1. Using the Born-Mayer-Huggins form of the potential energy, (a) calculate the equilibrium lattice constant (separation), \( r_0 \), and (b) the lattice energy, \( V(r_0) \), for BaO (Rocksalt structure). Compute for nearest neighbors only. (c) How do the values compare with Table 7.1 (course notes)?

2. Two possible configurations for the hypothetical Ar\(_3\) molecule are shown below.

![Diagram](image1.png)

(a) For each configuration compute the interatomic distance (separation) to 5 significant digits. Given constants \( A_{12} = 4.0005 \) and \( A_6 = 4.03 \) for the a. molecule and \( A_6 = A_{12} = 6 \) for b. molecule. You can leave your answers in terms of \( \sigma \).

(b) Compute their cohesive energies. You can leave your answers in terms of \( \varepsilon \).

(c) Based on your answers which configuration has the shorter bond length and which is more stable (i.e., has the larger cohesive/bond energy)?

(d) Plot the values you calculated on energy vs. separation (Condon-Morse) curves. Label the axes and the values on the two curves.

3. Calculate the Madelung constant for CsCl (just calculate for the first two summation terms, i.e., consider both first and second shells). The cubic CsCl crystal structure was discussed in class 3/slide 5, i.e. the first shell). Use \( r_0 \) for the anion–cation distance. The first shell (unit cell) and second shell (hint: consider atom labeled 2 as your origin and Cs and atom labeled 1 as Cl) are shown: