Report - 5

$$E_{ab} = \sum_{i}^{\text{on } a} \sum_{j}^{\text{on } b} \frac{k_C q_i q_j}{r_{ij}^2} + \frac{A}{r_{\text{OO}}^{12}} - \frac{B}{r_{\text{OO}}^{6}},$$

$$k_c = 332.1 \text{ Å} \cdot kcal/(mol \cdot e^2)$$

$$A = 582.0 * 10^3 kcal\text{Å}^{12}/mol$$

$$B = 595.0 \, kcal\text{Å}^6/mol$$

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Original configuration energy:  -5071.964855601935
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The energy obtained after applying the formula along with the periodic boundary condition