000000
N	-5.506000000	-5.656000000	0.000000000
B	-6.727000000	-4.951000000	0.000000000
B	-5.506000000	-2.836000000	0.000000000
N	-6.727000000	-3.541000000	0.000000000
N	-5.506000000	-1.426000000	0.000000000
B	-6.727000000	-0.721000000	0.000000000
B	-5.506000000	1.394000000	0.000000000
N	-6.727000000	0.689000000	0.000000000
N	-5.506000000	2.804000000	0.000000000
B	-6.727000000	3.509000000	0.000000000
B	-5.506000000	5.624000000	0.000000000
N	-6.727000000	4.919000000	0.000000000
N	-5.506000000	7.034000000	0.000000000
B	-6.727000000	7.739000000	0.000000000
B	-5.506000000	9.854000000	0.000000000
N	-6.727000000	9.149000000	0.000000000
N	-5.506000000	11.264000000	0.000000000
B	-6.727000000	11.969000000	0.000000000
B	-5.506000000	14.084000000	0.000000000
N	-6.727000000	13.379000000	0.000000000
N	-5.506000000	15.494000000	0.000000000
B	-6.727000000	16.199000000	0.000000000
B	-3.064000000	-15.526000000	0.000000000
N	-4.285000000	-16.231000000	0.000000000
N	-3.064000000	-14.116000000	0.000000000
B	-4.285000000	-13.411000000	0.000000000



B	-3.064000000	-11.296000000	0.000000000
N	-4.285000000	-12.001000000	0.000000000
N	-3.064000000	-9.886000000	0.000000000
B	-4.285000000	-9.181000000	0.000000000
B	-3.064000000	-7.066000000	0.000000000
N	-4.285000000	-7.771000000	0.000000000
N	-3.064000000	-5.656000000	0.000000000
B	-4.285000000	-4.951000000	0.000000000
N	-4.285000000	-3.541000000	0.000000000
N	-3.064000000	2.804000000	0.000000000
B	-4.285000000	3.509000000	0.000000000
B	-3.064000000	5.624000000	0.000000000
N	-4.285000000	4.919000000	0.000000000
N	-3.064000000	7.034000000	0.000000000
B	-4.285000000	7.739000000	0.000000000
B	-3.064000000	9.854000000	0.000000000
N	-4.285000000	9.149000000	0.000000000
N	-3.064000000	11.264000000	0.000000000
B	-4.285000000	11.969000000	0.000000000
B	-3.064000000	14.084000000	0.000000000
N	-4.285000000	13.379000000	0.000000000
N	-3.064000000	15.494000000	0.000000000
B	-4.285000000	16.199000000	0.000000000
B	-0.622000000	-15.526000000	0.000000000
N	-1.843000000	-16.231000000	0.000000000
N	-0.622000000	-14.116000000	0.000000000
B	-1.843000000	-13.411000000	0.000000000
B	-0.622000000	-11.296000000	0.000000000
N	-1.843000000	-12.001000000	0.000000000
N	-0.622000000	-9.886000000	0.000000000
B	-1.843000000	-9.181000000	0.000000000
B	-0.622000000	-7.066000000	0.000000000
N	-1.843000000	-7.771000000	0.000000000
N	-0.622000000	-5.656000000	0.000000000
B	-1.843000000	-4.951000000	0.000000000
N	-0.622000000	2.804000000	0.000000000
B	-1.843000000	3.509000000	0.000000000
B	-0.622000000	5.624000000	0.000000000
N	-1.843000000	4.919000000	0.000000000
N	-0.622000000	7.034000000	0.000000000
B	-1.843000000	7.739000000	0.000000000
B	-0.622000000	9.854000000	0.000000000
N	-1.843000000	9.149000000	0.000000000
N	-0.622000000	11.264000000	0.000000000
B	-1.843000000	11.969000000	0.000000000
B	-0.622000000	14.084000000	0.000000000
N	-1.843000000	13.379000000	0.000000000
N	-0.622000000	15.494000000	0.000000000
B	-1.843000000	16.199000000	0.000000000
B	1.820000000	-15.526000000	0.000000000
N	0.599000000	-16.231000000	0.000000000
N	1.820000000	-14.116000000	0.000000000
B	0.599000000	-13.411000000	0.000000000
B	1.820000000	-11.296000000	0.000000000
N	0.599000000	-12.001000000	0.000000000
N	1.820000000	-9.886000000	0.000000000
B	0.599000000	-9.181000000	0.000000000
B	1.820000000	-7.066000000	0.000000000
N	0.599000000	-7.771000000	0.000000000
N	1.820000000	-5.656000000	0.000000000
B	0.599000000	-4.951000000	0.000000000
N	1.820000000	2.804000000	0.000000000
