Implementation and performance evaluation of different cubic equations of state for the estimation of properties of organic mixtures

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Supplementary Informations to accompany Implementation and performance evaluation of different cubic equations of state for the estimation of properties of organic mixtures.

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1. Derivatives

The development of the derivatives is based on the source [**?**]. Only the derivatives affected by the volume translation are added here.

In this work, the volume translation is considered as a constant (it is not function of δ nor the composition).

1.1. Derivatives of $\psi^{(-)}$

$$\psi^{(-)} = -\ln\left(1-(b-c)\,\delta\rho_r\right) \tag{1}$$

$$\frac{\partial\psi^{(-)}}{\partial\delta} = \frac{(b-c)\,\rho_r}{1-(b-c)\,\delta\rho_r} \tag{2}$$

$$\frac{\partial^2\psi^{(-)}}{\partial\delta^2} = \left(\frac{(b-c)\,\rho_r}{1-(b-c)\,\delta\rho_r}\right)^2 \tag{3}$$

$$\frac{\partial^3\psi^{(-)}}{\partial\delta^3} = 2\left(\frac{(b-c)\,\rho_r}{1-(b-c)\,\delta\rho_r}\right)^3 \tag{4}$$

$$\frac{\partial^4\psi^{(-)}}{\partial\delta^4} = 6\left(\frac{(b-c)\,\rho_r}{1-(b-c)\,\delta\rho_r}\right)^4 \tag{5}$$

1.2. Composition derivatives of $\psi^{(-)}$

The derivatives of $\psi^{(-)}$ with respect to δ and one composition derivative:

$$\frac{\partial\psi^{(-)}}{\partial x_i} = \frac{\delta\rho_r\dfrac{\partial b}{\partial x_i}}{1-(b-c)\,\delta\rho_r} \tag{6}$$

$$\frac{\partial^2\psi^{(-)}}{\partial x_i\partial\delta} = \frac{\rho_r\dfrac{\partial b}{\partial x_i}}{\left(1-(b-c)\,\delta\rho_r\right)^2} \tag{7}$$

$$\frac{\partial^3\psi^{(-)}}{\partial x_i\partial\delta^2} = \frac{2\rho_r^2(b-c)\dfrac{\partial b}{\partial x_i}}{\left(1-(b-c)\,\delta\rho_r\right)^3} \tag{8}$$

$$\frac{\partial^4\psi^{(-)}}{\partial x_i\partial\delta^3} = \frac{6\rho_r^3(b-c)^2\dfrac{\partial b}{\partial x_i}}{\left(1-(b-c)\,\delta\rho_r\right)^4} \tag{9}$$

$$\frac{\partial^5\psi^{(-)}}{\partial x_i\partial\delta^4} = \frac{24\rho_r^4(b-c)^3\dfrac{\partial b}{\partial x_i}}{\left(1-(b-c)\,\delta\rho_r\right)^5} \tag{10}$$

The derivatives of $\psi^{(-)}$ with respect to δ and two composition derivatives:

$$\frac{\partial^2\psi^{(-)}}{\partial x_i\partial x_j} = \frac{\delta\rho_r\dfrac{\partial^2 b}{\partial x_i\partial x_j}}{1-\delta\rho_r(b-c)} + \frac{(\delta\rho_r)^2\dfrac{\partial b}{\partial x_i}\dfrac{\partial b}{\partial x_j}}{(1-\delta\rho_r(b-c))^2} \tag{11}$$

$$\frac{\partial^3\psi^{(-)}}{\partial x_i\partial x_j\partial\delta} = \frac{\rho_r\dfrac{\partial^2 b}{\partial x_i\partial x_j}}{(1-\delta\rho_r(b-c))^2} + \frac{2\delta\rho_r^2\dfrac{\partial b}{\partial x_i}\dfrac{\partial b}{\partial x_j}}{(1-\delta\rho_r(b-c))^3} \tag{12}$$

$$\frac{\partial^4\psi^{(-)}}{\partial x_i\partial x_j\partial\delta^2} = \frac{2\rho_r^2(b-c)\dfrac{\partial^2 b}{\partial x_i\partial x_j}}{(1-\delta\rho_r(b-c))^3} + \frac{2\rho_r^2\dfrac{\partial b}{\partial x_i}\dfrac{\partial b}{\partial x_j}}{(1-\delta\rho_r(b-c))^4}\left(2\delta\rho_r(b-c)+1\right) \tag{13}$$

$$\frac{\partial^5\psi^{(-)}}{\partial x_i\partial x_j\partial\delta^3} = \frac{6\rho_r^3(b-c)^2\dfrac{\partial^2 b}{\partial x_i\partial x_j}}{(1-\delta\rho_r(b-c))^4} + \frac{12\rho_r^3(b-c)\dfrac{\partial b}{\partial x_i}\dfrac{\partial b}{\partial x_j}}{(1-\delta\rho_r(b-c))^5}\left(\delta\rho_r(b-c)+1\right) \tag{14}$$

$$\frac{\partial^6\psi^{(-)}}{\partial x_i\partial x_j\partial\delta^4} = \frac{24\rho_r^4(b-c)^3\dfrac{\partial^2 b}{\partial x_i\partial x_j}}{(1-\delta\rho_r(b-c))^5} + \frac{24\rho_r^4(b-c)^2\dfrac{\partial b}{\partial x_i}\dfrac{\partial b}{\partial x_j}}{(1-\delta\rho_r(b-c))^6}\left(2\delta\rho_r(b-c)+3\right) \tag{15}$$

The derivatives of $\psi^{(-)}$ with respect to δ and three composition derivatives:

$$\frac{\partial^3\psi^{(-)}}{\partial x_i\partial x_j\partial x_k} = \frac{\delta\rho_r\dfrac{\partial^3 b}{\partial x_i\partial x_j\partial x_k}}{1-\delta\rho_r(b-c)} + \frac{(\delta\rho_r)^2\left(\dfrac{\partial b}{\partial x_i}\dfrac{\partial^2 b}{\partial x_j\partial x_k}+\dfrac{\partial b}{\partial x_j}\dfrac{\partial^2 b}{\partial x_i\partial x_k}+\dfrac{\partial b}{\partial x_k}\dfrac{\partial^2 b}{\partial x_i\partial x_j}\right)}{(1-\delta\rho_r(b-c))^2} + \frac{2(\delta\rho_r)^3\dfrac{\partial b}{\partial x_i}\dfrac{\partial b}{\partial x_j}\dfrac{\partial b}{\partial x_k}}{(1-\delta\rho_r(b-c))^3} \tag{16}$$

$$\frac{\partial^4\psi^{(-)}}{\partial x_i\partial x_j\partial x_k\partial\delta} = \frac{\rho_r\dfrac{\partial^3 b}{\partial x_i\partial x_j\partial x_k}}{(1-\delta\rho_r(b-c))^2} + \frac{2\delta\rho_r^2\left(\dfrac{\partial b}{\partial x_i}\dfrac{\partial^2 b}{\partial x_j\partial x_k}+\dfrac{\partial b}{\partial x_j}\dfrac{\partial^2 b}{\partial x_i\partial x_k}+\dfrac{\partial b}{\partial x_k}\dfrac{\partial^2 b}{\partial x_i\partial x_j}\right)}{(1-\delta\rho_r(b-c))^3} + \frac{6\delta^2\rho_r^3\dfrac{\partial b}{\partial x_i}\dfrac{\partial b}{\partial x_j}\dfrac{\partial b}{\partial x_k}}{(1-\delta\rho_r(b-c))^4} \tag{17}$$

1.3. Derivatives of $\psi^{(+)}$

$$\psi^{(+)} = \frac{\ln\left(\dfrac{1+(b\Delta_1+c)\delta\rho_r}{1+(b\Delta_2+c)\delta\rho_r}\right)}{b(\Delta_1-\Delta_2)} \tag{18}$$

$$\frac{\partial\psi^{(+)}}{\partial\delta} = \frac{\rho_r}{\left(1+(b\Delta_1+c)\delta\rho_r\right)\left(1+(b\Delta_2+c)\delta\rho_r\right)} \tag{19}$$

The term

$$\Pi_{12} = \left(1+(b\Delta_1+c)\delta\rho_r\right)\left(1+(b\Delta_2+c)\delta\rho_r\right) \tag{20}$$

is introduced to ease the next derivatives.

We have:

$$\frac{\partial \psi^{(+)}}{\partial \delta} = \frac{\rho_r}{\Pi_{12}} \tag{21}$$

$$\frac{\partial^2 \psi^{(+)}}{\partial \delta^2} = -\rho_r \frac{\frac{\partial \Pi_{12}}{\partial \delta}}{\Pi_{12}^2} \tag{22}$$

$$\frac{\partial^3 \psi^{(+)}}{\partial \delta^3} = \rho_r \frac{-\Pi_{12}\frac{\partial^2 \Pi_{12}}{\partial \delta^2} + 2\left(\frac{\partial \Pi_{12}}{\partial \delta}\right)^2}{\Pi_{12}^3} \tag{23}$$

$$\frac{\partial^4 \psi^{(+)}}{\partial \delta^4} = \rho_r \frac{\Pi_{12}^2 \frac{\partial^3 \Pi_{12}}{\partial \delta^3} + 6\Pi_{12}\frac{\partial \Pi_{12}}{\partial \delta}\frac{\partial^2 \Pi_{12}}{d\delta^2} - 6\left(\frac{\partial \Pi_{12}}{\partial \delta}\right)^3}{\Pi_{12}^4} \tag{24}$$

$$= \rho_r \frac{6\Pi_{12}\frac{\partial \Pi_{12}}{\partial \delta}\frac{\partial^2 \Pi_{12}}{d\delta^2} - 6\left(\frac{\partial \Pi_{12}}{\partial \delta}\right)^3}{\Pi_{12}^4} \tag{25}$$

With the derivatives of Π_{12}:

$$\Pi_{12} = (1 + (b\Delta_1 + c)\delta\rho_r)\,(1 + (b\Delta_2 + c)\delta\rho_r) \tag{26}$$

$$\frac{\partial \Pi_{12}}{\partial \delta} = \rho_r\,(2\,(b\Delta_1 + c)\,(b\Delta_2 + c)\,\delta\rho_r + (\Delta_1 + \Delta_2)\,b + 2c) \tag{27}$$

$$\frac{\partial^2 \Pi_{12}}{\partial \delta^2} = 2\rho_r^2\,(b\Delta_1 + c)\,(b\Delta_2 + c) \tag{28}$$

$$\frac{\partial^3 \Pi_{12}}{\partial \delta^3} = 0 \tag{29}$$

Note that equation 29 has been used to simplify equation 24 in equation 25.

1.4. Composition derivatives of Π_{12}

The derivatives of Π_{12} with respect to δ and one composition derivative:

$$\frac{\partial \Pi_{12}}{\partial x_i} = \delta\rho_r \frac{\partial b}{\partial x_i}\,(2\Delta_1\Delta_2\delta\rho_r b + (\Delta_1 + \Delta_2)\,(1 + c\delta\rho_r)) \tag{30}$$

$$\frac{\partial^2 \Pi_{12}}{\partial x_i \partial \delta} = \rho_r \frac{\partial b}{\partial x_i}\,(4\Delta_1\Delta_2\delta\rho_r b + (\Delta_1 + \Delta_2)\,(1 + 2c\delta\rho_r)) \tag{31}$$

$$\frac{\partial^3 \Pi_{12}}{\partial x_i \partial \delta^2} = 2\rho_r^2 \frac{\partial b}{\partial x_i}\,(2\Delta_1\Delta_2 b + (\Delta_1 + \Delta_2)\,c) \tag{32}$$

$$\frac{\partial^4 \Pi_{12}}{\partial x_i \partial \delta^3} = 0 \tag{33}$$

$$\frac{\partial^5 \Pi_{12}}{\partial x_i \partial \delta^4} = 0 \tag{34}$$

The derivatives of Π_{12} with respect to δ and two composition derivatives:

$$\frac{\partial^2 \Pi_{12}}{\partial x_i \partial x_j} = \delta\rho_r \left(2\Delta_1\Delta_2\delta\rho_r \frac{\partial b}{\partial x_i}\frac{\partial b}{\partial x_j} + \left(2\Delta_1\Delta_2\delta\rho_r b + (\Delta_1+\Delta_2)(1+c\delta\rho_r)\right)\frac{\partial^2 b}{\partial x_i \partial x_j} \right) \tag{35}$$

$$\frac{\partial^3 \Pi_{12}}{\partial x_i \partial x_j \partial\delta} = \rho_r \left(4\Delta_1\Delta_2\delta\rho_r \frac{\partial b}{\partial x_i}\frac{\partial b}{\partial x_j} + \left(4\Delta_1\Delta_2\delta\rho_r b + (\Delta_1+\Delta_2)(1+2c\delta\rho_r)\right)\frac{\partial^2 b}{\partial x_i \partial x_j} \right) \tag{36}$$

$$\frac{\partial^4 \Pi_{12}}{\partial x_i \partial x_j \partial\delta^2} = 2\rho_r^2 \left(2\Delta_1\Delta_2 \frac{\partial b}{\partial x_i}\frac{\partial b}{\partial x_j} + \left(2\Delta_1\Delta_2 b + (\Delta_1+\Delta_2)\, c\right)\frac{\partial^2 b}{\partial x_i \partial x_j} \right) \tag{37}$$

$$\frac{\partial^5 \Pi_{12}}{\partial x_i \partial x_j \partial\delta^3} = 0 \tag{38}$$

$$\frac{\partial^6 \Pi_{12}}{\partial x_i \partial x_j \partial\delta^4} = 0 \tag{39}$$

The derivatives of Π_{12} with respect to δ and three composition derivatives:

$$\frac{\partial^3 \Pi_{12}}{\partial x_i \partial x_j \partial x_k} = \delta\rho_r \left(\begin{array}{l} 2\Delta_1\Delta_2\delta\rho_r \left(\frac{\partial b}{\partial x_i}\frac{\partial^2 b}{\partial x_j \partial x_k} + \frac{\partial b}{\partial x_j}\frac{\partial^2 b}{\partial x_i \partial x_k} + \frac{\partial b}{\partial x_k}\frac{\partial^2 b}{\partial x_i \partial x_j} \right) \\ + \left(2\Delta_1\Delta_2\delta\rho_r b + (\Delta_1+\Delta_2)(1+c\delta\rho_r)\right)\frac{\partial^3 b}{\partial x_i \partial x_j \partial x_k} \end{array} \right) \tag{40}$$

$$\frac{\partial^4 \Pi_{12}}{\partial x_i \partial x_j \partial x_k \partial\delta} = \rho_r \left(\begin{array}{l} 4\Delta_1\Delta_2\delta\rho_r \left(\frac{\partial b}{\partial x_i}\frac{\partial^2 b}{\partial x_j \partial x_k} + \frac{\partial b}{\partial x_j}\frac{\partial^2 b}{\partial x_i \partial x_k} + \frac{\partial b}{\partial x_k}\frac{\partial^2 b}{\partial x_i \partial x_j} \right) \\ + \left(4\Delta_1\Delta_2\delta\rho_r b + (\Delta_1+\Delta_2)(1+2c\delta\rho_r)\right)\frac{\partial^3 b}{\partial x_i \partial x_j \partial x_k} \end{array} \right) \tag{41}$$

1.5. Composition derivatives of $\psi^{(+)}$

To simplify the composition derivatives of $\psi^{(+)}$, the term $A = \ln\left(\frac{1+(b\Delta_1+c)\delta\rho_r}{1+(b\Delta_2+c)\delta\rho_r}\right)$ is introduced. Equation 18 becomes:

$$\psi^{(+)} = \frac{A}{b(\Delta_1-\Delta_2)} \tag{42}$$

The derivatives of A with respect to the compositions ends up being the same as in the case without the volume translation.

All the unaffected derivatives are found in source [**?**].

2. Comparison

2.1. Deviation definition

The deviation used in this work is the relative deviation without sign.
Applied to the case of the molar volume[1]:

$$E_v = \frac{\left\| v_{ref} - v_{calc} \right\|}{v_{ref}} \tag{43}$$

The temperature, pressure and density deviations are computed as:

$$E_T = \frac{\| T_{data} - T_{calc} \|}{T_{data}} \tag{44}$$

$$E_p = \frac{\| p_{data} - p_{calc} \|}{p_{data}} \tag{45}$$

$$E_\rho = \frac{\| \rho_{data} - \rho_{calc} \|}{\rho_{data}} \tag{46}$$

The average deviations are computed as:

$$\bar{E}_T = \frac{1}{n} \sum_{1}^{n} E_T \tag{47}$$

$$\bar{E}_p = \frac{1}{n} \sum_{1}^{n} E_p \tag{48}$$

$$\bar{E}_\rho = \frac{1}{n} \sum_{1}^{n} E_\rho \tag{49}$$

The box plot represent five values: the minimal value, the first quartile (25% of the data have smaller values), the median (50% of the data have smaller values, 50% have higher value), the third quartile (75% of the data have smaller values), and the maximum (100% of the data have smaller or equal values).
This is a convenient way to represent the repartition of the deviation.

2.2. Volume isobars comparison

2.2.1. Pure

Here is an example with different pure fluids. The deviation here are relative to RefProp's values.

[1]The volume, pressure and temperature are on absolute scale, thus never negative. This allows to drop the absolute value on the denominator.

Fluid BUTANE.

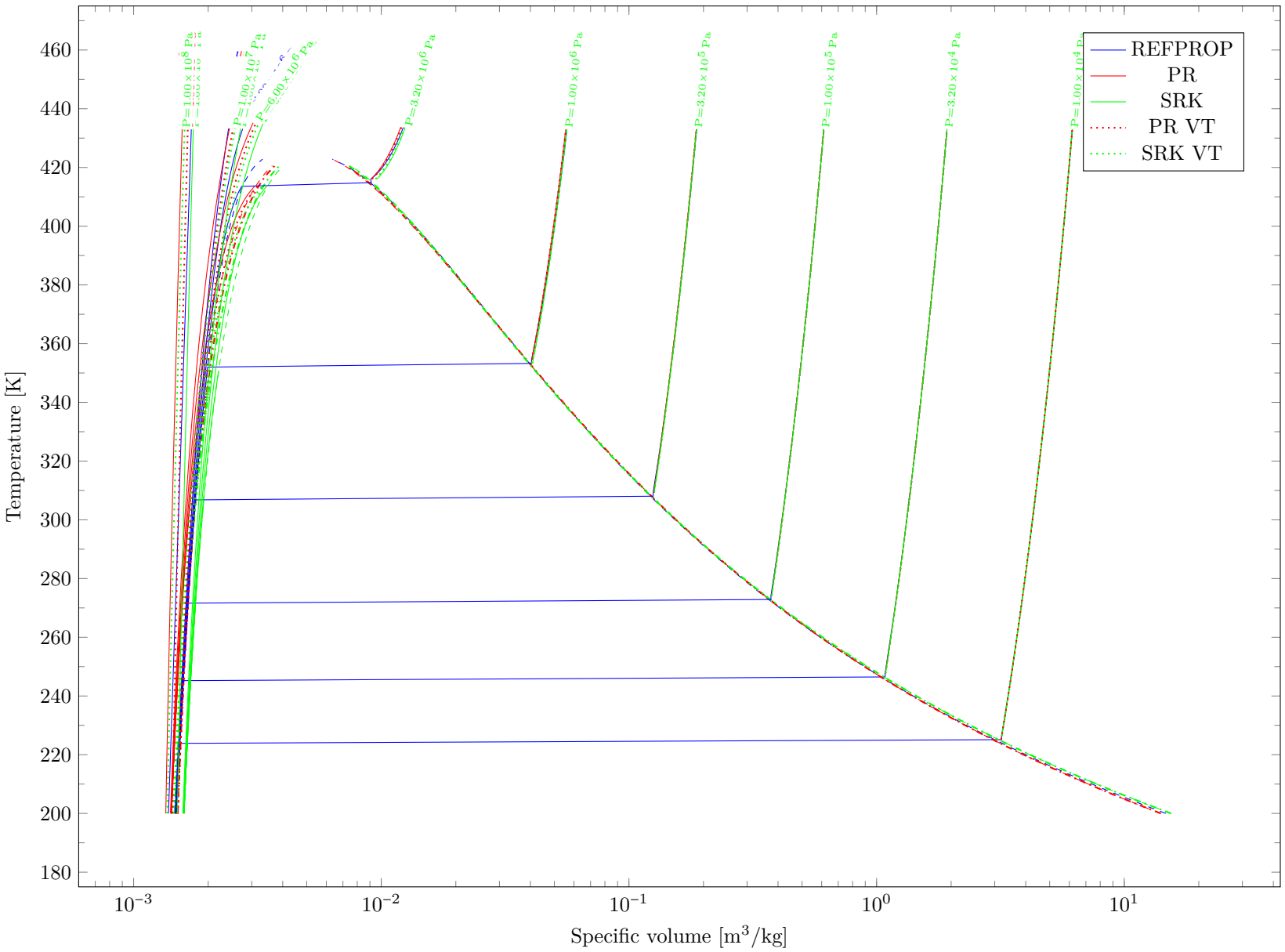


Figure 1: Isobar curves and saturation curve (dashed) on temperature/volume plot, fluid BUTANE

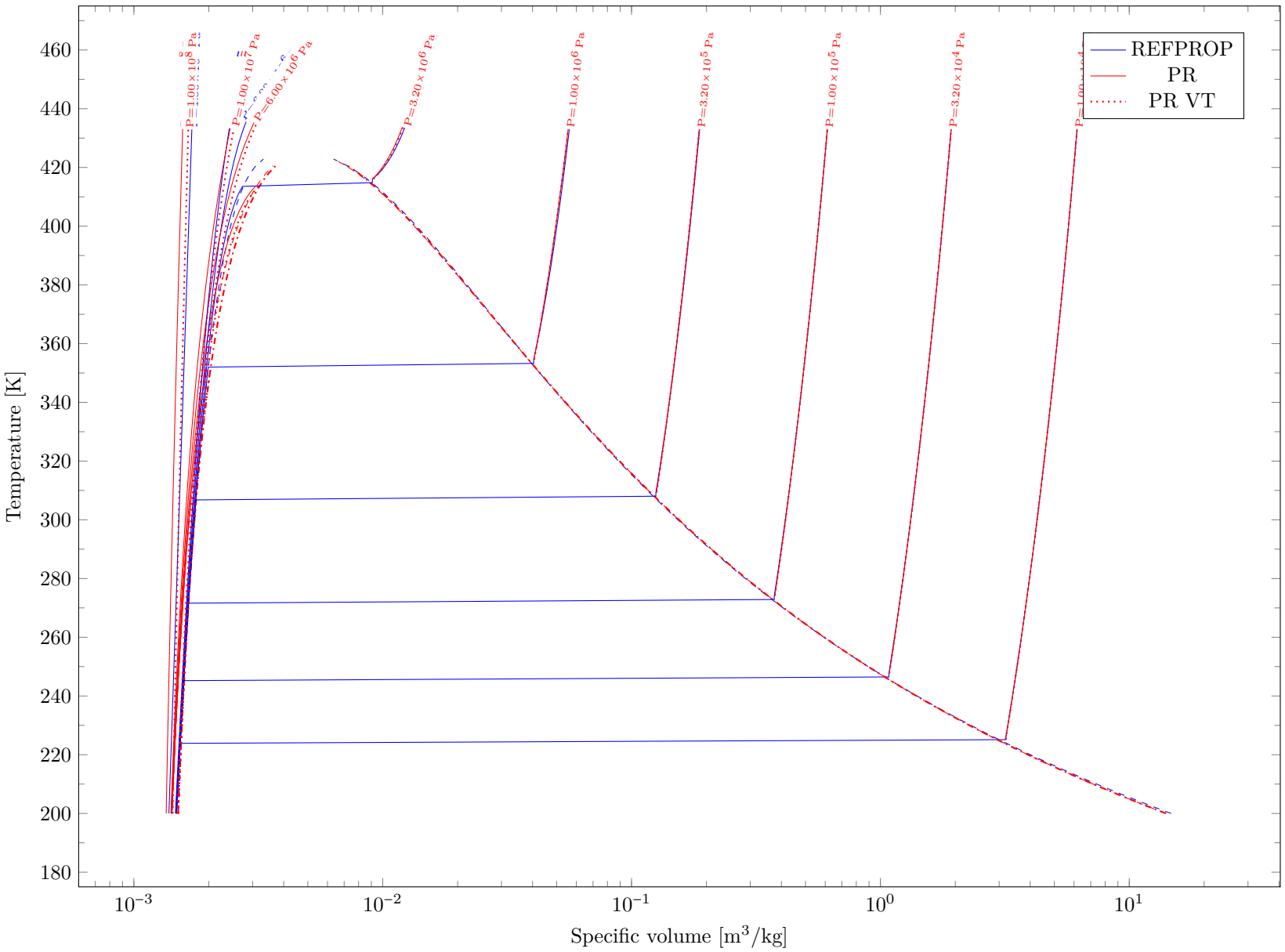


Figure 2: Isobar curves and saturation curve (dashed) on temperature/volume plot, comparison of PR with REFPROP, fluid BUTANE

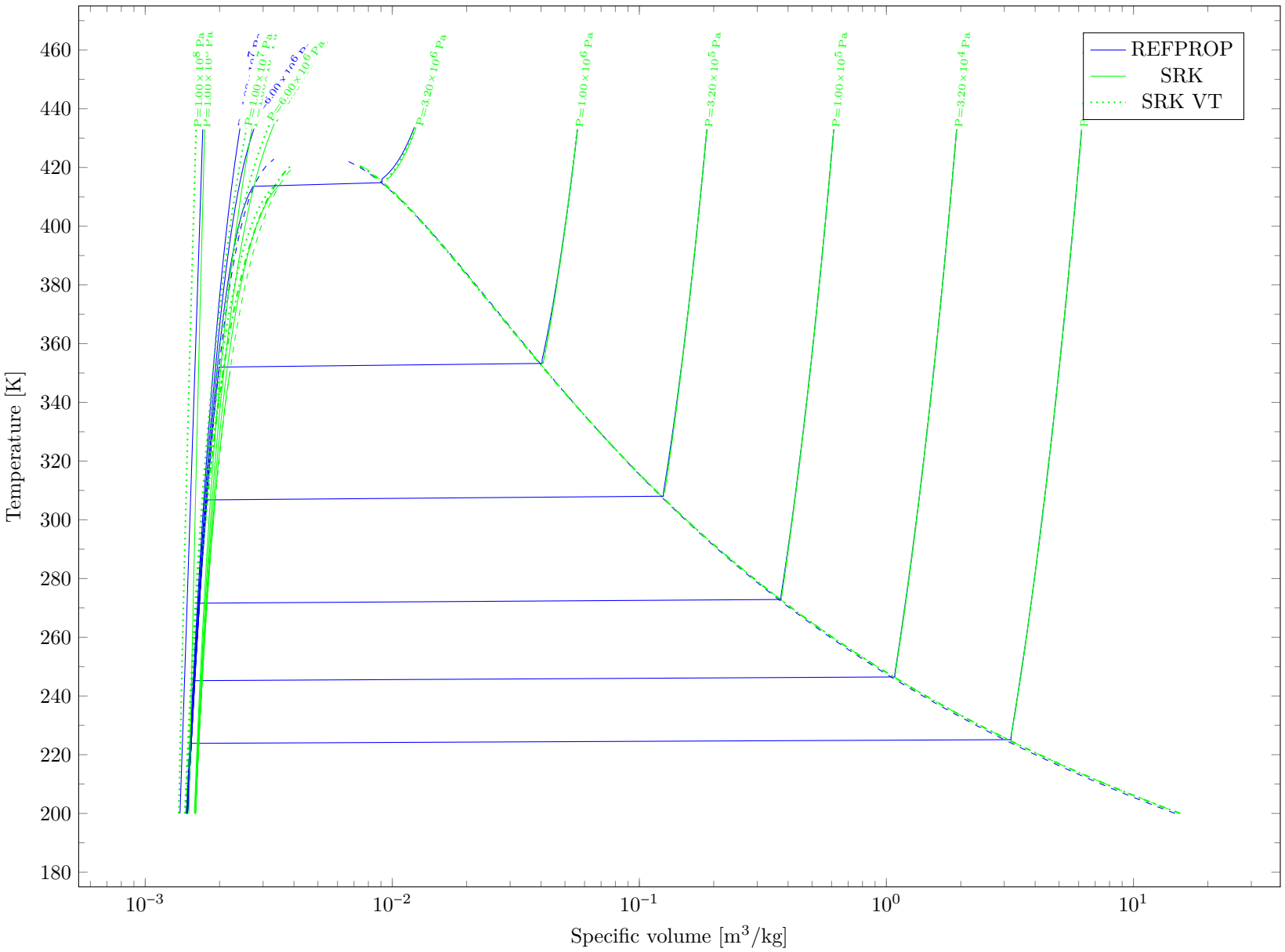


Figure 3: Isobar curves and saturation curve (dashed) on temperature/volume plot, comparison of SRK with REFPROP, fluid BUTANE

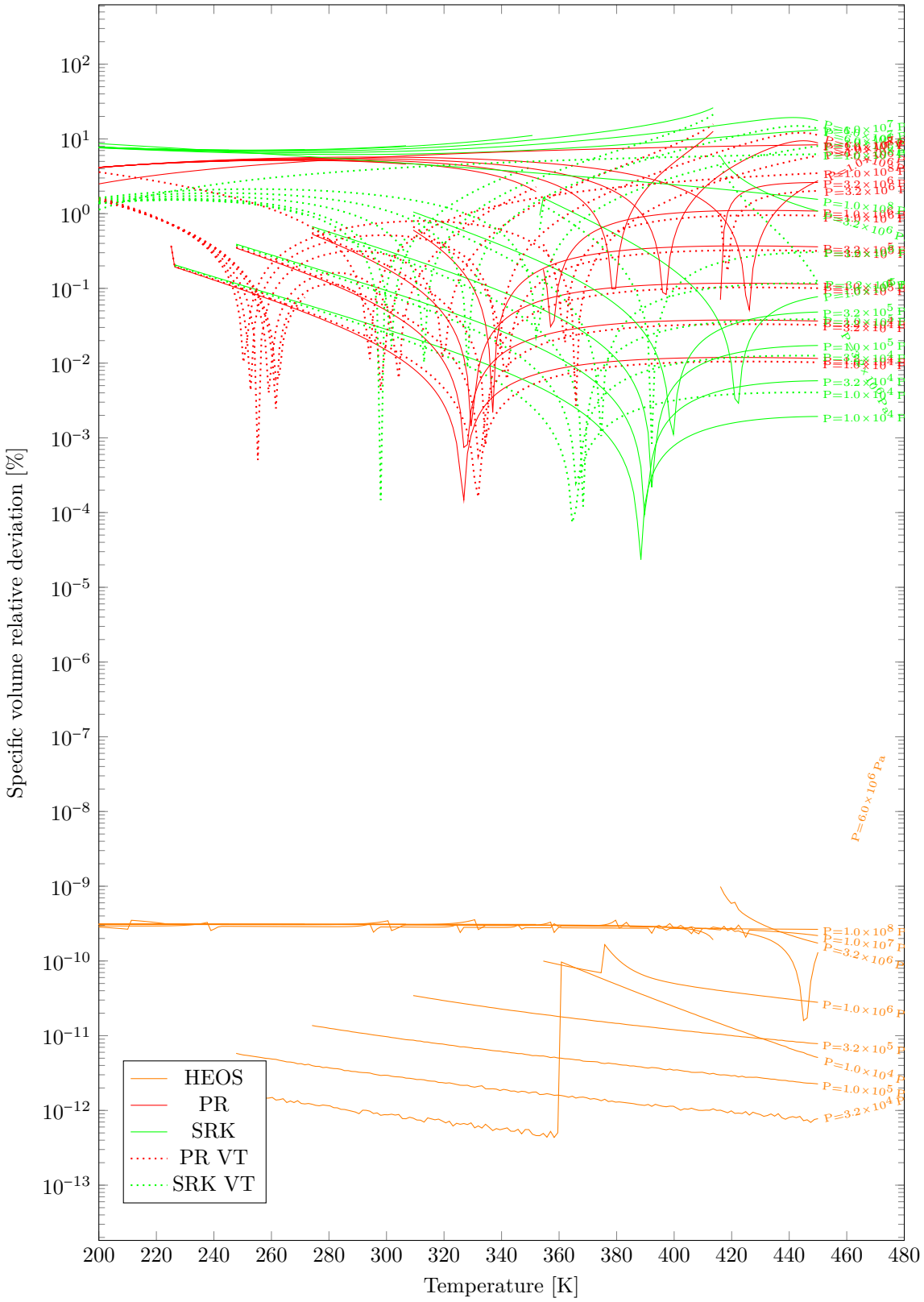


Figure 4: Deviation with the reference for each isobar, fluid BUTANE

Fluid R32.

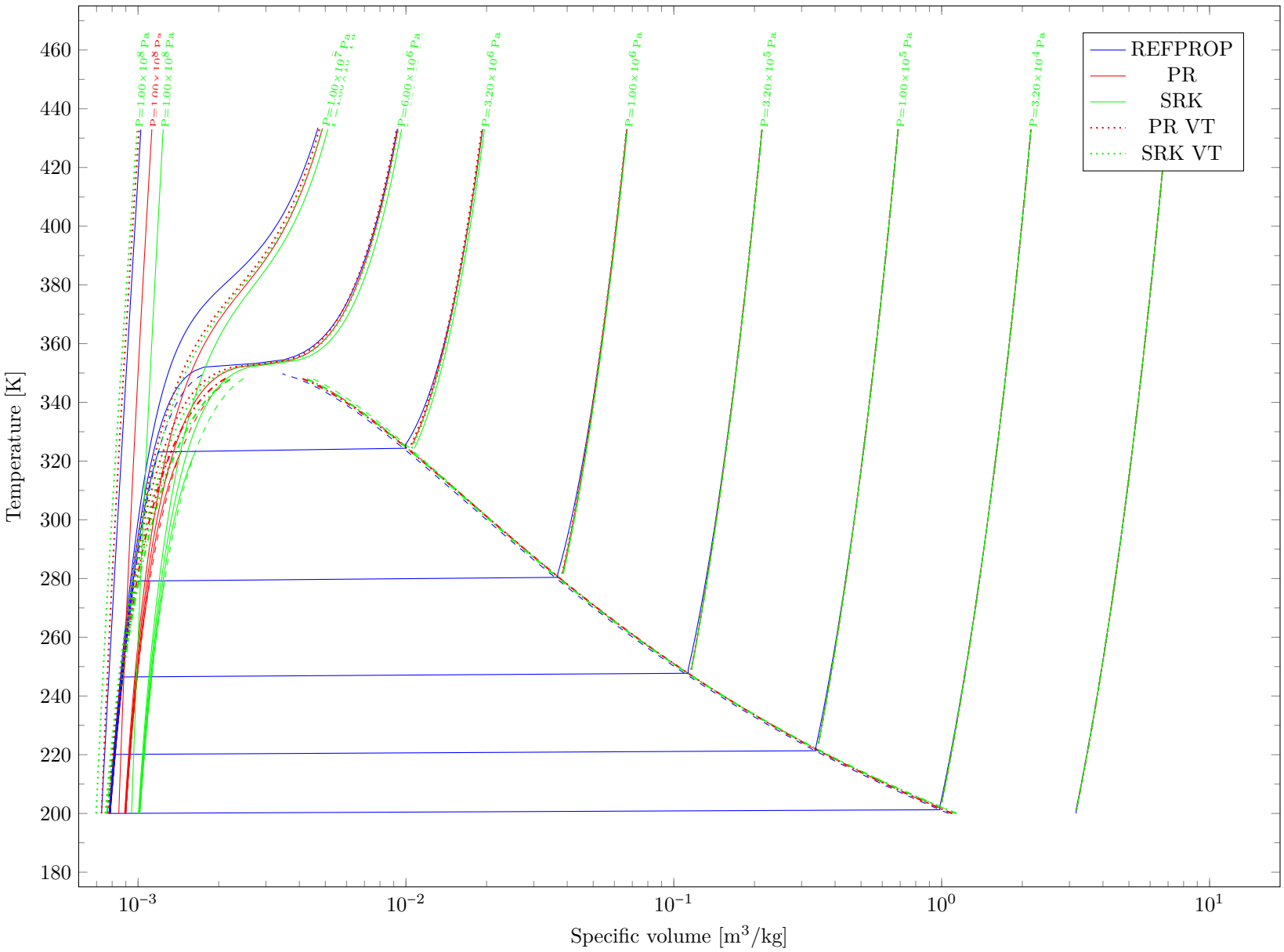


Figure 5: Isobar curves and saturation curve (dashed) on temperature/volume plot, fluid R32

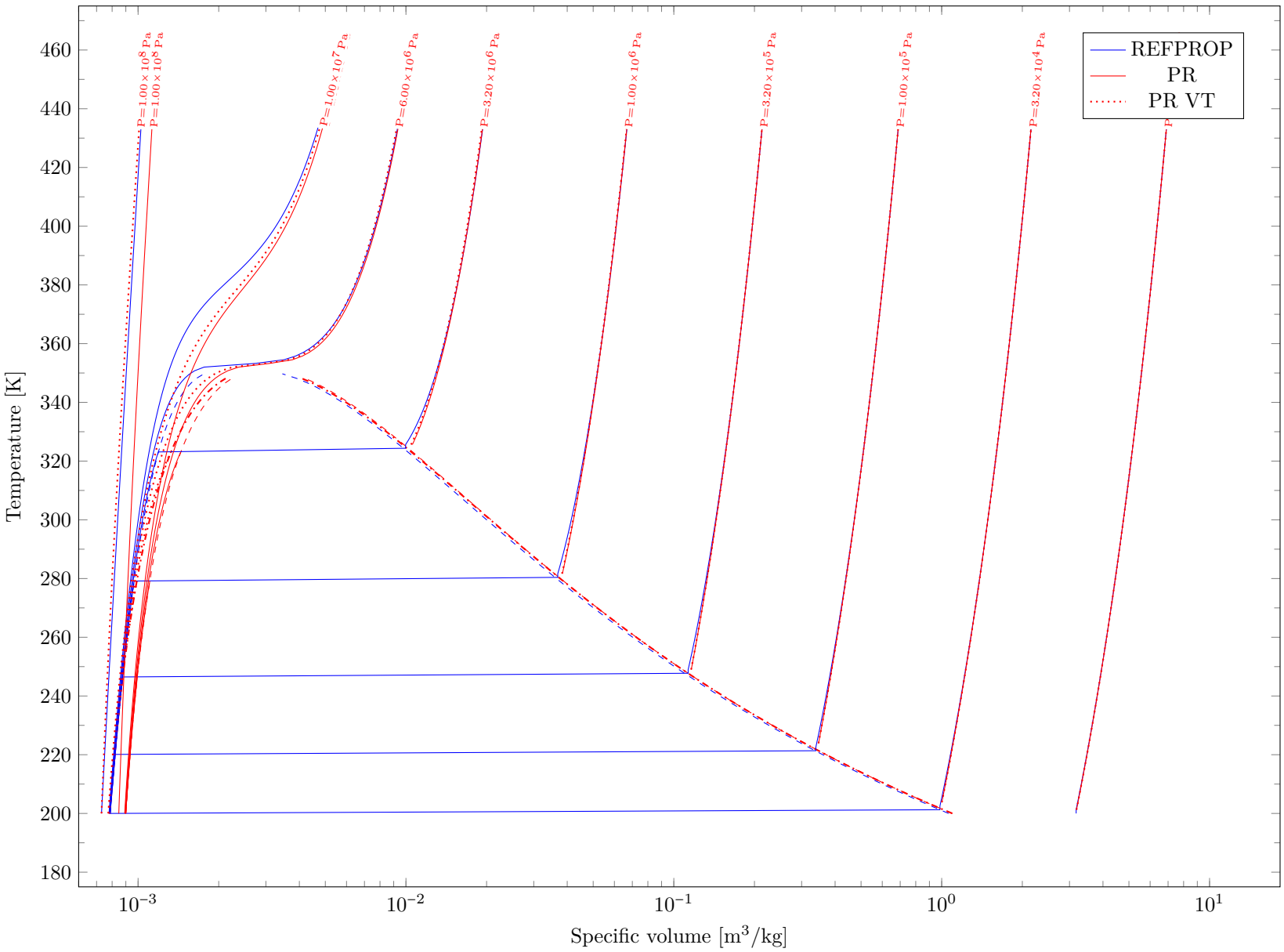


Figure 6: Isobar curves and saturation curve (dashed) on temperature/volume plot, comparison of PR with REFPROP, fluid R32

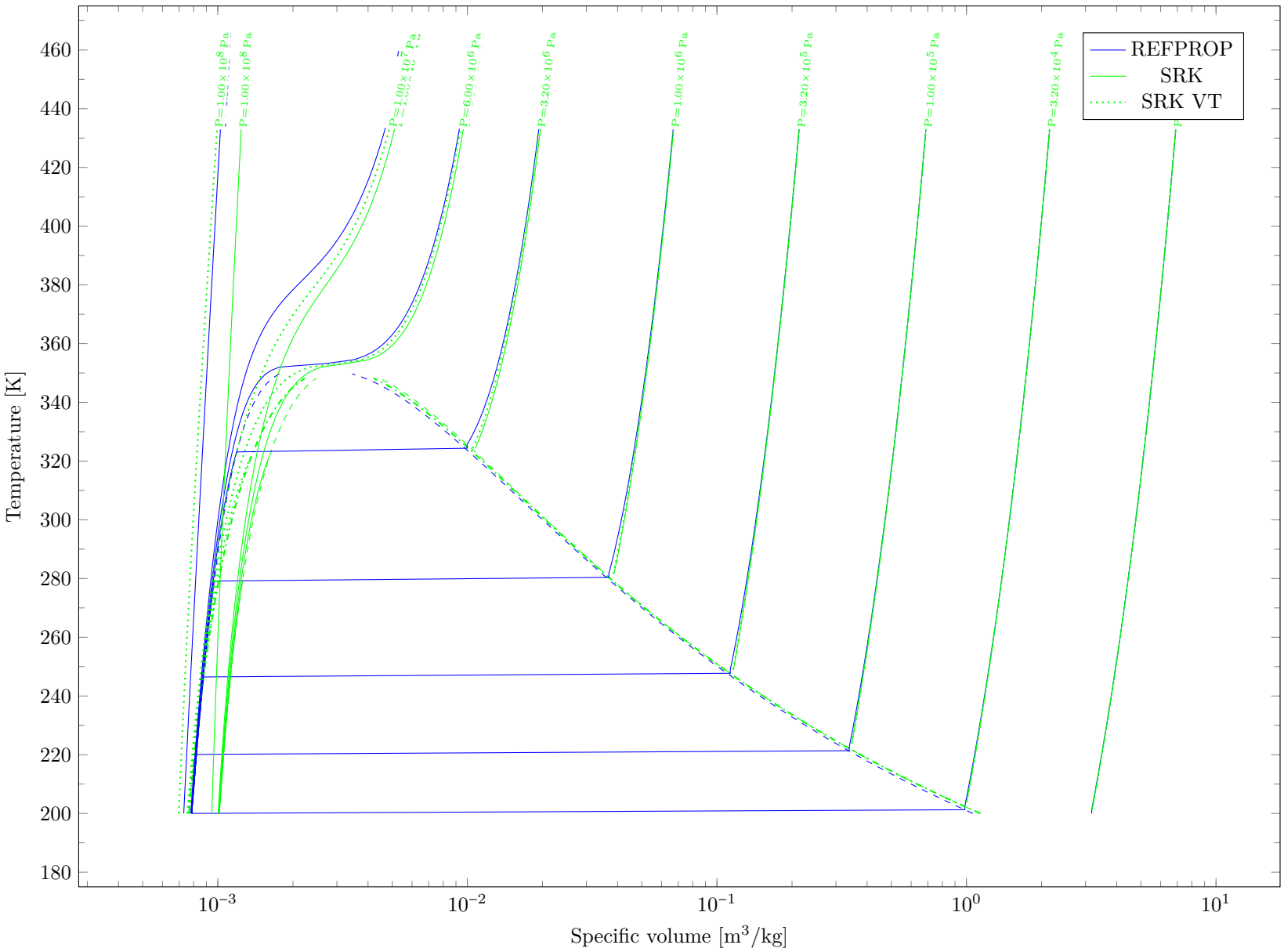


Figure 7: Isobar curves and saturation curve (dashed) on temperature/volume plot, comparison of SRK with REFPROP, fluid R32

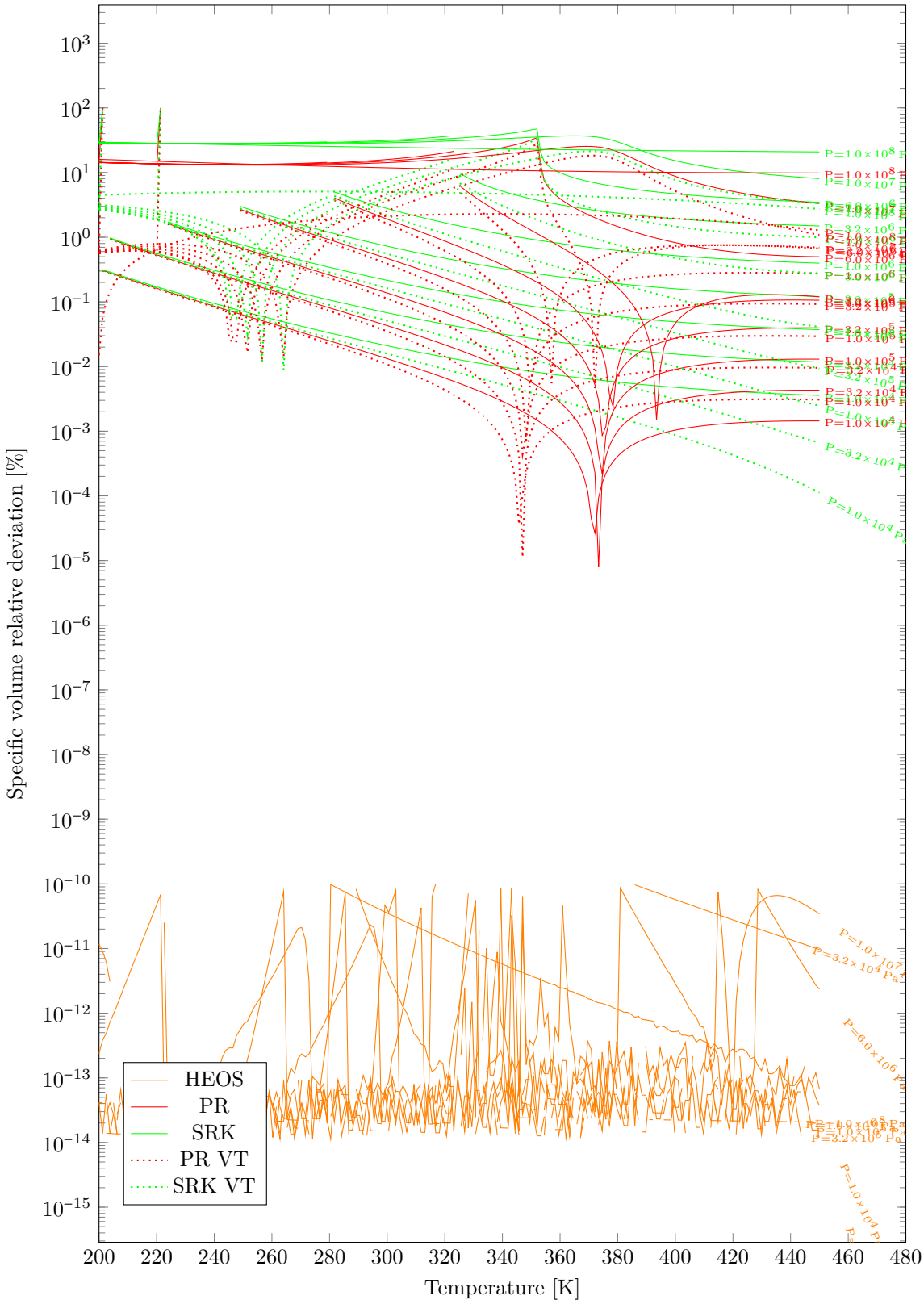


Figure 8: Deviation with the reference for each isobar, fluid R32

Fluid R125.

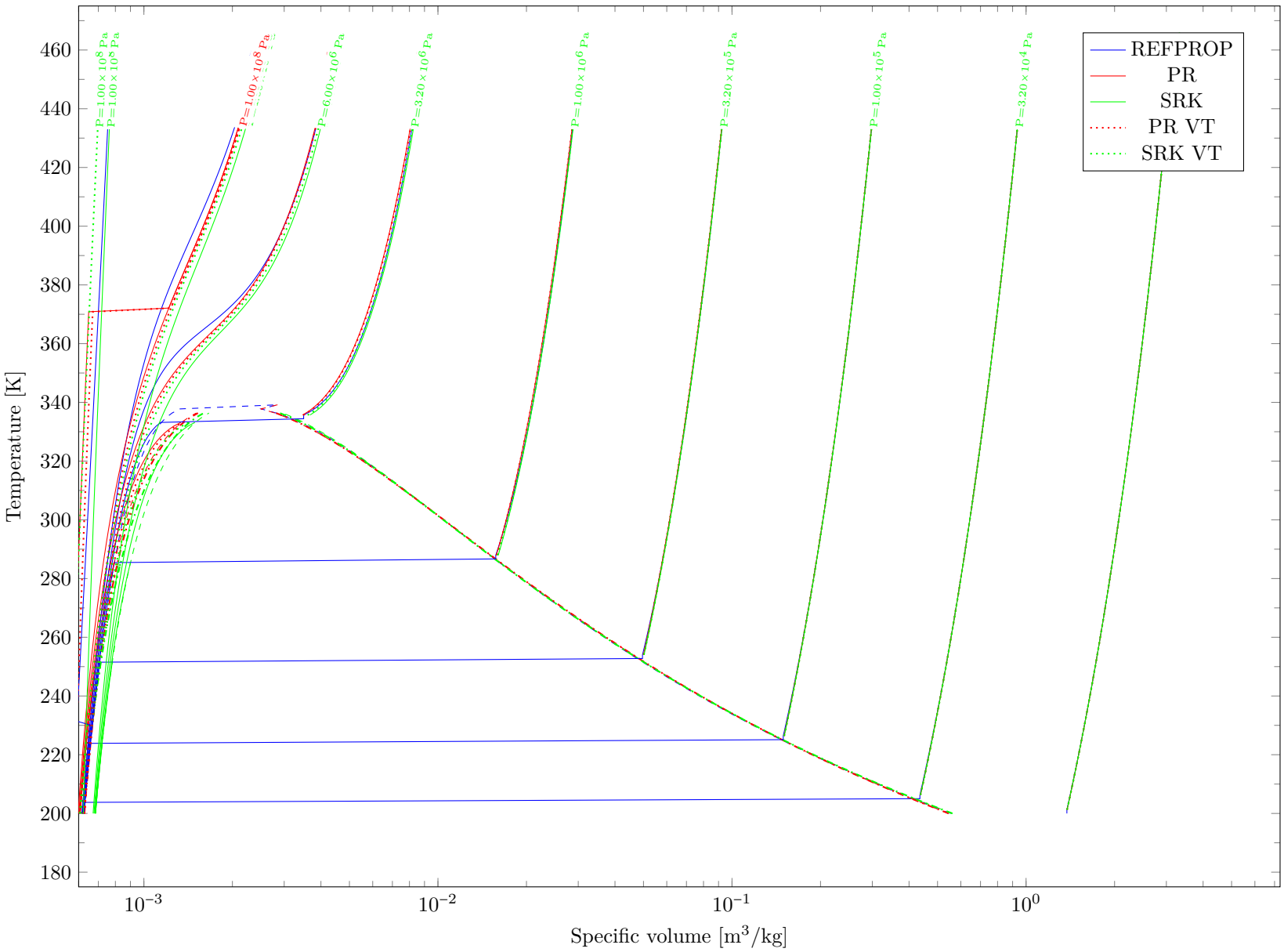


Figure 9: Isobar curves and saturation curve (dashed) on temperature/volume plot, fluid R125

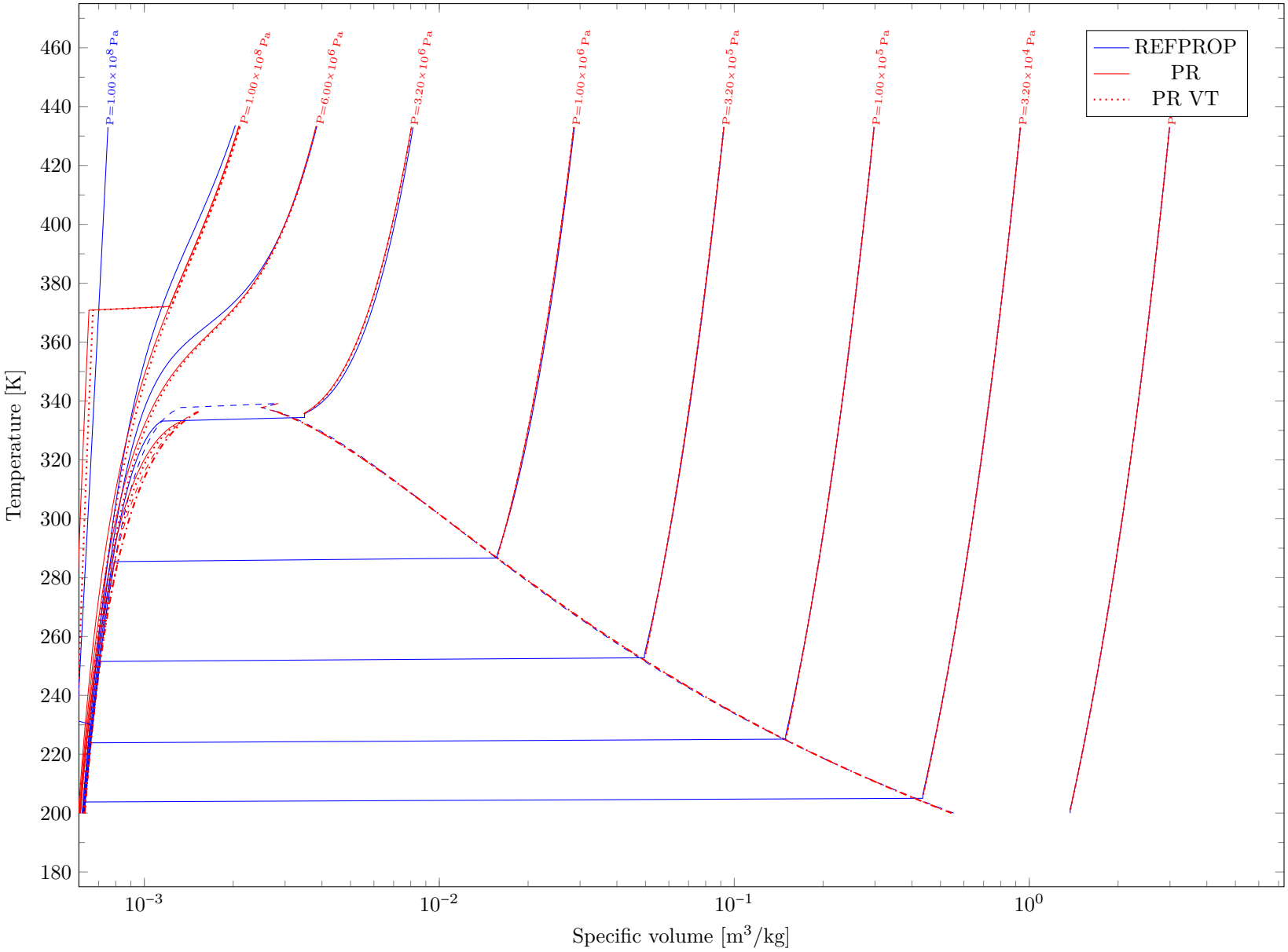


Figure 10: Isobar curves and saturation curve (dashed) on temperature/volume plot, comparison of PR with REFPROP, fluid R125

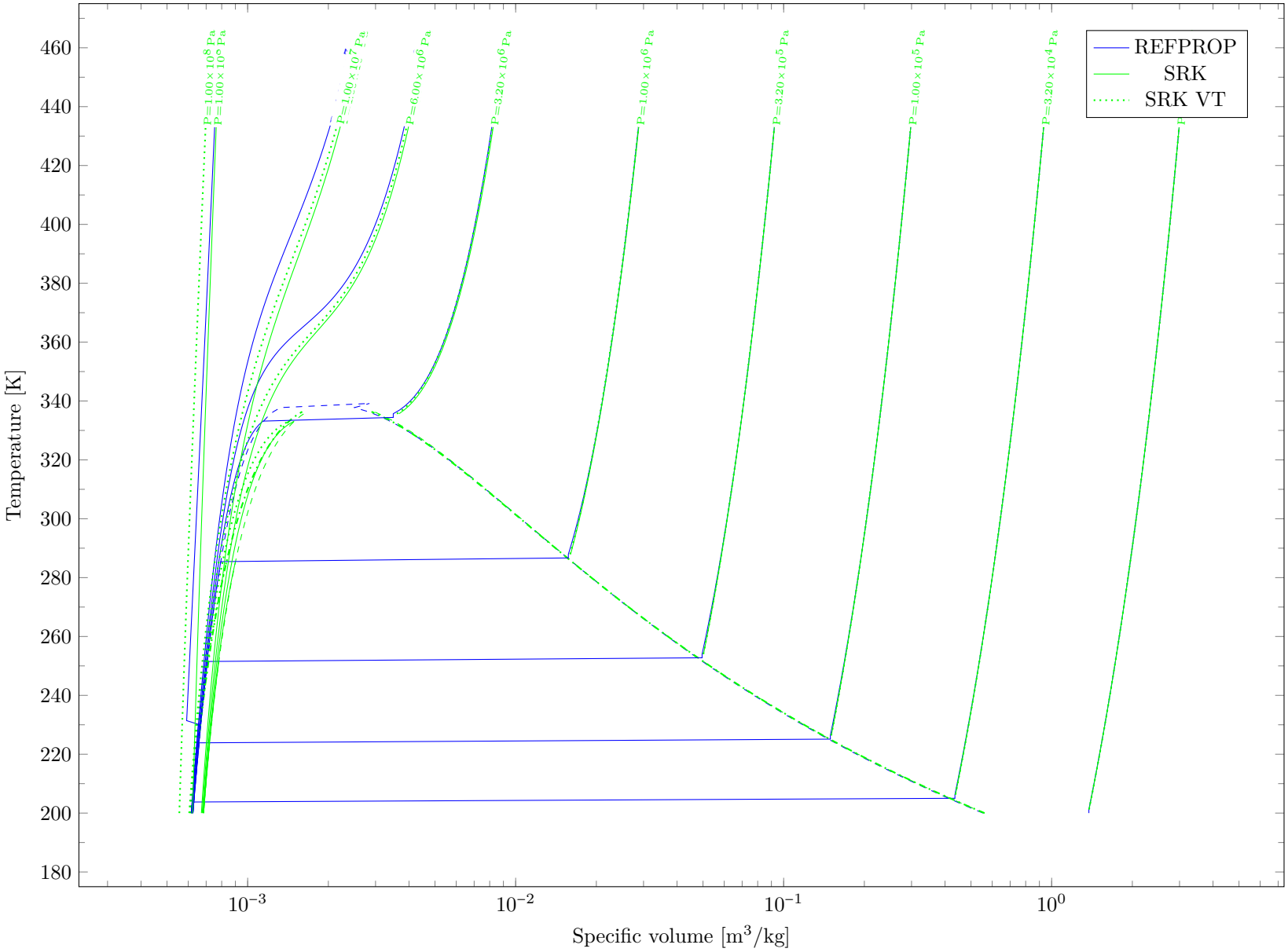


Figure 11: Isobar curves and saturation curve (dashed) on temperature/volume plot, comparison of SRK with REFPROP, fluid R125

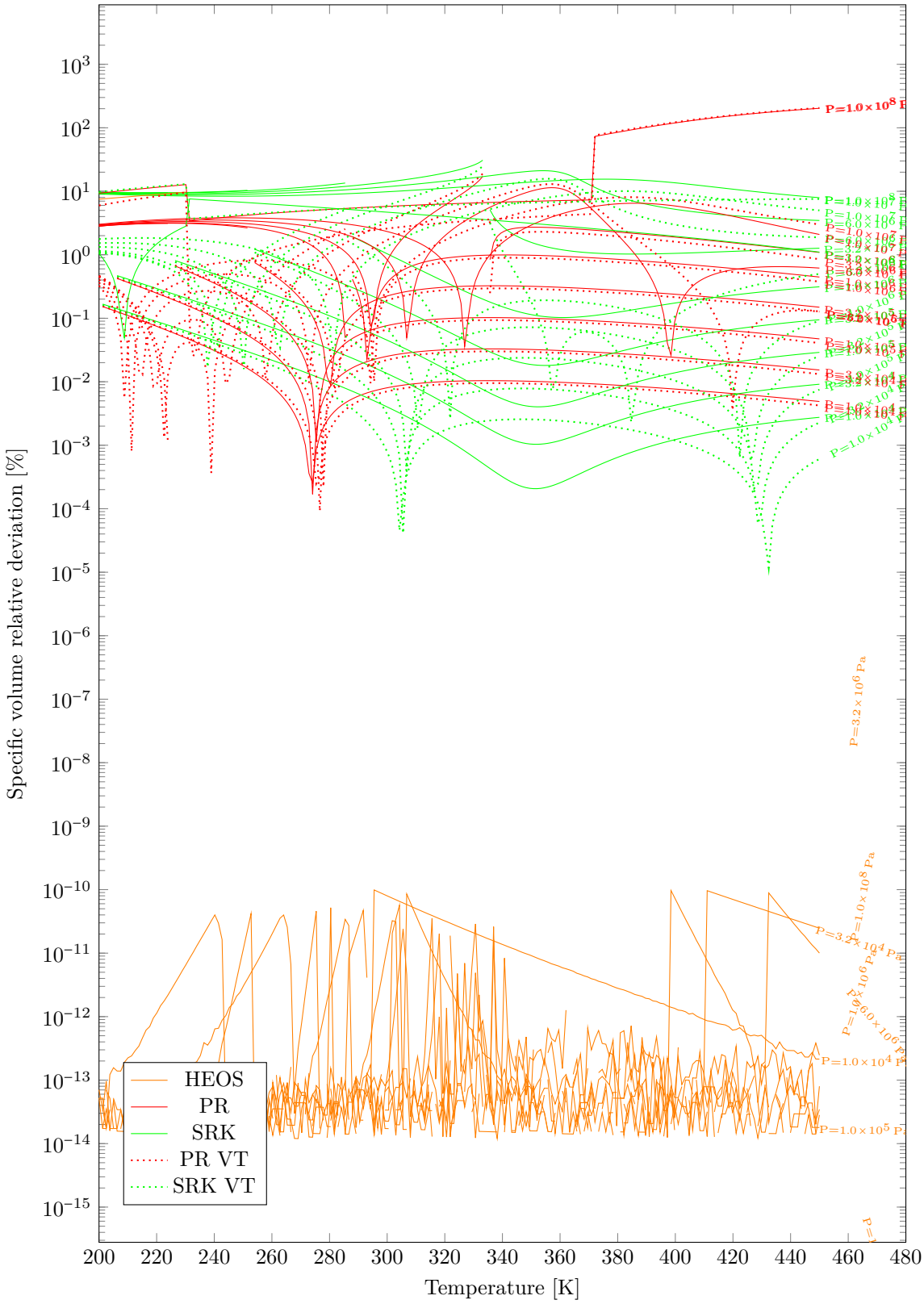


Figure 12: Deviation with the reference for each isobar, fluid R125

Fluid R134A.

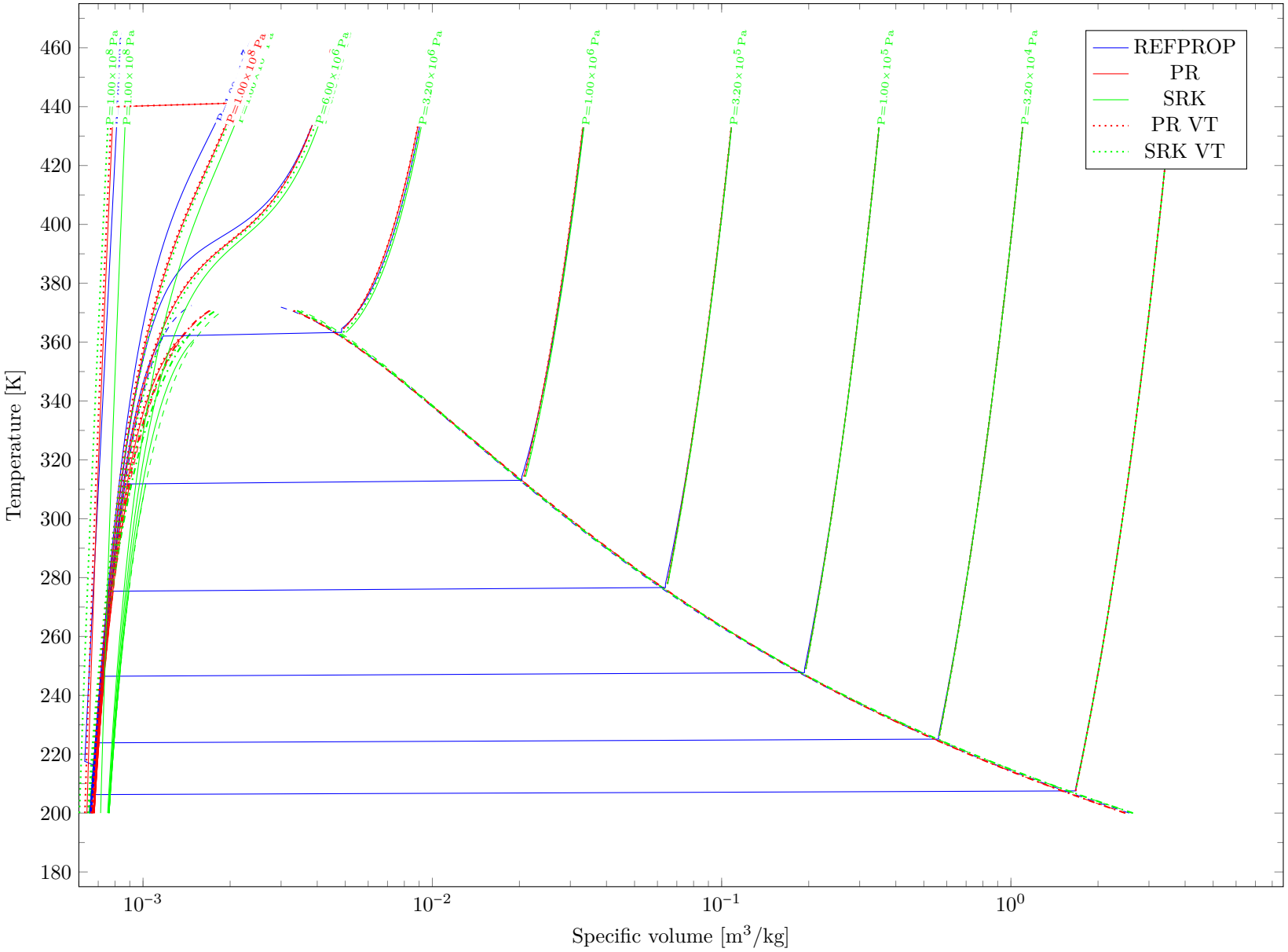


Figure 13: Isobar curves and saturation curve (dashed) on temperature/volume plot, fluid R134A

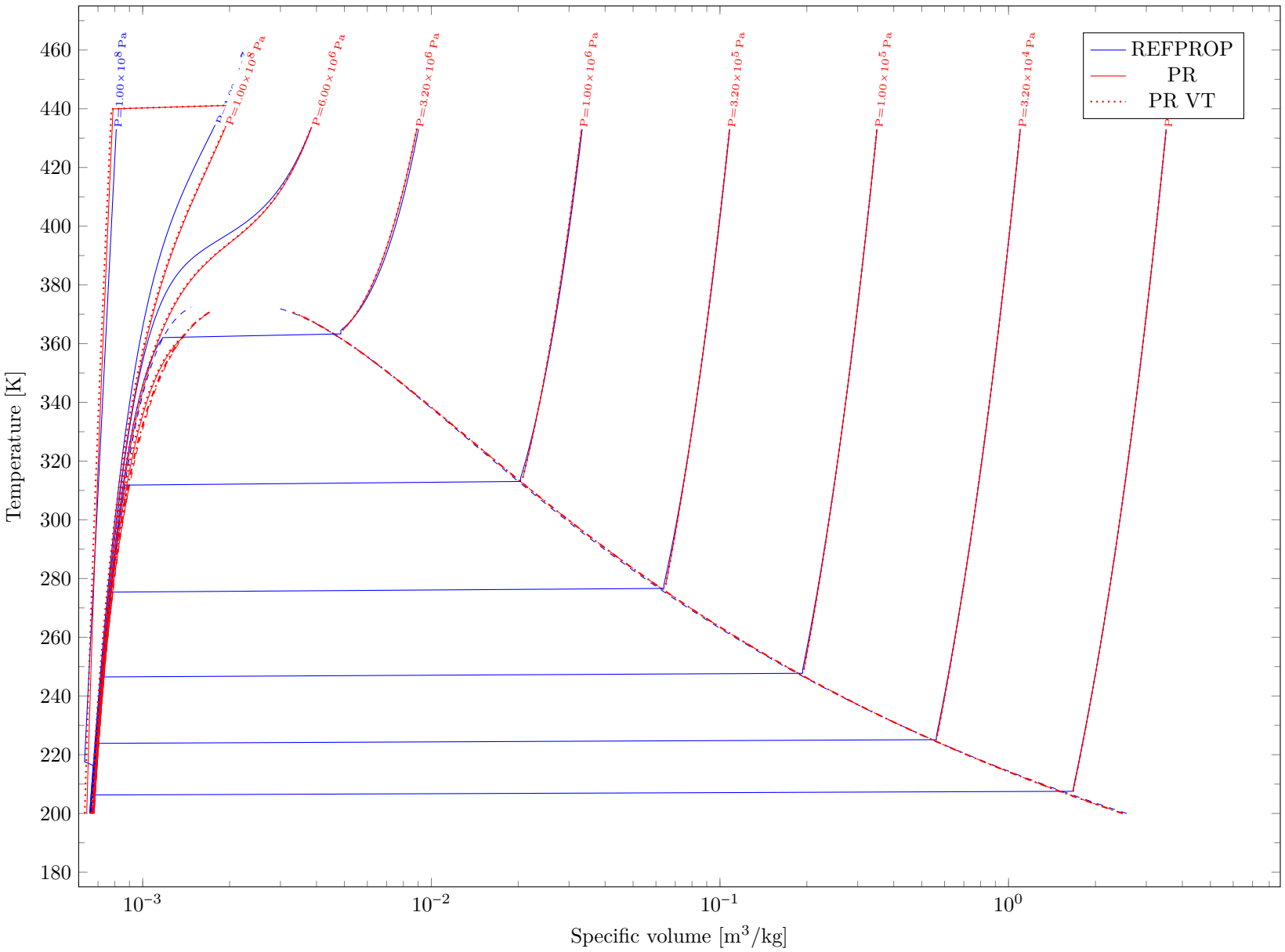


Figure 14: Isobar curves and saturation curve (dashed) on temperature/volume plot, comparison of PR with REFPROP, fluid R134A

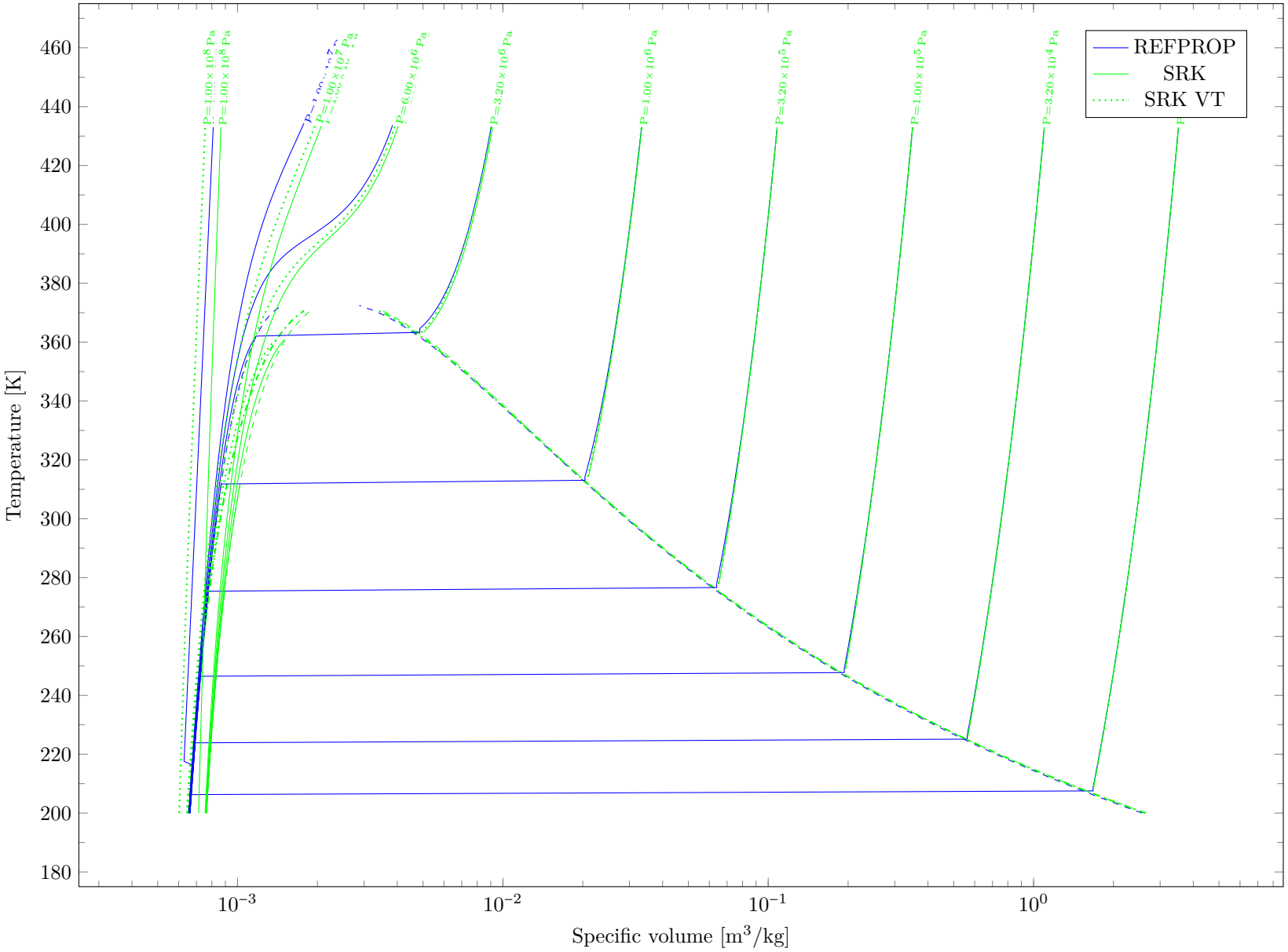


Figure 15: Isobar curves and saturation curve (dashed) on temperature/volume plot, comparison of SRK with REFPROP, fluid R134A

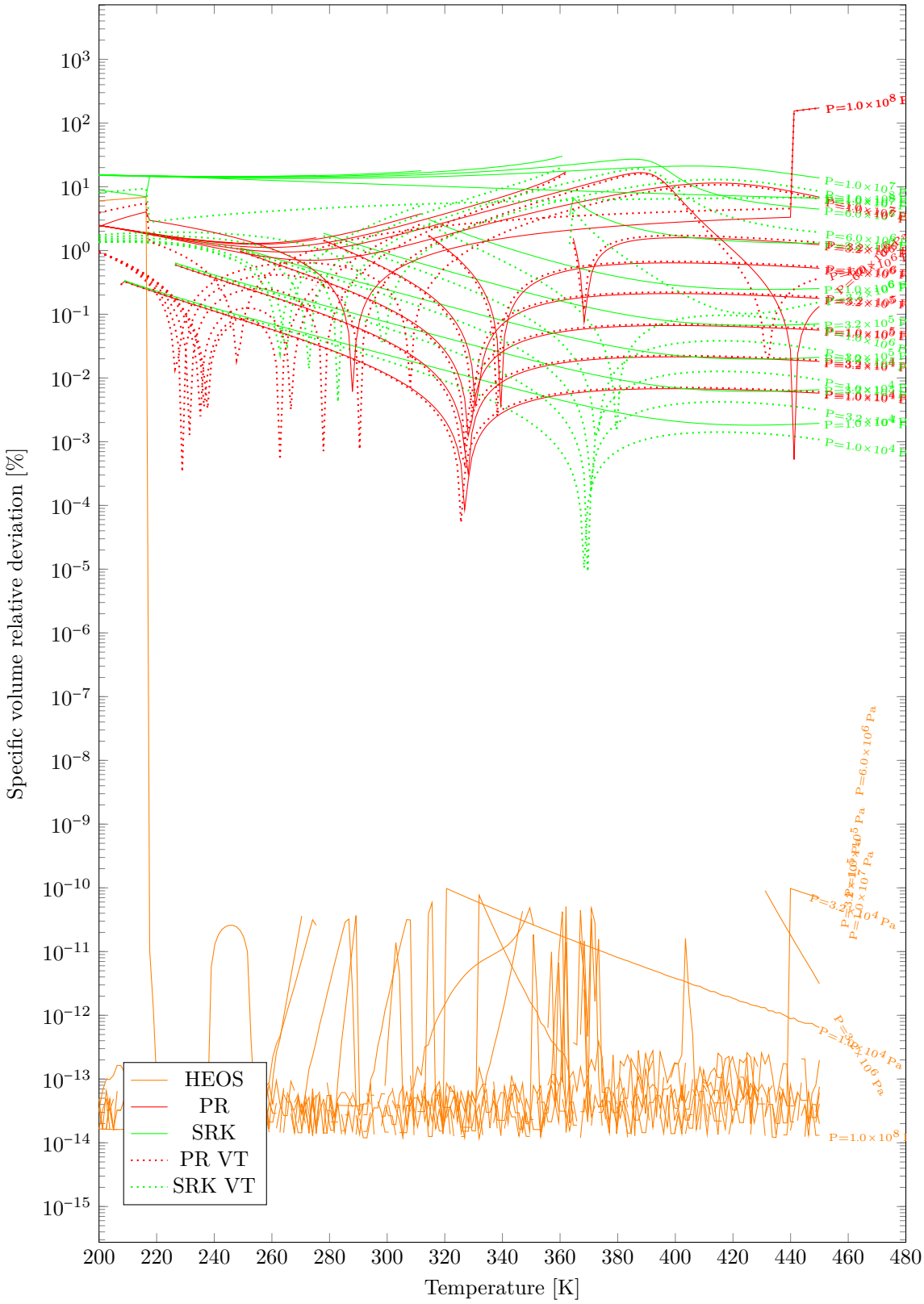


Figure 16: Deviation with the reference for each isobar, fluid R134A

Fluid R143A.

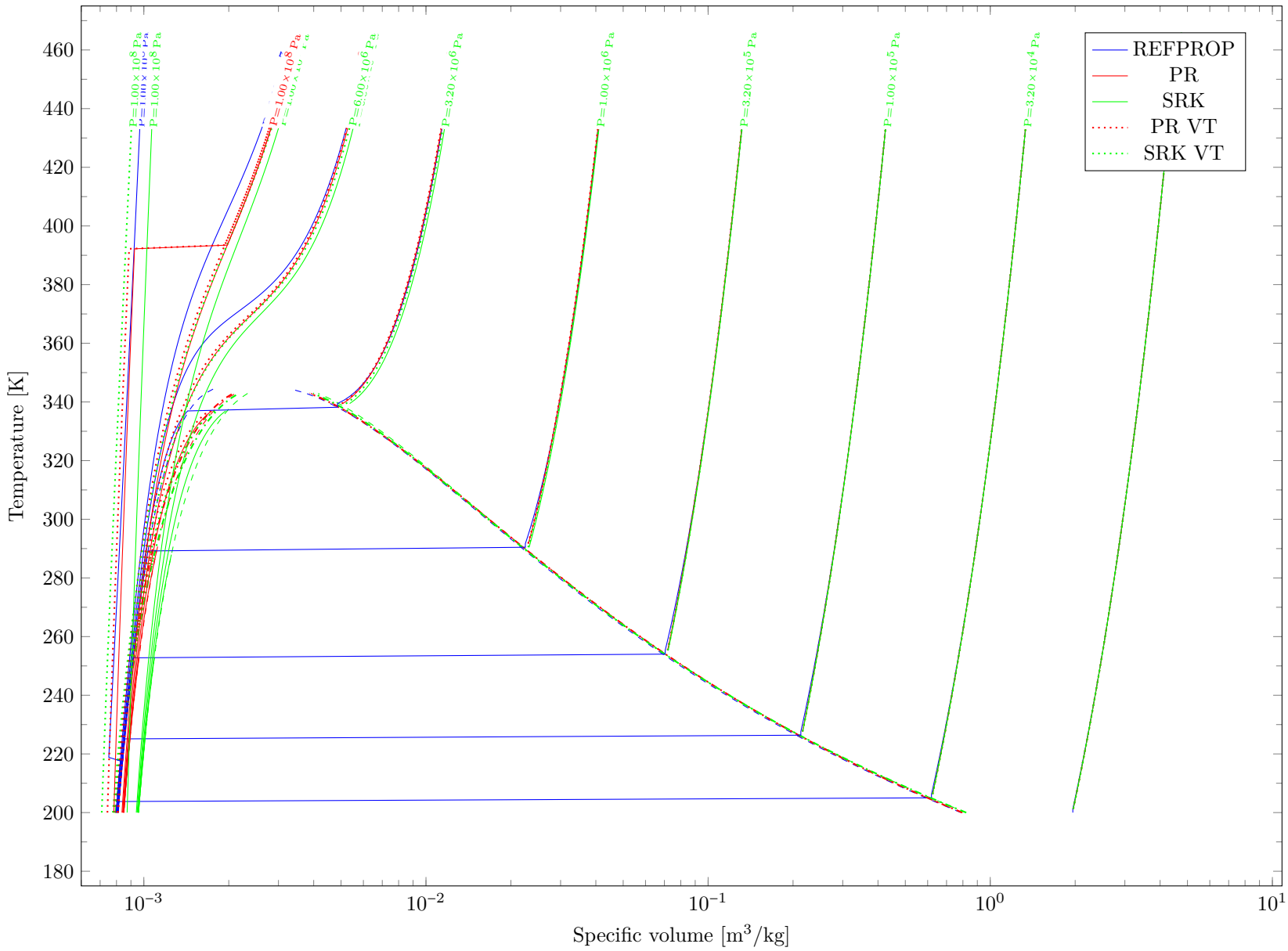


Figure 17: Isobar curves and saturation curve (dashed) on temperature/volume plot, fluid R143A

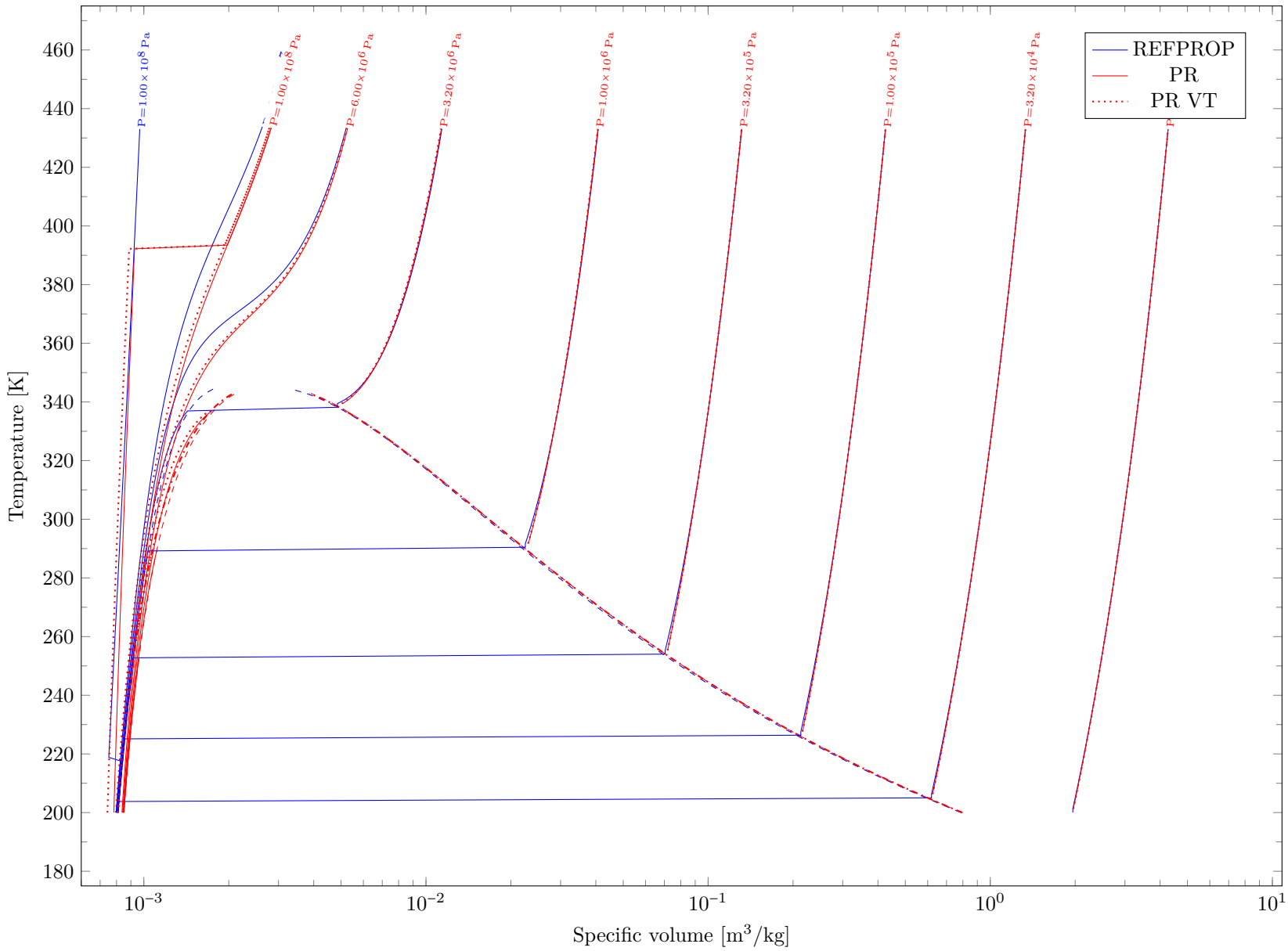


Figure 18: Isobar curves and saturation curve (dashed) on temperature/volume plot, comparison of PR with REFPROP, fluid R143A

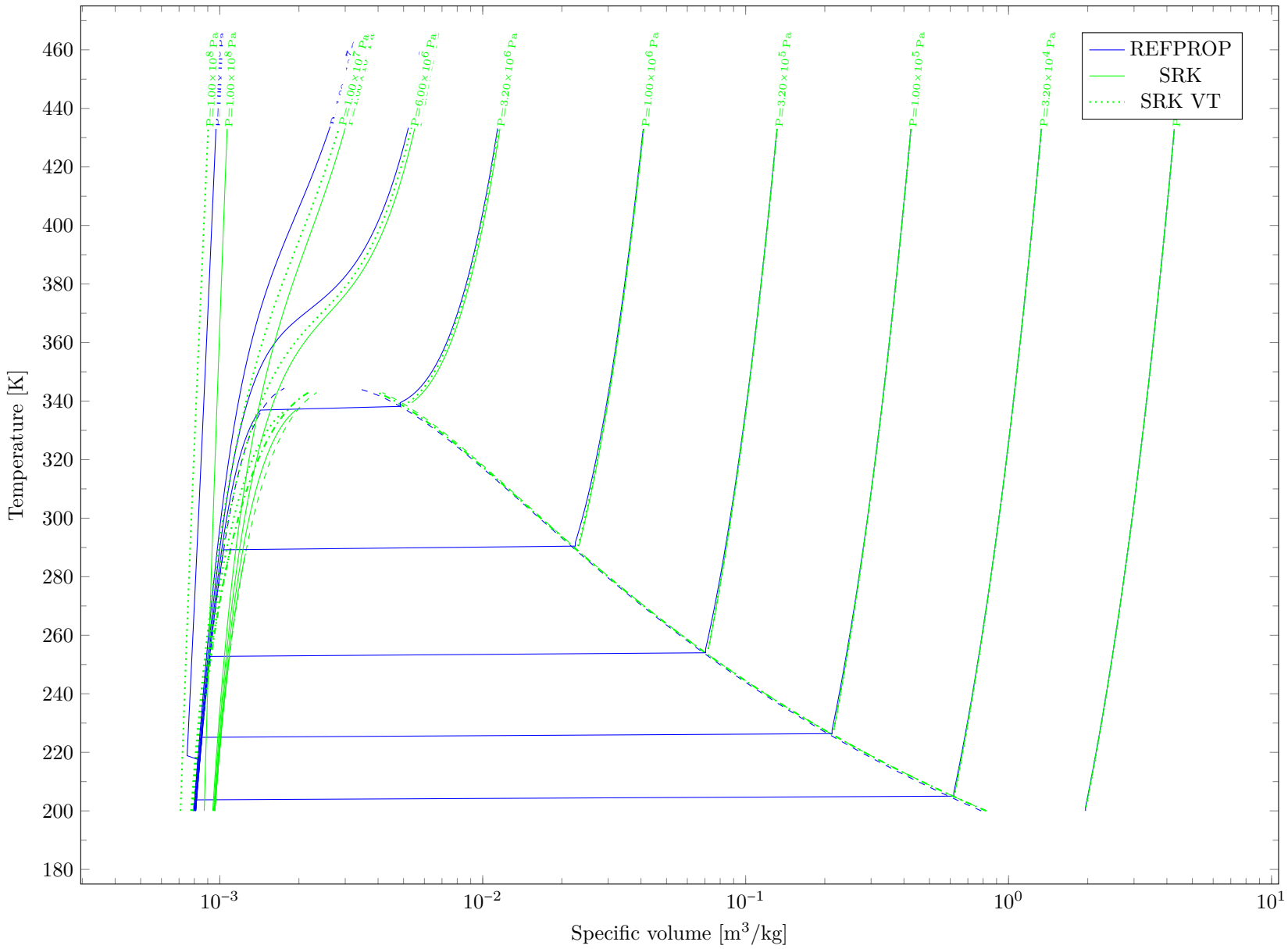


Figure 19: Isobar curves and saturation curve (dashed) on temperature/volume plot, comparison of SRK with REFPROP, fluid R143A

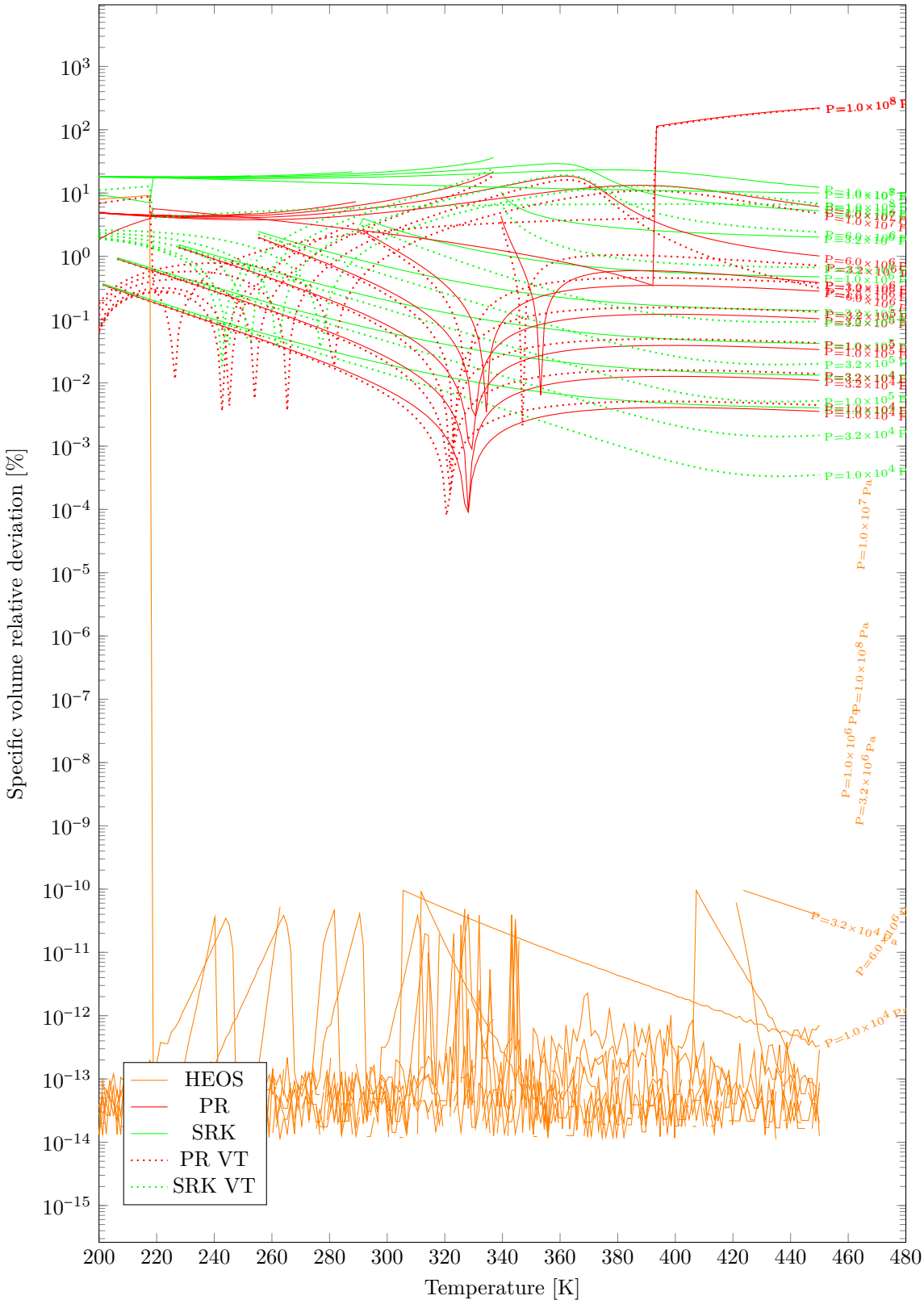


Figure 20: Deviation with the reference for each isobar, fluid R143A

Fluid R1234YF.

