

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	1
2	Procedure	2
3	Evaluation	2
4	Error Analysis	2
5	Conclusion	2
6	References	2

1 Theory

[1]

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

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

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

$$\Delta U_s = U_{\text{Gitter}} + U_{\text{vib}} \quad (4)$$

$$U_s = \frac{5}{2}RT - \Delta H \quad (5)$$

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

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

$$T^* = \frac{k_B T}{\varepsilon_0} \quad (8)$$

$$p^* = \frac{p \sigma_0^3}{\varepsilon_0} \quad (9)$$

2 Procedure

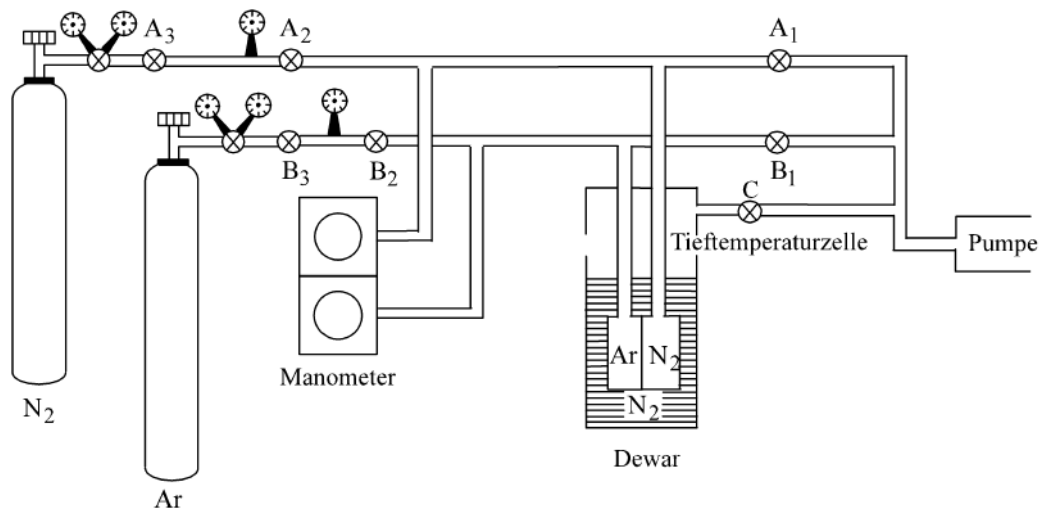


Abb. 1: Scheme of the measuring apparatus.

3 Evaluation

4 Error Analysis

5 Conclusion

6 References

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