B	0.599000000	3.509000000	0.000000000
B	1.820000000	5.624000000	0.000000000
N	0.599000000	4.919000000	0.000000000
N	1.820000000	7.034000000	0.000000000
B	0.599000000	7.739000000	0.000000000
B	1.820000000	9.854000000	0.000000000
N	0.599000000	9.149000000	0.000000000
N	1.820000000	11.264000000	0.000000000
B	0.599000000	11.969000000	0.000000000
B	1.820000000	14.084000000	0.000000000
N	0.599000000	13.379000000	0.000000000
N	1.820000000	15.494000000	0.000000000
B	0.599000000	16.199000000	0.000000000

B	4.263000000	-15.526000000	0.000000000
N	3.042000000	-16.231000000	0.000000000
N	4.263000000	-14.116000000	0.000000000
B	3.042000000	-13.411000000	0.000000000
B	4.263000000	-11.296000000	0.000000000
N	3.042000000	-12.001000000	0.000000000
N	4.263000000	-9.886000000	0.000000000
B	3.042000000	-9.181000000	0.000000000
B	4.263000000	-7.066000000	0.000000000
N	3.042000000	-7.771000000	0.000000000
N	4.263000000	-5.656000000	0.000000000
B	3.042000000	-4.951000000	0.000000000
B	4.263000000	-2.836000000	0.000000000
N	3.042000000	-3.541000000	0.000000000
N	4.263000000	-1.426000000	0.000000000
B	4.263000000	1.394000000	0.000000000
N	4.263000000	2.804000000	0.000000000
B	3.042000000	3.509000000	0.000000000
B	4.263000000	5.624000000	0.000000000
N	3.042000000	4.919000000	0.000000000
N	4.263000000	7.034000000	0.000000000
B	3.042000000	7.739000000	0.000000000
B	4.263000000	9.854000000	0.000000000
N	3.042000000	9.149000000	0.000000000
N	4.263000000	11.264000000	0.000000000
B	3.042000000	11.969000000	0.000000000
B	4.263000000	14.084000000	0.000000000
N	3.042000000	13.379000000	0.000000000
N	4.263000000	15.494000000	0.000000000
B	3.042000000	16.199000000	0.000000000
B	6.705000000	-15.526000000	0.000000000
N	5.484000000	-16.231000000	0.000000000
N	6.705000000	-14.116000000	0.000000000
B	5.484000000	-13.411000000	0.000000000
B	6.705000000	-11.296000000	0.000000000
N	5.484000000	-12.001000000	0.000000000
N	6.705000000	-9.886000000	0.000000000
B	5.484000000	-9.181000000	0.000000000
B	6.705000000	-7.066000000	0.000000000
N	5.484000000	-7.771000000	0.000000000
N	6.705000000	-5.656000000	0.000000000
B	5.484000000	-4.951000000	0.000000000
B	6.705000000	-2.836000000	0.000000000
N	5.484000000	-3.541000000	0.000000000
N	6.705000000	-1.426000000	0.000000000
B	5.484000000	-0.721000000	0.000000000
B	6.705000000	1.394000000	0.000000000
N	5.484000000	0.689000000	0.000000000
N	6.705000000	2.804000000	0.000000000
B	5.484000000	3.509000000	0.000000000
B	6.705000000	5.624000000	0.000000000
N	5.484000000	4.919000000	0.000000000
N	6.705000000	7.034000000	0.000000000
B	5.484000000	7.739000000	0.000000000
B	6.705000000	9.854000000	0.000000000
N	5.484000000	9.149000000	0.000000000
N	6.705000000	11.264000000	0.000000000
B	5.484000000	11.969000000	0.000000000
B	6.705000000	14.084000000	0.000000000
N	5.484000000	13.379000000	0.000000000
N	6.705000000	15.494000000	0.000000000
B	5.484000000	16.199000000	0.000000000
B	9.147000000	-15.526000000	0.000000000
N	7.926000000	-16.231000000	0.000000000
N	9.147000000	-14.116000000	0.000000000
B	7.926000000	-13.411000000	0.000000000
B	9.147000000	-11.296000000	0.000000000
N	7.926000000	-12.001000000	0.000000000
N	9.147000000	-9.886000000	0.000000000
B	7.926000000	-9.181000000	0.000000000
B	9.147000000	-7.066000000	0.000000000
N	7.926000000	-7.771000000	0.000000000
N	9.147000000	-5.656000000	0.000000000
B	7.926000000	-4.951000000	0.000000000
B	9.147000000	-2.836000000	0.000000000

N	7.926000000	-3.541000000	0.000000000