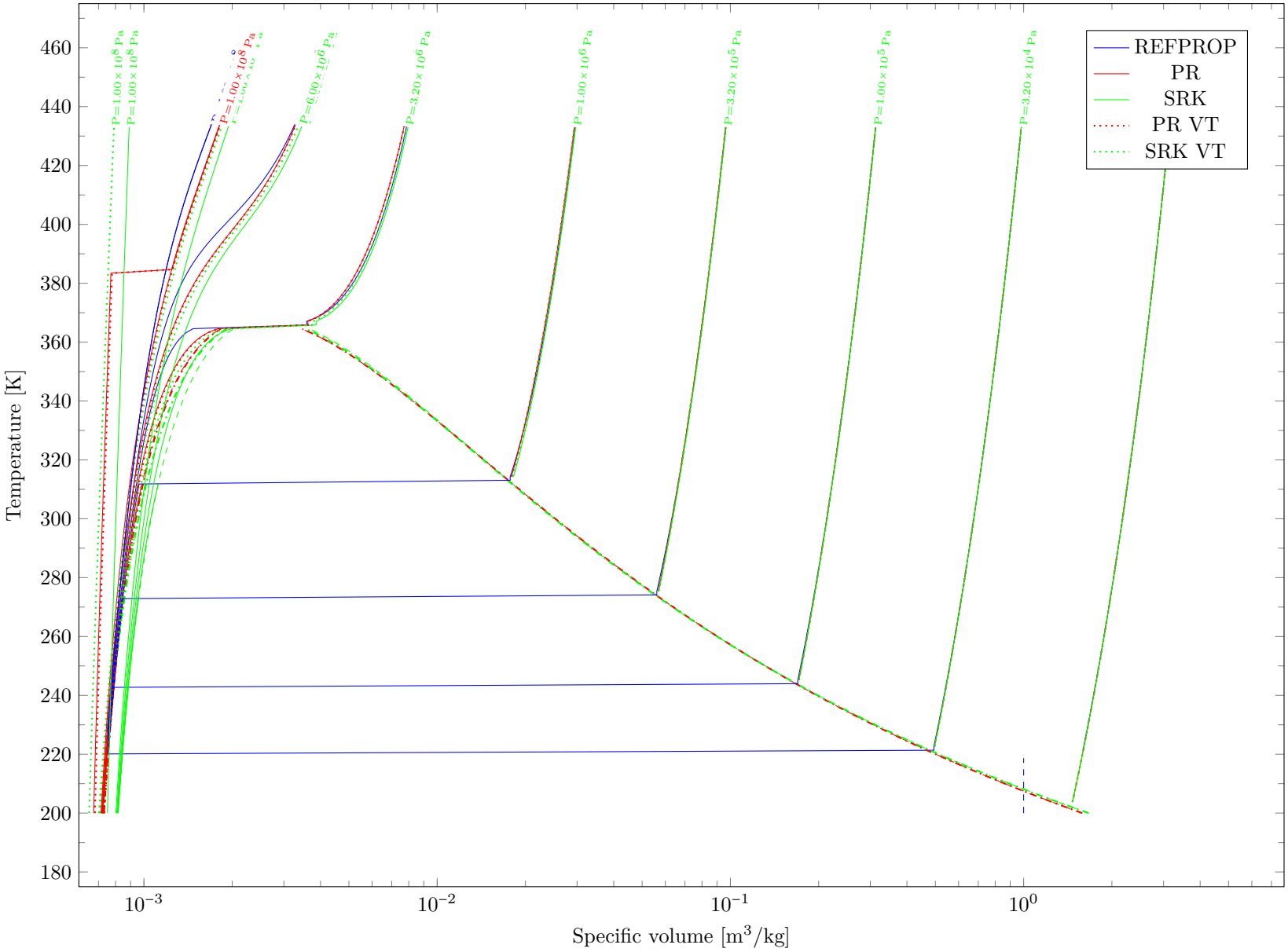


Figure 21: Isobar curves and saturation curve (dashed) on temperature/volume plot, fluid R1234YF

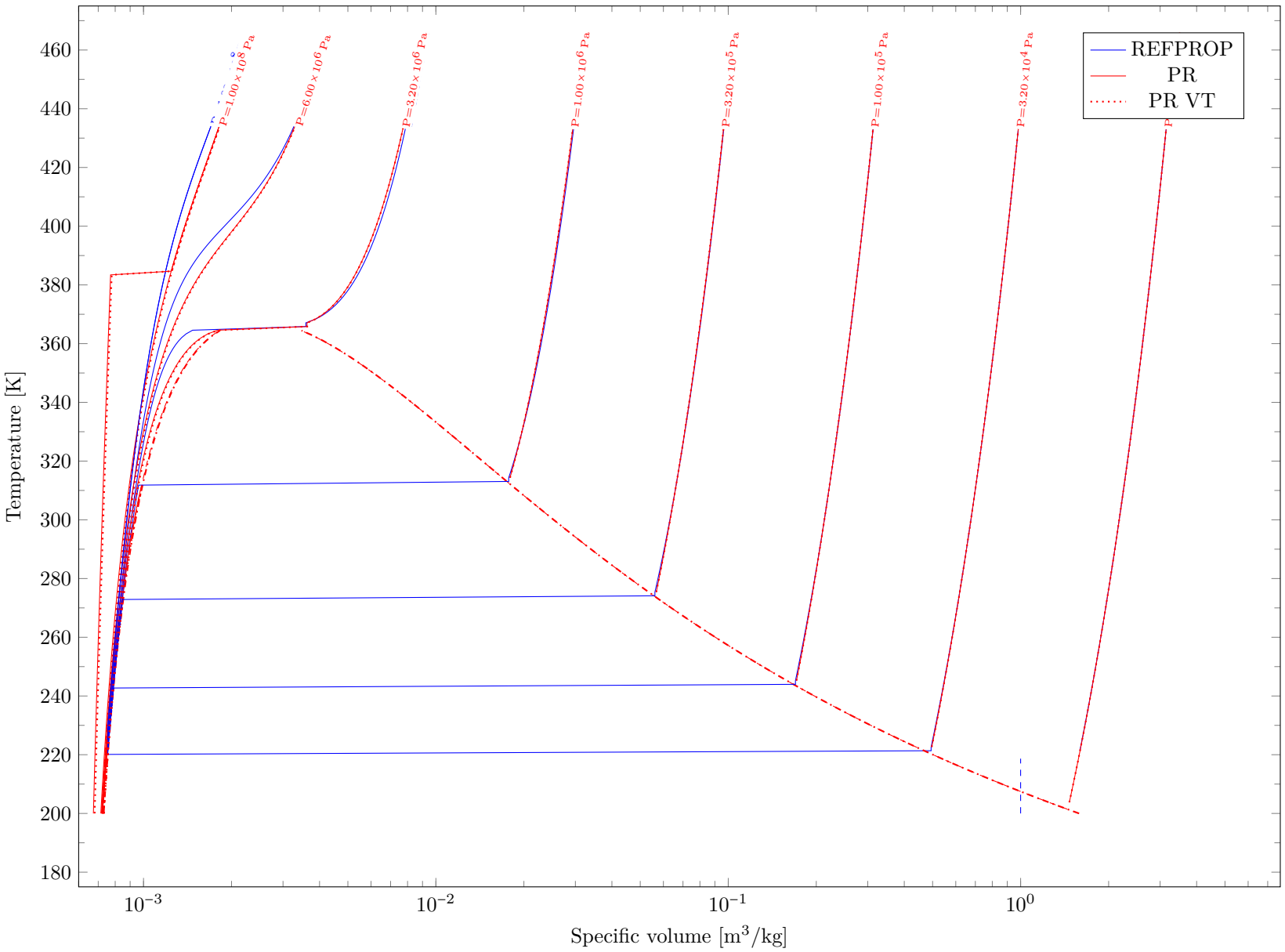


Figure 22: Isobar curves and saturation curve (dashed) on temperature/volume plot, comparison of PR with REFPROP, fluid R1234YF

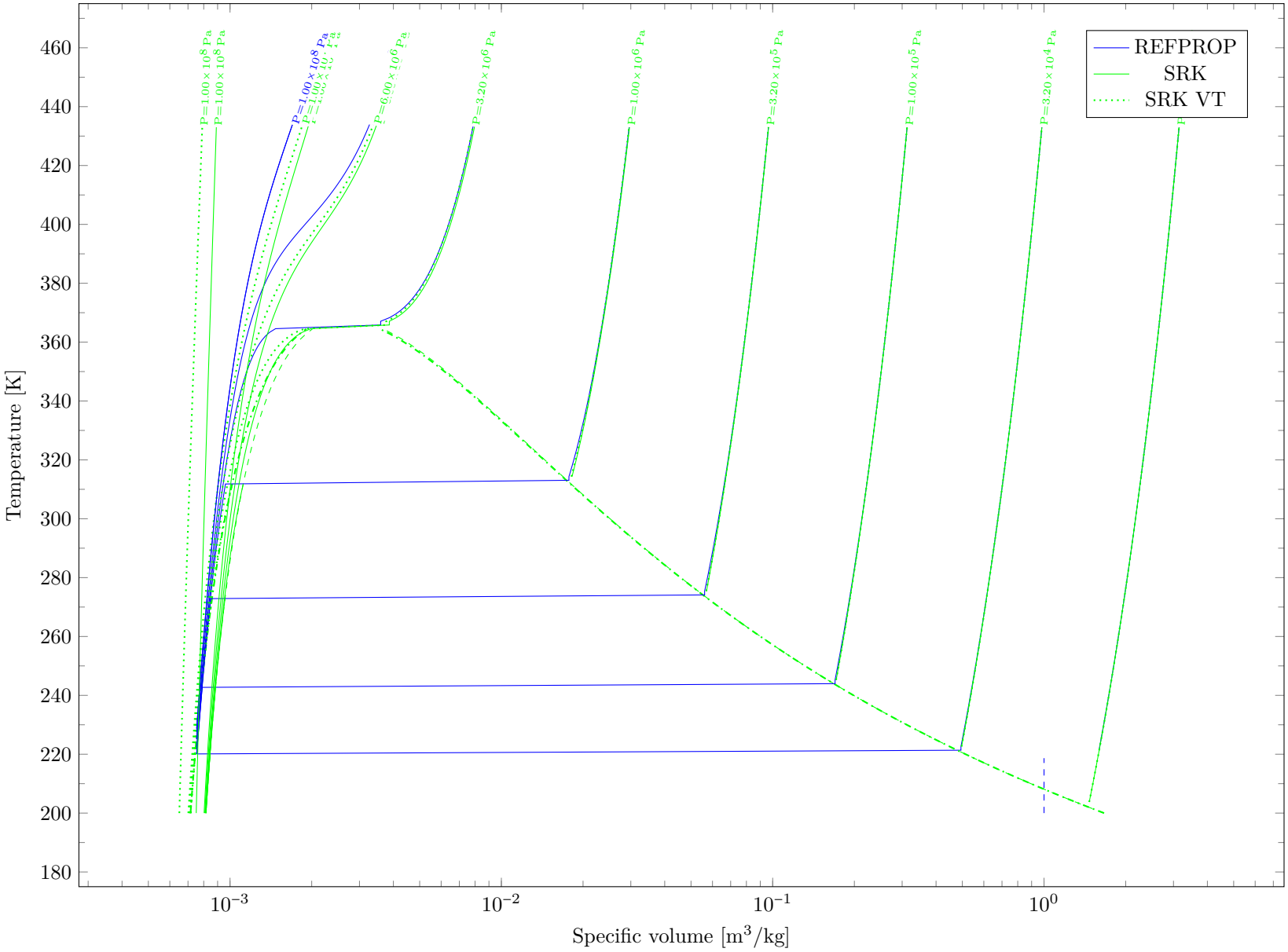


Figure 23: Isobar curves and saturation curve (dashed) on temperature/volume plot, comparison of SRK with REFPROP, fluid R1234YF

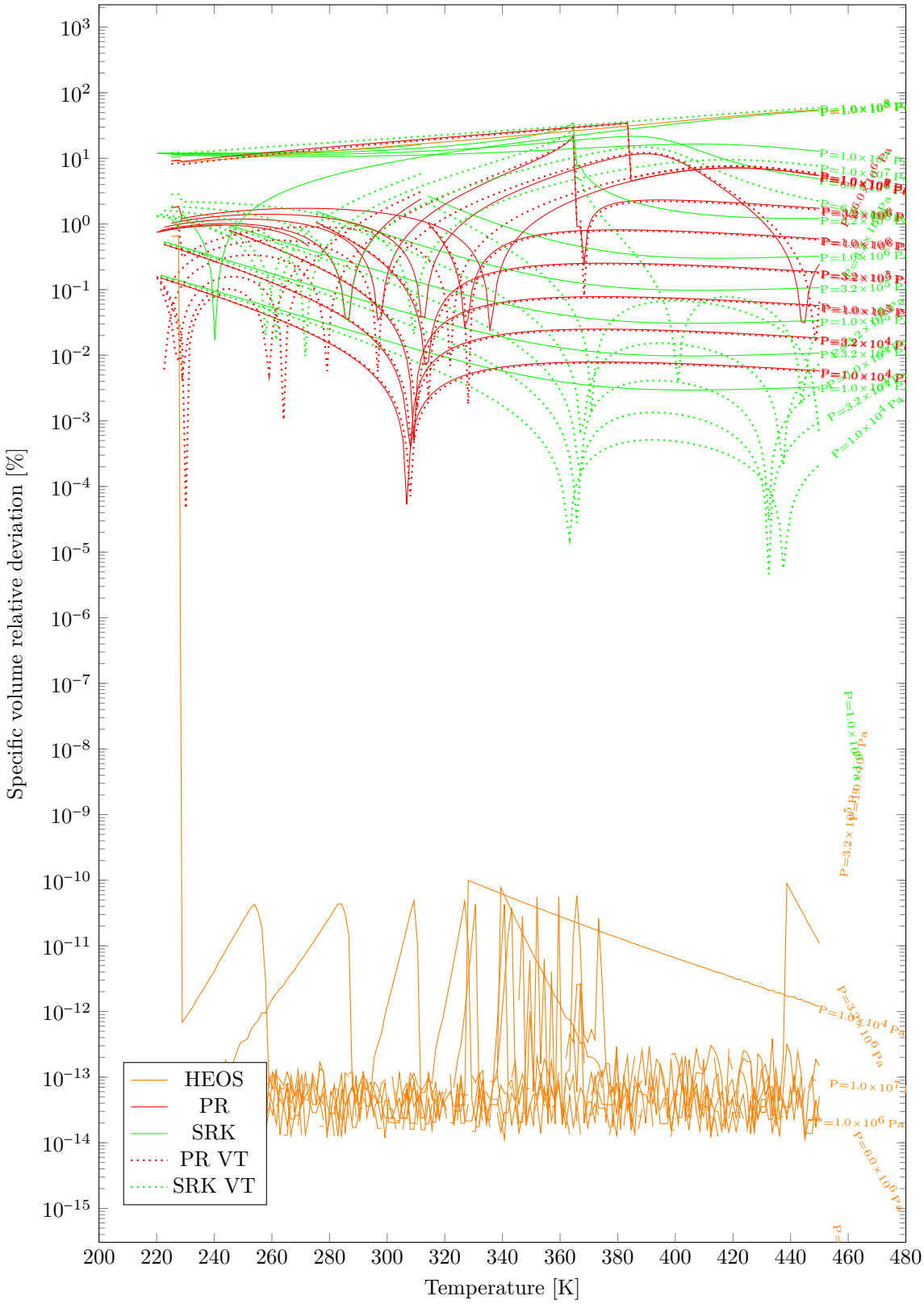


Figure 24: Deviation with the reference for each isobar, fluid R1234YF

2.2.2. Mixture

Here are some temperature-volume isobar (between 1×10^4 Pa and 1×10^8 Pa plots for the mixture R407C. This is a mixture of the fluids R125 (Pentafluoroethane), R134A (1,1,1,2-Tetrafluoroethan) and R32 (Difluoromethane). The mass fractions are respectively 25%, 52% and 23%, and molar fractions 17.956%, 43.933% and 38.111% [**?**].

They are compared to REFPROP who has an Helmholtz equation of state for R-407C.

All the other values are from CoolProp. The HEOS series is obtained with the predefined mixture R407C and the cubic with fluid specified as `"R125&R134a&R32"`, with the molar fractions `[0.17956,0.43933,0.38111]`. When interaction parameter k_{ij} is used, it has been obtained by fitting to vapour-liquid equilibrium data.

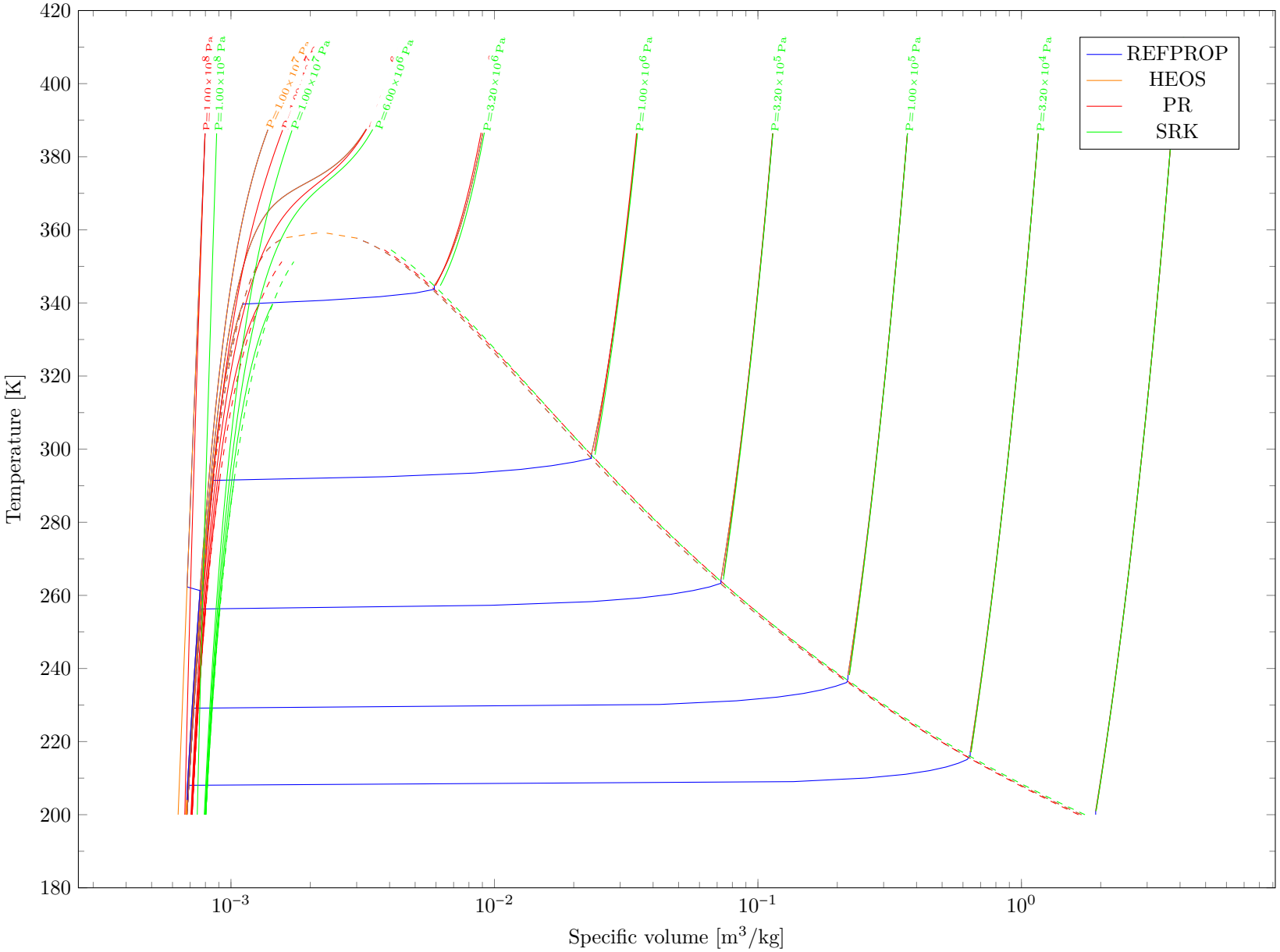


Figure 25: Isobar curves and saturation curve (dashed) on temperature/volume plot, fluid R407C

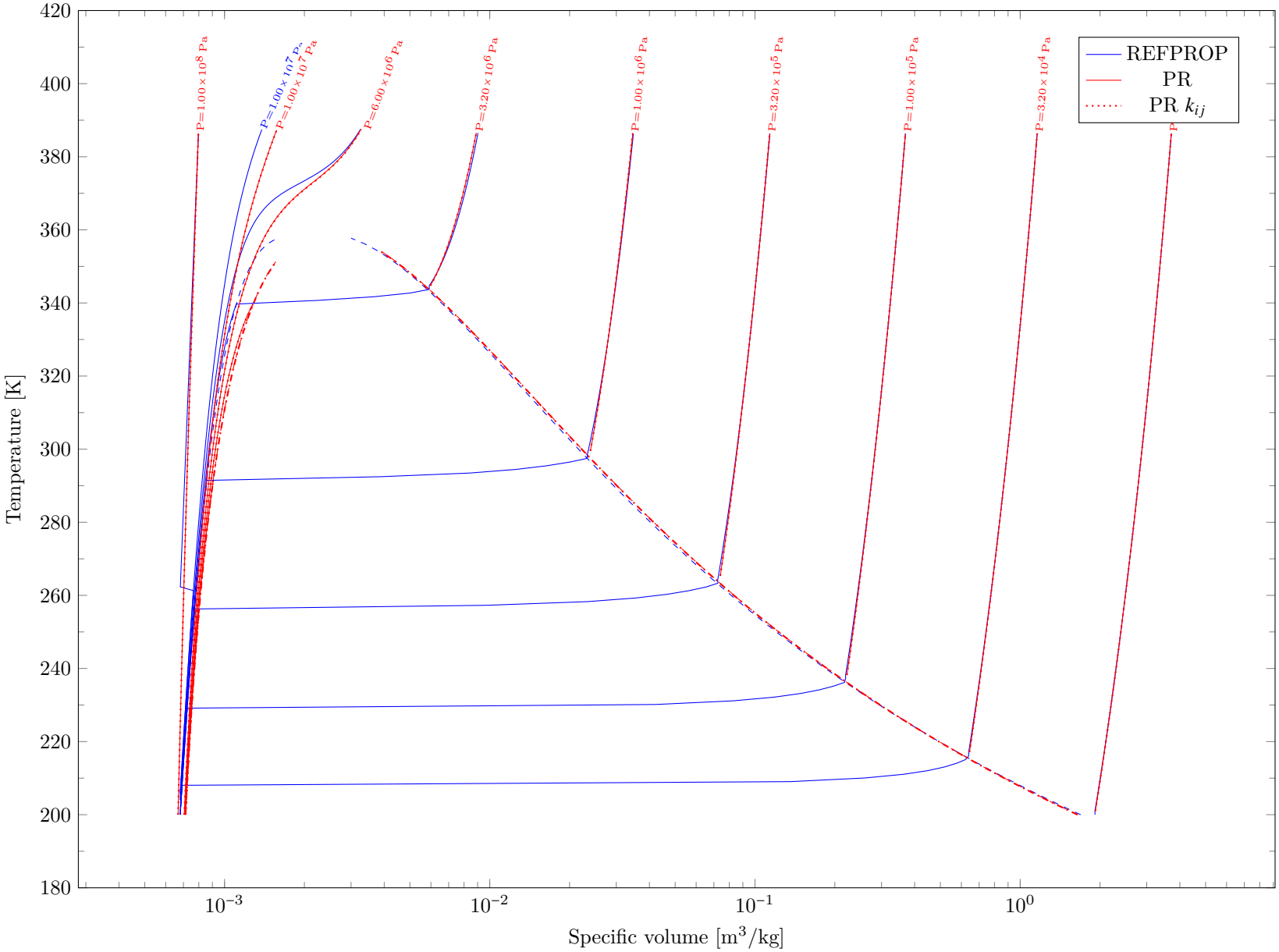


Figure 26: Isobar curves and saturation curve (dashed) on temperature/volume plot, comparison of PR with REFPROP, fluid R407C

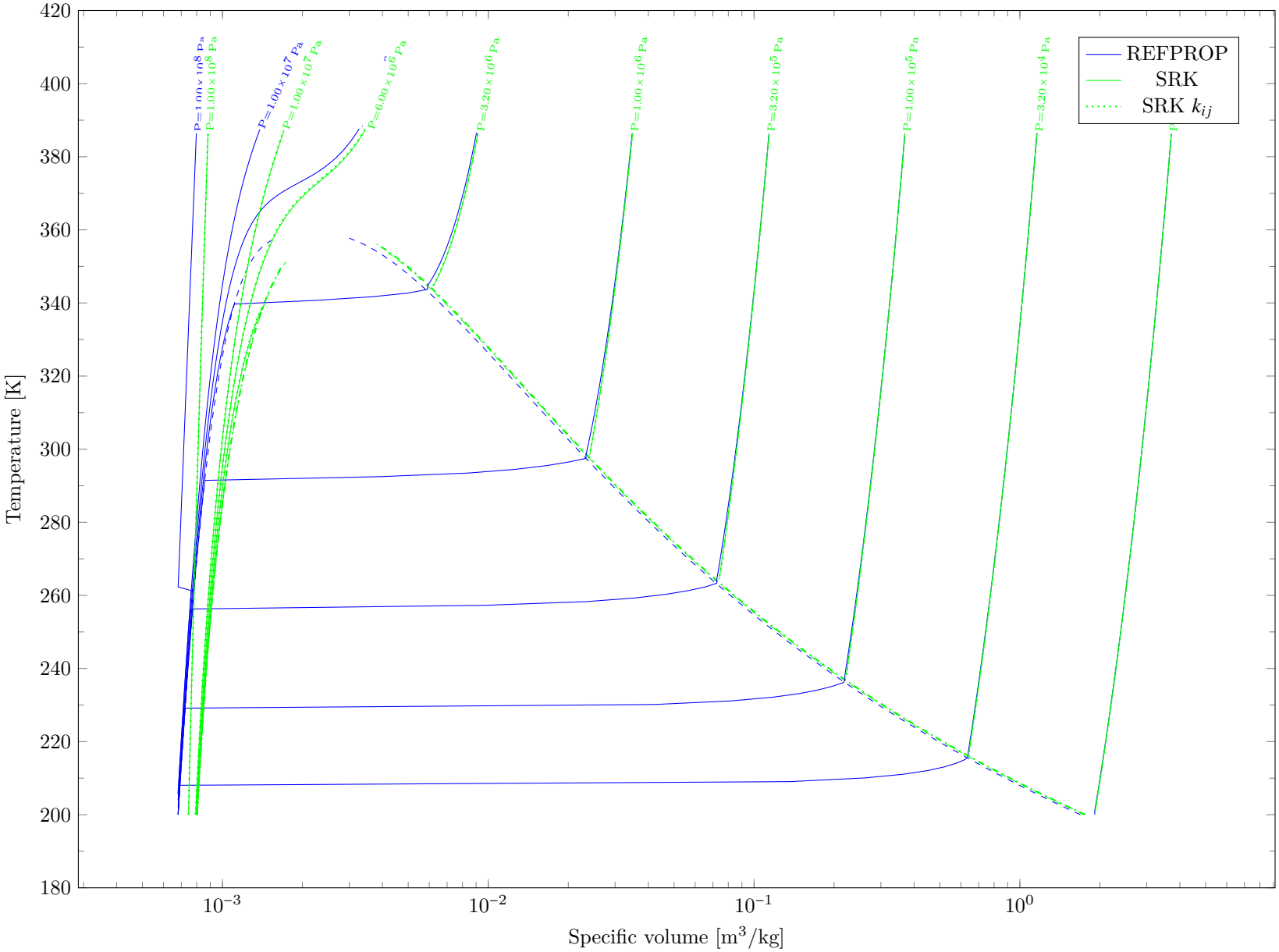


Figure 27: Isobar curves and saturation curve (dashed) on temperature/volume plot, comparison of SRK with REFPROP, fluid R407C

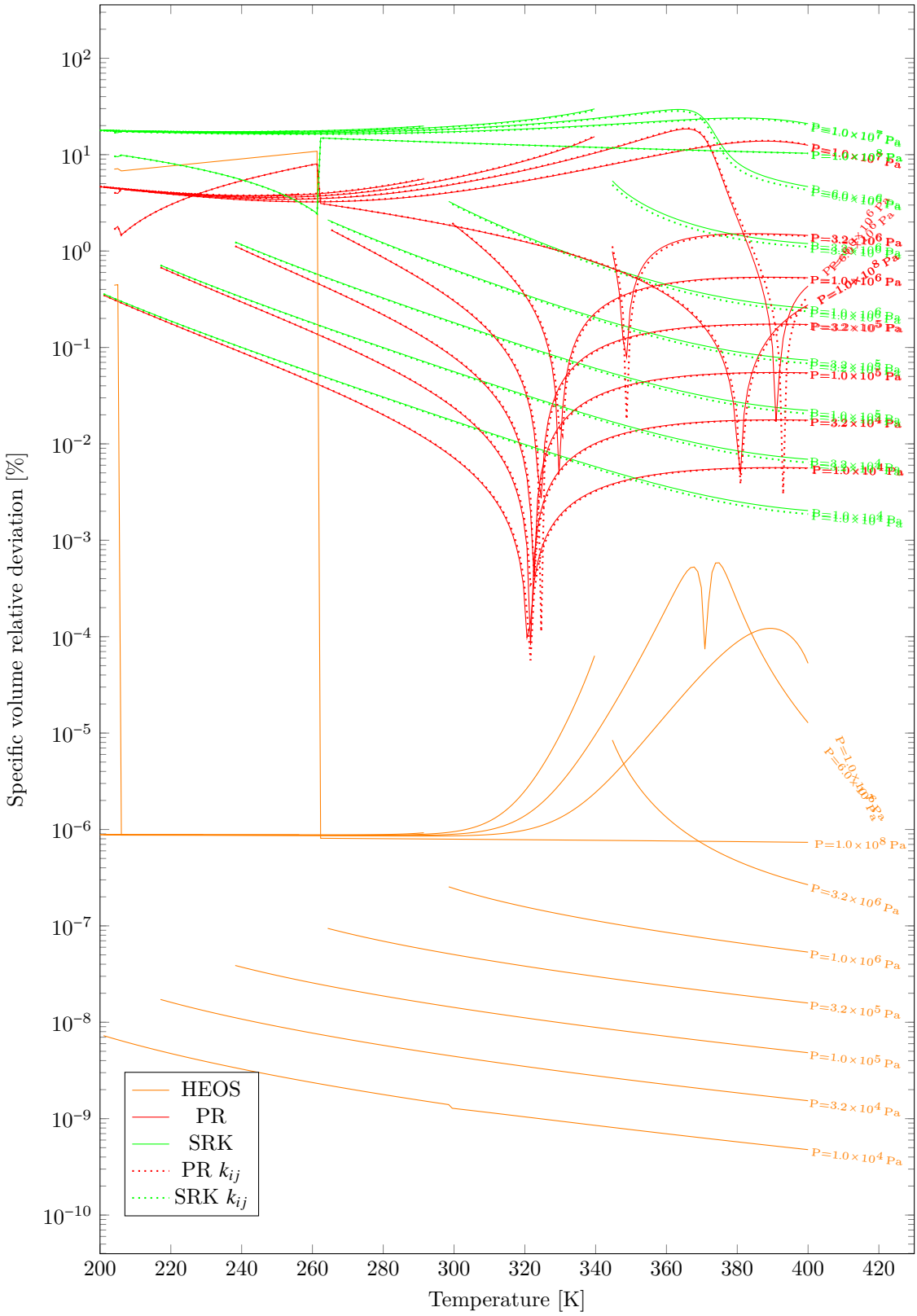


Figure 28: Deviation with the reference for each isobar, fluid R407C

2.3. Pure fluid data

Here are a series of deviation plot comparing the density deviation obtained with the different equations of states to experimental values[2]. These experimental values where gracefully provided by NIST which collected them from the many references you can find at the end of this document.

These data contains liquid, vapour and saturation data but no two phase points. The deviation value is obtained by applying equation 46 to the result obtained when computing the density from the temperature and pressure. The phase was imposed for non RefProp calls (the interface to impose phase to RefProp from CoolProp's call was not available at that time). The reference densities are the one provided by the experimental data. For vapour-liquid equilibrium data, only the temperature was provided. In this case, the values where computed from the temperature and the vapour quality (0 or 1).

Some of the fluid computed here where not available with RefProp which lead to empty result for that model.

The volume translation parameter is approximated by making the difference with the molar volume of RefProp at the reduce temperature $T_r = 0.7T_{\text{crit}}$. If the this temperature was out of range of RefProp, a reduce temperature of $T_r = 0.8T_{\text{crit}}$ was used instead. When the fluid was not available in RefProp, the HEOS model of CoolProp was used.

For each fluid, the first one compare the range of deviation obtained for each EOS with all the data point provided (minimum, 1er quartile, median, 3rd quartile, maximum). The second plot compares the evolution of the density deviation with the temperature, and the third one the evolution with the pressure.

[2]These plots are generated automatically with imposed range to ease comparison, it can happens part of the data are out of the displayed range.

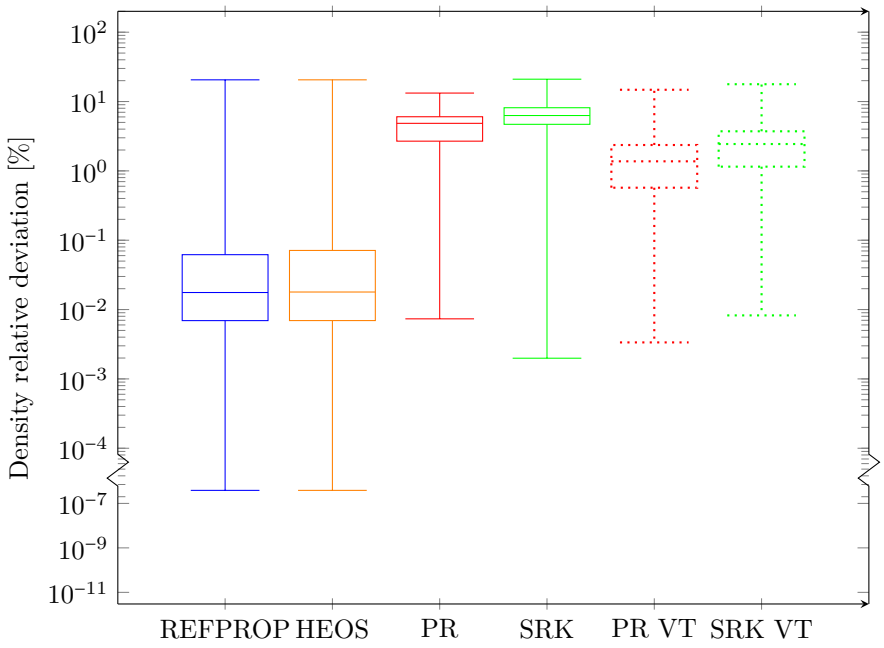


Figure 29: Relative density deviation to experimental data for fluid 1-Butene

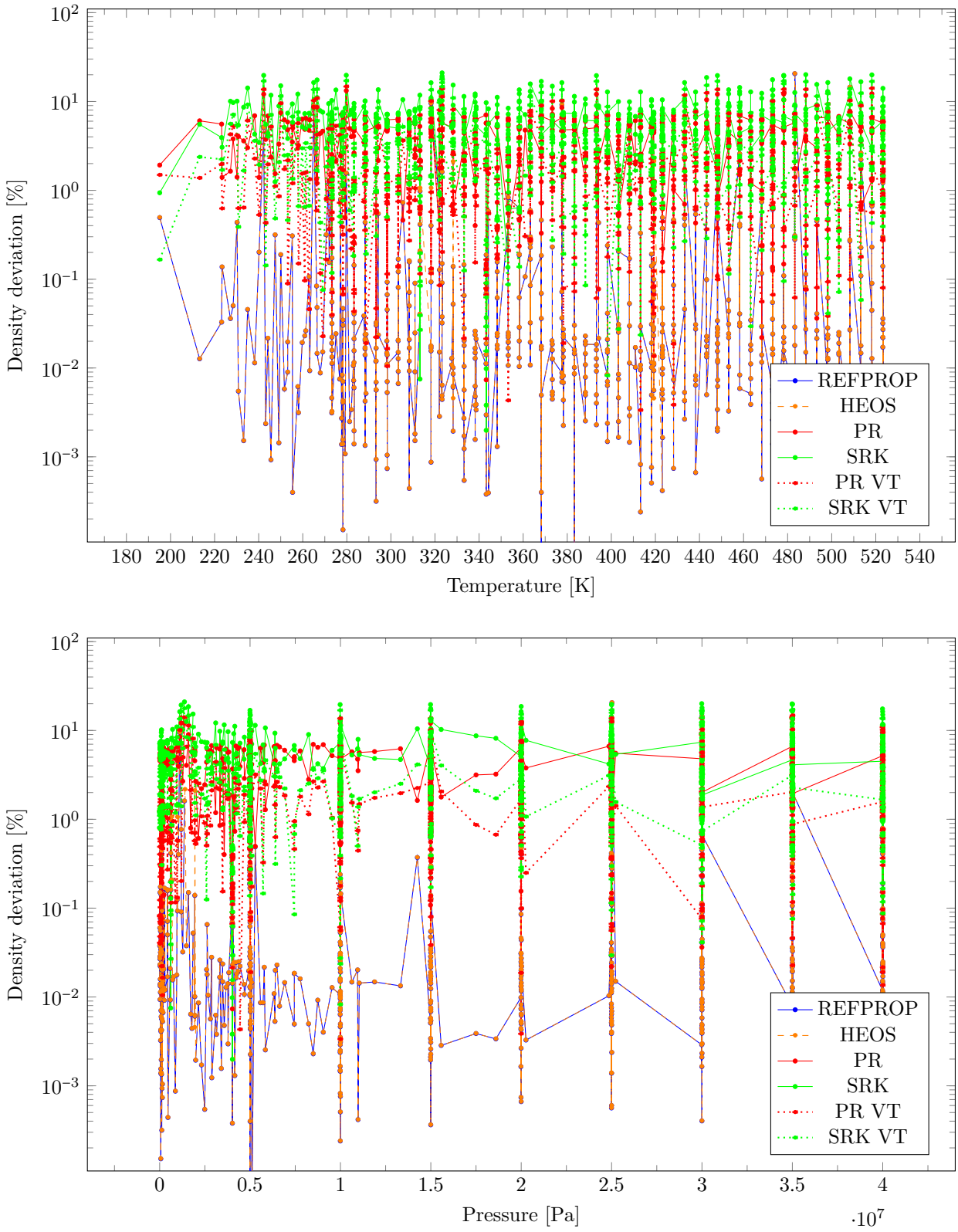


Figure 30: Density dependence on the temperature and pressure for fluid 1-Butene

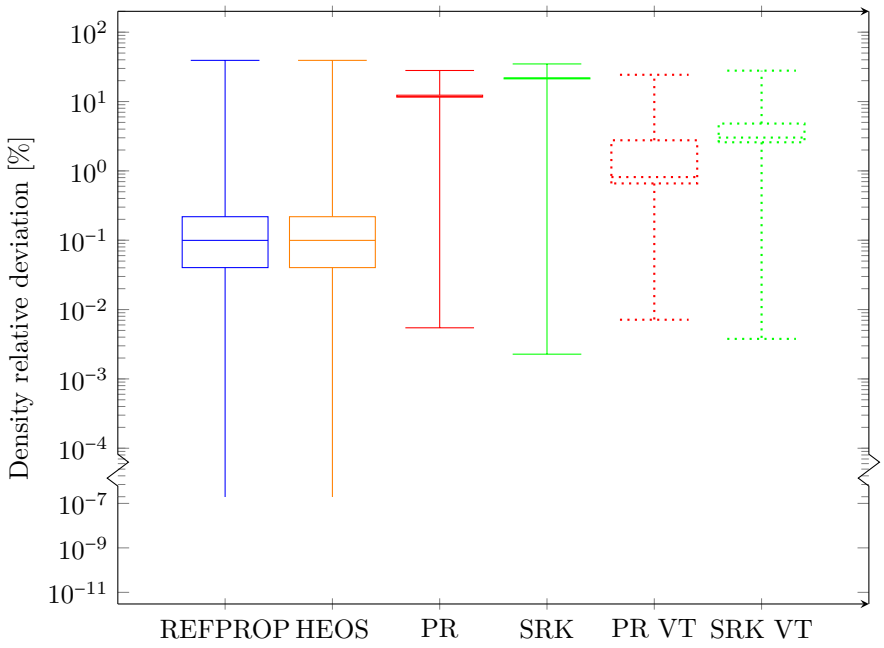


Figure 31: Relative density deviation to experimental data for fluid Acetone

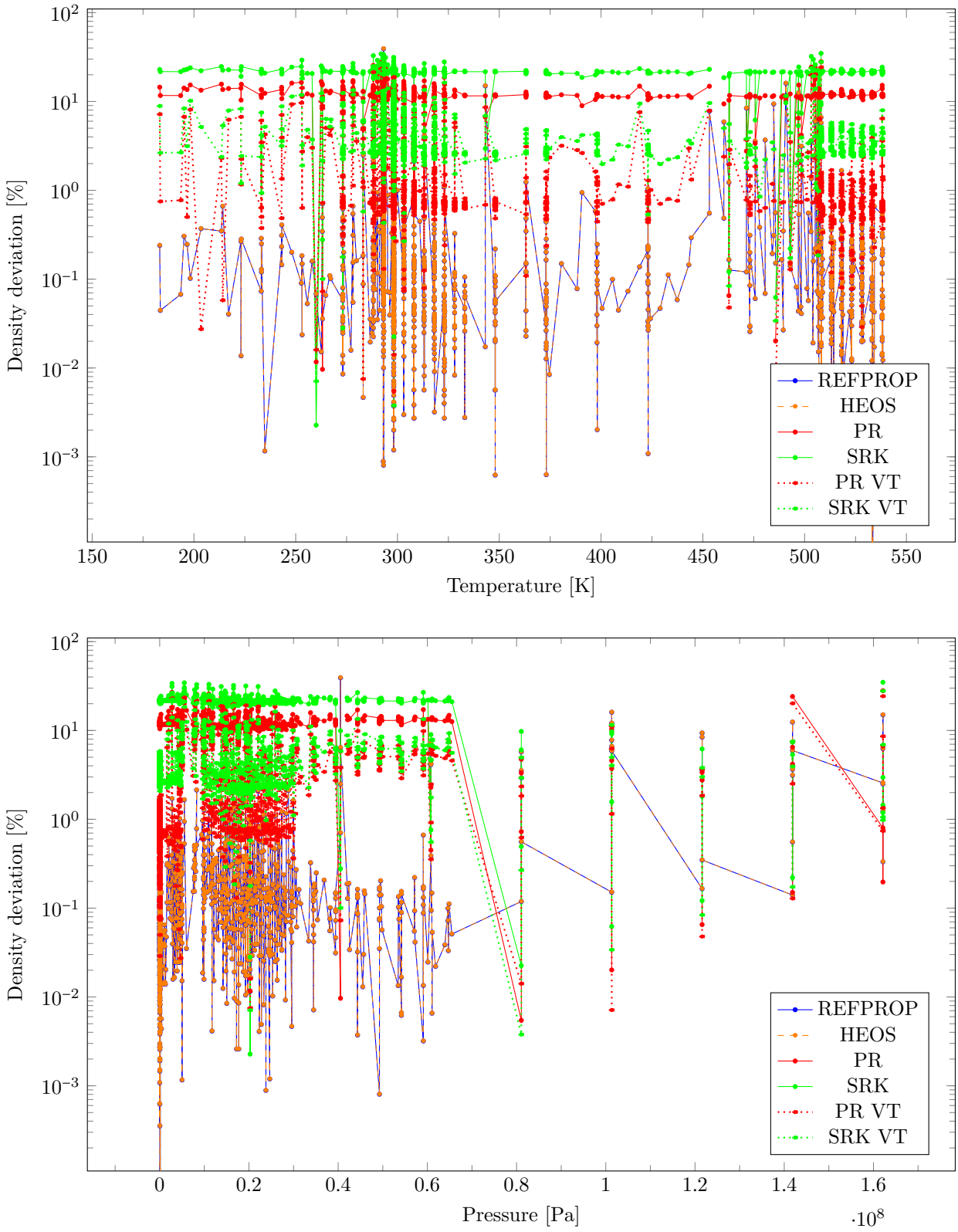


Figure 32: Density dependence on the temperature and pressure for fluid Acetone

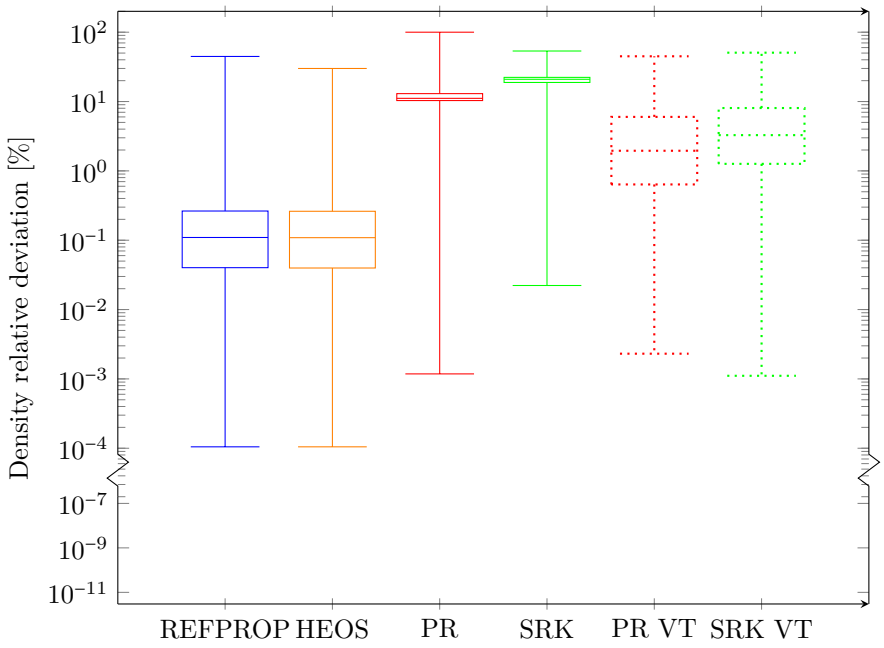


Figure 33: Relative density deviation to experimental data for fluid Ammonia

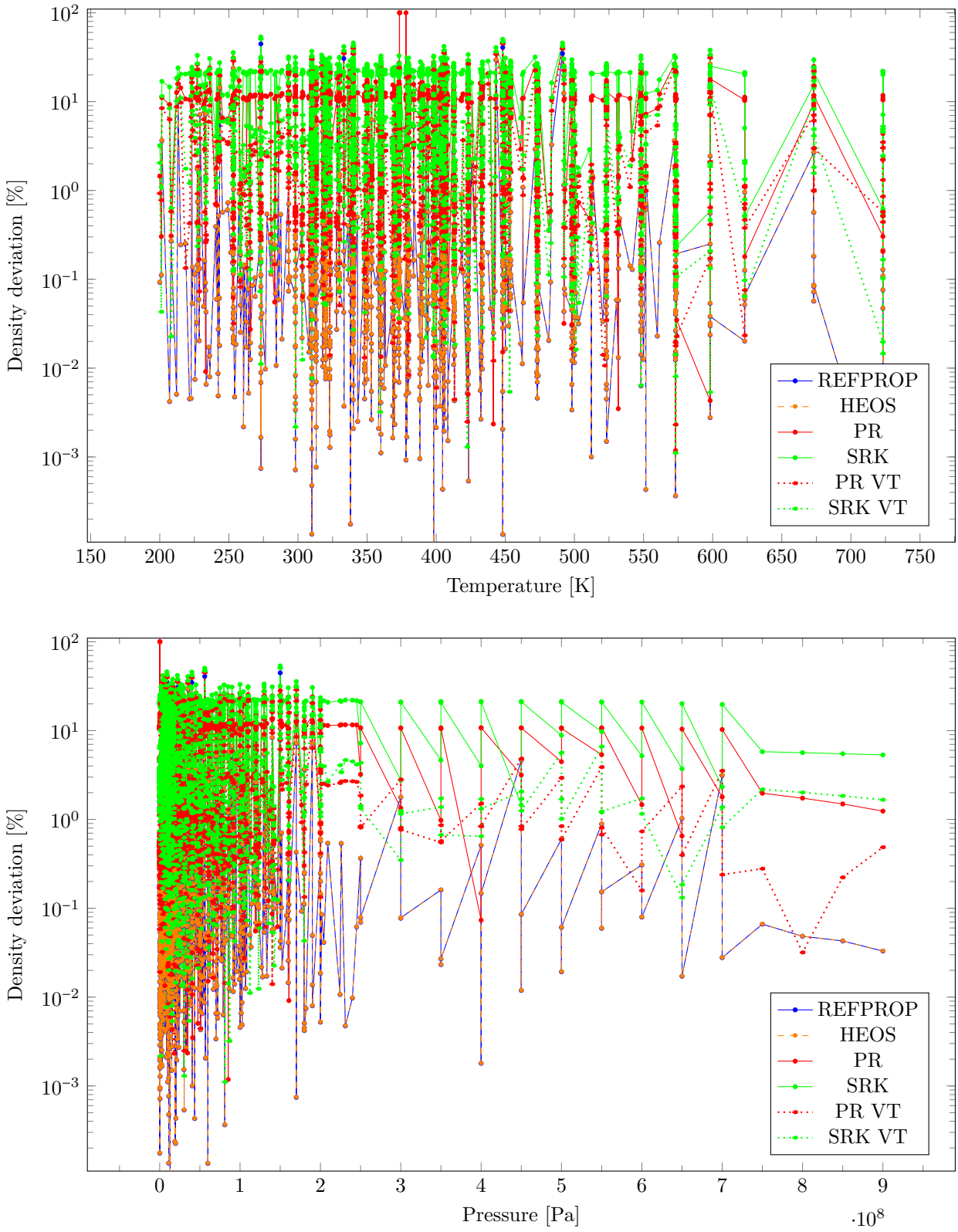


Figure 34: Density dependence on the temperature and pressure for fluid Ammonia

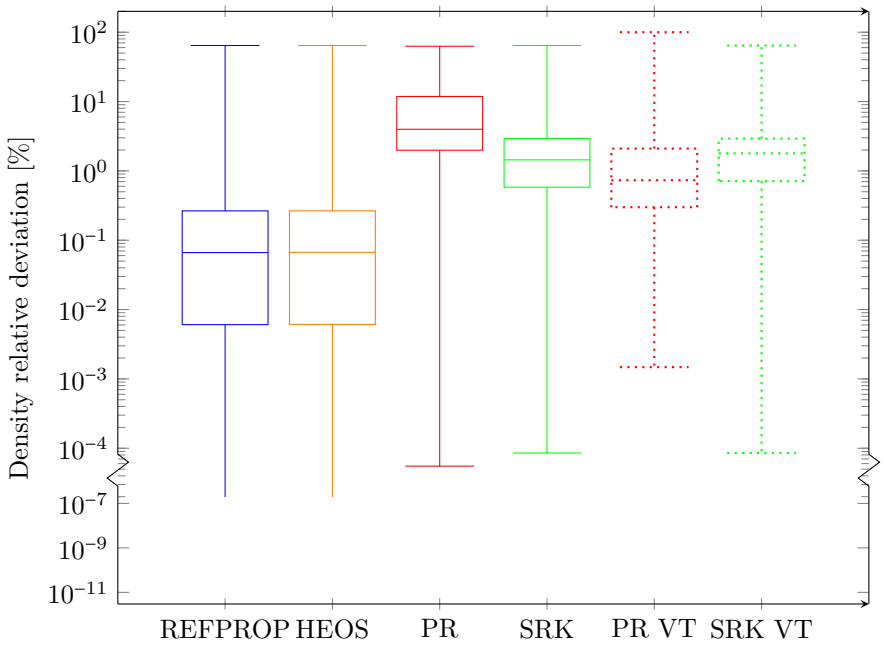


Figure 35: Relative density deviation to experimental data for fluid Argon

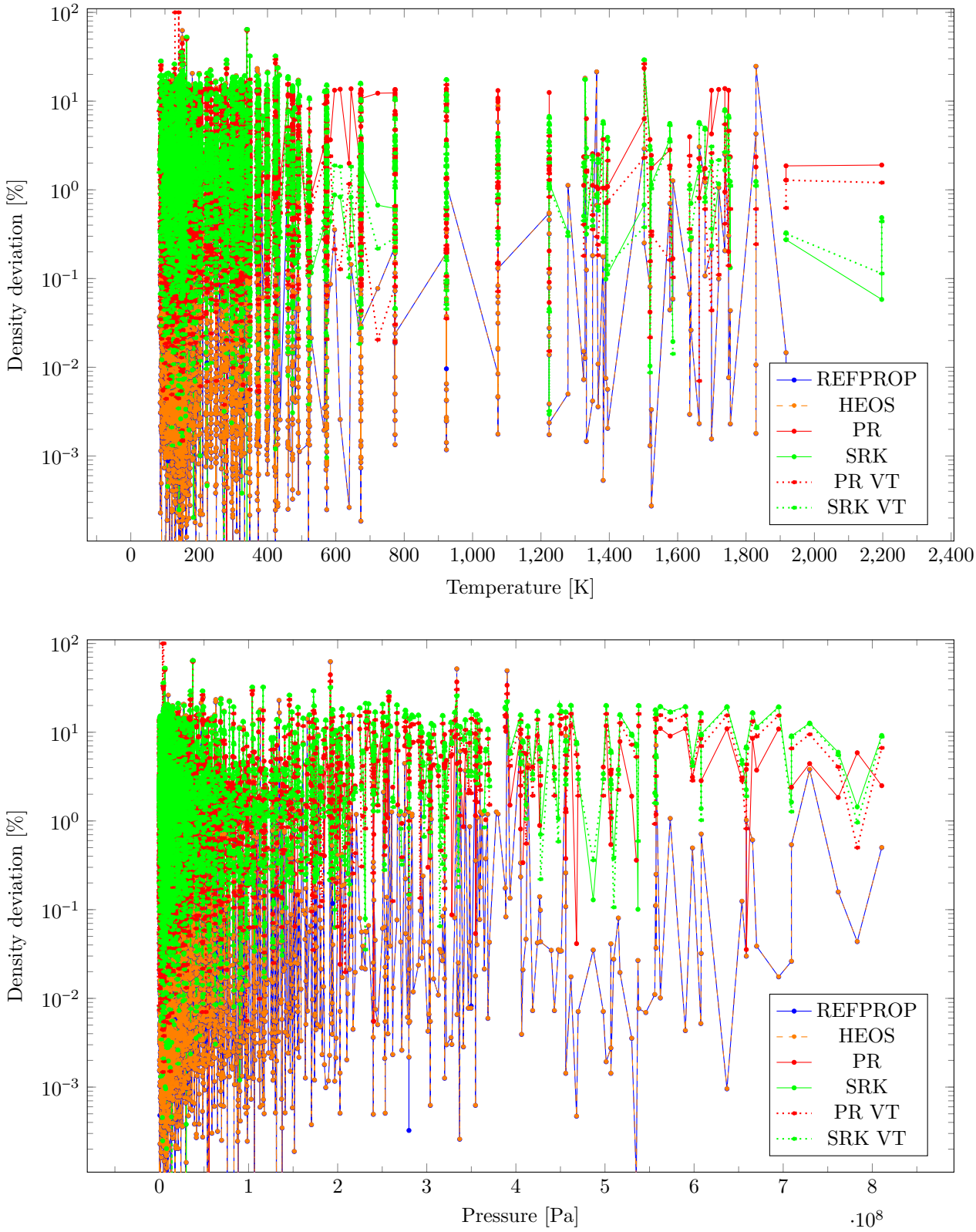


Figure 36: Density dependence on the temperature and pressure for fluid Argon

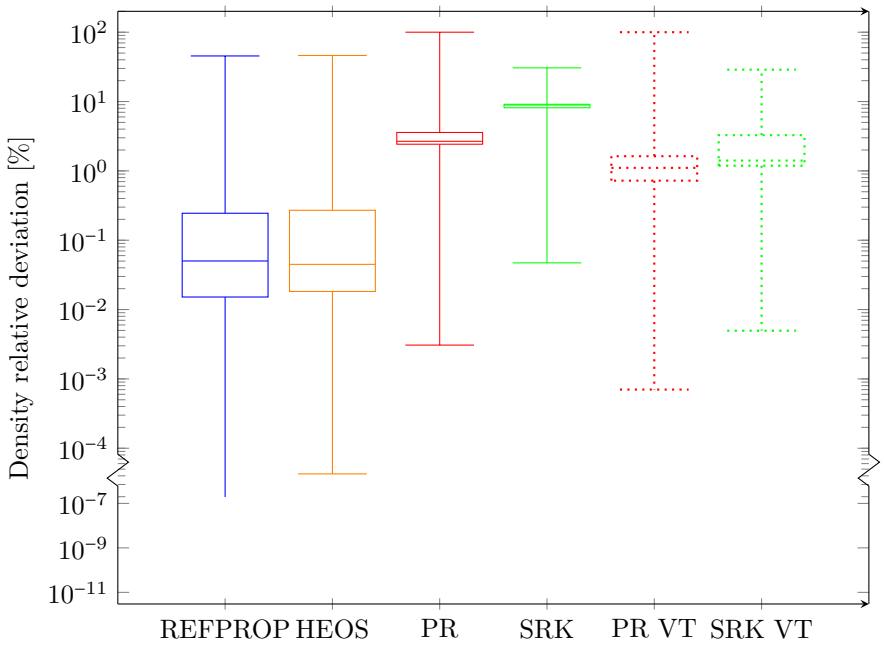


Figure 37: Relative density deviation to experimental data for fluid Benzene

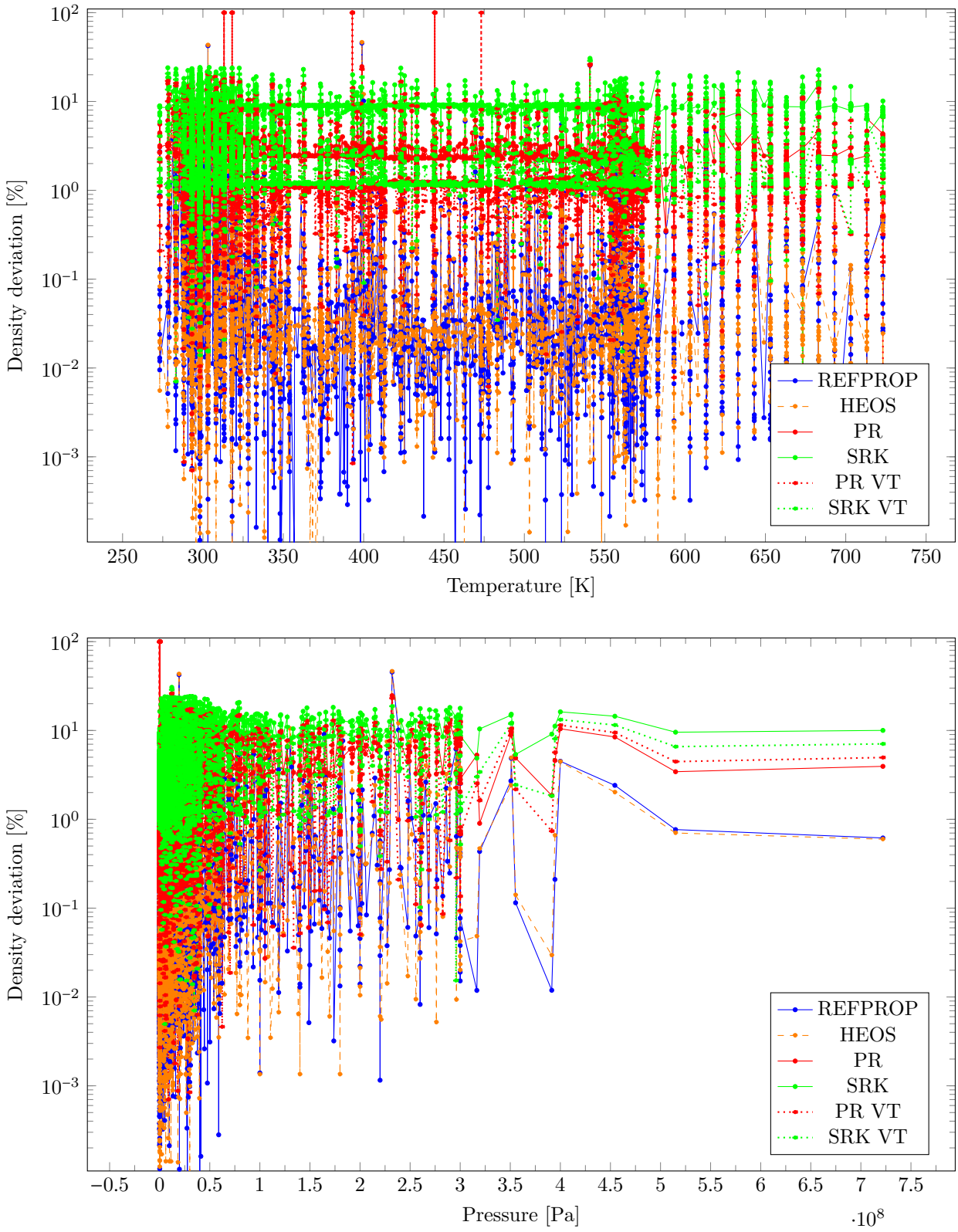


Figure 38: Density dependence on the temperature and pressure for fluid Benzene

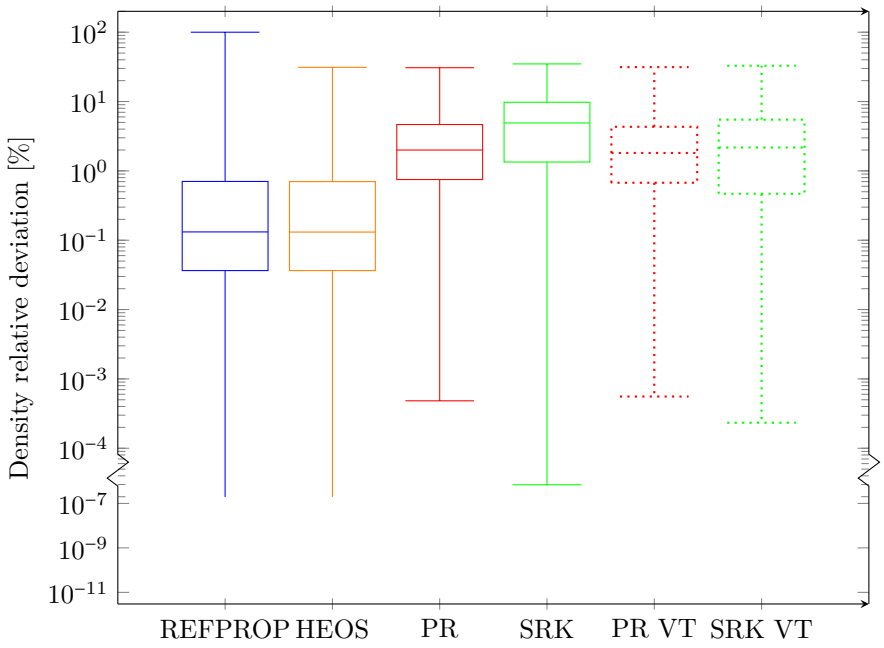


Figure 39: Relative density deviation to experimental data for fluid CarbonDioxide

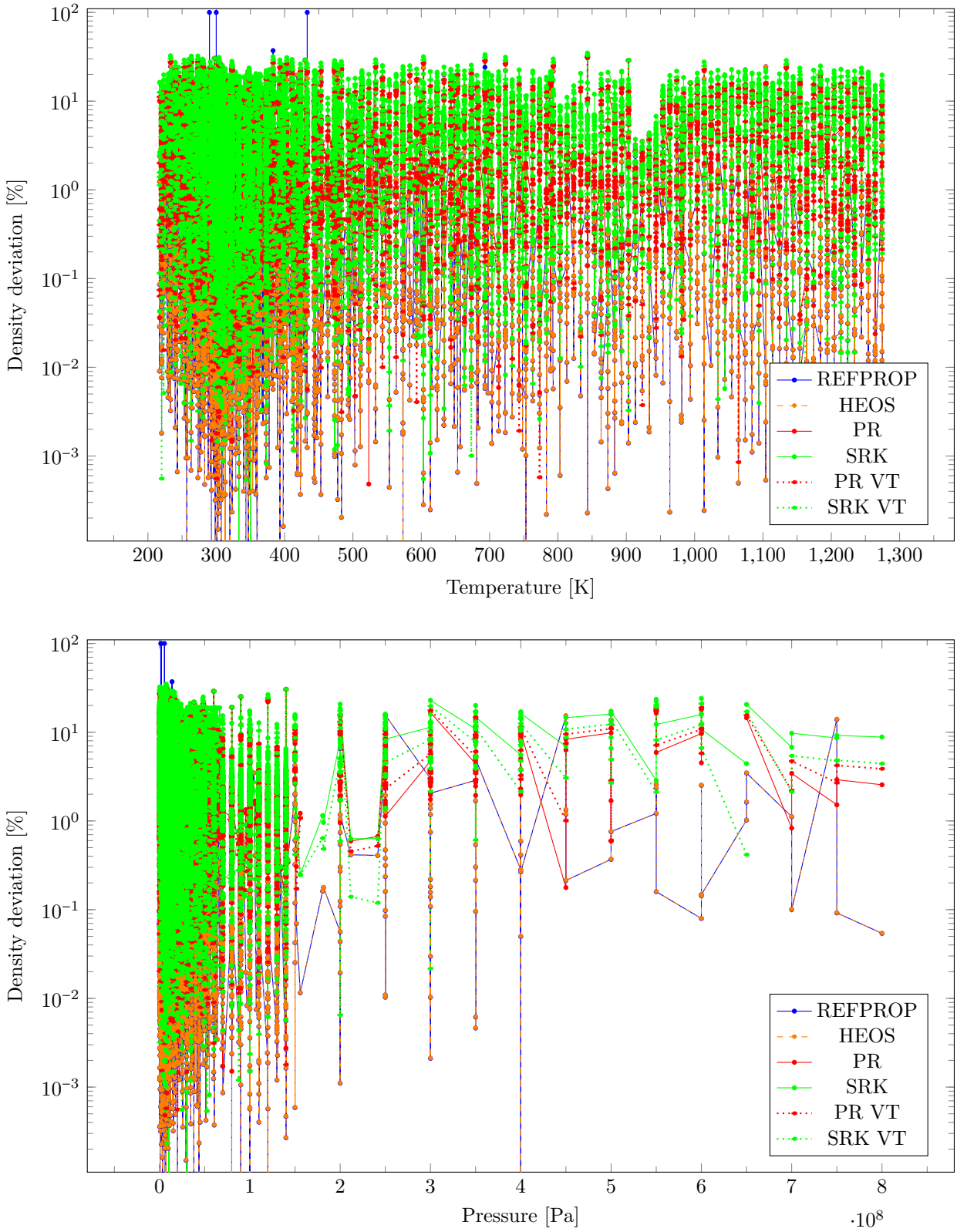


Figure 40: Density dependence on the temperature and pressure for fluid CarbonDioxide

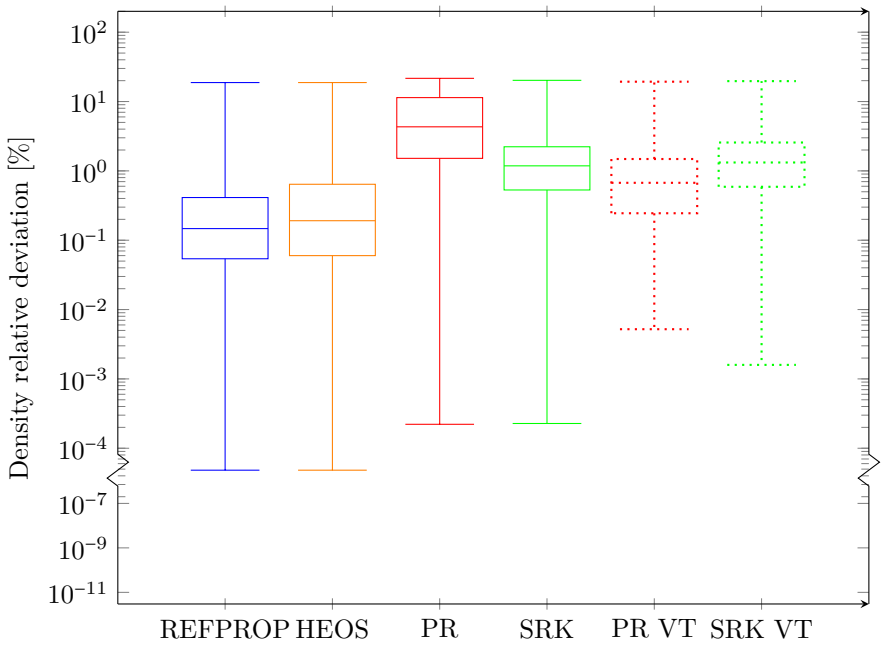


Figure 41: Relative density deviation to experimental data for fluid CarbonMonoxide

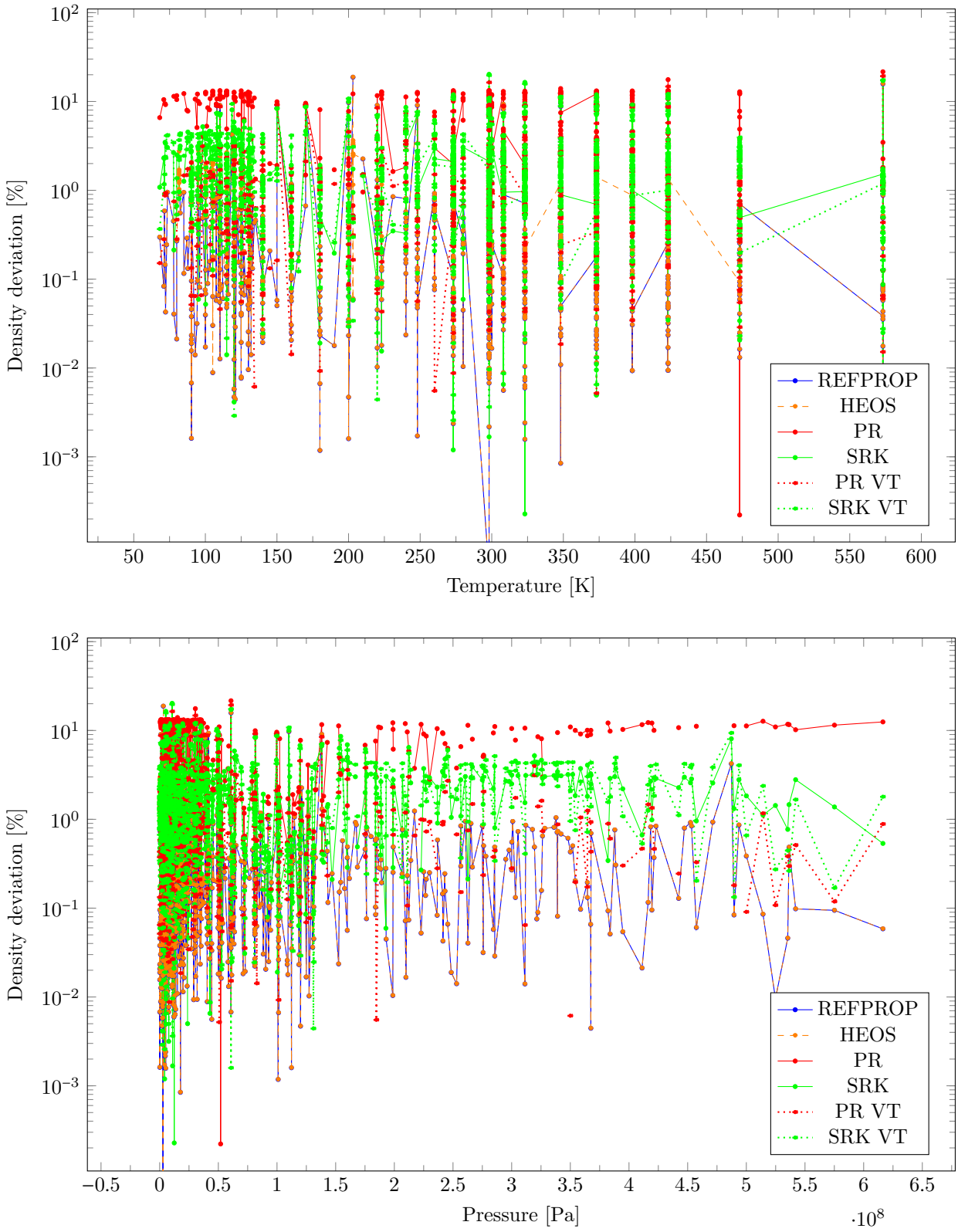


Figure 42: Density dependence on the temperature and pressure for fluid CarbonMonoxide

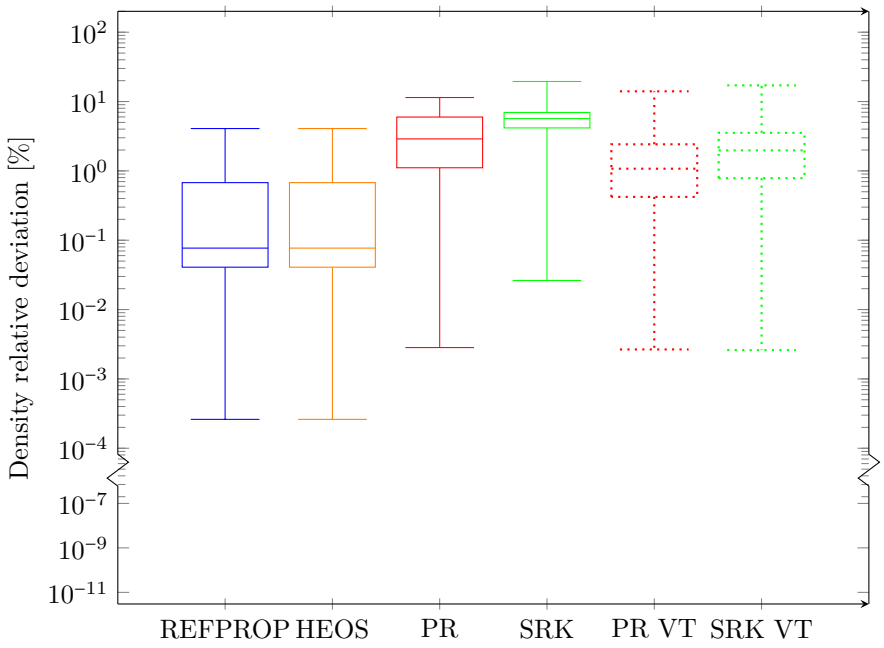


Figure 43: Relative density deviation to experimental data for fluid CarbonylSulfide

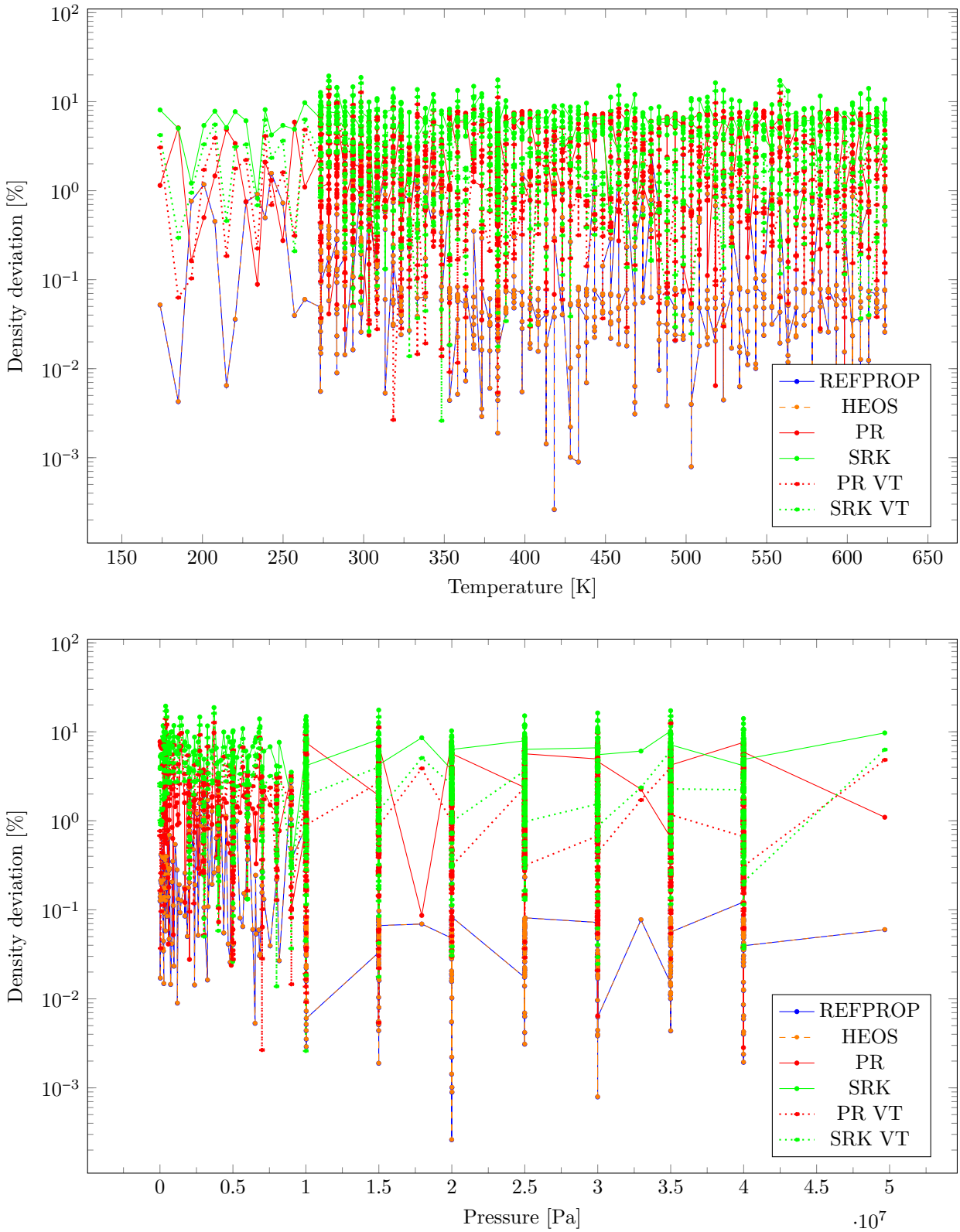


Figure 44: Density dependence on the temperature and pressure for fluid CarbonylSulfide

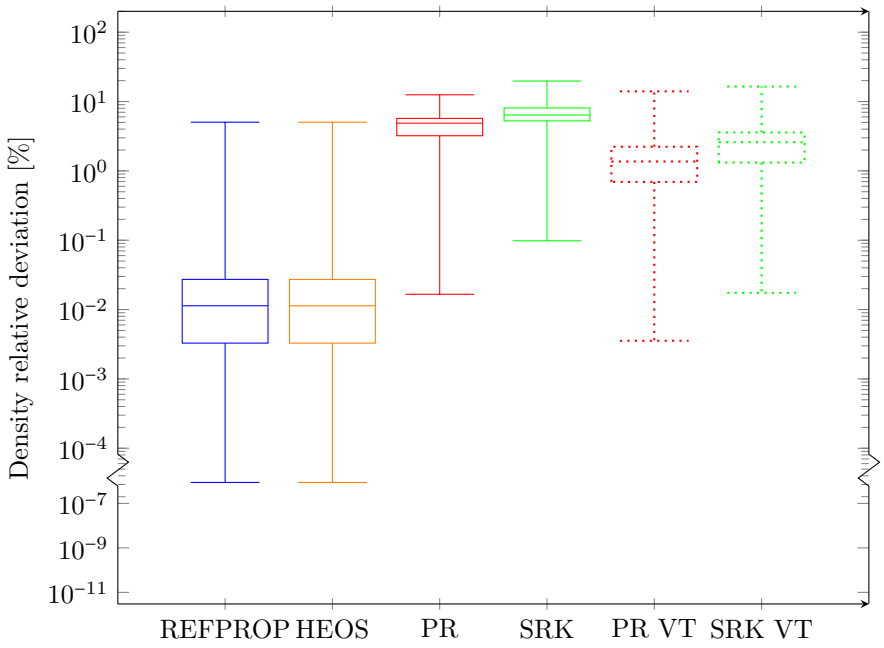


Figure 45: Relative density deviation to experimental data for fluid CIS-2-BUTENE

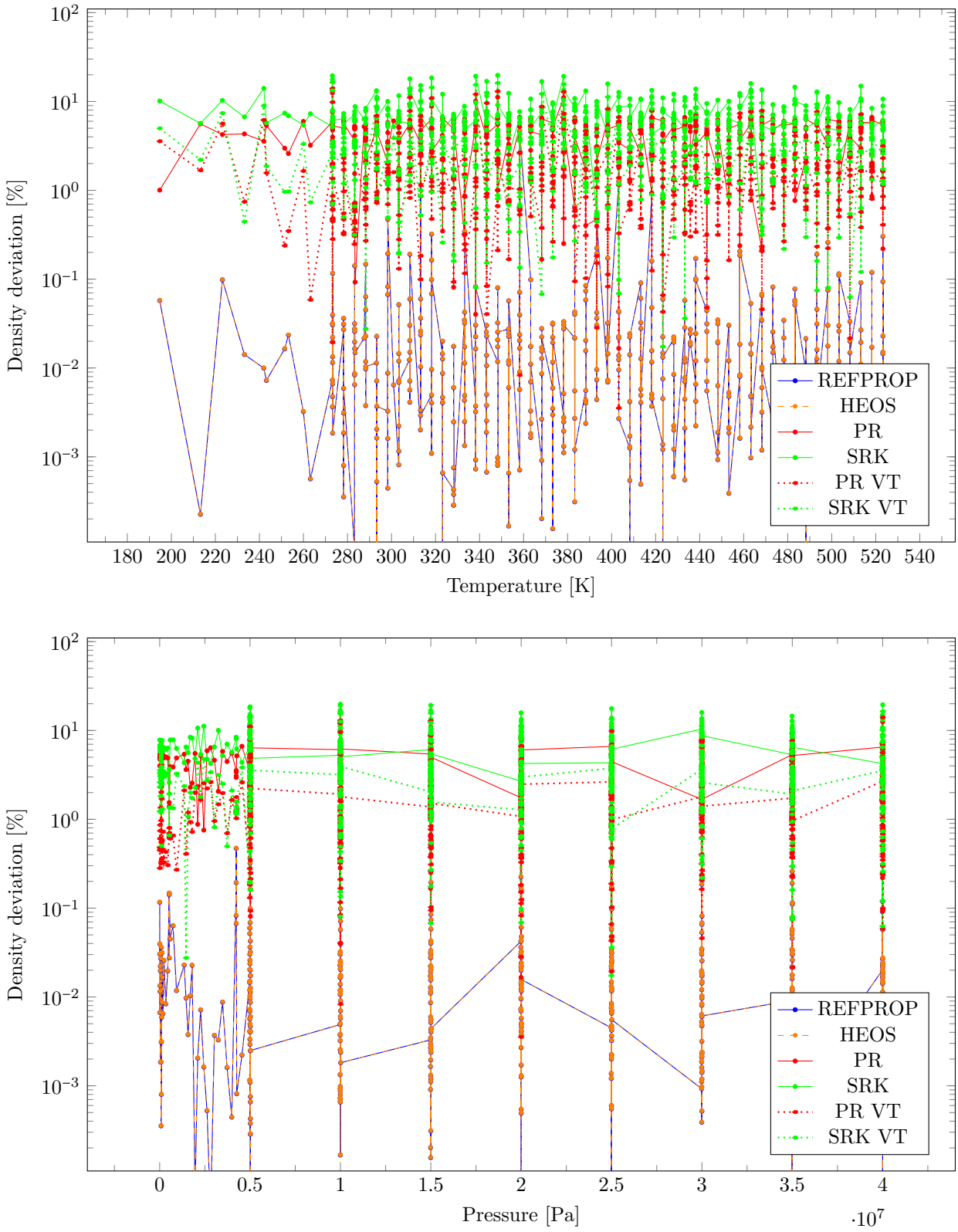


Figure 46: Density dependence on the temperature and pressure for fluid cis-2-Butene

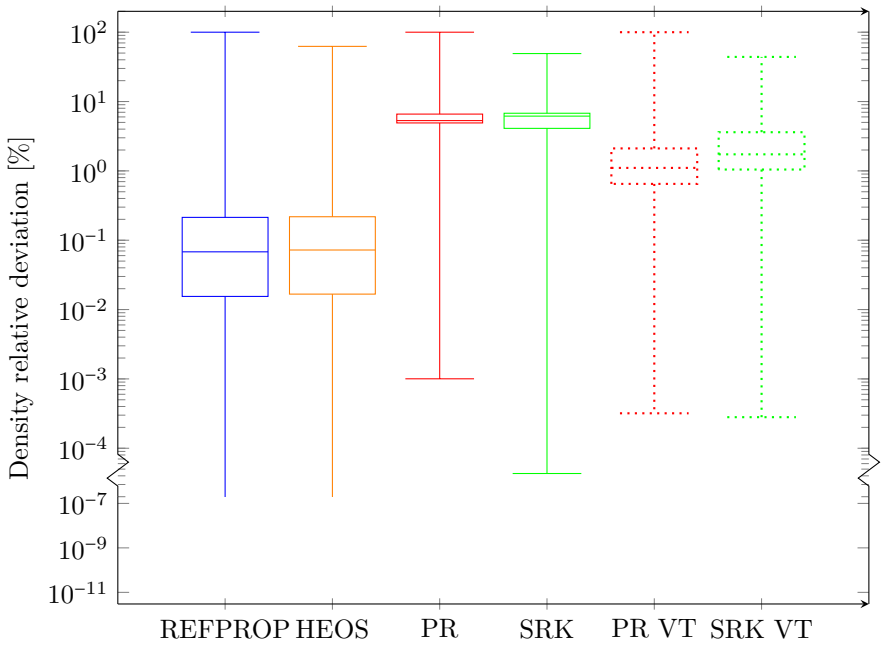


Figure 47: Relative density deviation to experimental data for fluid CycloHexane

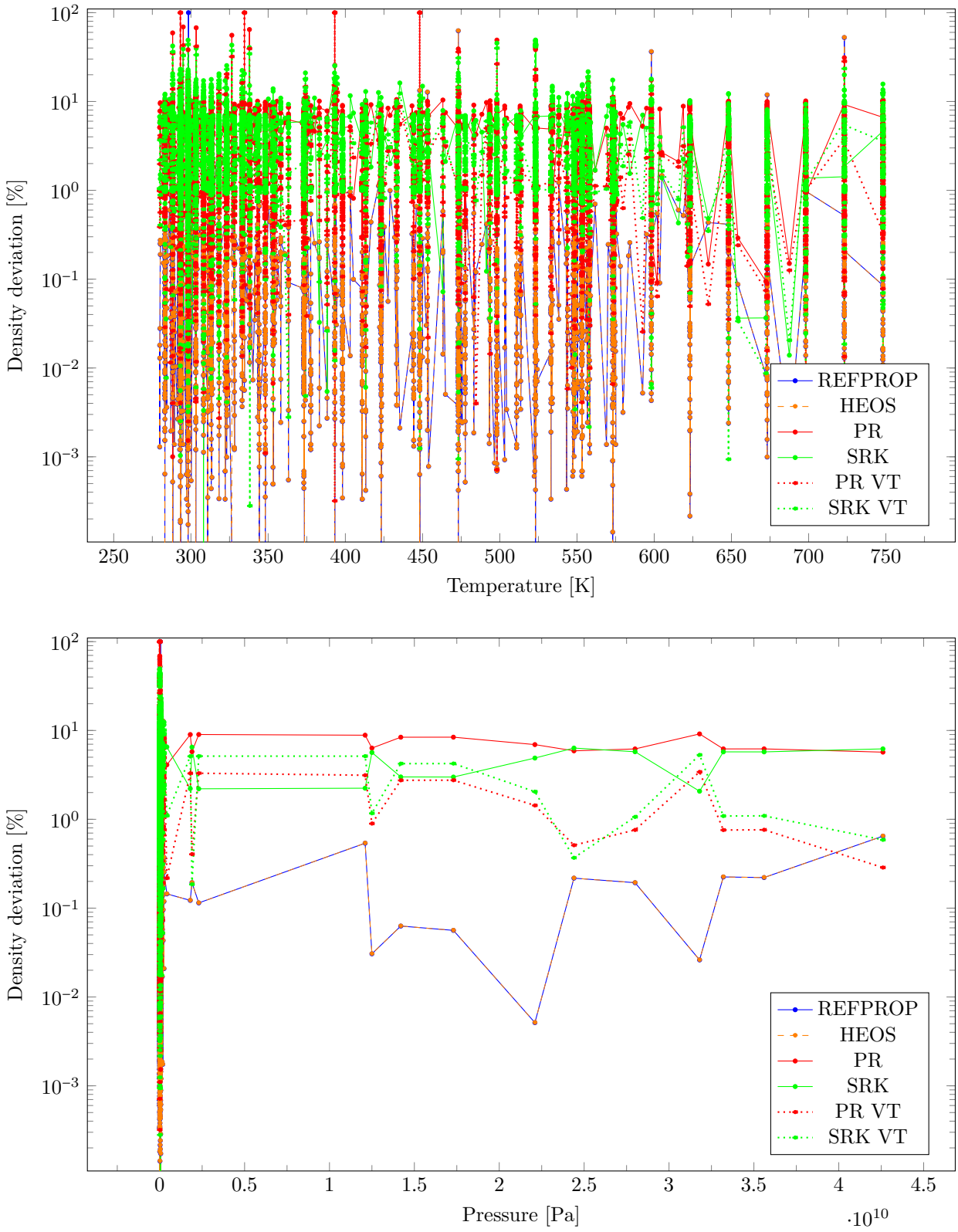


Figure 48: Density dependence on the temperature and pressure for fluid CycloHexane

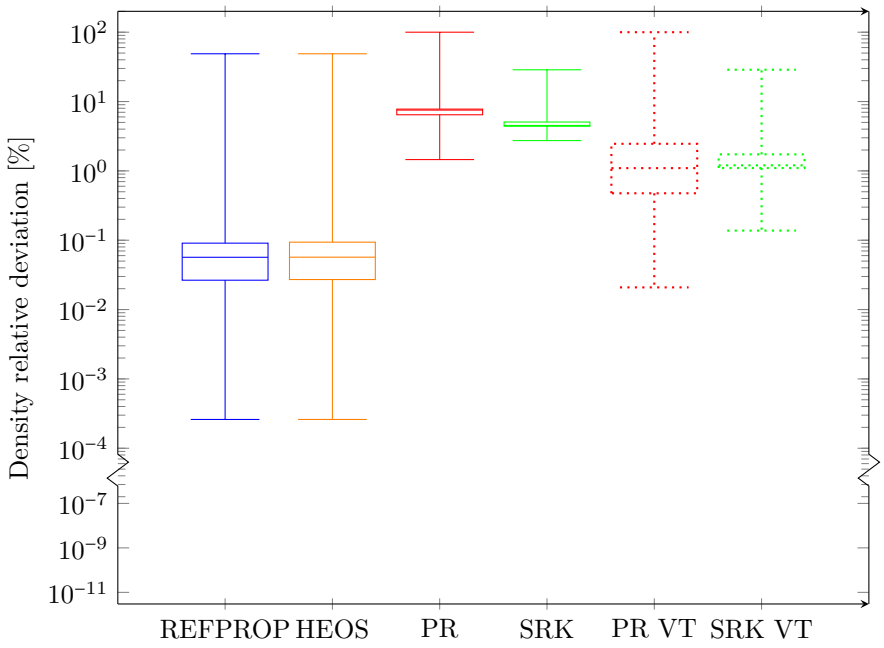


Figure 49: Relative density deviation to experimental data for fluid Cyclopentane

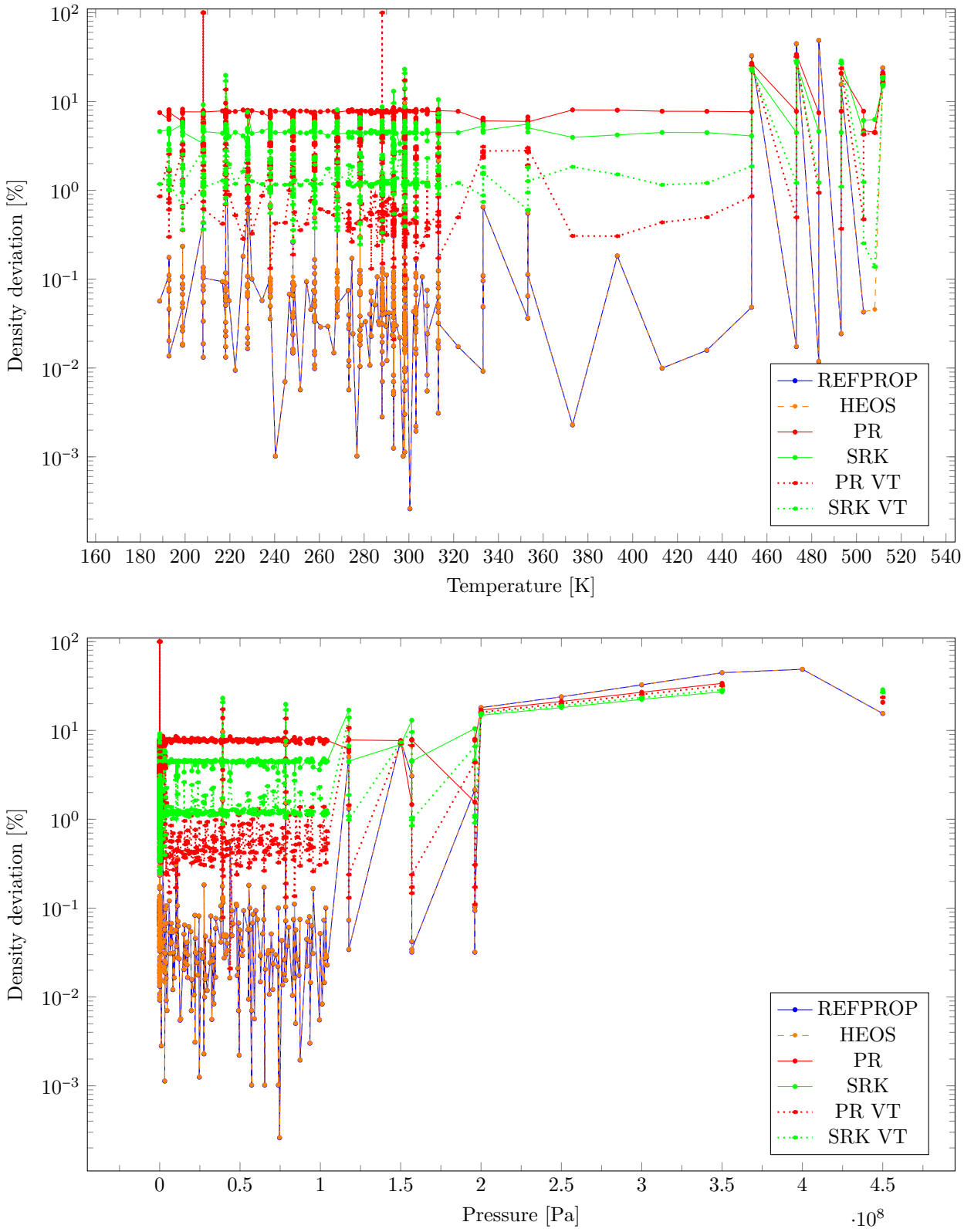


Figure 50: Density dependence on the temperature and pressure for fluid Cyclopentane

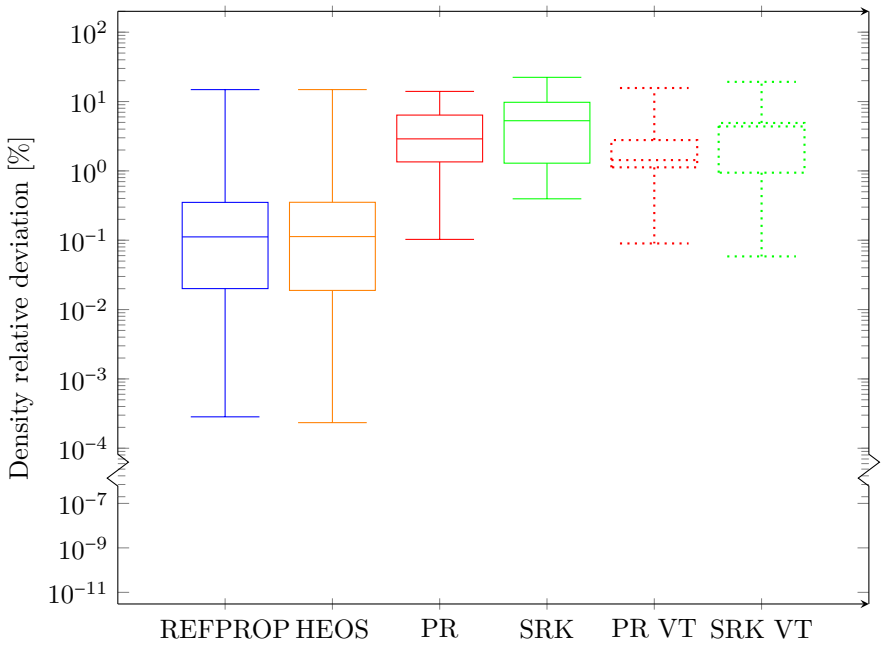


Figure 51: Relative density deviation to experimental data for fluid CycloPropane

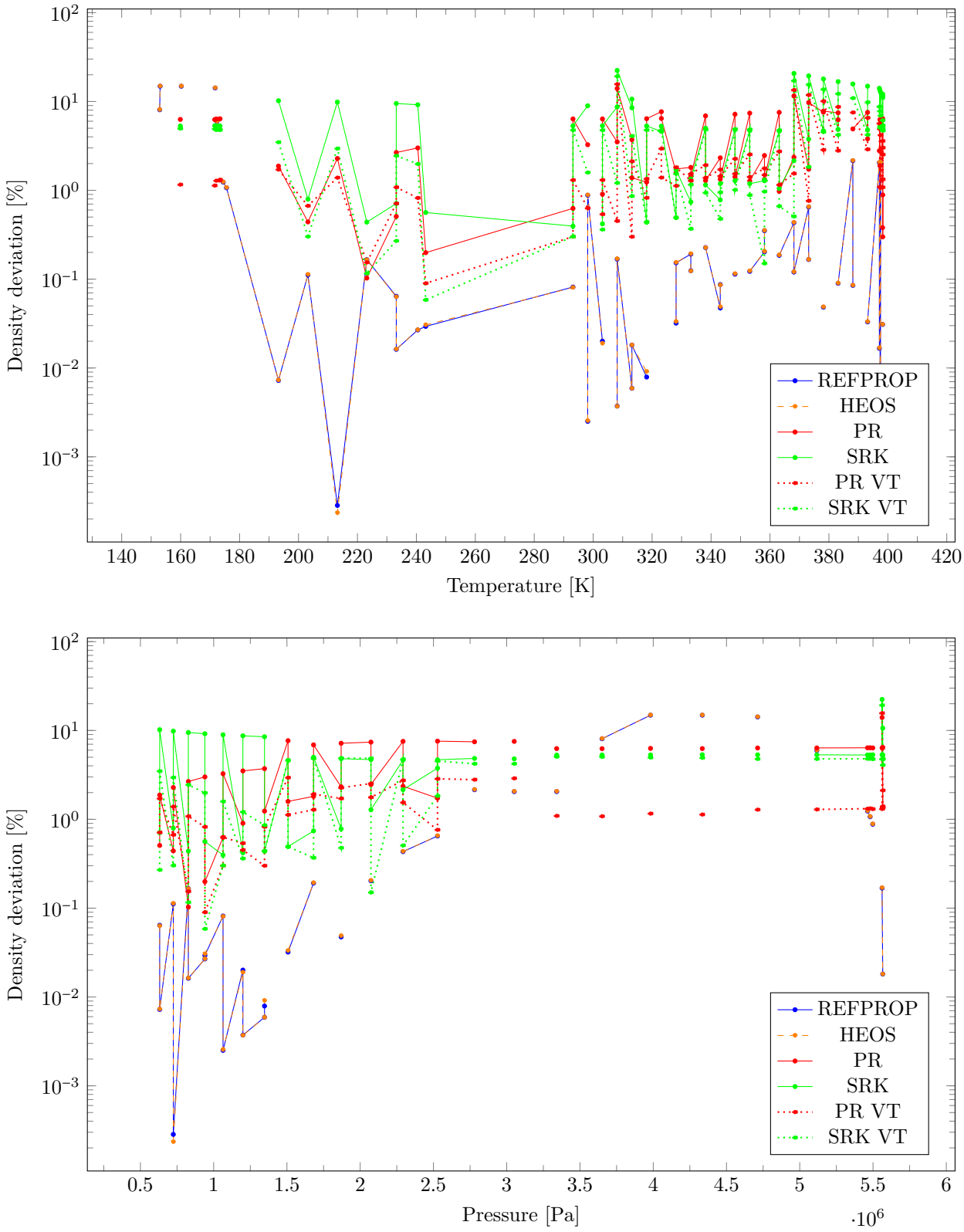


Figure 52: Density dependence on the temperature and pressure for fluid CycloPropane

