The Improved Lennard-Jones (ILJ) potential is given by

$$V_{ILJ}(r) = \epsilon \left[\frac{m}{n(r) - m} \cdot \left(\frac{r_0}{r} \right)^{n(r)} - \frac{n(r)}{n(r) - m} \cdot \left(\frac{r_0}{r} \right)^{m} \right], \tag{1}$$

where

$$n(r) = \beta + 4.0 \cdot \left(\frac{r}{r_0} \right)^2 \tag{2}$$

and $r = R_{i,j}$ is the distance between carbon atom i and nitrogen atom j. The parameters r_0, ϵ and β are set according to the atoms interacting, while m is set according the to the partial charges of the interacting species. The induction potential term for a N_3^- anion interacting with carbon atoms is given by (in meV)

$$V_{ind}(R_{i,1}, R_{i,2}, R_{i,3}) = -7200 \cdot \alpha_c \cdot \frac{n_2(R_{i,2})}{n_2(R_{i,2}) - 4} \left[\frac{q_1}{R_{i,1}^2} + \frac{q_2}{R_{i,2}^2} + \frac{q_3}{R_{i,3}^2} \right]^2, \tag{3}$$

where $R_{i,1}$, $R_{i,2}$ and $R_{i,3}$ are the distances between the carbon atom i and the three nitrogen atoms, q_1, q_2 and q_3 are the partial charges on the nitrogen atoms, α_c is the polarizability of the carbon atoms and $n_2(R_{i,2})$ is equal to $n(r)$ using r_0 according to the interaction between $C - N_2$. The interaction energy between a trinitrogen anion confined inside a carbon nanotube is given by

$$E_{int} = \sum_{i=1}^{N_C} V_{ILJ}^{C-N_{1,3}}(R_{i,1}) + V_{ILJ}^{C-N_2}(R_{i,2}) V_{ILJ}^{C-N_{1,3}}(R_{i,3}) + V_{ind}(R_{i,1}, R_{i,2}, R_{i,3}), \tag{4}$$

where N_C corresponds to the total number of carbon atoms, the ILJ potentials $V_{ILJ}^{C-N_{1,3}}$ and $V_{ILJ}^{C-N_2}$ are defined according to the parameters given in Table 1 and the polarizability α_c appearing in V_{ind} is set to 1.2, the partial charges as $q_1 = q_3 = -0.56$ and $q_2 = 0.12$ and finally the term $\frac{n_2}{n_2 - 4}$ is simplified to 1.0 for the time being. Table 2 shows the interaction energies

atom types	ϵ	r_0	β	m
C-$N_{1,3}$	5.205	3.994	6–9	6.0
C-N_2	3.536	3.828	6–9	6.0

Table 1: ILJ parameters for the interaction of N_3^- confined inside a carbon nanotube. Different values of β are tested.

computed using the above formula and different values of β for a representative geometry. A second series of test has been done by resetting the term $\frac{n_2}{n_2 - 4}$, which depends on β and therefore will change accordingly. Table 3 shows the results in this case.

E_{int}	$\beta = 6.0$	$\beta = 7.0$	$\beta = 8.0$	$\beta = 9.0$
V_{ILJ} [meV]	-569.17	-517.63	-462.66	-403.66
V_{ILJ} [kcal/mol]	-13.12	-11.94	-10.67	-9.31
V_{ind} [meV]	-2493.52	-2493.52	-2493.52	-2493.52
V_{ind} [kcal/mol]	-57.50	-57.50	-57.50	-57.50
E_{int} [meV]	-3062.68	-3011.15	-2956.18	-2897.18
E_{int} [kcal/mol]	-70.63	-69.44	-68.17	-66.81

Table 2: Interaction energies computed using ILJ and the induction term for different β values. The term $\frac{n_2}{n_2-4}$ in the induction potential was kept fixed equal one. The reference MP2 value is -32.31 kcal/mol (-1401.13 meV).

E_{int}	$\beta = 6.0$	$\beta = 7.0$	$\beta = 8.0$	$\beta = 9.0$
V_{ILJ} [meV]	-569.17	-517.63	-462.66	-403.66
V_{ILJ} [kcal/mol]	-13.12	-11.94	-10.67	-9.31
V_{ind} [meV]	-4033.24	-3818.14	-3657.00	-3531.54
V_{ind} [kcal/mol]	-93.01	-88.05	-84.33	-81.44
E_{int} [meV]	-4602.40	-4335.77	-4119.67	-3935.20
E_{int} [kcal/mol]	-106.13	-99.98	-95.00	-90.75

Table 3: Interaction energies computed using ILJ and the induction term for different β values. The term $\frac{n_2}{n_2-4}$ in the induction potential was let free to vary. The reference MP2 value is -32.31 kcal/mol (-1401.13 meV).