N	9.147000000	-1.426000000	0.000000000
B	7.926000000	-0.721000000	0.000000000
B	9.147000000	1.394000000	0.000000000
N	7.926000000	0.689000000	0.000000000
N	9.147000000	2.804000000	0.000000000
B	7.926000000	3.509000000	0.000000000
B	9.147000000	5.624000000	0.000000000
N	7.926000000	4.919000000	0.000000000
N	9.147000000	7.034000000	0.000000000
B	7.926000000	7.739000000	0.000000000
B	9.147000000	9.854000000	0.000000000
N	7.926000000	9.149000000	0.000000000
N	9.147000000	11.264000000	0.000000000
B	7.926000000	11.969000000	0.000000000
B	9.147000000	14.084000000	0.000000000
N	7.926000000	13.379000000	0.000000000
N	9.147000000	15.494000000	0.000000000
B	7.926000000	16.199000000	0.000000000
B	11.589000000	-15.526000000	0.000000000
N	10.368000000	-16.231000000	0.000000000
N	11.589000000	-14.116000000	0.000000000
B	10.368000000	-13.411000000	0.000000000
B	11.589000000	-11.296000000	0.000000000
N	10.368000000	-12.001000000	0.000000000
N	11.589000000	-9.886000000	0.000000000
B	10.368000000	-9.181000000	0.000000000
B	11.589000000	-7.066000000	0.000000000
N	10.368000000	-7.771000000	0.000000000
N	11.589000000	-5.656000000	0.000000000
B	10.368000000	-4.951000000	0.000000000
B	11.589000000	-2.836000000	0.000000000
N	10.368000000	-3.541000000	0.000000000
N	11.589000000	-1.426000000	0.000000000
B	10.368000000	-0.721000000	0.000000000
B	11.589000000	1.394000000	0.000000000
N	10.368000000	0.689000000	0.000000000
N	11.589000000	2.804000000	0.000000000
B	10.368000000	3.509000000	0.000000000
B	11.589000000	5.624000000	0.000000000
N	10.368000000	4.919000000	0.000000000
N	11.589000000	7.034000000	0.000000000
B	10.368000000	7.739000000	0.000000000
B	11.589000000	9.854000000	0.000000000
N	10.368000000	9.149000000	0.000000000
N	11.589000000	11.264000000	0.000000000
B	10.368000000	11.969000000	0.000000000
B	11.589000000	14.084000000	0.000000000
N	10.368000000	13.379000000	0.000000000
N	11.589000000	15.494000000	0.000000000
B	10.368000000	16.199000000	0.000000000
B	14.031000000	-15.526000000	0.000000000
N	12.810000000	-16.231000000	0.000000000
N	14.031000000	-14.116000000	0.000000000
B	12.810000000	-13.411000000	0.000000000
B	14.031000000	-11.296000000	0.000000000
N	12.810000000	-12.001000000	0.000000000
N	14.031000000	-9.886000000	0.000000000
B	12.810000000	-9.181000000	0.000000000
B	14.031000000	-7.066000000	0.000000000
N	12.810000000	-7.771000000	0.000000000
N	14.031000000	-5.656000000	0.000000000
B	12.810000000	-4.951000000	0.000000000
B	14.031000000	-2.836000000	0.000000000
N	12.810000000	-3.541000000	0.000000000
N	14.031000000	-1.426000000	0.000000000
B	12.810000000	-0.721000000	0.000000000
B	14.031000000	1.394000000	0.000000000
N	12.810000000	0.689000000	0.000000000
N	14.031000000	2.804000000	0.000000000
B	12.810000000	3.509000000	0.000000000
B	14.031000000	5.624000000	0.000000000
N	12.810000000	4.919000000	0.000000000
N	14.031000000	7.034000000	0.000000000
B	12.810000000	7.739000000	0.000000000

B	14.0310000000	9.8540000000	0.0000000000
N	12.8100000000	9.1490000000	0.0000000000
N	14.0310000000	11.2640000000	0.0000000000
B	12.8100000000	11.9690000000	0.0000000000
B	14.0310000000	14.0840000000	0.0000000000
N	12.8100000000	13.3790000000	0.0000000000
N	14.0310000000	15.4940000000	0.0000000000
B	12.8100000000	16.1990000000	0.0000000000
B	16.4740000000	-15.5260000000	0.0000000000
N	15.2520000000	-16.2310000000	0.0000000000
N	16.4740000000	-14.1160000000	0.0000000000
B	15.2520000000	-13.4110000000	0.0000000000
B	16.4740000000	-11.2960000000	0.0000000000