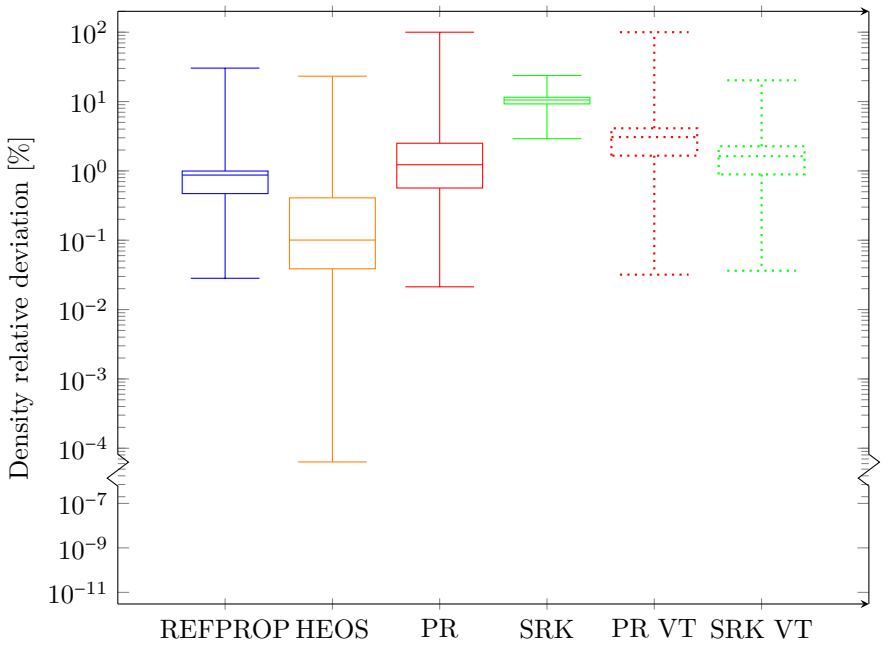


Figure 53: Relative density deviation to experimental data for fluid D4

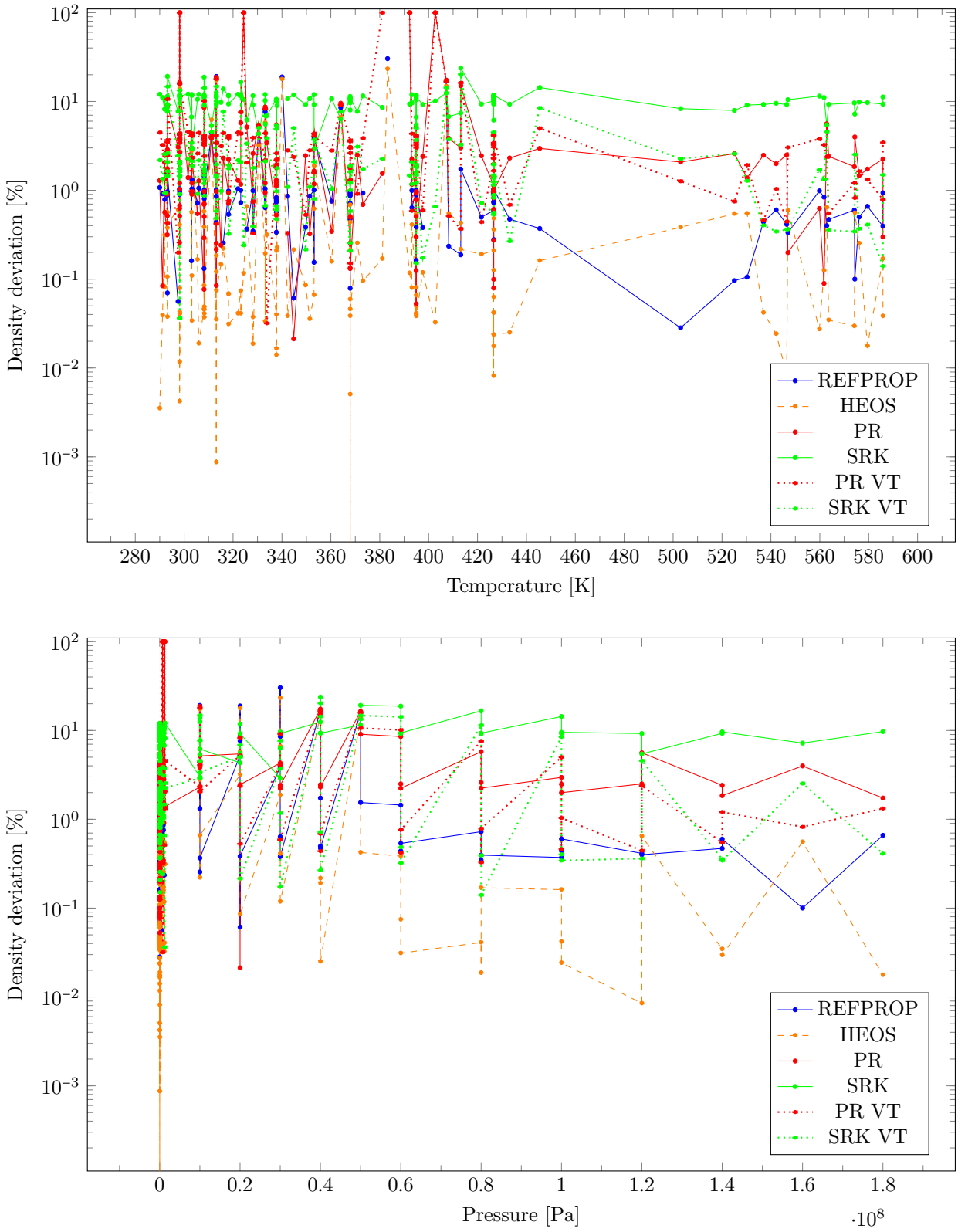


Figure 54: Density dependence on the temperature and pressure for fluid D4

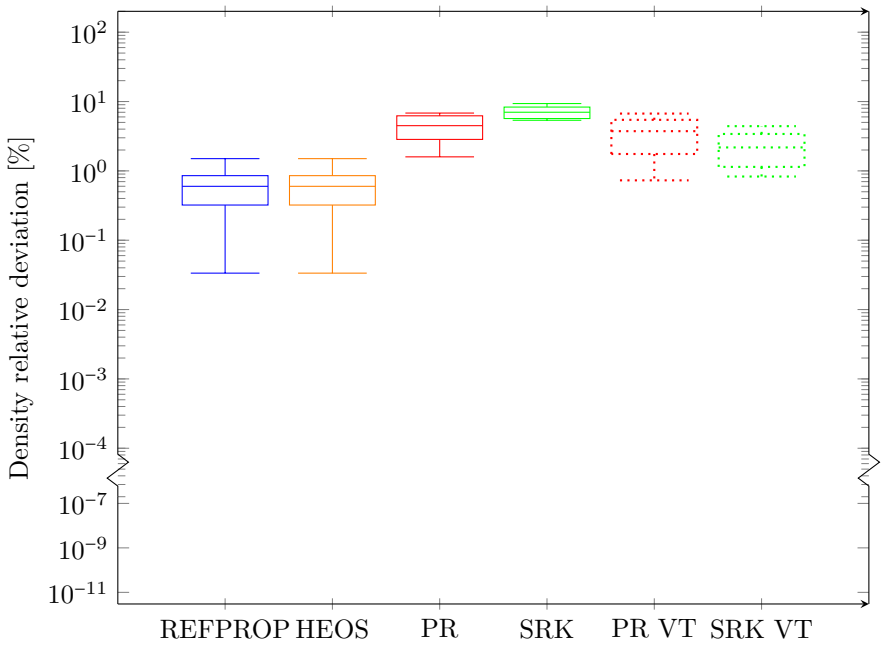


Figure 55: Relative density deviation to experimental data for fluid D5

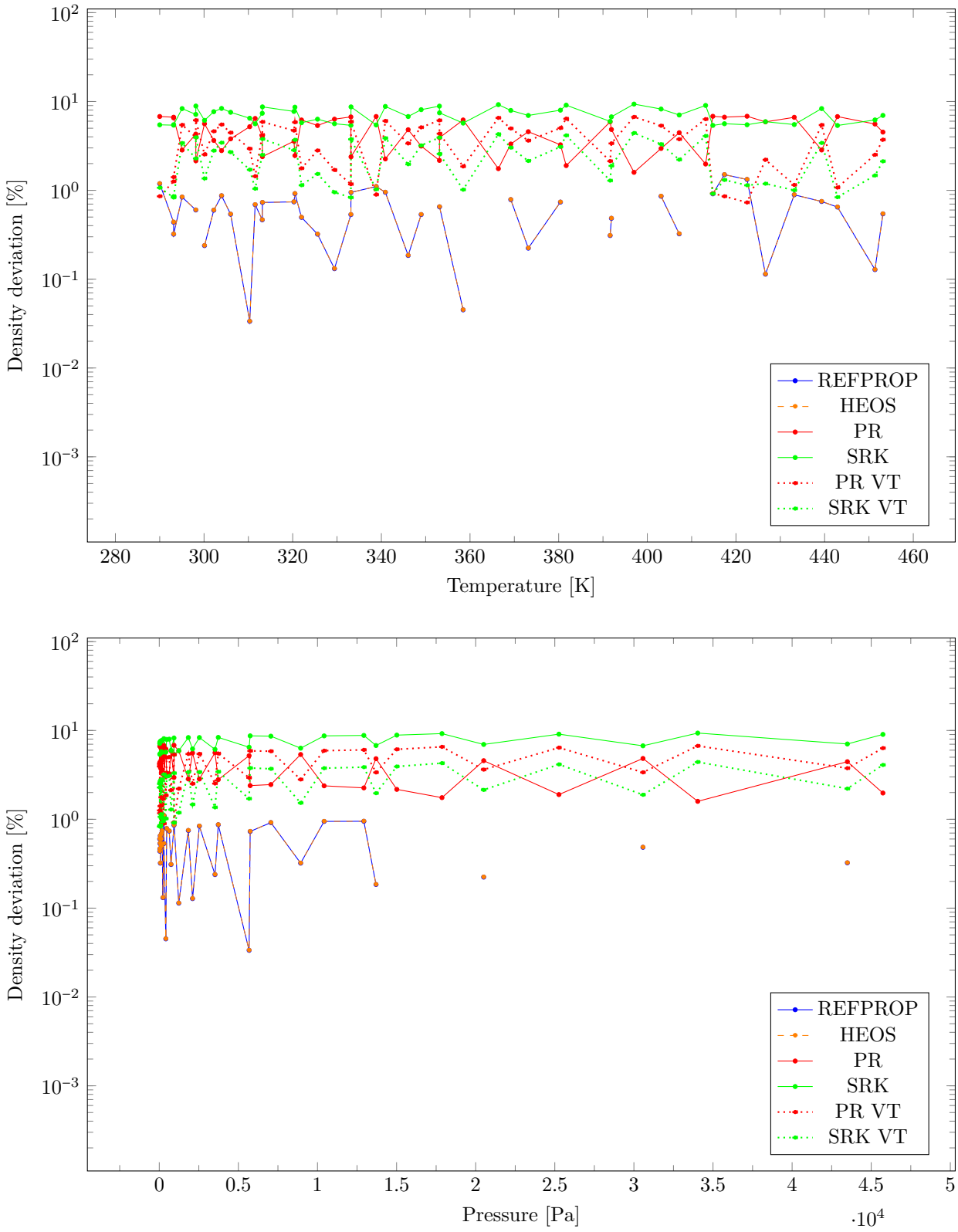


Figure 56: Density dependence on the temperature and pressure for fluid D5

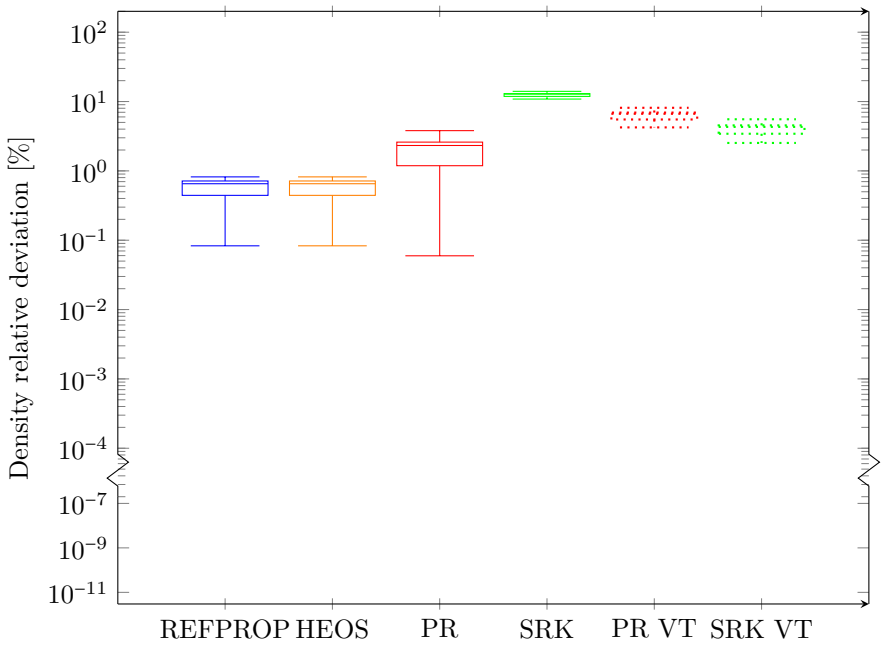


Figure 57: Relative density deviation to experimental data for fluid D6

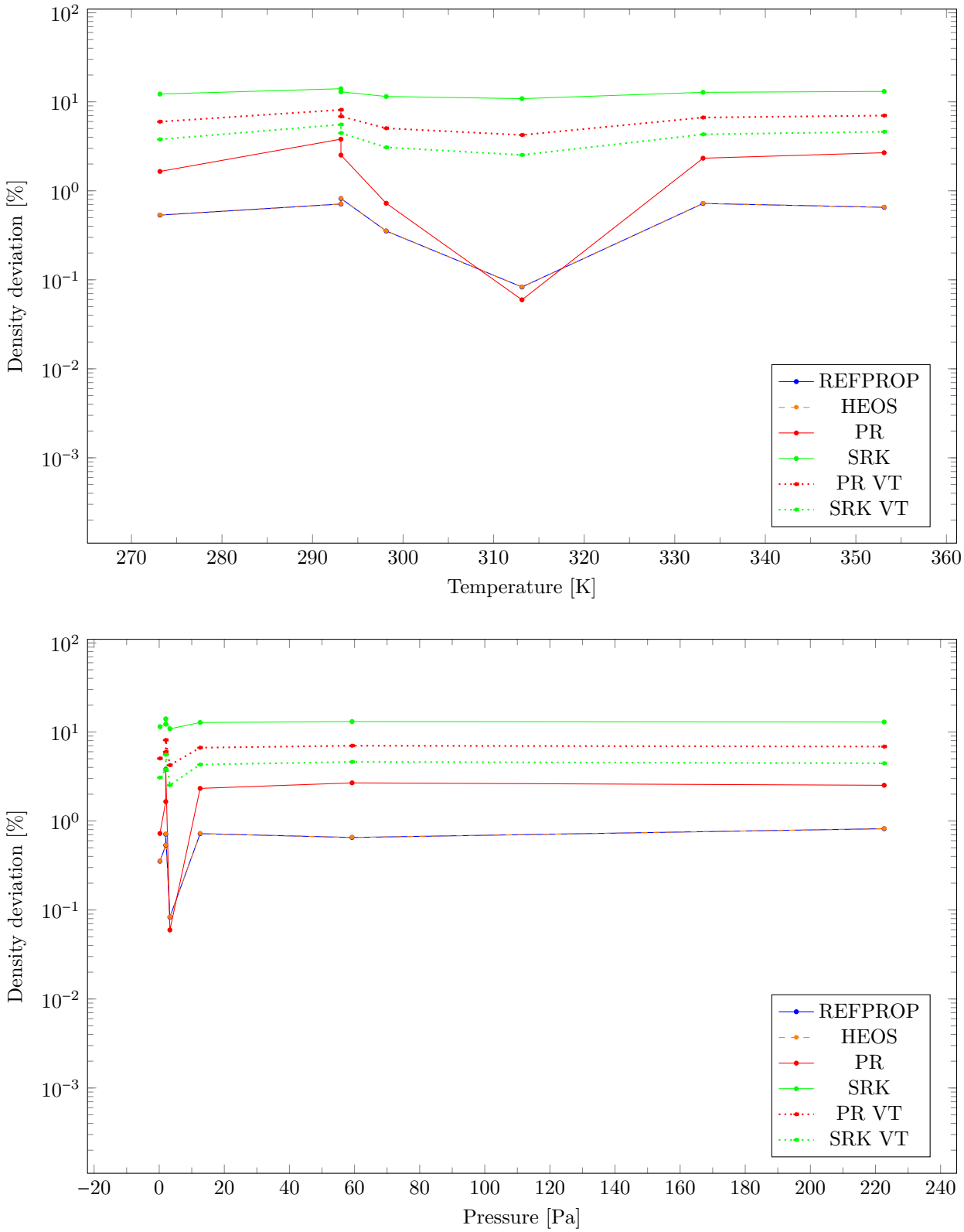


Figure 58: Density dependence on the temperature and pressure for fluid D6

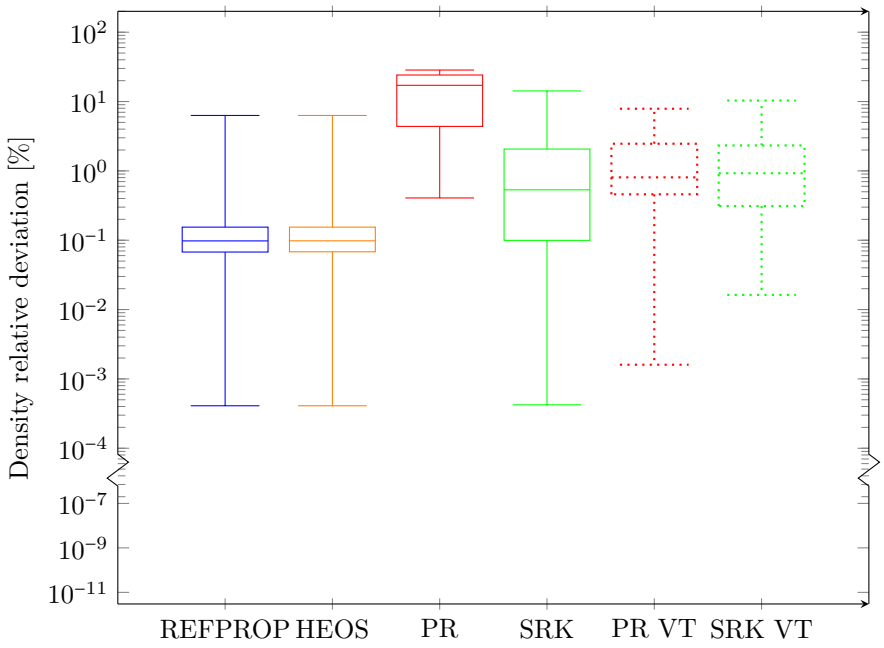


Figure 59: Relative density deviation to experimental data for fluid Deuterium

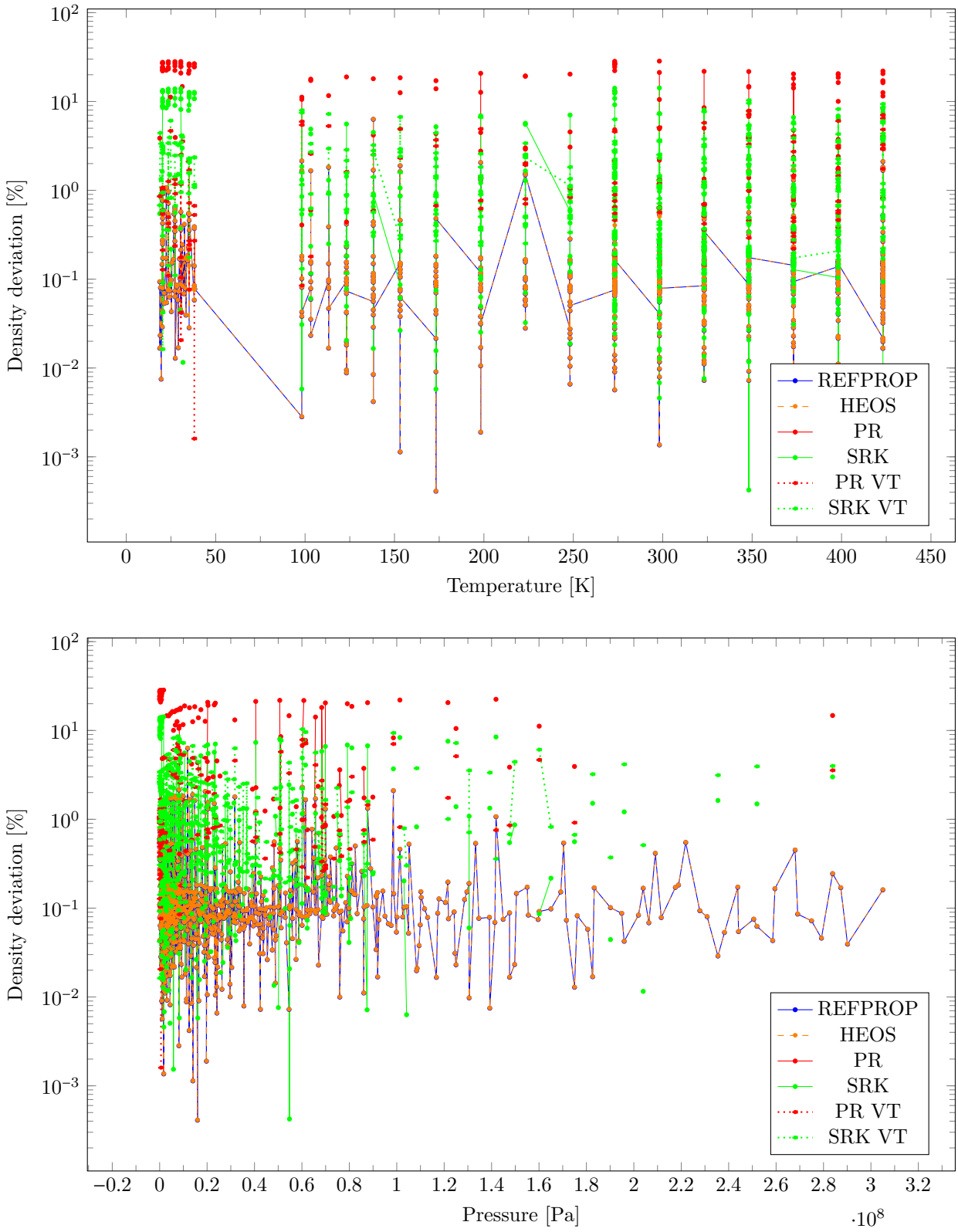


Figure 60: Density dependence on the temperature and pressure for fluid Deuterium

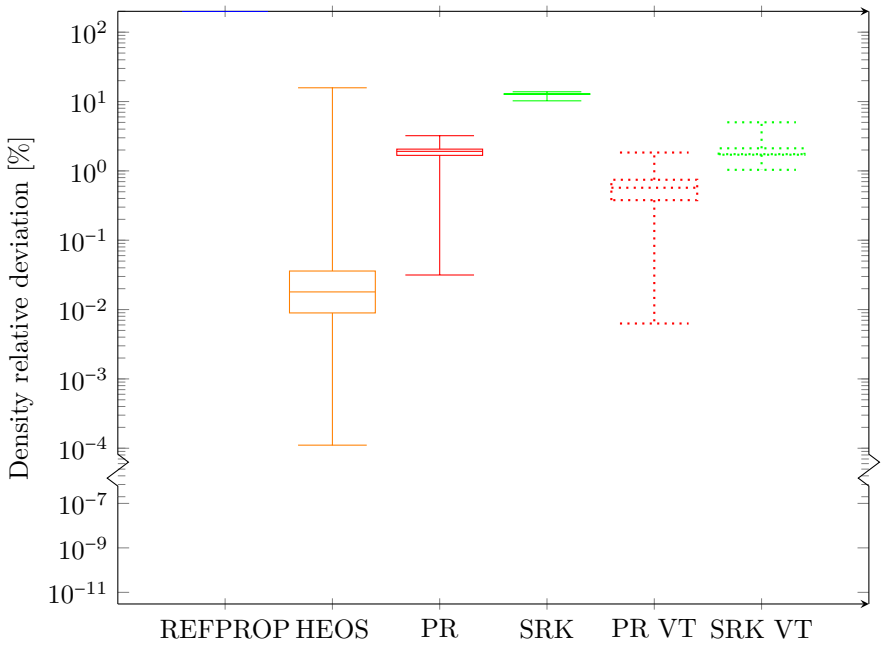


Figure 61: Relative density deviation to experimental data for fluid Dichloroethane

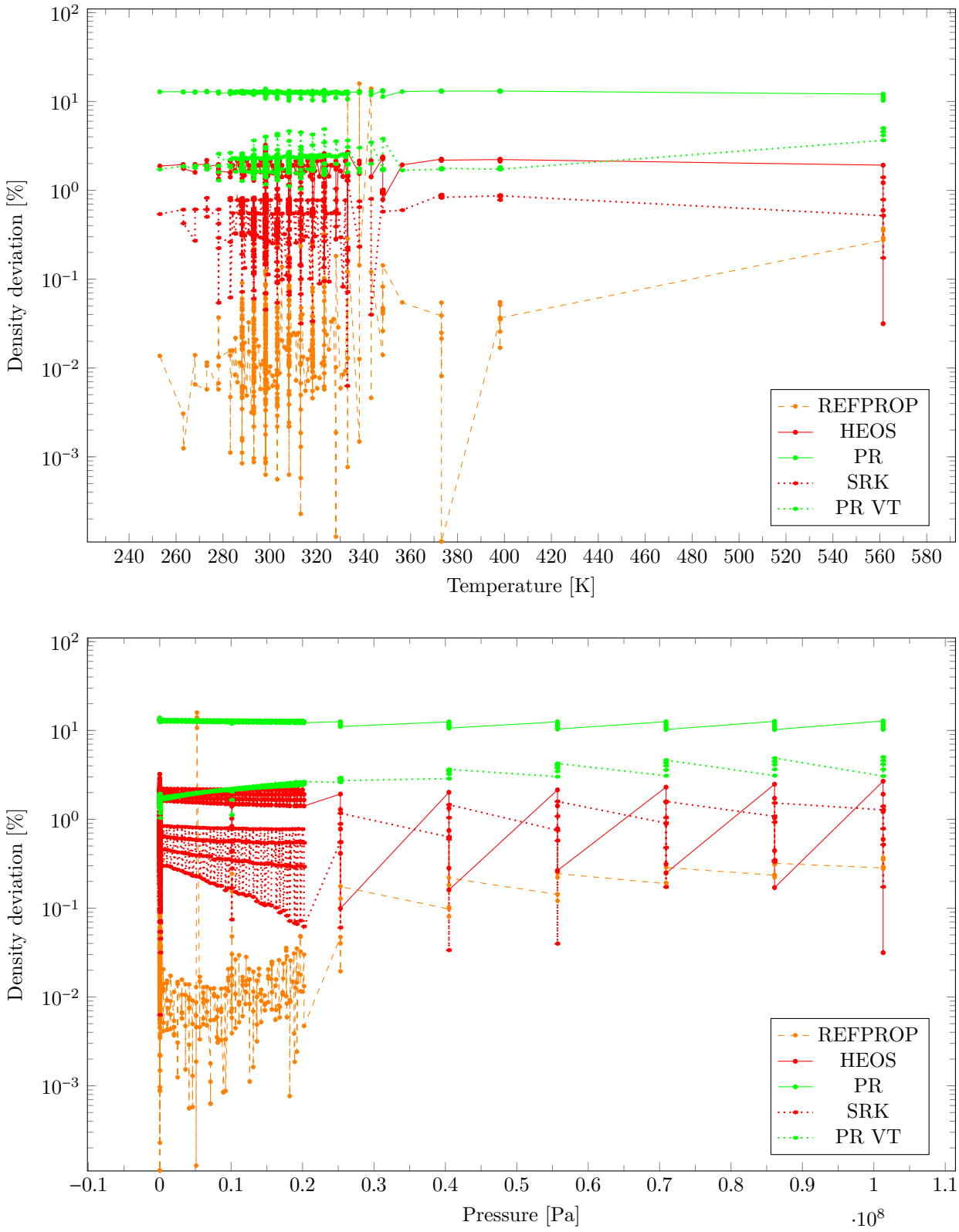


Figure 62: Density dependence on the temperature and pressure for fluid Dichloroethane

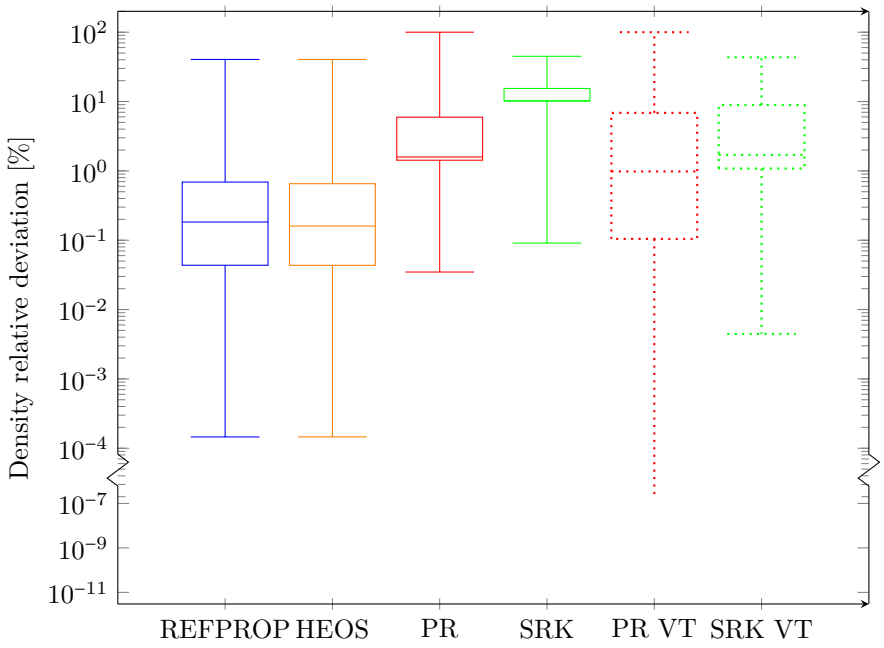


Figure 63: Relative density deviation to experimental data for fluid DiethylEther

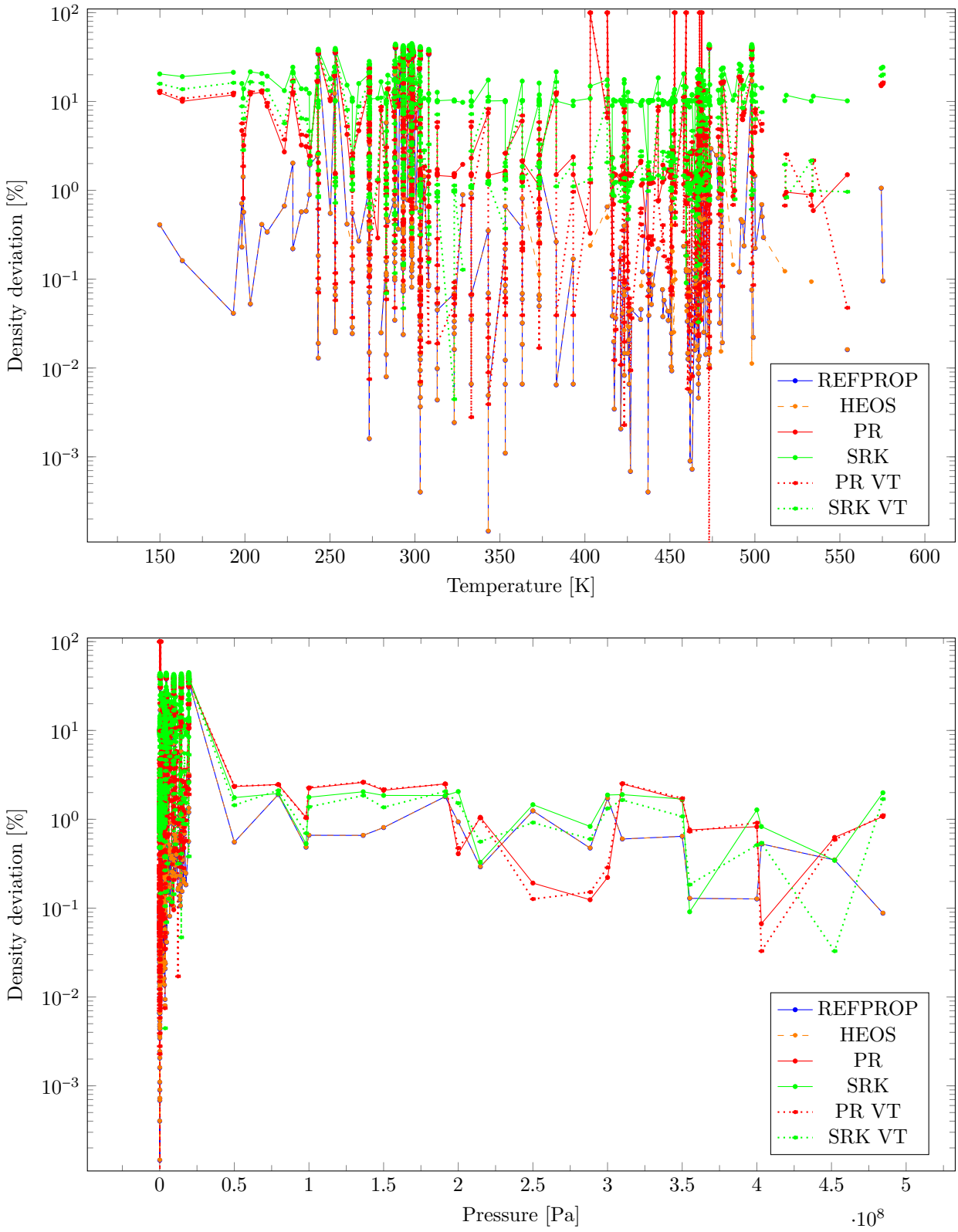


Figure 64: Density dependence on the temperature and pressure for fluid DiethylEther

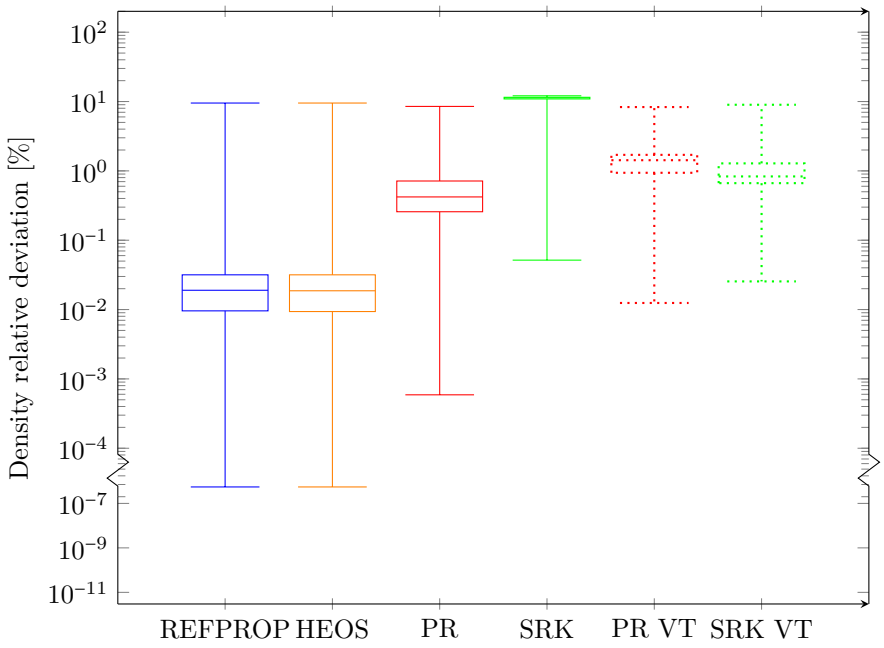


Figure 65: Relative density deviation to experimental data for fluid DimethylCarbonate

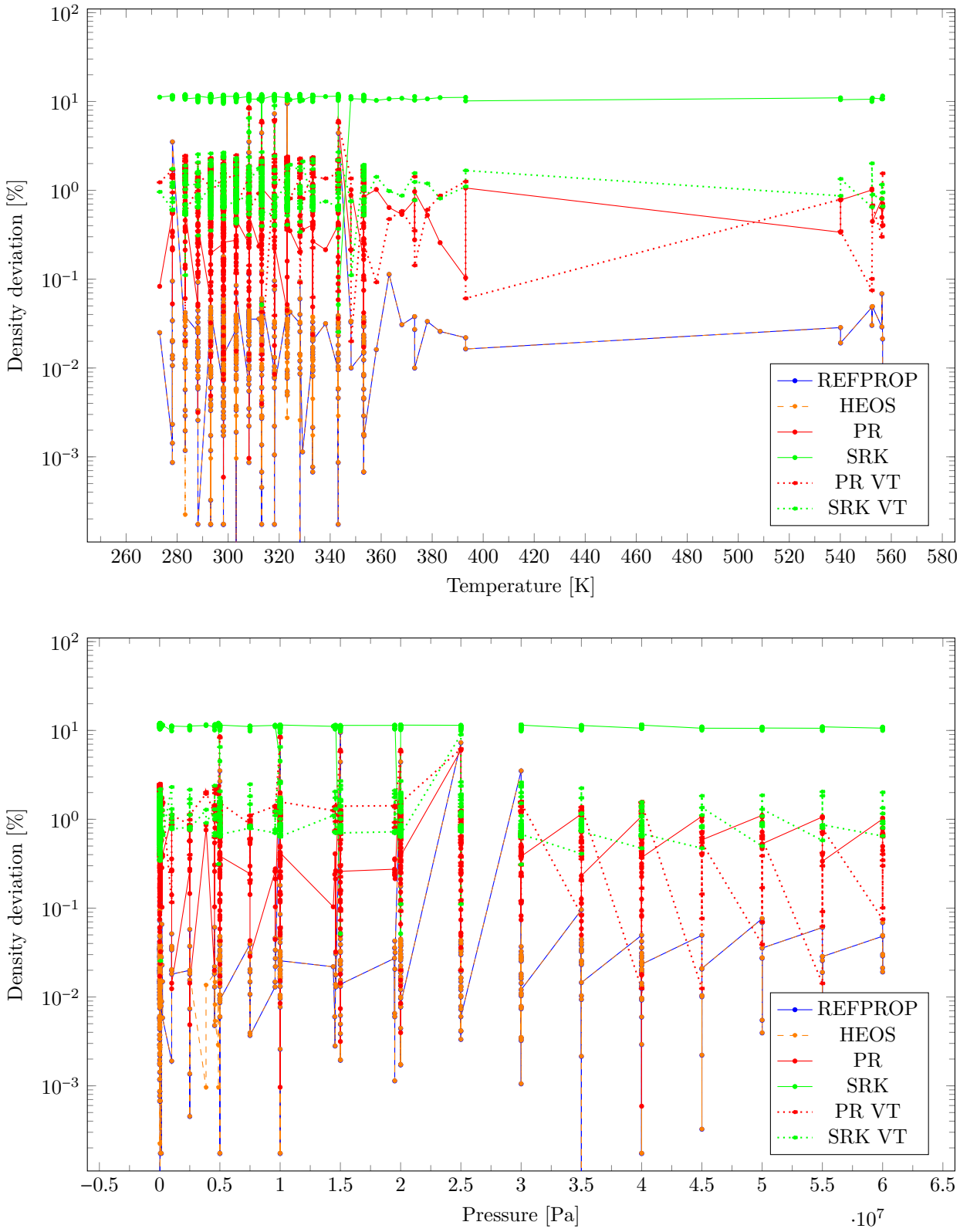


Figure 66: Density dependence on the temperature and pressure for fluid DimethylCarbonate

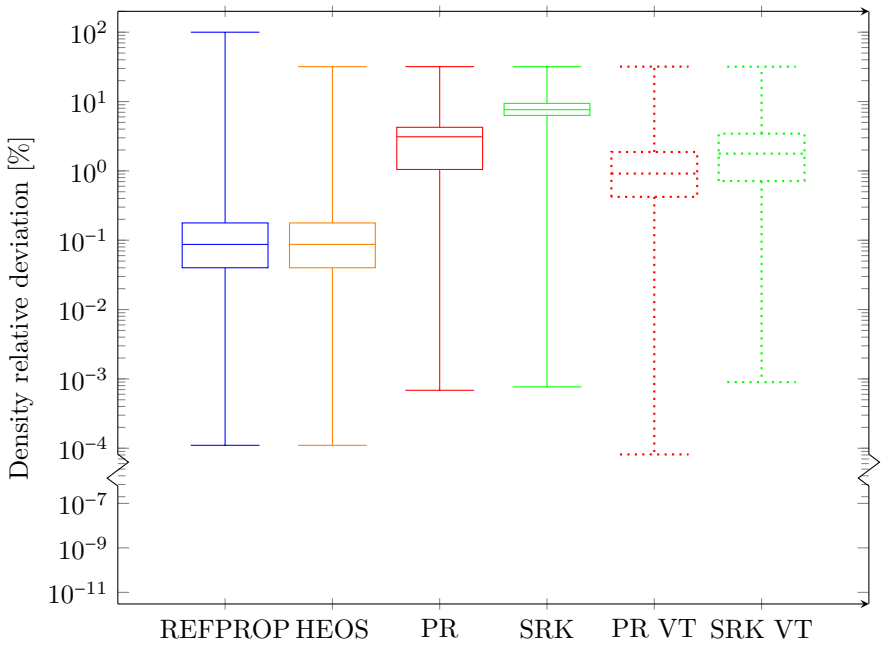


Figure 67: Relative density deviation to experimental data for fluid DimethylEther

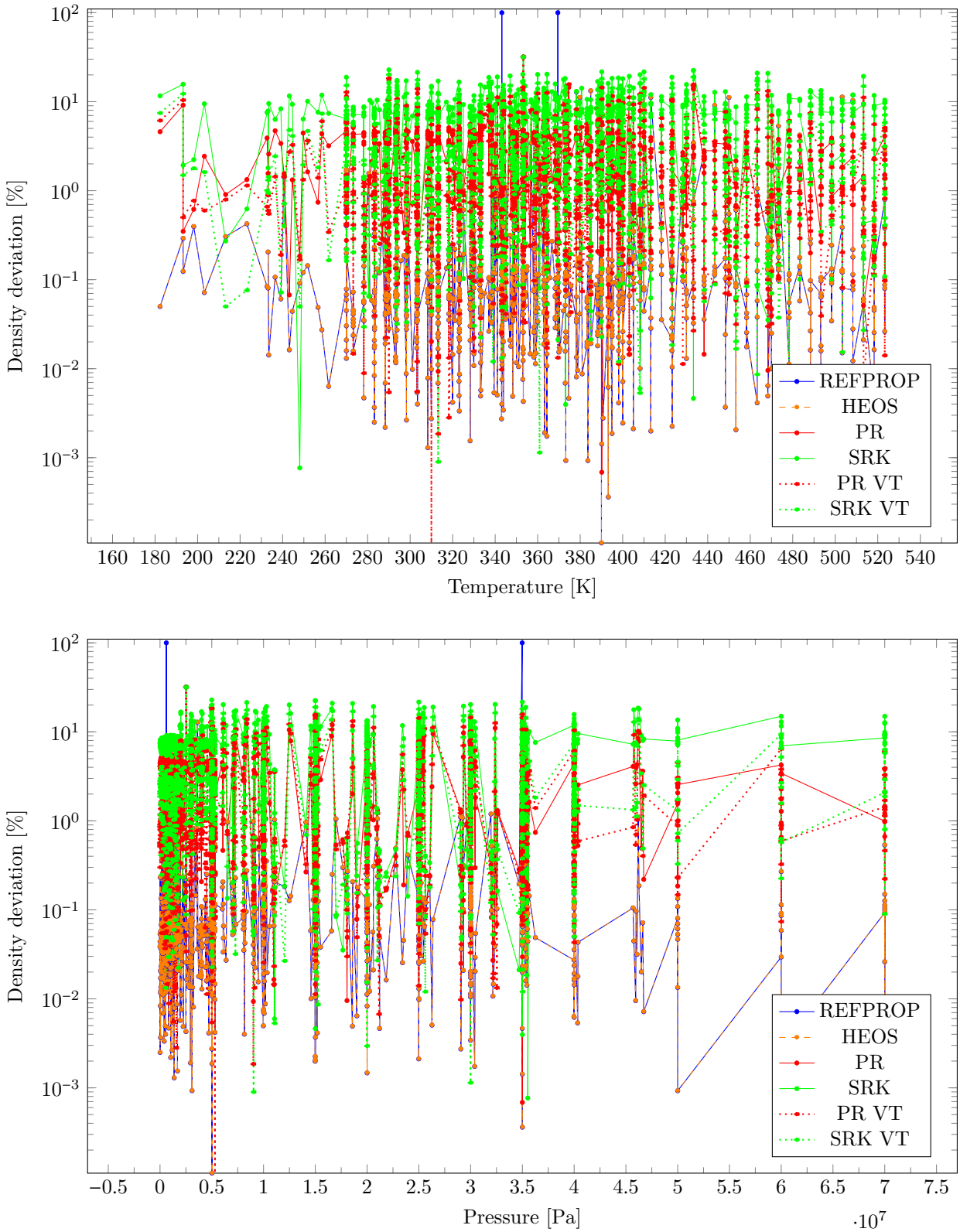


Figure 68: Density dependence on the temperature and pressure for fluid DimethylEther

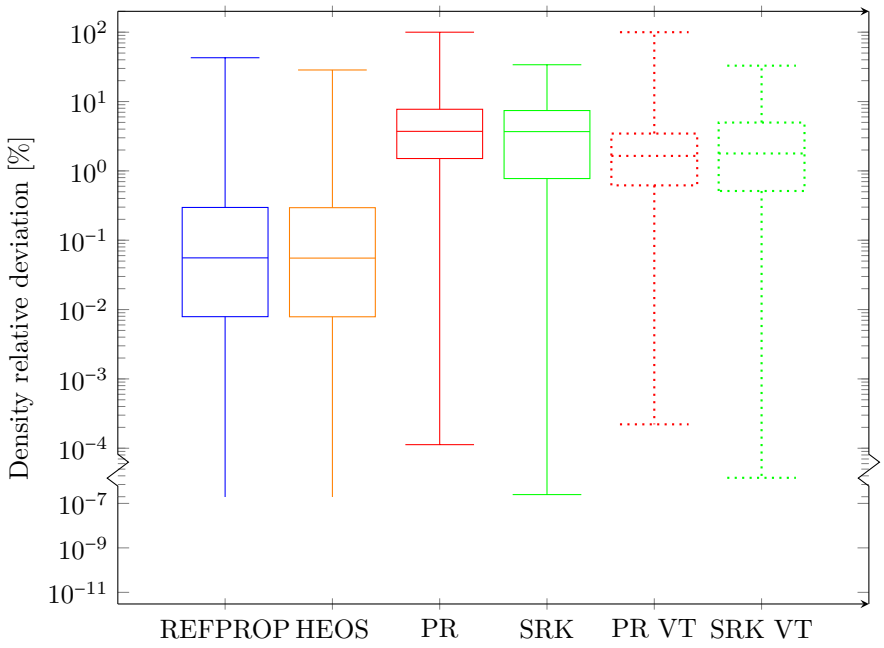


Figure 69: Relative density deviation to experimental data for fluid Ethane

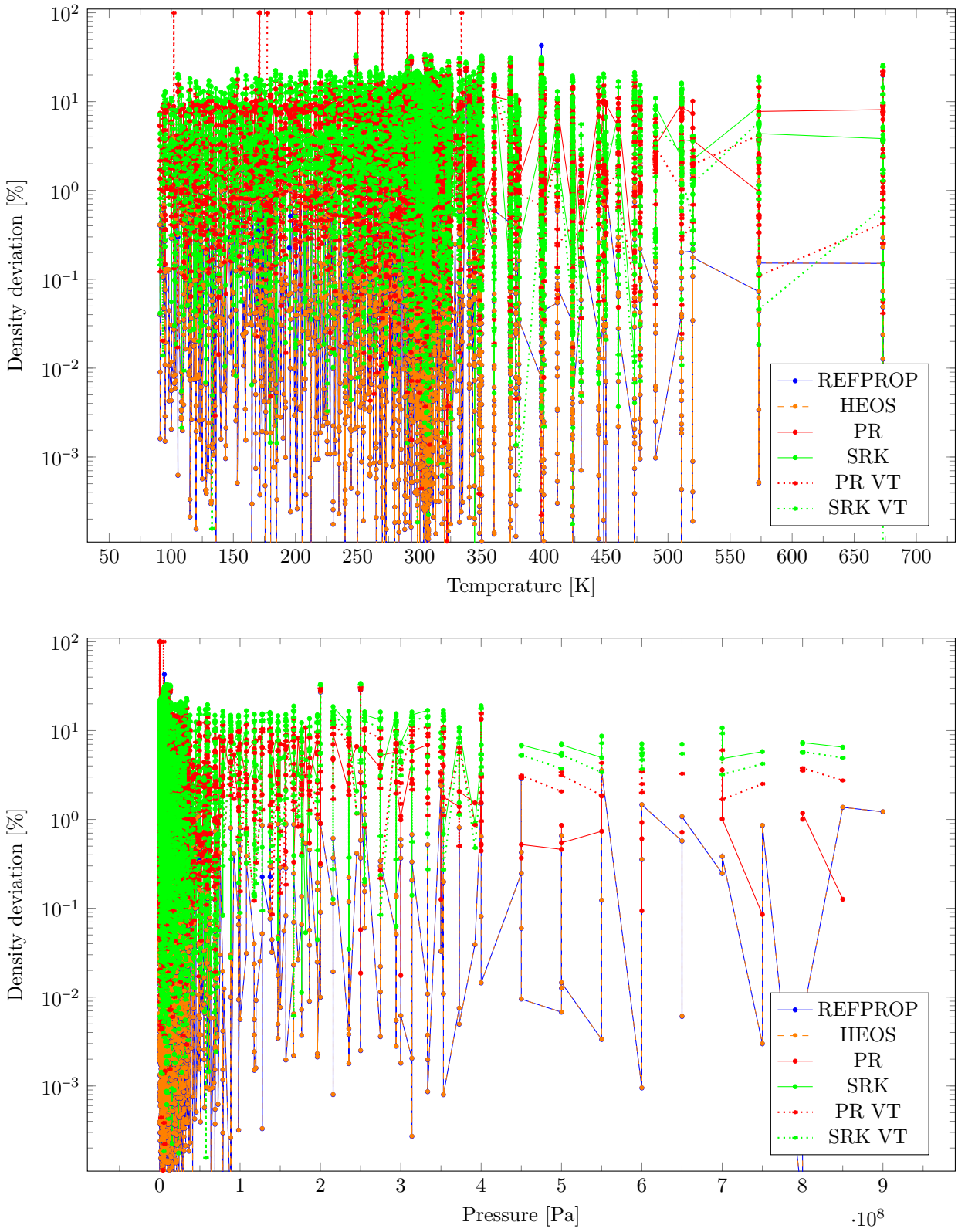


Figure 70: Density dependence on the temperature and pressure for fluid Ethane

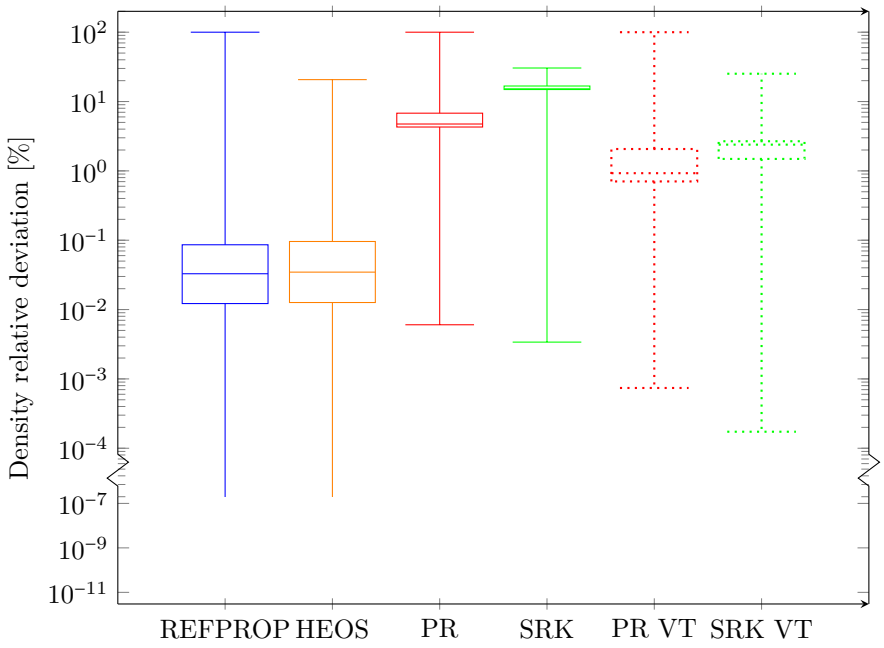


Figure 71: Relative density deviation to experimental data for fluid Ethanol

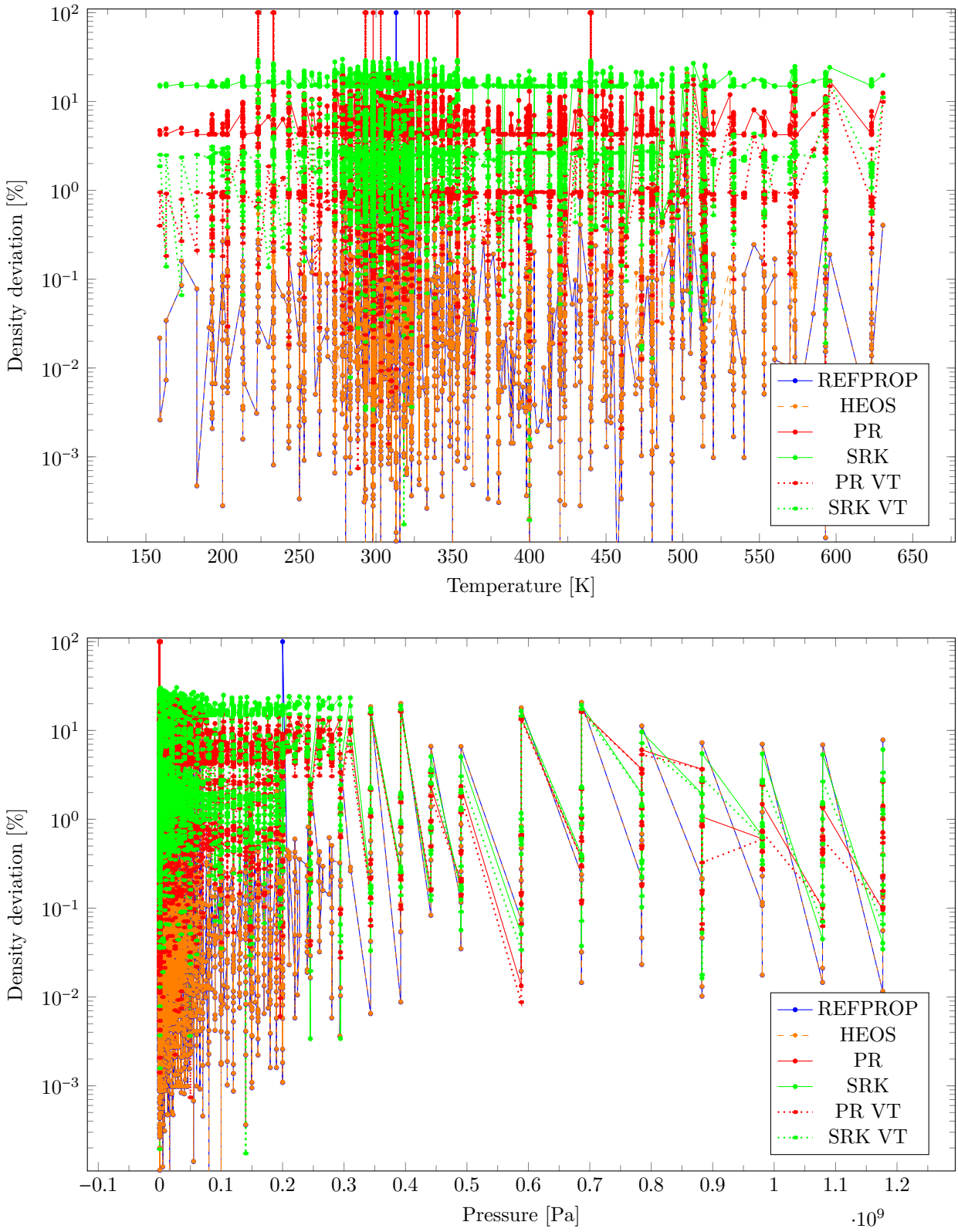


Figure 72: Density dependence on the temperature and pressure for fluid Ethanol

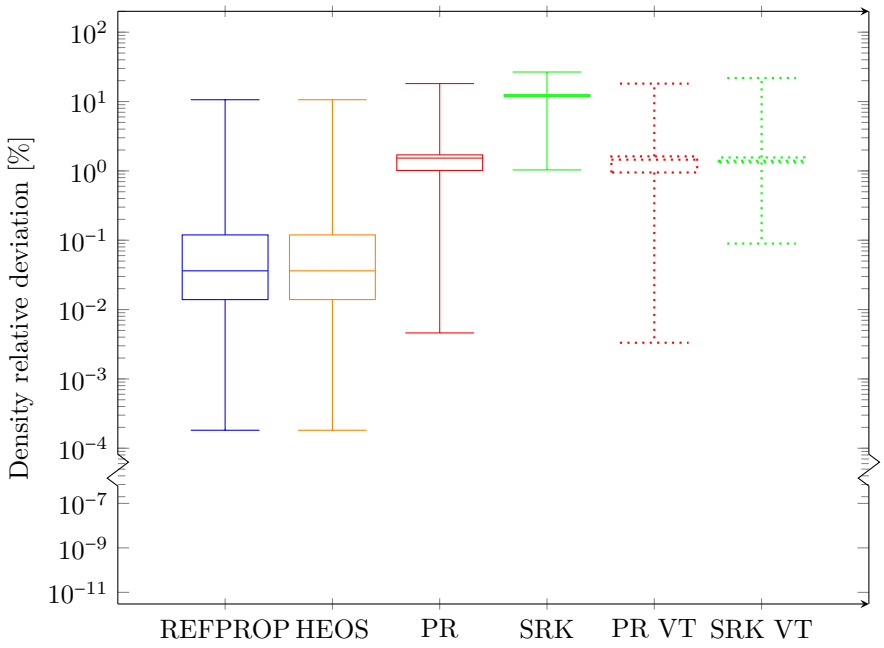


Figure 73: Relative density deviation to experimental data for fluid EthylBenzene

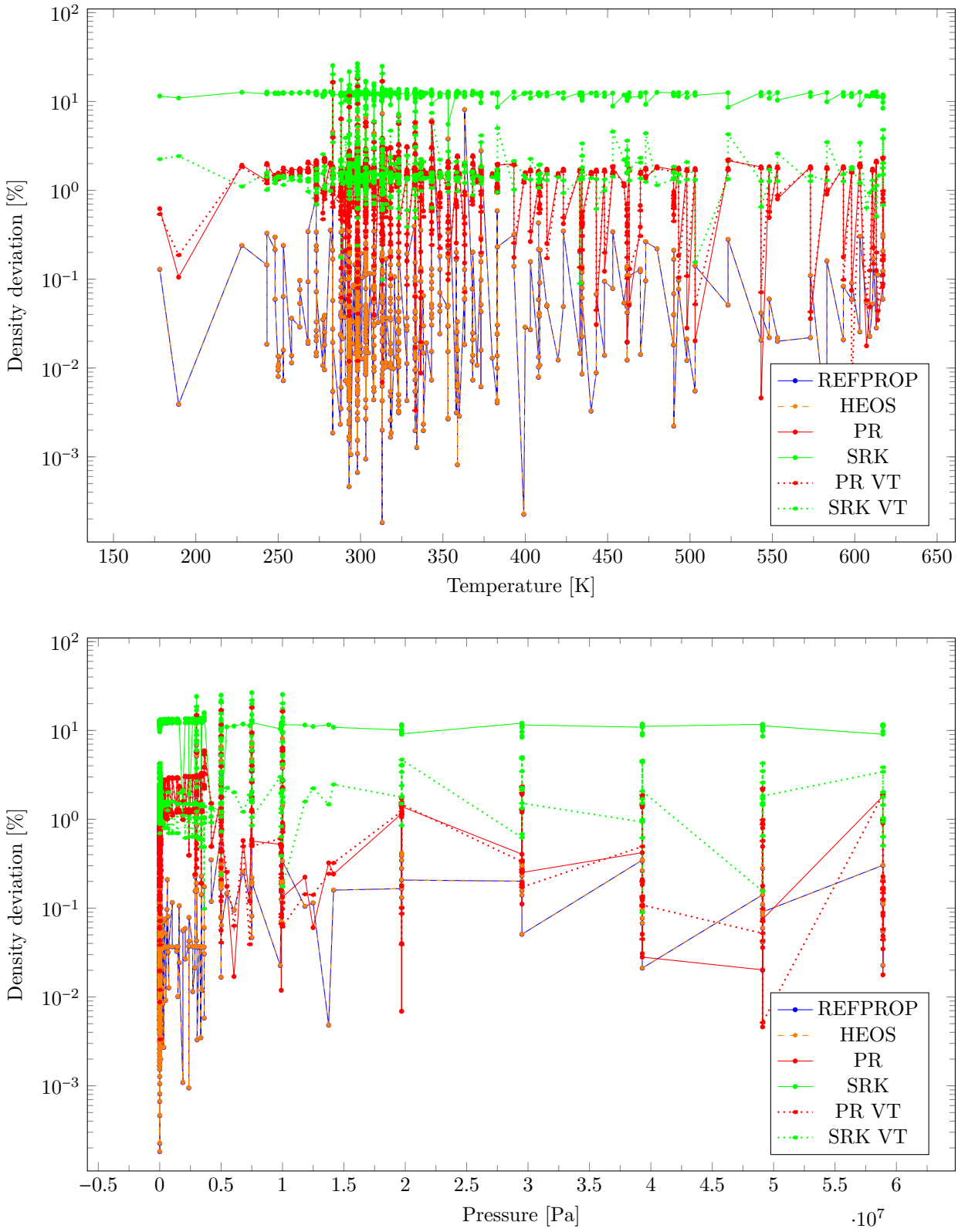


Figure 74: Density dependence on the temperature and pressure for fluid EthylBenzene

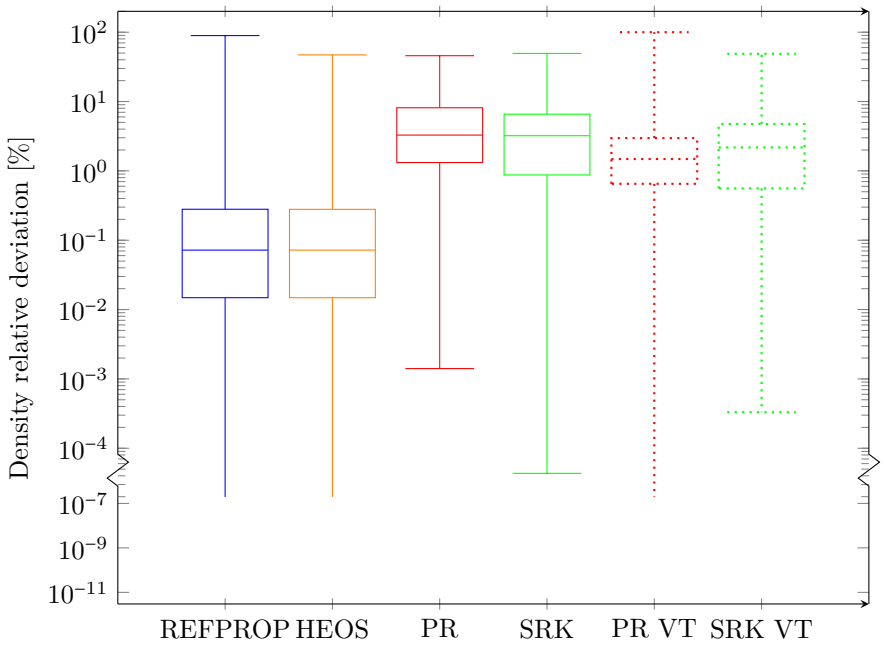


Figure 75: Relative density deviation to experimental data for fluid Ethylene

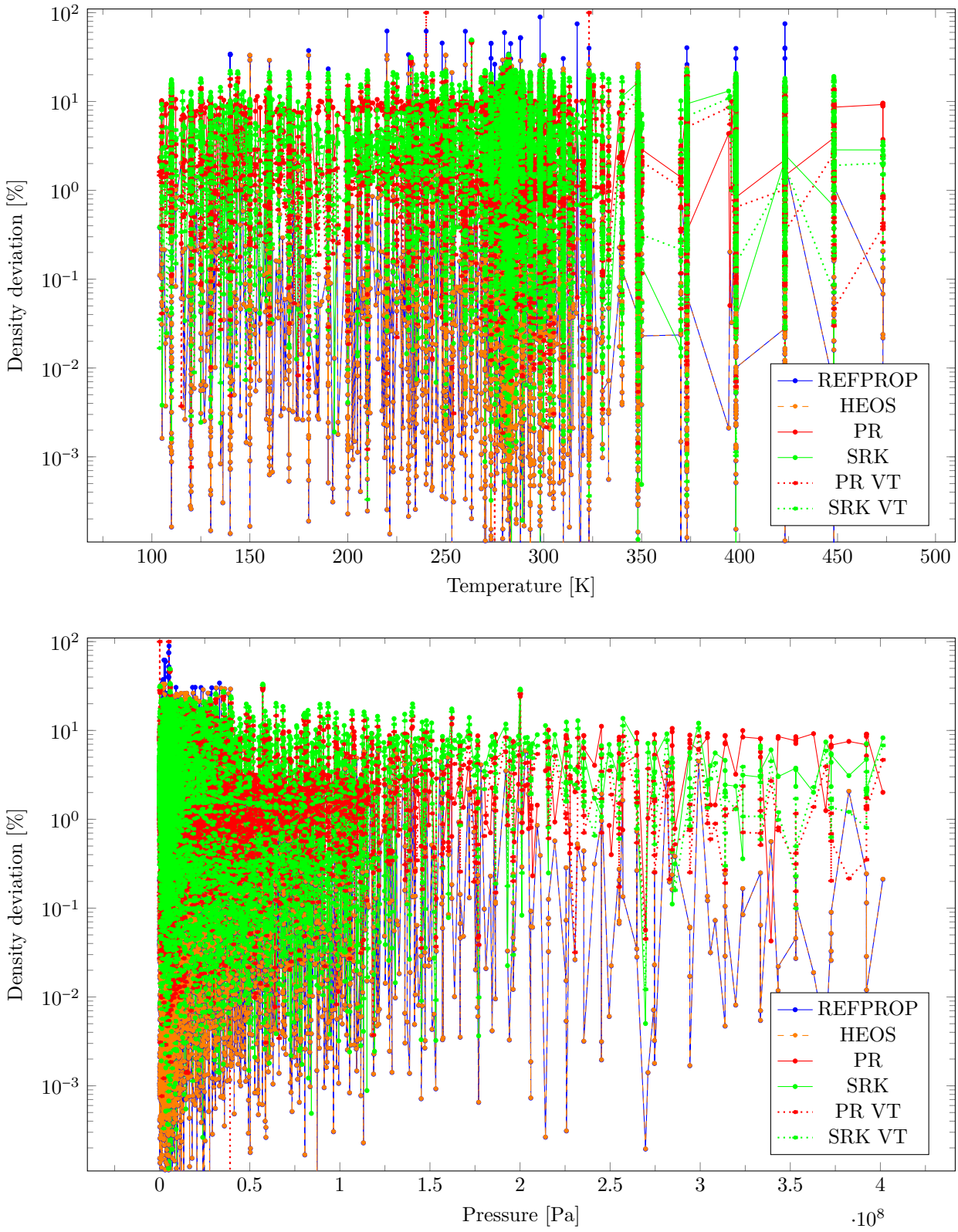


Figure 76: Density dependence on the temperature and pressure for fluid Ethylene

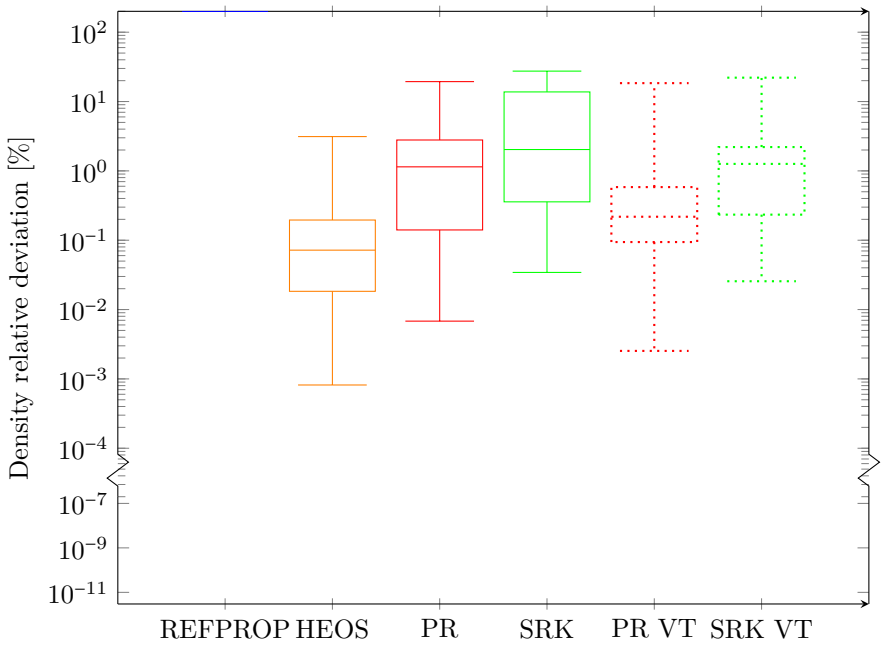


Figure 77: Relative density deviation to experimental data for fluid EthyleneOxide

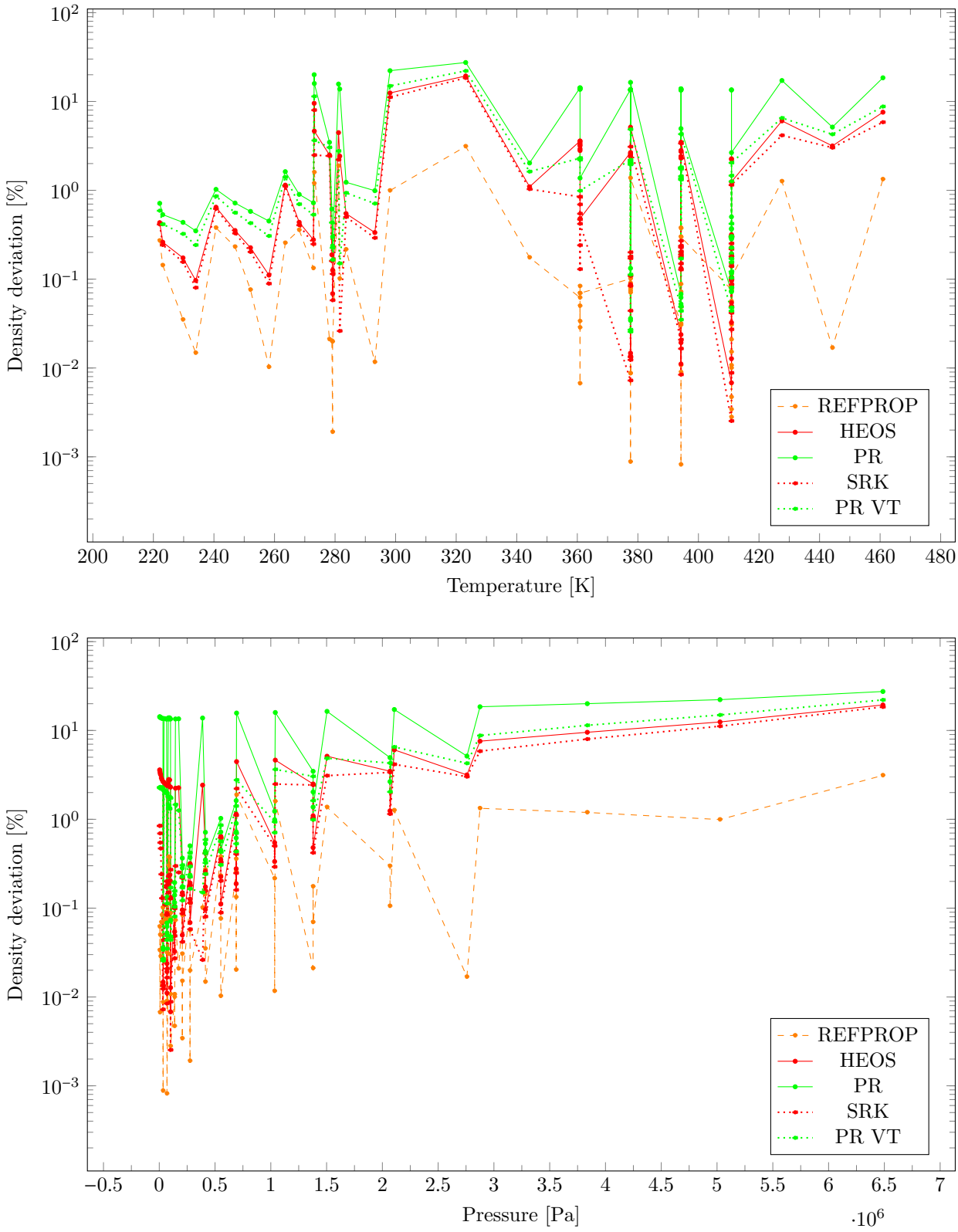


Figure 78: Density dependence on the temperature and pressure for fluid EthyleneOxide

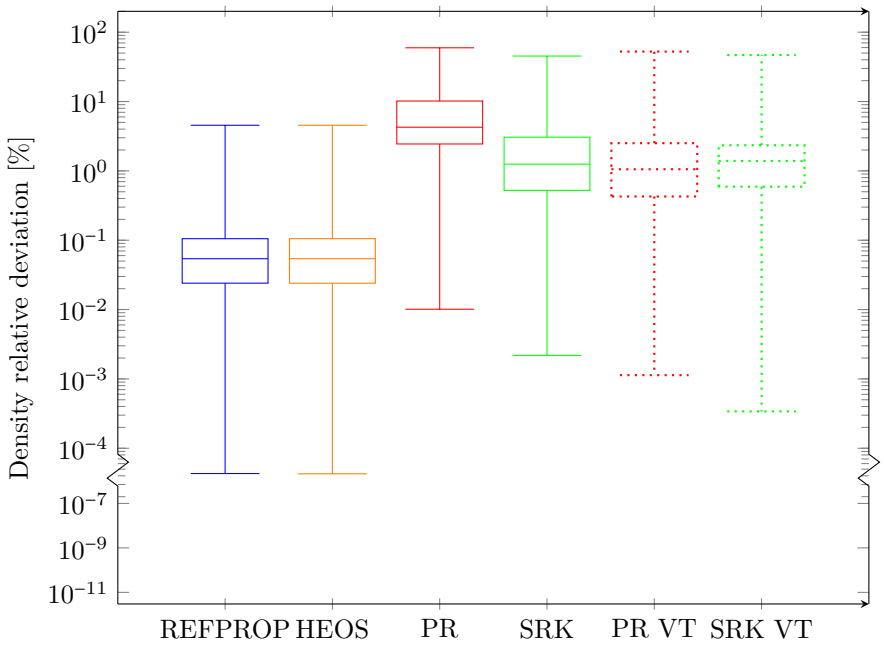


Figure 79: Relative density deviation to experimental data for fluid Fluorine

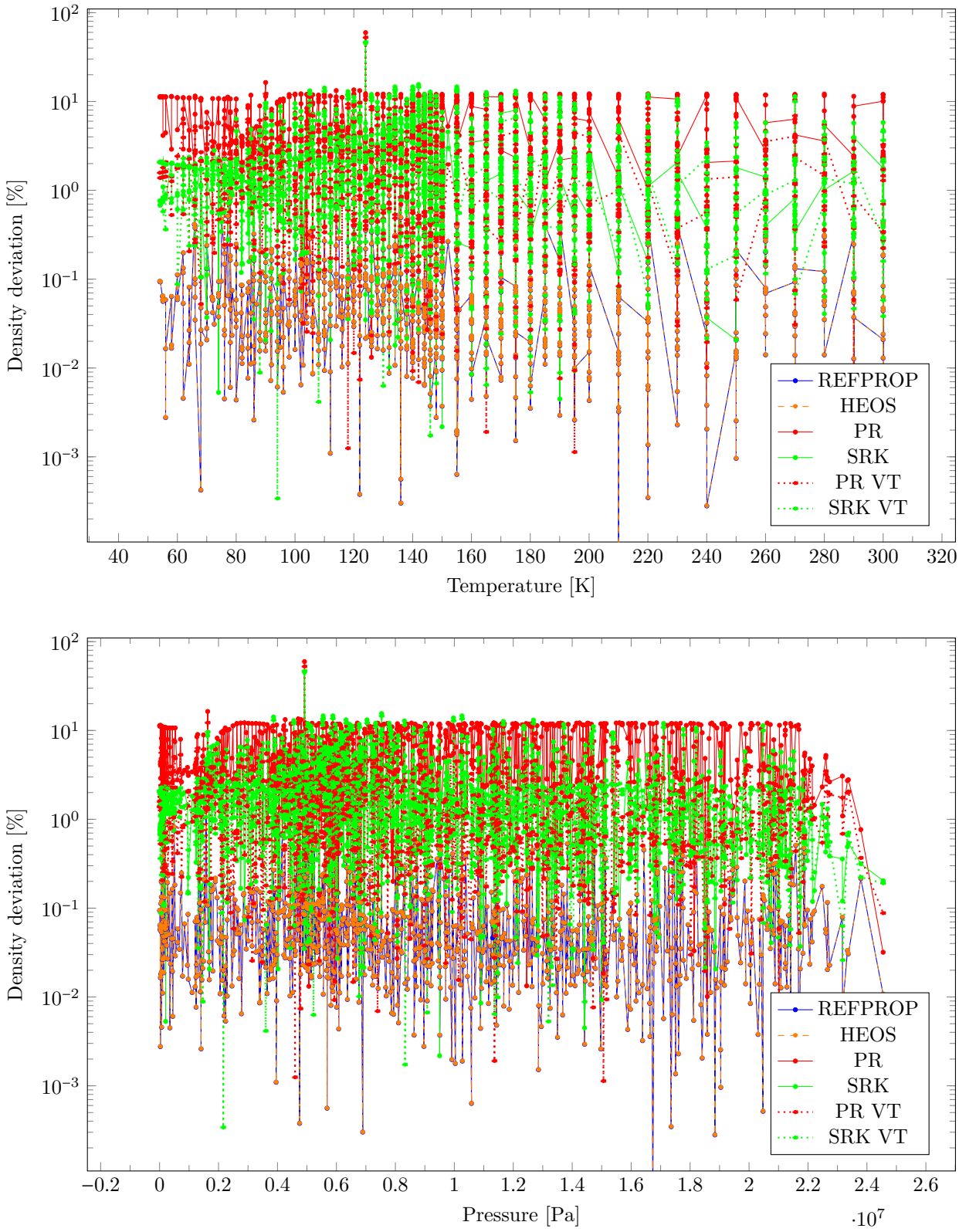


Figure 80: Density dependence on the temperature and pressure for fluid Fluorine

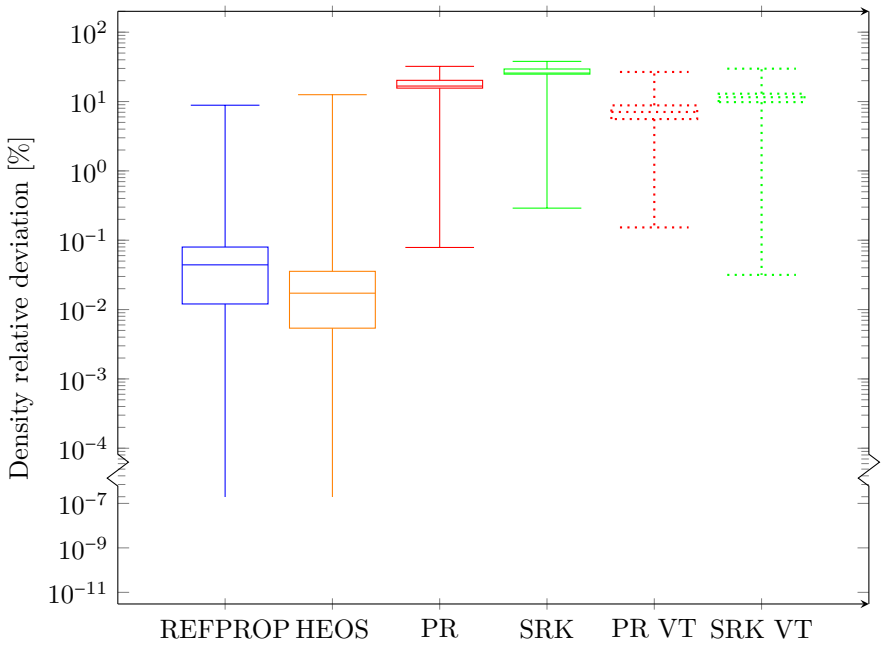


Figure 81: Relative density deviation to experimental data for fluid HeavyWater

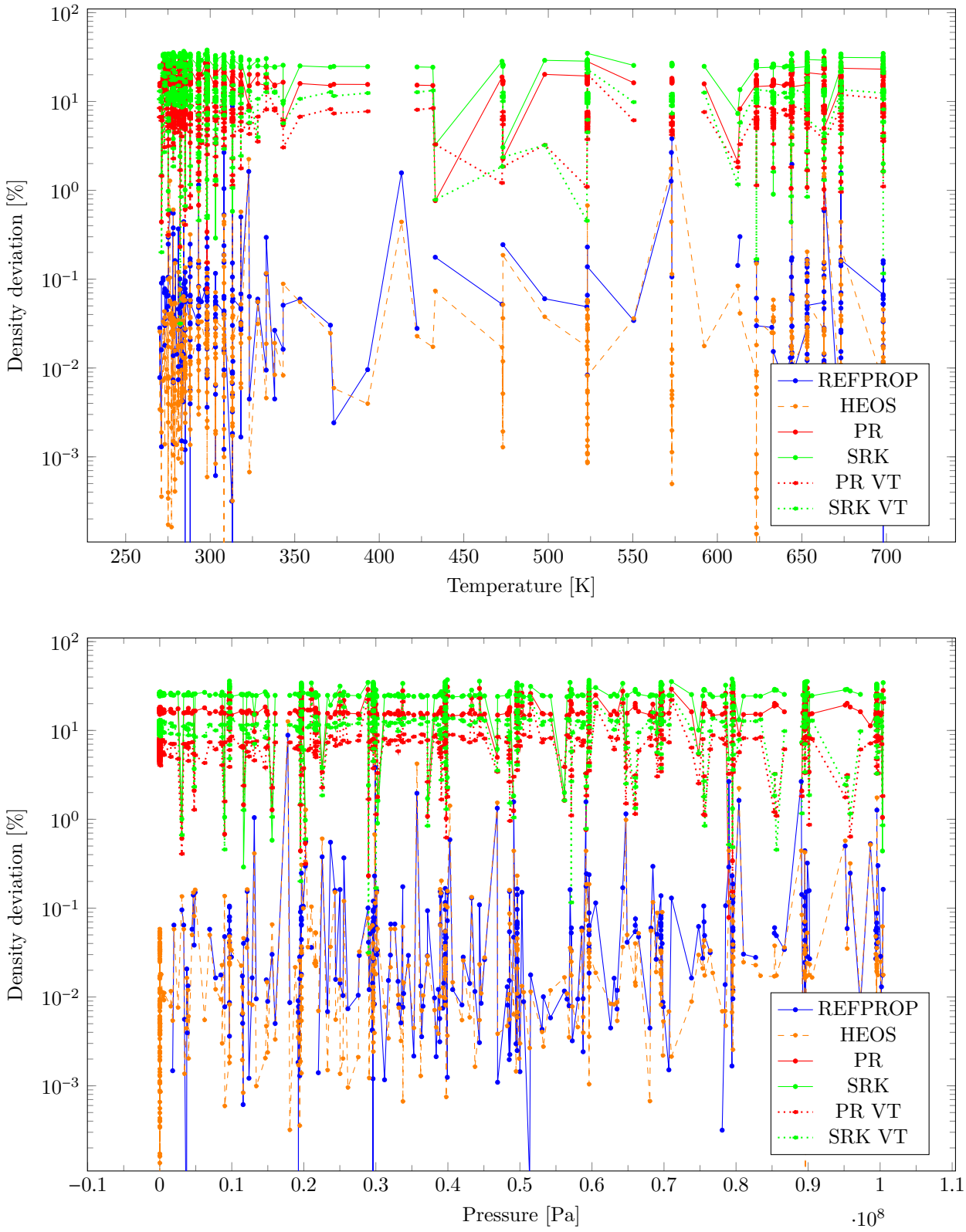


Figure 82: Density dependence on the temperature and pressure for fluid HeavyWater

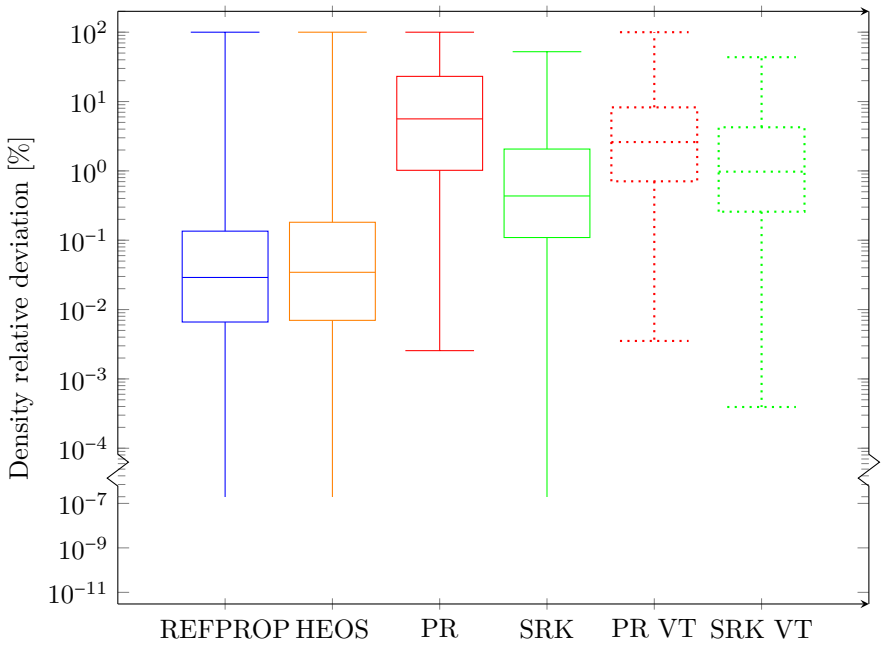


Figure 83: Relative density deviation to experimental data for fluid Helium

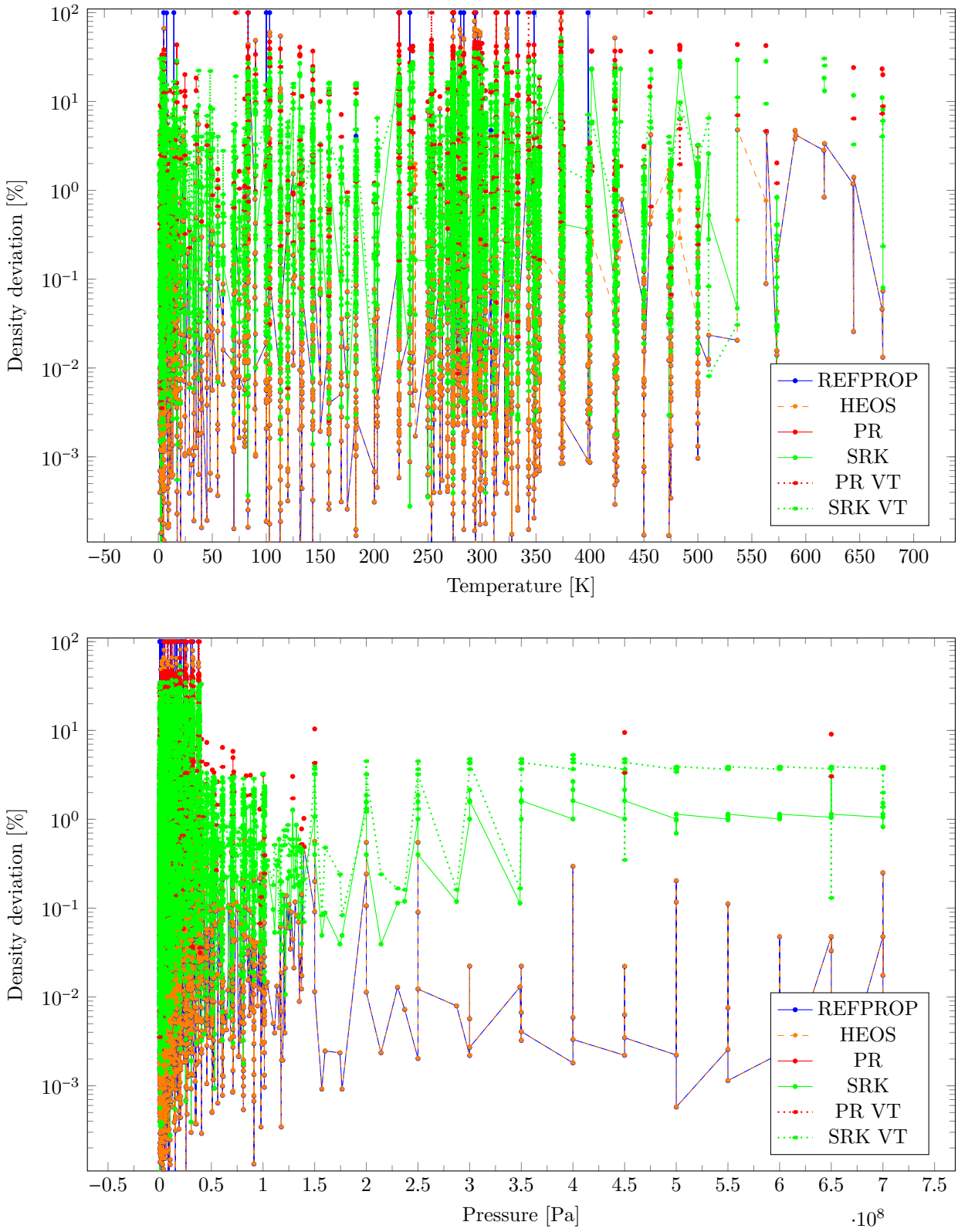


Figure 84: Density dependence on the temperature and pressure for fluid Helium

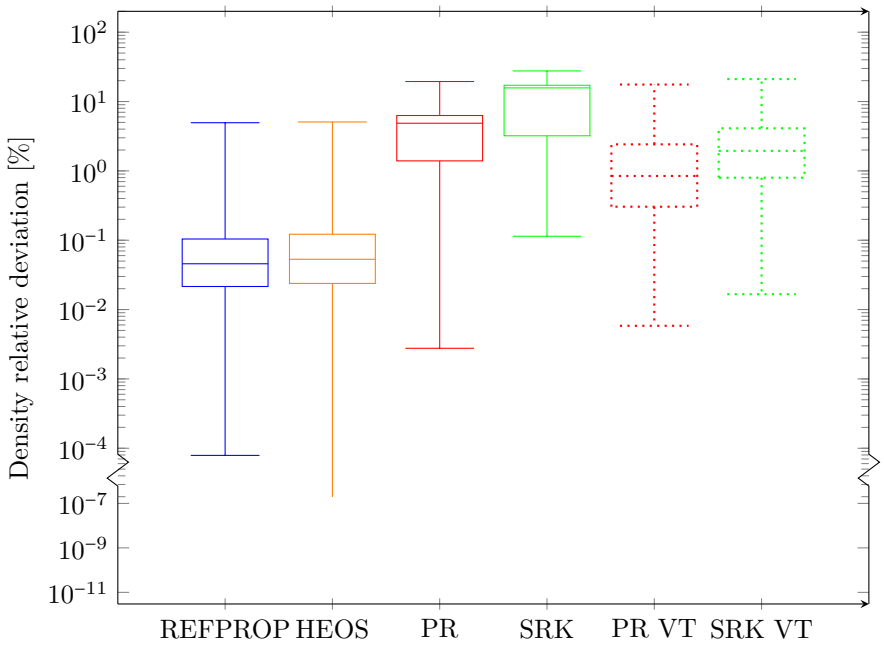


Figure 85: Relative density deviation to experimental data for fluid HFE143M

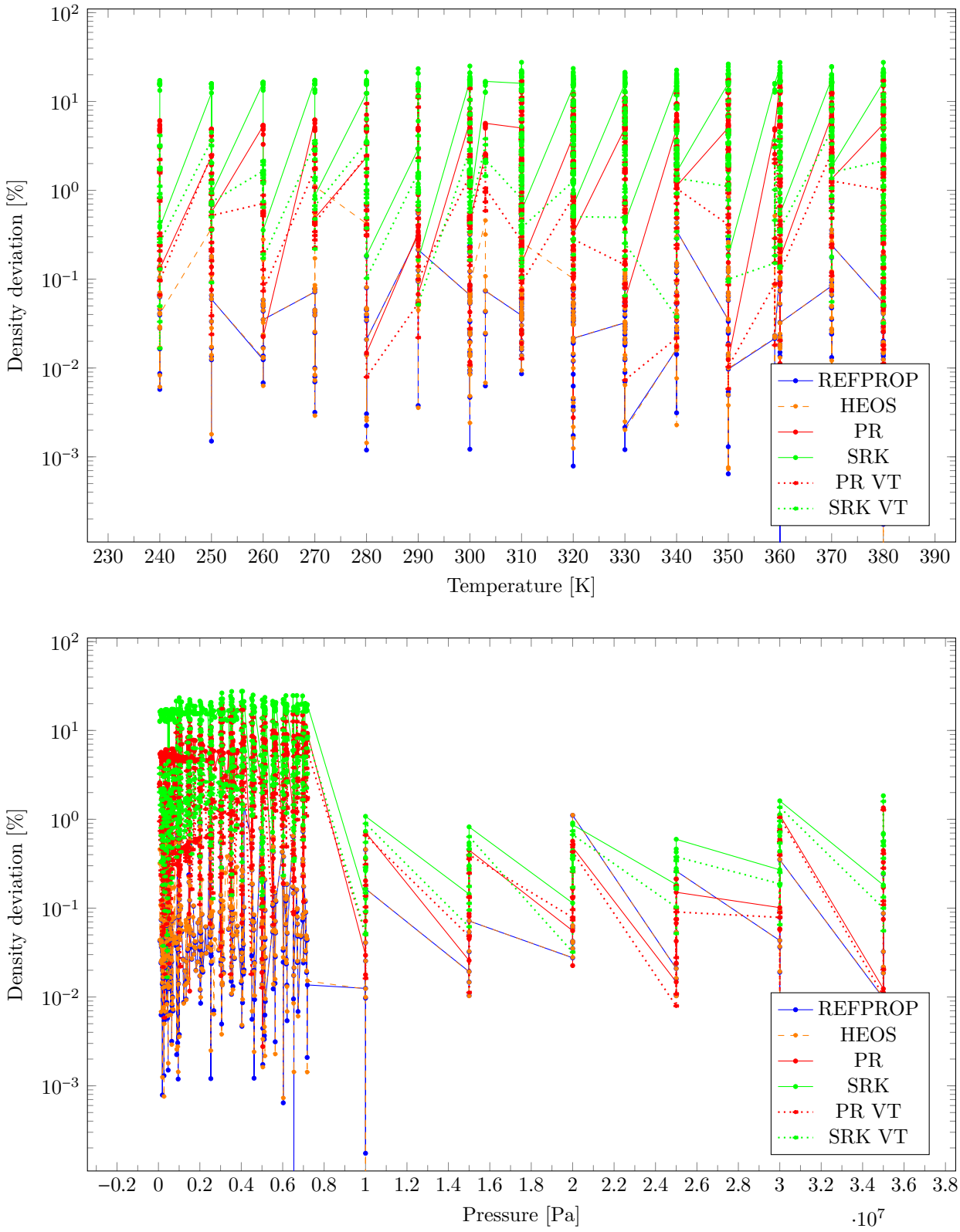


Figure 86: Density dependence on the temperature and pressure for fluid HFE143M

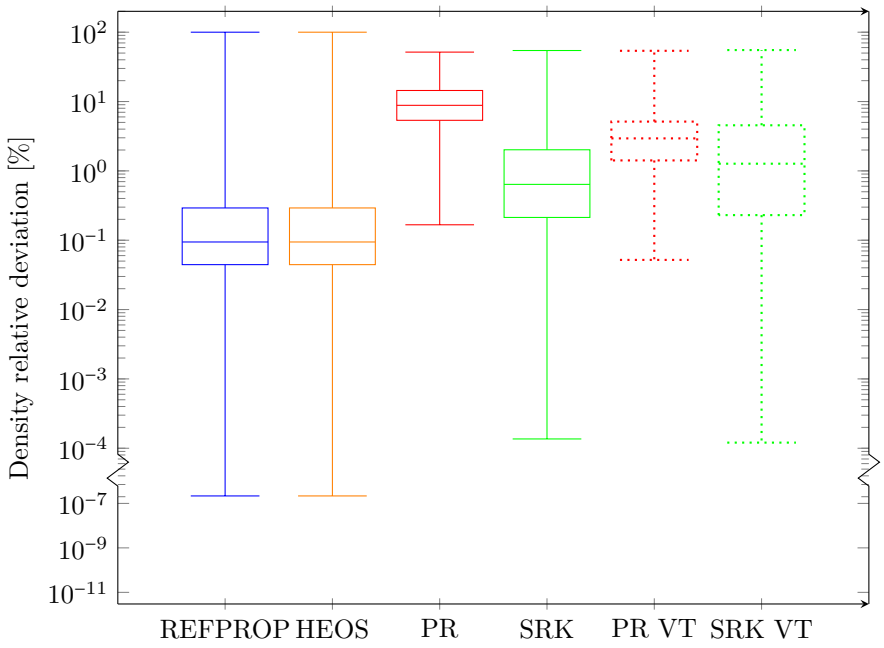


Figure 87: Relative density deviation to experimental data for fluid Hydrogen

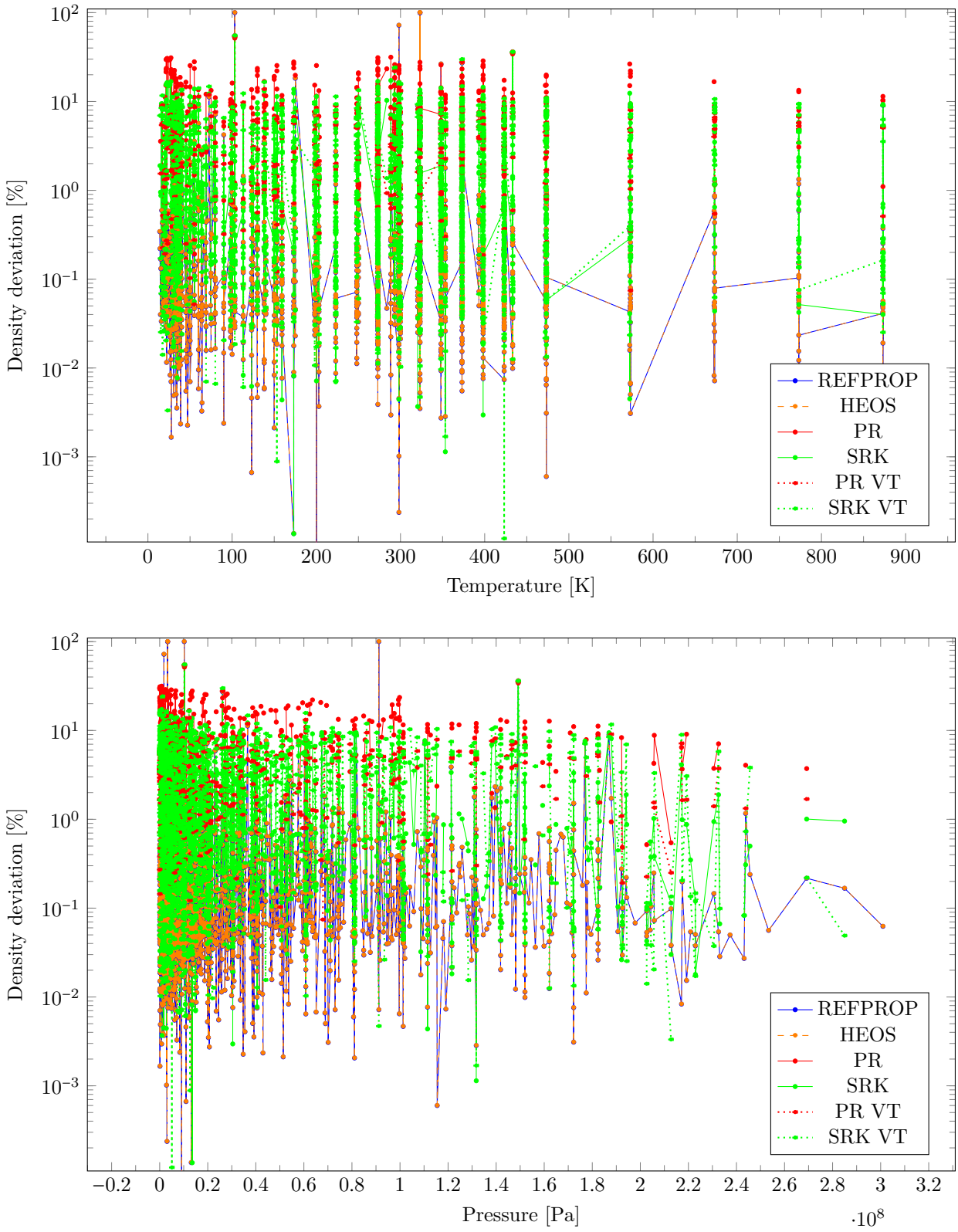


Figure 88: Density dependence on the temperature and pressure for fluid Hydrogen

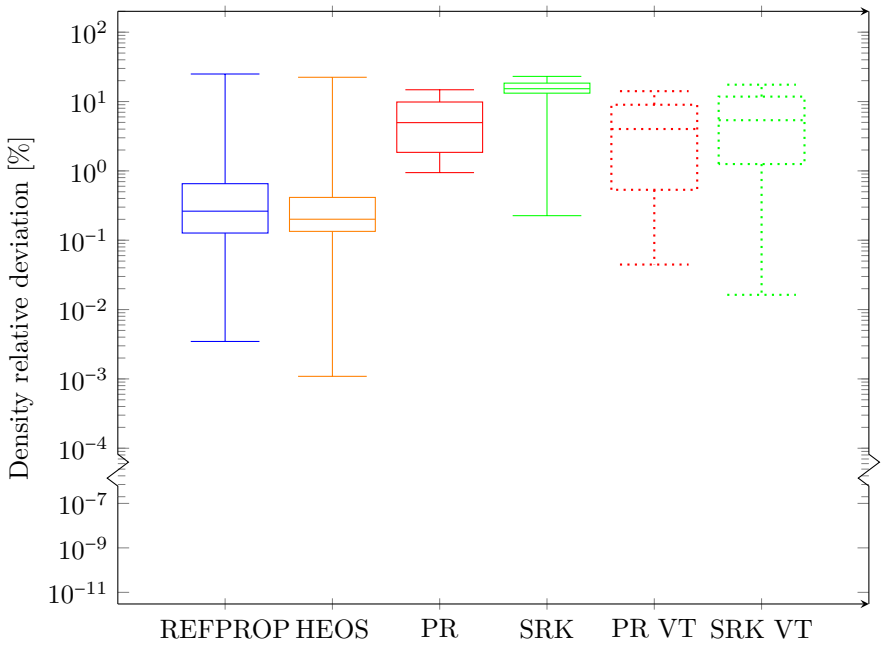


Figure 89: Relative density deviation to experimental data for fluid HydrogenChloride

