MD/GE - Molecular dynamics simulation and lattice energy of argon

Protocol for the Physical chemistry lab course PC 2 by
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1 Theory

[1]

$$V(r_{ij}) = 4\varepsilon_0 \left[\left(\frac{\sigma_0}{r_{ij}} \right)^{12} - \left(\frac{\sigma_0}{r_{ij}} \right)^{6} \right] \tag{1}$$

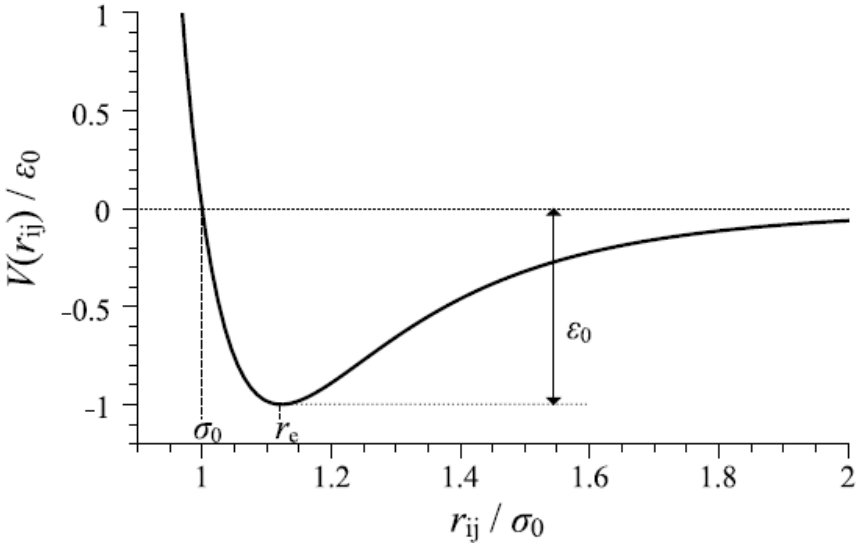

Abb. 1: .

$$T^* = \frac{k_B T}{\varepsilon_0} \tag{2}$$

$$p^* = \frac{p \sigma_0^3}{\varepsilon_0} \tag{3}$$

$$\ln p = -\frac{\Delta H_{sub}}{RT} + C \tag{4}$$

$$\Delta U_s = U_{lattice} + U_{vib} \tag{5}$$

$$U_s = \frac{5}{2} RT - \Delta H \tag{6}$$

$$U_{vib} = \frac{9}{8} R\Theta_D + 3RT \tag{7}$$

$$U_{lattice}(s) = 2N_A \varepsilon_0 \left[12.132 \left(\frac{\sigma_0}{a} \right)^{12} - 14.454 \left(\frac{\sigma_0}{a} \right)^{6} \right] \tag{8}$$

$$\log(p/\text{Torr}) = 7.781845 - \frac{341.619\ \text{K}}{T} - 0.0062649\frac{T}{\text{K}} \tag{9}$$

2 Procedure

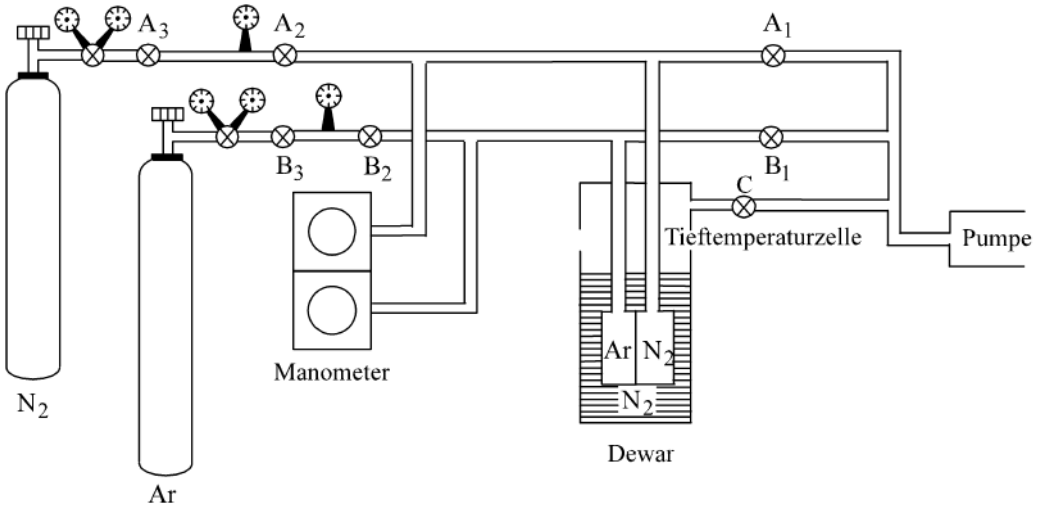

Abb. 2: Scheme of the measuring apparatus.

3 Evaluation

4 Error Analysis

5 Conclusion

6 References

[1] H. Dilger, *2025-pc2-script-en*, **2025**.