N	15.2520000000	-12.0010000000	0.0000000000
N	16.4740000000	-9.8860000000	0.0000000000
B	15.2520000000	-9.1810000000	0.0000000000
B	16.4740000000	-7.0660000000	0.0000000000
N	15.2520000000	-7.7710000000	0.0000000000
N	16.4740000000	-5.6560000000	0.0000000000
B	15.2520000000	-4.9510000000	0.0000000000
B	16.4740000000	-2.8360000000	0.0000000000
N	15.2520000000	-3.5410000000	0.0000000000
N	16.4740000000	-1.4260000000	0.0000000000
B	15.2520000000	-0.7210000000	0.0000000000
B	16.4740000000	1.3940000000	0.0000000000
N	15.2520000000	0.6890000000	0.0000000000
N	16.4740000000	2.8040000000	0.0000000000
B	15.2520000000	3.5090000000	0.0000000000
B	16.4740000000	5.6240000000	0.0000000000
N	15.2520000000	4.9190000000	0.0000000000
N	16.4740000000	7.0340000000	0.0000000000
B	15.2520000000	7.7390000000	0.0000000000
B	16.4740000000	9.8540000000	0.0000000000
N	15.2520000000	9.1490000000	0.0000000000
N	16.4740000000	11.2640000000	0.0000000000
B	15.2520000000	11.9690000000	0.0000000000
B	16.4740000000	14.0840000000	0.0000000000
N	15.2520000000	13.3790000000	0.0000000000
N	16.4740000000	15.4940000000	0.0000000000
B	15.2520000000	16.1990000000	0.0000000000
F	-3.0760000000	1.4280000000	0.0000000000
F	-0.6150000000	1.4260000000	0.0000000000
F	1.8300000000	1.4150000000	0.0000000000
F	-4.3280000000	-0.7310000000	0.0000000000
F	-3.1370000000	-2.8460000000	0.0000000000
F	1.8430000000	-2.8550000000	0.0000000000
F	3.0820000000	-0.7670000000	0.0000000000
H	-4.4830000000	0.8230000000	0.0000000000
H	3.2620000000	0.7990000000	0.0000000000
H	0.5870000000	-3.7740000000	0.0000000000
H	-1.8360000000	-3.7550000000	0.0000000000

**Pore 4.** (The final potential energy from DFT calculations: -14935.12 Hartree)

B	15.6770000000	-15.5640000000	0.0000000000
B	13.1670000000	-15.5640000000	0.0000000000
B	10.6570000000	-15.5640000000	0.0000000000
B	8.1470000000	-15.5640000000	0.0000000000
N	14.4190000000	-14.8380000000	0.0000000000
B	5.6370000000	-15.5640000000	0.0000000000
N	11.9090000000	-14.8380000000	0.0000000000
B	3.1270000000	-15.5640000000	0.0000000000
N	9.3990000000	-14.8380000000	0.0000000000
B	0.6170000000	-15.5640000000	0.0000000000
N	6.8890000000	-14.8380000000	0.0000000000
B	-1.8930000000	-15.5640000000	0.0000000000
N	4.3790000000	-14.8380000000	0.0000000000
B	-4.4030000000	-15.5640000000	0.0000000000
N	1.8690000000	-14.8380000000	0.0000000000
B	-6.9130000000	-15.5640000000	0.0000000000
B	14.4220000000	-13.3900000000	0.0000000000

N	-0.6410000000	-14.8380000000	0.0000000000
B	-9.4230000000	-15.5640000000	0.0000000000
N	11.9120000000	-13.3900000000	0.0000000000
B	-3.1510000000	-14.8380000000	0.0000000000
N	-11.9330000000	-15.5640000000	0.0000000000
B	9.4020000000	-13.3900000000	0.0000000000
N	-5.6610000000	-14.8380000000	0.0000000000
B	15.6740000000	-12.6640000000	0.0000000000
N	-14.4430000000	-15.5640000000	0.0000000000
B	6.8920000000	-13.3900000000	0.0000000000
N	-8.1710000000	-14.8380000000	0.0000000000
B	13.1640000000	-12.6640000000	0.0000000000
N	4.3820000000	-13.3900000000	0.0000000000
B	-10.6810000000	-14.8380000000	0.0000000000
N	10.6540000000	-12.6640000000	0.0000000000
B	1.8720000000	-13.3900000000	0.0000000000
N	-13.1910000000	-14.8380000000	0.0000000000
B	8.1440000000	-12.6640000000	0.0000000000
N	-0.6380000000	-13.3900000000	0.0000000000
B	-15.7010000000	-14.8380000000	0.0000000000
N	5.6340000000	-12.6640000000	0.0000000000
B	-3.1480000000	-13.3900000000	0.0000000000
N	3.1240000000	-12.6640000000	0.0000000000
B	-5.6580000000	-13.3900000000	0.0000000000