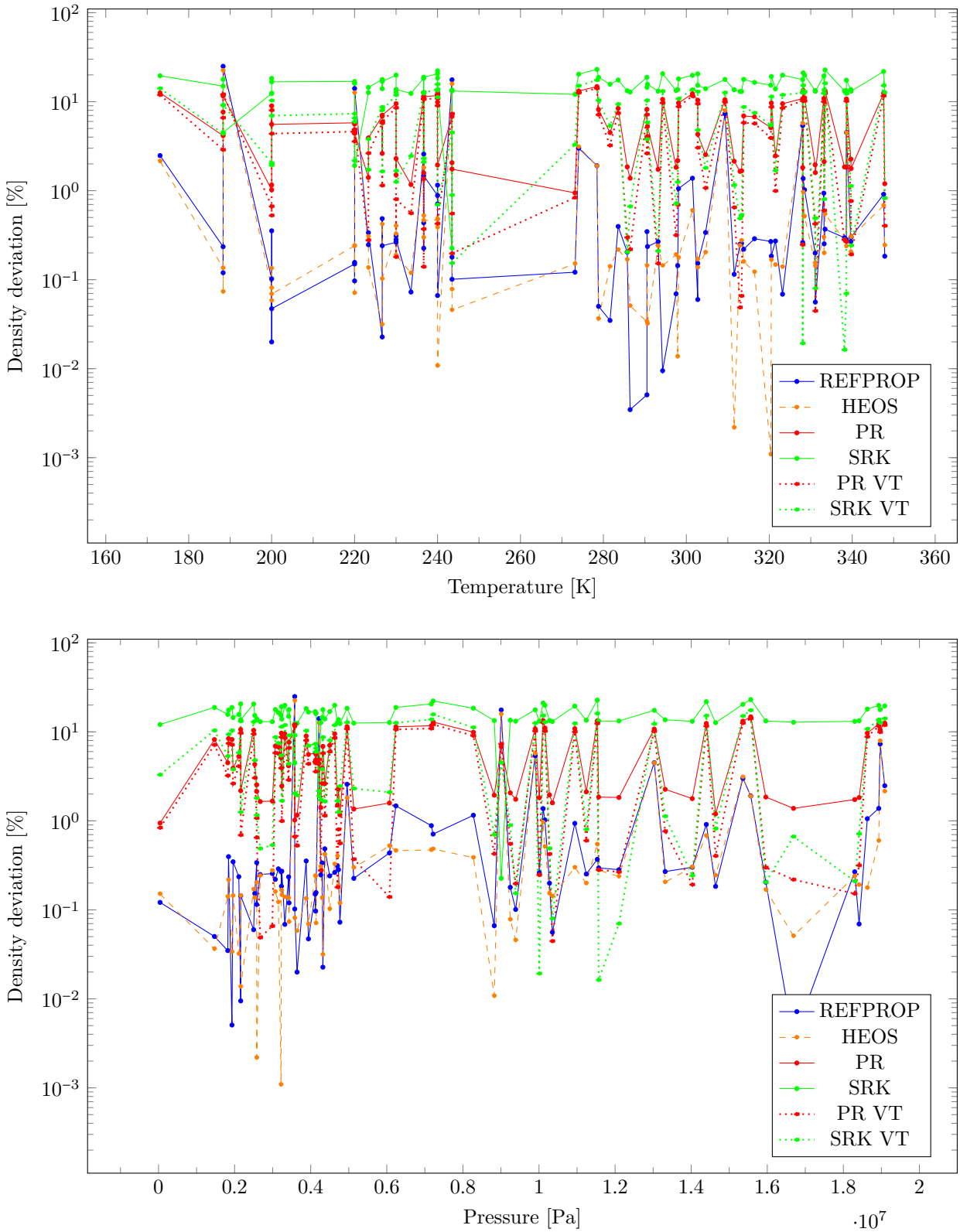


Figure 90: Density dependence on the temperature and pressure for fluid HydrogenChloride

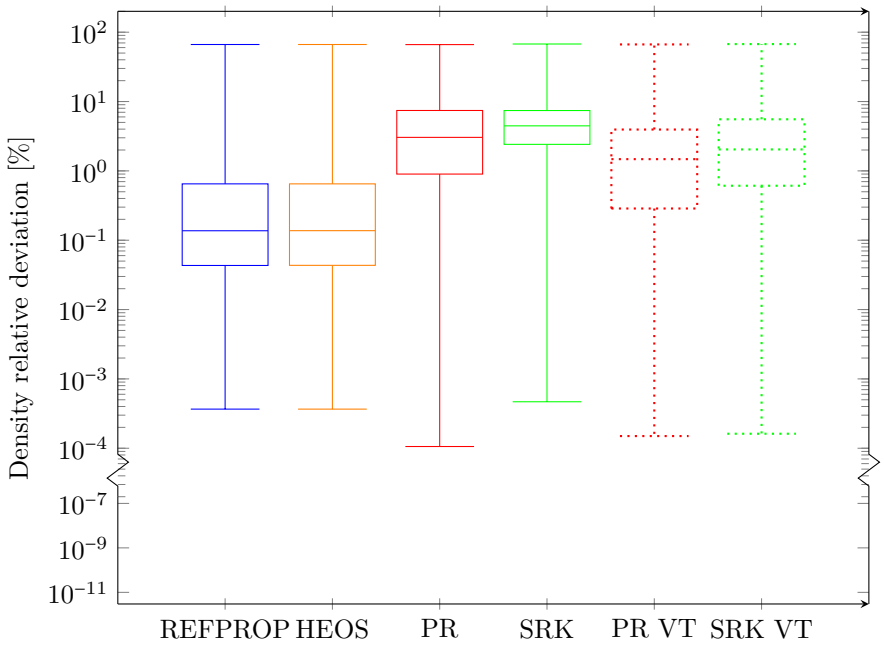


Figure 91: Relative density deviation to experimental data for fluid HydrogenSulfide

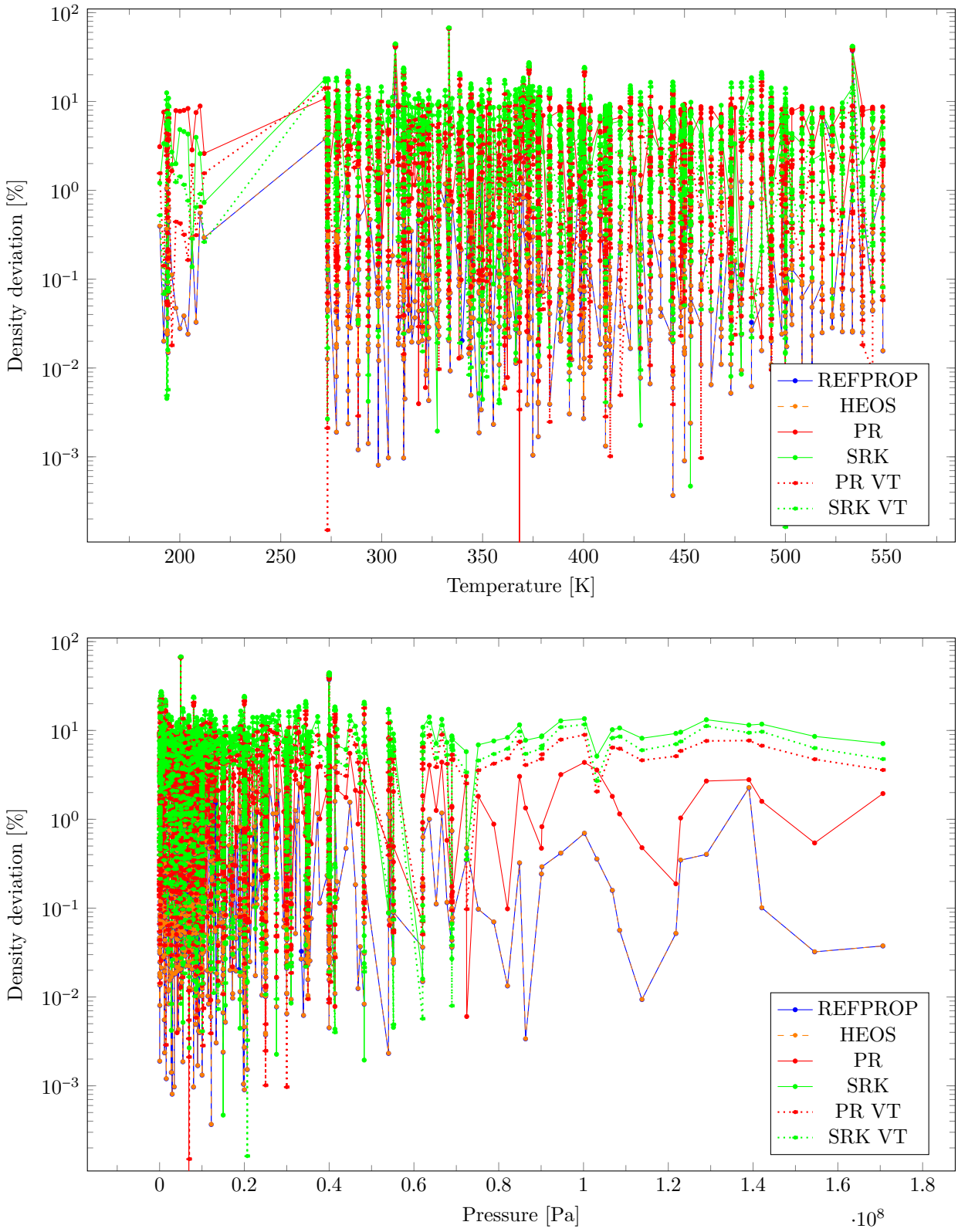


Figure 92: Density dependence on the temperature and pressure for fluid HydrogenSulfide

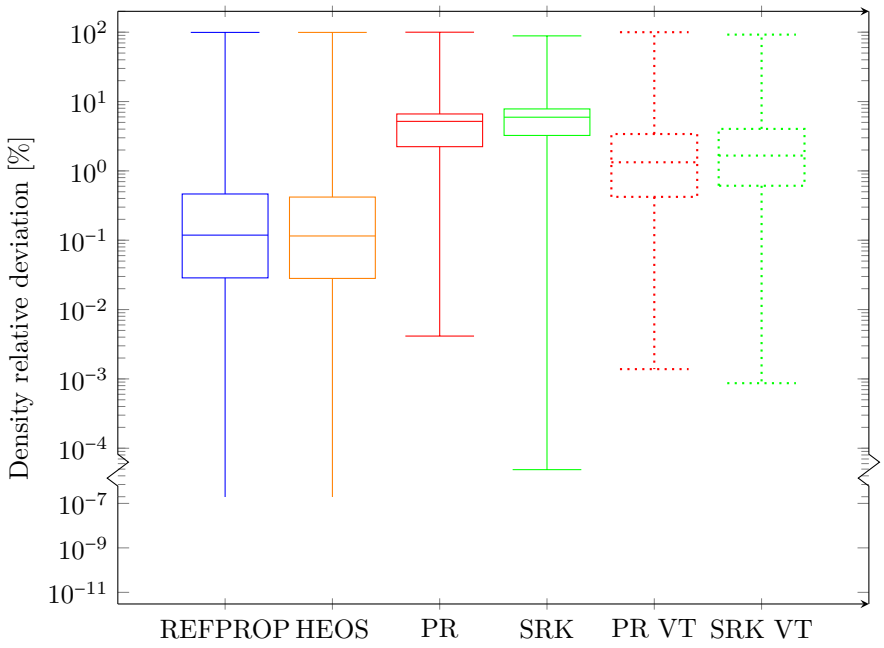


Figure 93: Relative density deviation to experimental data for fluid IsoButane

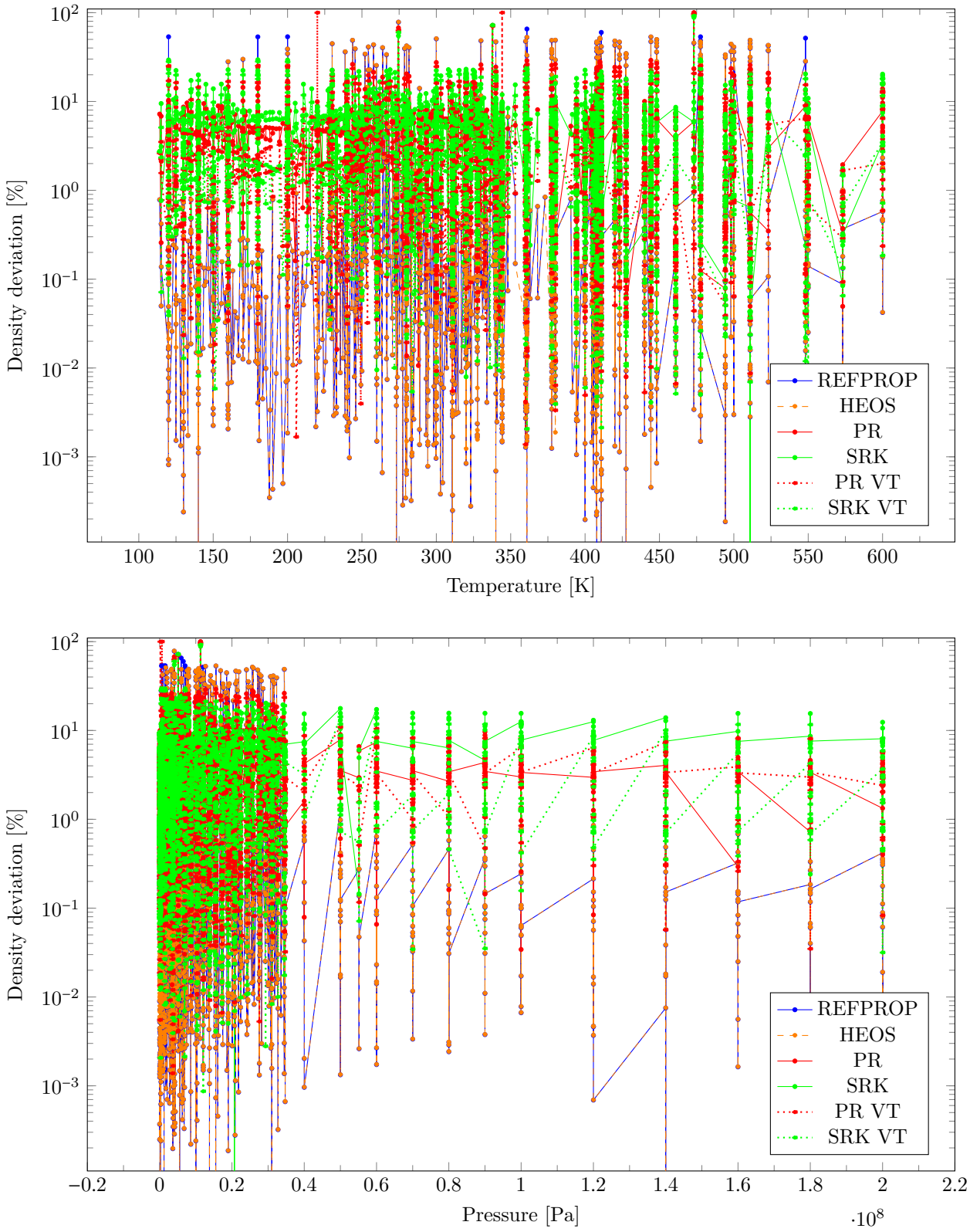


Figure 94: Density dependence on the temperature and pressure for fluid IsoButane

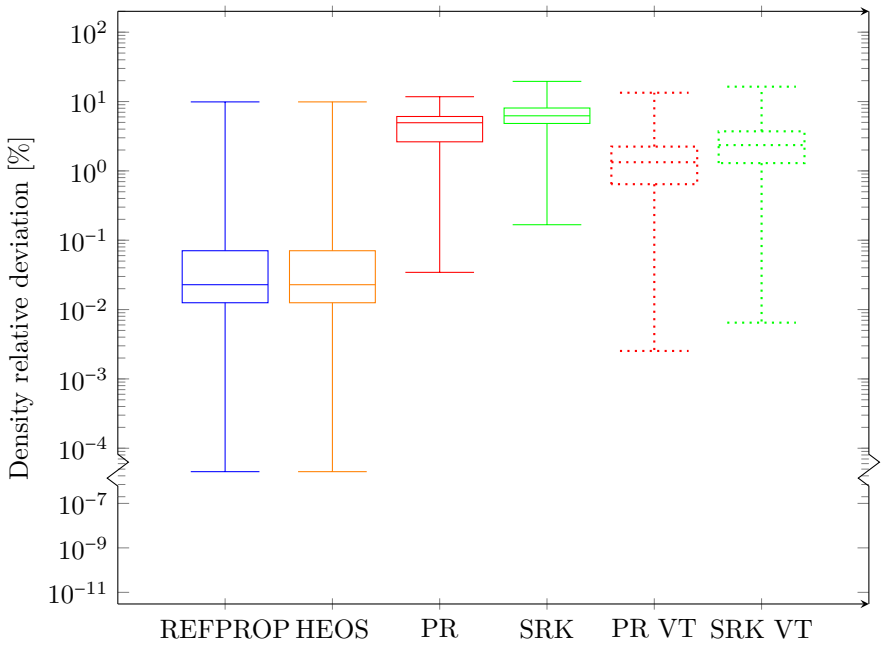


Figure 95: Relative density deviation to experimental data for fluid IsoButene

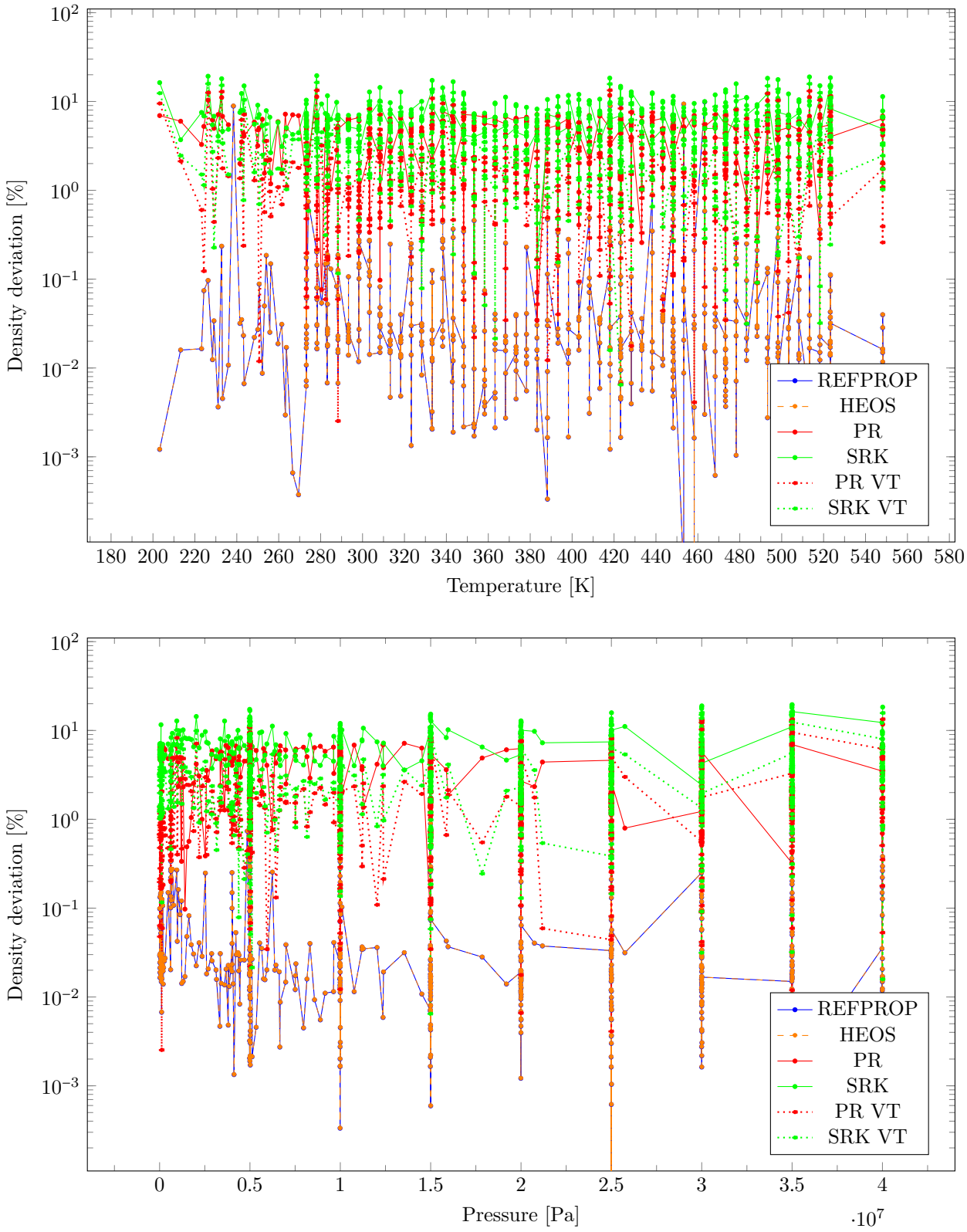


Figure 96: Density dependence on the temperature and pressure for fluid IsoButene

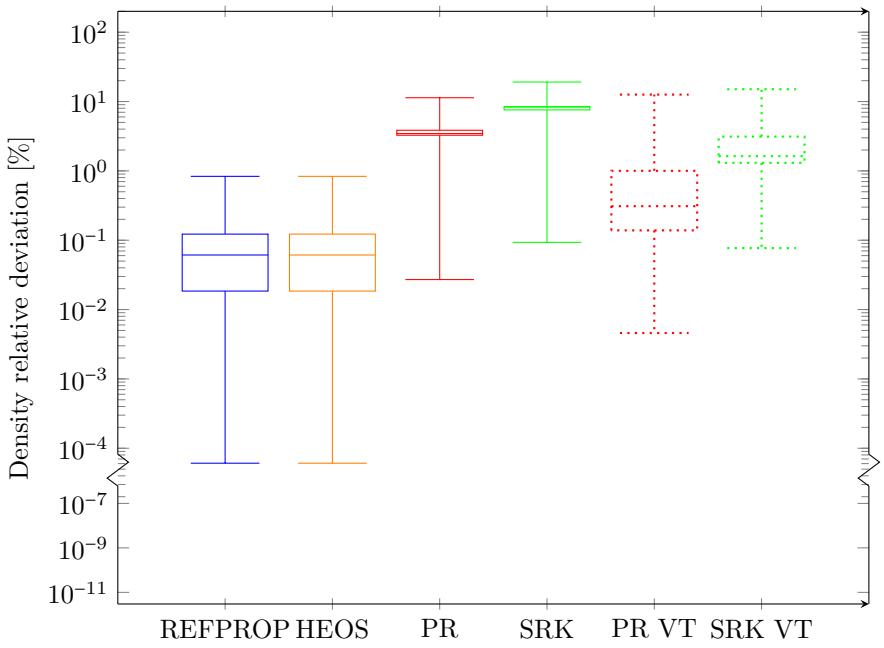


Figure 97: Relative density deviation to experimental data for fluid Isohexane

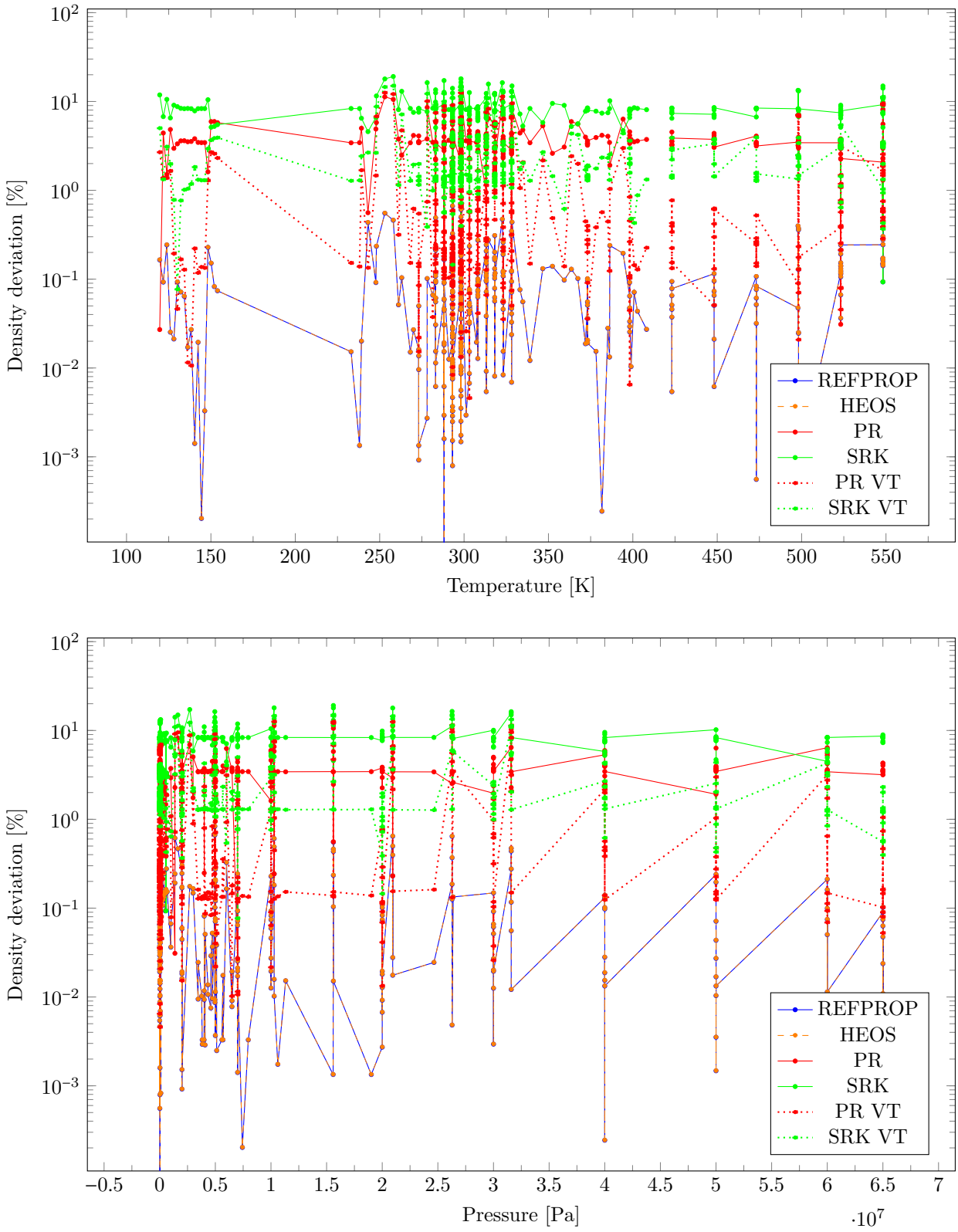


Figure 98: Density dependence on the temperature and pressure for fluid Isohexane

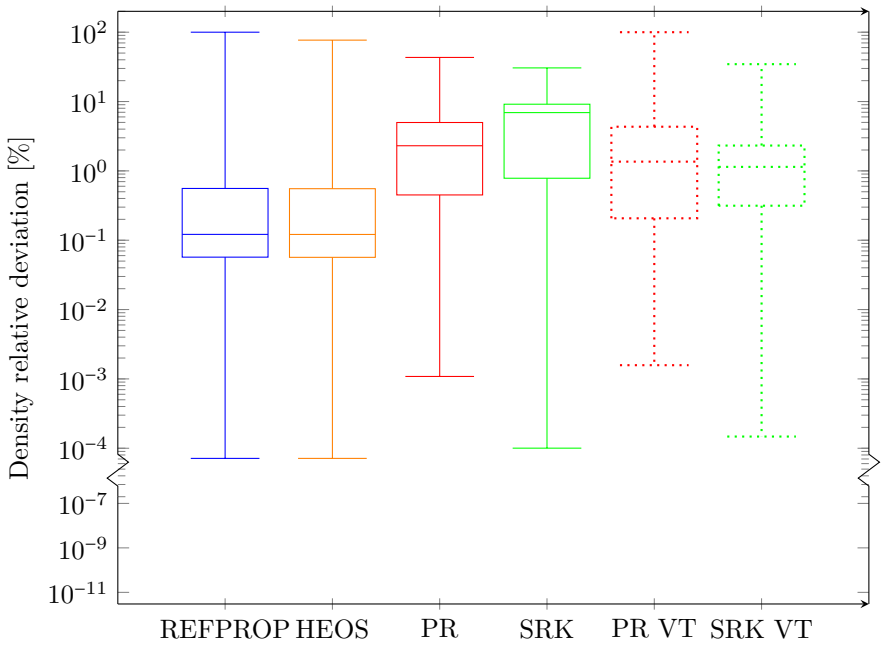


Figure 99: Relative density deviation to experimental data for fluid Isopentane

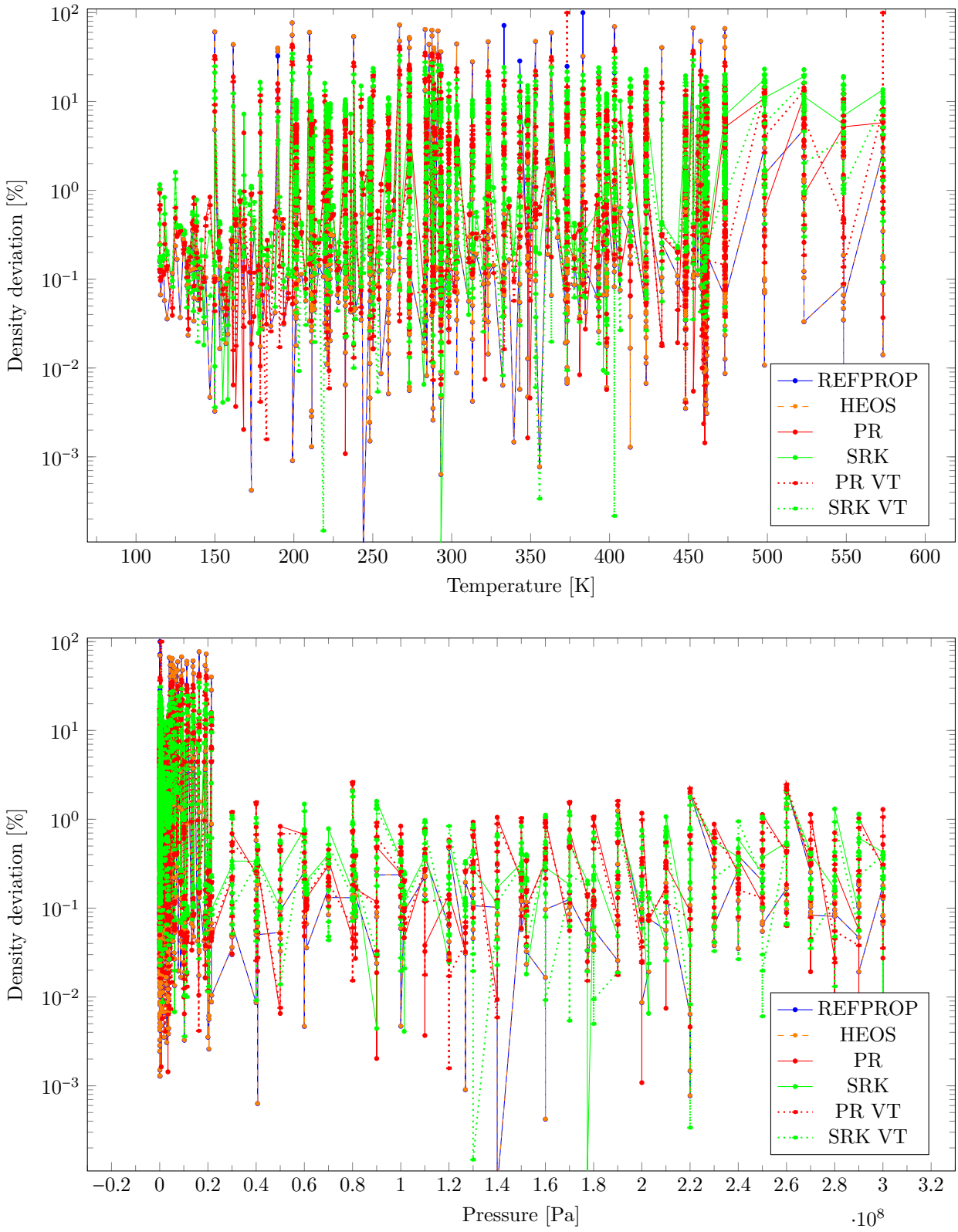


Figure 100: Density dependence on the temperature and pressure for fluid Isopentane

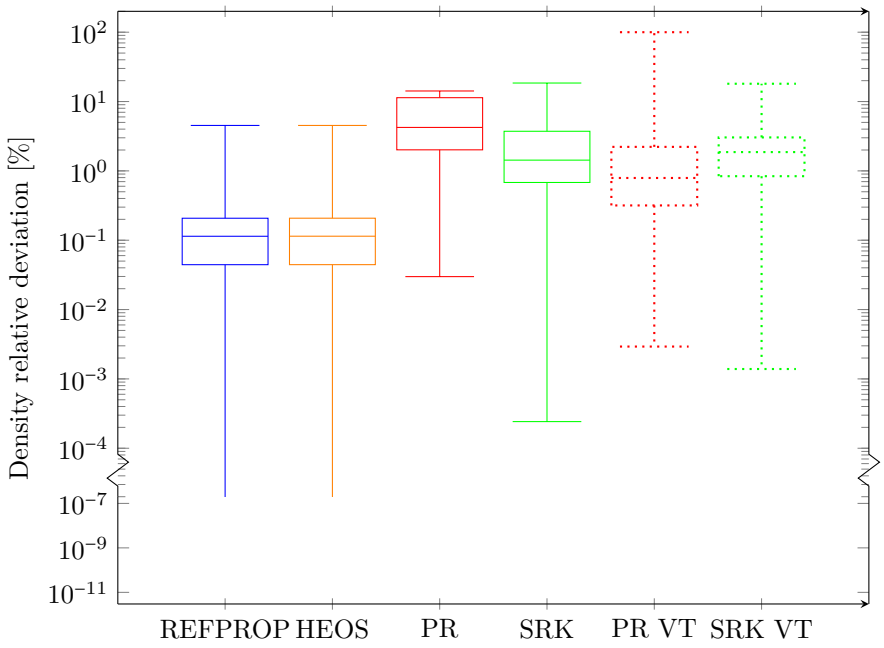


Figure 101: Relative density deviation to experimental data for fluid Krypton

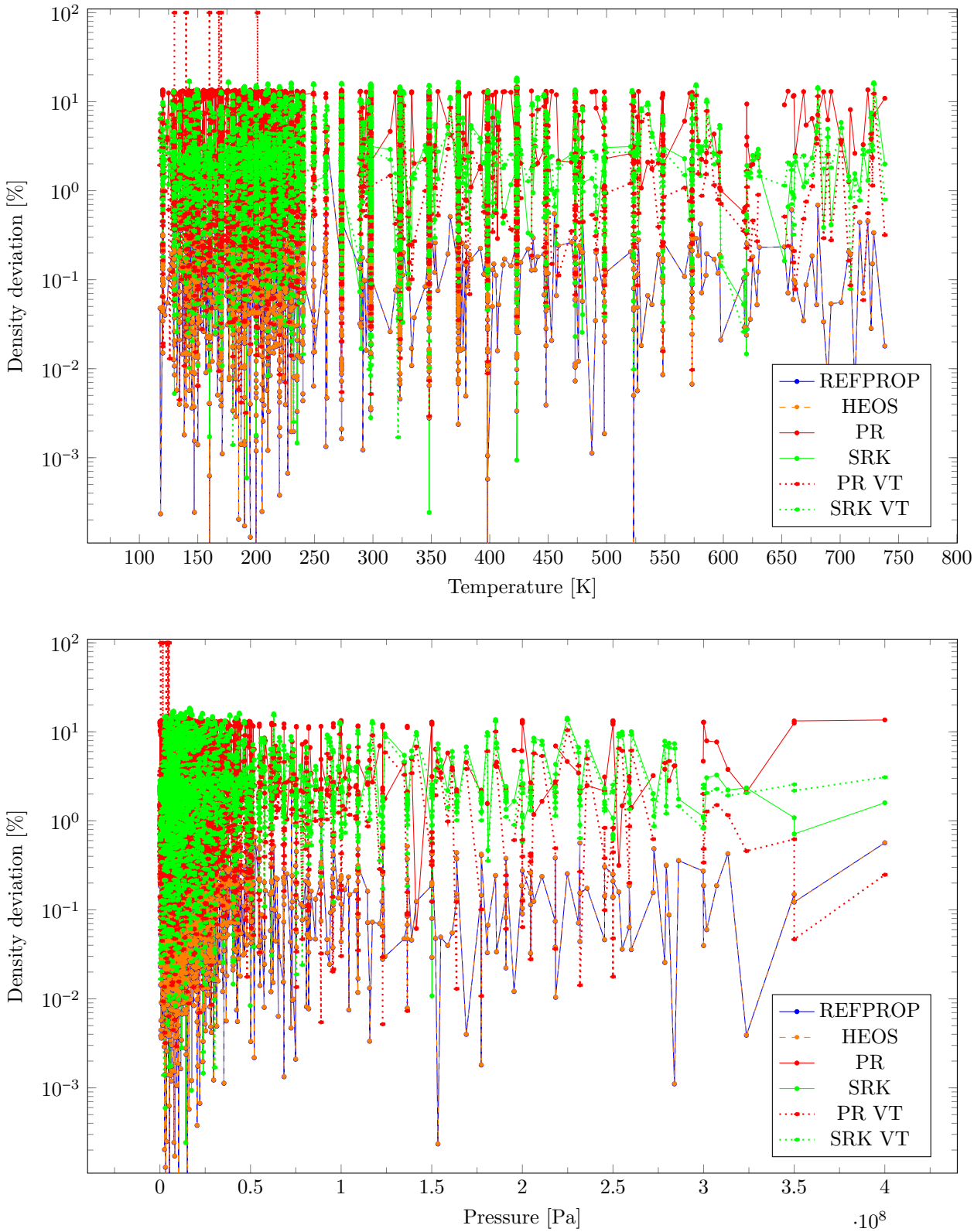


Figure 102: Density dependence on the temperature and pressure for fluid Krypton

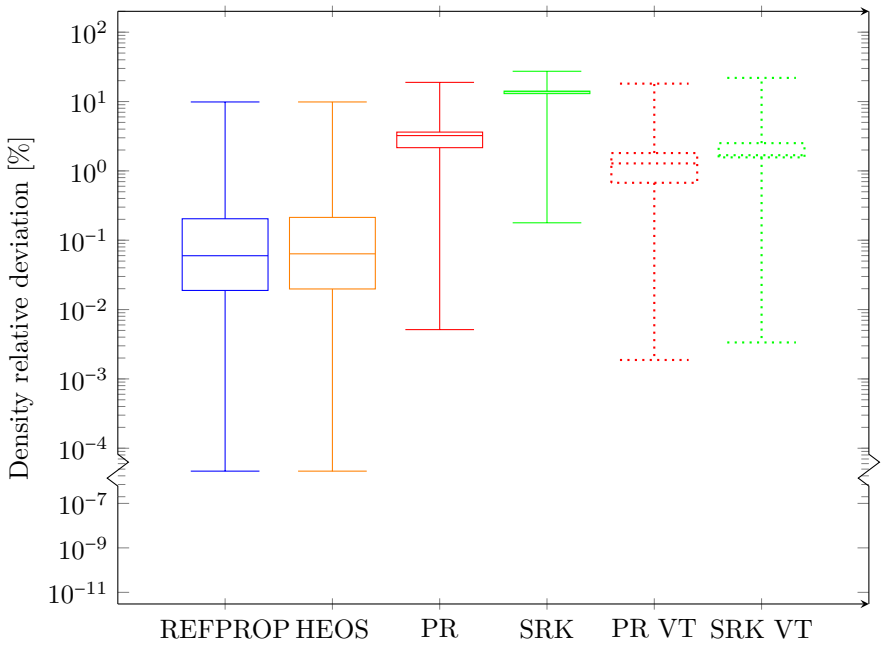


Figure 103: Relative density deviation to experimental data for fluid m-Xylene

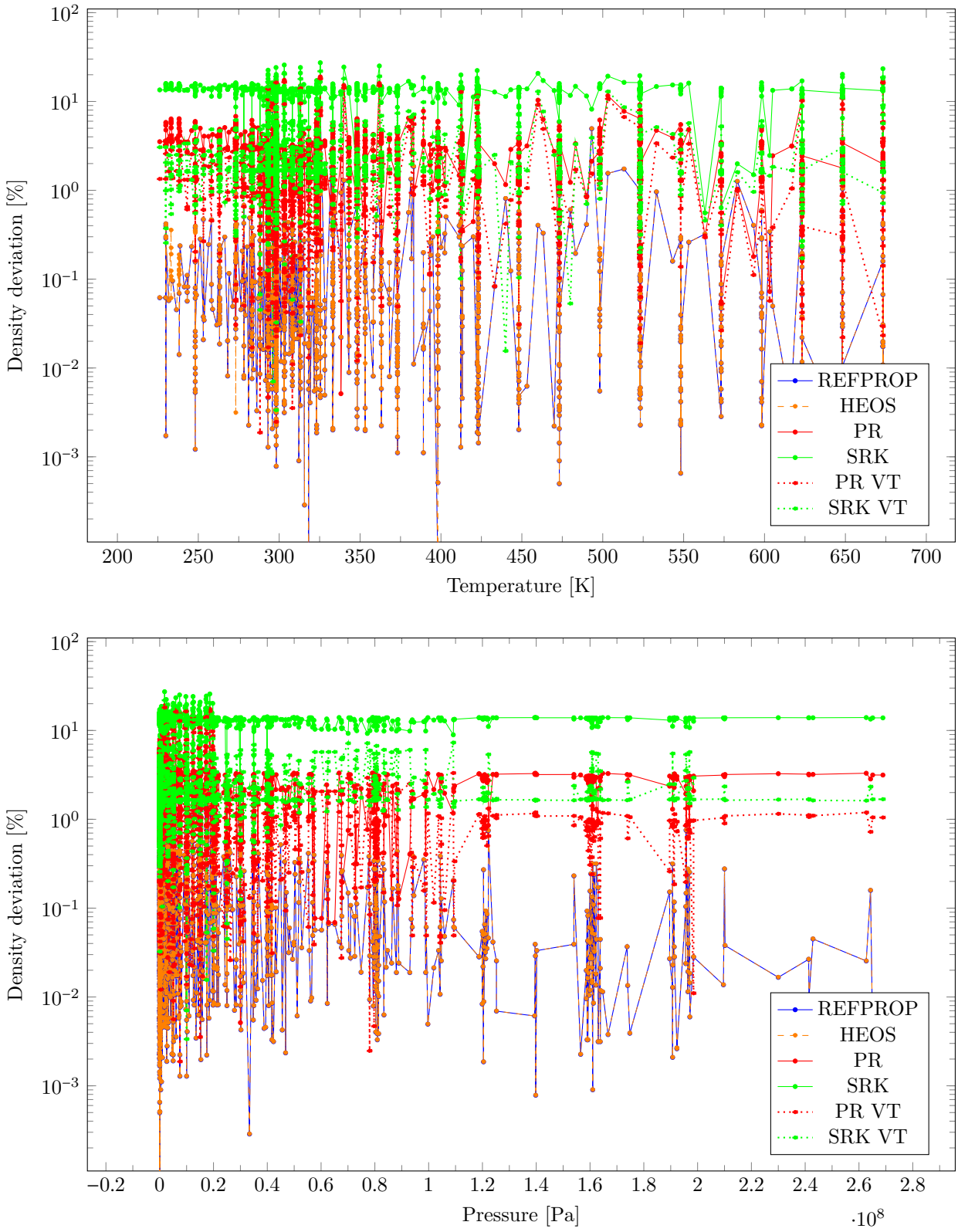


Figure 104: Density dependence on the temperature and pressure for fluid m-Xylene

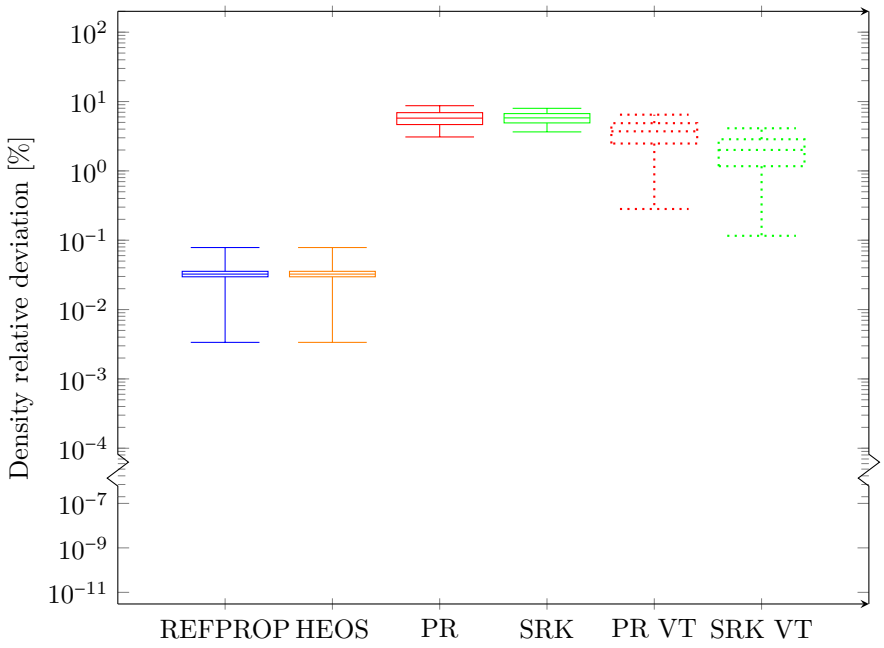


Figure 105: Relative density deviation to experimental data for fluid MD2M

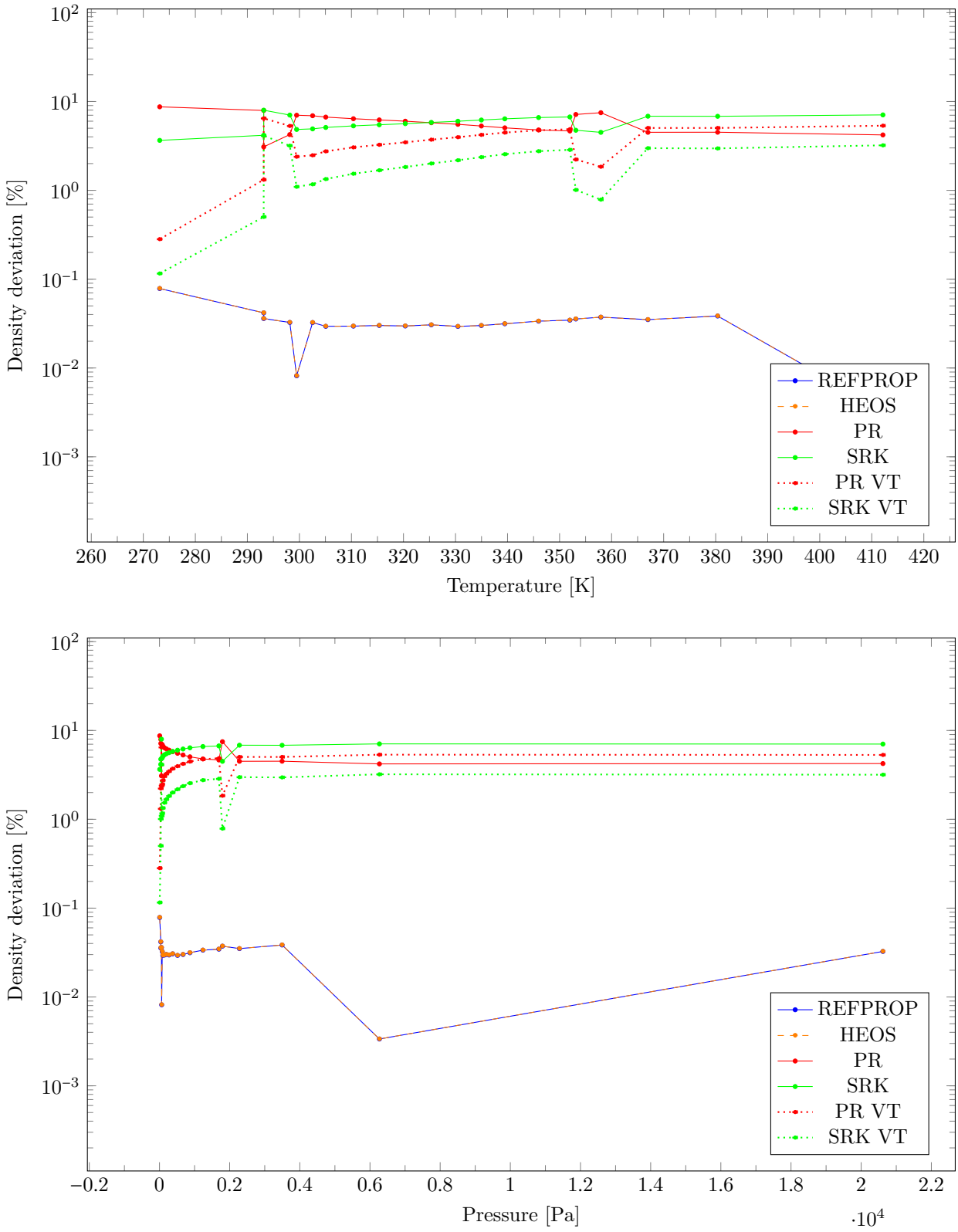


Figure 106: Density dependence on the temperature and pressure for fluid MD2M

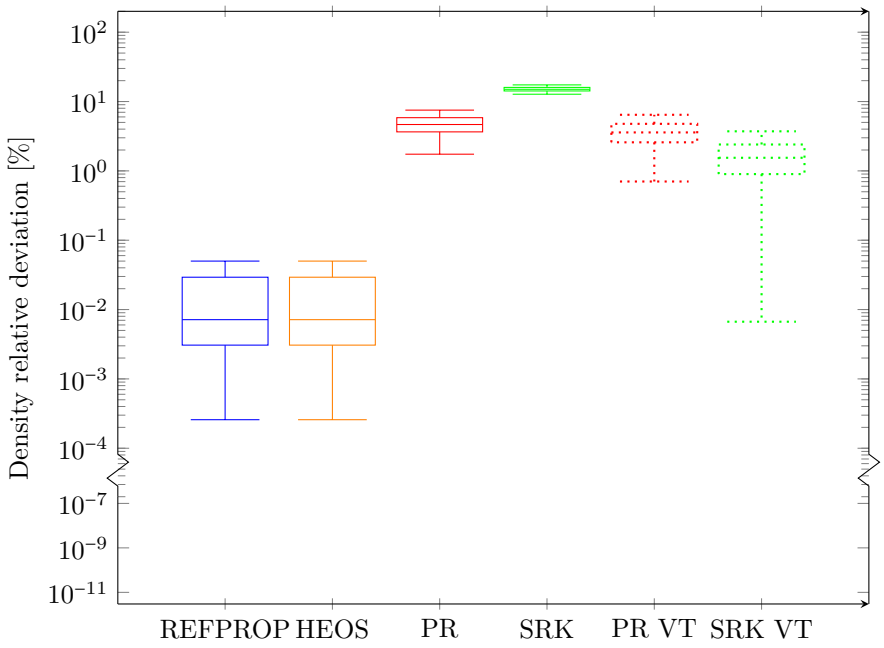


Figure 107: Relative density deviation to experimental data for fluid MD3M

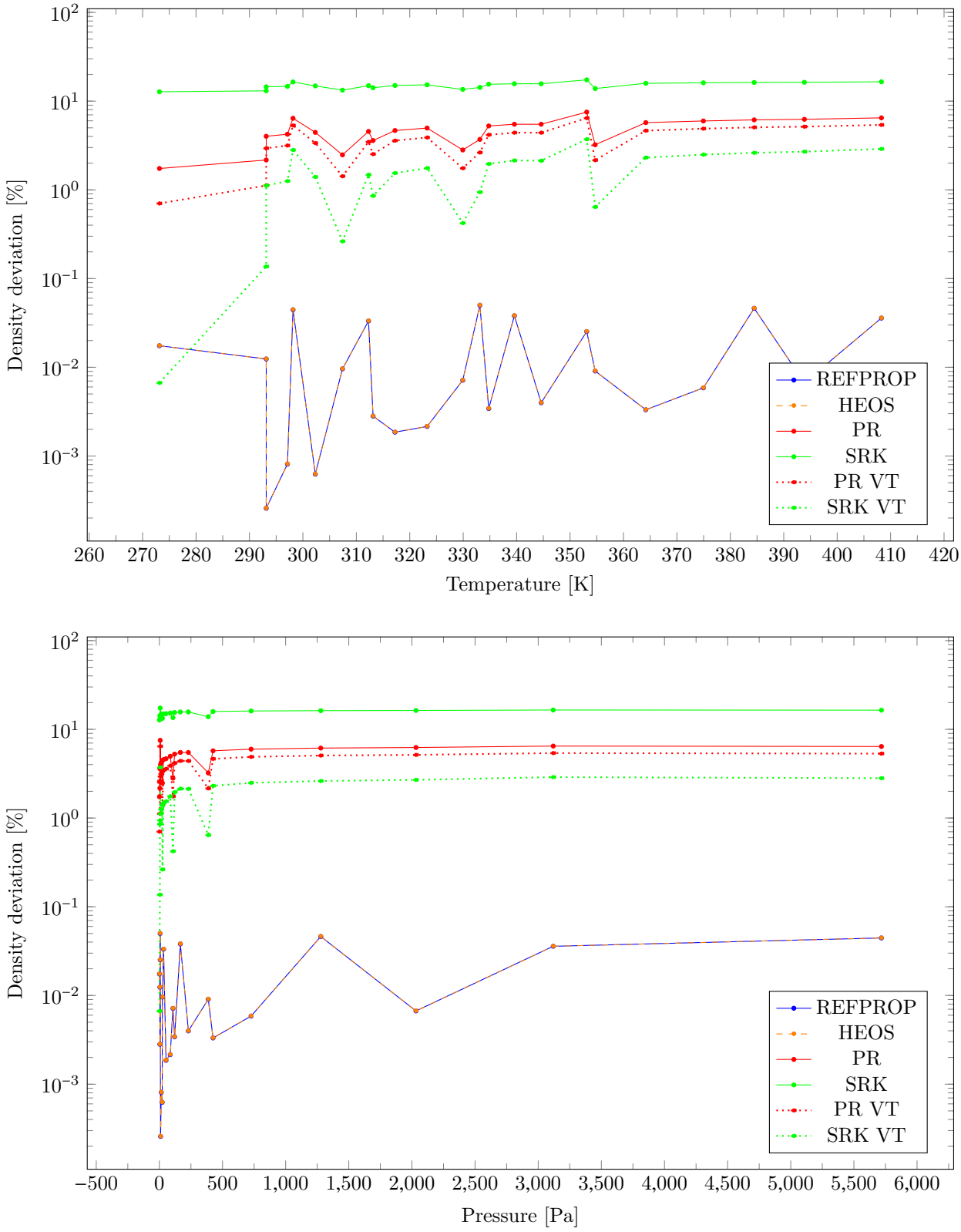


Figure 108: Density dependence on the temperature and pressure for fluid MD3M

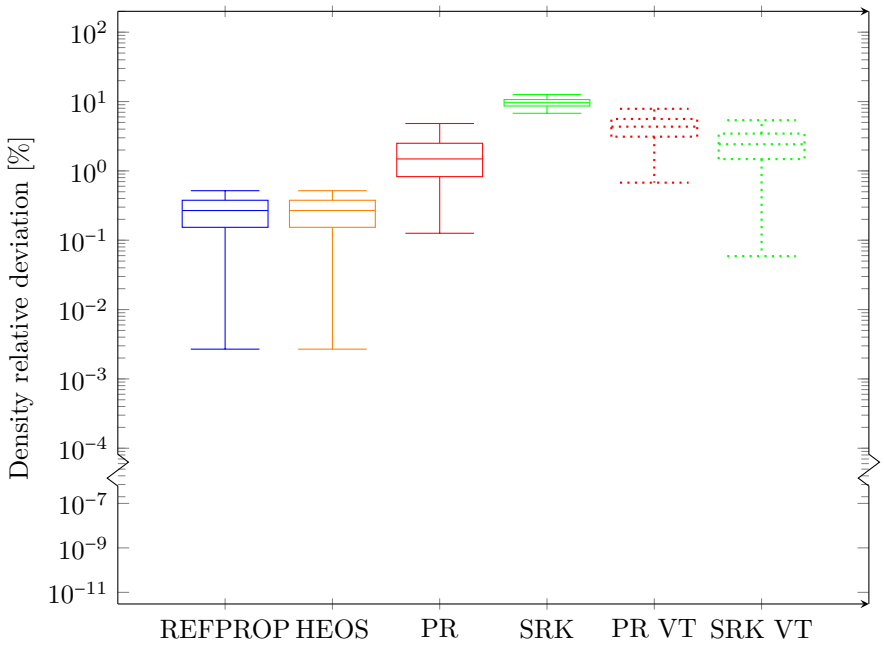


Figure 109: Relative density deviation to experimental data for fluid MD4M

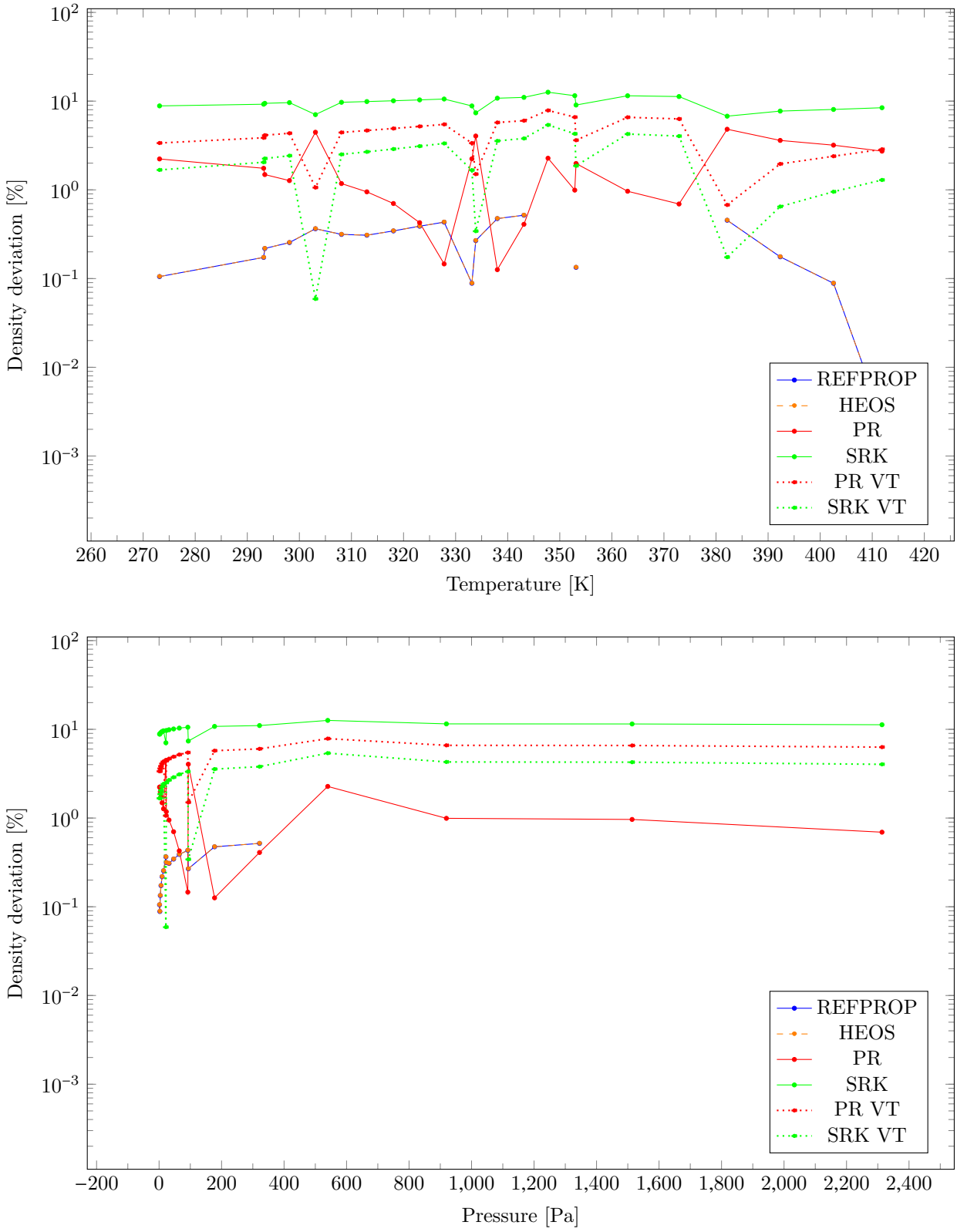


Figure 110: Density dependence on the temperature and pressure for fluid MD4M

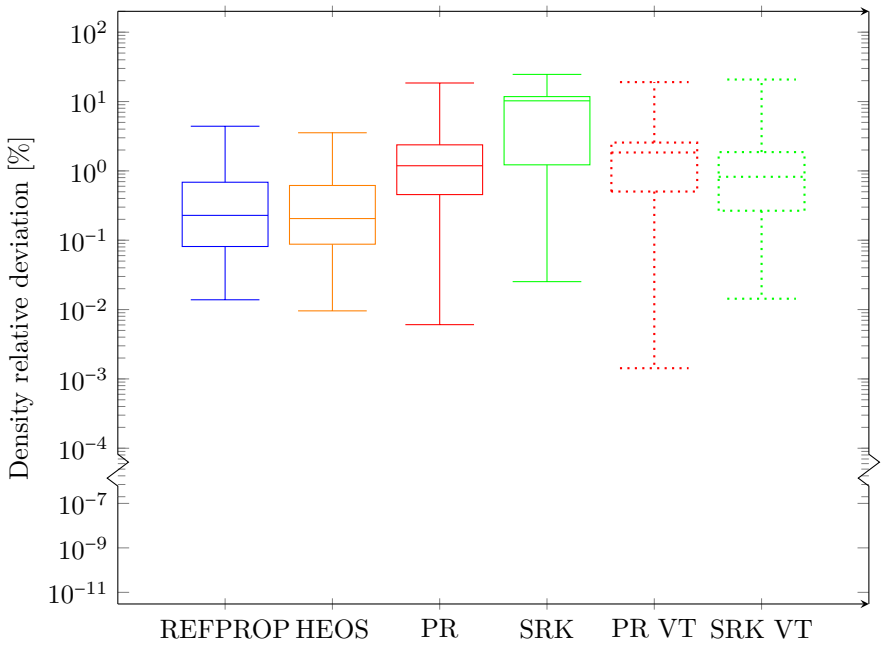


Figure 111: Relative density deviation to experimental data for fluid MDM

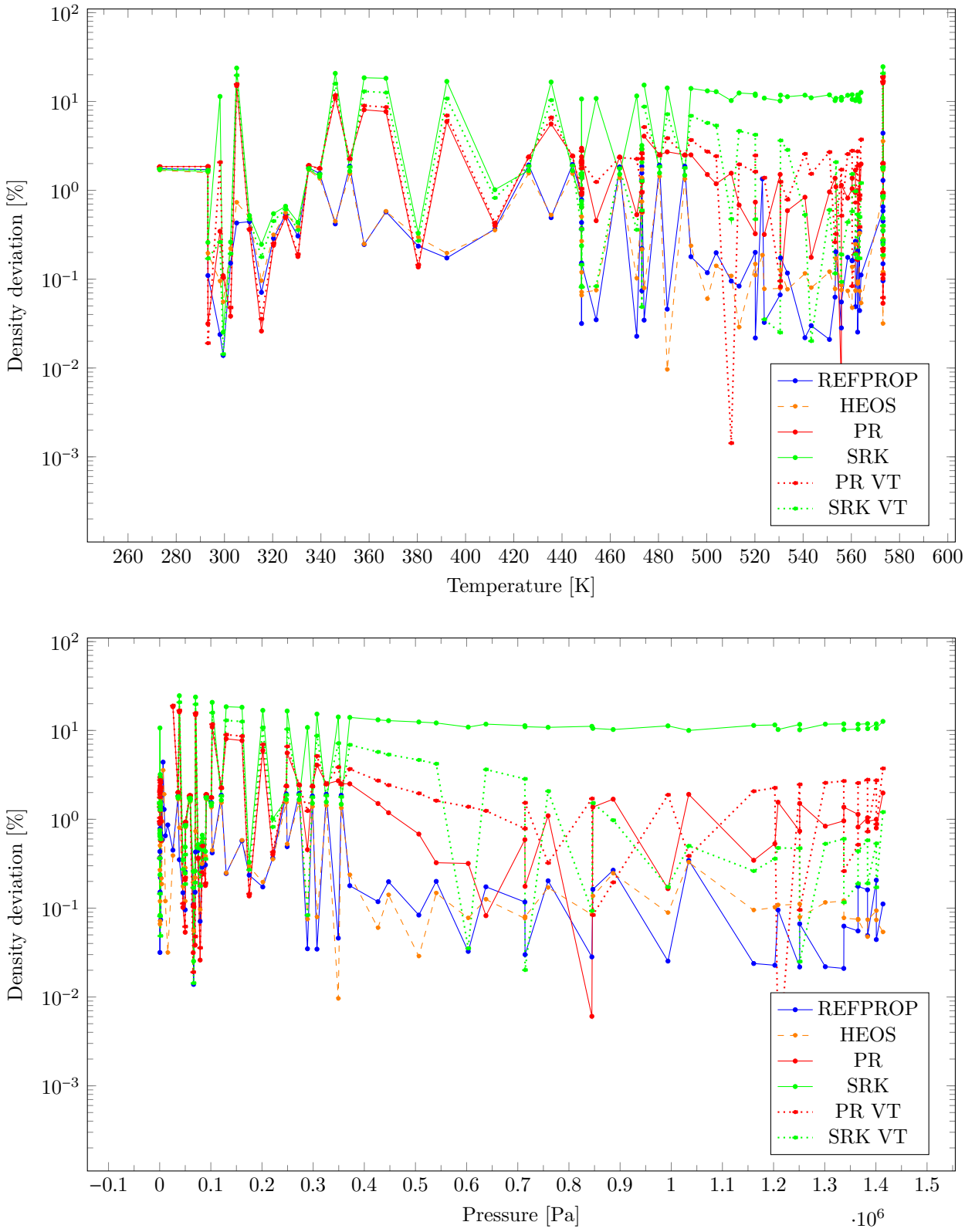


Figure 112: Density dependence on the temperature and pressure for fluid MDM

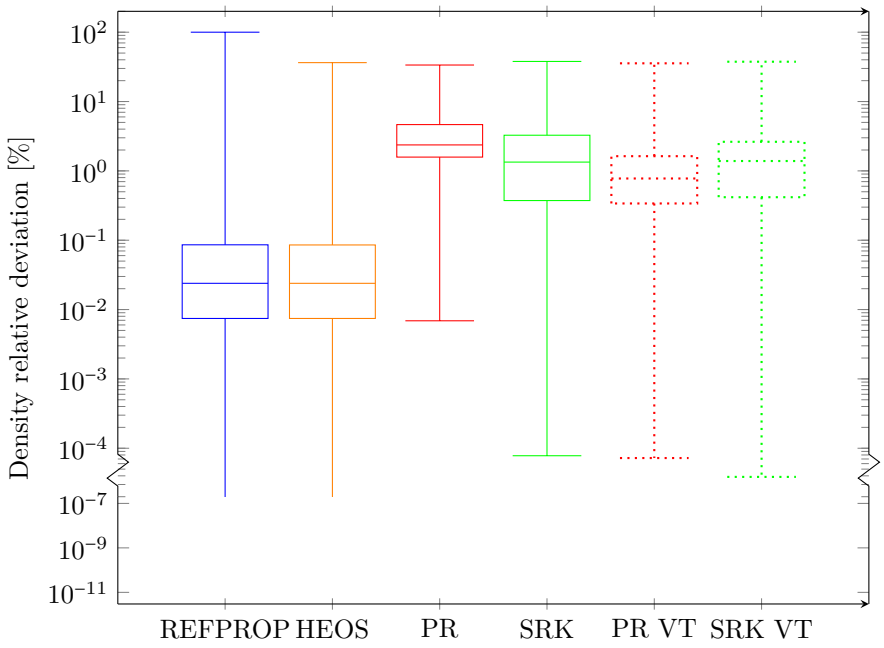


Figure 113: Relative density deviation to experimental data for fluid METHANE

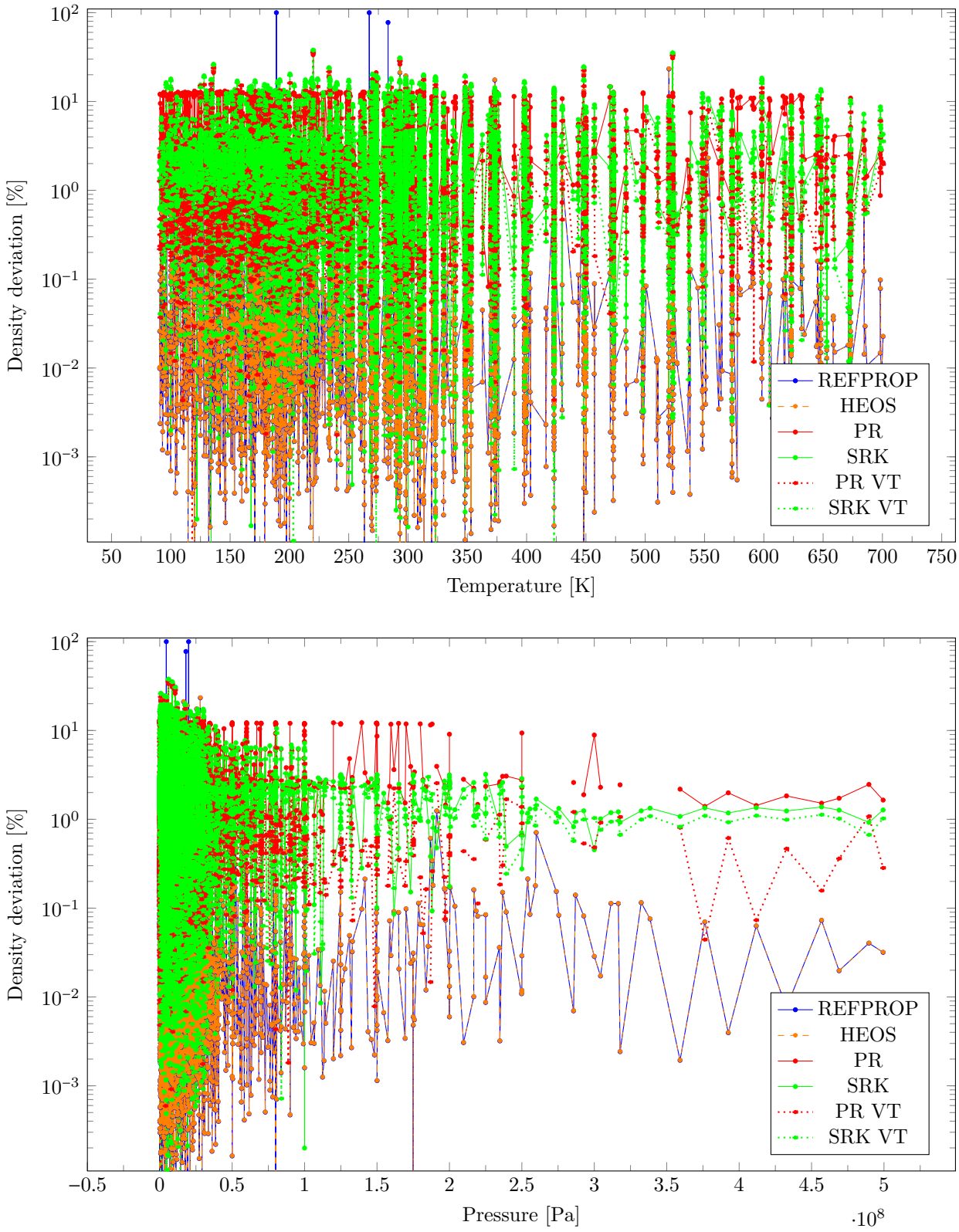


Figure 114: Density dependence on the temperature and pressure for fluid Methane

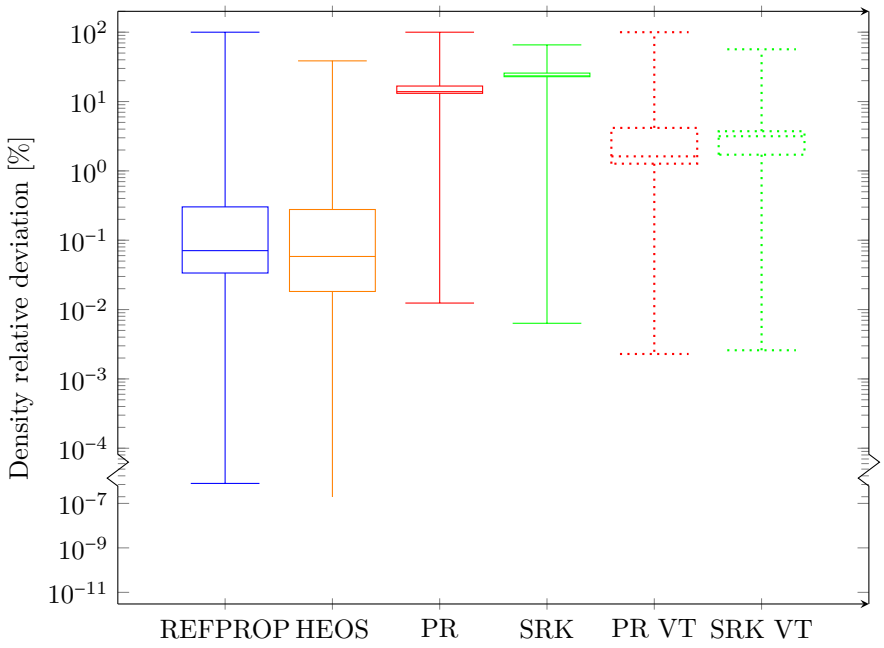


Figure 115: Relative density deviation to experimental data for fluid Methanol

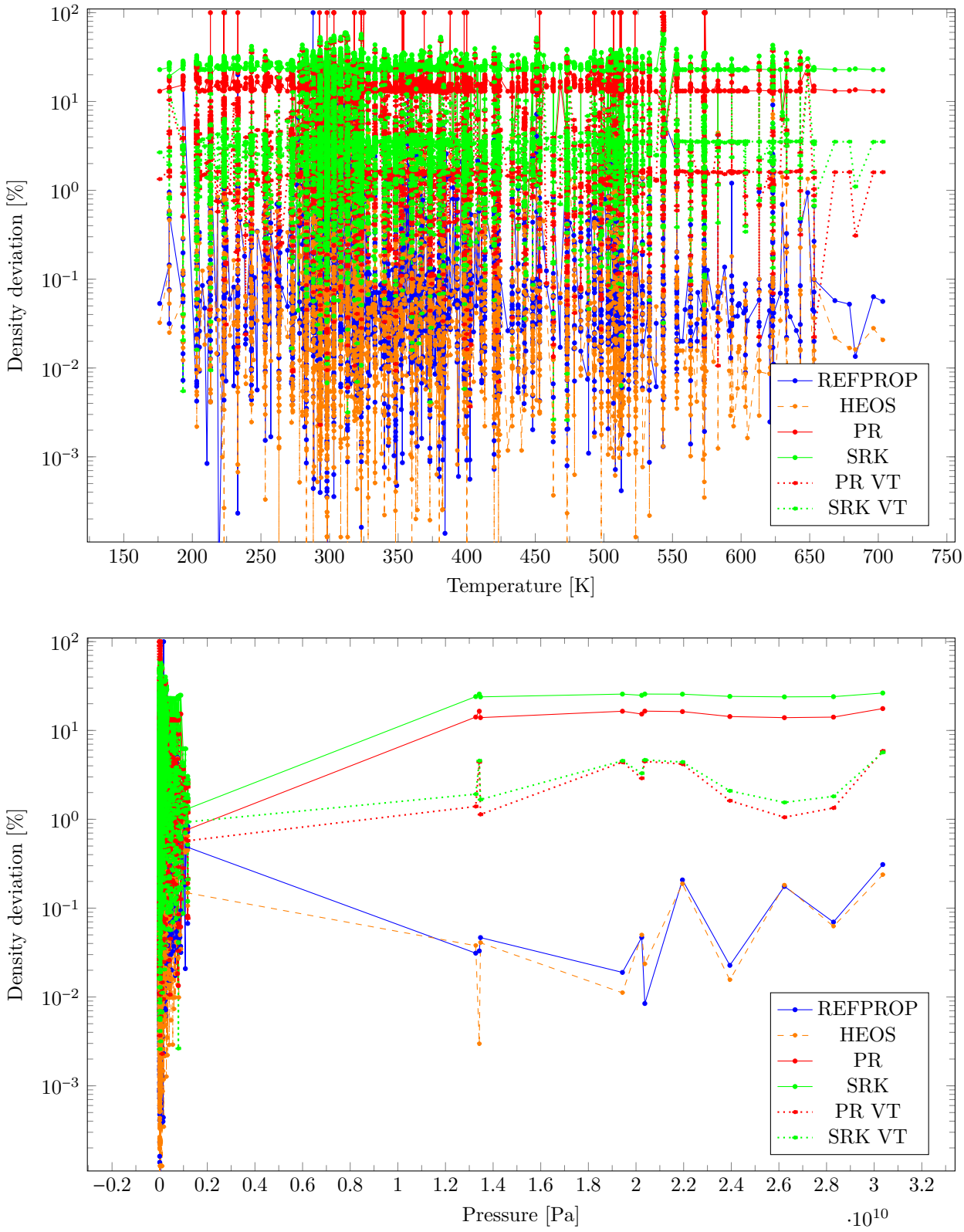


Figure 116: Density dependence on the temperature and pressure for fluid Methanol

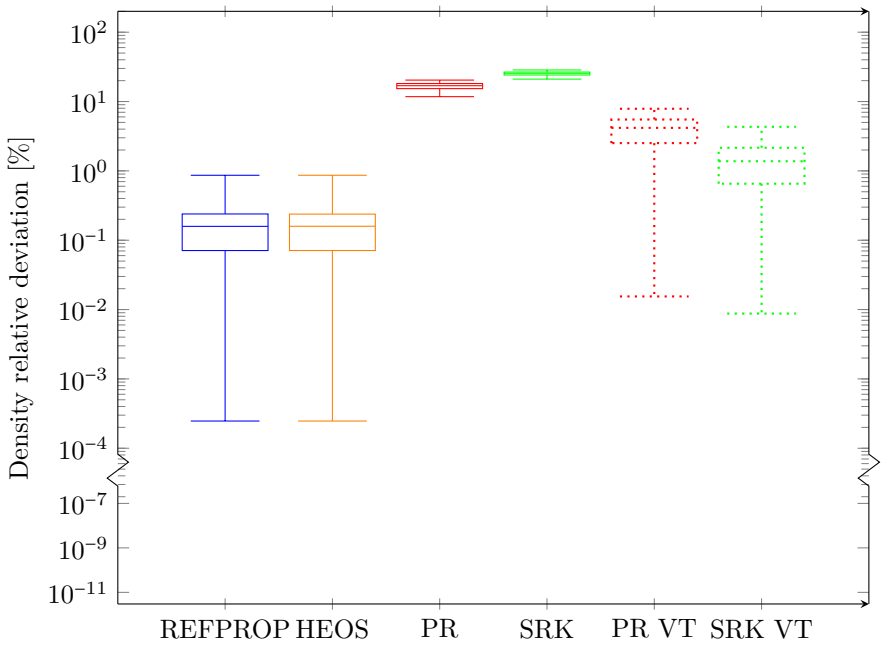


Figure 117: Relative density deviation to experimental data for fluid MethylLinoleate

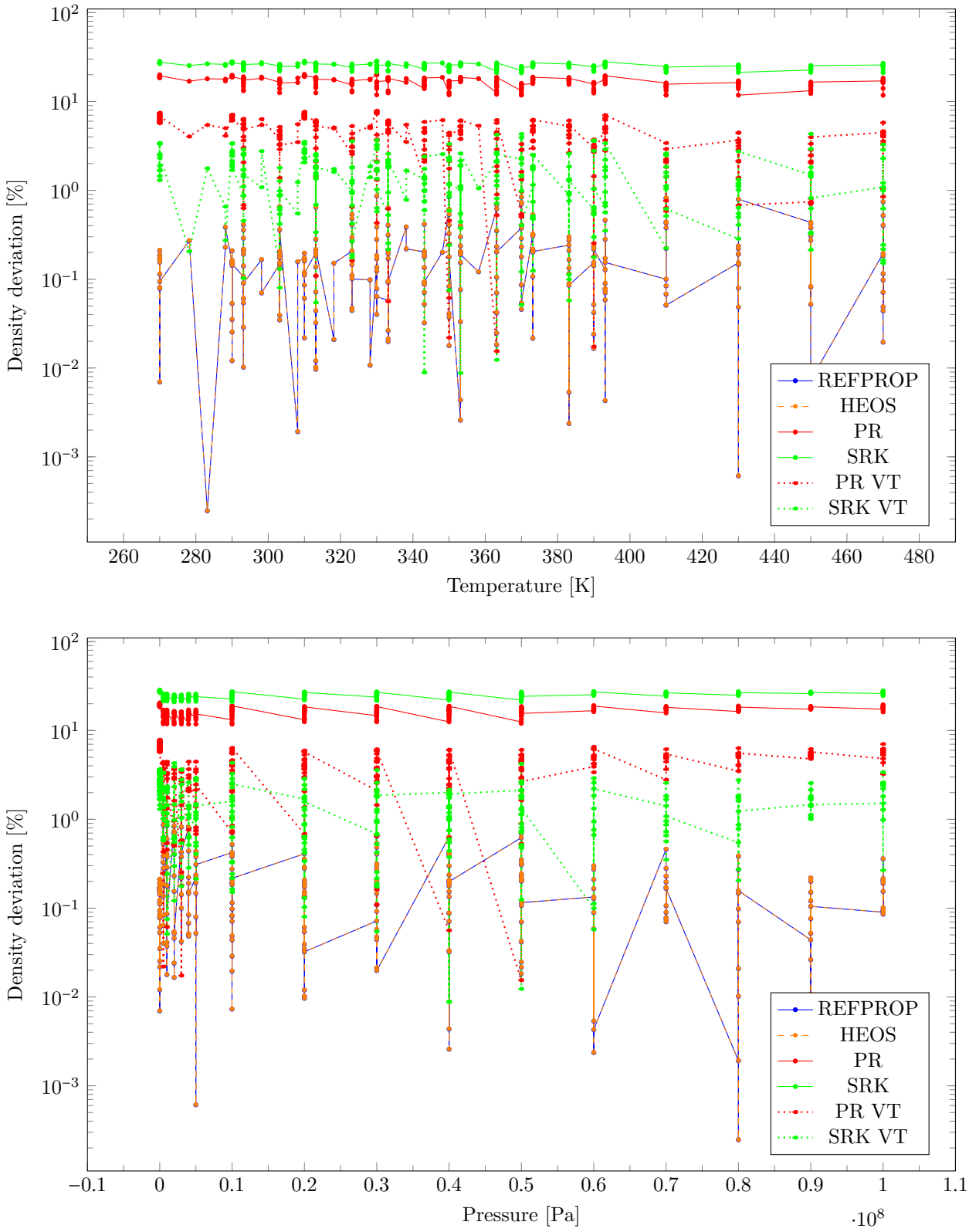


Figure 118: Density dependence on the temperature and pressure for fluid MethylLinoleate

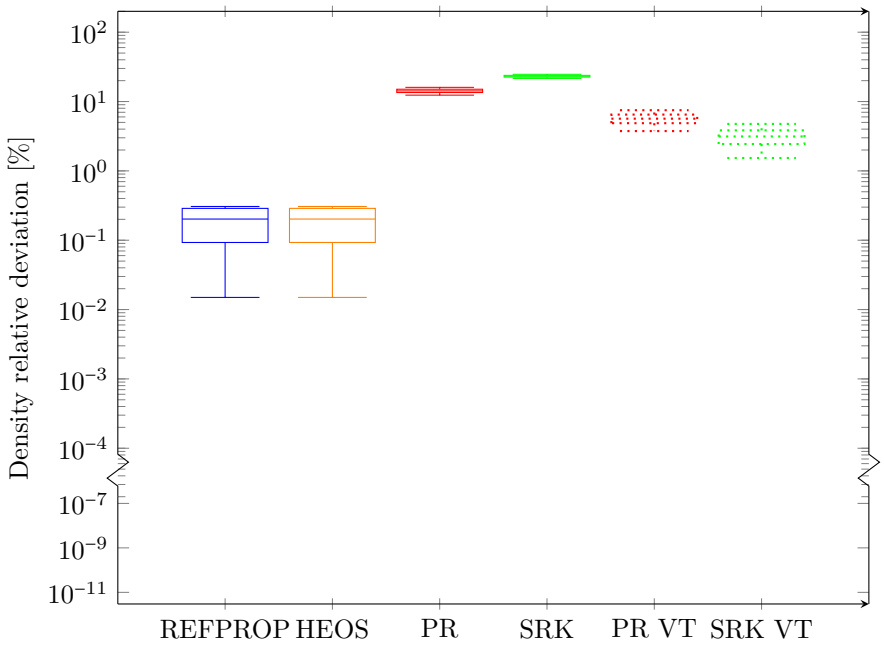


Figure 119: Relative density deviation to experimental data for fluid MethylLinolenate

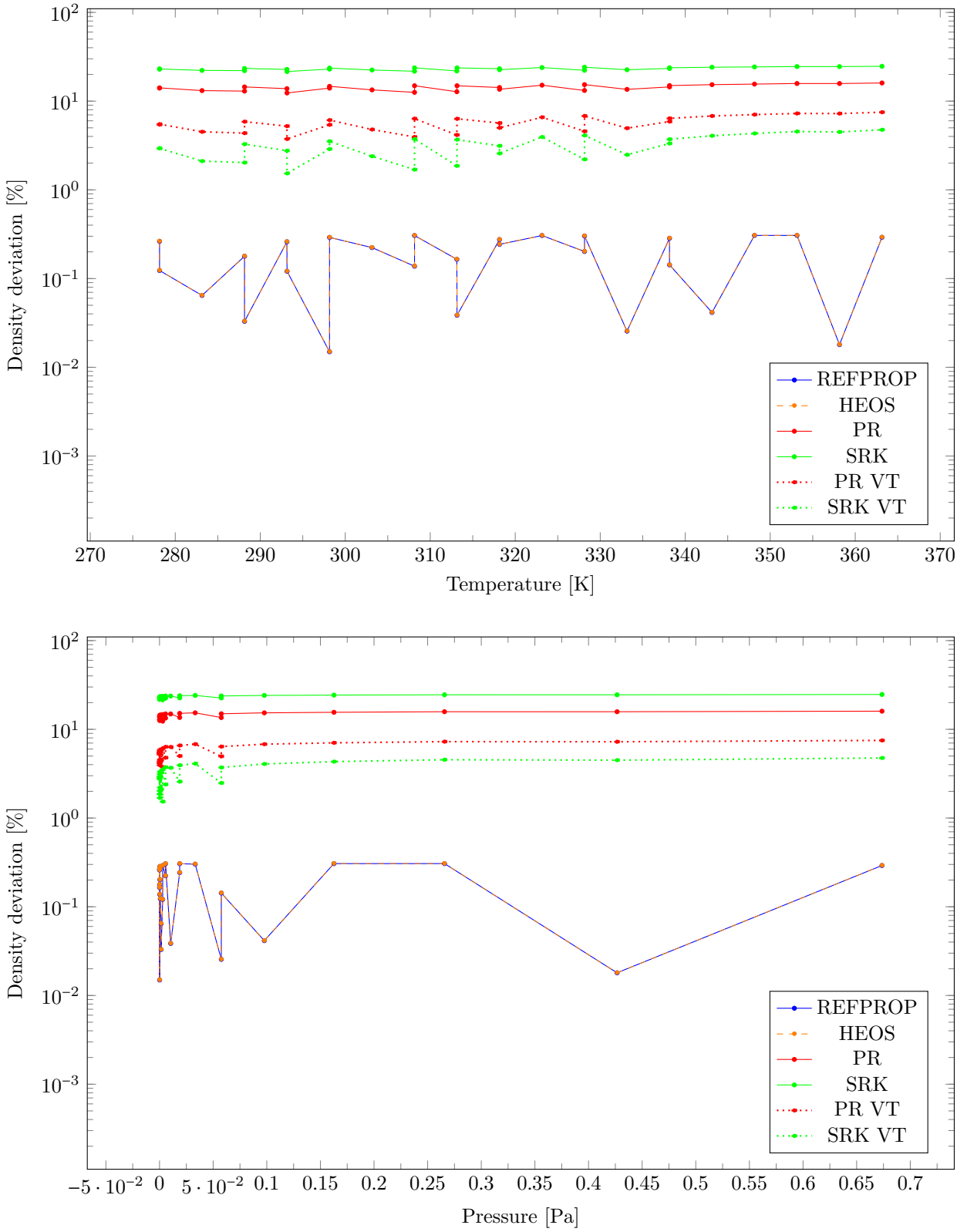


Figure 120: Density dependence on the temperature and pressure for fluid MethylLinolenate

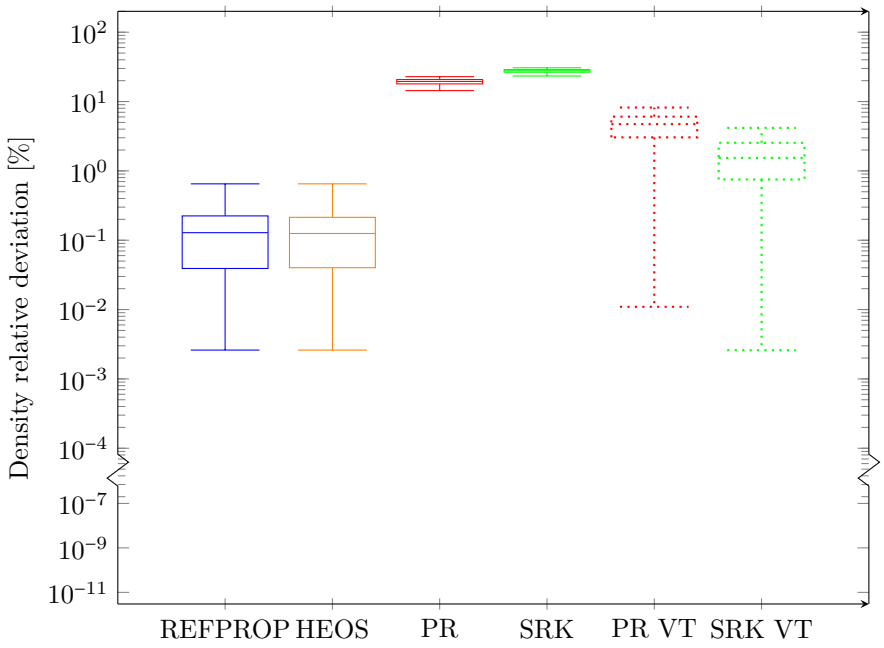


Figure 121: Relative density deviation to experimental data for fluid MethylOleate

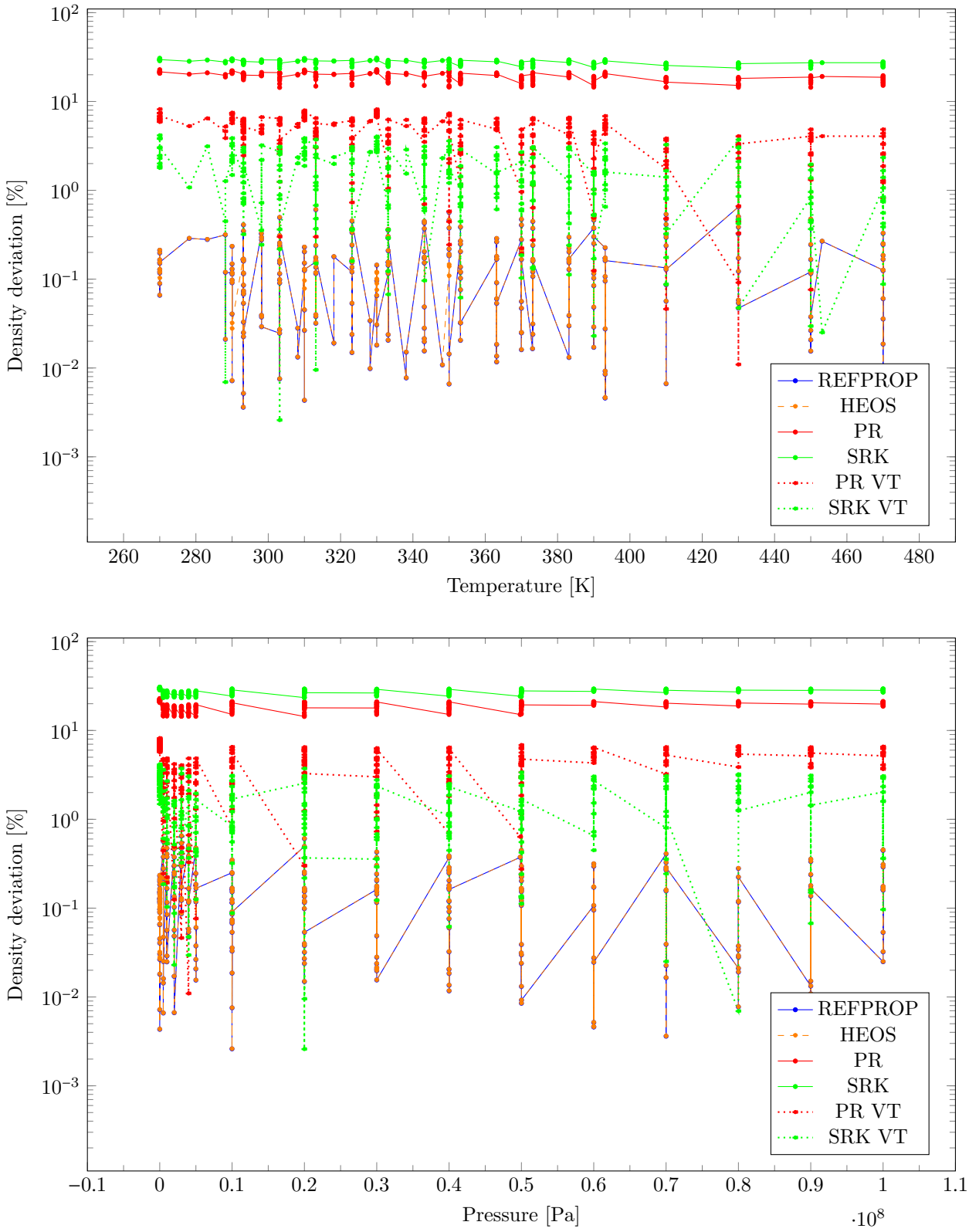


Figure 122: Density dependence on the temperature and pressure for fluid MethylOleate

