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

Protocol for the Physical chemistry lab course PC 2 by
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Inhaltsverzeichnis

1 Theory

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

$$\ln p = -\frac{\Delta H_{\text{sub}}}{RT} + C \tag{2}$$

$$U_{\text{Gitter}}(s) = 2N_A\varepsilon_0 \left[12.132 \left(\frac{\sigma_0}{a} \right)^{12} - 14.454 \left(\frac{\sigma_0}{a} \right)^6 \right] \tag{3}$$

$$\Delta U_s = U_{\text{Gitter}} + U_{\text{vib}} \tag{4}$$

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

$$U_{\text{vib}} = \frac{9}{8}R\Theta_D + 3RT \tag{6}$$

$$\log(p/\text{Torr}) = 7.781845 - \frac{341.619 \text{ K}}{T} - 0.0062649\frac{T}{\text{K}} \tag{7}$$

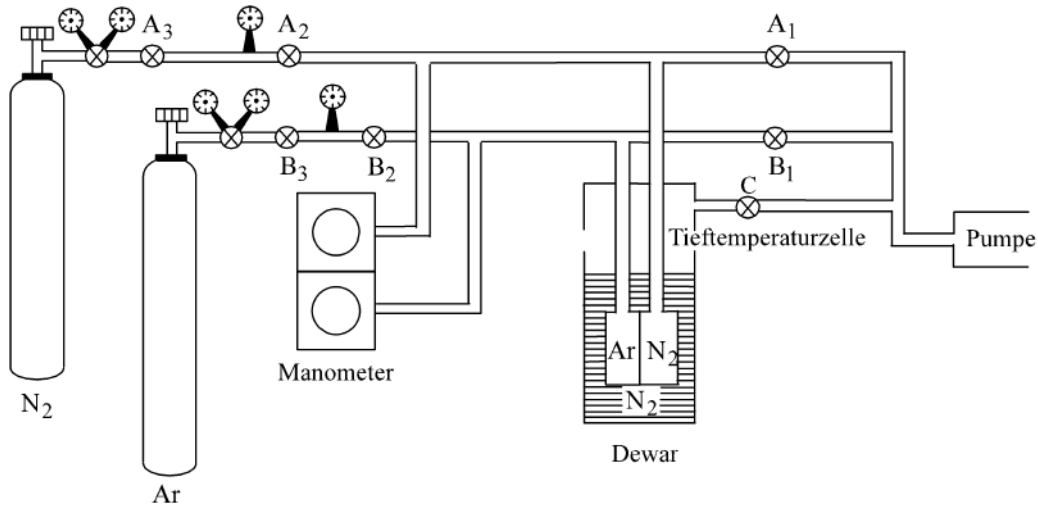Abb. 1: Scheme of the measuring apparatus.

2 Procedure

3 Evaluation

4 Error Analysis

5 Conclusion