N	15.6770000000	-11.2160000000	0.0000000000
B	0.6140000000	-12.6640000000	0.0000000000
N	-8.1680000000	-13.3900000000	0.0000000000
B	13.1670000000	-11.2160000000	0.0000000000
N	-1.8960000000	-12.6640000000	0.0000000000
B	-10.6780000000	-13.3900000000	0.0000000000
N	10.6570000000	-11.2160000000	0.0000000000
B	-4.4060000000	-12.6640000000	0.0000000000
N	-13.1880000000	-13.3900000000	0.0000000000
B	8.1470000000	-11.2160000000	0.0000000000
N	-6.9160000000	-12.6640000000	0.0000000000
B	14.4190000000	-10.4900000000	0.0000000000
N	-15.6980000000	-13.3900000000	0.0000000000
B	5.6370000000	-11.2160000000	0.0000000000
N	-9.4260000000	-12.6640000000	0.0000000000
B	11.9090000000	-10.4900000000	0.0000000000
N	3.1270000000	-11.2160000000	0.0000000000
B	-11.9360000000	-12.6640000000	0.0000000000
N	9.3990000000	-10.4900000000	0.0000000000
B	0.6170000000	-11.2160000000	0.0000000000
N	-14.4460000000	-12.6640000000	0.0000000000
B	6.8890000000	-10.4900000000	0.0000000000
N	-1.8930000000	-11.2160000000	0.0000000000
B	4.3790000000	-10.4900000000	0.0000000000
N	-4.4030000000	-11.2160000000	0.0000000000
B	1.8690000000	-10.4900000000	0.0000000000
N	-6.9130000000	-11.2160000000	0.0000000000
B	14.4220000000	-9.0420000000	0.0000000000
N	-0.6410000000	-10.4900000000	0.0000000000
B	-9.4230000000	-11.2160000000	0.0000000000
N	11.9120000000	-9.0420000000	0.0000000000
B	-3.1510000000	-10.4900000000	0.0000000000
N	-11.9330000000	-11.2160000000	0.0000000000
B	9.4020000000	-9.0420000000	0.0000000000
N	-5.6610000000	-10.4900000000	0.0000000000
B	15.6740000000	-8.3160000000	0.0000000000
N	-14.4430000000	-11.2160000000	0.0000000000
B	6.8920000000	-9.0420000000	0.0000000000
N	-8.1710000000	-10.4900000000	0.0000000000
B	13.1640000000	-8.3160000000	0.0000000000
N	4.3820000000	-9.0420000000	0.0000000000
B	-10.6810000000	-10.4900000000	0.0000000000
N	10.6540000000	-8.3160000000	0.0000000000
B	1.8720000000	-9.0420000000	0.0000000000
N	-13.1910000000	-10.4900000000	0.0000000000
B	8.1440000000	-8.3160000000	0.0000000000
N	-0.6380000000	-9.0420000000	0.0000000000
B	-15.7010000000	-10.4900000000	0.0000000000
N	5.6340000000	-8.3160000000	0.0000000000
B	-3.1480000000	-9.0420000000	0.0000000000
N	3.1240000000	-8.3160000000	0.0000000000

B	-5.658000000	-9.042000000	0.000000000
B	15.677000000	-6.869000000	0.000000000
N	0.614000000	-8.316000000	0.000000000
B	-8.168000000	-9.042000000	0.000000000
B	13.167000000	-6.869000000	0.000000000
N	-1.896000000	-8.316000000	0.000000000
B	-10.678000000	-9.042000000	0.000000000
B	10.657000000	-6.869000000	0.000000000
N	-4.406000000	-8.316000000	0.000000000
B	-13.188000000	-9.042000000	0.000000000
B	8.147000000	-6.869000000	0.000000000
N	-6.916000000	-8.316000000	0.000000000
N	14.419000000	-6.143000000	0.000000000
B	-15.698000000	-9.042000000	0.000000000
B	5.637000000	-6.869000000	0.000000000
N	-9.426000000	-8.316000000	0.000000000
N	11.909000000	-6.143000000	0.000000000
B	3.127000000	-6.869000000	0.000000000
N	-11.936000000	-8.316000000	0.000000000
N	9.399000000	-6.143000000	0.000000000
B	0.617000000	-6.869000000	0.000000000
N	-14.446000000	-8.316000000	0.000000000
N	6.889000000	-6.143000000	0.000000000
B	-1.893000000	-6.869000000	0.000000000
N	4.379000000	-6.143000000	0.000000000
B	-4.403000000	-6.869000000	0.000000000
N	1.869000000	-6.143000000	0.000000000
B	-6.913000000	-6.869000000	0.000000000
B	14.422000000	-4.695000000	0.000000000
N	-0.641000000	-6.143000000	0.000000000
B	-9.423000000	-6.869000000	0.000000000
B	11.912000000	-4.695000000	0.000000000