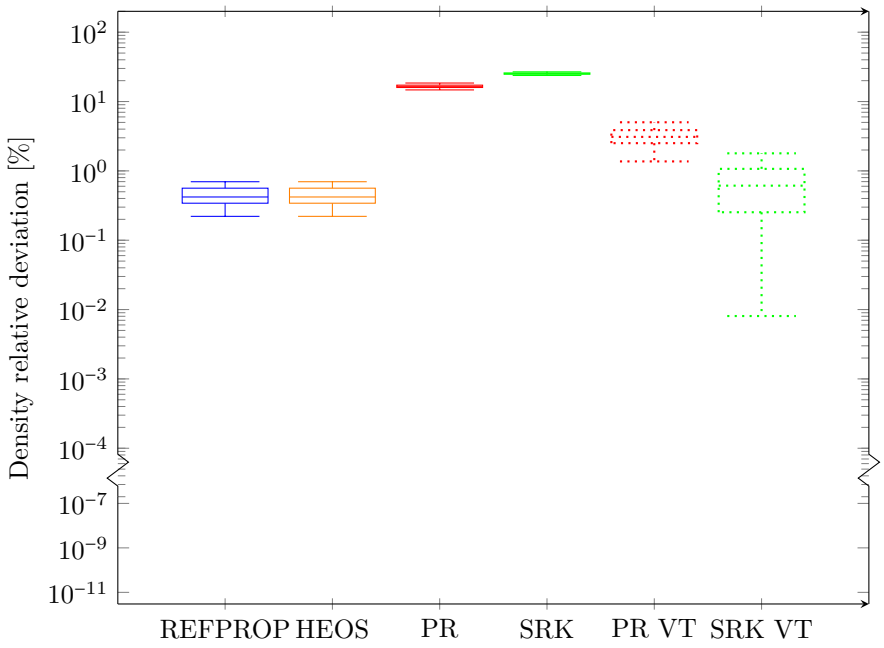


Figure 123: Relative density deviation to experimental data for fluid MethylPalmitate

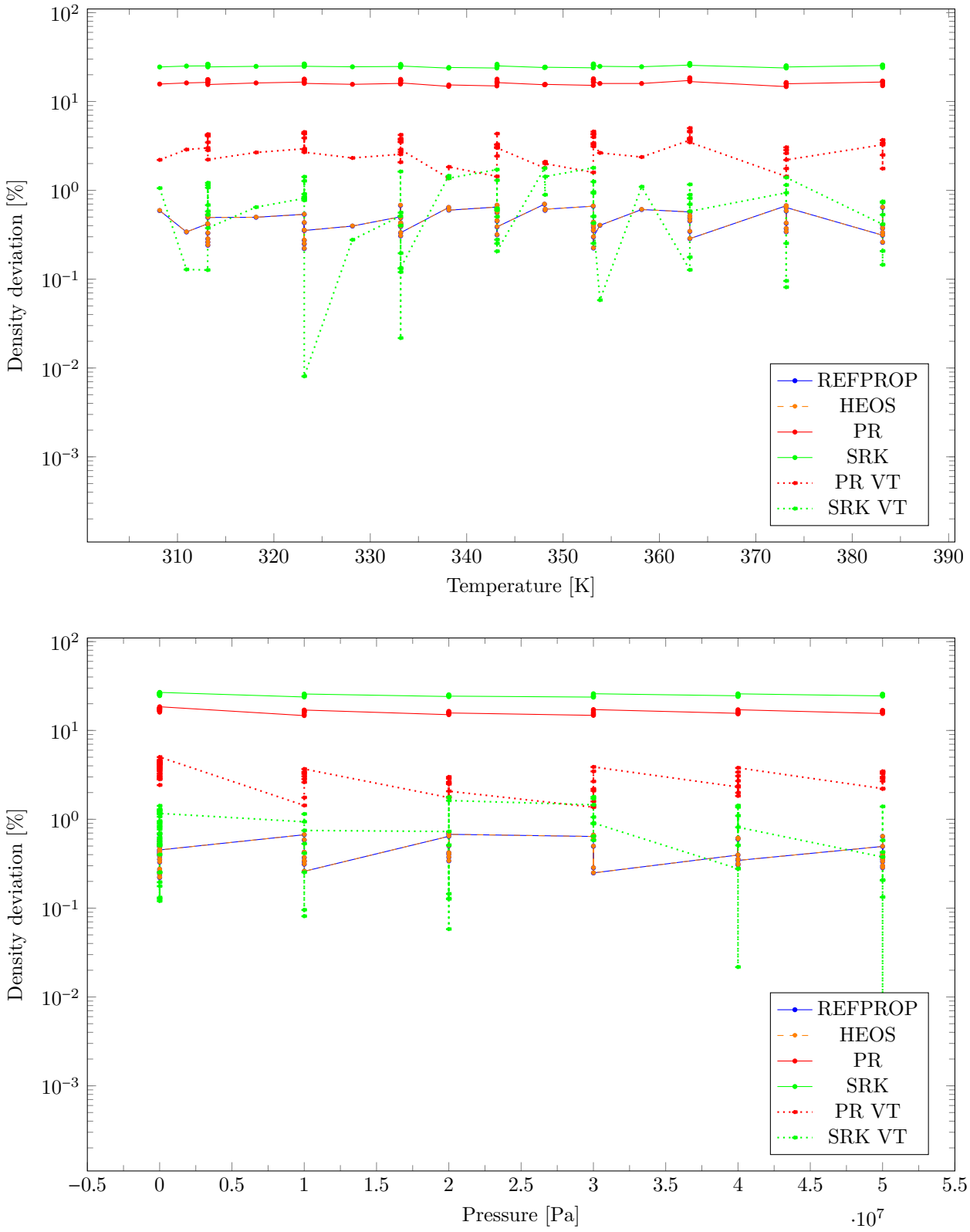


Figure 124: Density dependence on the temperature and pressure for fluid MethylPalmitate

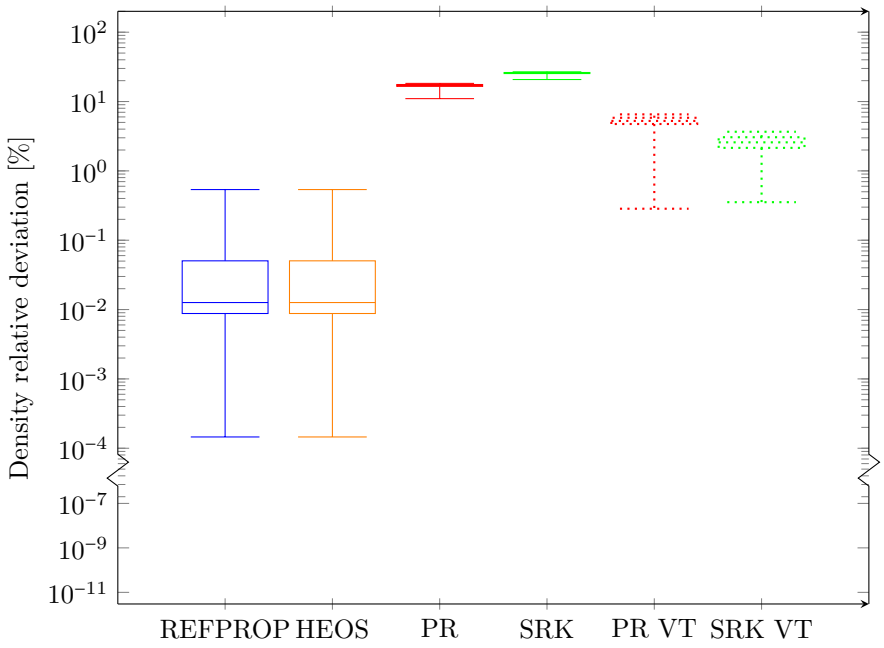
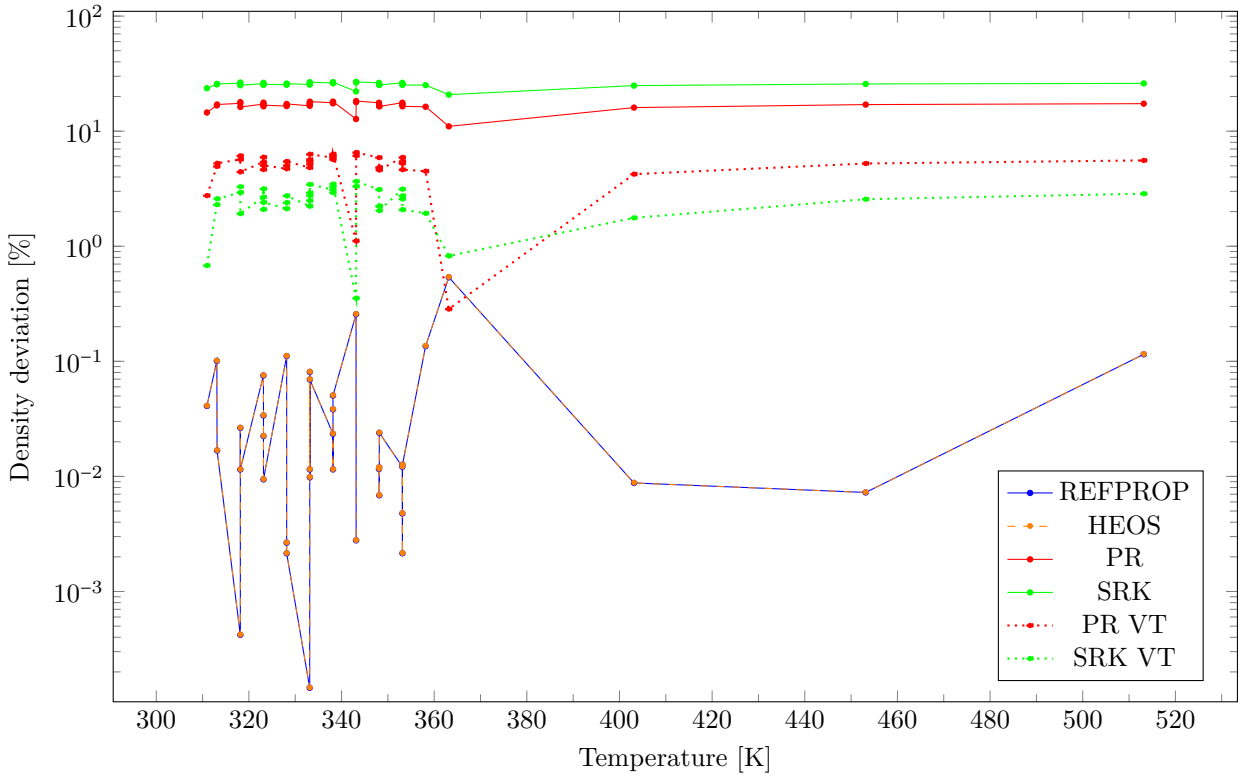


Figure 125: Relative density deviation to experimental data for fluid MethylStearate



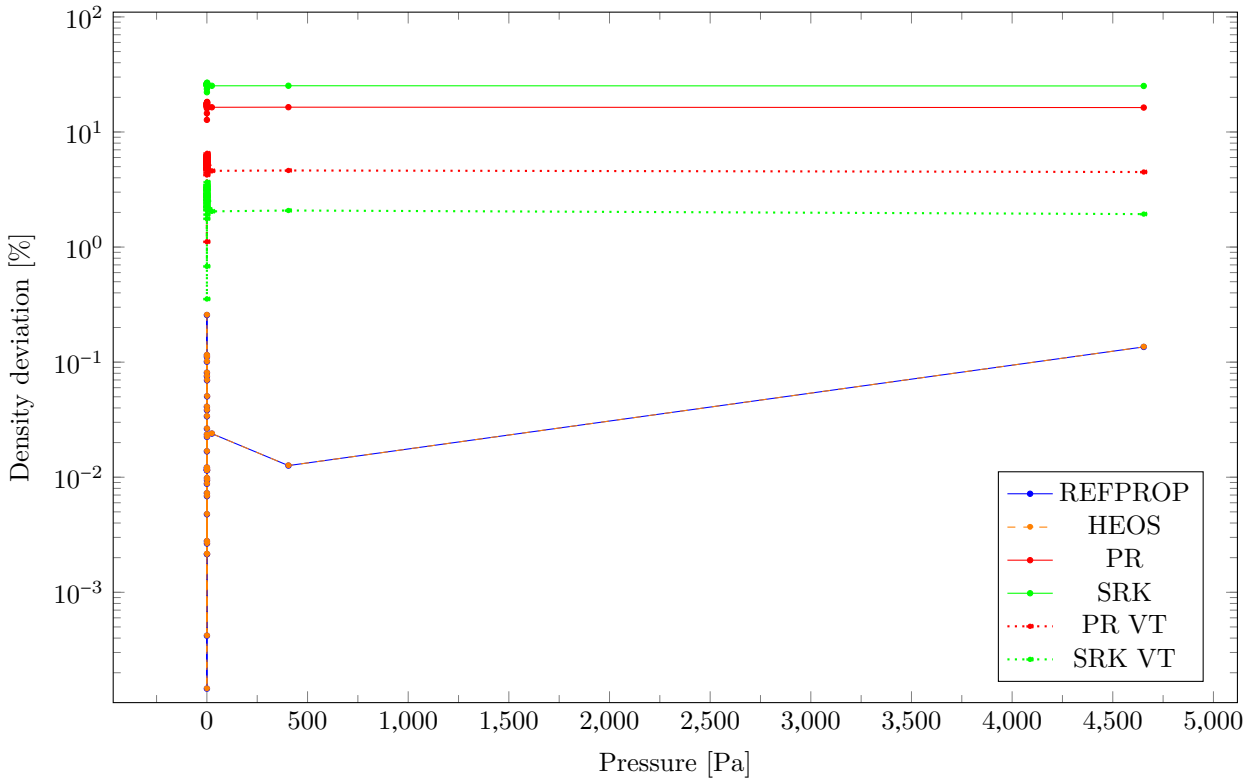


Figure 126: Density dependence on the temperature and pressure for fluid MethylStearate

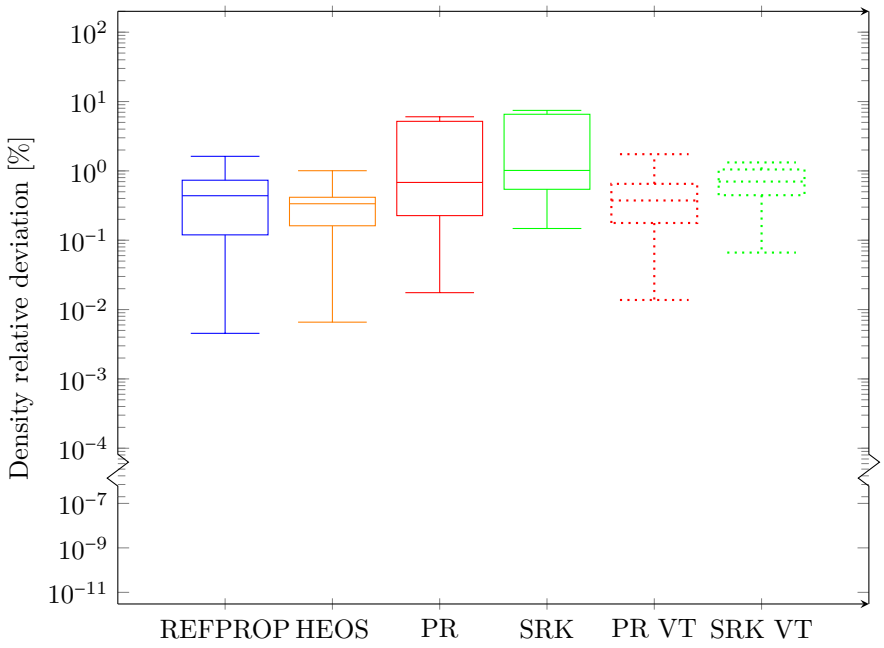


Figure 127: Relative density deviation to experimental data for fluid MM

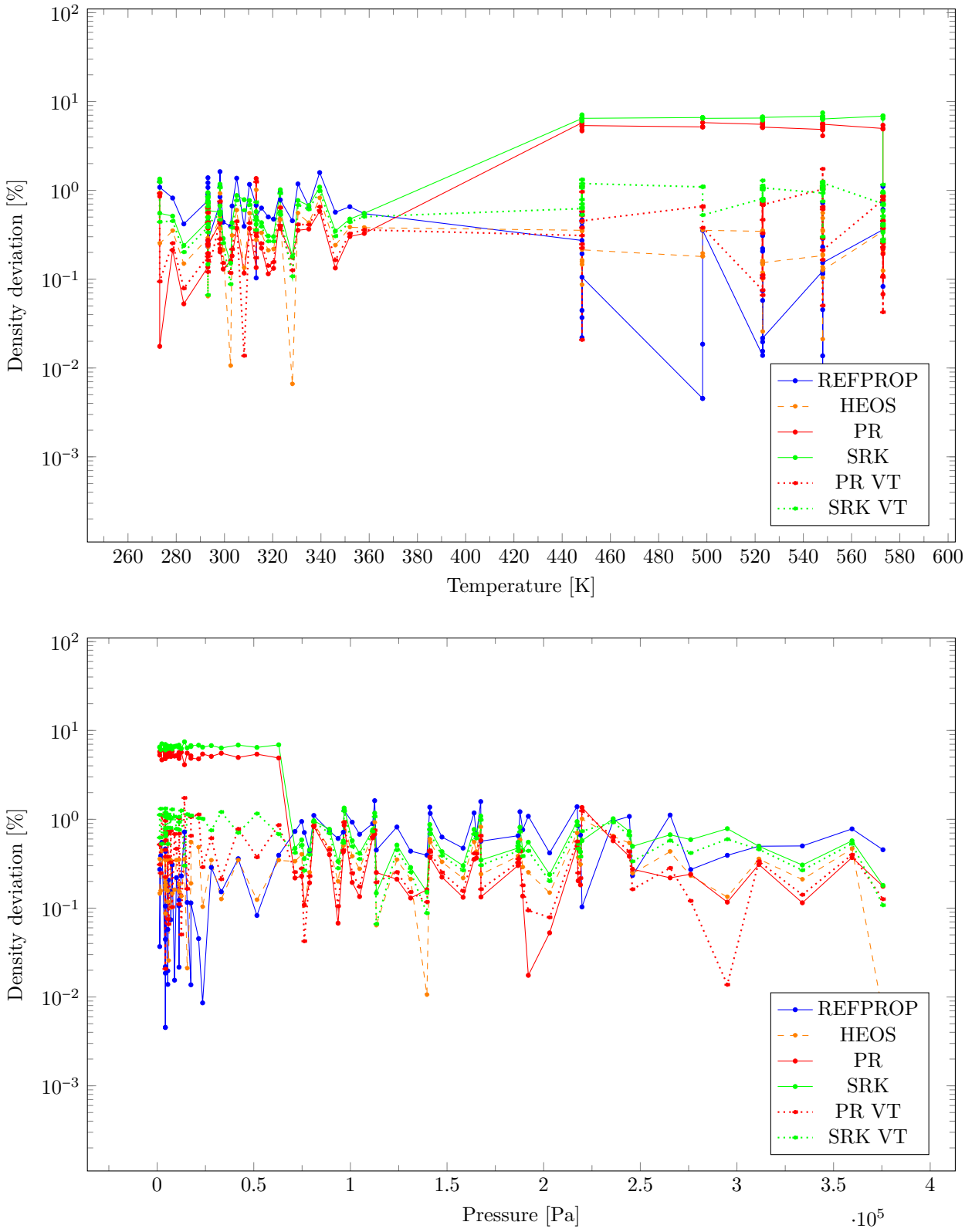


Figure 128: Density dependence on the temperature and pressure for fluid MM

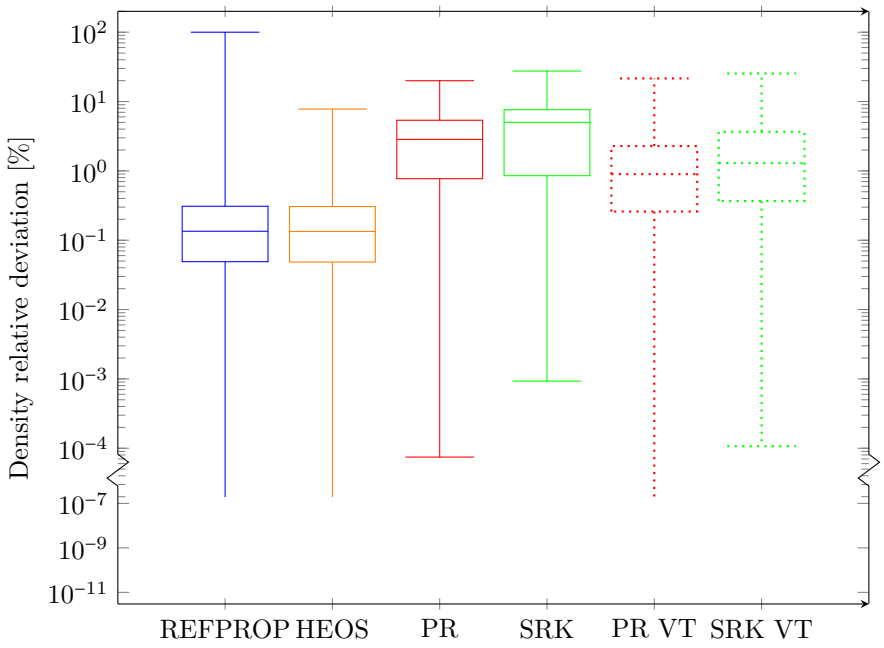


Figure 129: Relative density deviation to experimental data for fluid n-Butane

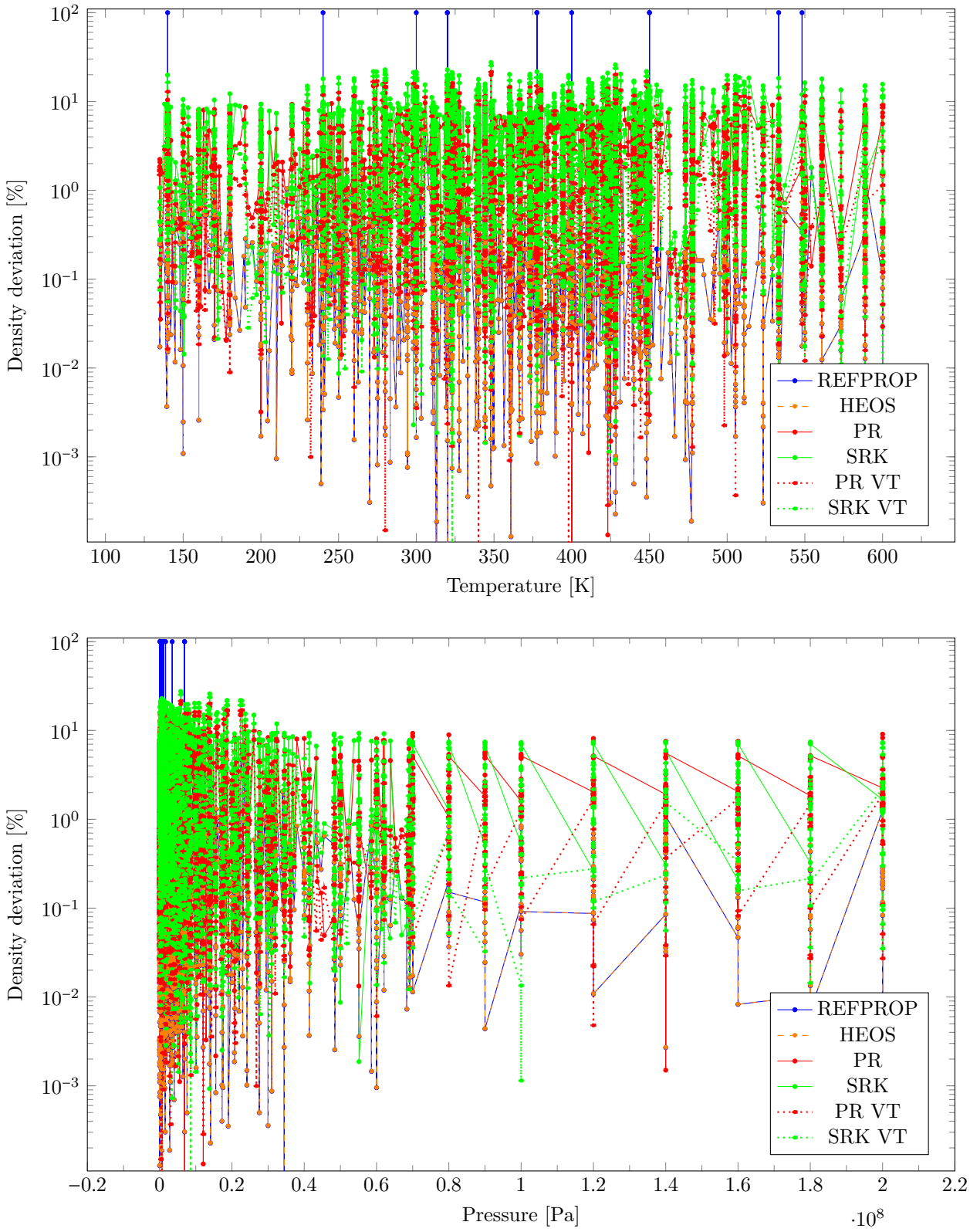


Figure 130: Density dependence on the temperature and pressure for fluid n-Butane

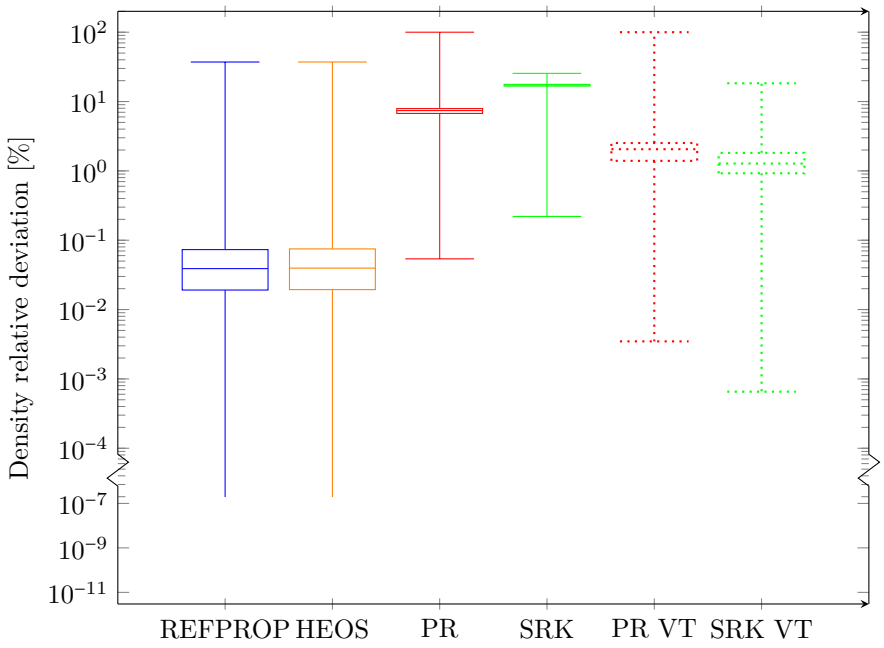


Figure 131: Relative density deviation to experimental data for fluid n-Decane

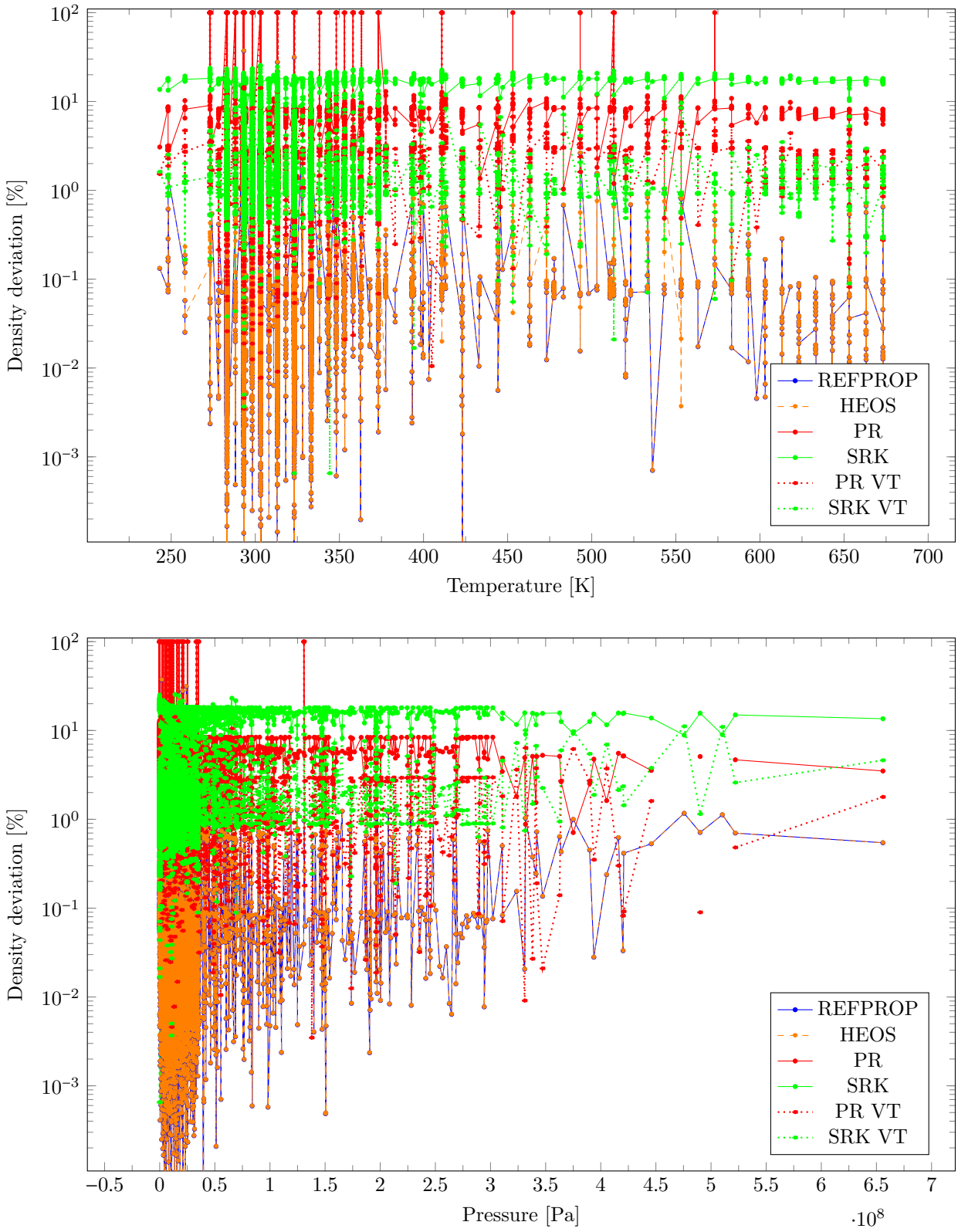


Figure 132: Density dependence on the temperature and pressure for fluid n-Decane

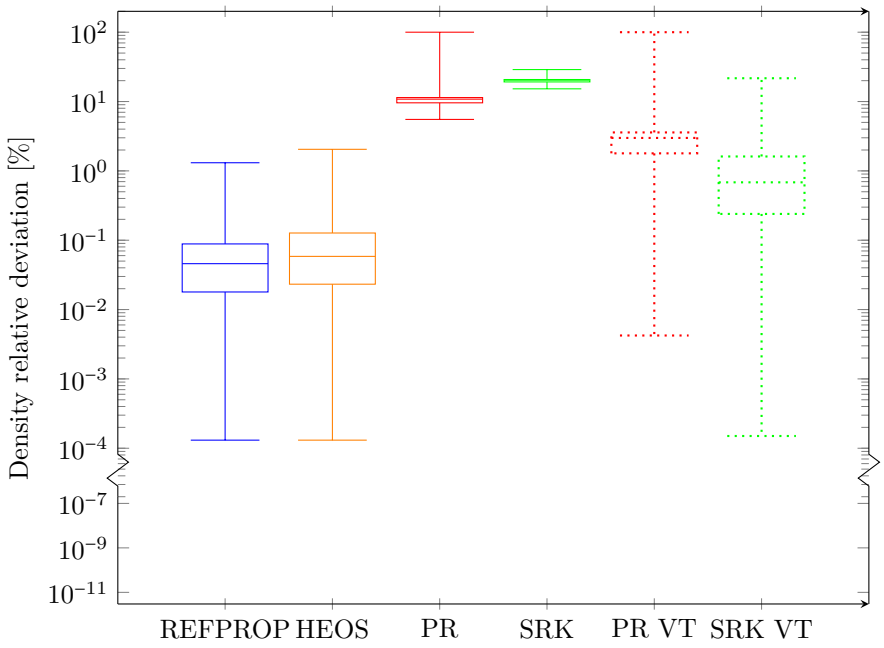


Figure 133: Relative density deviation to experimental data for fluid n-Dodecane

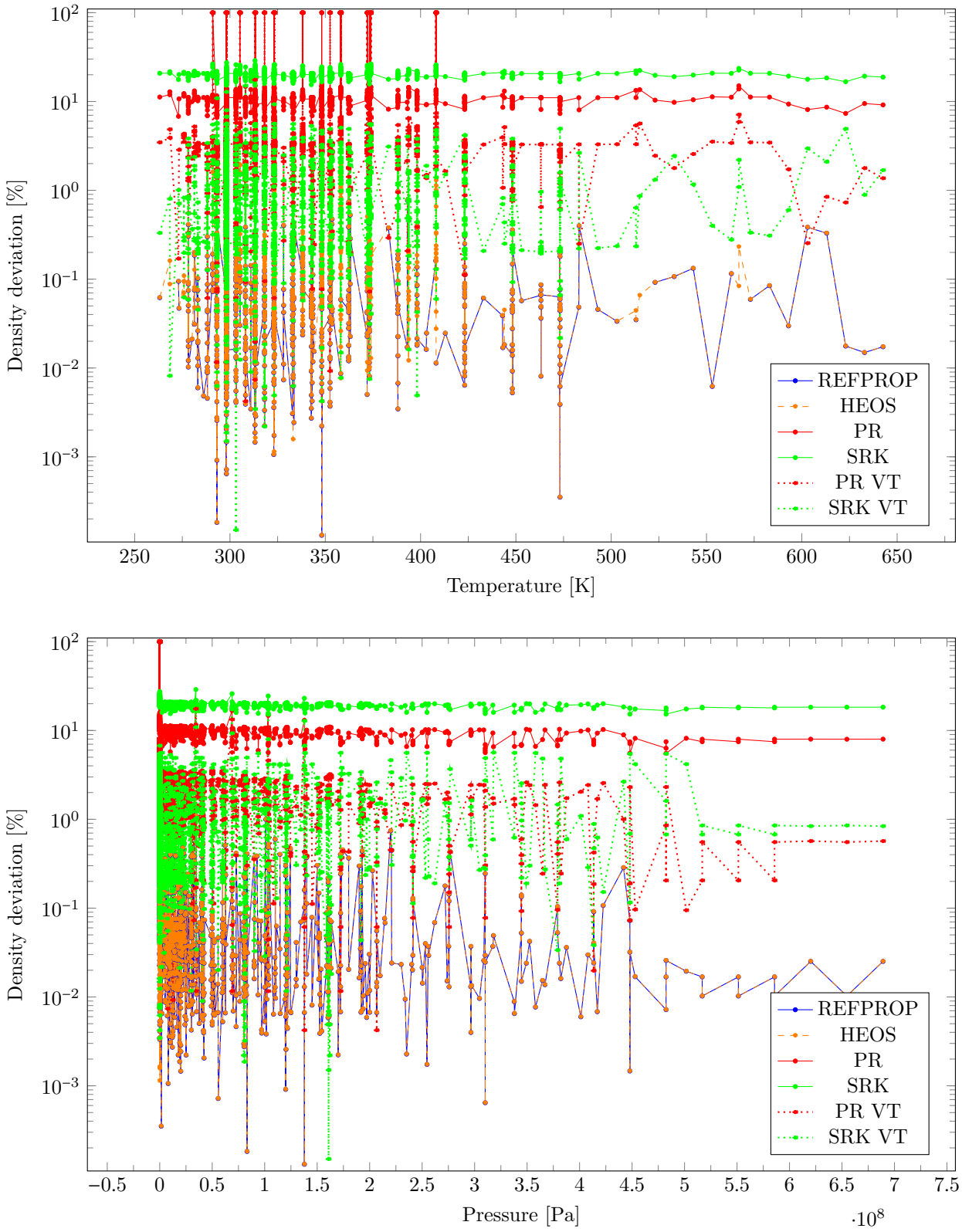


Figure 134: Density dependence on the temperature and pressure for fluid n-Dodecane

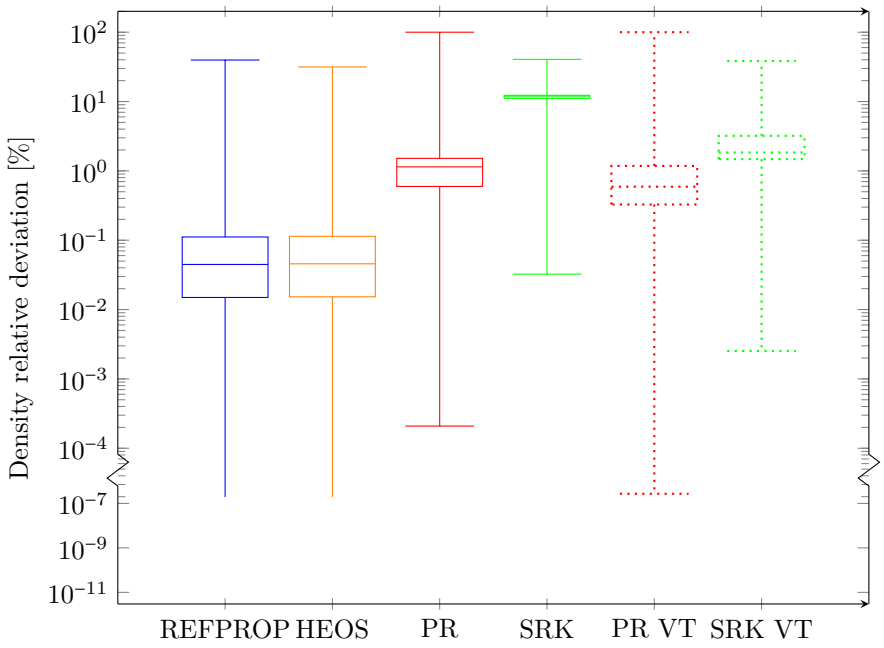


Figure 135: Relative density deviation to experimental data for fluid n-Heptane

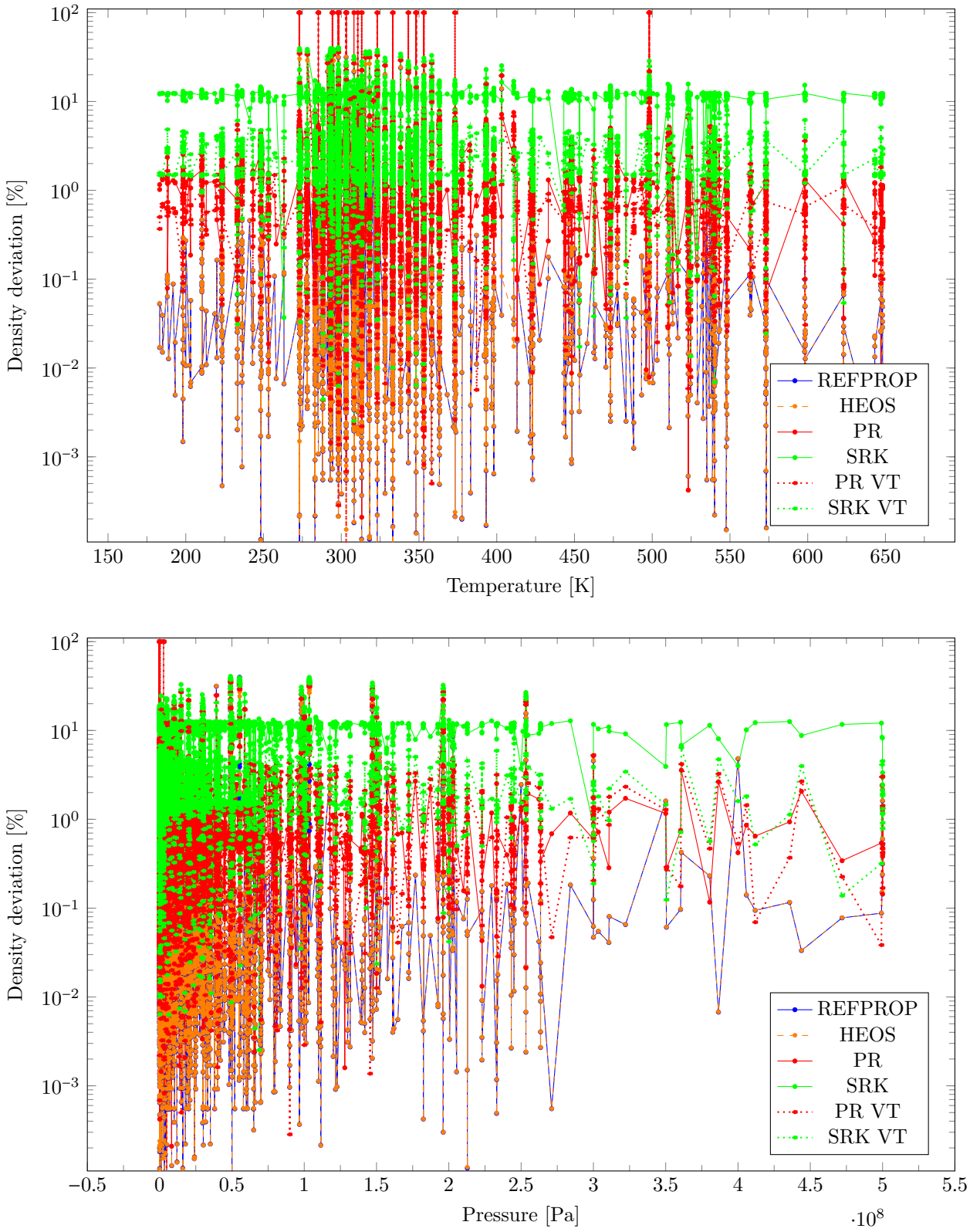


Figure 136: Density dependence on the temperature and pressure for fluid n-Heptane

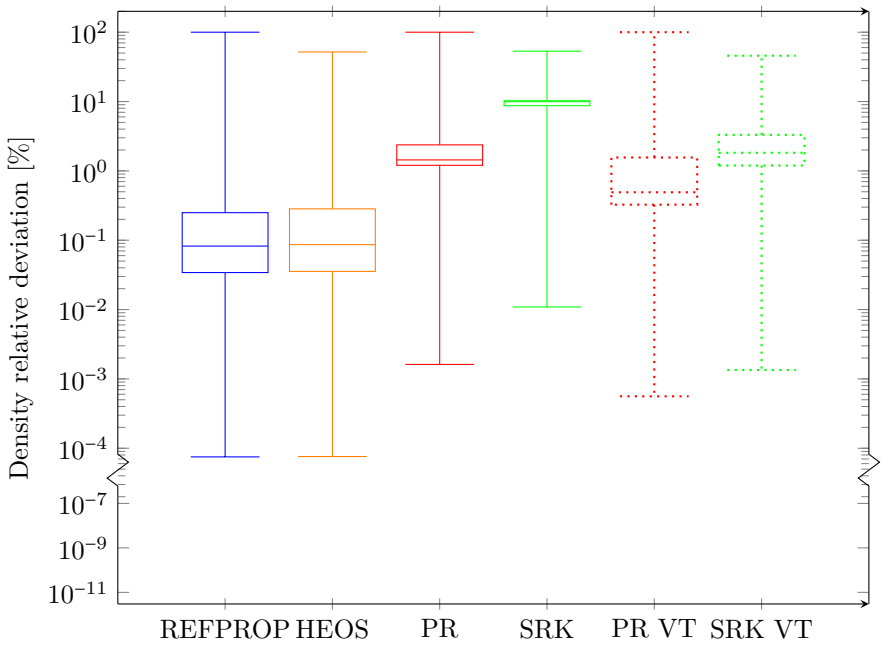


Figure 137: Relative density deviation to experimental data for fluid n-Hexane

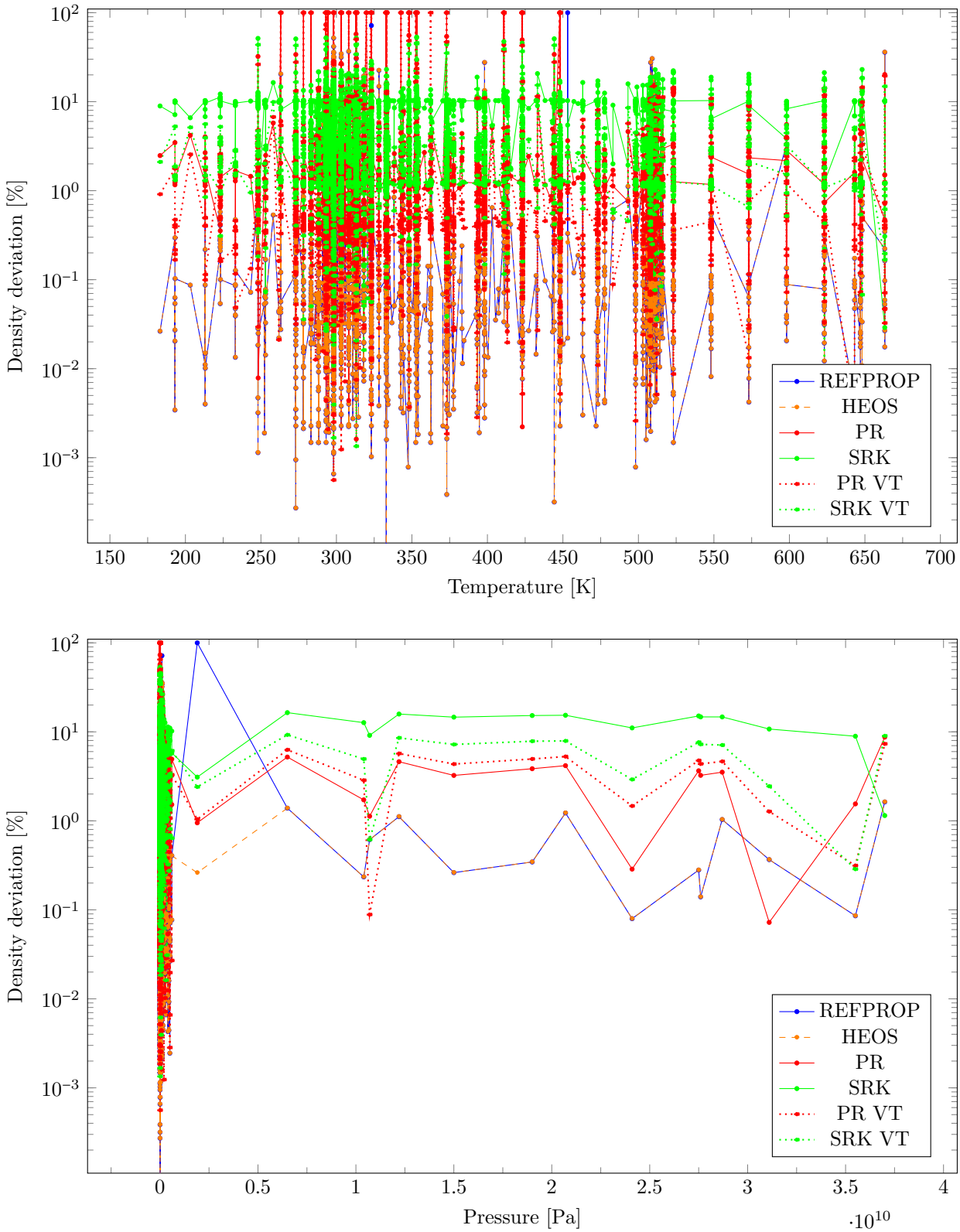


Figure 138: Density dependence on the temperature and pressure for fluid n-Hexane

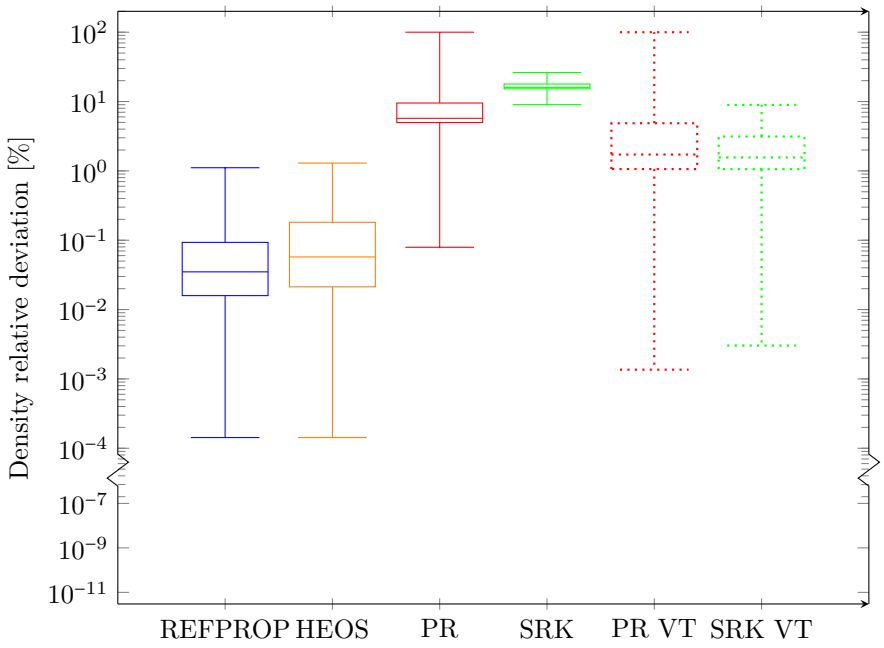


Figure 139: Relative density deviation to experimental data for fluid n-Nonane

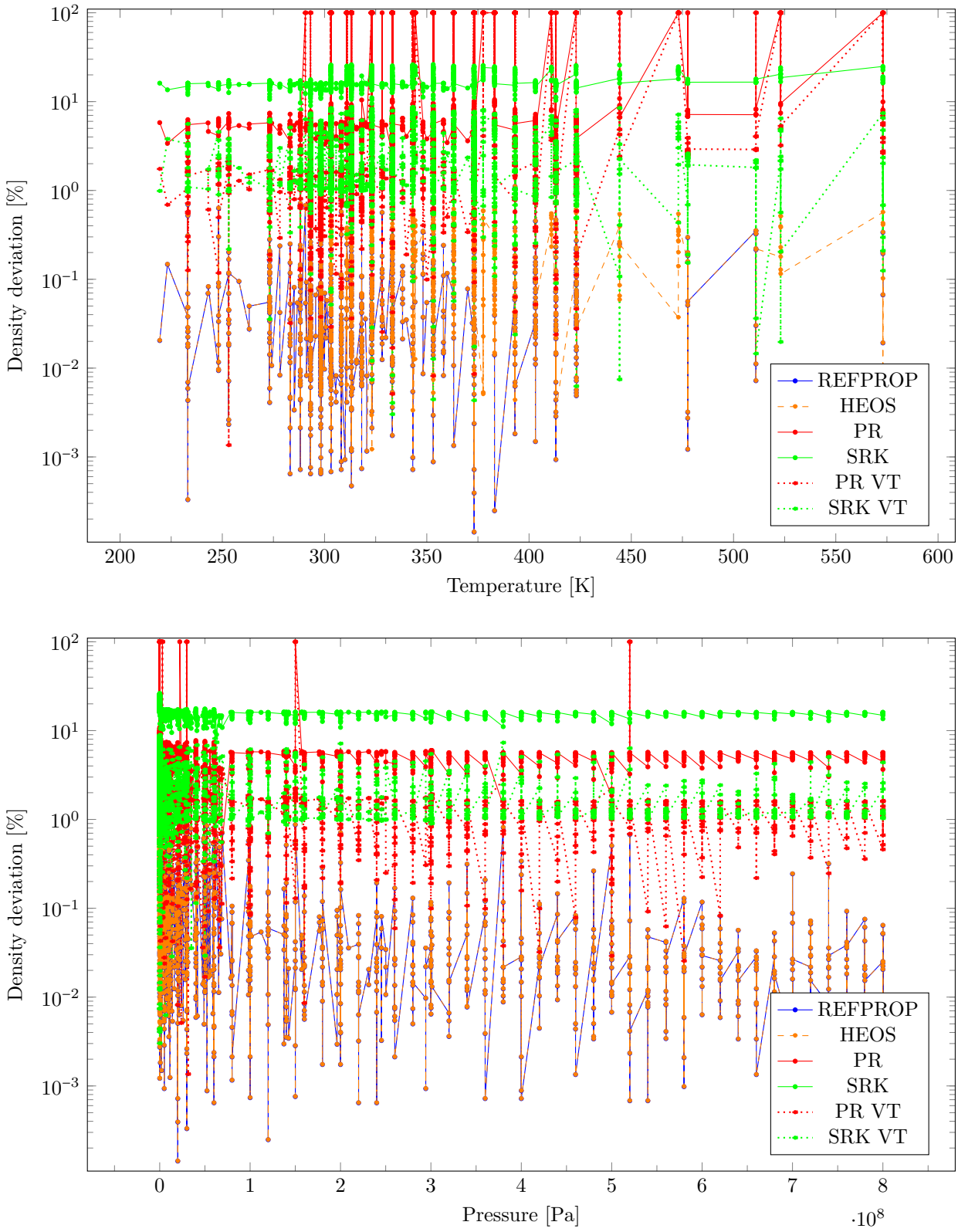


Figure 140: Density dependence on the temperature and pressure for fluid n-Nonane

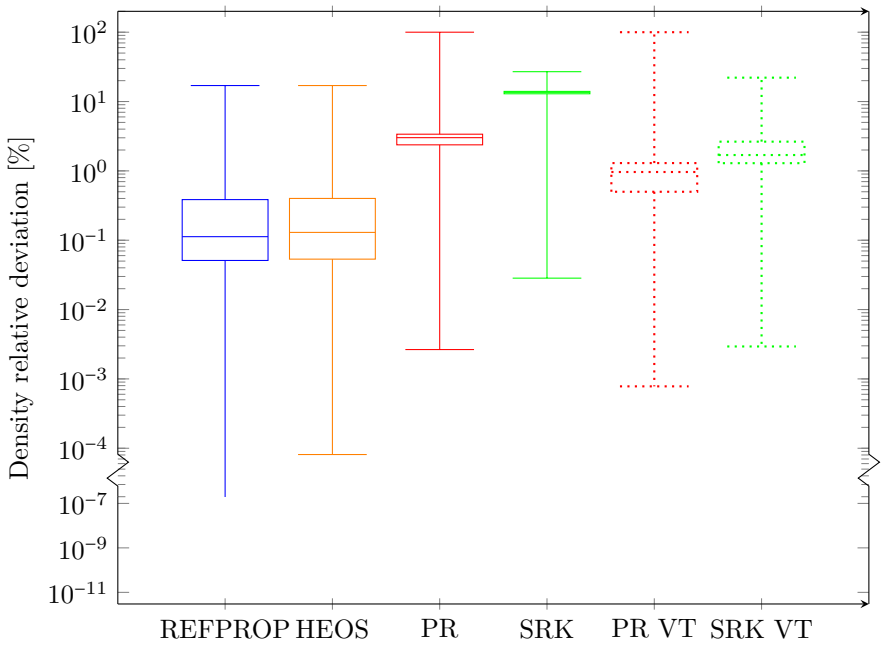


Figure 141: Relative density deviation to experimental data for fluid n-Octane

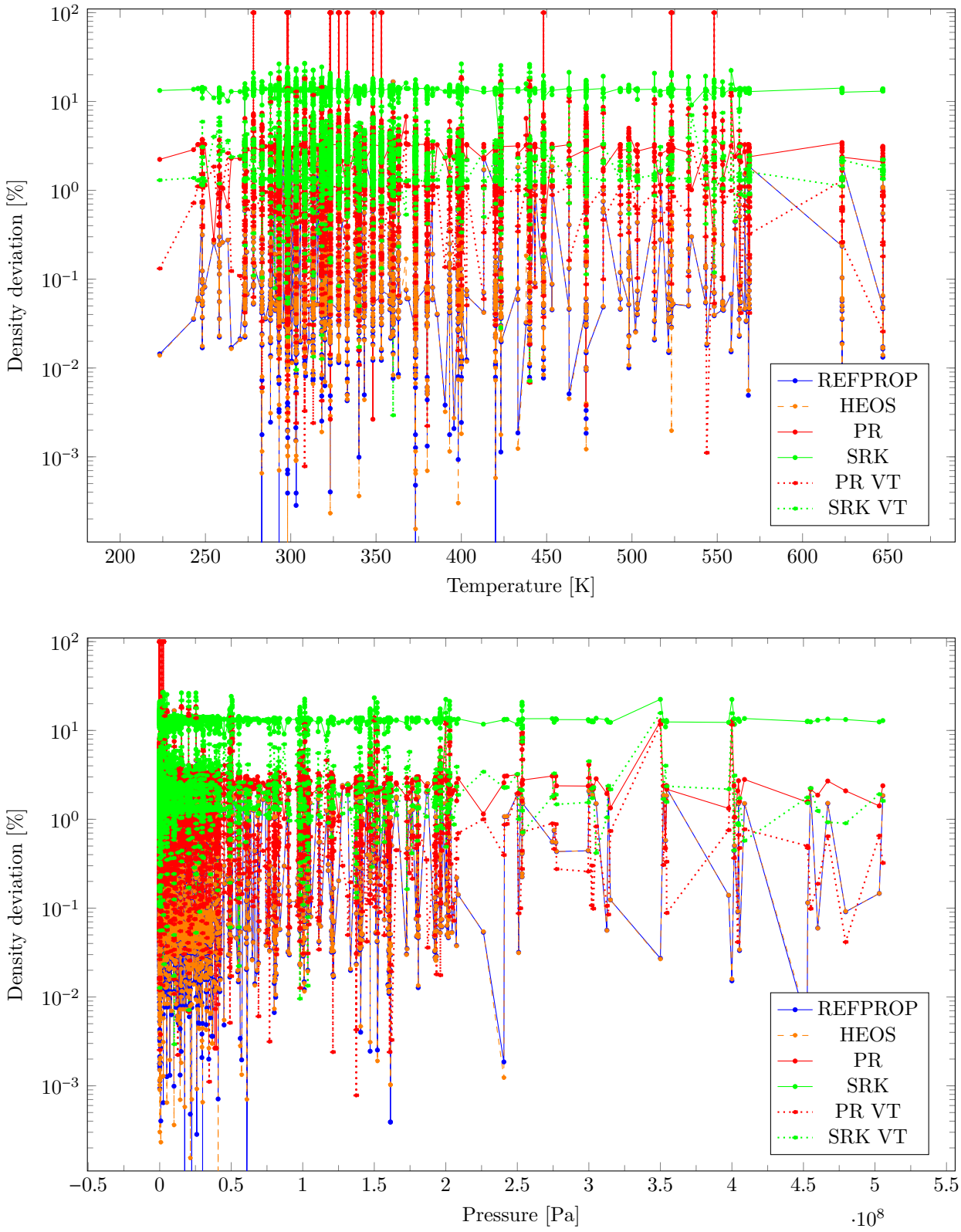


Figure 142: Density dependence on the temperature and pressure for fluid n-Octane

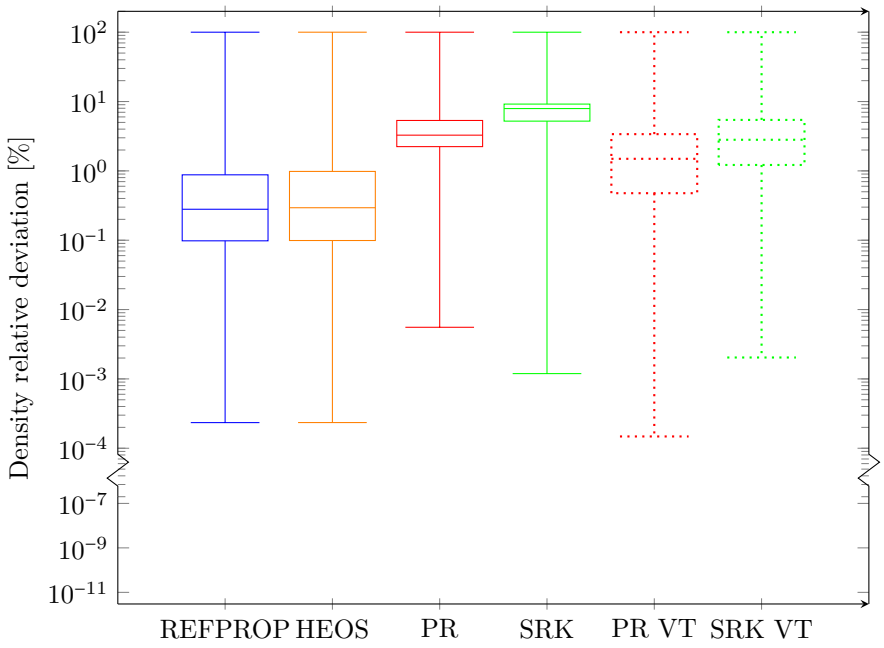


Figure 143: Relative density deviation to experimental data for fluid n-Pentane

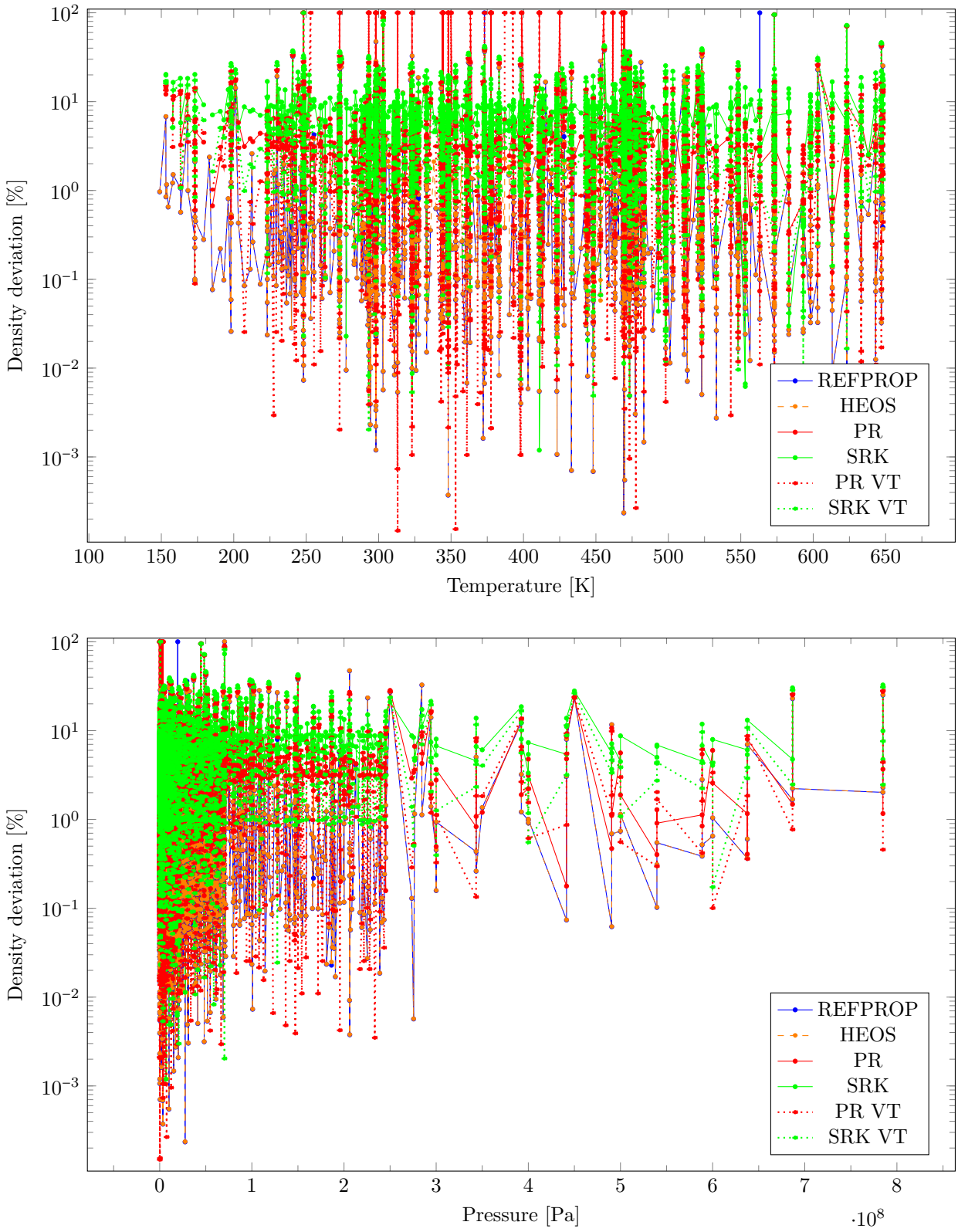


Figure 144: Density dependence on the temperature and pressure for fluid n-Pentane

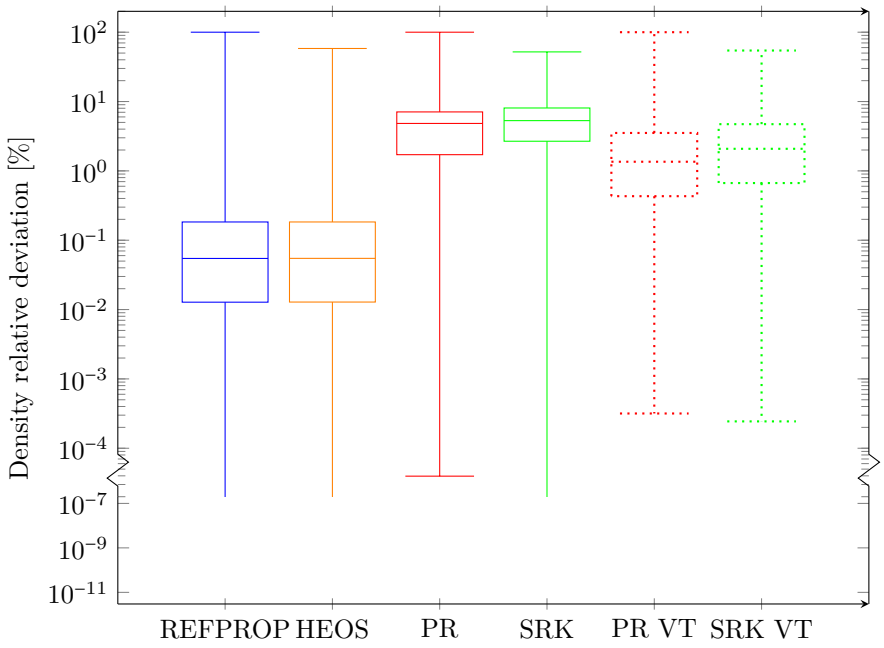


Figure 145: Relative density deviation to experimental data for fluid n-Propane

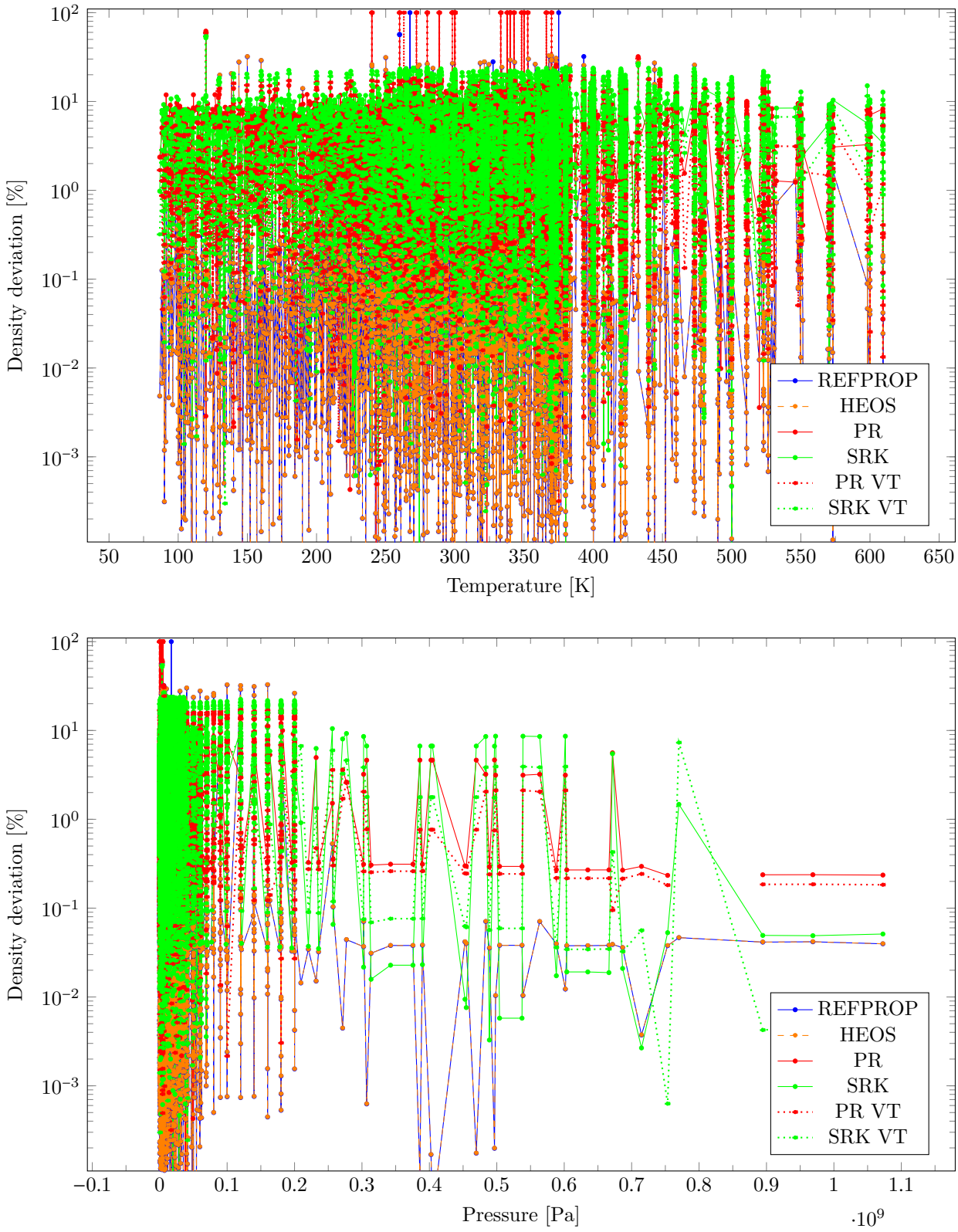


Figure 146: Density dependence on the temperature and pressure for fluid n-Propane

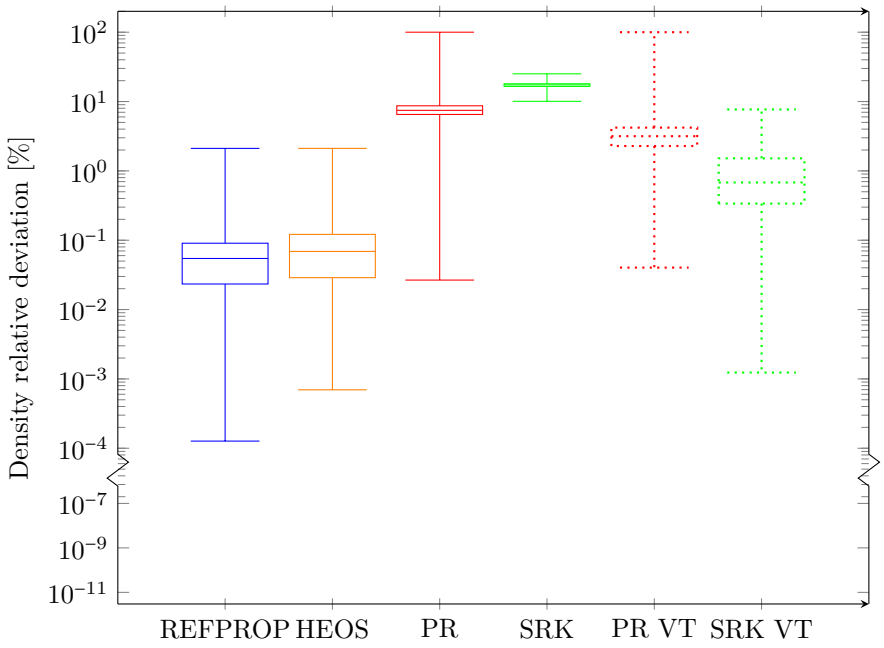


Figure 147: Relative density deviation to experimental data for fluid n-Undecane

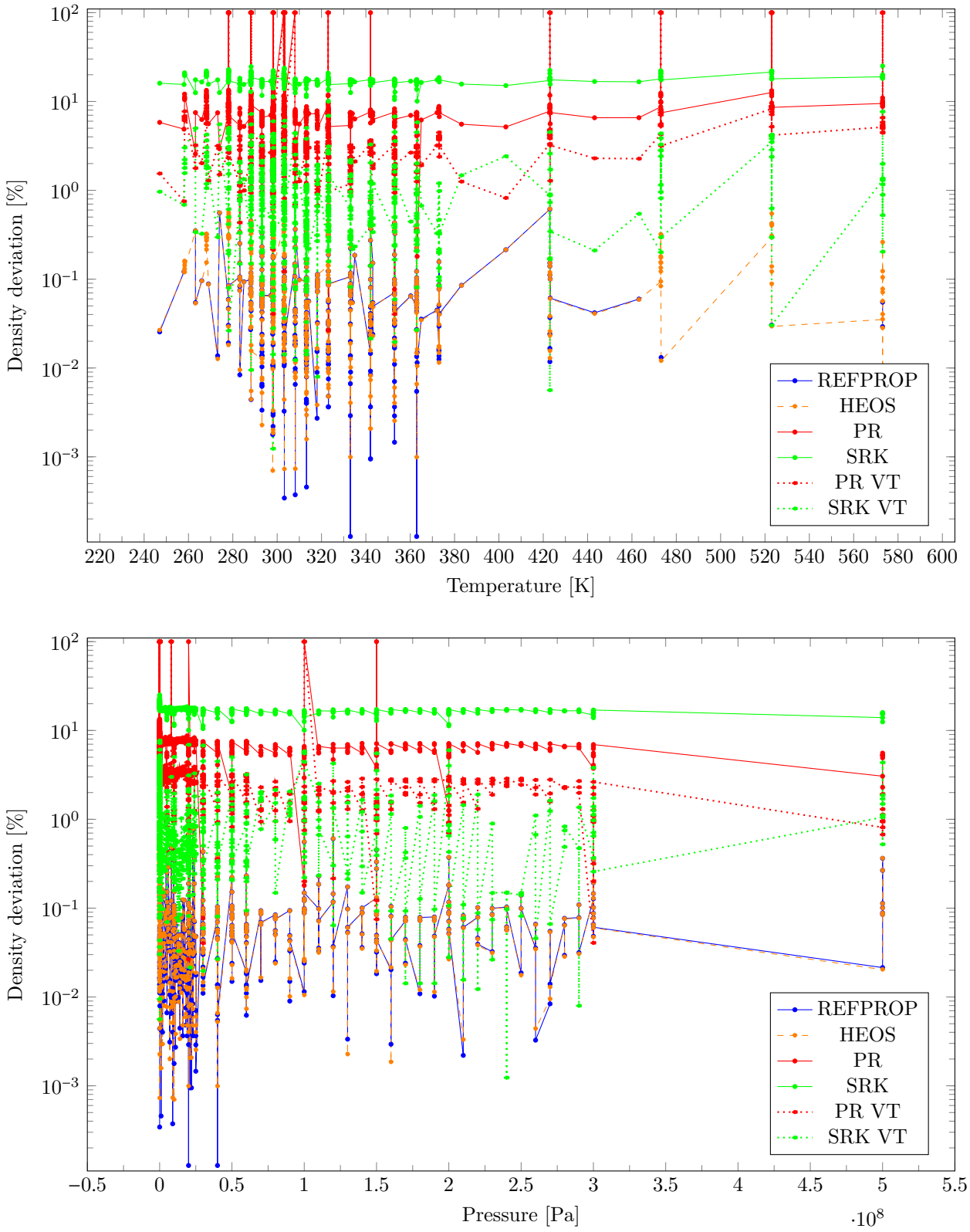


Figure 148: Density dependence on the temperature and pressure for fluid n-Undecane

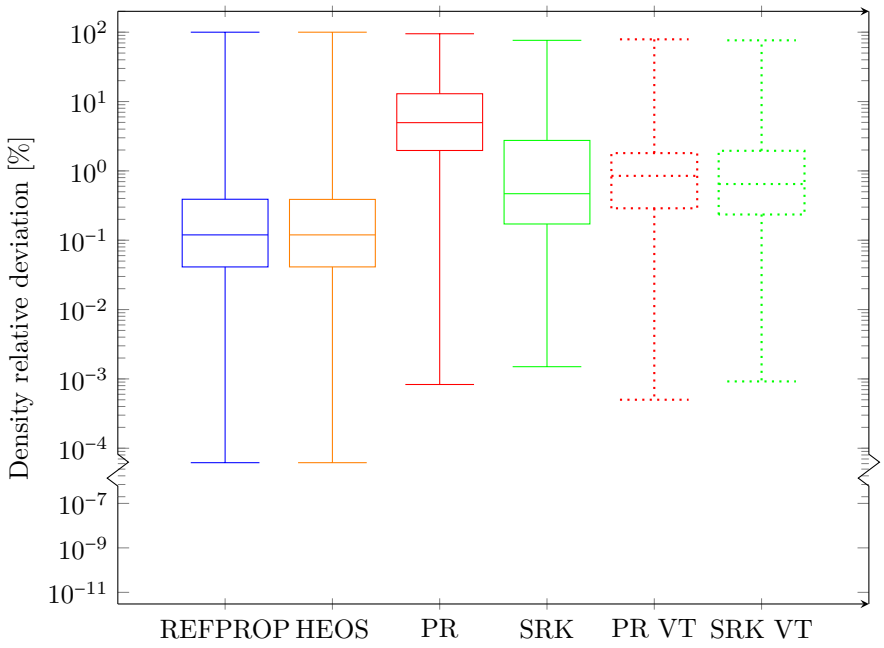


Figure 149: Relative density deviation to experimental data for fluid Neon

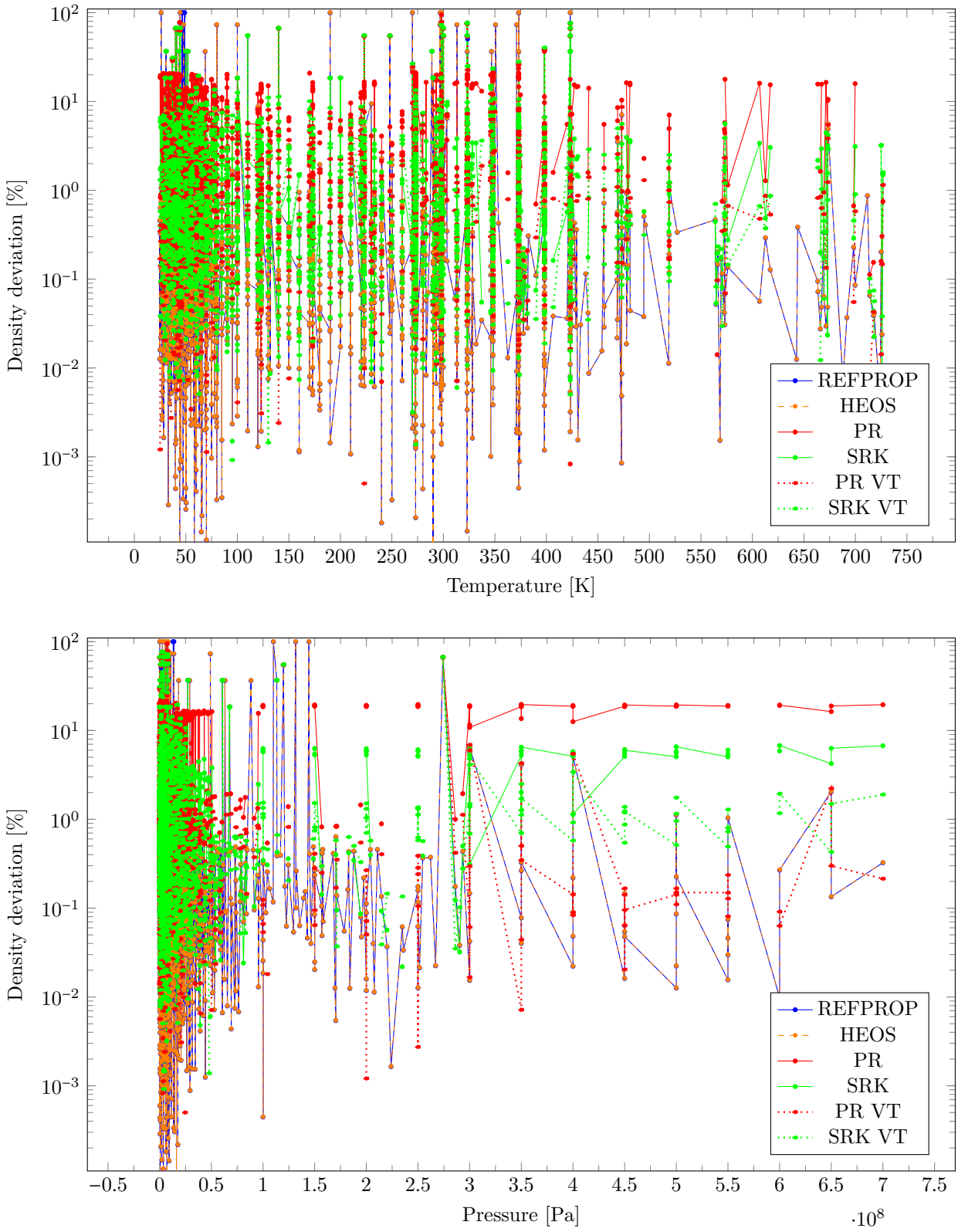


Figure 150: Density dependence on the temperature and pressure for fluid Neon

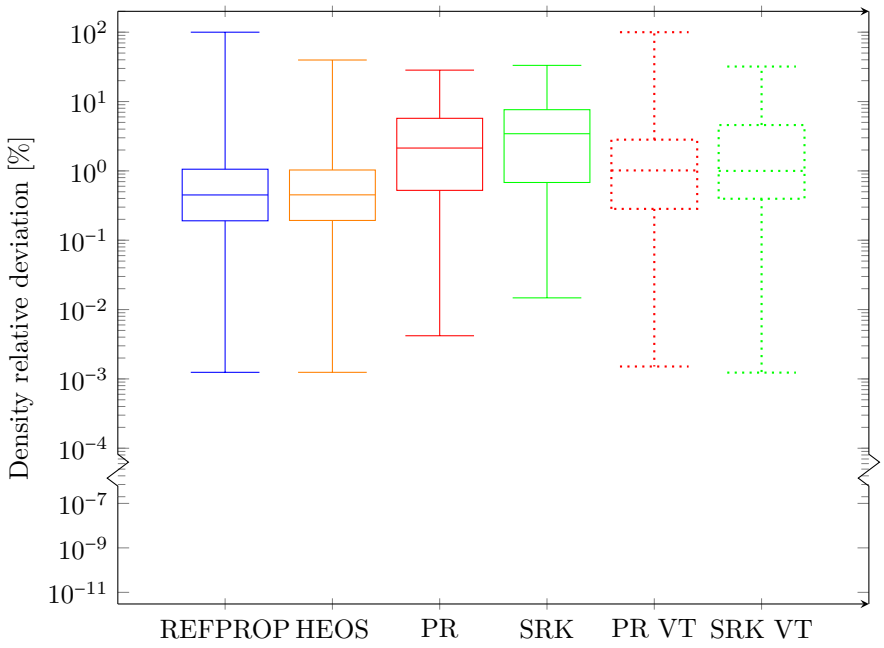


Figure 151: Relative density deviation to experimental data for fluid NEOPENTANE

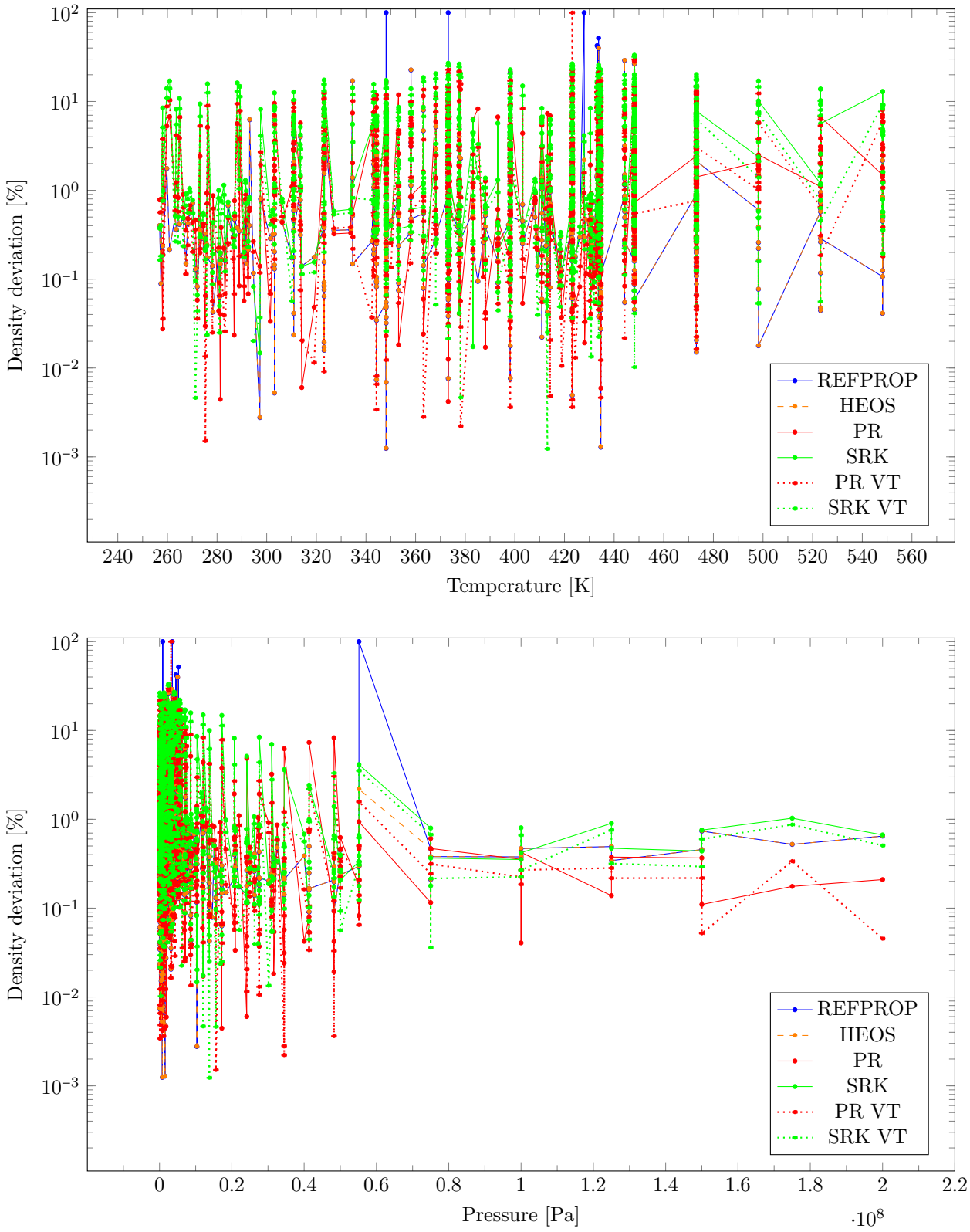


Figure 152: Density dependence on the temperature and pressure for fluid Neopentane

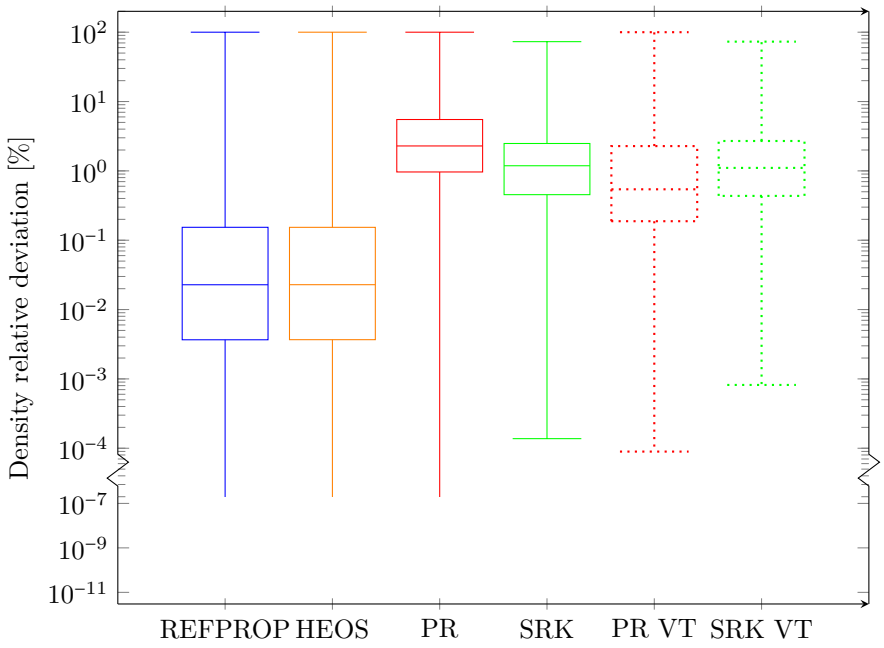
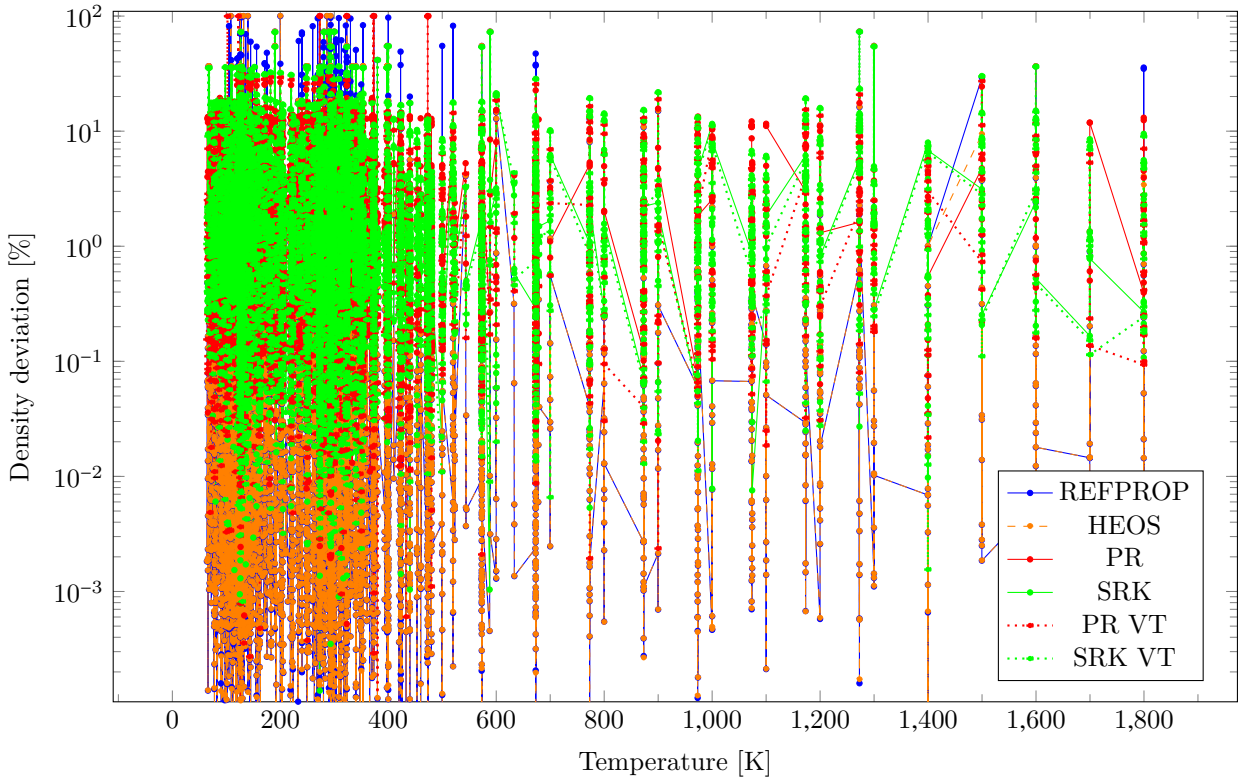


Figure 153: Relative density deviation to experimental data for fluid Nitrogen



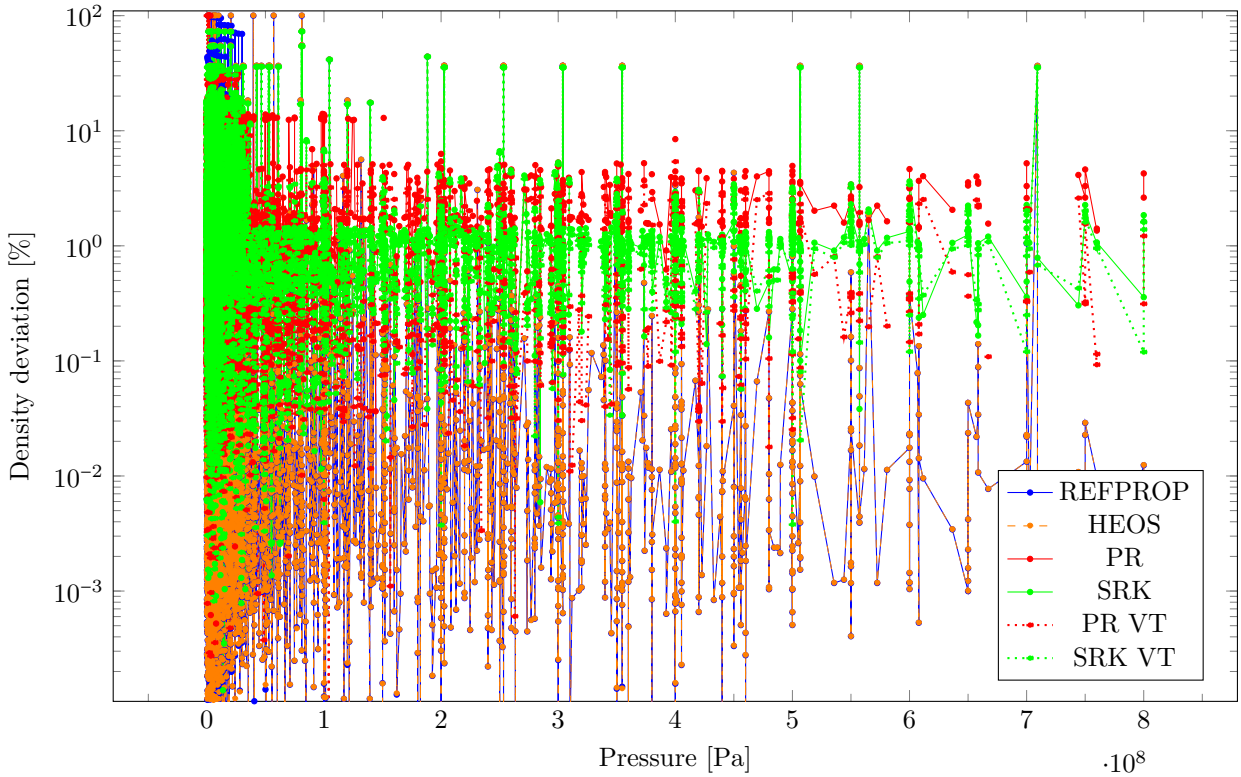


Figure 154: Density dependence on the temperature and pressure for fluid Nitrogen

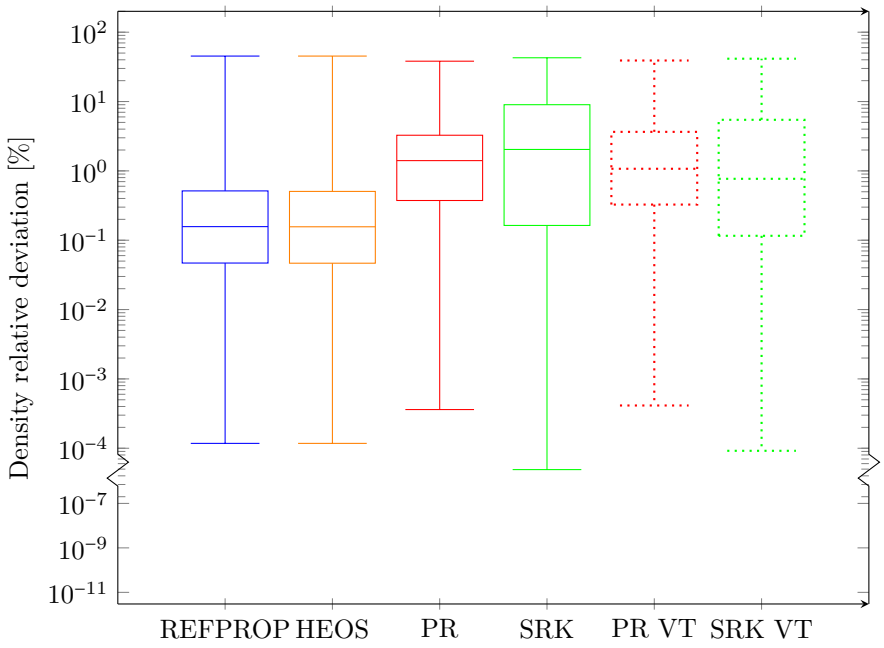


Figure 155: Relative density deviation to experimental data for fluid NitrousOxide