N	-3.151000000	-6.143000000	0.000000000
B	-11.933000000	-6.869000000	0.000000000
B	9.402000000	-4.695000000	0.000000000
N	-5.661000000	-6.143000000	0.000000000
N	15.674000000	-3.969000000	0.000000000
B	-14.443000000	-6.869000000	0.000000000
B	6.892000000	-4.695000000	0.000000000
N	-8.171000000	-6.143000000	0.000000000
N	13.164000000	-3.969000000	0.000000000
B	4.382000000	-4.695000000	0.000000000
N	-10.681000000	-6.143000000	0.000000000
N	10.654000000	-3.969000000	0.000000000
B	1.872000000	-4.695000000	0.000000000
N	-13.191000000	-6.143000000	0.000000000
N	8.144000000	-3.969000000	0.000000000
B	-0.638000000	-4.695000000	0.000000000
N	-15.701000000	-6.143000000	0.000000000
N	5.634000000	-3.969000000	0.000000000
B	-3.148000000	-4.695000000	0.000000000
N	3.124000000	-3.969000000	0.000000000
B	-5.658000000	-4.695000000	0.000000000
B	15.677000000	-2.521000000	0.000000000
N	0.614000000	-3.969000000	0.000000000
B	-8.168000000	-4.695000000	0.000000000
B	13.167000000	-2.521000000	0.000000000
N	-1.896000000	-3.969000000	0.000000000
B	-10.678000000	-4.695000000	0.000000000
B	10.657000000	-2.521000000	0.000000000
N	-4.406000000	-3.969000000	0.000000000
B	-13.188000000	-4.695000000	0.000000000
B	8.147000000	-2.521000000	0.000000000
N	-6.916000000	-3.969000000	0.000000000
N	14.419000000	-1.795000000	0.000000000
B	-15.698000000	-4.695000000	0.000000000
B	5.637000000	-2.521000000	0.000000000
N	-9.426000000	-3.969000000	0.000000000
N	11.909000000	-1.795000000	0.000000000
B	3.127000000	-2.521000000	0.000000000
N	-11.936000000	-3.969000000	0.000000000
N	9.399000000	-1.795000000	0.000000000
N	-14.446000000	-3.969000000	0.000000000
N	6.889000000	-1.795000000	0.000000000
N	4.379000000	-1.795000000	0.000000000

B	-4.403000000	-2.521000000	0.000000000
B	-6.913000000	-2.521000000	0.000000000
B	14.422000000	-0.348000000	0.000000000
B	-9.423000000	-2.521000000	0.000000000
B	11.912000000	-0.348000000	0.000000000
B	-11.933000000	-2.521000000	0.000000000
B	9.402000000	-0.348000000	0.000000000
N	-5.661000000	-1.795000000	0.000000000
N	15.674000000	0.379000000	0.000000000
B	-14.443000000	-2.521000000	0.000000000
B	6.892000000	-0.348000000	0.000000000
N	-8.171000000	-1.795000000	0.000000000
N	13.164000000	0.379000000	0.000000000
B	4.382000000	-0.348000000	0.000000000
N	-10.681000000	-1.795000000	0.000000000
N	10.654000000	0.379000000	0.000000000
N	-13.191000000	-1.795000000	0.000000000
N	8.144000000	0.379000000	0.000000000
N	-15.701000000	-1.795000000	0.000000000
N	5.634000000	0.379000000	0.000000000
B	-5.658000000	-0.348000000	0.000000000
B	15.677000000	1.826000000	0.000000000
B	-8.168000000	-0.348000000	0.000000000
B	13.167000000	1.826000000	0.000000000
B	-10.678000000	-0.348000000	0.000000000
B	10.657000000	1.826000000	0.000000000
B	-13.188000000	-0.348000000	0.000000000
B	8.147000000	1.826000000	0.000000000
N	-6.916000000	0.379000000	0.000000000
N	14.419000000	2.552000000	0.000000000
B	-15.698000000	-0.348000000	0.000000000
B	5.637000000	1.826000000	0.000000000
N	-9.426000000	0.379000000	0.000000000
N	11.909000000	2.552000000	0.000000000
N	-11.936000000	0.379000000	0.000000000
N	9.399000000	2.552000000	0.000000000
N	-14.446000000	0.379000000	0.000000000
N	6.889000000	2.552000000	0.000000000
N	4.379000000	2.552000000	0.000000000
B	-6.913000000	1.826000000	0.000000000
B	14.422000000	4.000000000	0.000000000
B	-9.423000000	1.826000000	0.000000000
B	11.912000000	4.000000000	0.000000000
B	-11.933000000	1.826000000	0.000000000
B	9.402000000	4.000000000	0.000000000
N	-5.661000000	2.552000000	0.000000000
N	15.674000000	4.726000000	0.000000000
B	-14.443000000	1.826000000	0.000000000
B	6.892000000	4.000000000	0.000000000
N	-8.171000000	2.552000000	0.000000000
N	13.164000000	4.726000000	0.000000000
B	4.382000000	4.000000000	0.000000000
N	-10.681000000	2.552000000	0.000000000
N	10.654000000	4.726000000	0.000000000
N	-13.191000000	2.552000000	0.000000000
N	8.144000000	4.726000000	0.000000000
N	-15.701000000	2.552000000	0.000000000
N	5.634000000	4.726000000	0.000000000
N	3.124000000	4.726000000	0.000000000
B	-5.658000000	4.000000000	0.000000000
B	15.677000000	6.174000000	0.000000000
B	-8.168000000	4.000000000	0.000000000
B	13.167000000	6.174000000	0.000000000
B	-10.678000000	4.000000000	0.000000000
B	10.657000000	6.174000000	0.000000000
N	-4.406000000	4.726000000	0.000000000
B	-13.188000000	4.000000000	0.000000000
B	8.147000000	6.174000000	0.000000000
N	-6.916000000	4.726000000	0.000000000
N	14.419000000	6.900000000	0.000000000
B	-15.698000000	4.000000000	0.000000000
B	5.637000000	6.174000000	0.000000000
N	-9.426000000	4.726000000	0.000000000
N	11.909000000	6.900000000	0.000000000
B	3.127000000	6.174000000	0.000000000

N	-11.9360000000	4.7260000000	0.0000000000
N	9.3990000000	6.9000000000	0.0000000000
B	0.6170000000	6.1740000000	0.0000000000
N	-14.4460000000	4.7260000000	0.0000000000
N	6.8890000000	6.9000000000	0.0000000000
B	-1.8930000000	6.1740000000	0.0000000000
N	4.3790000000	6.9000000000	0.0000000000
B	-4.4030000000	6.1740000000	0.0000000000
N	1.8690000000	6.9000000000	0.0000000000
B	-6.9130000000	6.1740000000	0.0000000000
B	14.4220000000	8.3470000000	0.0000000000
N	-0.6410000000	6.9000000000	0.0000000000
B	-9.4230000000	6.1740000000	0.0000000000
B	11.9120000000	8.3470000000	0.0000000000
N	-3.1510000000	6.9000000000	0.0000000000
B	-11.9330000000	6.1740000000	0.0000000000
B	9.4020000000	8.3470000000	0.0000000000
N	-5.6610000000	6.9000000000	0.0000000000
N	15.6740000000	9.0730000000	0.0000000000
B	-14.4430000000	6.1740000000	0.0000000000
B	6.8920000000	8.3470000000	0.0000000000
N	-8.1710000000	6.9000000000	0.0000000000
N	13.1640000000	9.0730000000	0.0000000000
B	4.3820000000	8.3470000000	0.0000000000
N	-10.6810000000	6.9000000000	0.0000000000
N	10.6540000000	9.0730000000	0.0000000000
B	1.8720000000	8.3470000000	0.0000000000
N	-13.1910000000	6.9000000000	0.0000000000
N	8.1440000000	9.0730000000	0.0000000000
B	-0.6380000000	8.3470000000	0.0000000000
N	-15.7010000000	6.9000000000	0.0000000000
N	5.6340000000	9.0730000000	0.0000000000
B	-3.1480000000	8.3470000000	0.0000000000
N	3.1240000000	9.0730000000	0.0000000000
B	-5.6580000000	8.3470000000	0.0000000000
B	15.6770000000	10.5210000000	0.0000000000
N	0.6140000000	9.0730000000	0.0000000000
B	-8.1680000000	8.3470000000	0.0000000000
B	13.1670000000	10.5210000000	0.0000000000
N	-1.8960000000	9.0730000000	0.0000000000
B	-10.6780000000	8.3470000000	0.0000000000
B	10.6570000000	10.5210000000	0.0000000000
N	-4.4060000000	9.0730000000	0.0000000000
B	-13.1880000000	8.3470000000	0.0000000000
B	8.1470000000	10.5210000000	0.0000000000
N	-6.9160000000	9.0730000000	0.0000000000
N	14.4190000000	11.2470000000	0.0000000000
B	-15.6980000000	8.3470000000	0.0000000000
B	5.6370000000	10.5210000000	0.0000000000
N	-9.4260000000	9.0730000000	0.0000000000
N	11.9090000000	11.2470000000	0.0000000000
B	3.1270000000	10.5210000000	0.0000000000
N	-11.9360000000	9.0730000000	0.0000000000
N	9.3990000000	11.2470000000	0.0000000000
B	0.6170000000	10.5210000000	0.0000000000
N	-14.4460000000	9.0730000000	0.0000000000