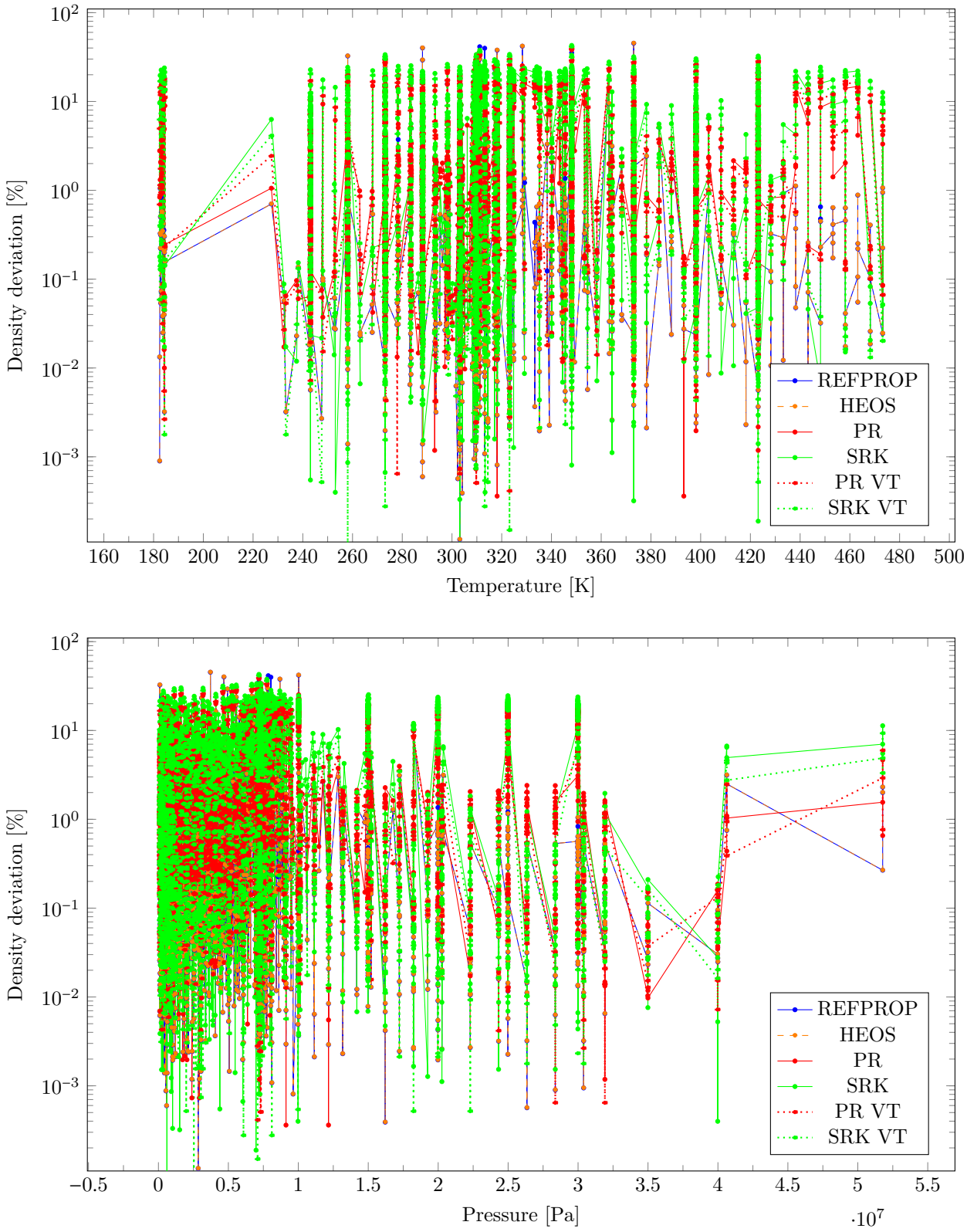


Figure 156: Density dependence on the temperature and pressure for fluid NitrousOxide

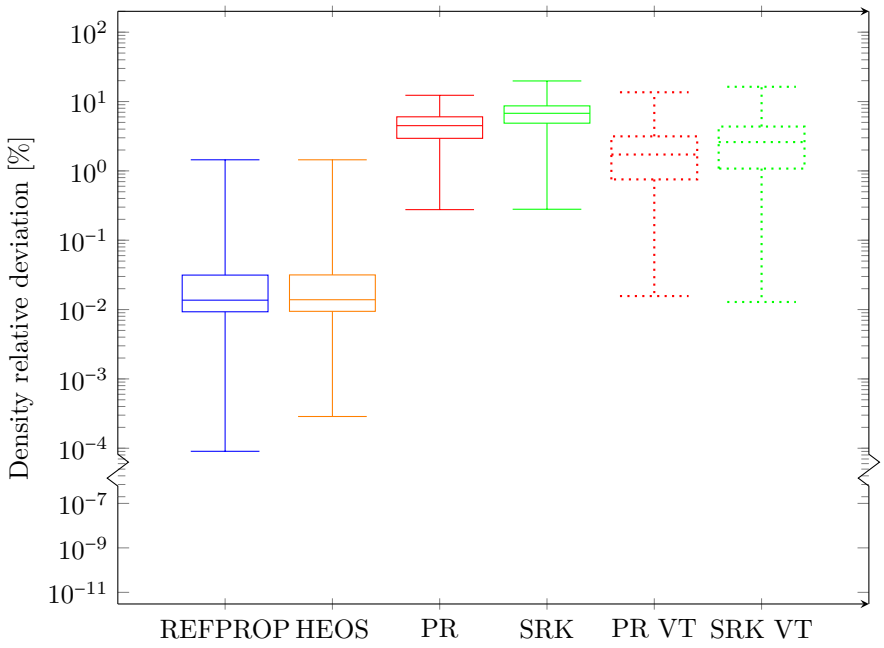


Figure 157: Relative density deviation to experimental data for fluid Novec649

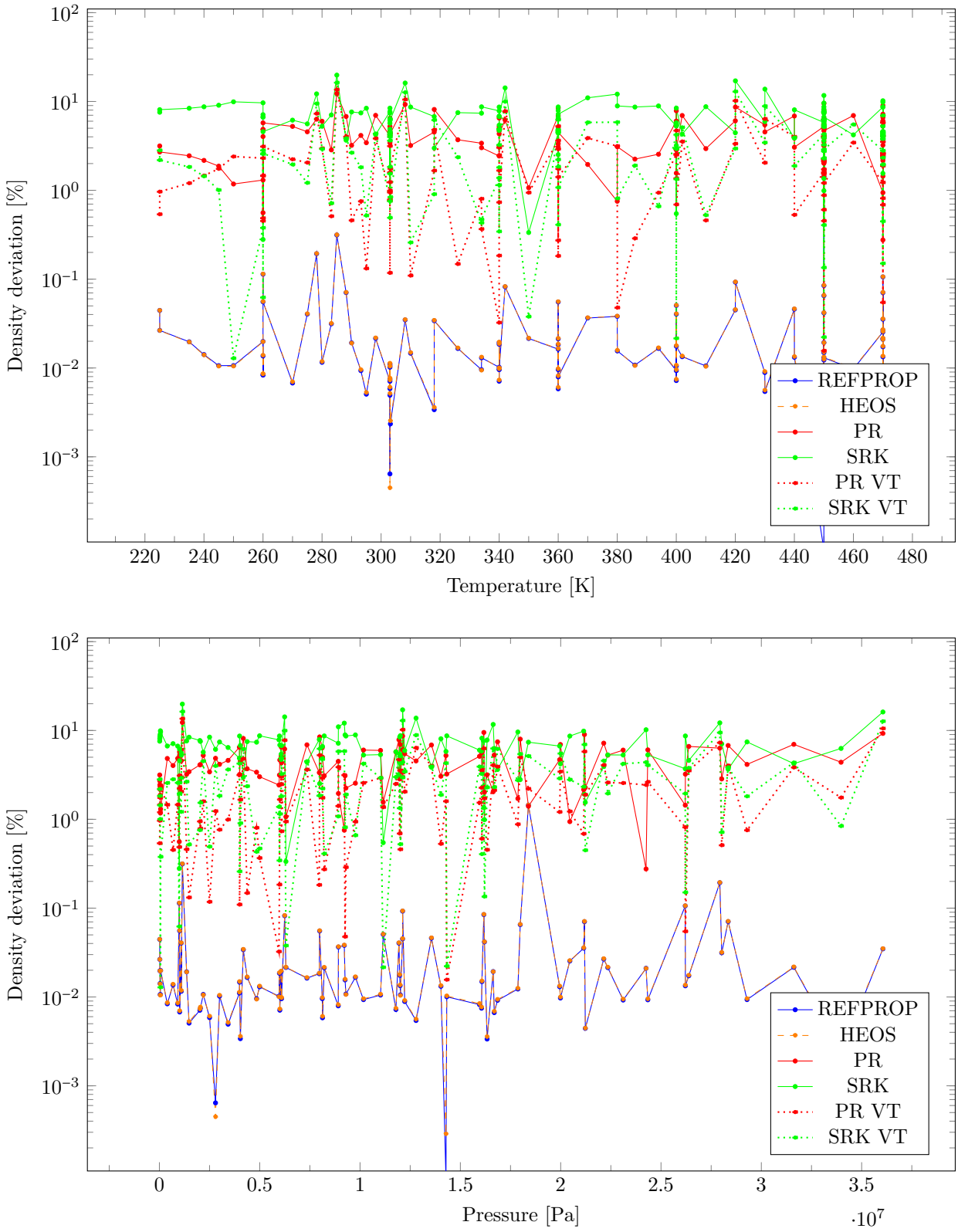


Figure 158: Density dependence on the temperature and pressure for fluid Novec649

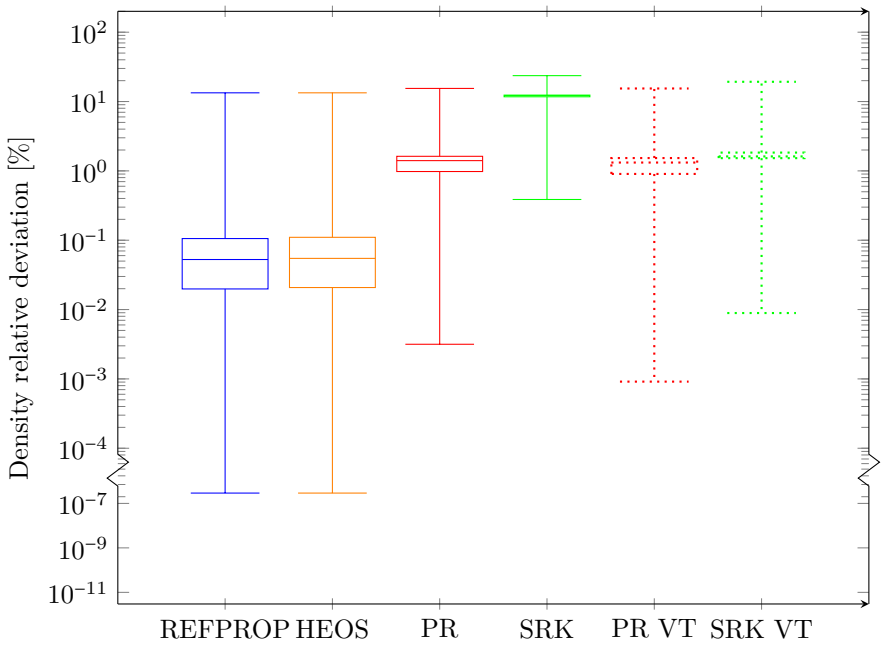


Figure 159: Relative density deviation to experimental data for fluid o-Xylene

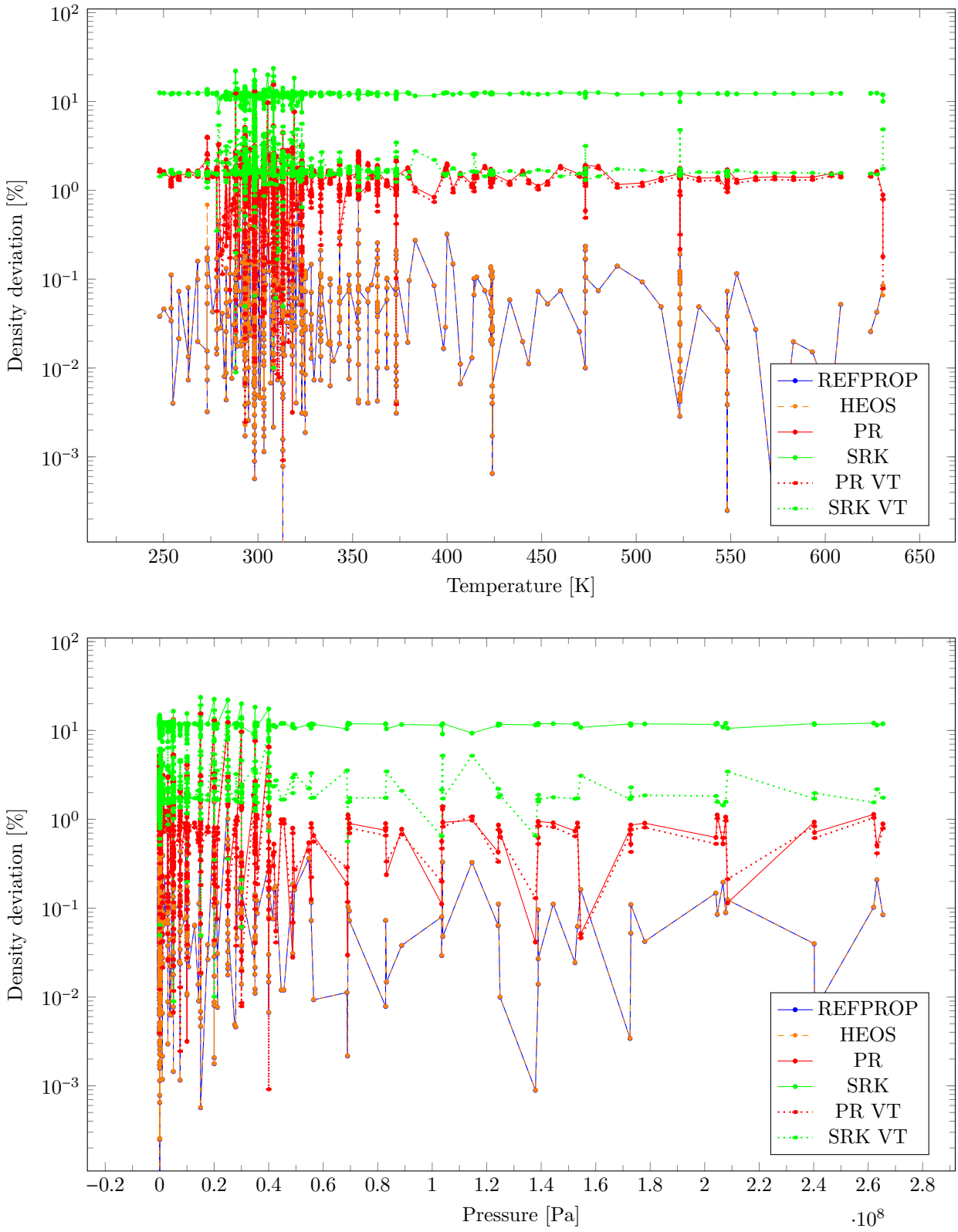


Figure 160: Density dependence on the temperature and pressure for fluid o-Xylene

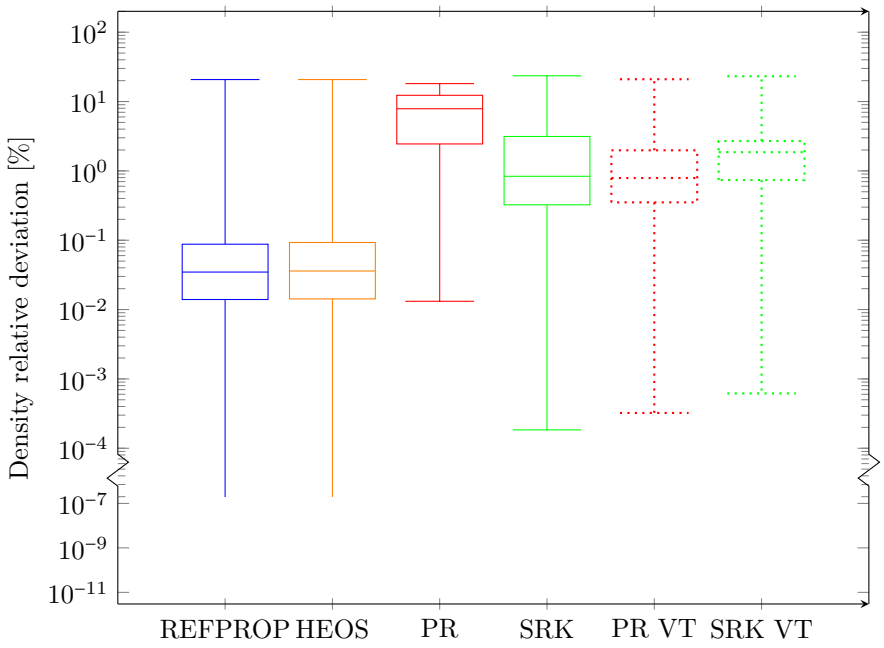


Figure 161: Relative density deviation to experimental data for fluid Oxygen

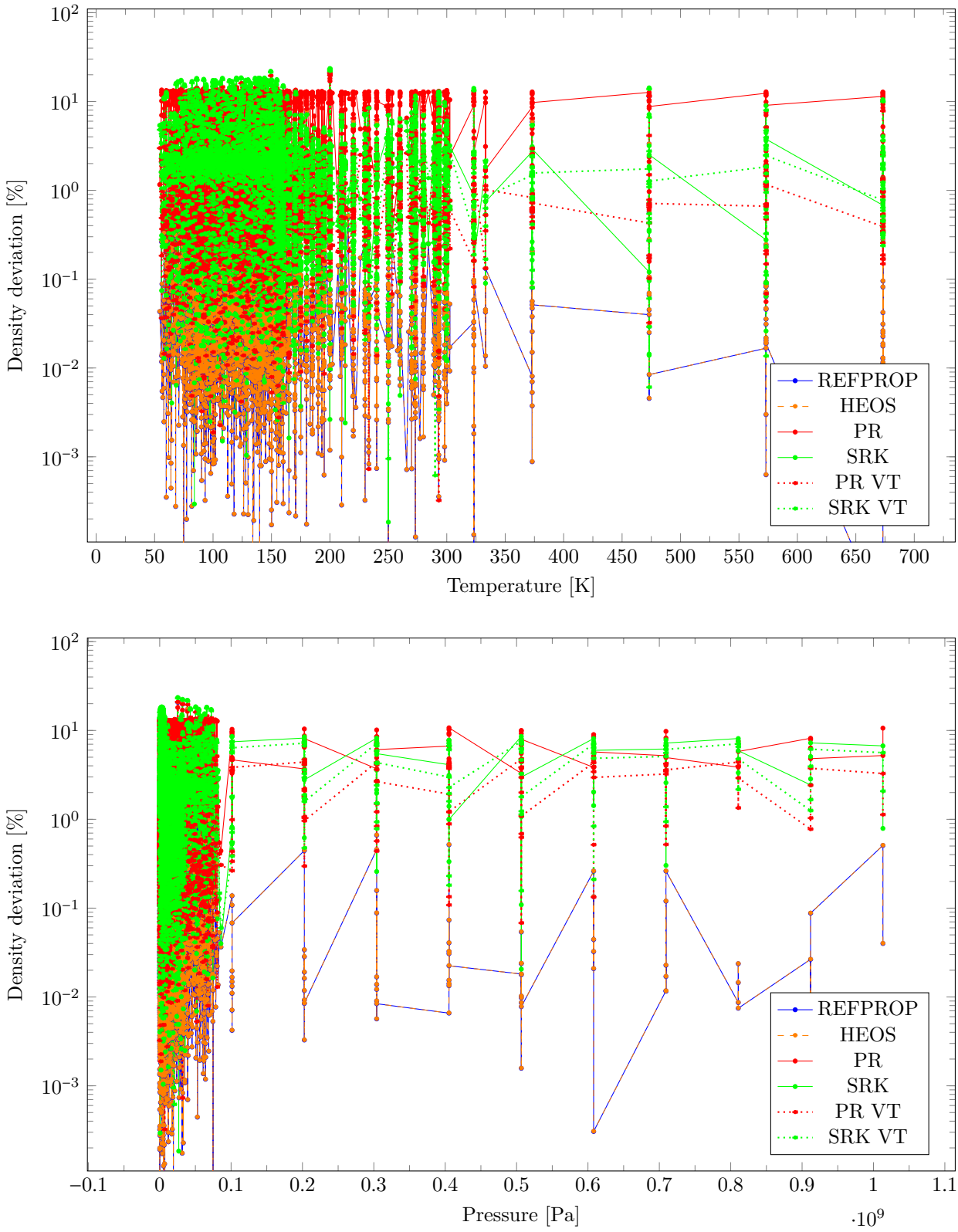


Figure 162: Density dependence on the temperature and pressure for fluid Oxygen

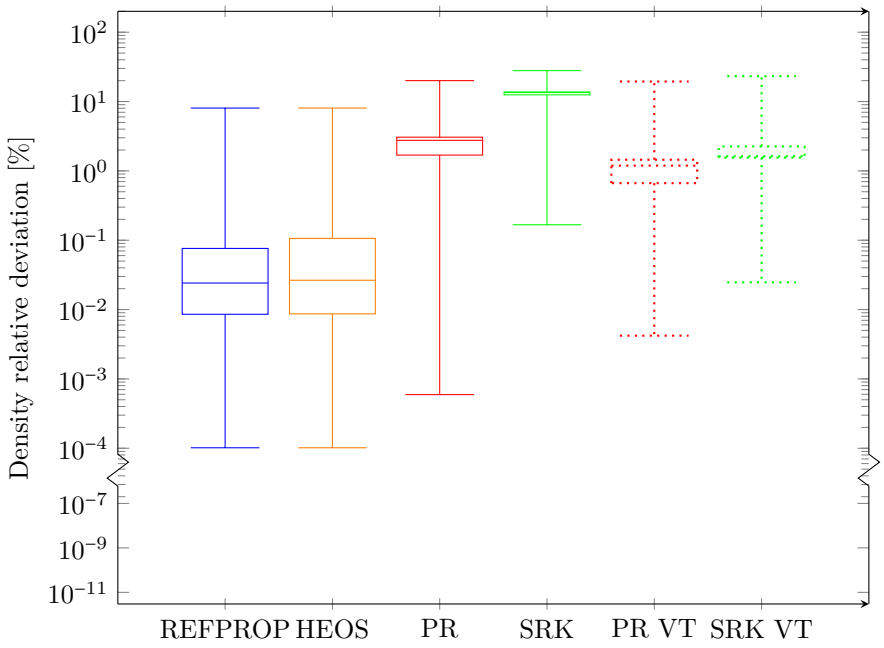


Figure 163: Relative density deviation to experimental data for fluid p-Xylene

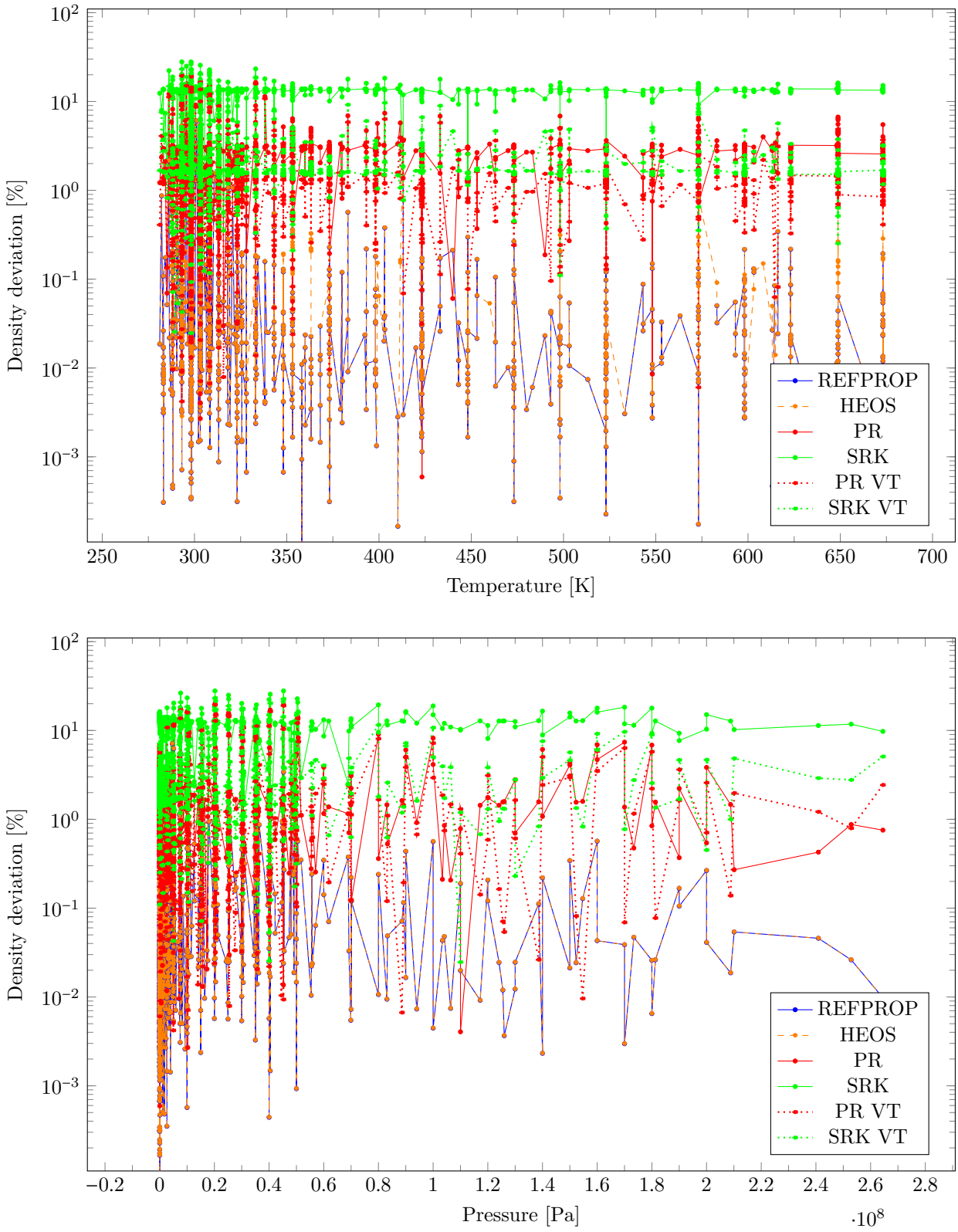


Figure 164: Density dependence on the temperature and pressure for fluid p-Xylene

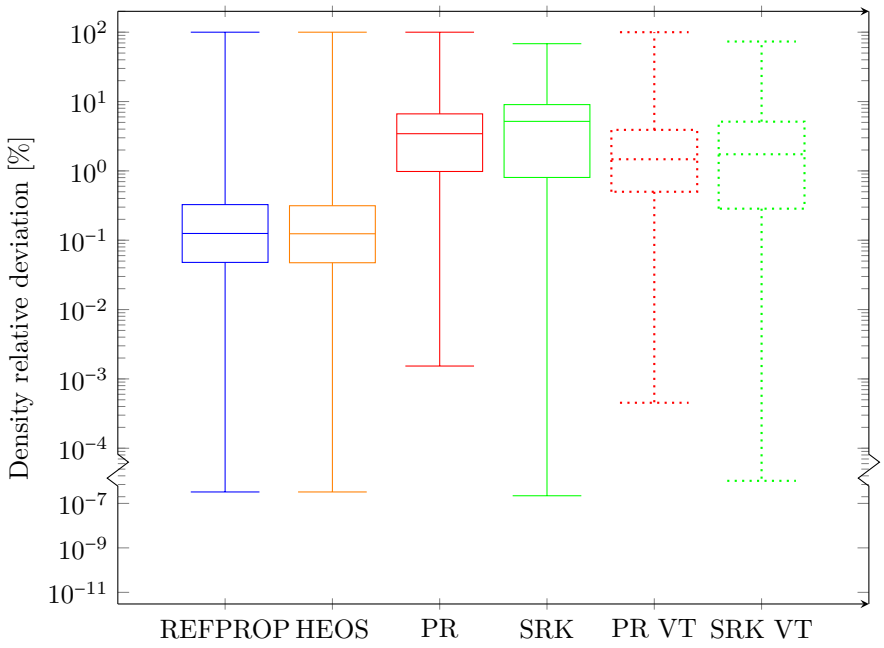


Figure 165: Relative density deviation to experimental data for fluid Propylene

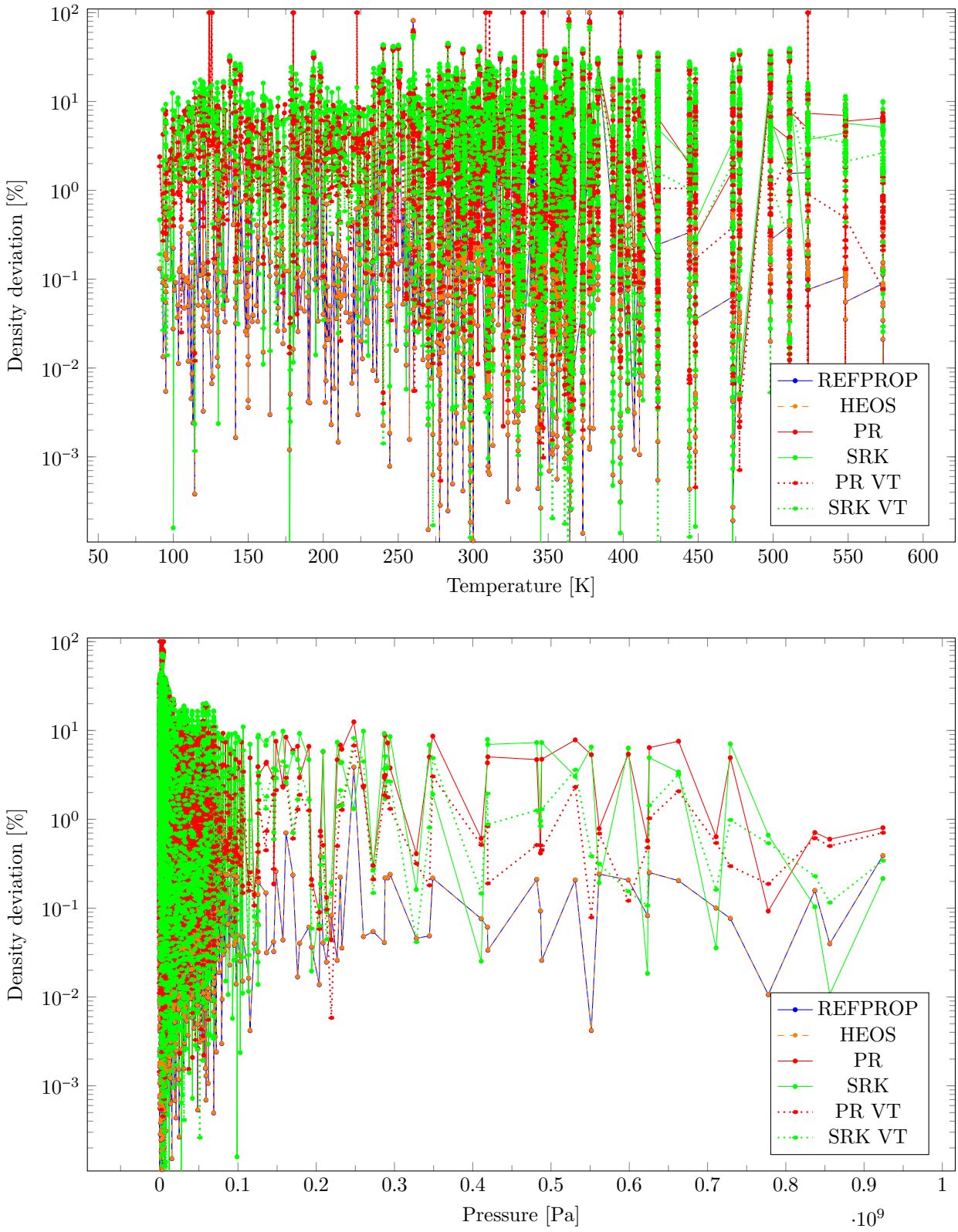


Figure 166: Density dependence on the temperature and pressure for fluid Propylene

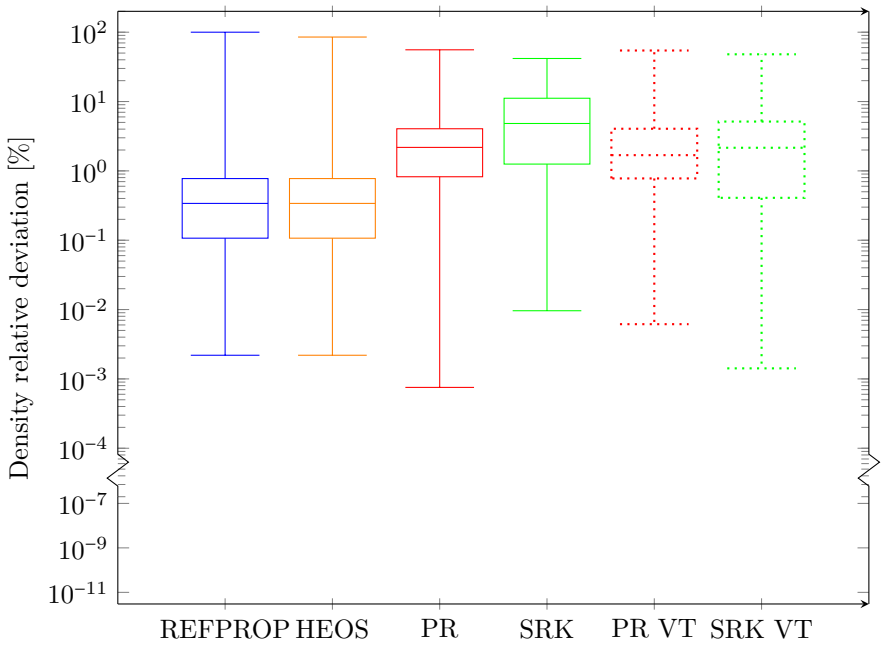


Figure 167: Relative density deviation to experimental data for fluid Propyne

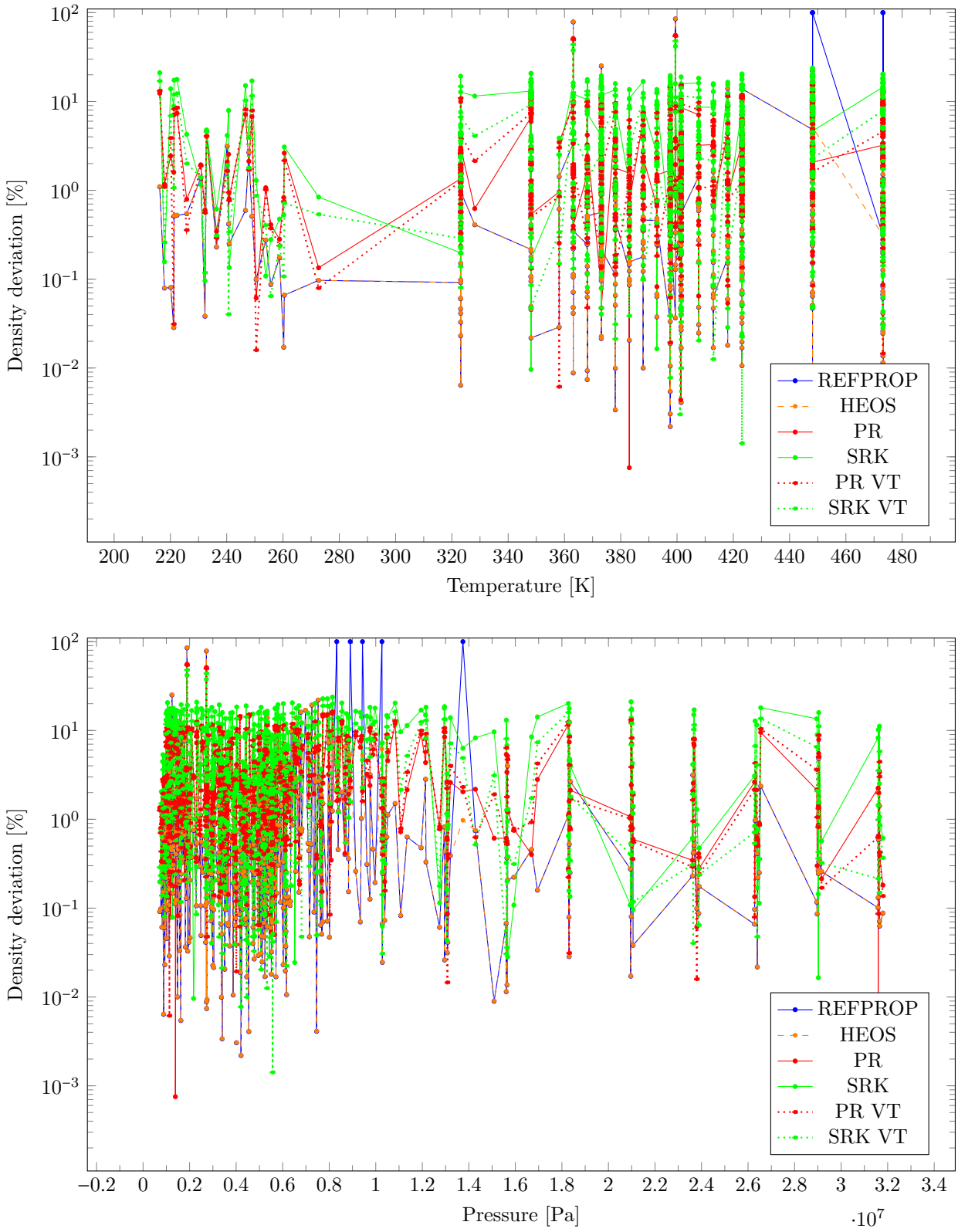


Figure 168: Density dependence on the temperature and pressure for fluid Propyne

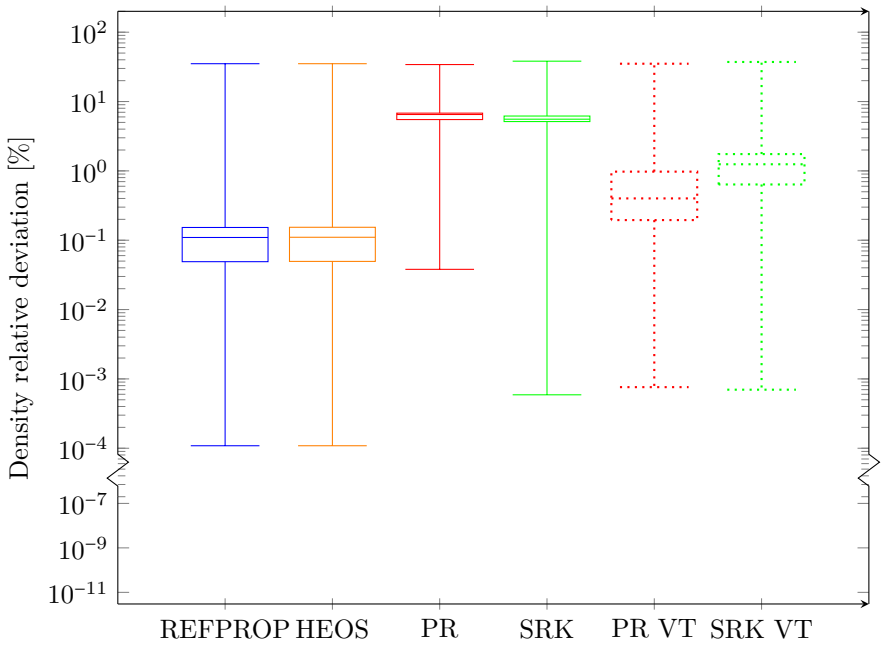


Figure 169: Relative density deviation to experimental data for fluid R11

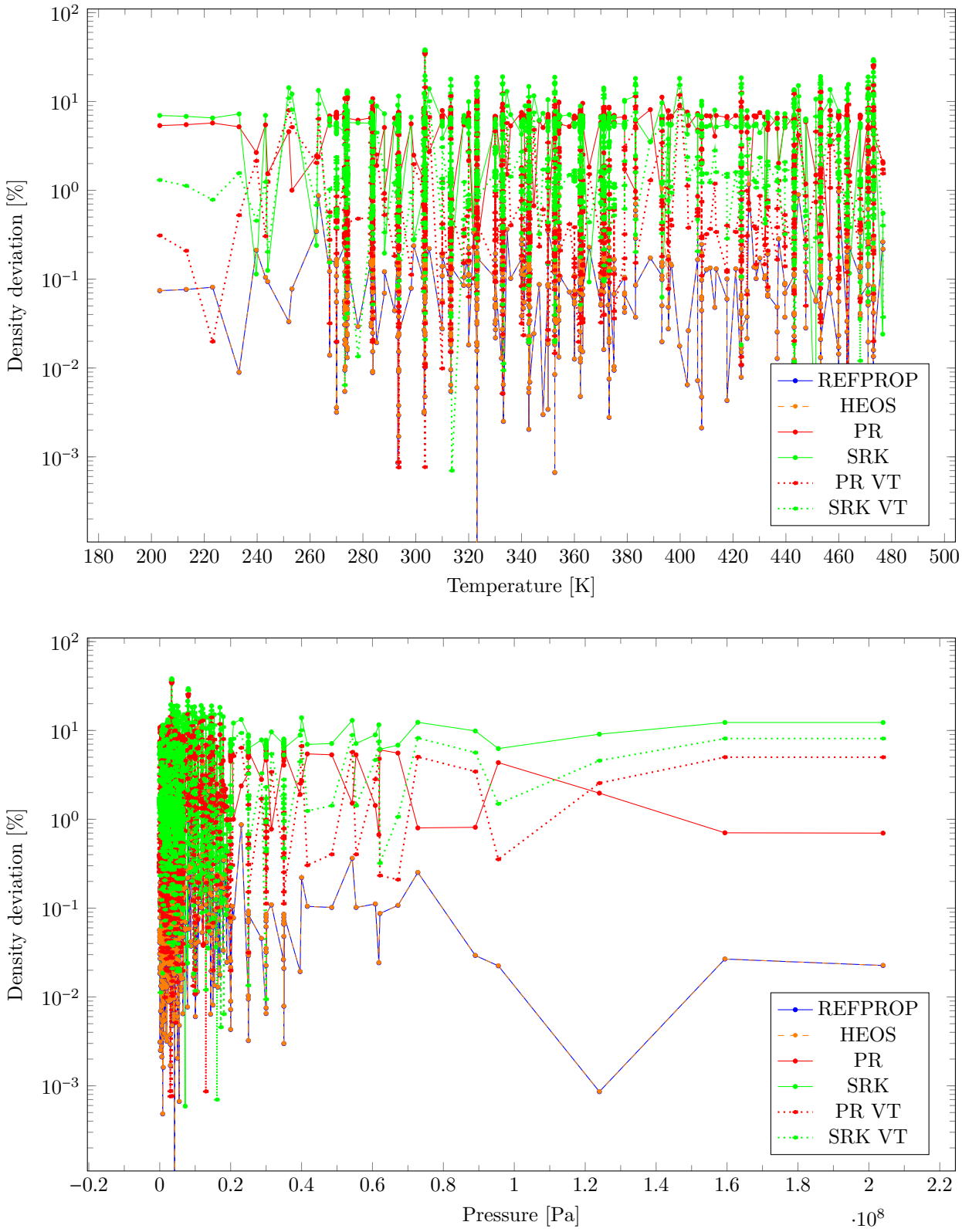


Figure 170: Density dependence on the temperature and pressure for fluid R11

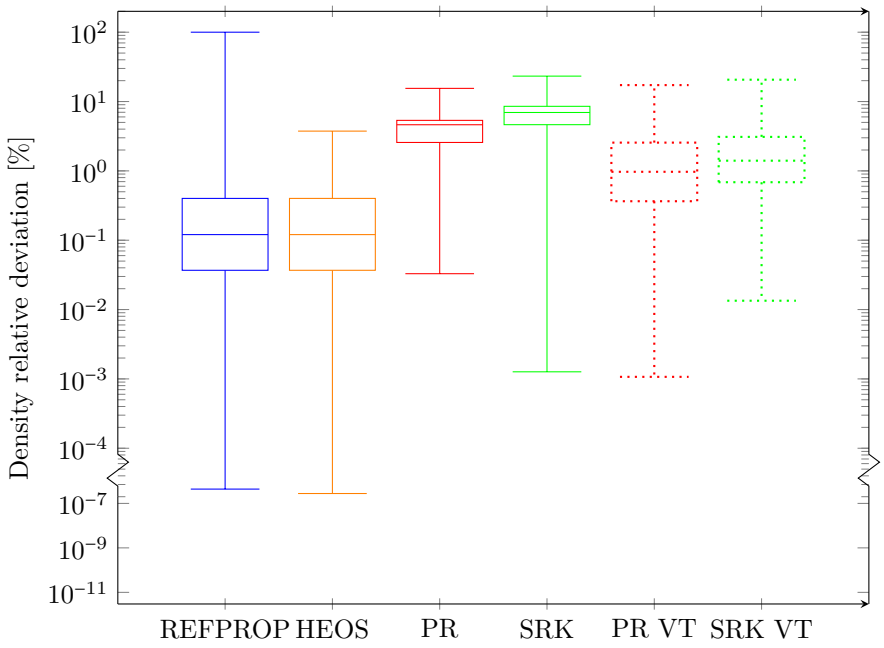


Figure 171: Relative density deviation to experimental data for fluid R113

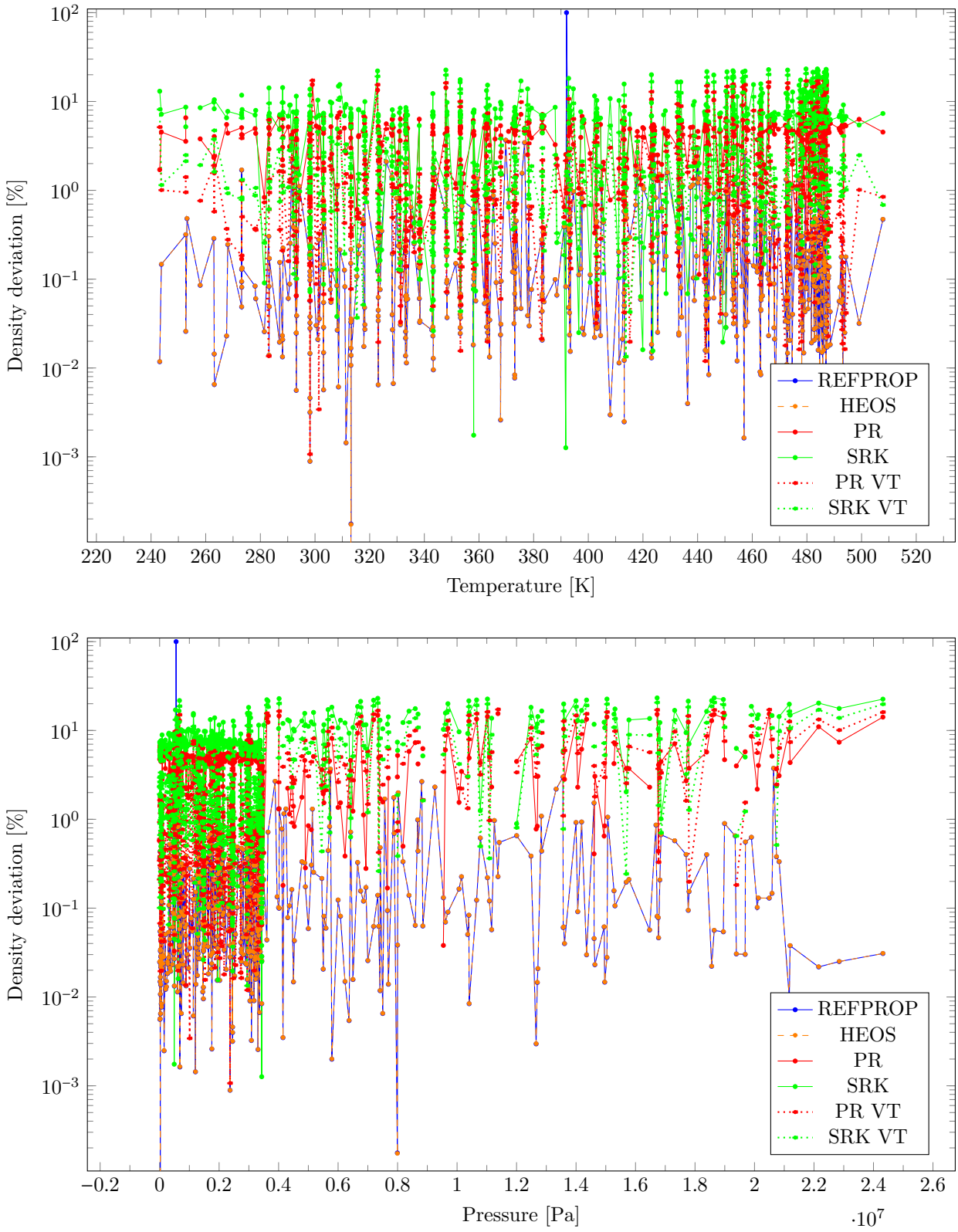


Figure 172: Density dependence on the temperature and pressure for fluid R113

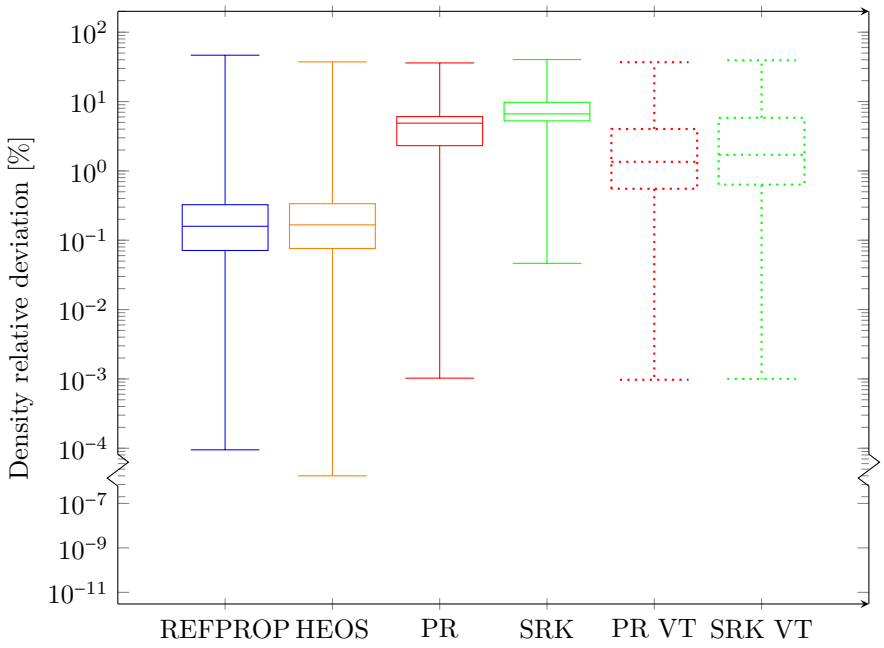


Figure 173: Relative density deviation to experimental data for fluid R114

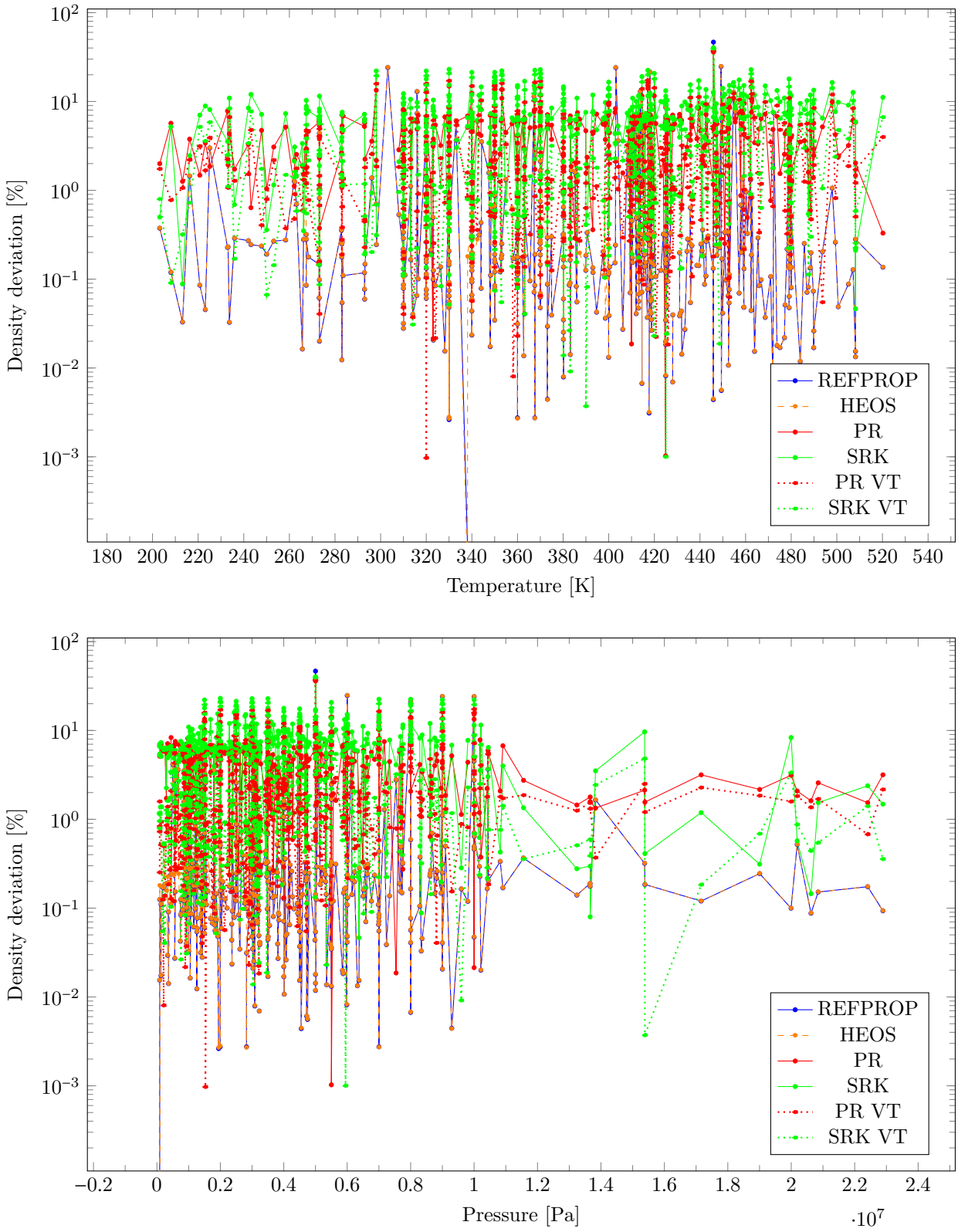


Figure 174: Density dependence on the temperature and pressure for fluid R114

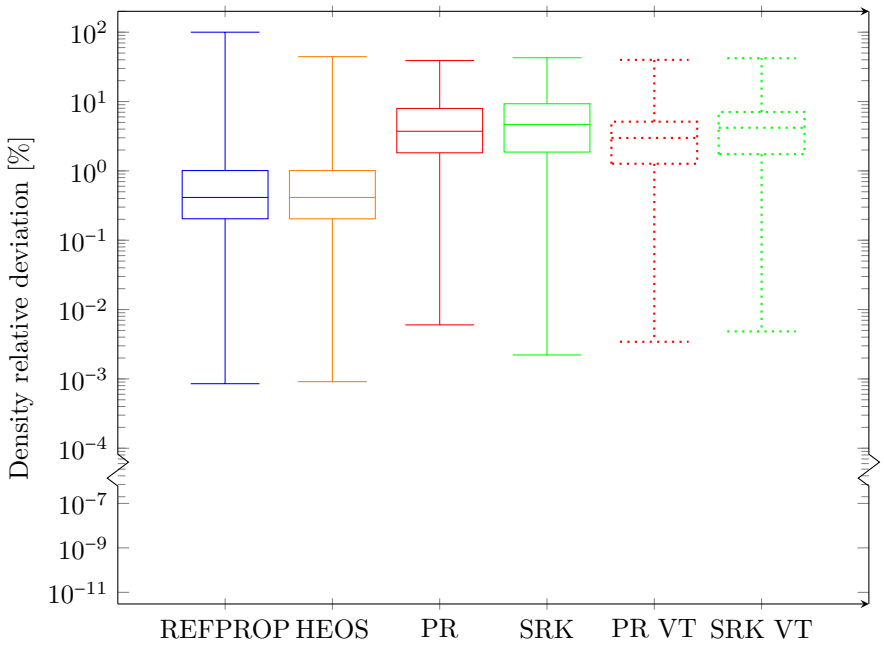


Figure 175: Relative density deviation to experimental data for fluid R115

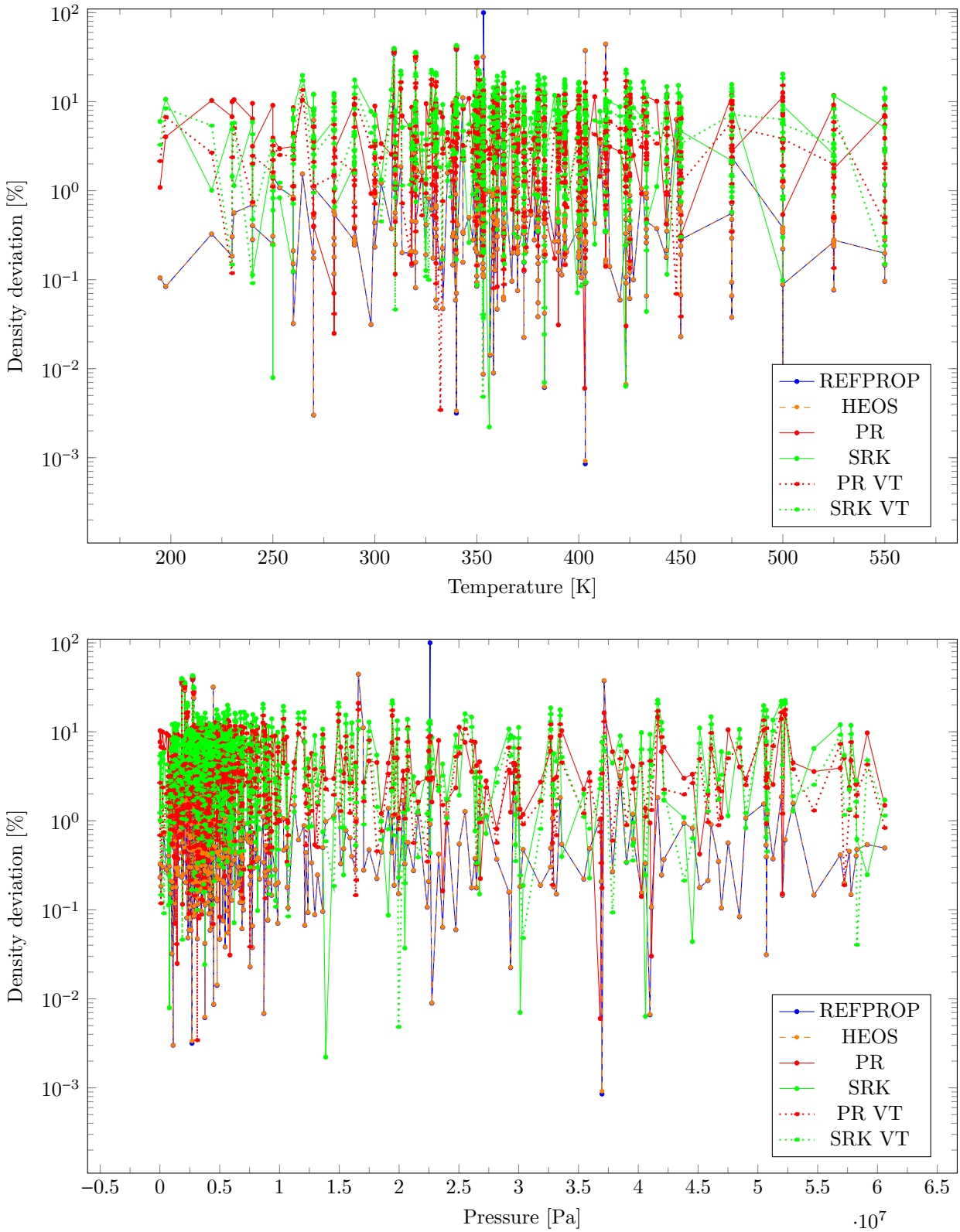


Figure 176: Density dependence on the temperature and pressure for fluid R115

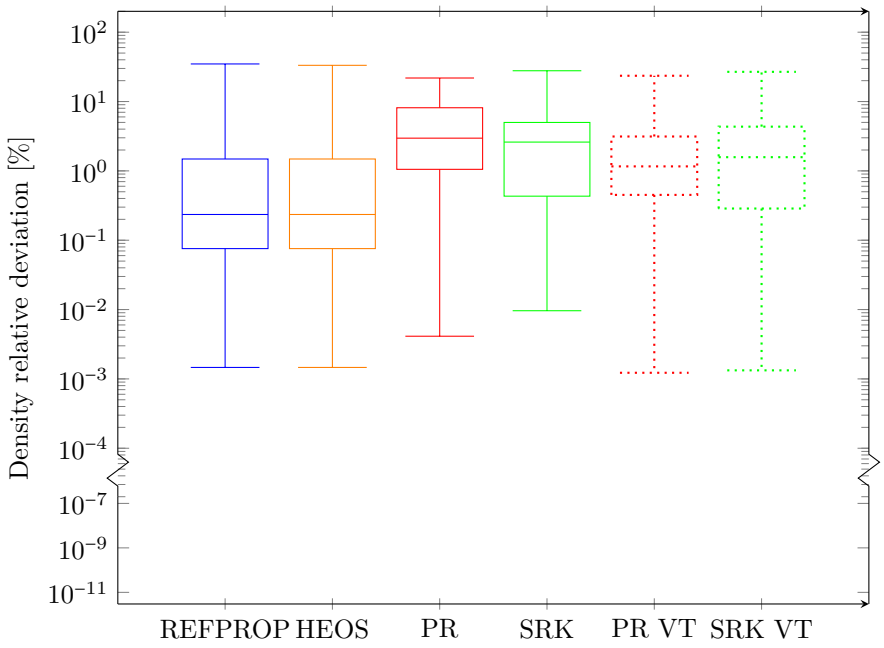


Figure 177: Relative density deviation to experimental data for fluid R116

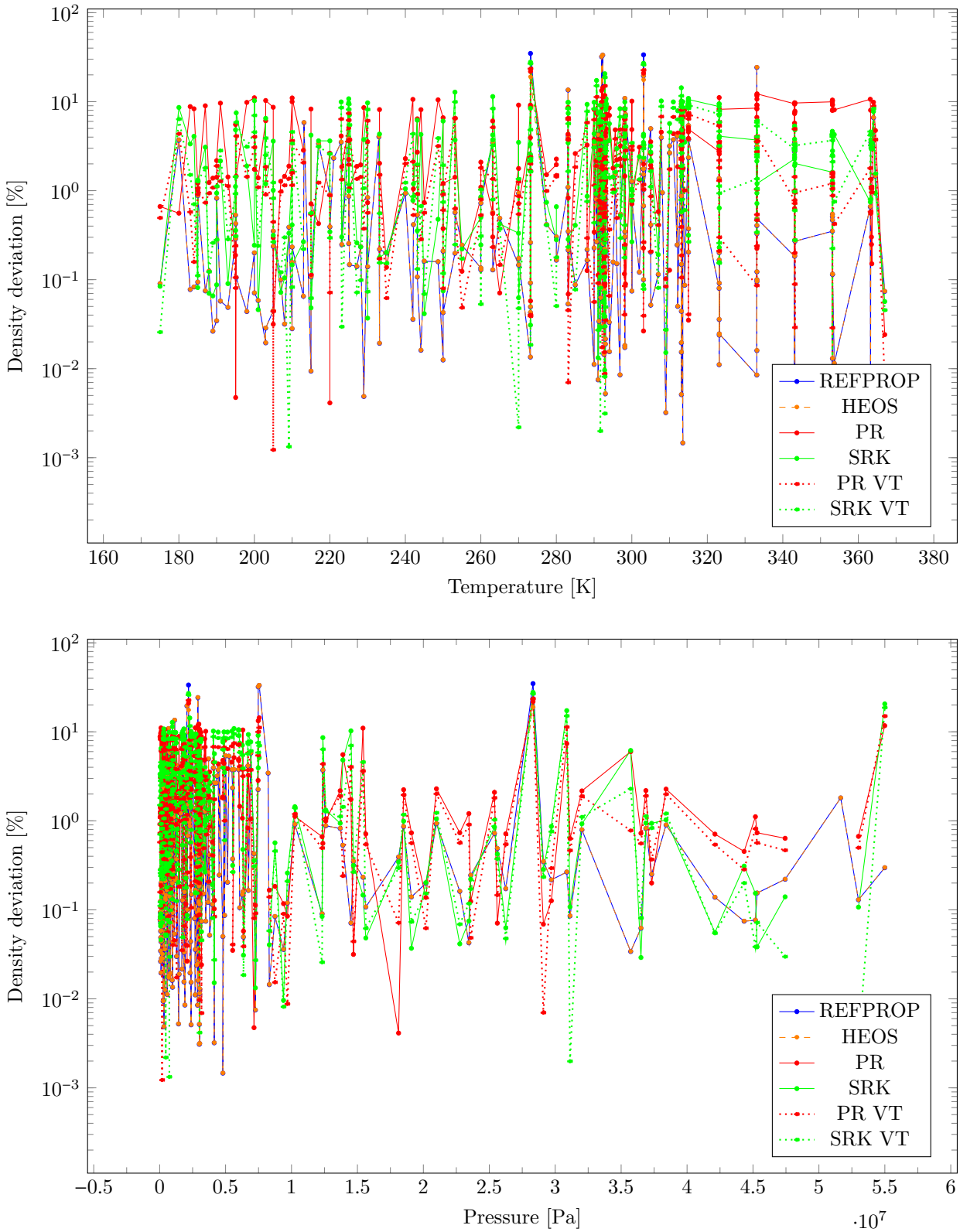


Figure 178: Density dependence on the temperature and pressure for fluid R116

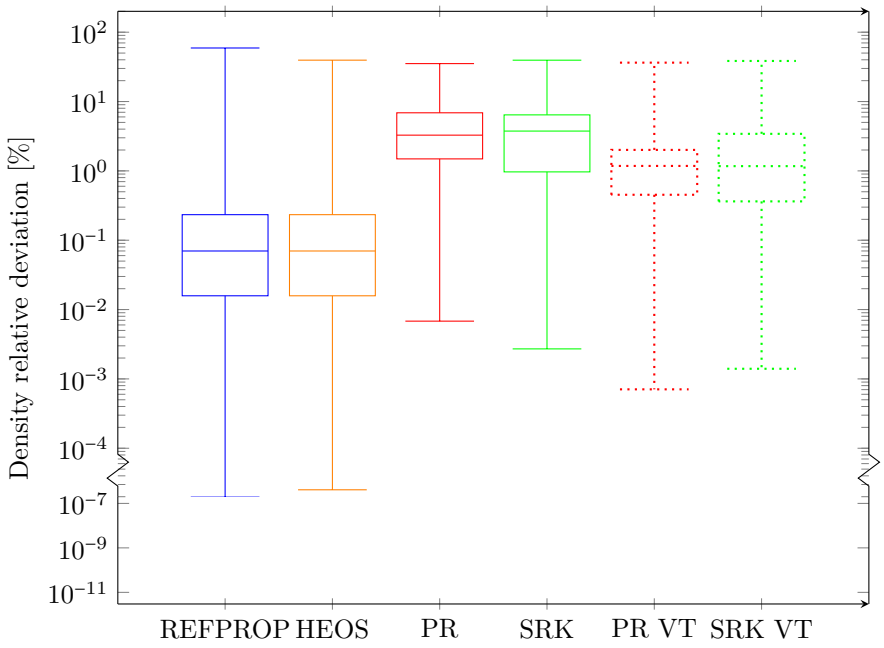


Figure 179: Relative density deviation to experimental data for fluid R12

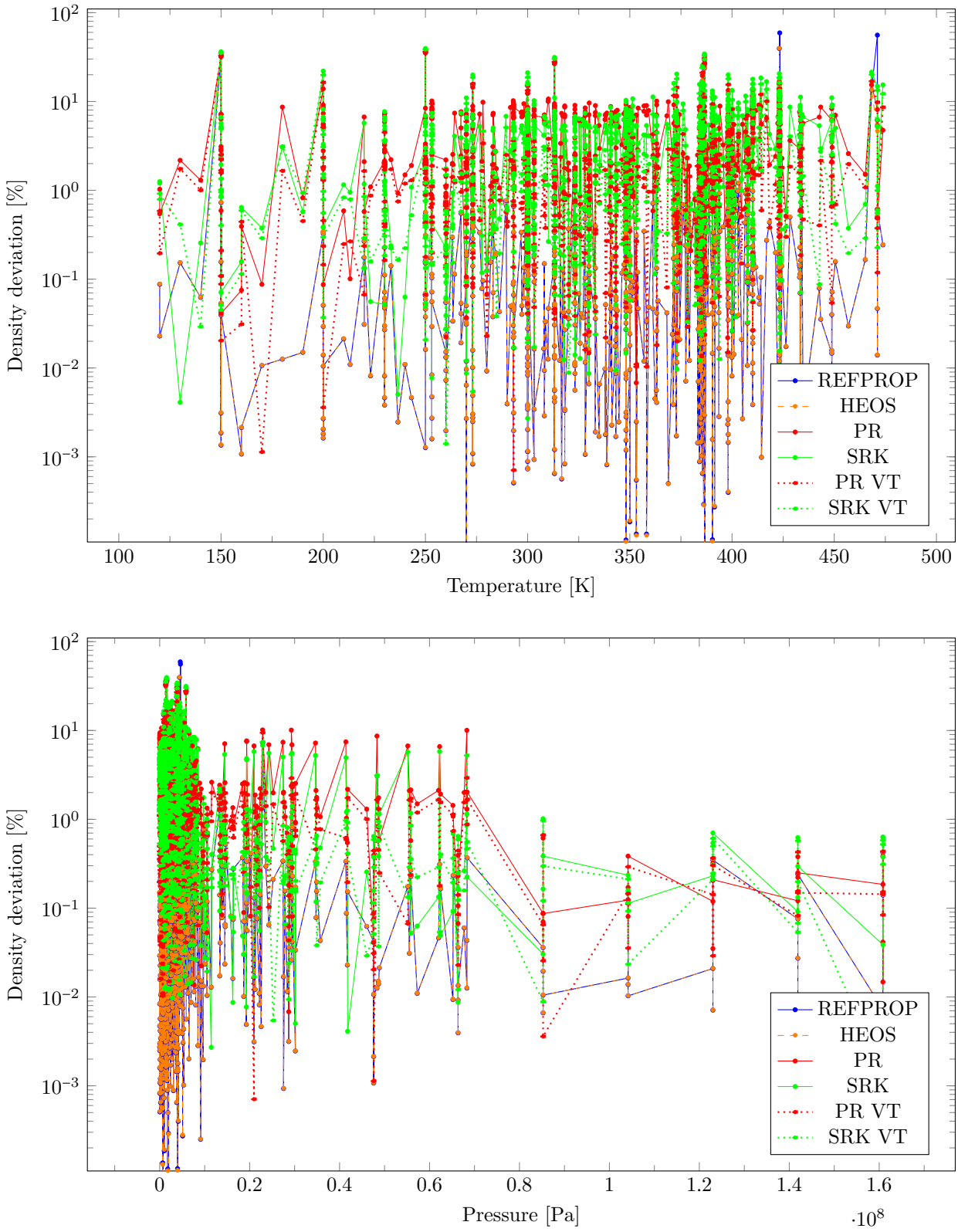


Figure 180: Density dependence on the temperature and pressure for fluid R12

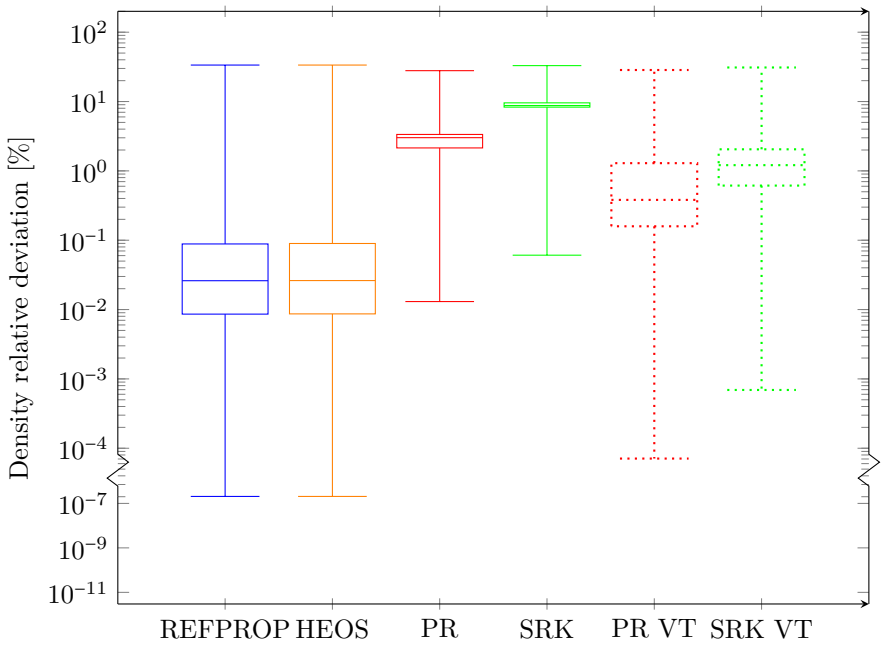


Figure 181: Relative density deviation to experimental data for fluid R123

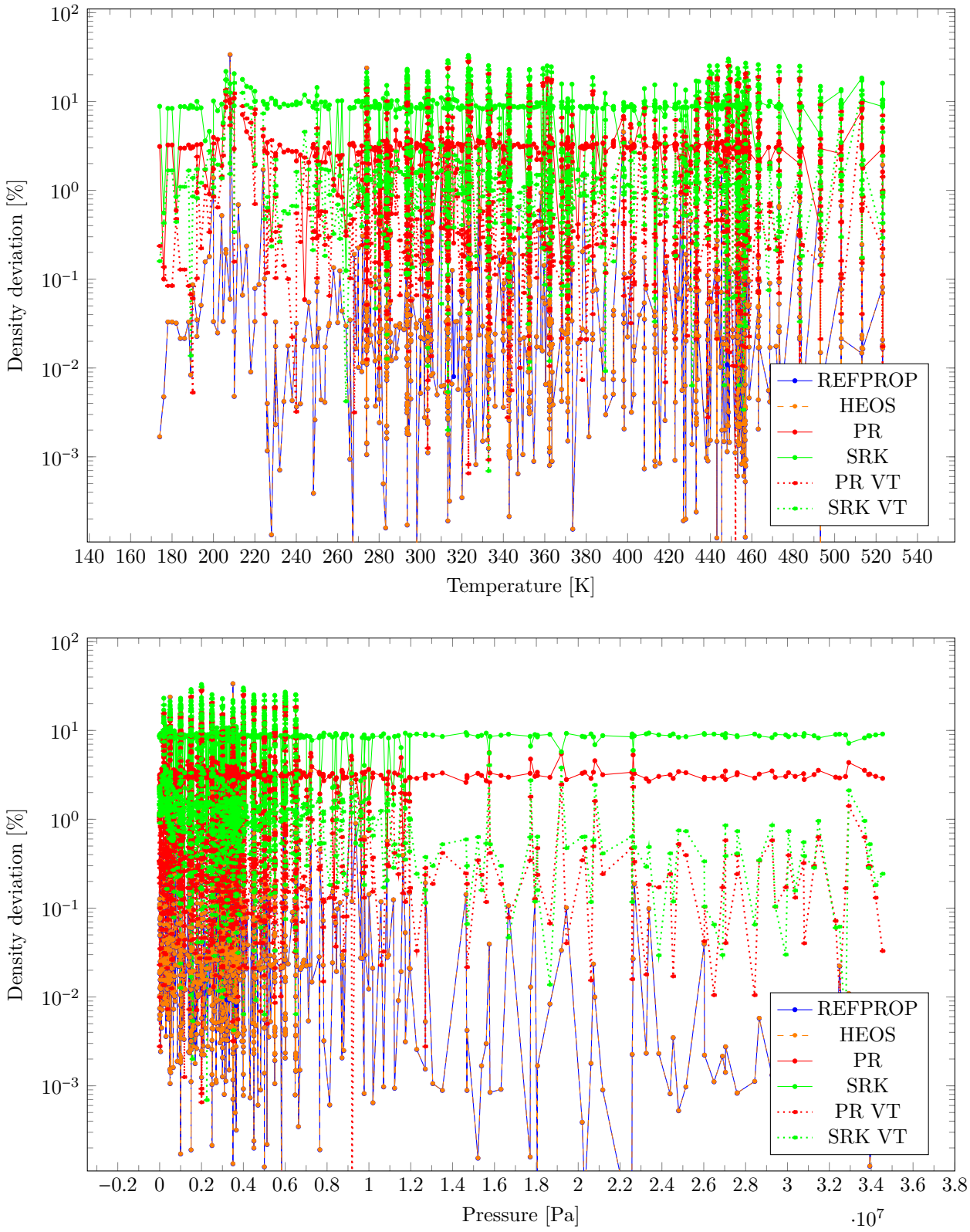


Figure 182: Density dependence on the temperature and pressure for fluid R123

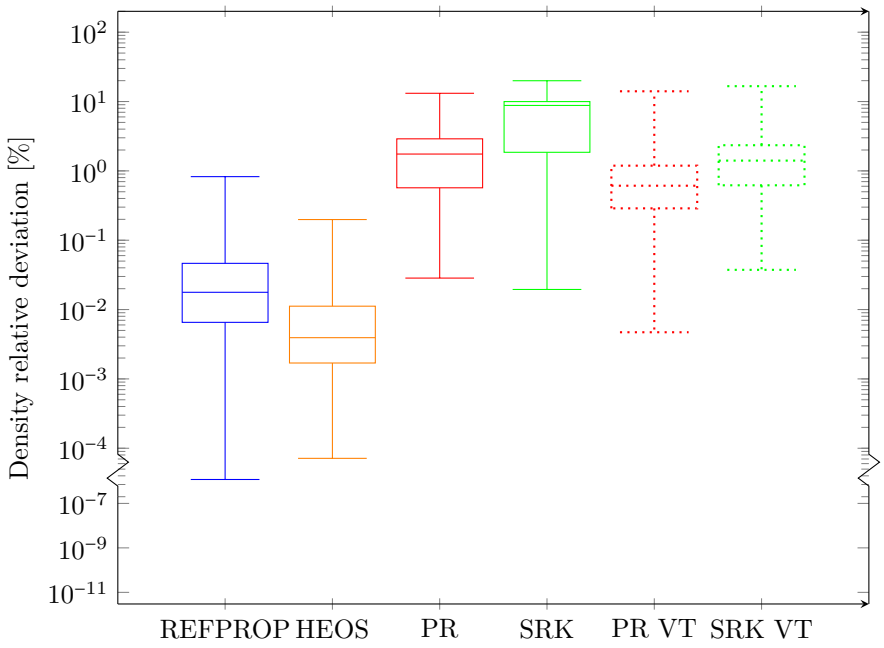


Figure 183: Relative density deviation to experimental data for fluid R1233zd(E)

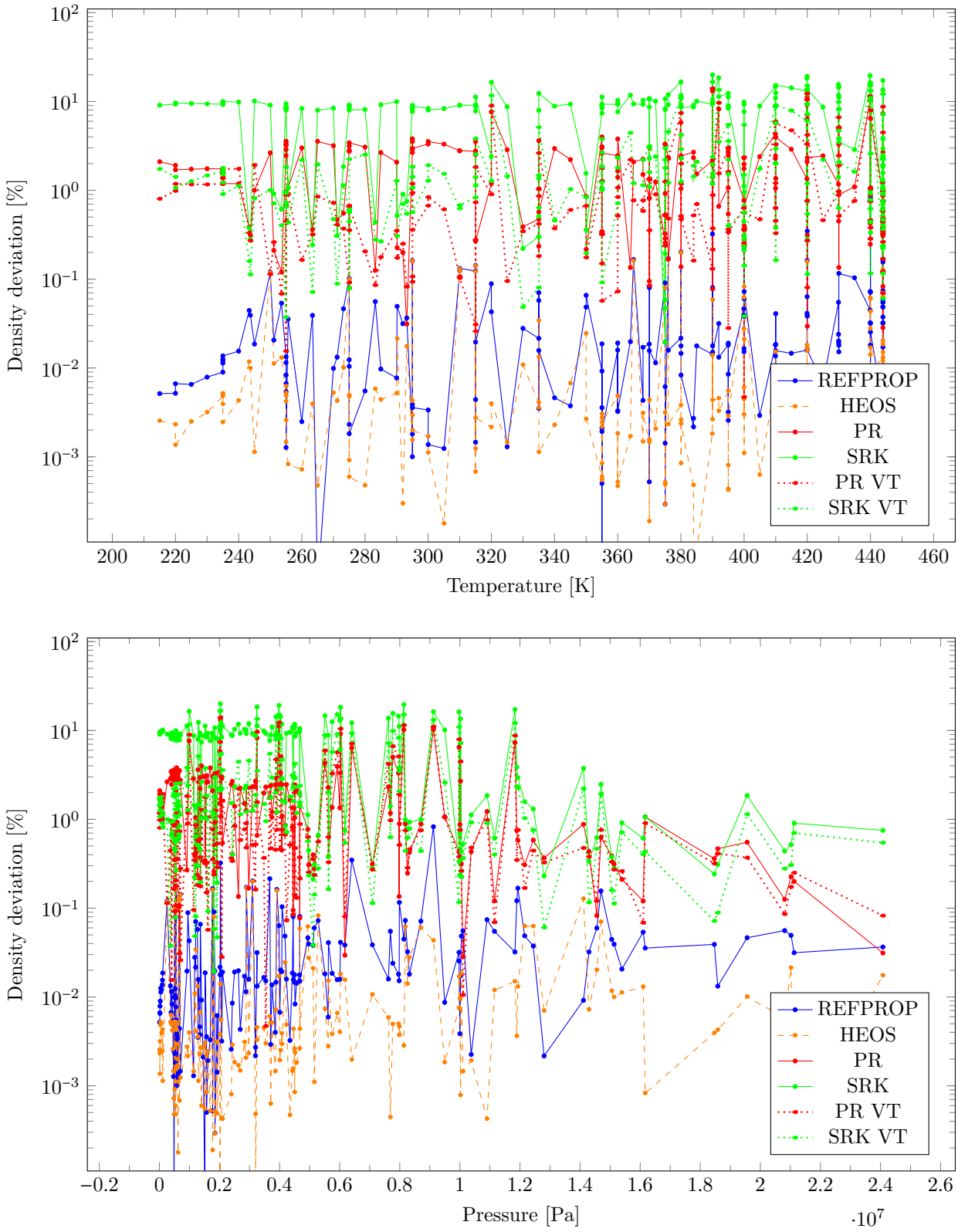


Figure 184: Density dependence on the temperature and pressure for fluid R1233zd(E)

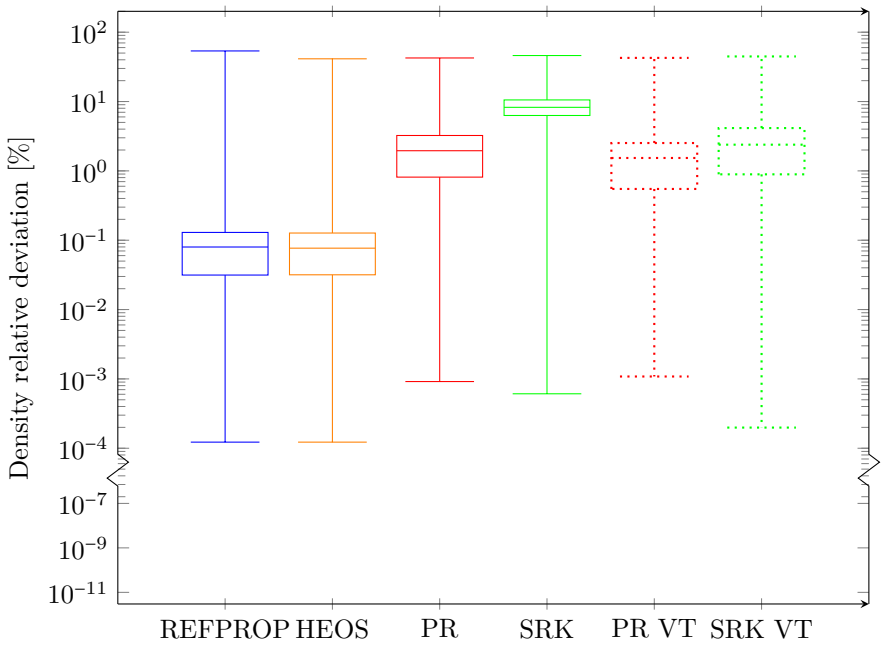


Figure 185: Relative density deviation to experimental data for fluid R1234YF

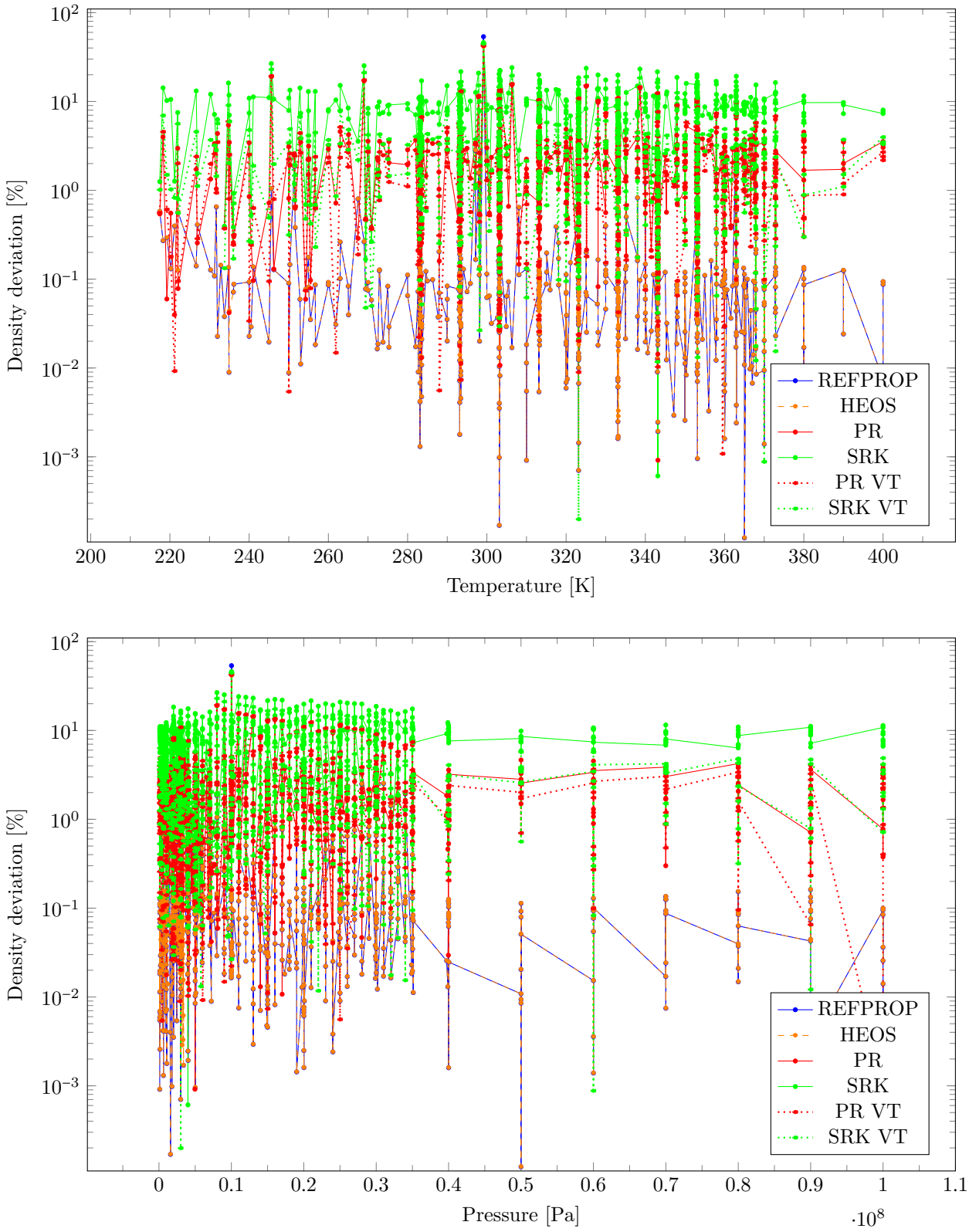


Figure 186: Density dependence on the temperature and pressure for fluid R1234YF

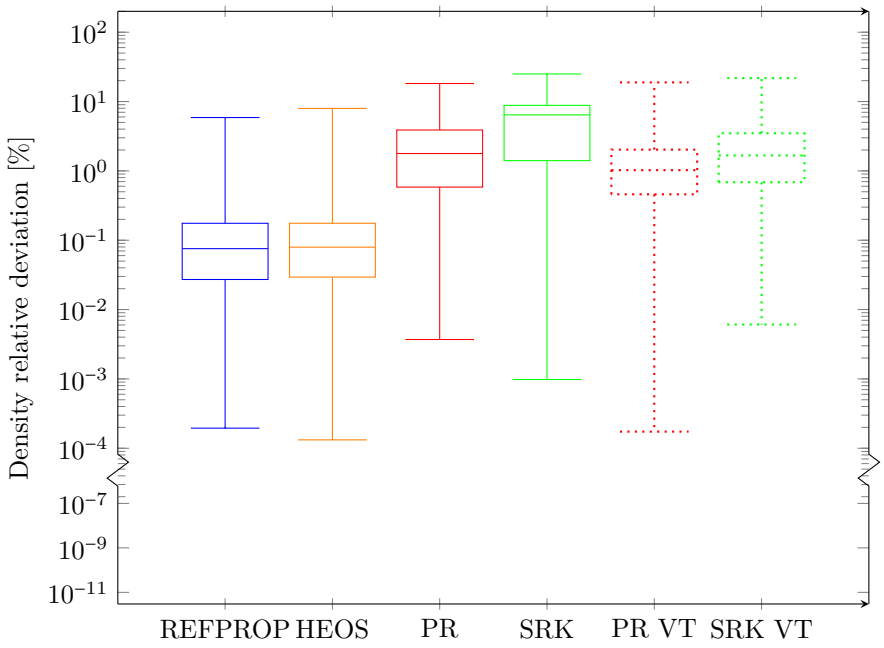


Figure 187: Relative density deviation to experimental data for fluid R1234ZE(E)

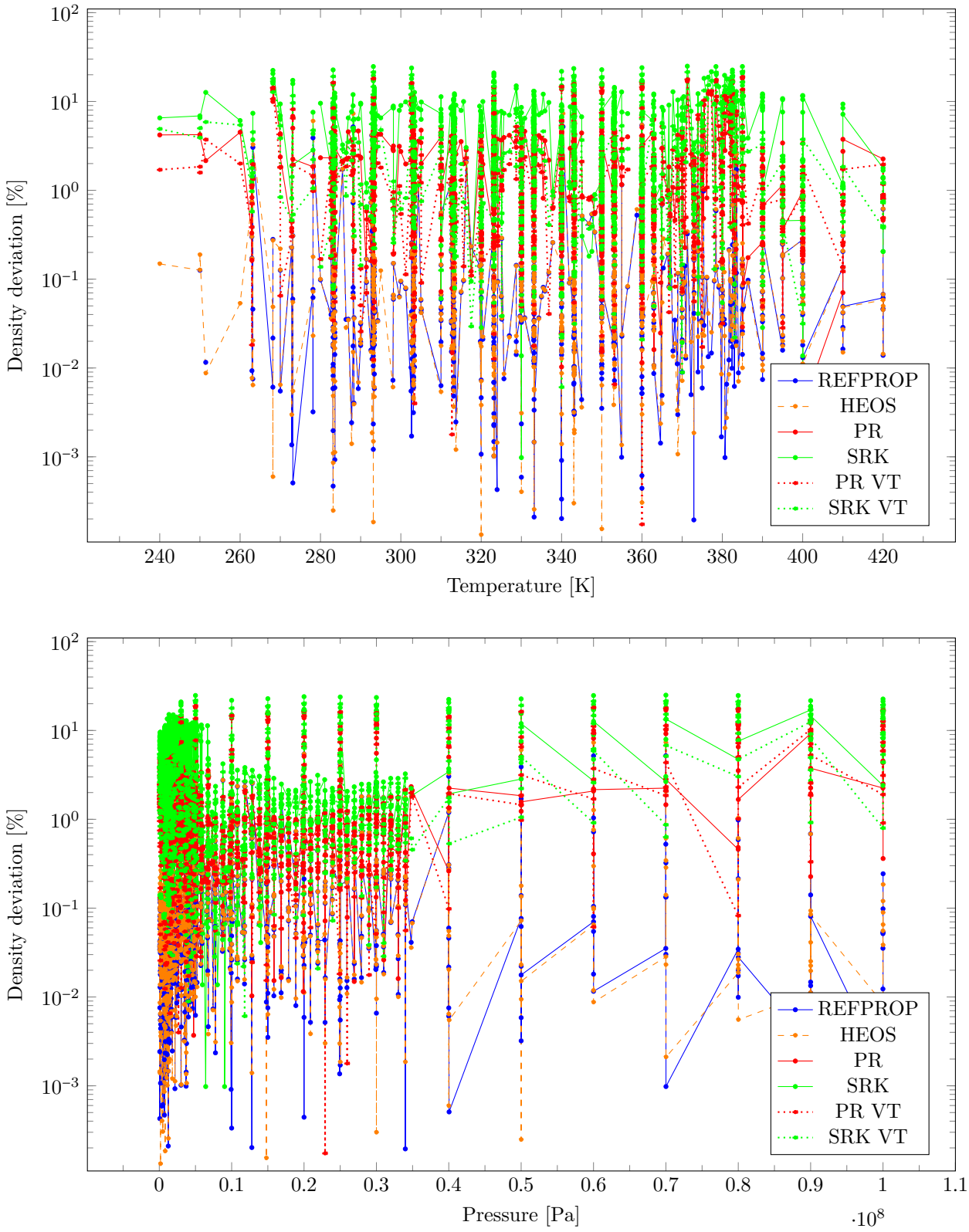


Figure 188: Density dependence on the temperature and pressure for fluid R1234ZE(E)

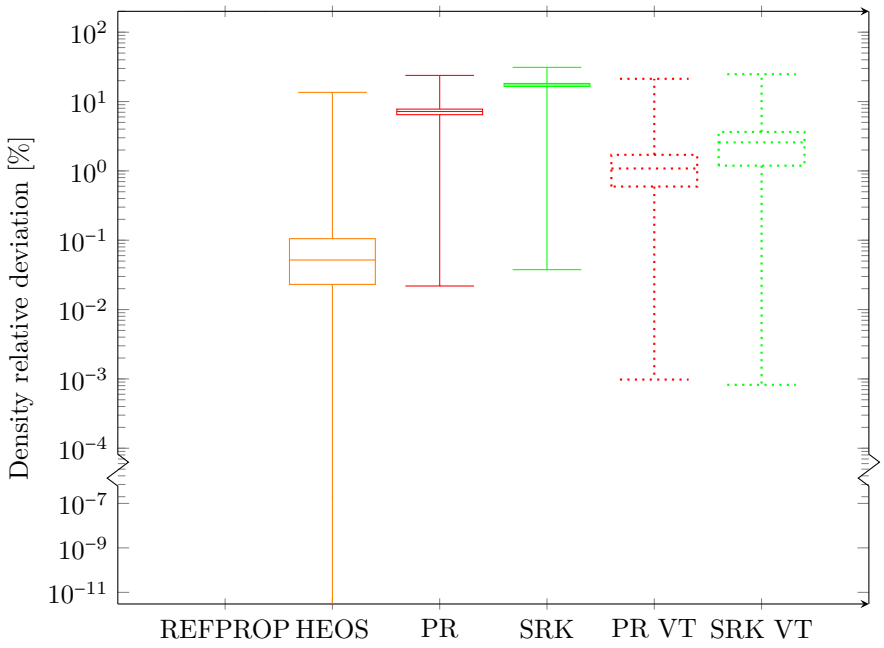


Figure 189: Relative density deviation to experimental data for fluid R1234ZE(Z)

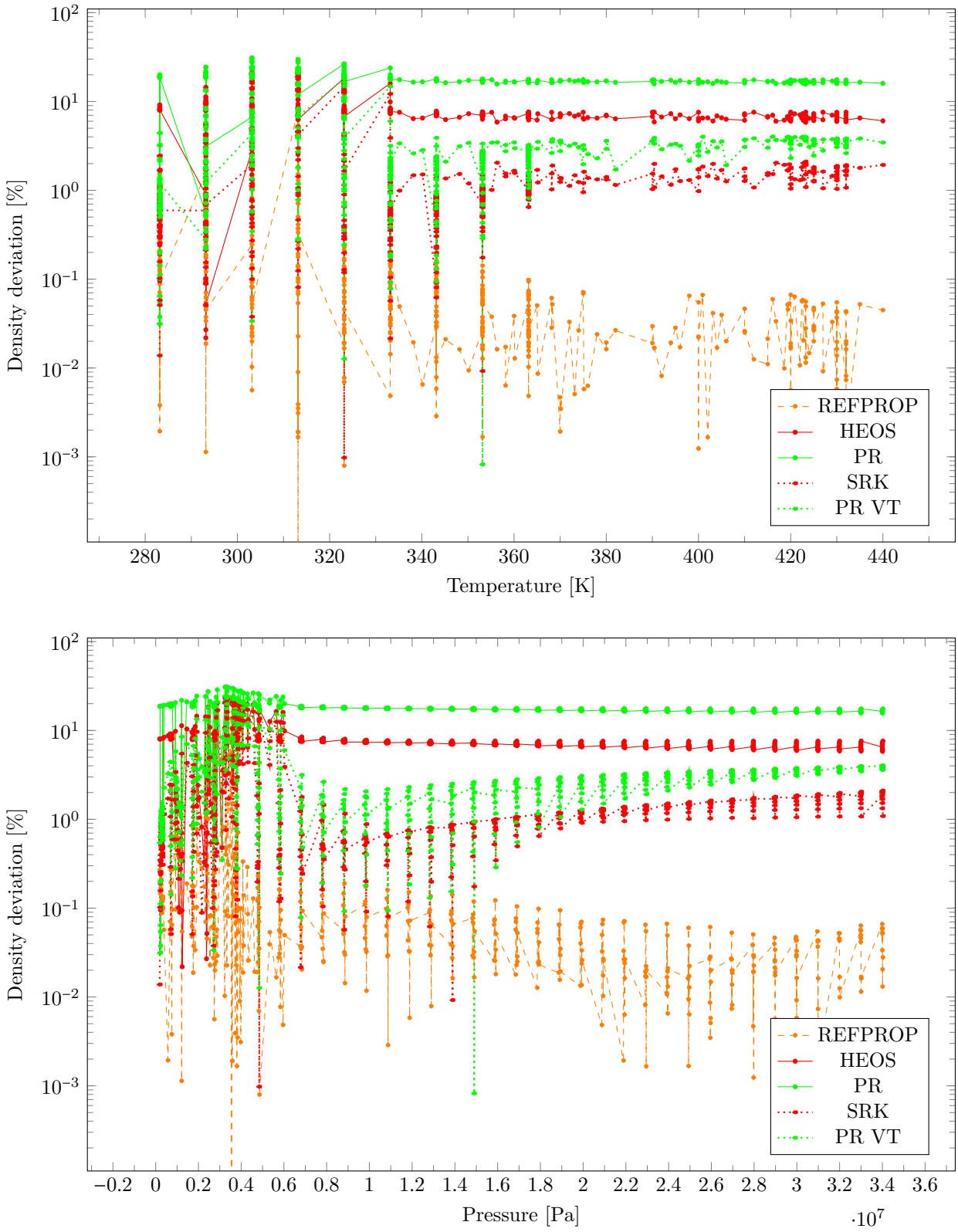


Figure 190: Density dependence on the temperature and pressure for fluid R1234ze(Z)