N	6.8890000000	11.2470000000	0.0000000000
B	-1.8930000000	10.5210000000	0.0000000000
N	4.3790000000	11.2470000000	0.0000000000
B	-4.4030000000	10.5210000000	0.0000000000
N	1.8690000000	11.2470000000	0.0000000000
B	-6.9130000000	10.5210000000	0.0000000000
B	14.4220000000	12.6950000000	0.0000000000
N	-0.6410000000	11.2470000000	0.0000000000
B	-9.4230000000	10.5210000000	0.0000000000
B	11.9120000000	12.6950000000	0.0000000000
N	-3.1510000000	11.2470000000	0.0000000000
B	-11.9330000000	10.5210000000	0.0000000000
B	9.4020000000	12.6950000000	0.0000000000
N	-5.6610000000	11.2470000000	0.0000000000
N	15.6740000000	13.4210000000	0.0000000000
B	-14.4430000000	10.5210000000	0.0000000000
B	6.8920000000	12.6950000000	0.0000000000
N	-8.1710000000	11.2470000000	0.0000000000
N	13.1640000000	13.4210000000	0.0000000000



B	4.382000000	12.695000000	0.000000000
N	-10.681000000	11.247000000	0.000000000
N	10.654000000	13.421000000	0.000000000
B	1.872000000	12.695000000	0.000000000
N	-13.191000000	11.247000000	0.000000000
N	8.144000000	13.421000000	0.000000000
B	-0.638000000	12.695000000	0.000000000
N	-15.701000000	11.247000000	0.000000000
N	5.634000000	13.421000000	0.000000000
B	-3.148000000	12.695000000	0.000000000
N	3.124000000	13.421000000	0.000000000
B	-5.658000000	12.695000000	0.000000000
B	15.677000000	14.869000000	0.000000000
N	0.614000000	13.421000000	0.000000000
B	-8.168000000	12.695000000	0.000000000
B	13.167000000	14.869000000	0.000000000
N	-1.896000000	13.421000000	0.000000000
B	-10.678000000	12.695000000	0.000000000
B	10.657000000	14.869000000	0.000000000
N	-4.406000000	13.421000000	0.000000000
B	-13.188000000	12.695000000	0.000000000
B	8.147000000	14.869000000	0.000000000
N	-6.916000000	13.421000000	0.000000000
N	14.419000000	15.595000000	0.000000000
B	-15.698000000	12.695000000	0.000000000
B	5.637000000	14.869000000	0.000000000
N	-9.426000000	13.421000000	0.000000000
N	11.909000000	15.595000000	0.000000000
B	3.127000000	14.869000000	0.000000000
N	-11.936000000	13.421000000	0.000000000
N	9.399000000	15.595000000	0.000000000
B	0.617000000	14.869000000	0.000000000
N	-14.446000000	13.421000000	0.000000000
N	6.889000000	15.595000000	0.000000000
B	-1.893000000	14.869000000	0.000000000
N	4.379000000	15.595000000	0.000000000
B	-4.403000000	14.869000000	0.000000000
N	1.869000000	15.595000000	0.000000000
B	-6.913000000	14.869000000	0.000000000
N	-0.641000000	15.595000000	0.000000000
B	-9.423000000	14.869000000	0.000000000
N	-3.151000000	15.595000000	0.000000000
B	-11.933000000	14.869000000	0.000000000
N	-5.661000000	15.595000000	0.000000000
B	-14.443000000	14.869000000	0.000000000
N	-8.171000000	15.595000000	0.000000000
N	-10.681000000	15.595000000	0.000000000
N	-13.191000000	15.595000000	0.000000000
N	-15.701000000	15.595000000	0.000000000
H	0.618000000	4.974000000	0.000000000
H	-1.892000000	4.974000000	0.000000000
H	-4.618000000	0.251000000	0.000000000
H	-3.363000000	-1.922000000	0.000000000
H	2.088000000	-1.921000000	0.000000000
H	3.343000000	0.252000000	0.000000000
O	-3.201000000	4.033000000	0.000000000
O	-4.456000000	1.859000000	0.000000000
O	-1.896000000	-2.579000000	0.000000000
O	0.614000000	-2.579000000	0.000000000
O	3.374000000	1.971000000	0.000000000
O	2.087000000	4.127000000	0.000000000
H	-3.434000000	1.271000000	0.000000000
H	-2.179000000	3.445000000	0.000000000
H	1.066000000	3.537000000	0.000000000
H	2.353000000	1.381000000	0.000000000
H	0.614000000	-1.400000000	0.000000000
H	-1.896000000	-1.400000000	0.000000000