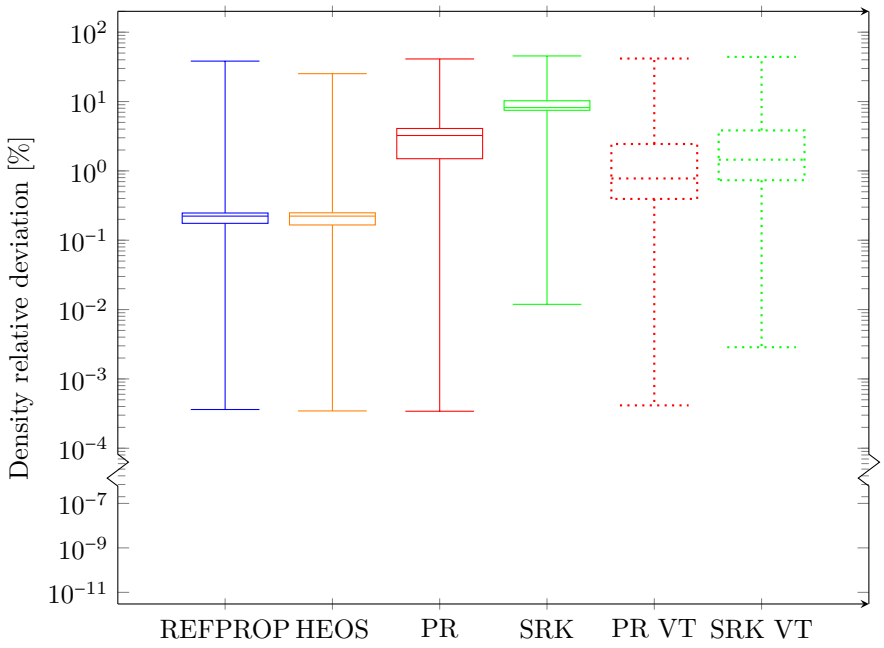


Figure 191: Relative density deviation to experimental data for fluid R124

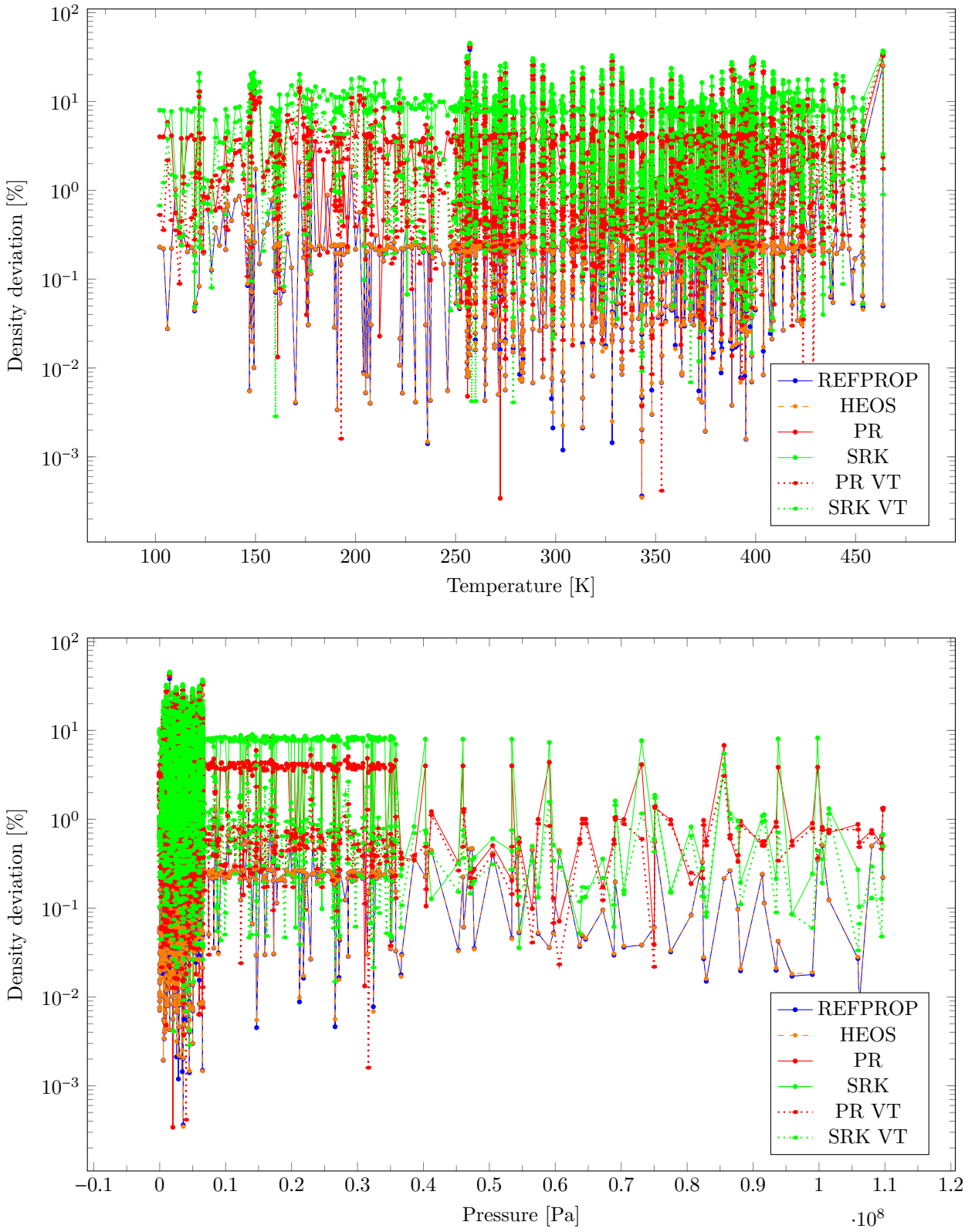


Figure 192: Density dependence on the temperature and pressure for fluid R124

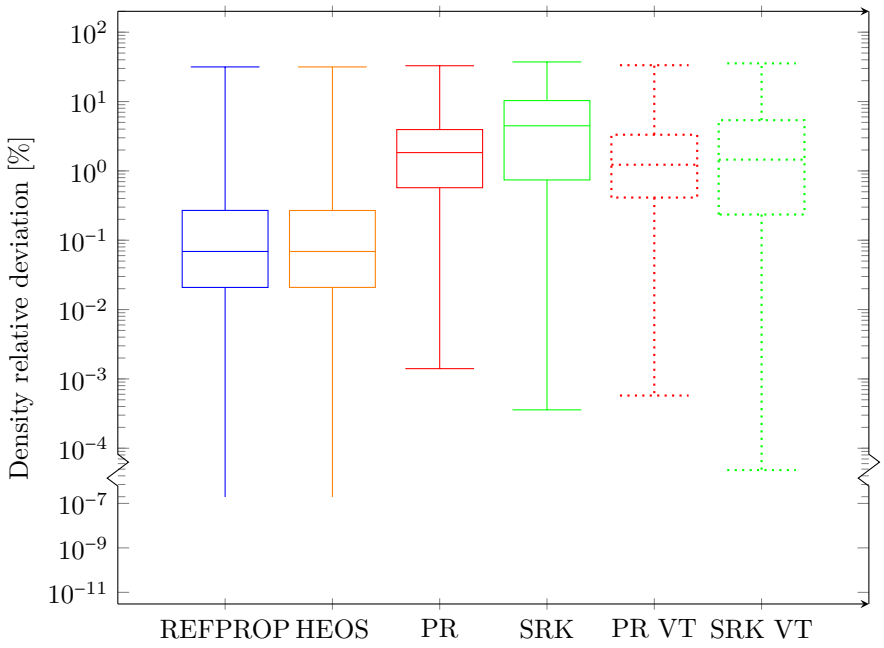


Figure 193: Relative density deviation to experimental data for fluid R125

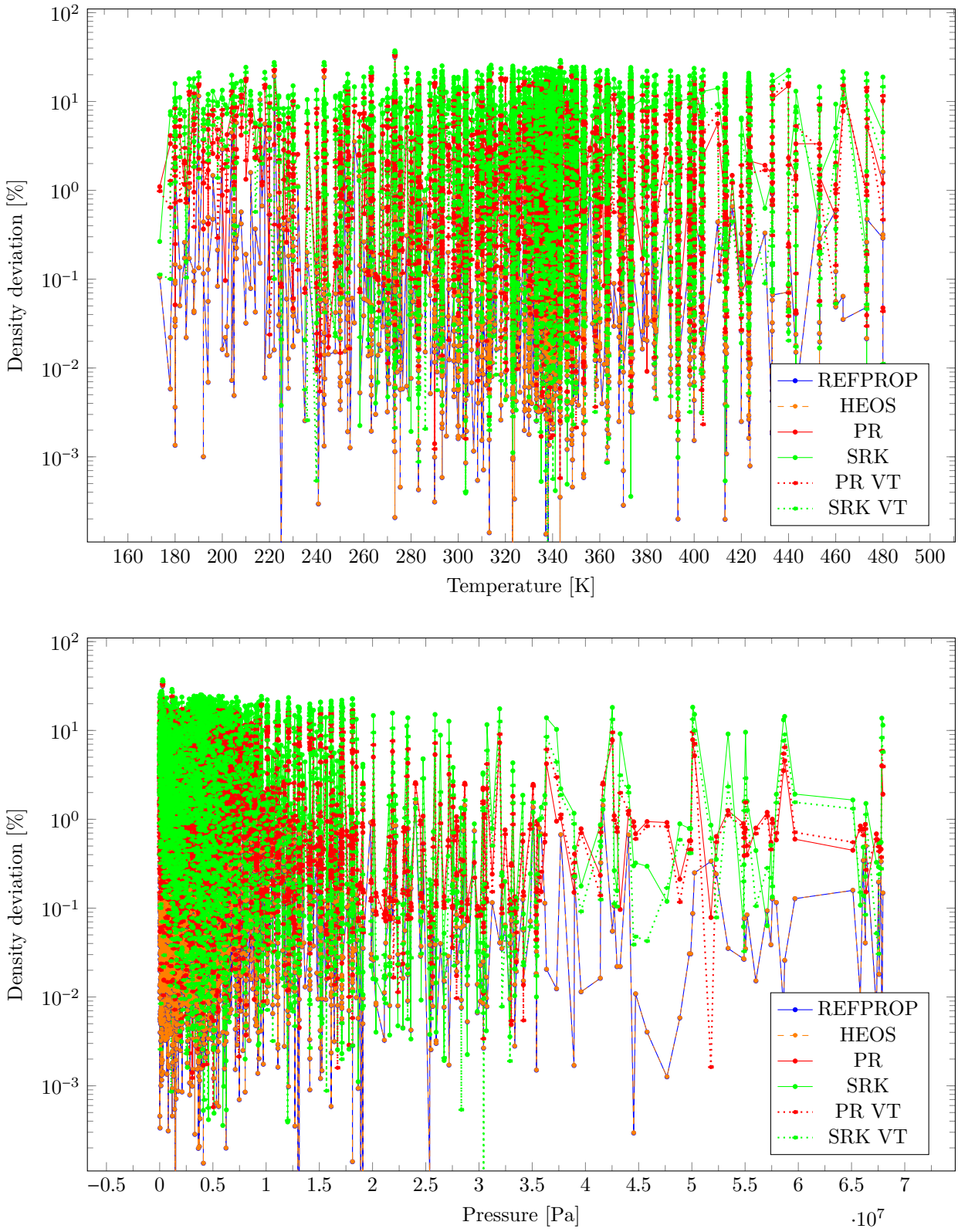


Figure 194: Density dependence on the temperature and pressure for fluid R125

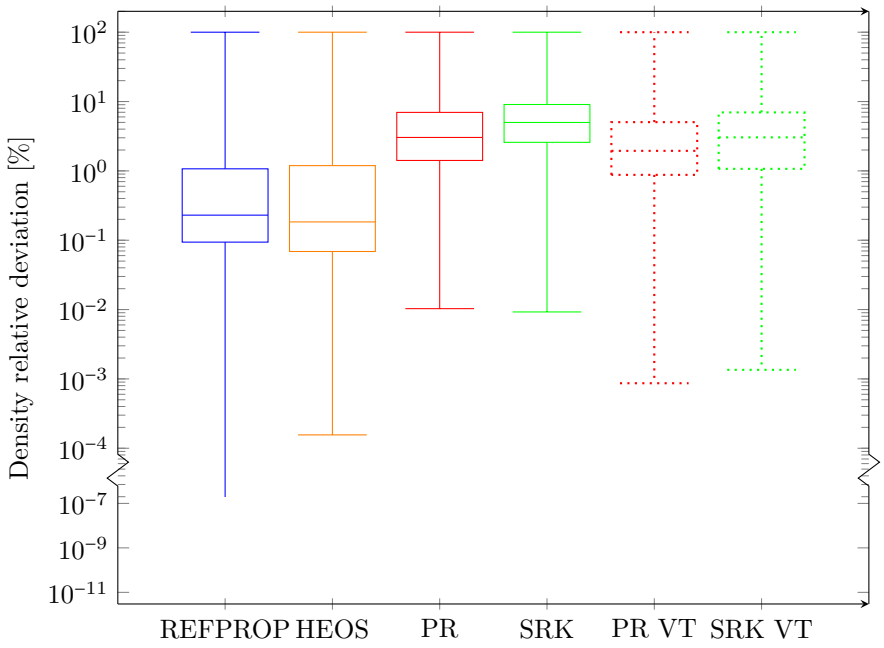


Figure 195: Relative density deviation to experimental data for fluid R13

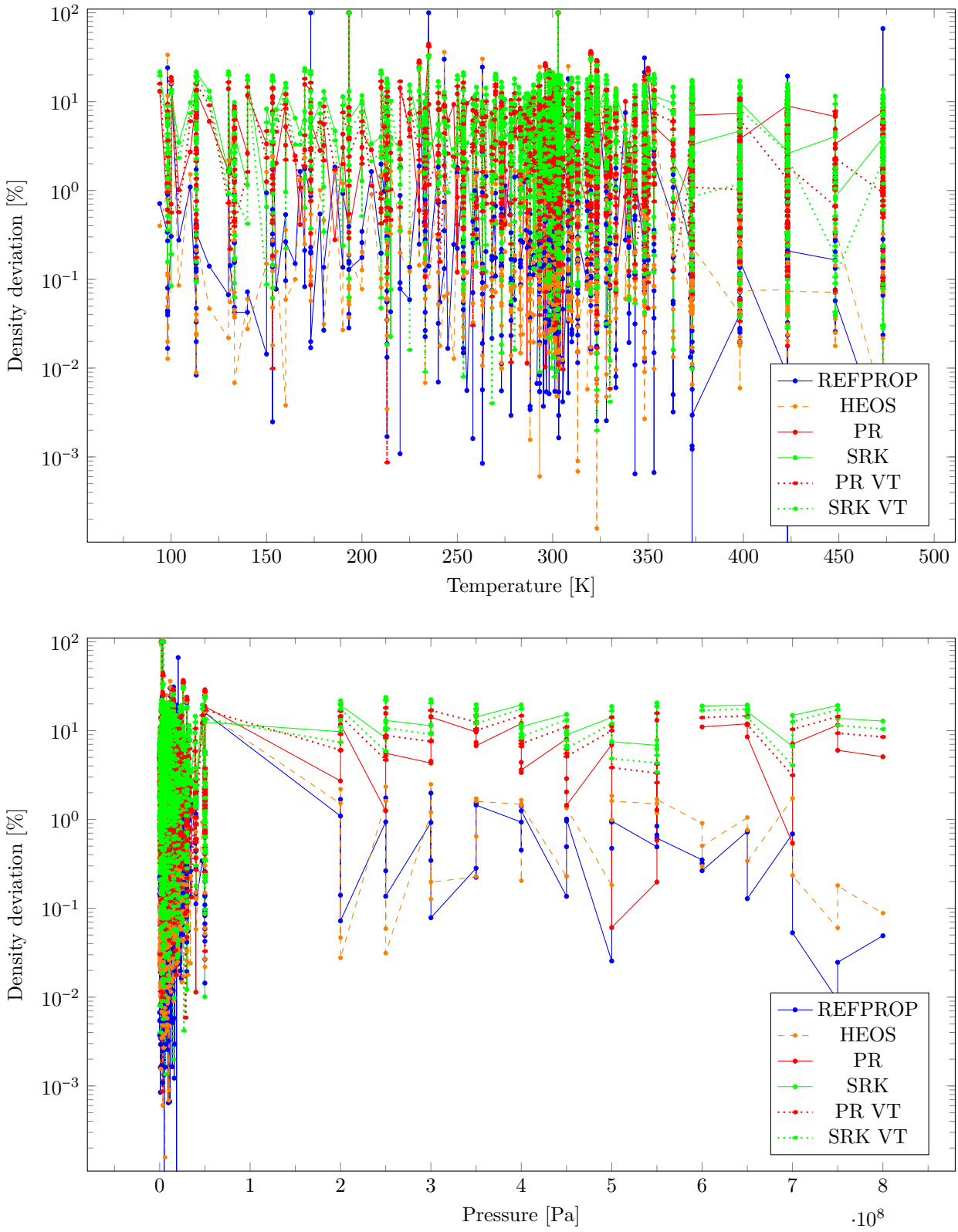


Figure 196: Density dependence on the temperature and pressure for fluid R13

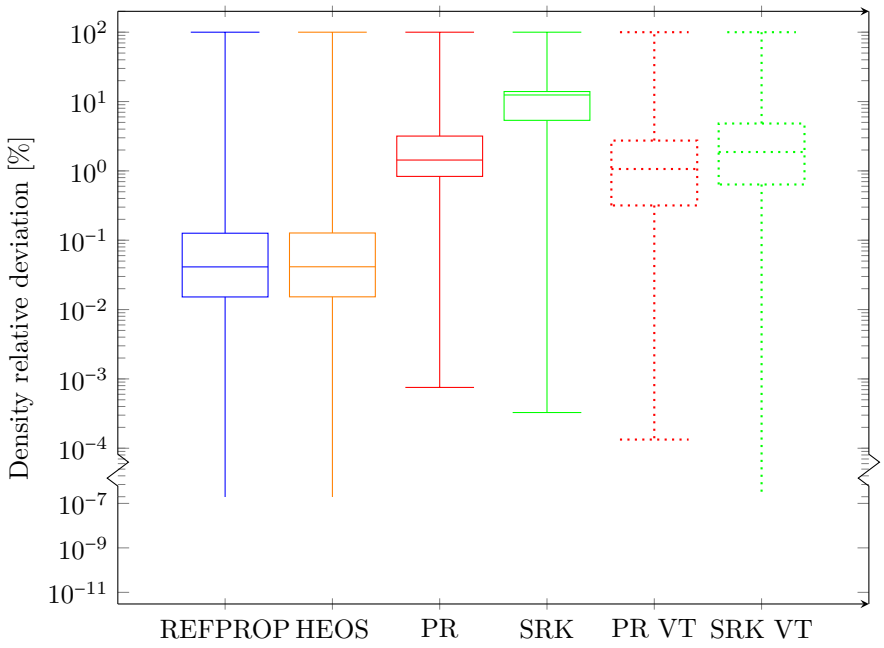


Figure 197: Relative density deviation to experimental data for fluid R134A

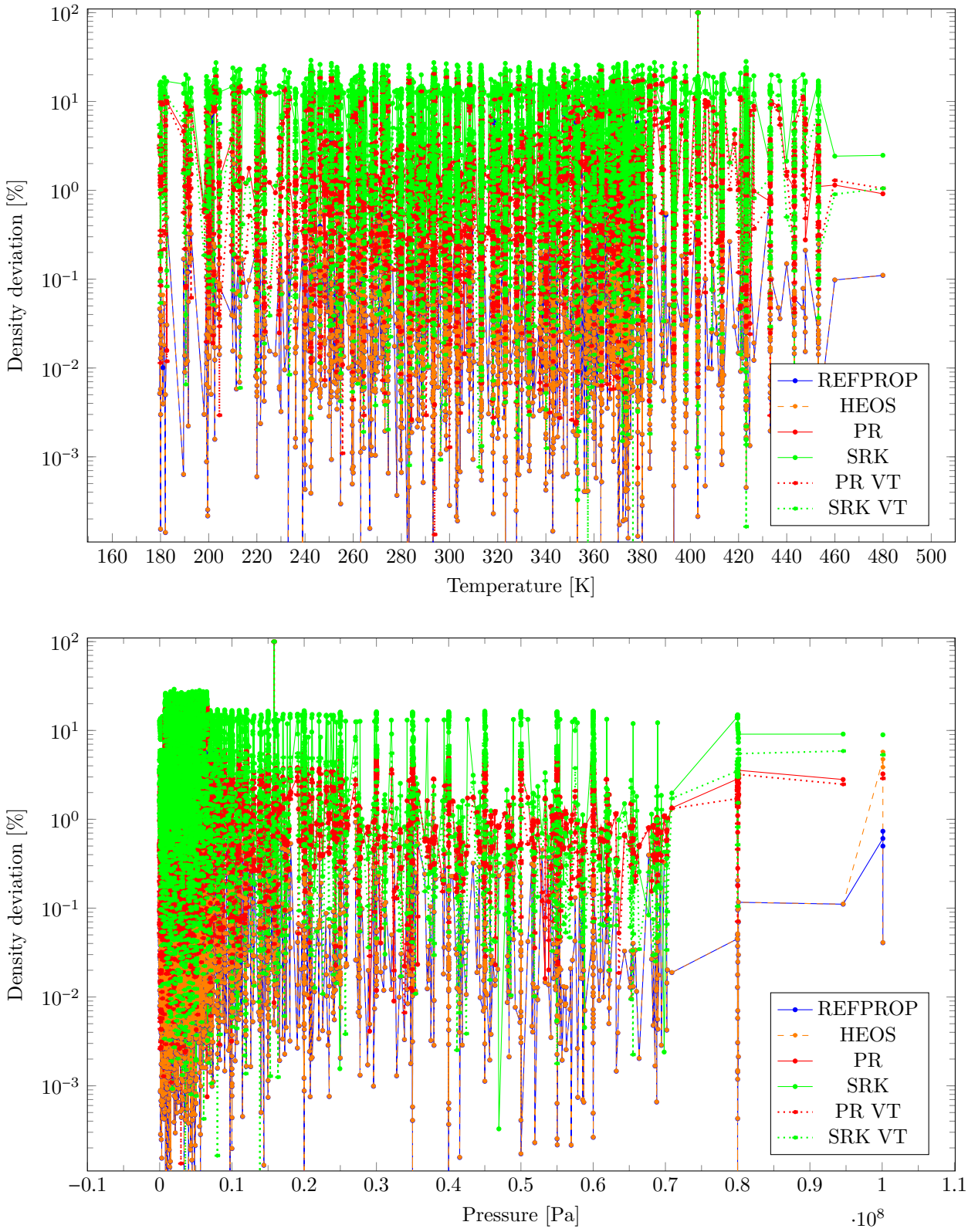


Figure 198: Density dependence on the temperature and pressure for fluid R134A

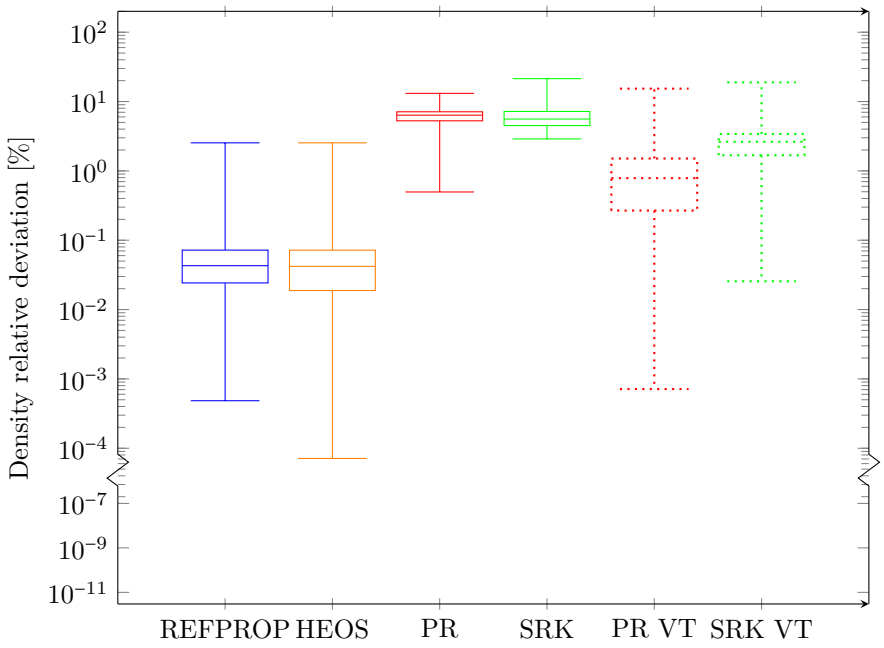


Figure 199: Relative density deviation to experimental data for fluid R13I1

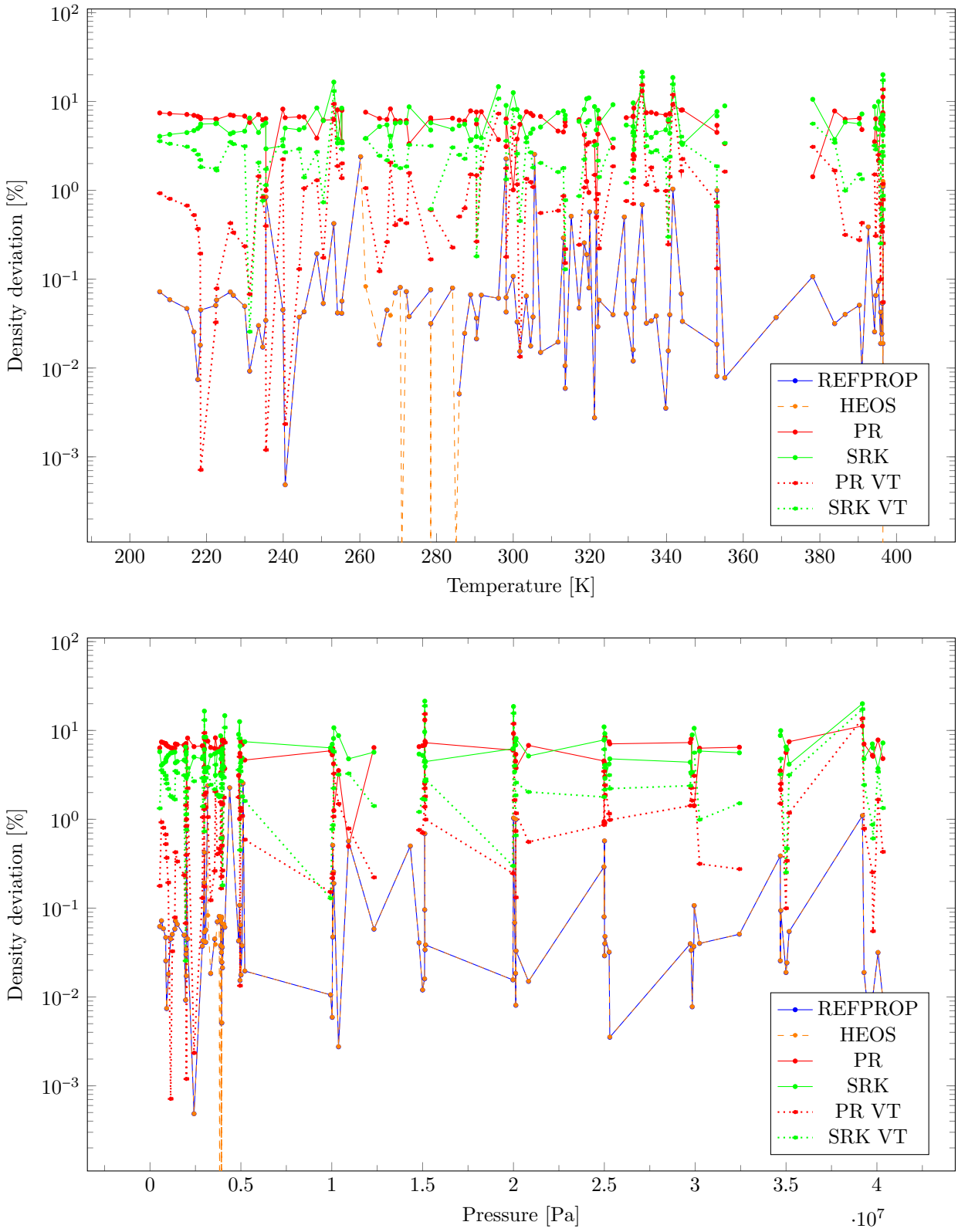


Figure 200: Density dependence on the temperature and pressure for fluid R13I1

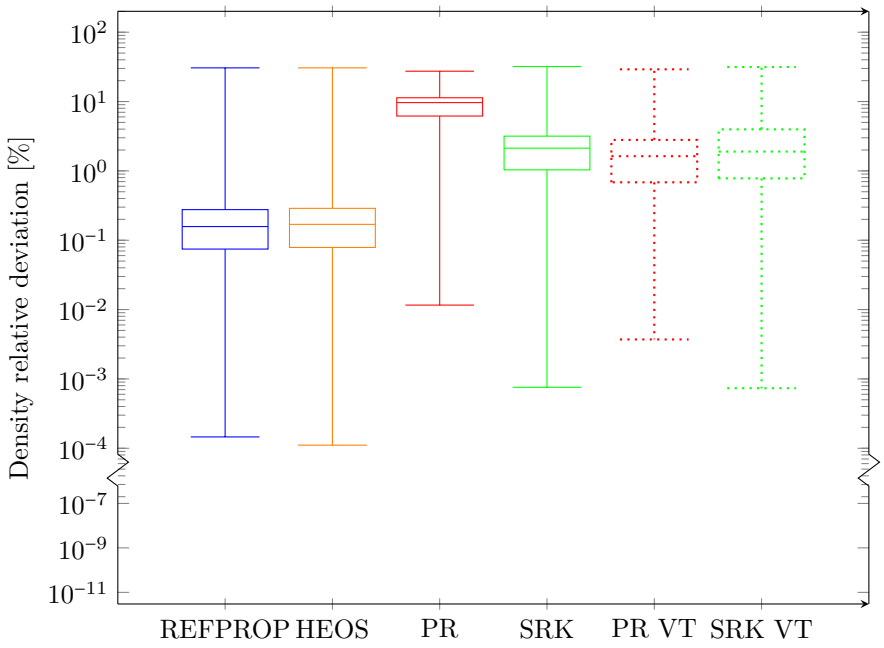


Figure 201: Relative density deviation to experimental data for fluid R14

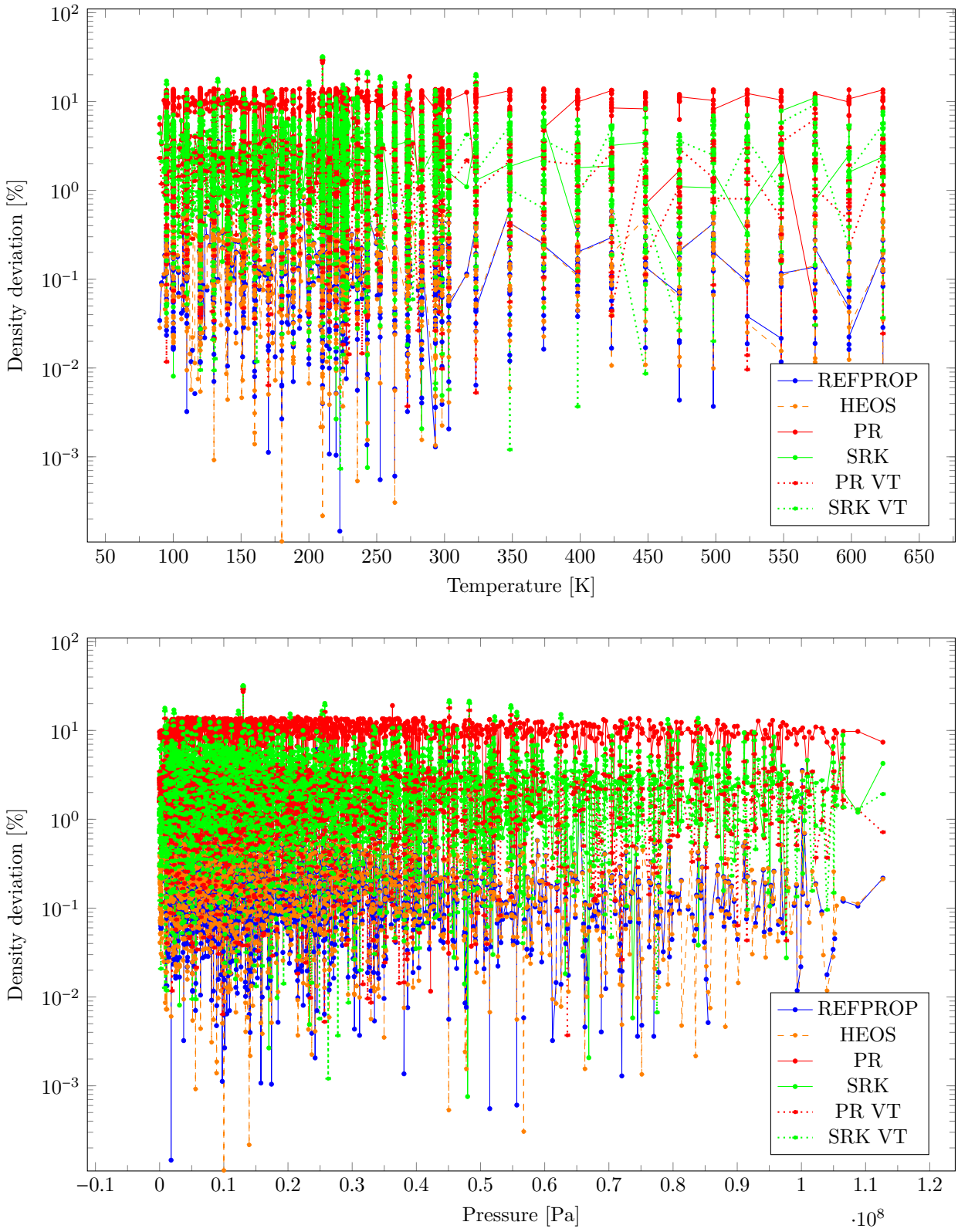


Figure 202: Density dependence on the temperature and pressure for fluid R14

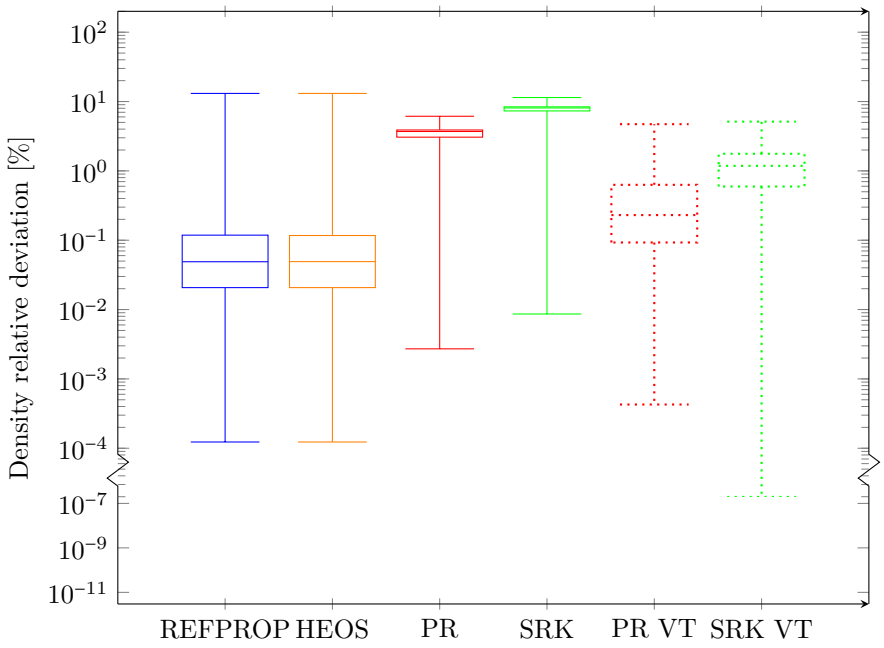


Figure 203: Relative density deviation to experimental data for fluid R141B

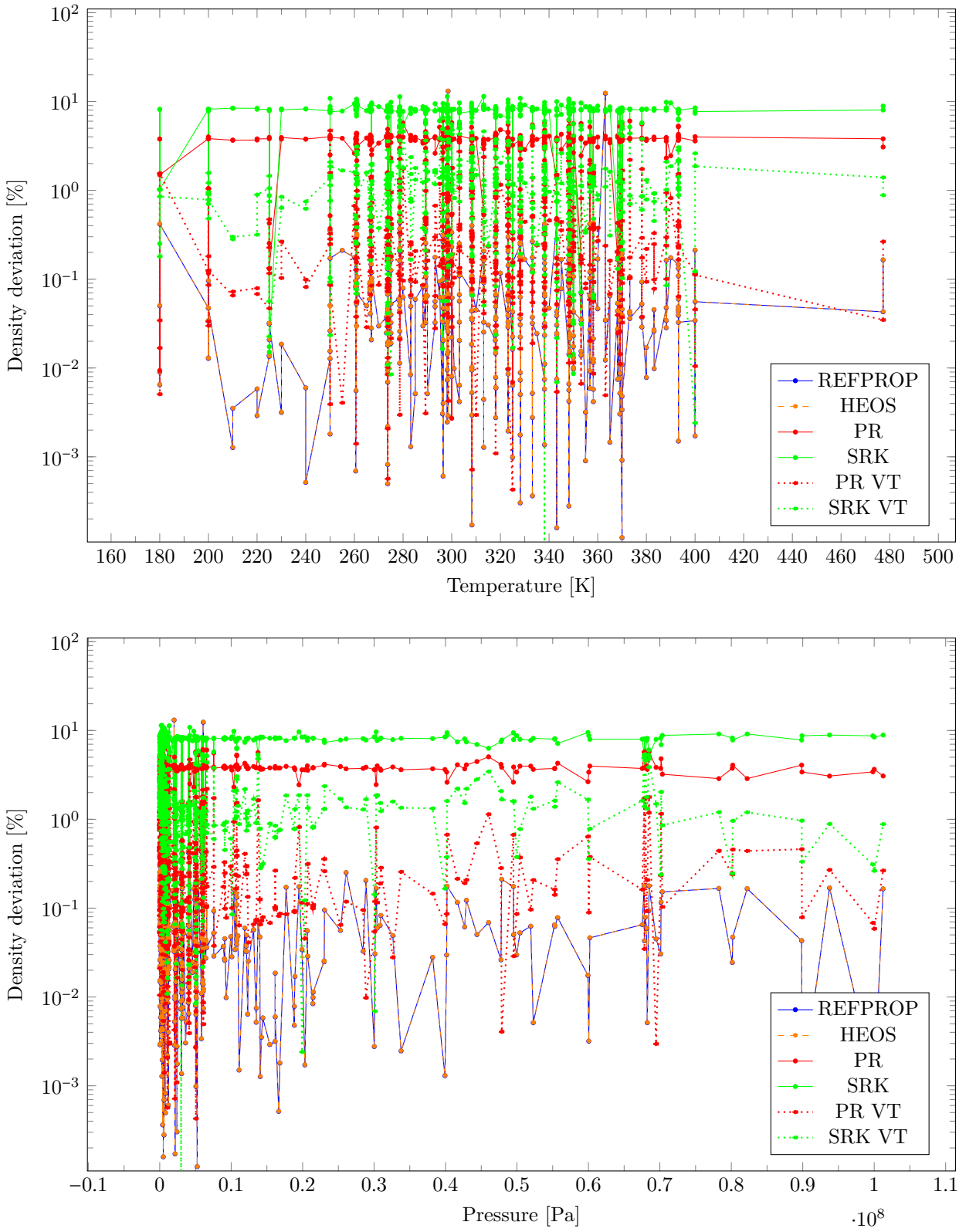


Figure 204: Density dependence on the temperature and pressure for fluid R141B

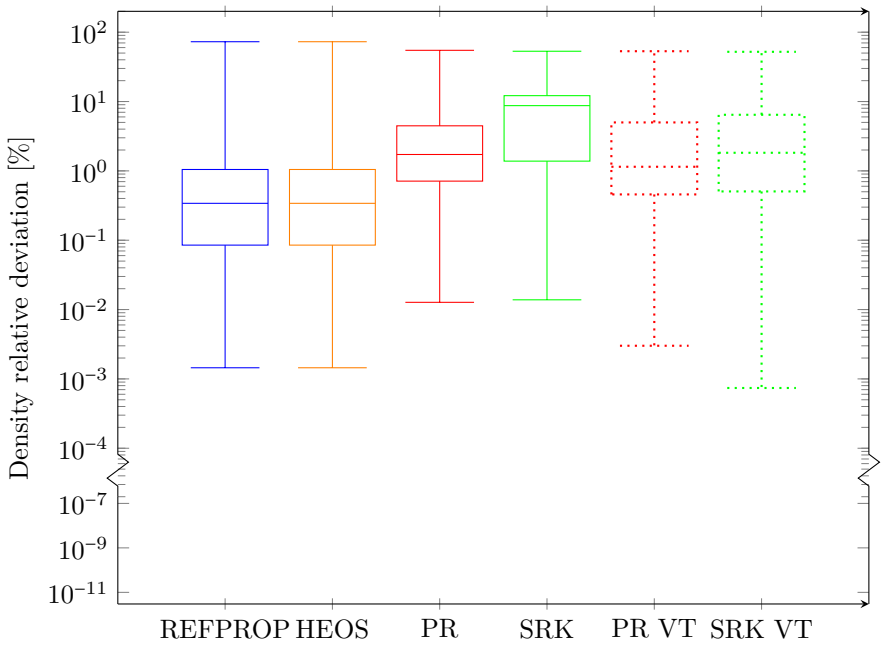


Figure 205: Relative density deviation to experimental data for fluid R142B

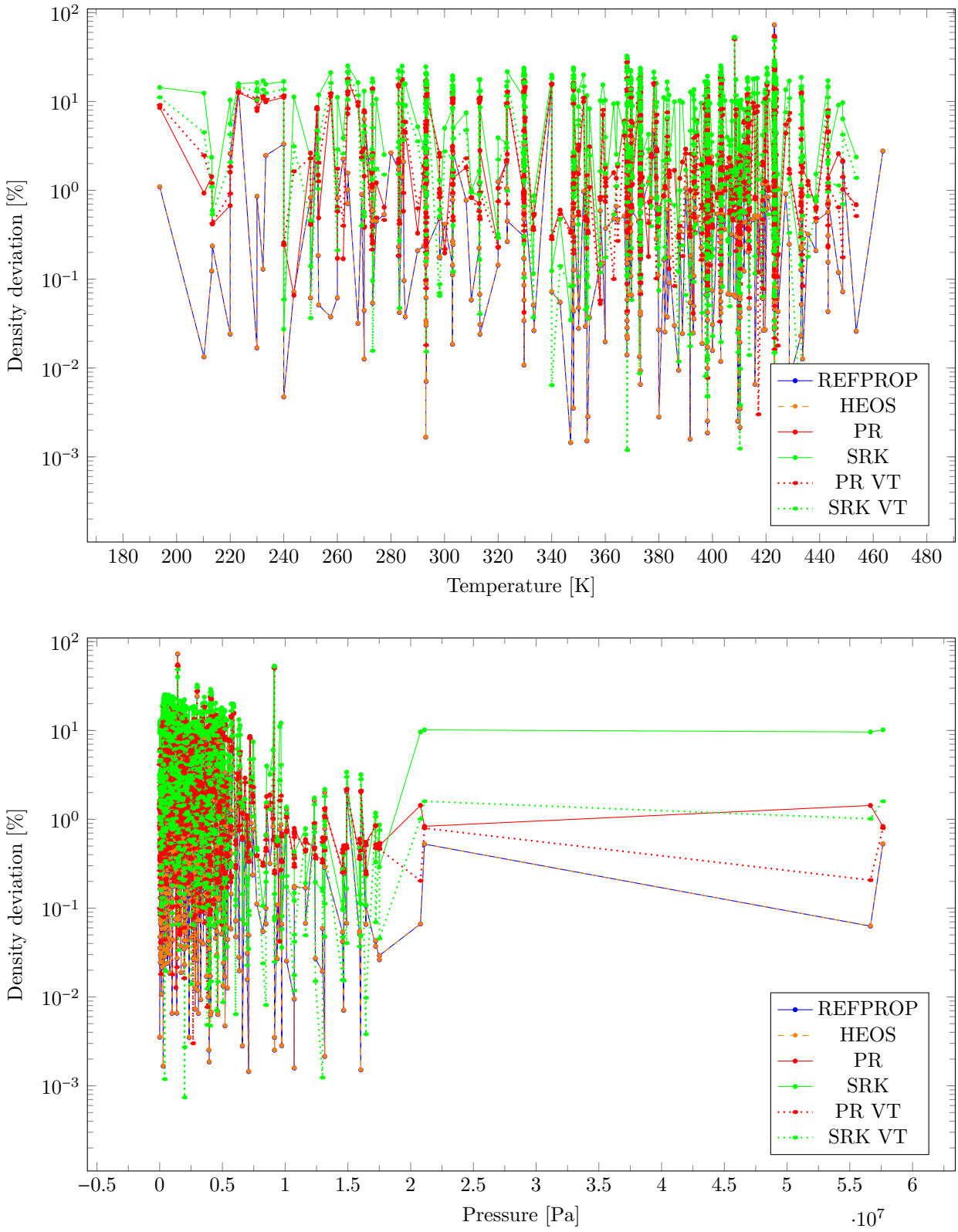


Figure 206: Density dependence on the temperature and pressure for fluid R142B

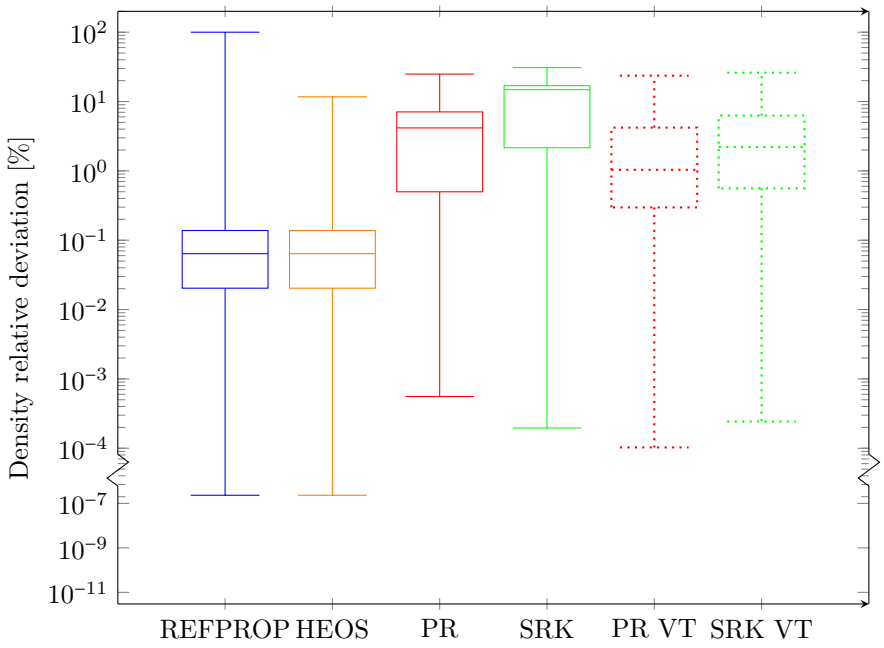


Figure 207: Relative density deviation to experimental data for fluid R143A

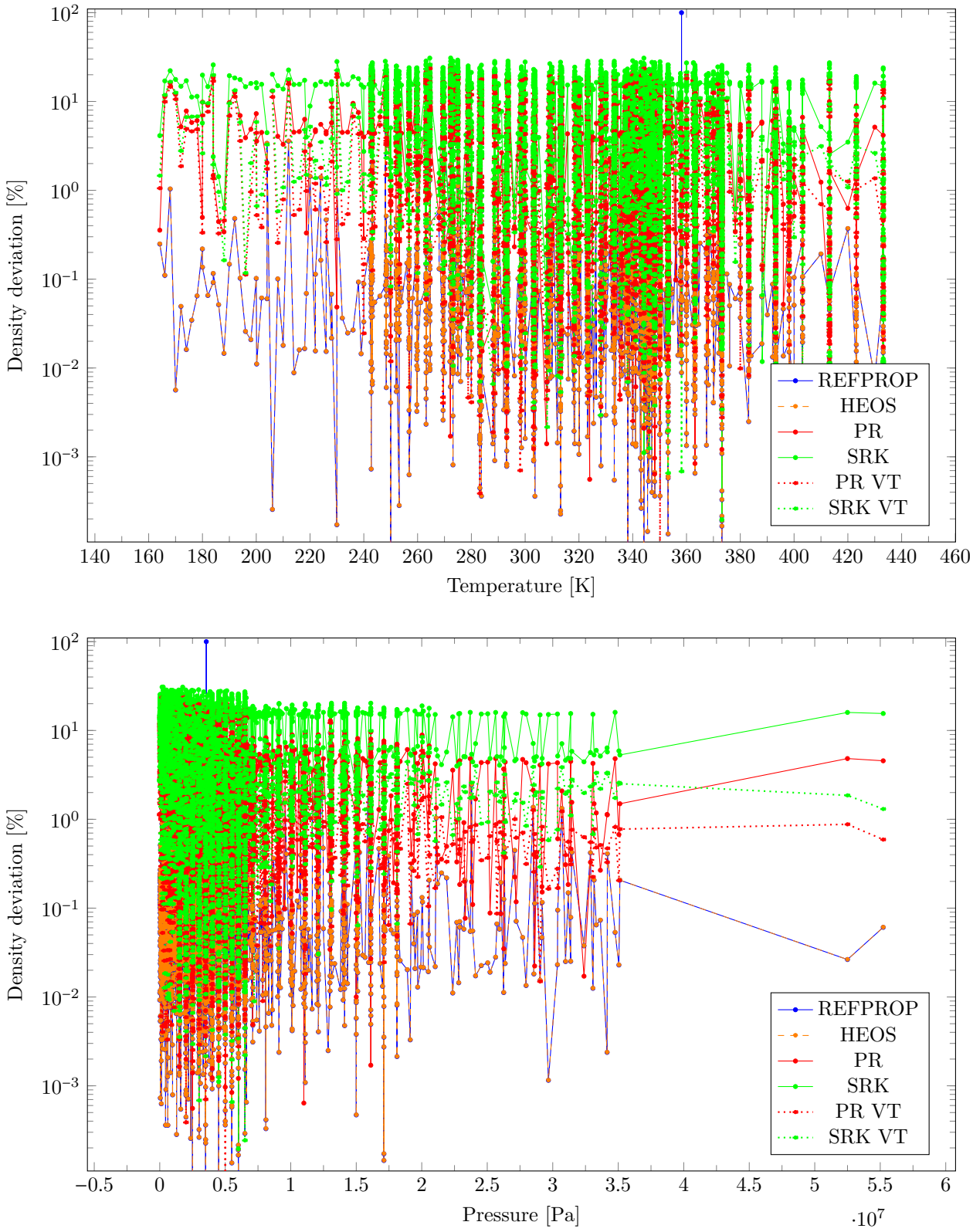


Figure 208: Density dependence on the temperature and pressure for fluid R143A

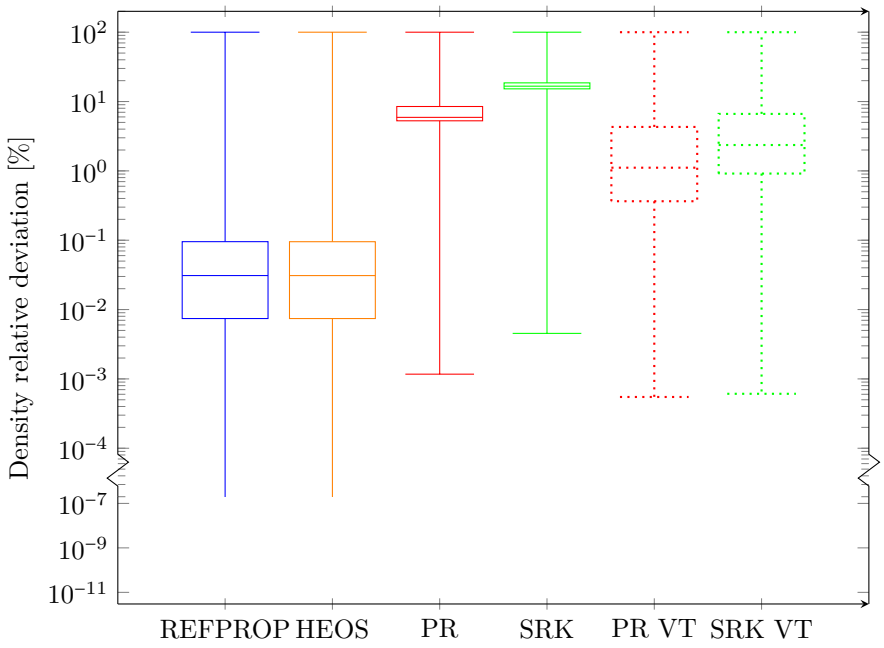


Figure 209: Relative density deviation to experimental data for fluid R152A

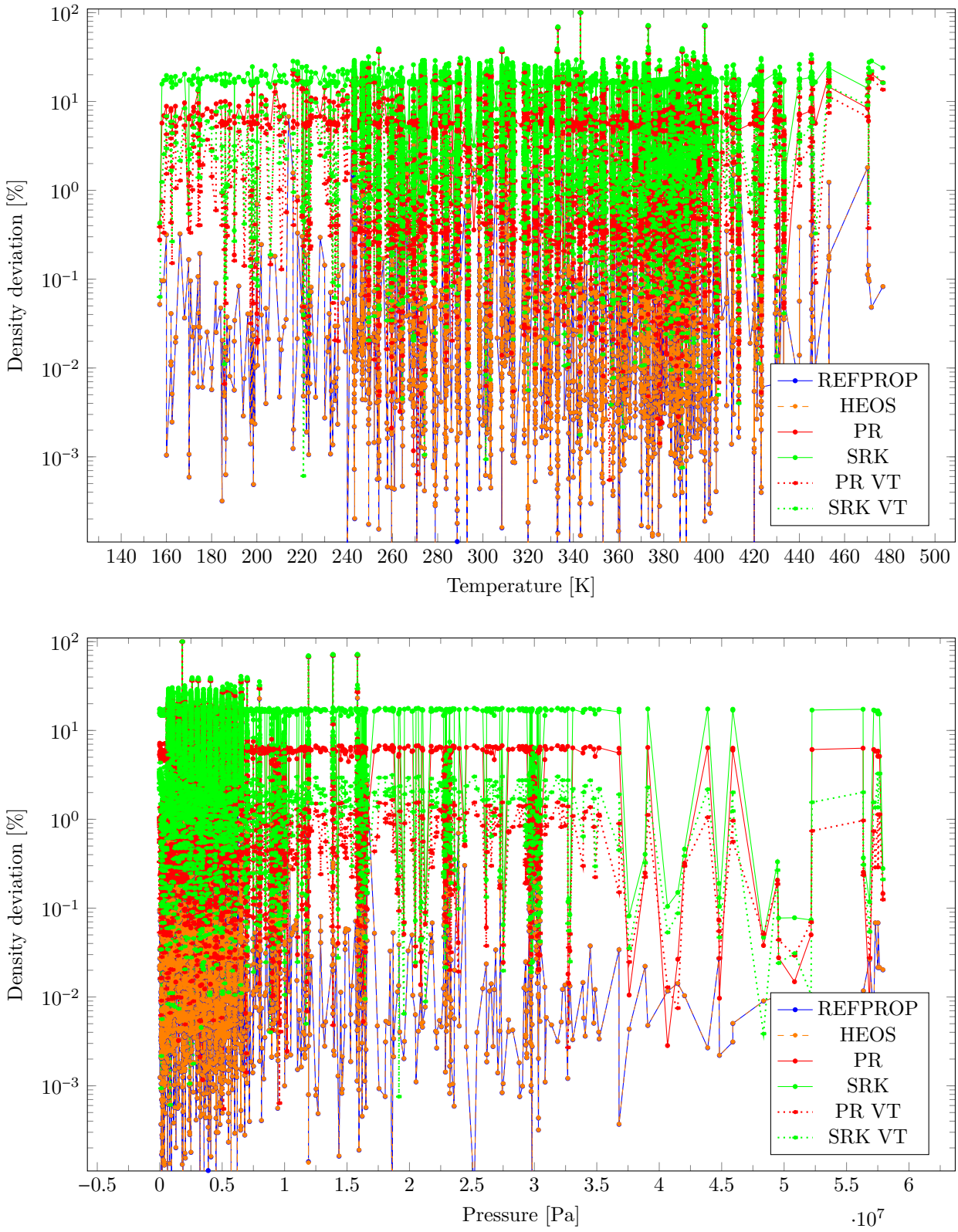


Figure 210: Density dependence on the temperature and pressure for fluid R152A

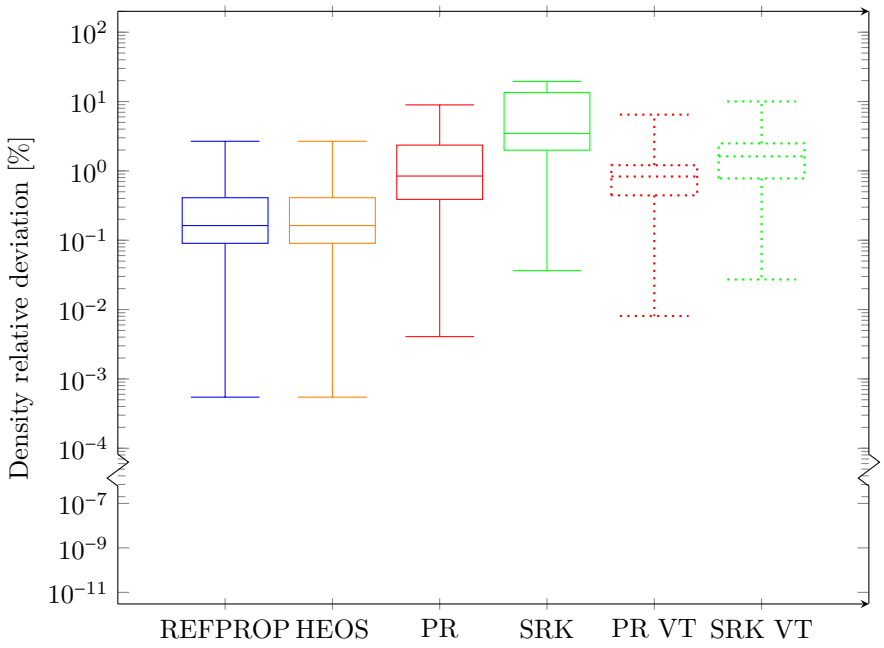


Figure 211: Relative density deviation to experimental data for fluid R161

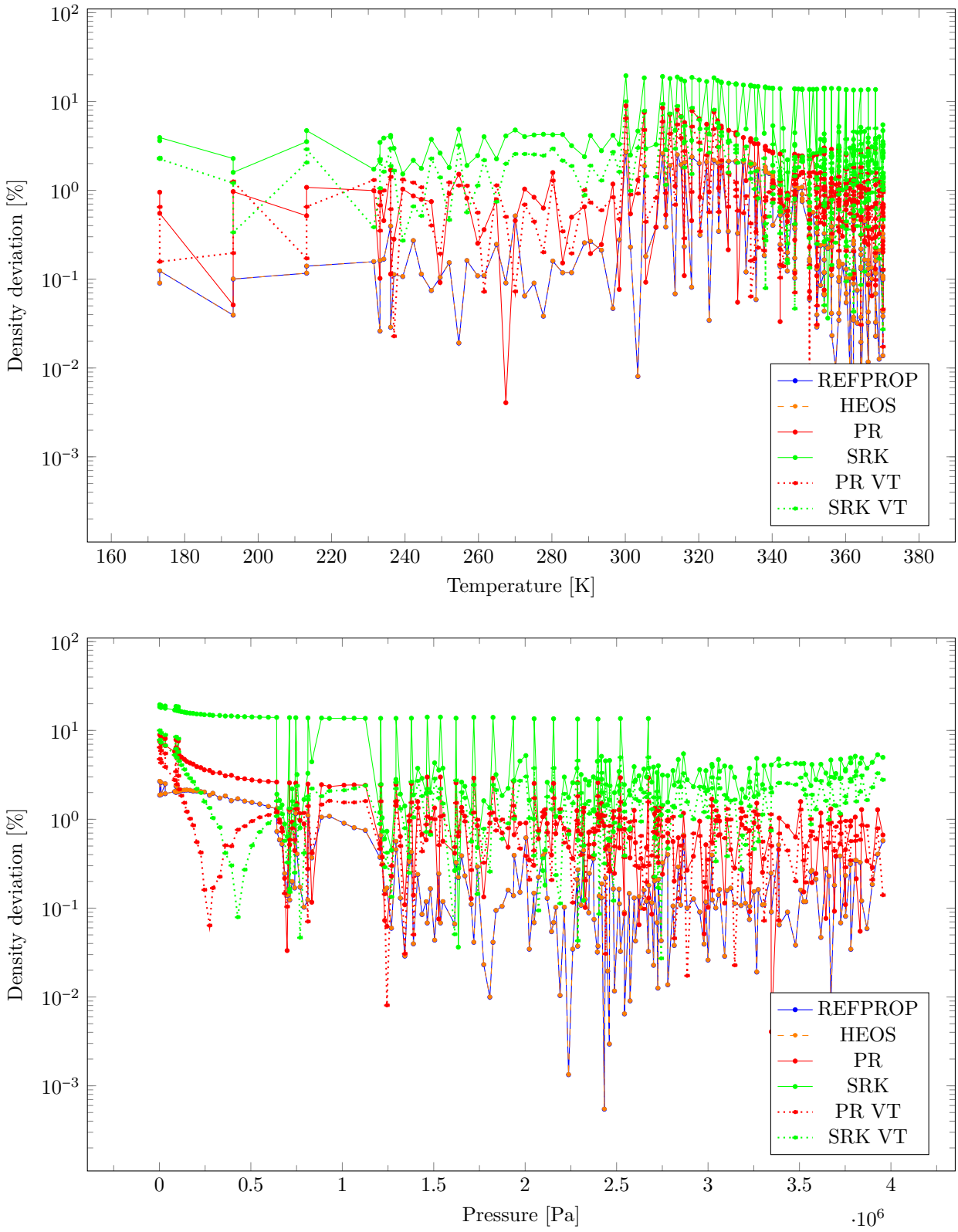


Figure 212: Density dependence on the temperature and pressure for fluid R161

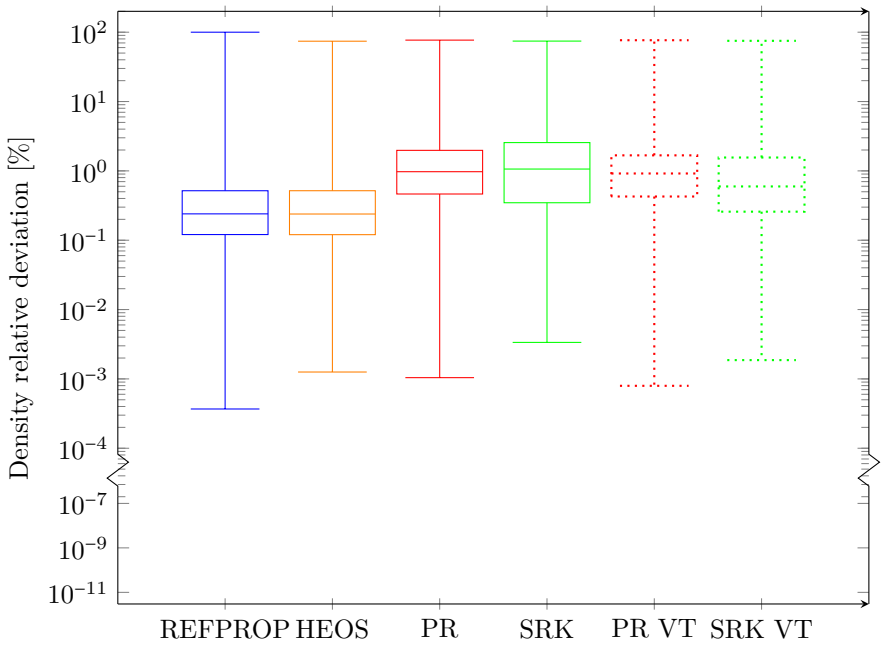


Figure 213: Relative density deviation to experimental data for fluid R21

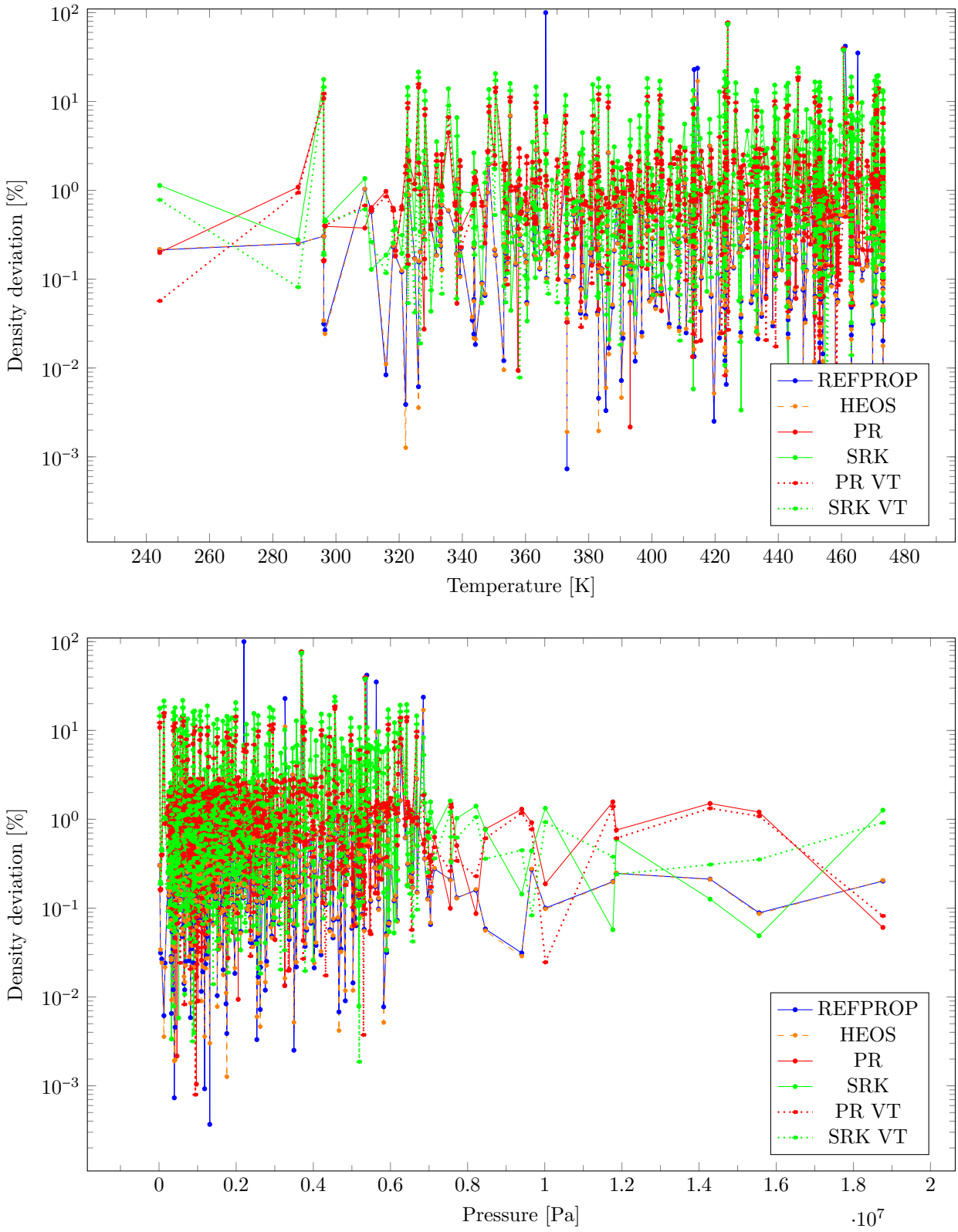


Figure 214: Density dependence on the temperature and pressure for fluid R21

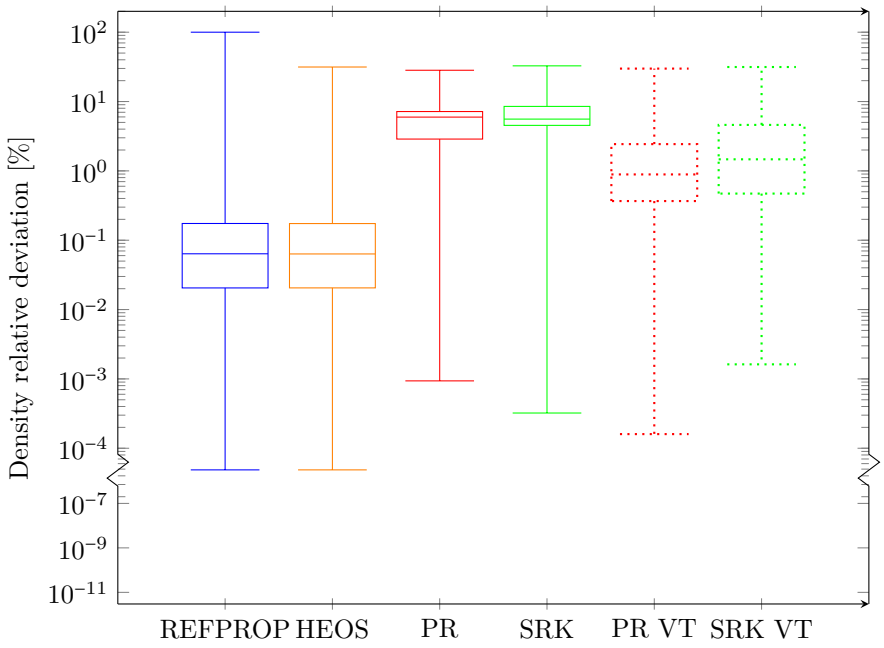


Figure 215: Relative density deviation to experimental data for fluid R218

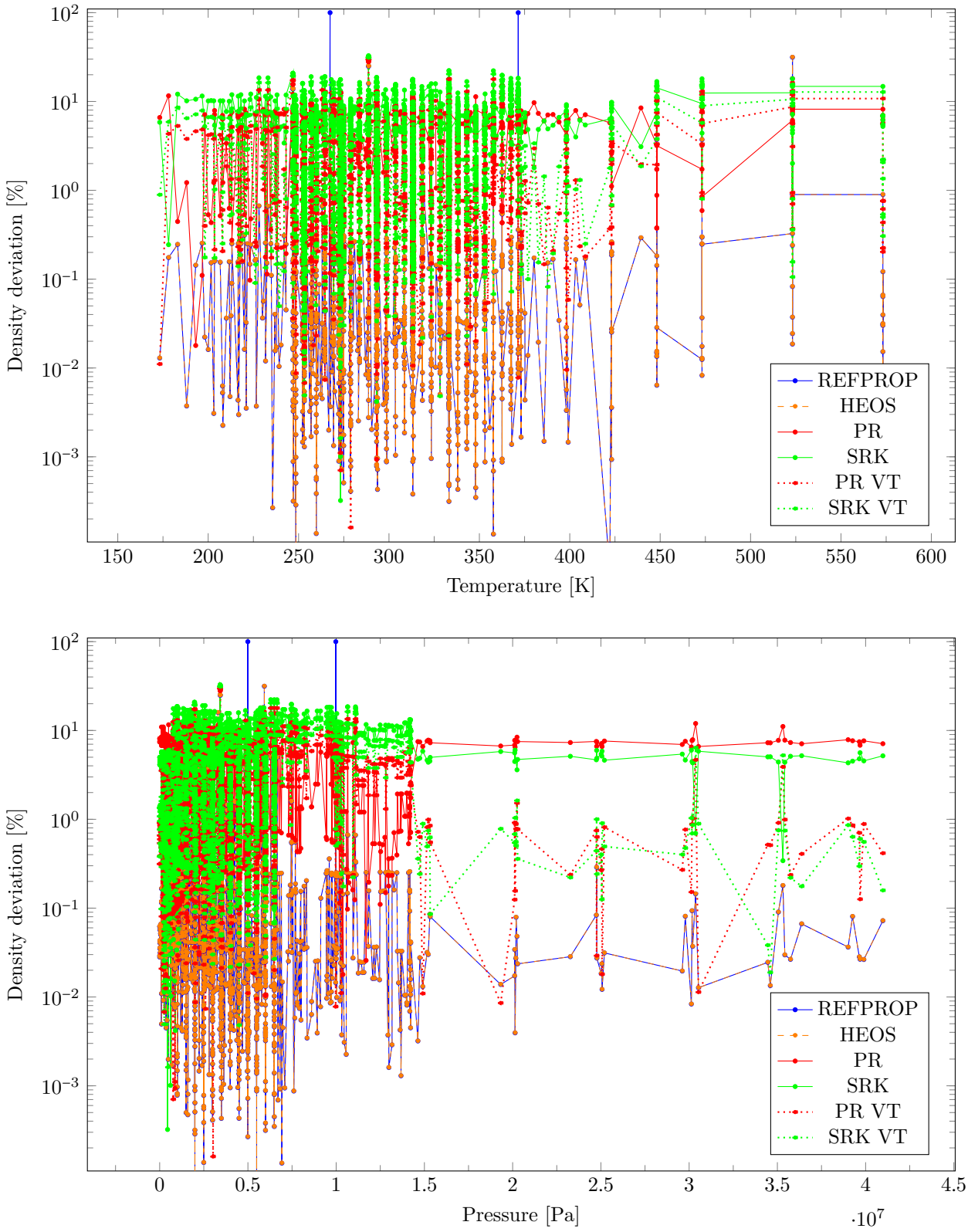


Figure 216: Density dependence on the temperature and pressure for fluid R218

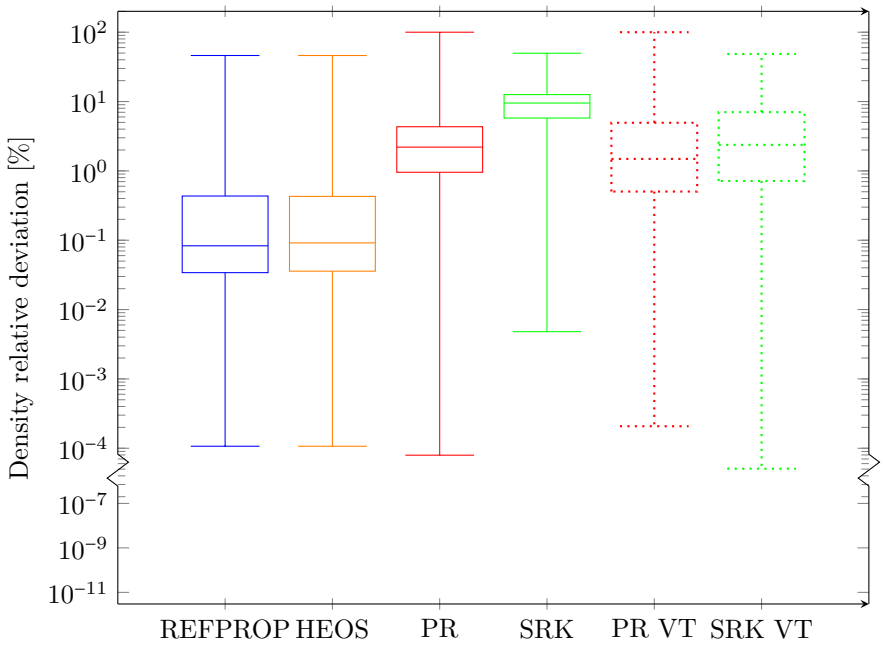


Figure 217: Relative density deviation to experimental data for fluid R22

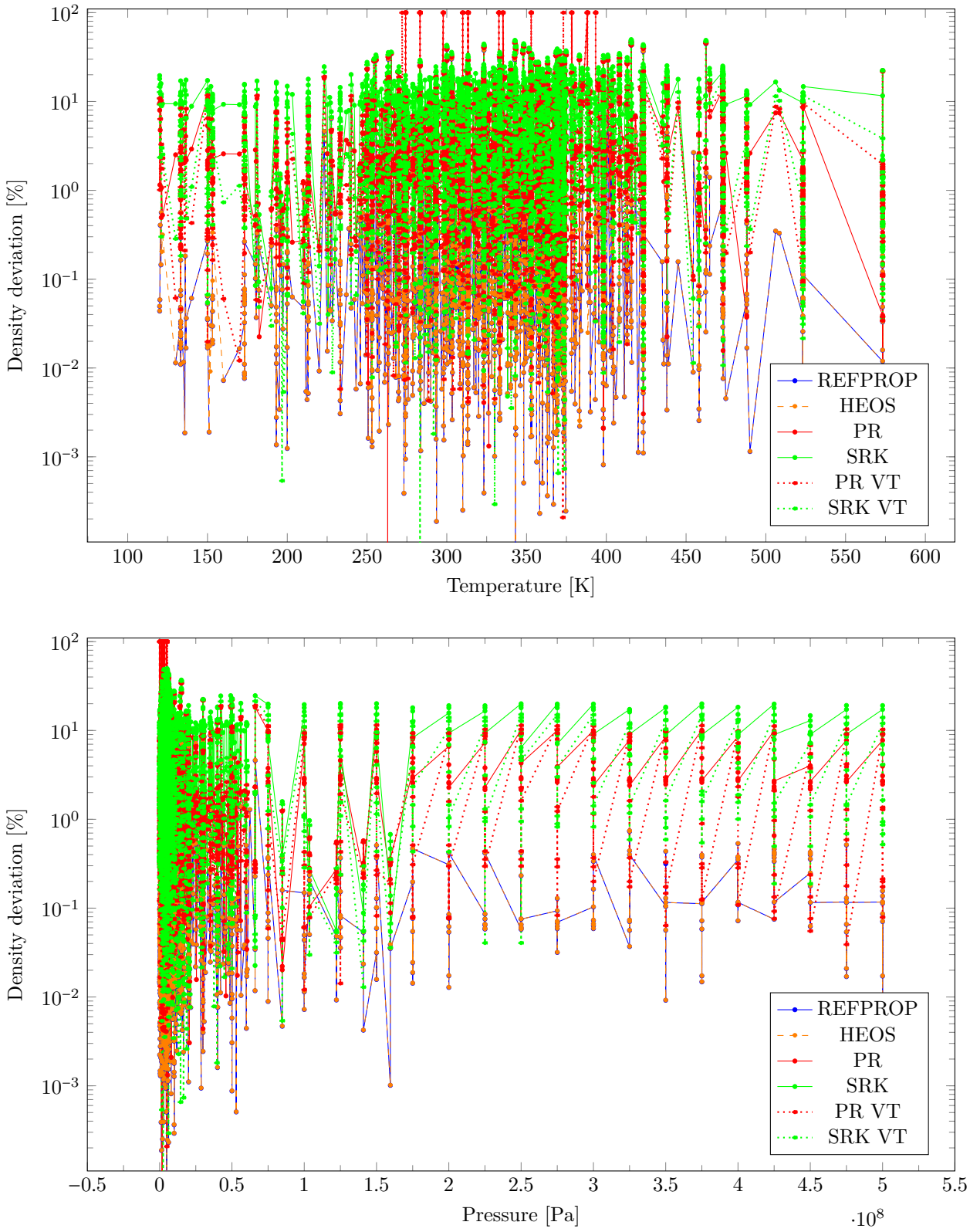


Figure 218: Density dependence on the temperature and pressure for fluid R22

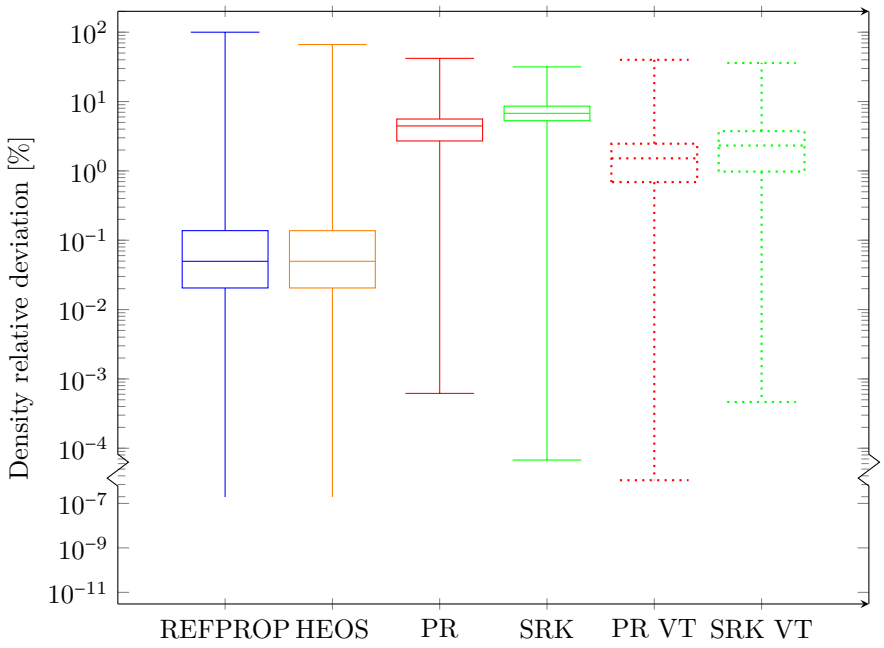


Figure 219: Relative density deviation to experimental data for fluid R227EA

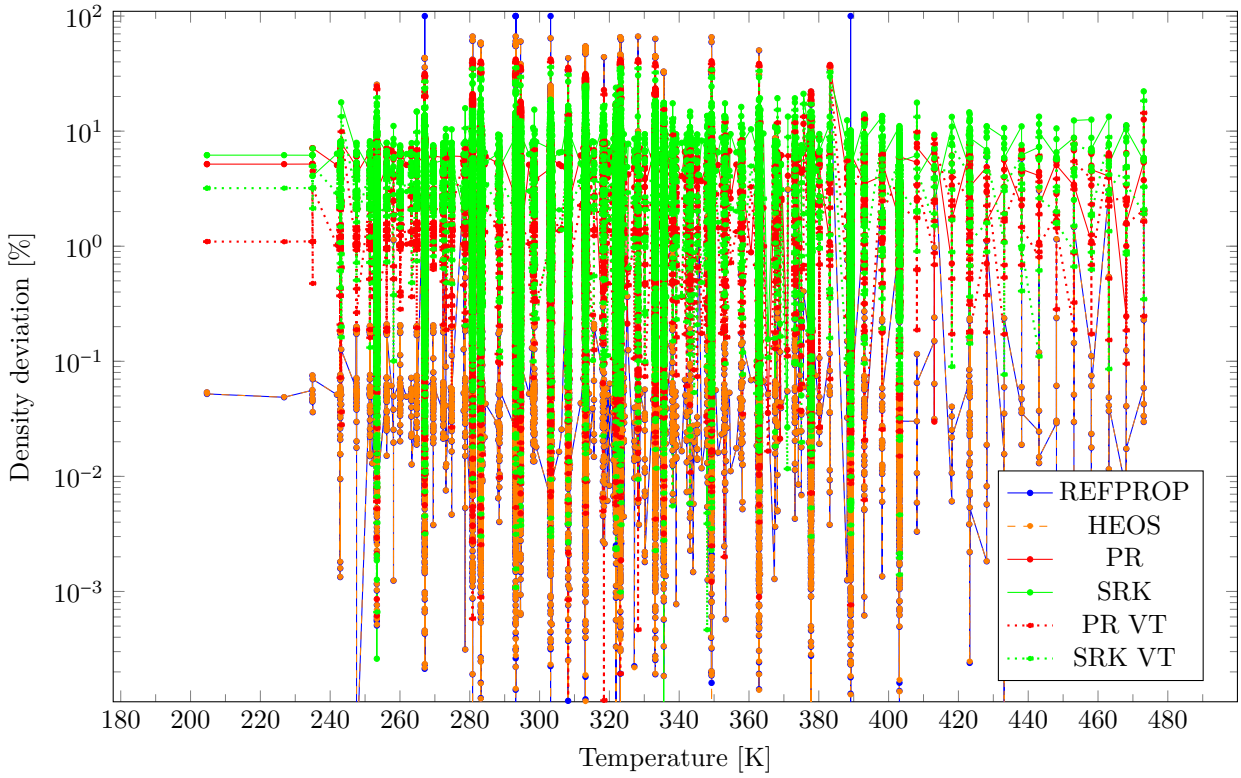


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Figure 220: Density dependence on the temperature and pressure for fluid R227EA

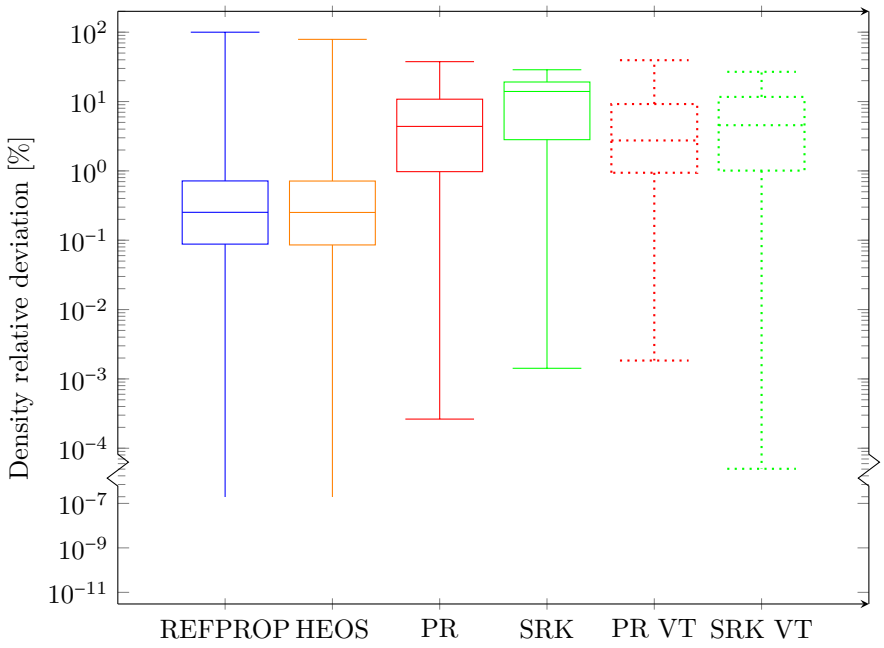


Figure 221: Relative density deviation to experimental data for fluid R23

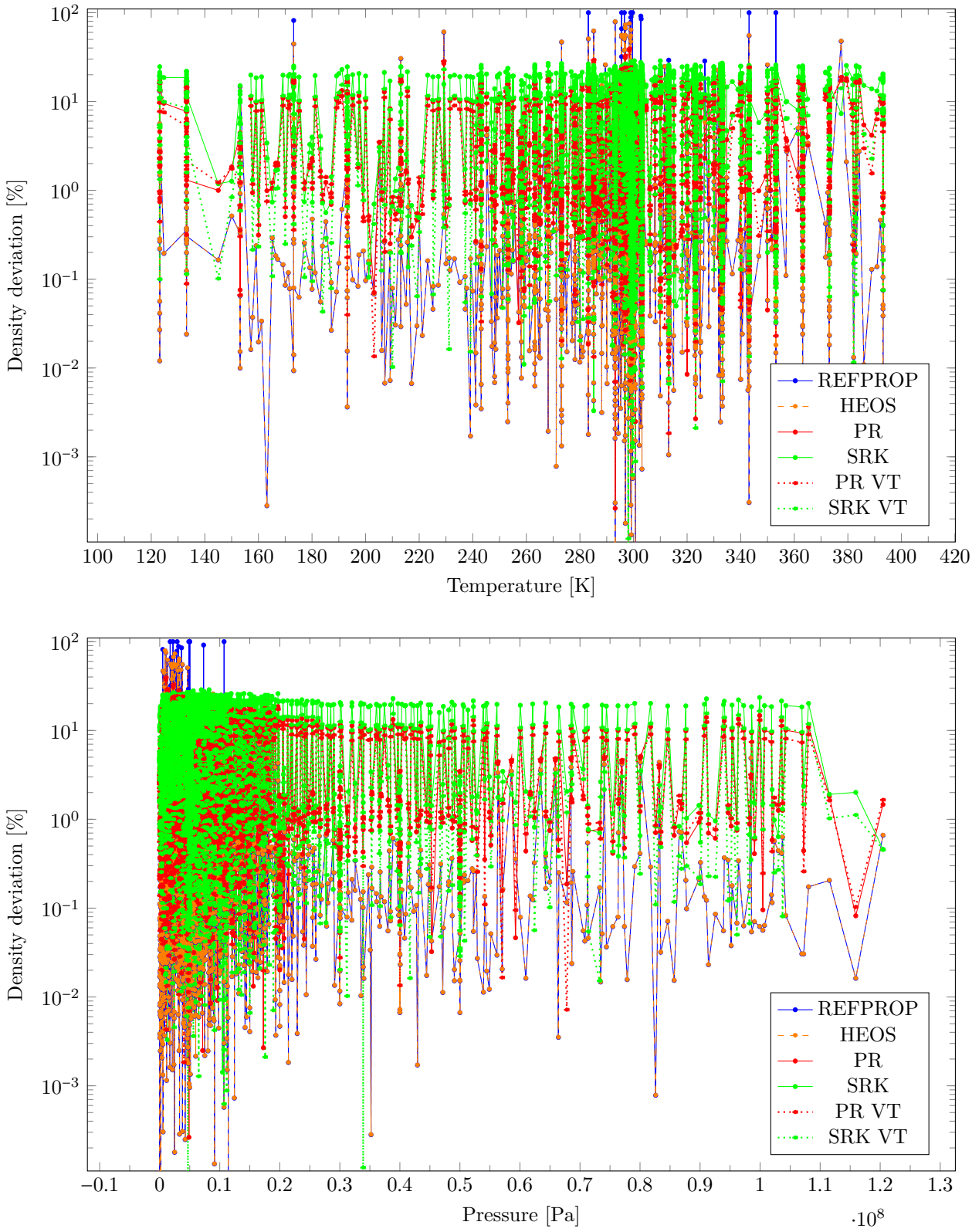


Figure 222: Density dependence on the temperature and pressure for fluid R23

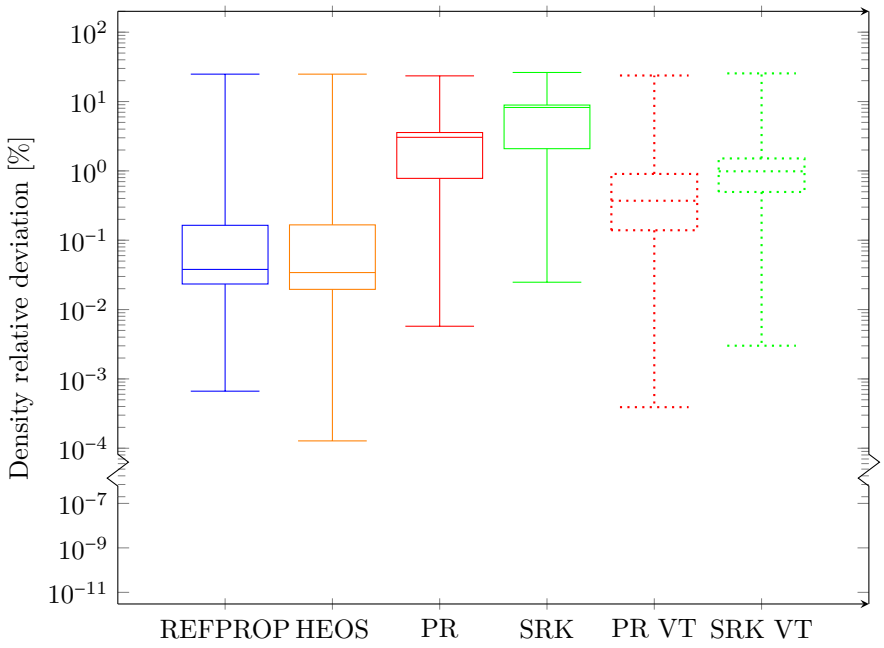


Figure 223: Relative density deviation to experimental data for fluid R236EA

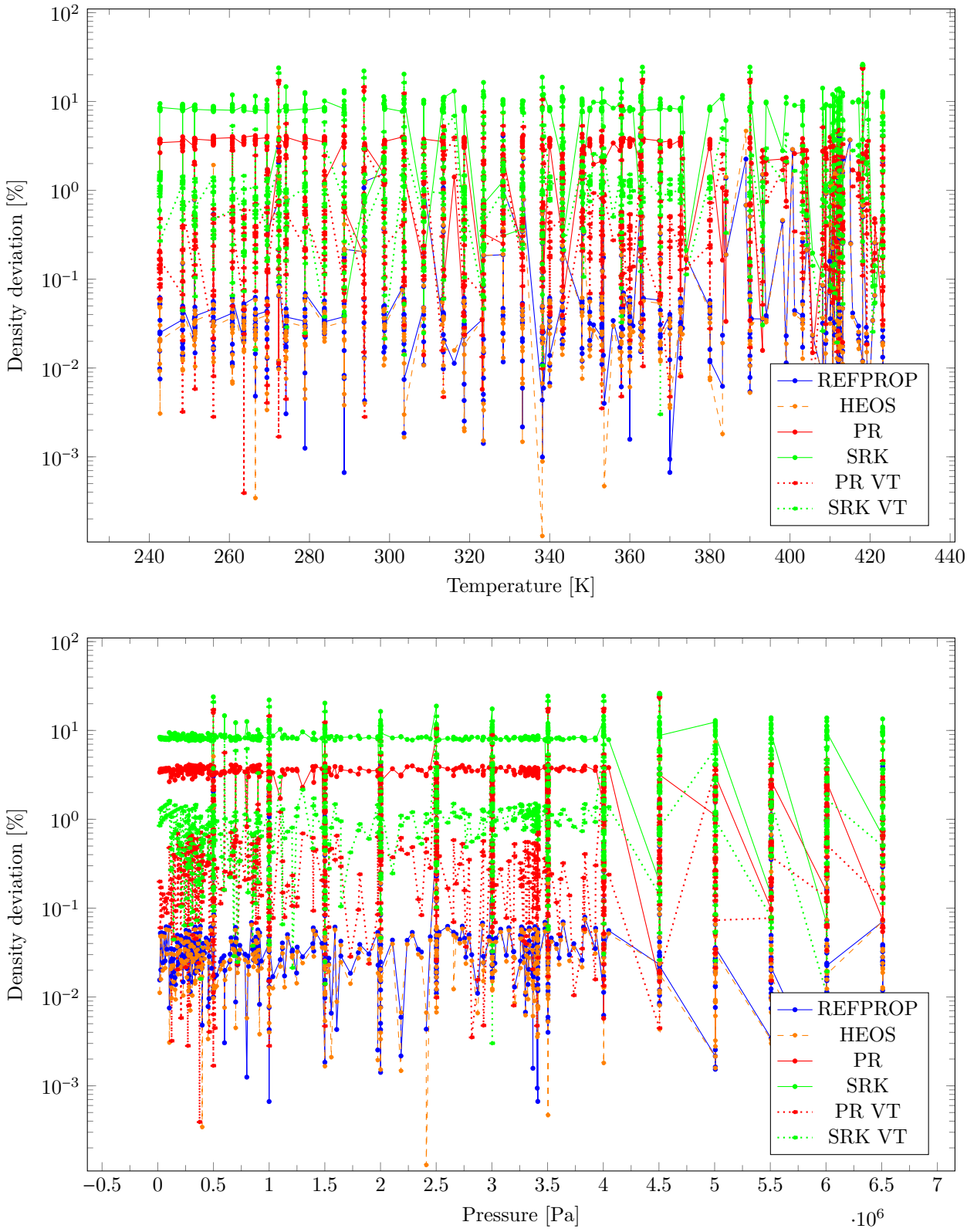


Figure 224: Density dependence on the temperature and pressure for fluid R236EA

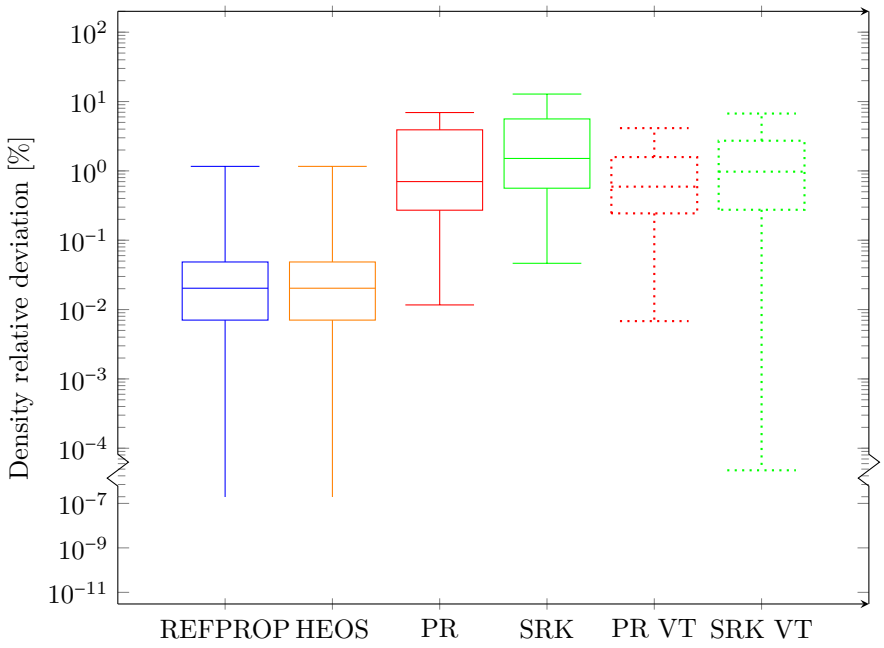


Figure 225: Relative density deviation to experimental data for fluid R236FA

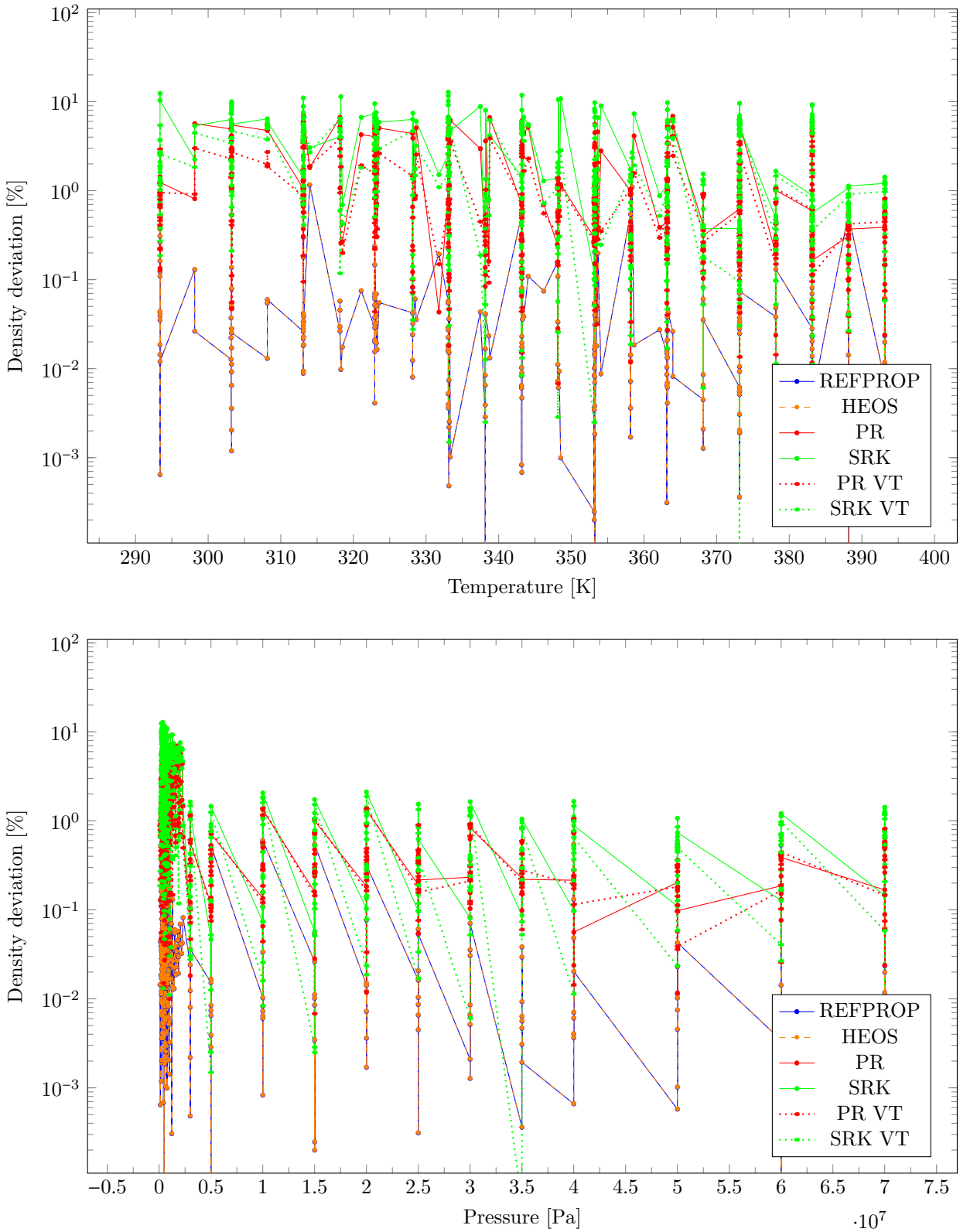


Figure 226: Density dependence on the temperature and pressure for fluid R236FA

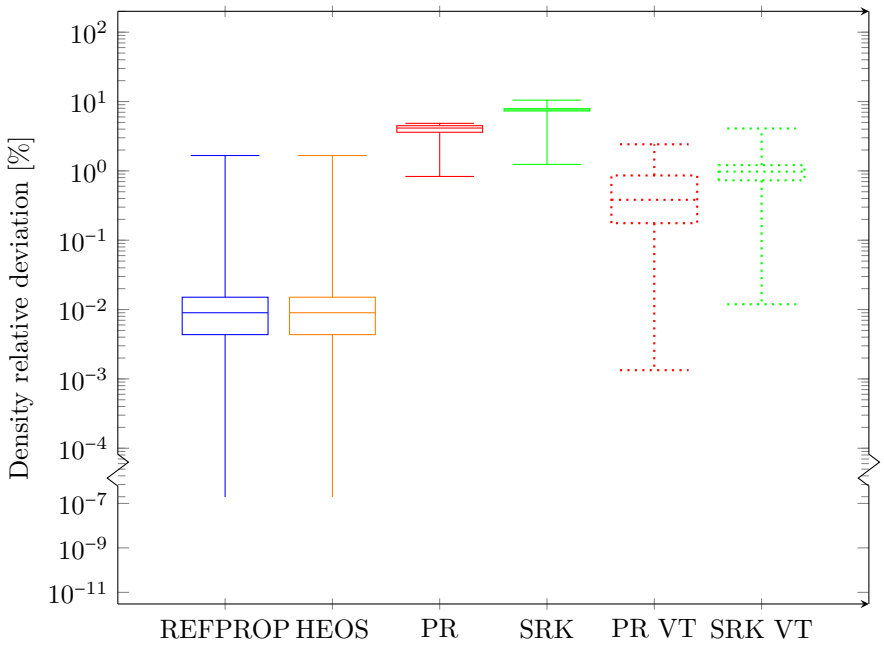


Figure 227: Relative density deviation to experimental data for fluid R245CA

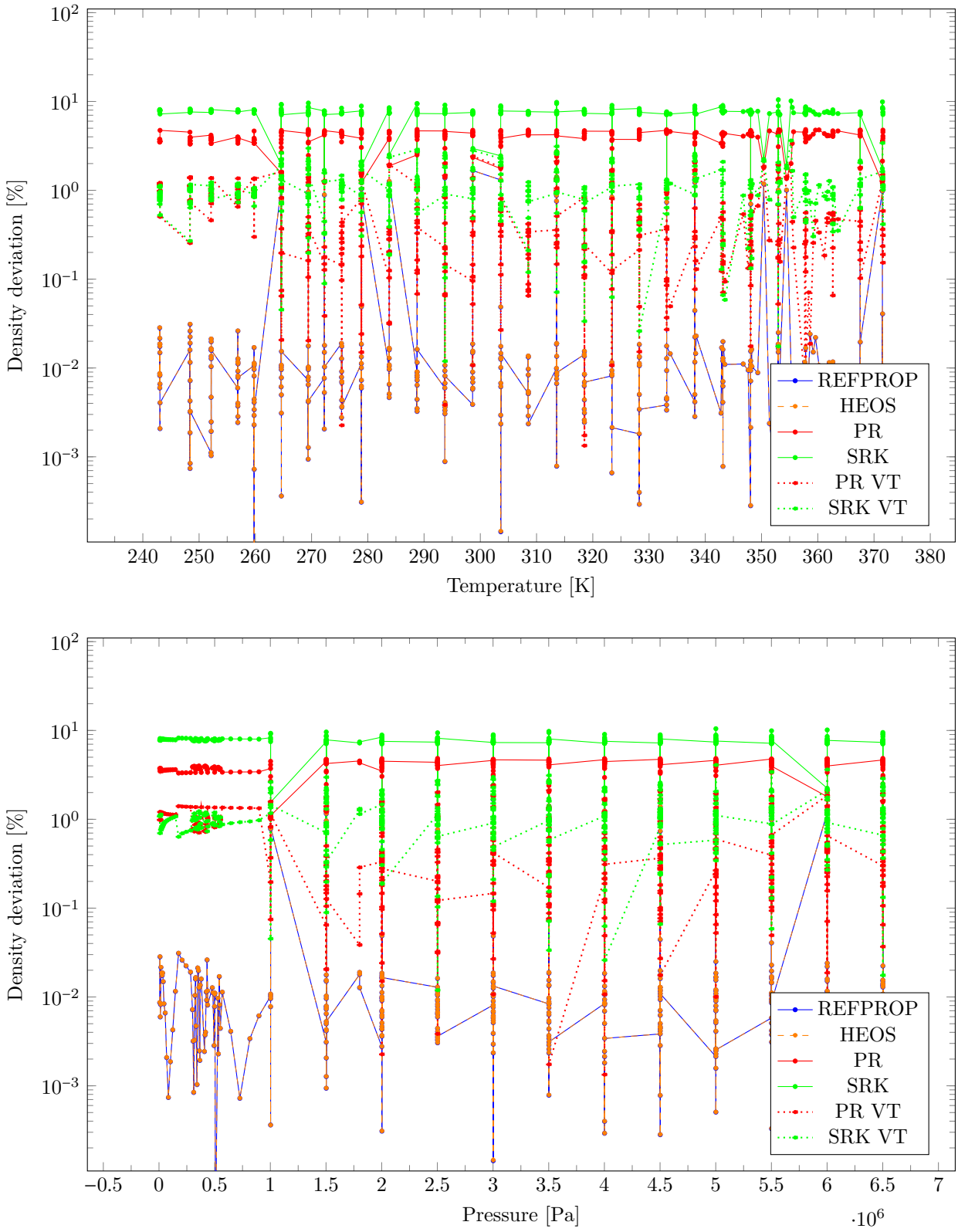


Figure 228: Density dependence on the temperature and pressure for fluid R245CA

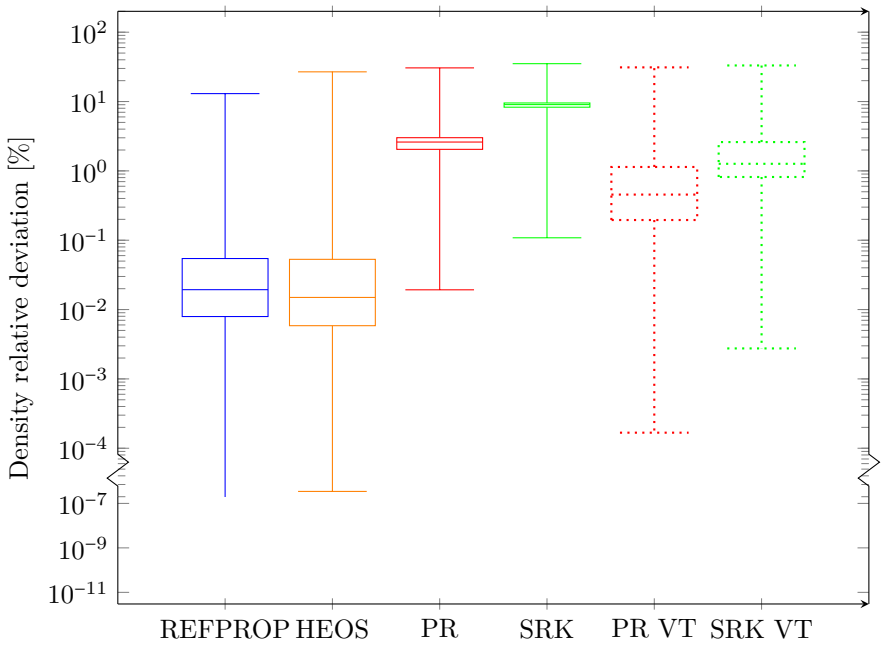


Figure 229: Relative density deviation to experimental data for fluid R245FA

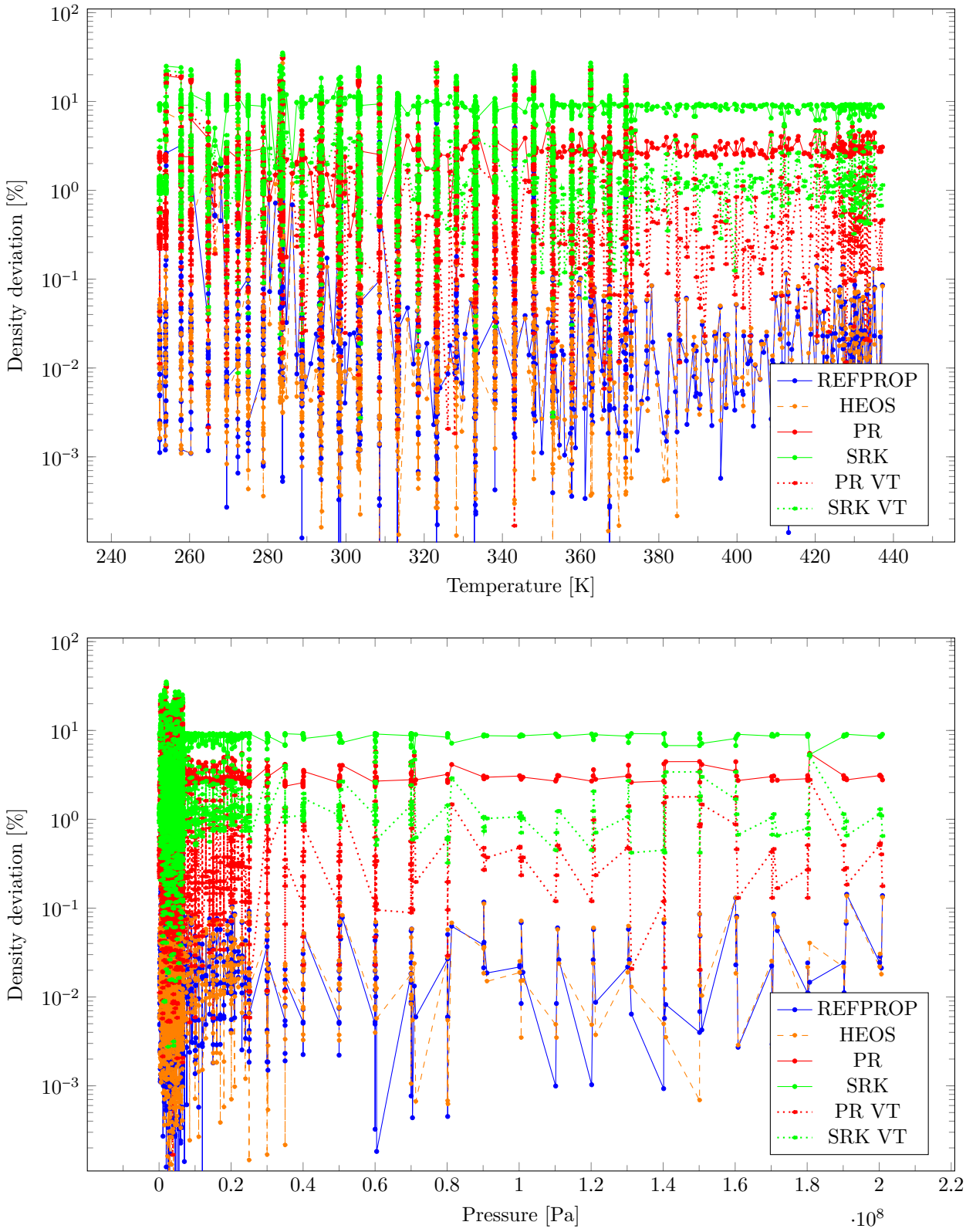


Figure 230: Density dependence on the temperature and pressure for fluid R245FA

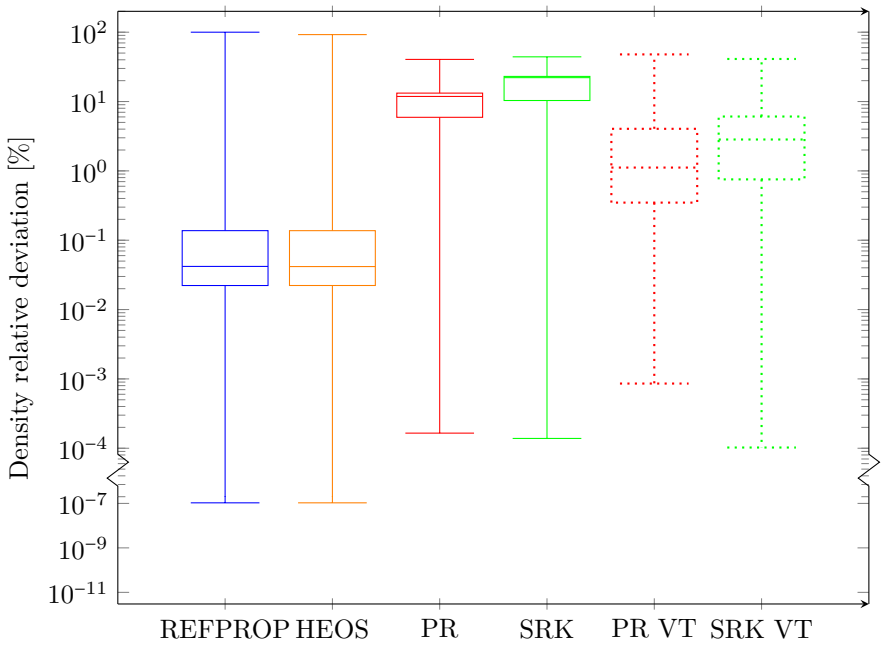


Figure 231: Relative density deviation to experimental data for fluid R32

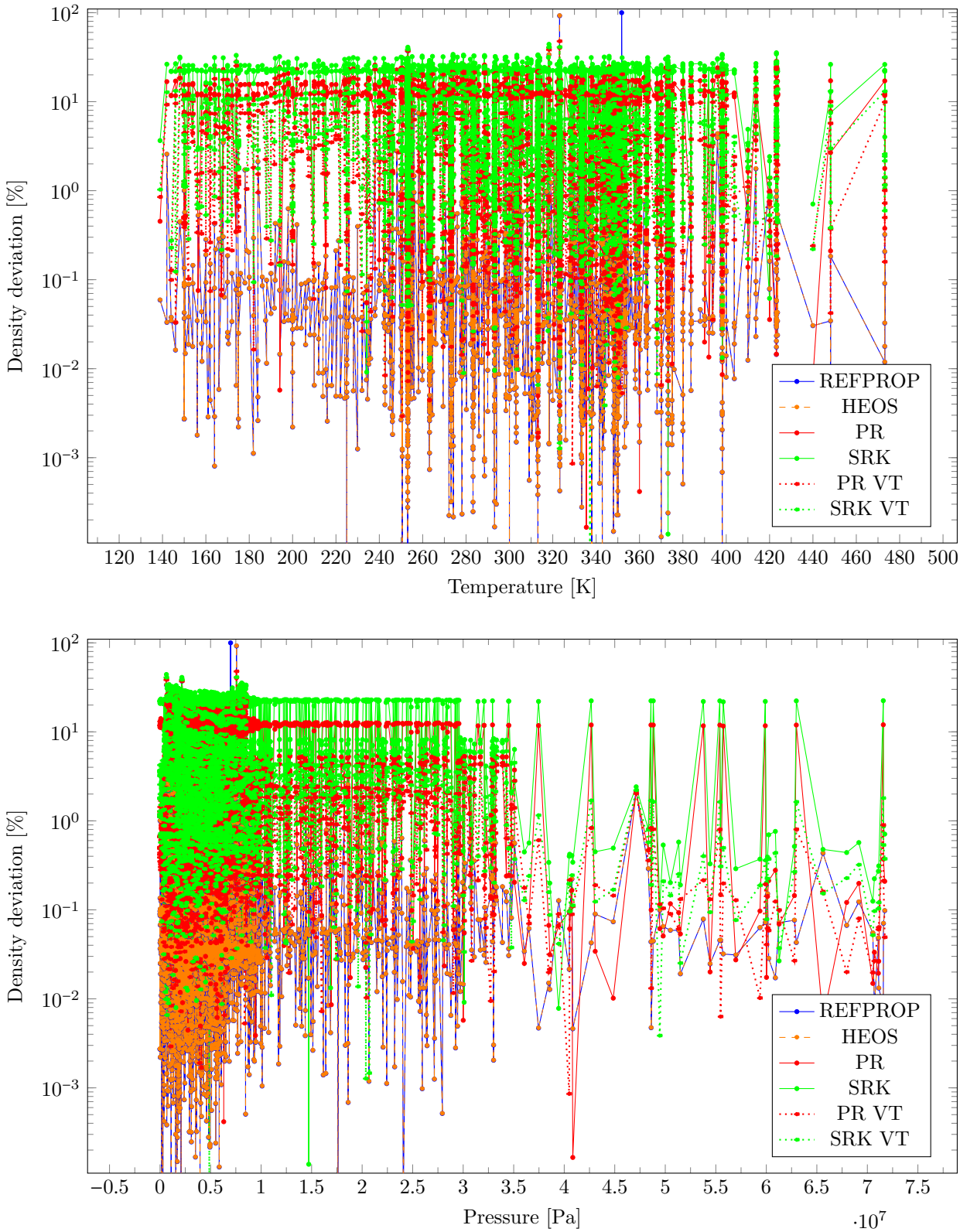


Figure 232: Density dependence on the temperature and pressure for fluid R32

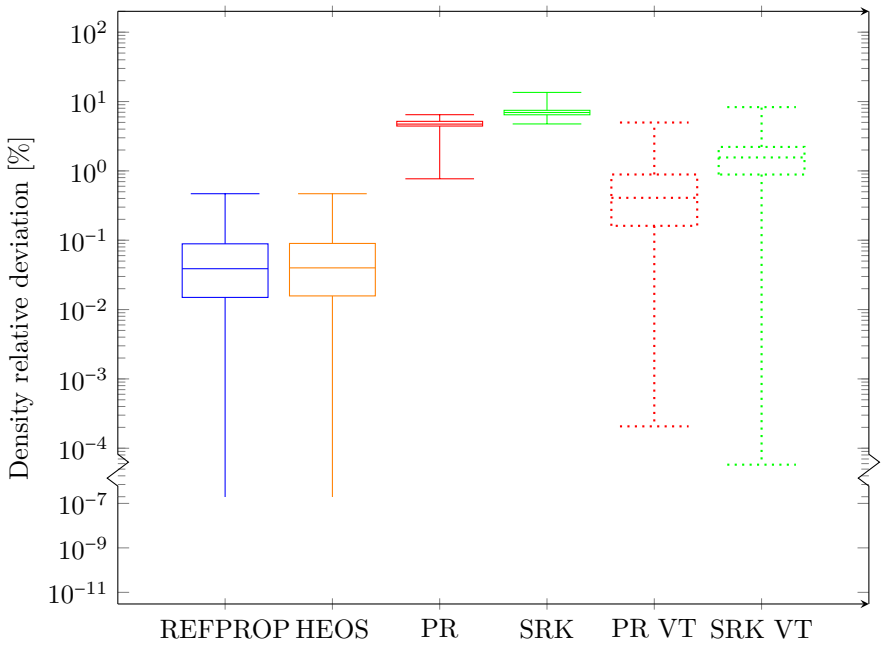


Figure 233: Relative density deviation to experimental data for fluid R365MFC

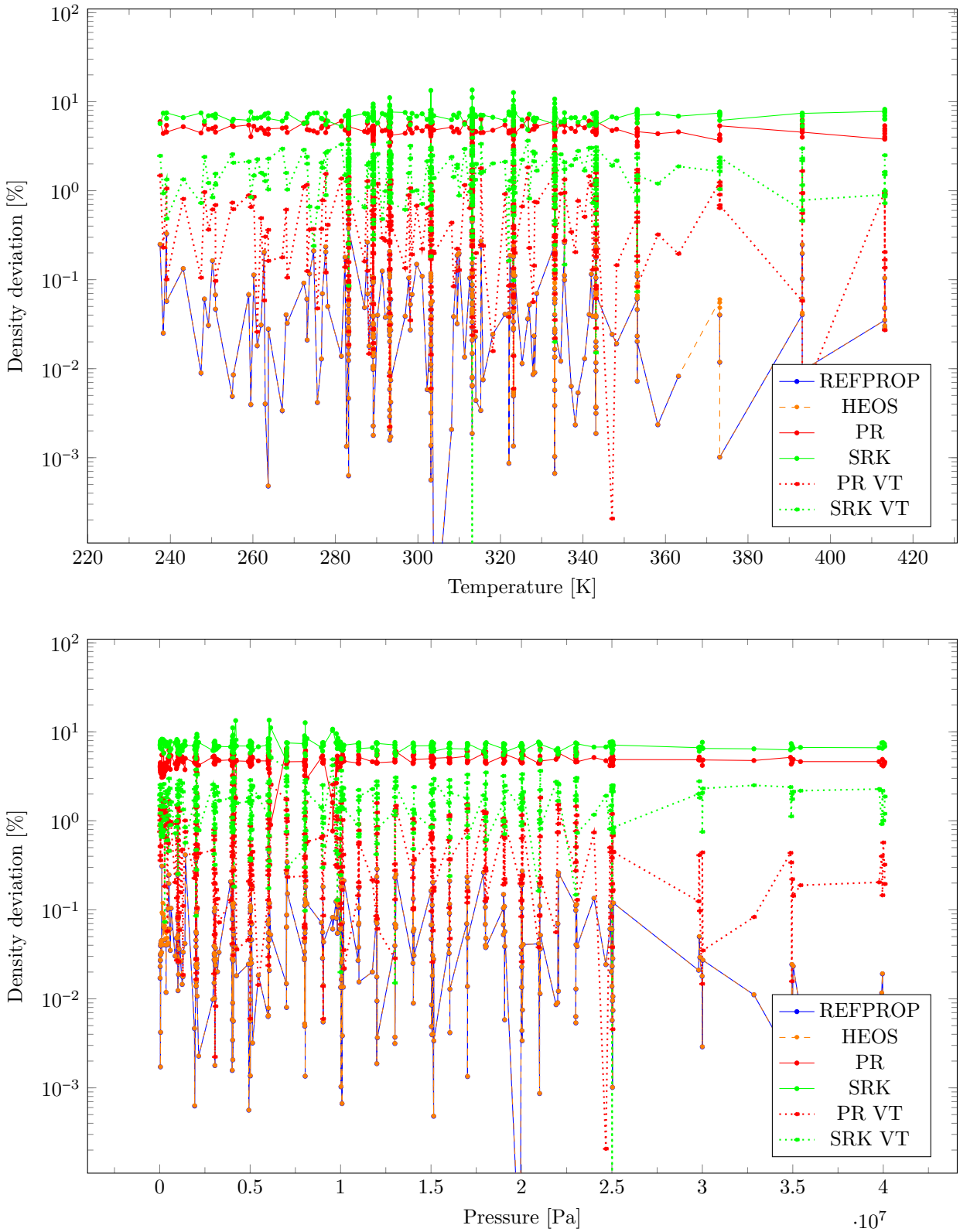


Figure 234: Density dependence on the temperature and pressure for fluid R365MFC

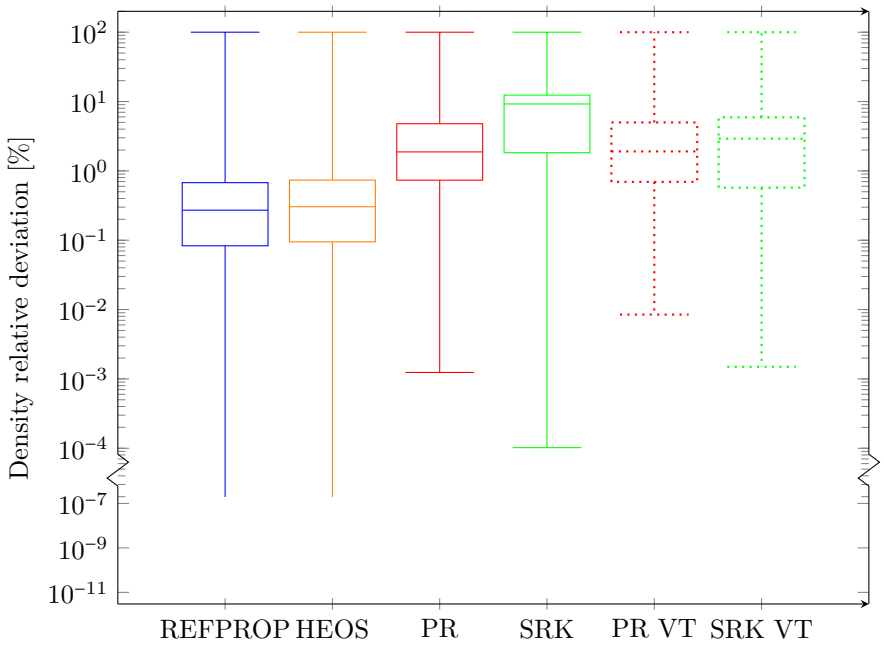


Figure 235: Relative density deviation to experimental data for fluid R40

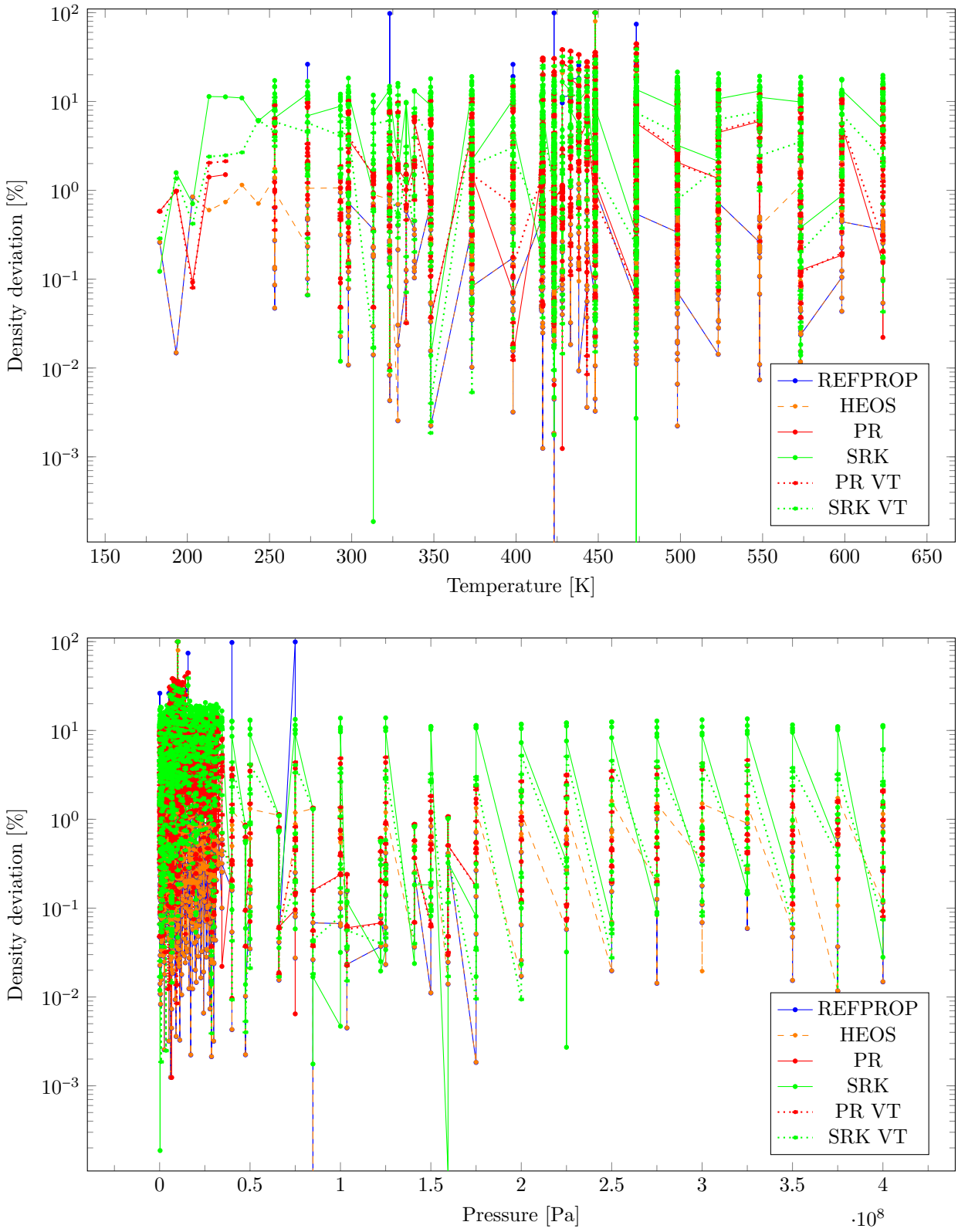


Figure 236: Density dependence on the temperature and pressure for fluid R40

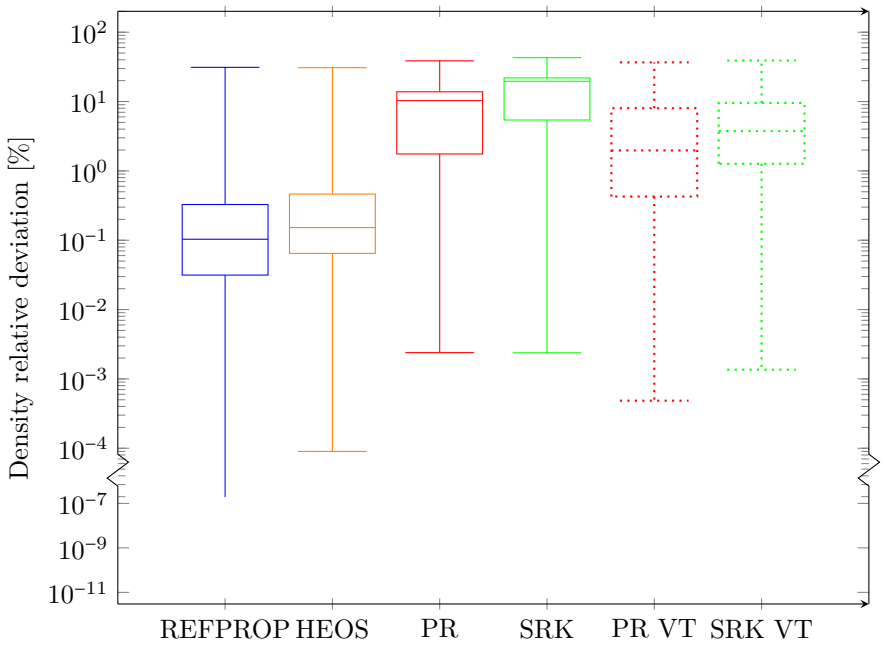


Figure 237: Relative density deviation to experimental data for fluid R41

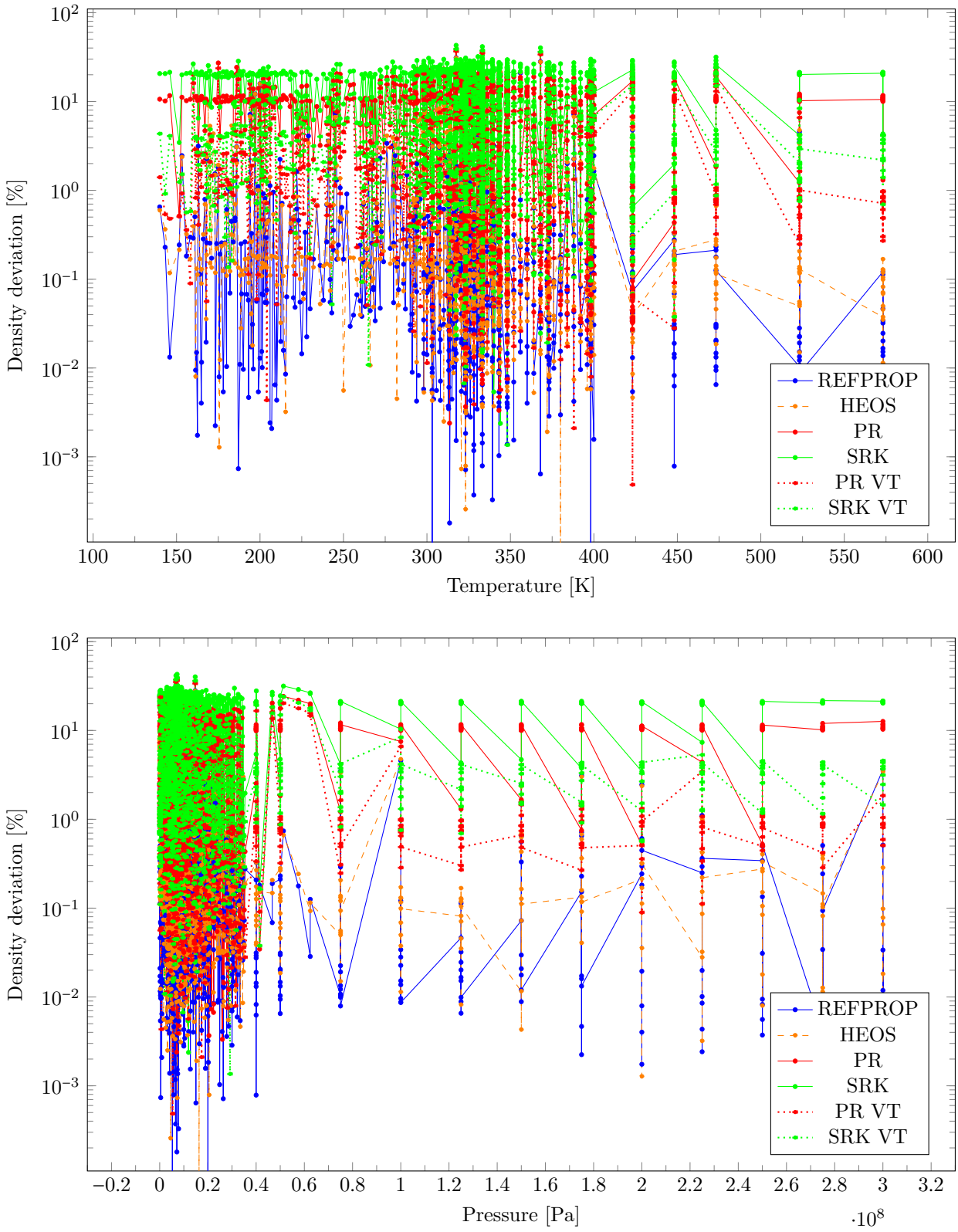


Figure 238: Density dependence on the temperature and pressure for fluid R41

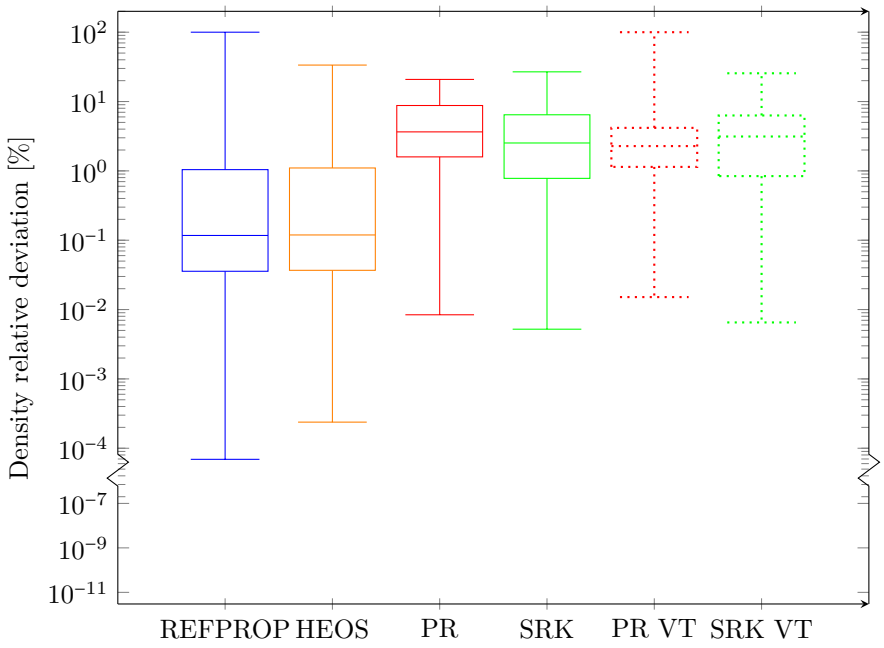


Figure 239: Relative density deviation to experimental data for fluid RC318

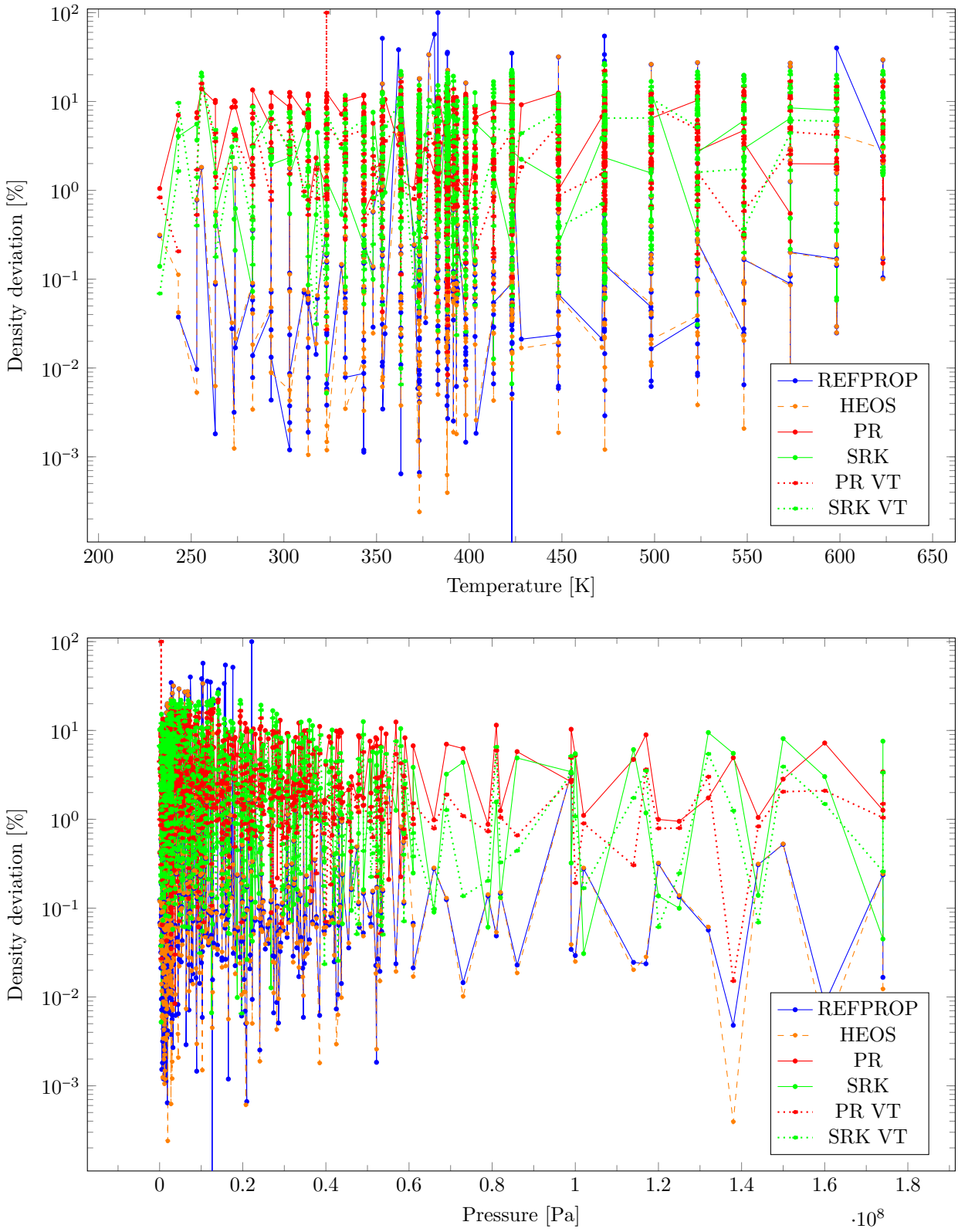


Figure 240: Density dependence on the temperature and pressure for fluid RC318

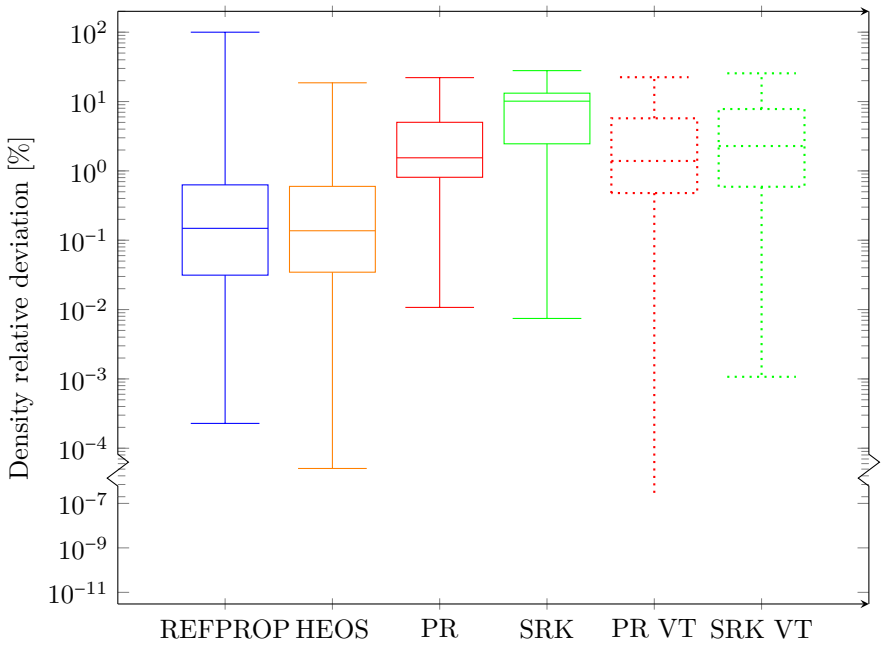


Figure 241: Relative density deviation to experimental data for fluid SulfurDioxide

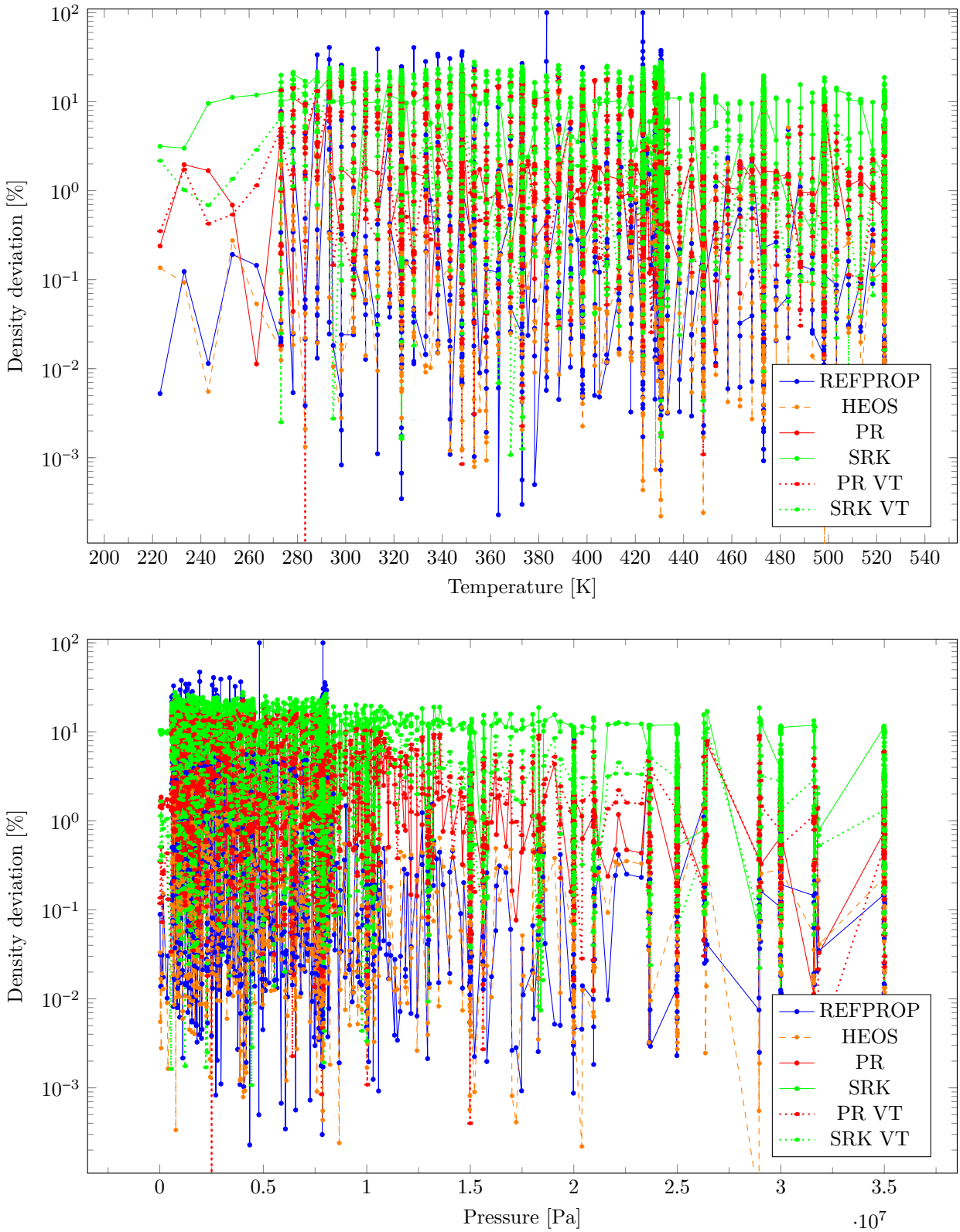


Figure 242: Density dependence on the temperature and pressure for fluid SulfurDioxide

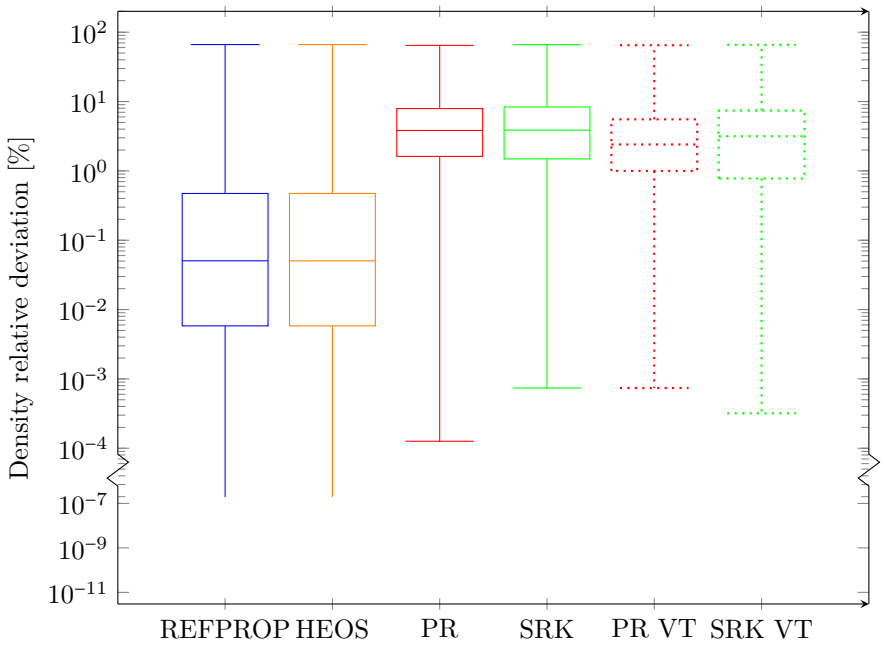


Figure 243: Relative density deviation to experimental data for fluid SulfurHexafluoride

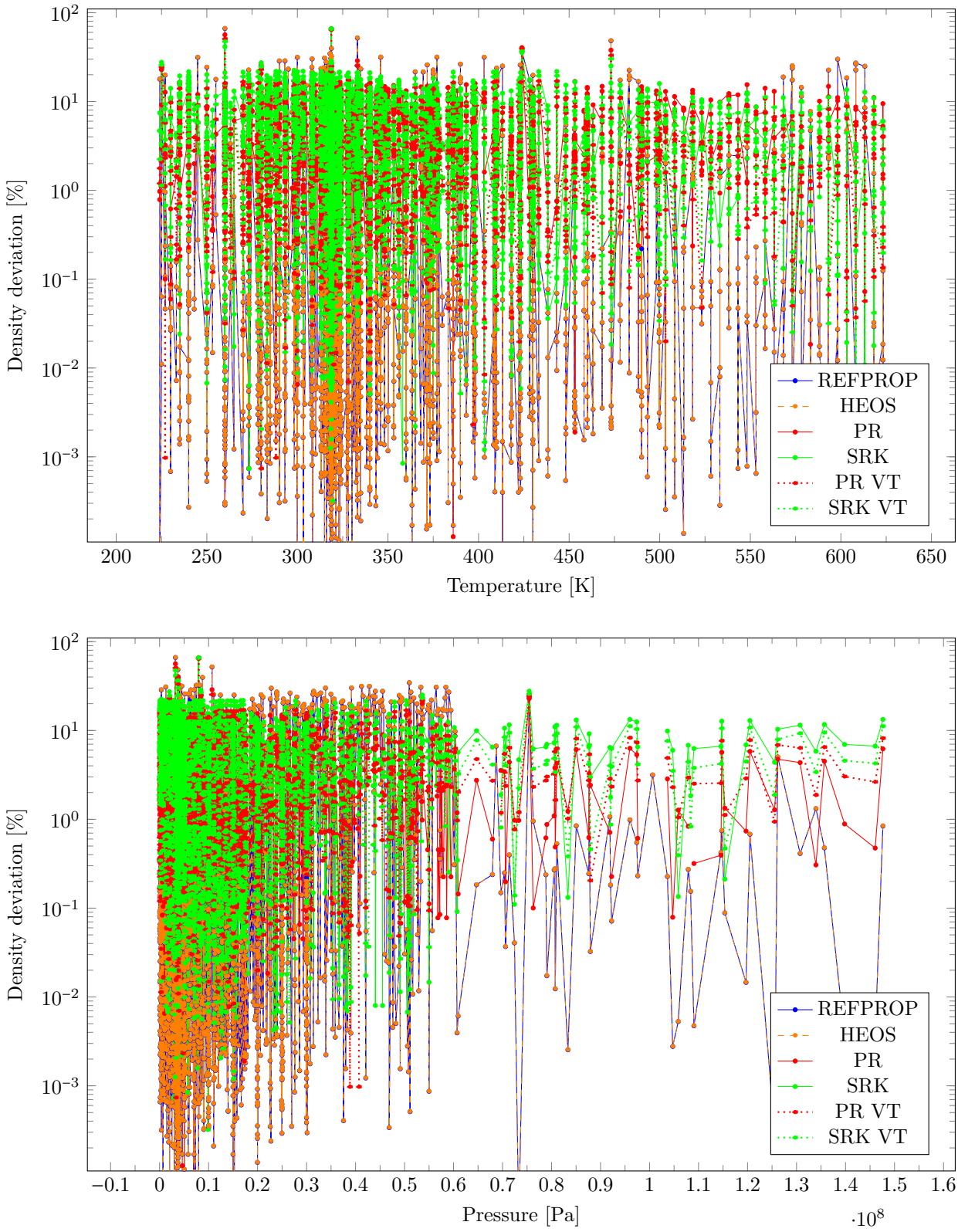


Figure 244: Density dependence on the temperature and pressure for fluid SulfurHexafluoride

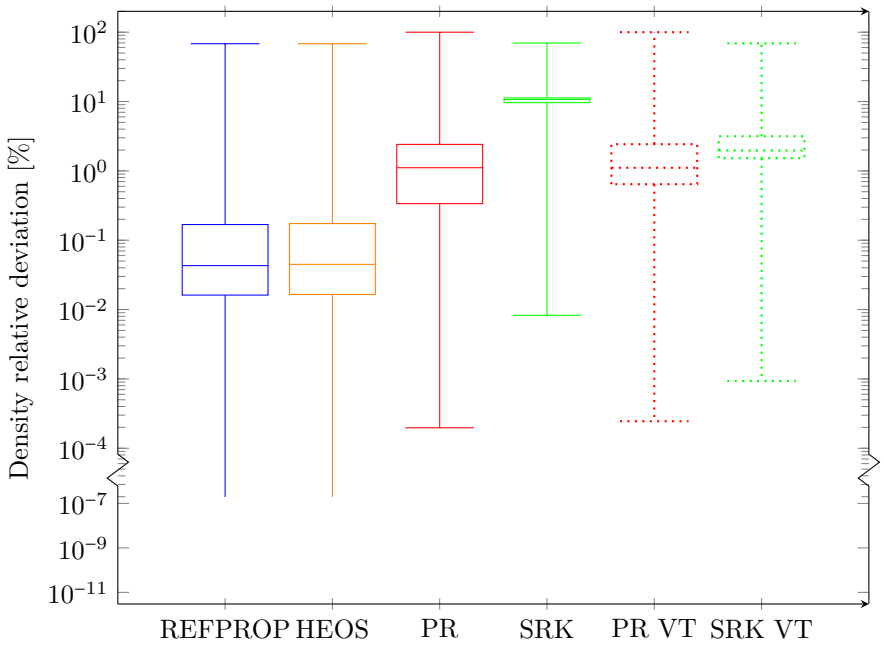


Figure 245: Relative density deviation to experimental data for fluid Toluene

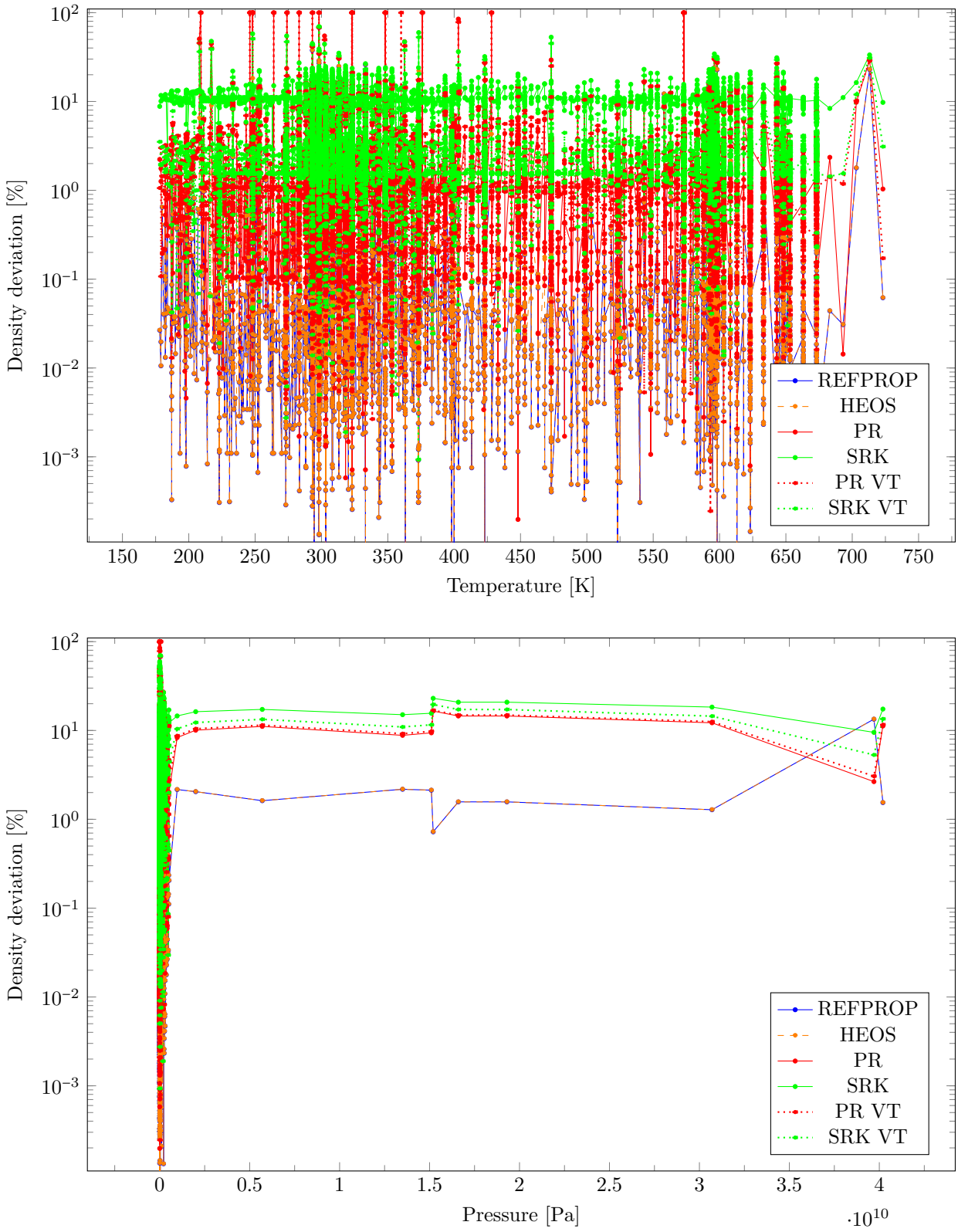


Figure 246: Density dependence on the temperature and pressure for fluid Toluene

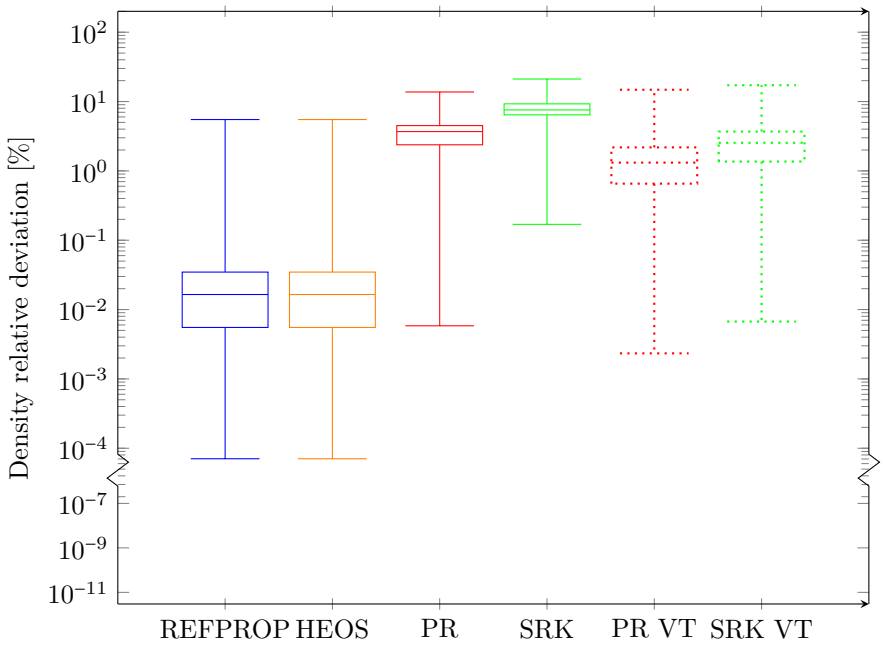
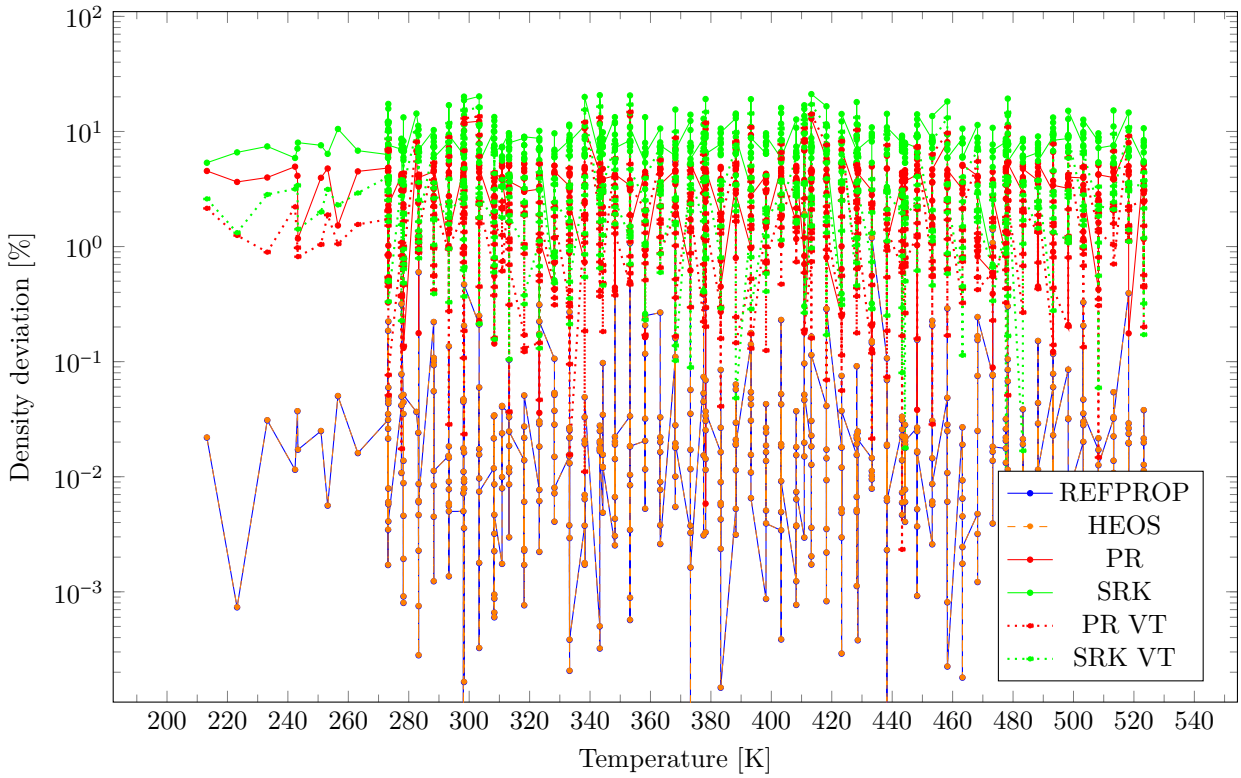


Figure 247: Relative density deviation to experimental data for fluid TRANS-2-BUTENE



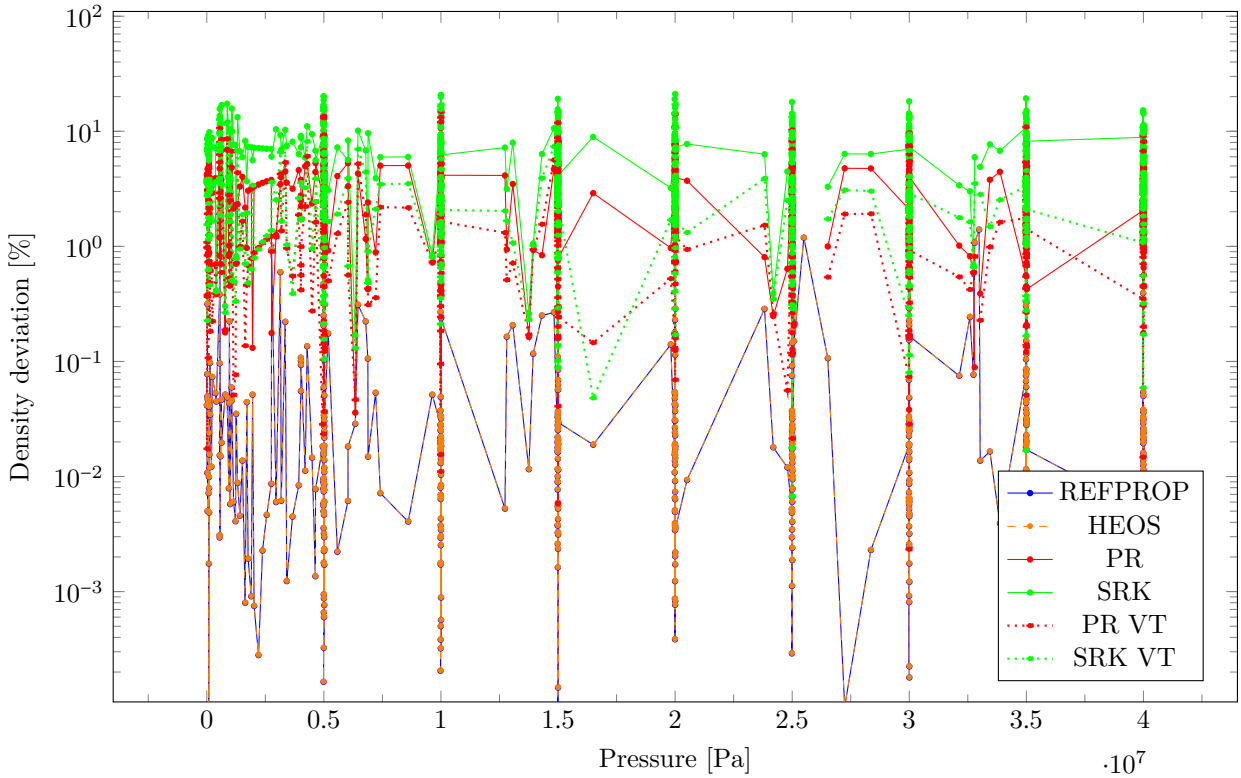


Figure 248: Density dependence on the temperature and pressure for fluid TRANS-2-BUTENE

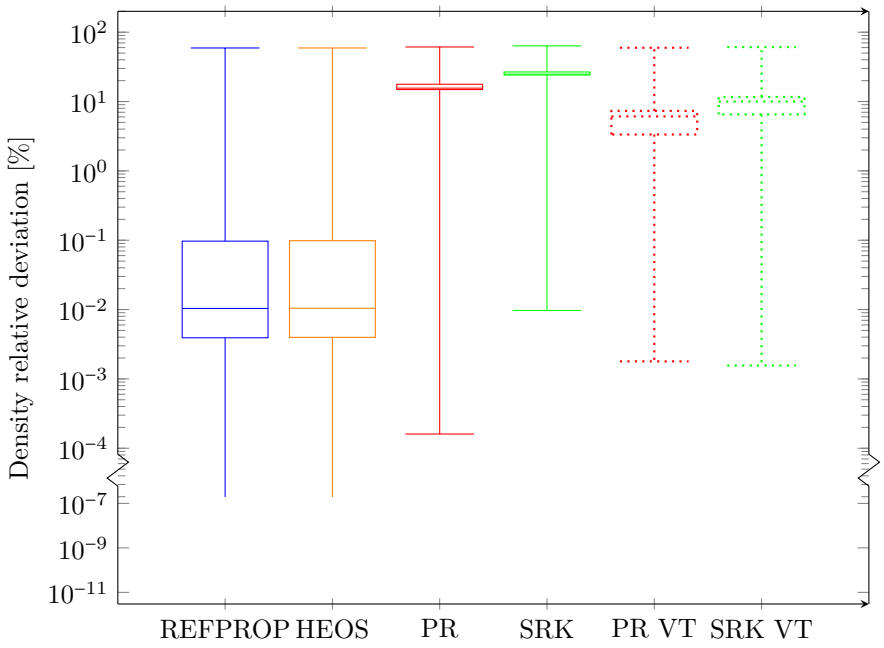


Figure 249: Relative density deviation to experimental data for fluid Water

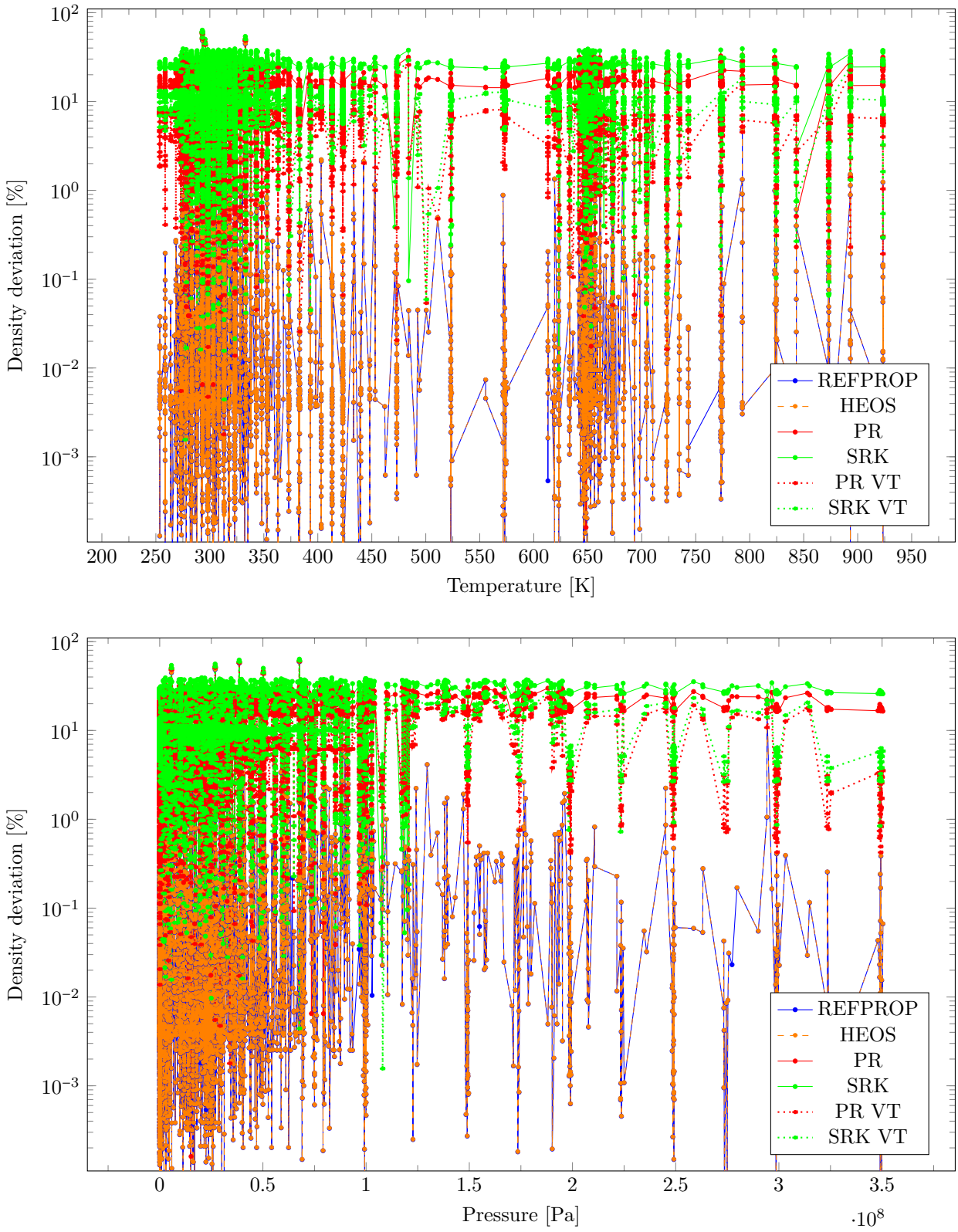


Figure 250: Density dependence on the temperature and pressure for fluid Water

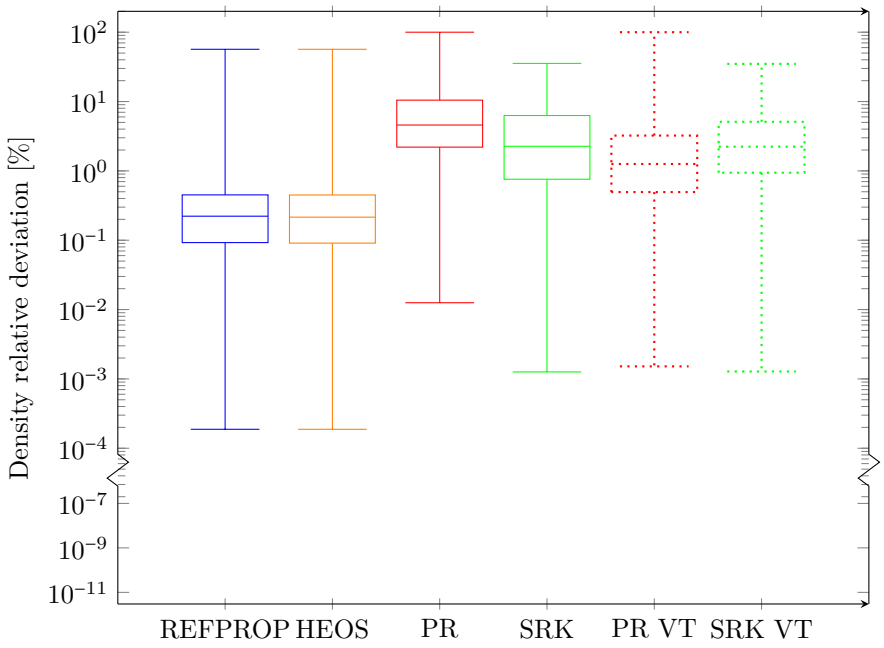


Figure 251: Relative density deviation to experimental data for fluid Xenon

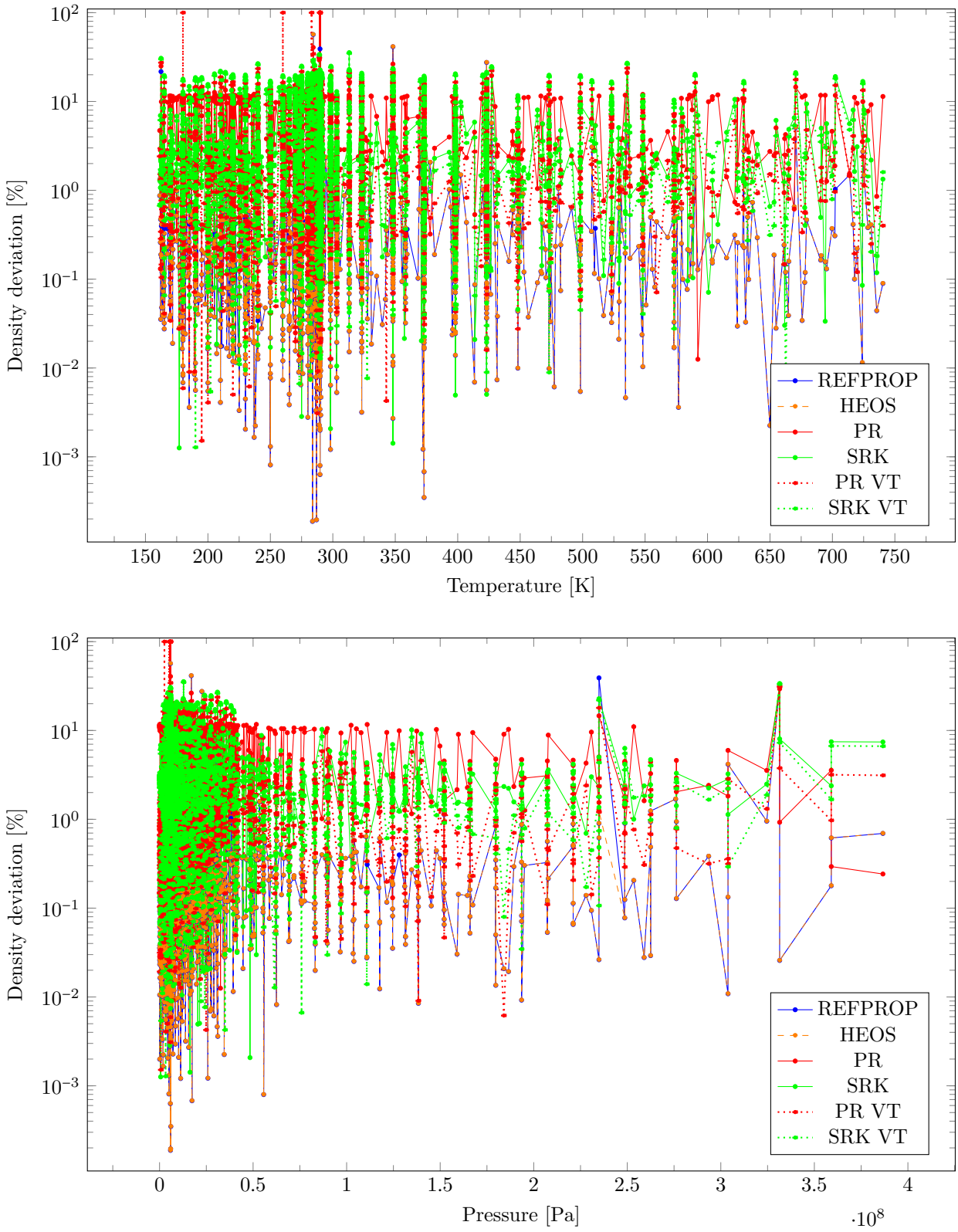


Figure 252: Density dependence on the temperature and pressure for fluid Xenon

2.4. Saturation data

For mixtures, vapour-liquid equilibrium data where provided by NIST. These data consist of different molar fraction of the mixture and the temperature and pressure corresponding to the saturation curve.

The temperature was computed from the pressure and quality input. The pressure was computed from the temperature and quality. The deviations where than computed according to equations 44 and 45.

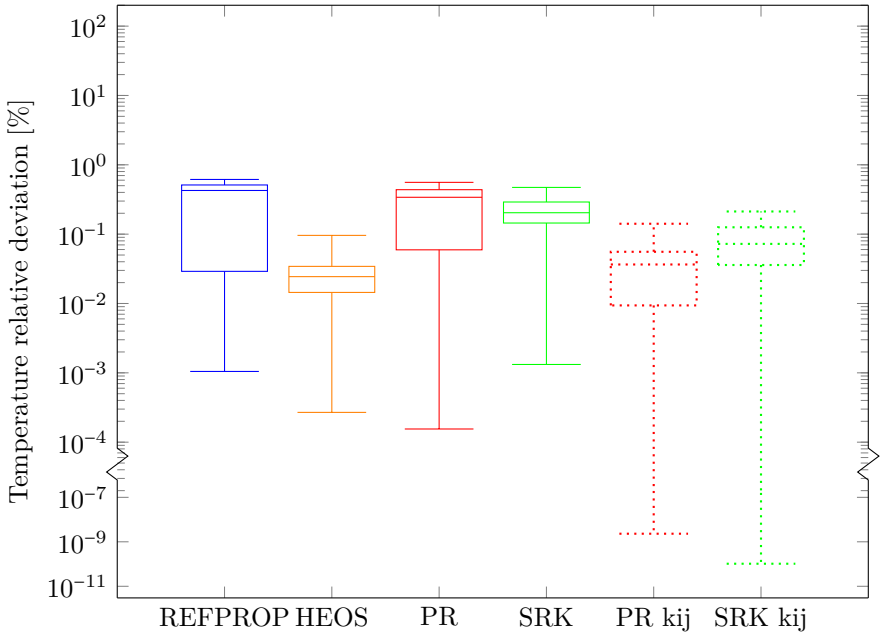
The volume translation has not been tested here (no density data to compare too), but the interaction parameter k_{ij} has been used. This parameter has been computed by fitting to the experimental data with Brent's method. The error function used for this fitting was:

$$\bar{E} = \sum \left| E_T + 0.1 E_p \right| \tag{50}$$

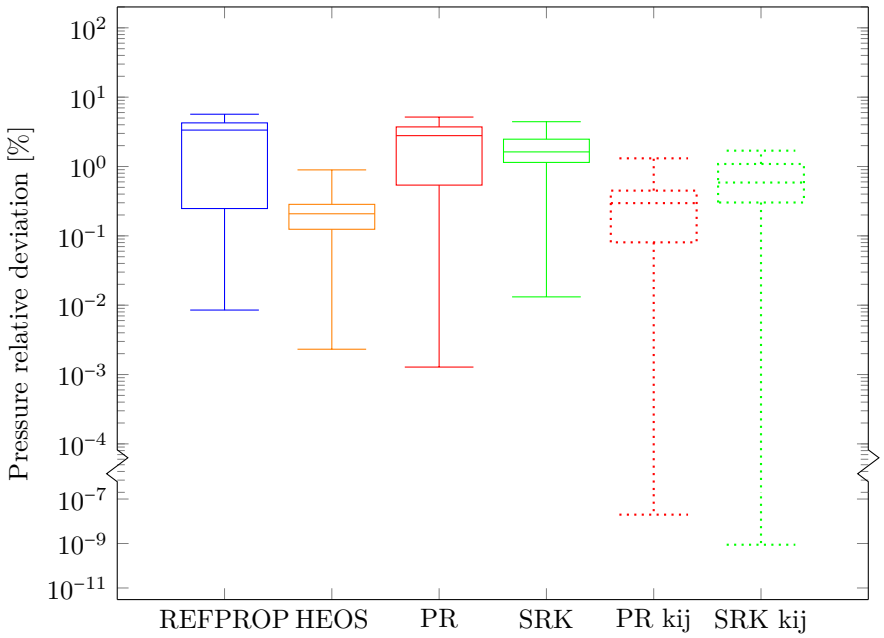
were E_T and E_p are from equations 44 and 45.

2.4.1. Binary mixture

Mixture R1234YF-R134A.



(a) Temperature deviation



(b) Pressure deviation

Figure 253: Relative deviation to experimental saturation data for mixtures based on R1234YF and R134A

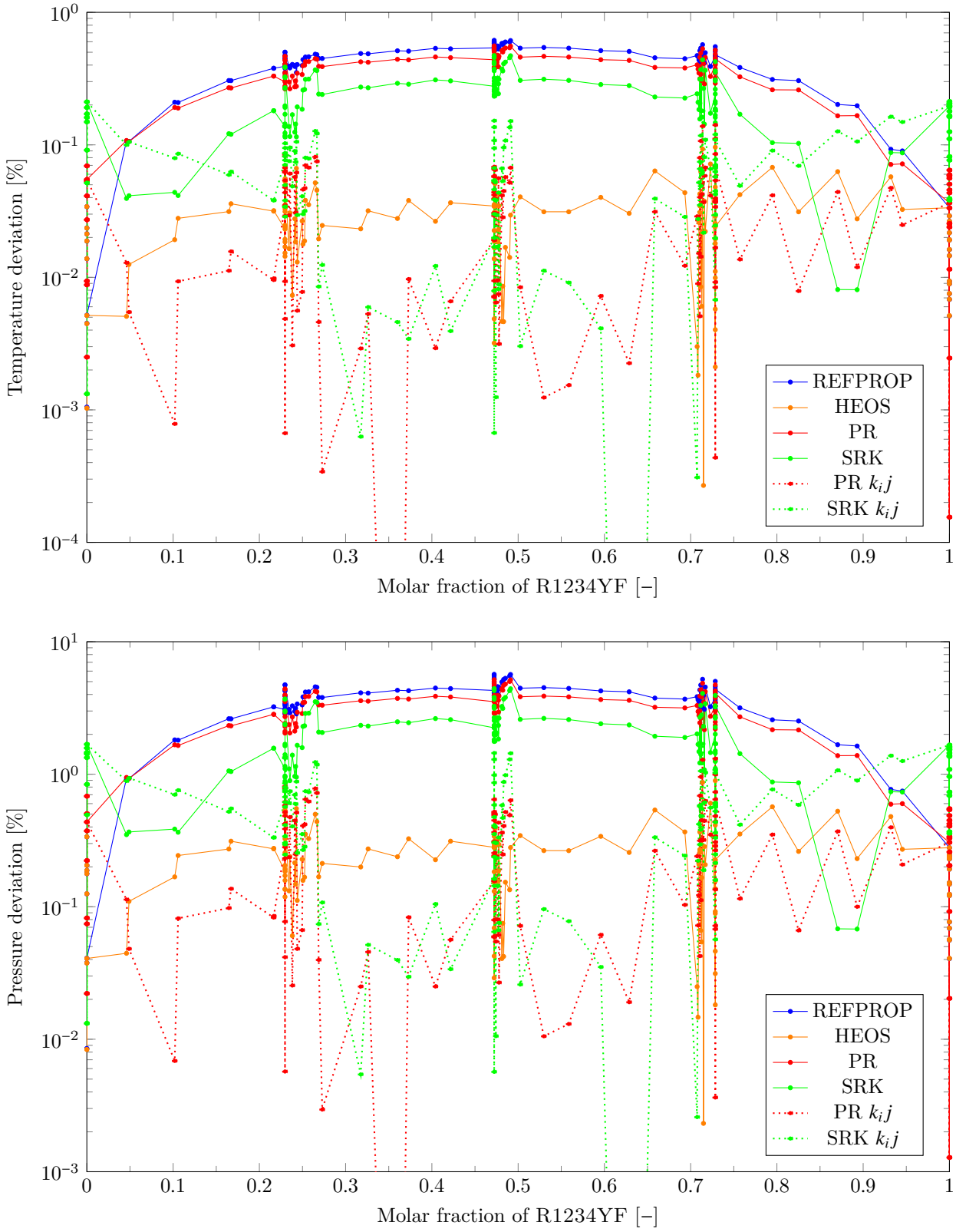


Figure 254: Dependence on the molar fraction for the binary mixture R1234YF-R134A

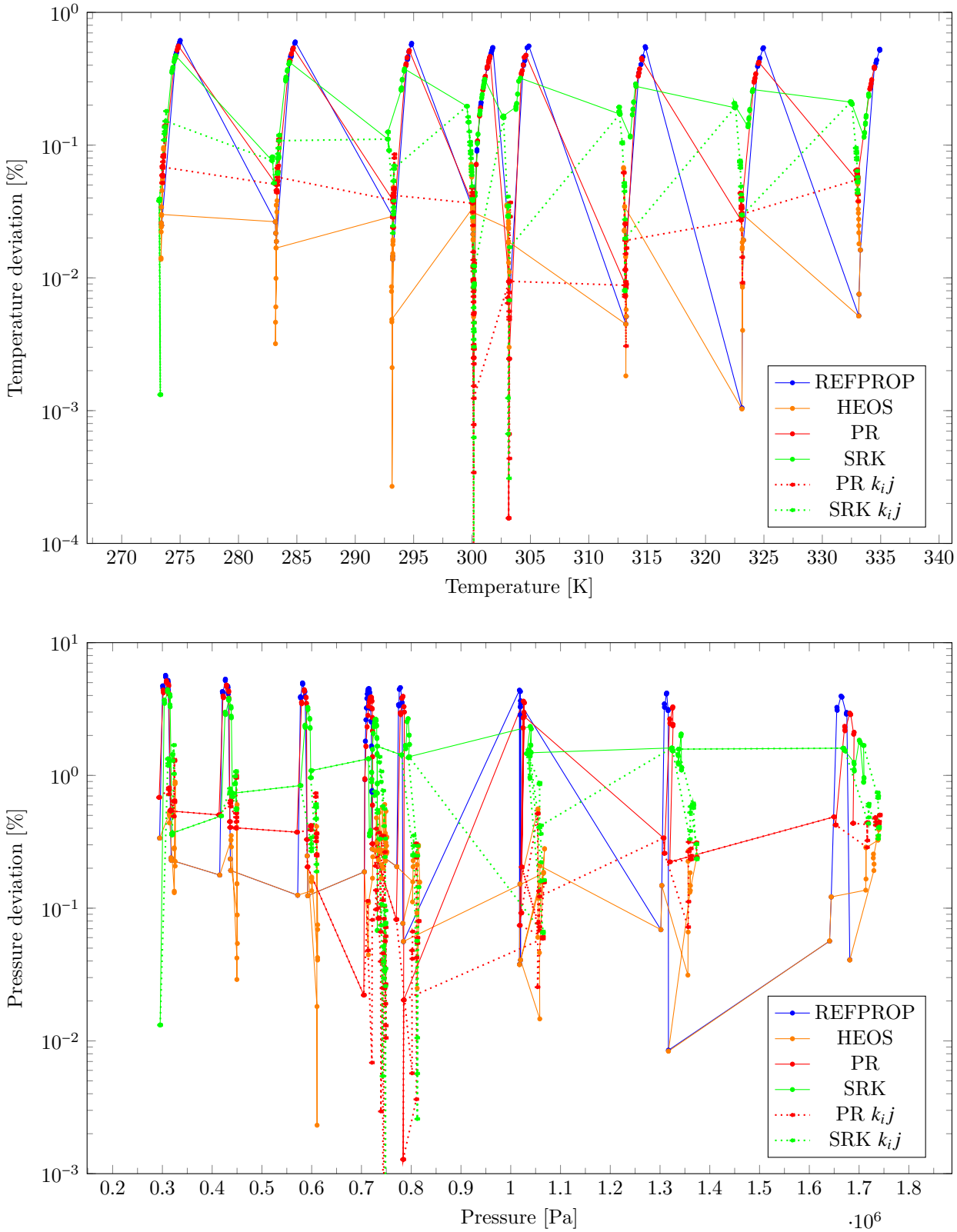
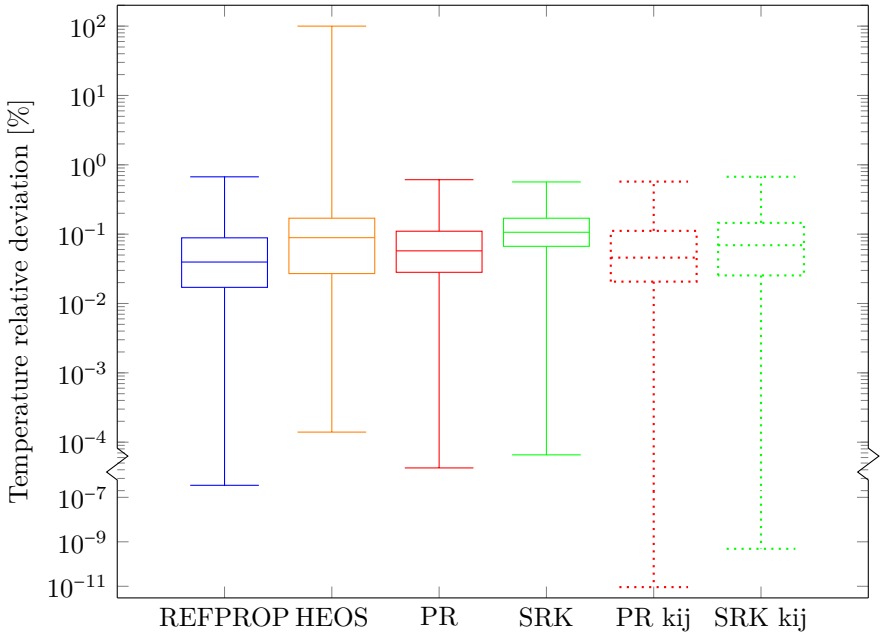
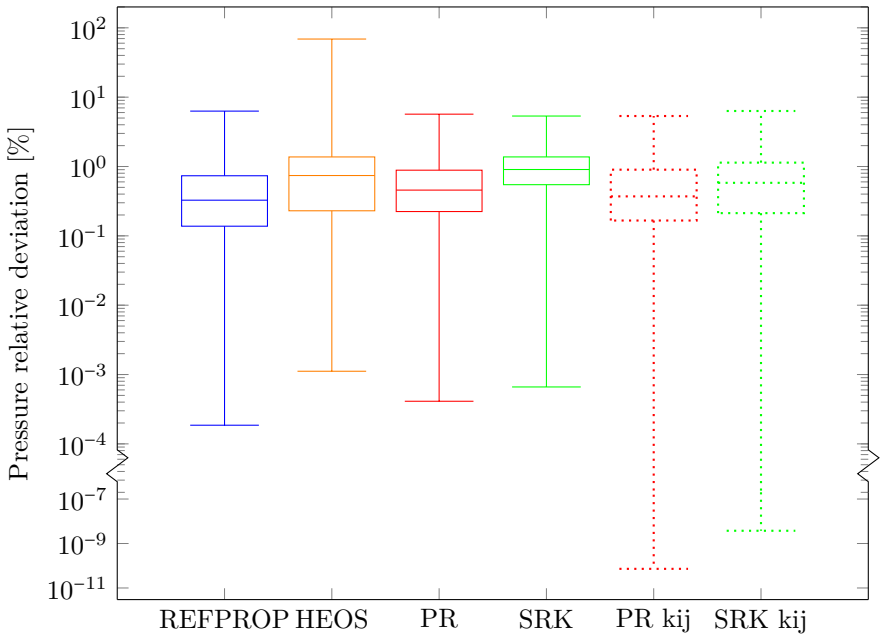


Figure 255: Dependence on the temperature and pressure for the binary mixture R1234YF-R134A

Mixture R125-R32.



(a) Temperature deviation



(b) Pressure deviation

Figure 256: Relative deviation to experimental saturation data for mixtures based on R125 and R32

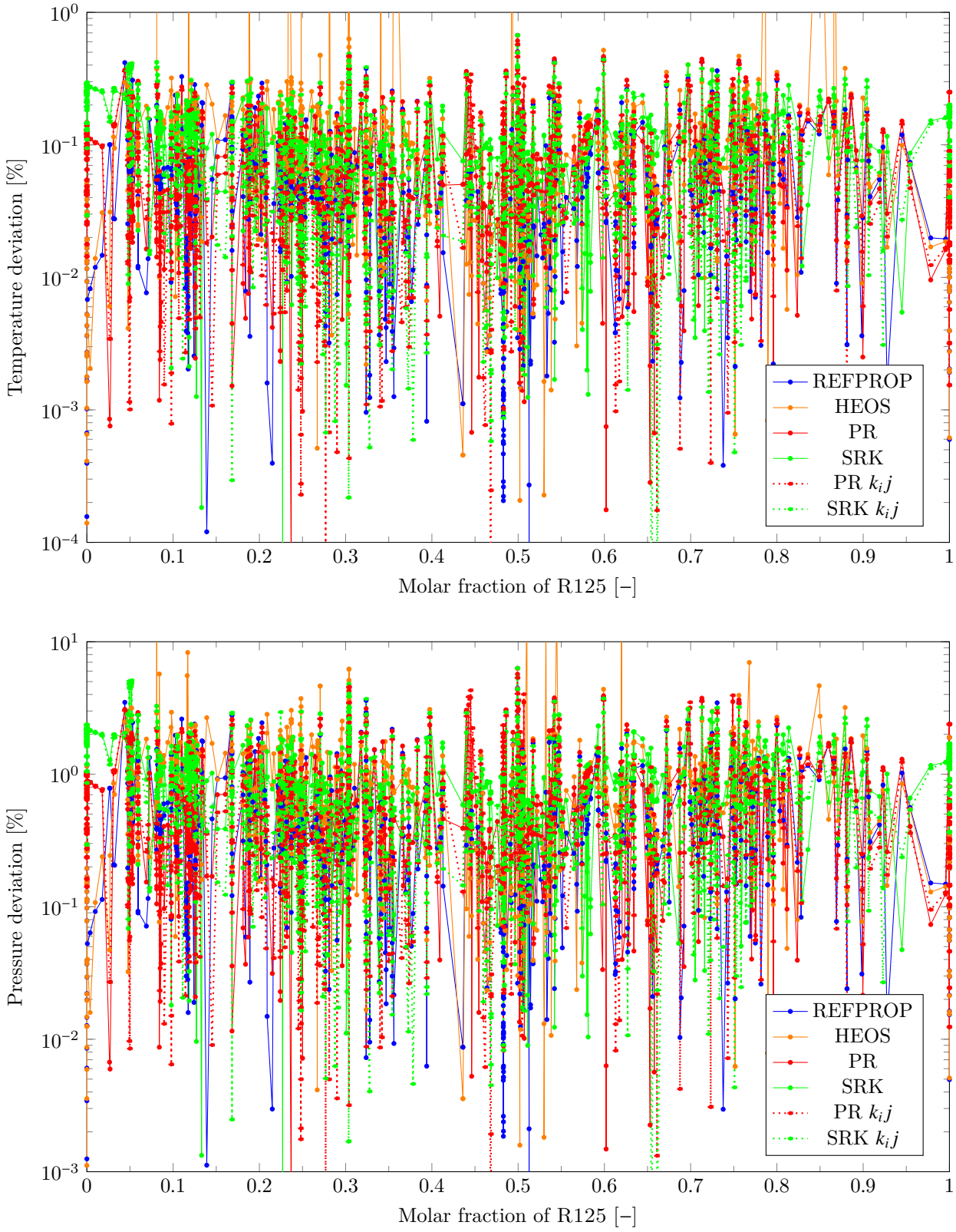


Figure 257: Dependence on the molar fraction for the binary mixture R125-R32

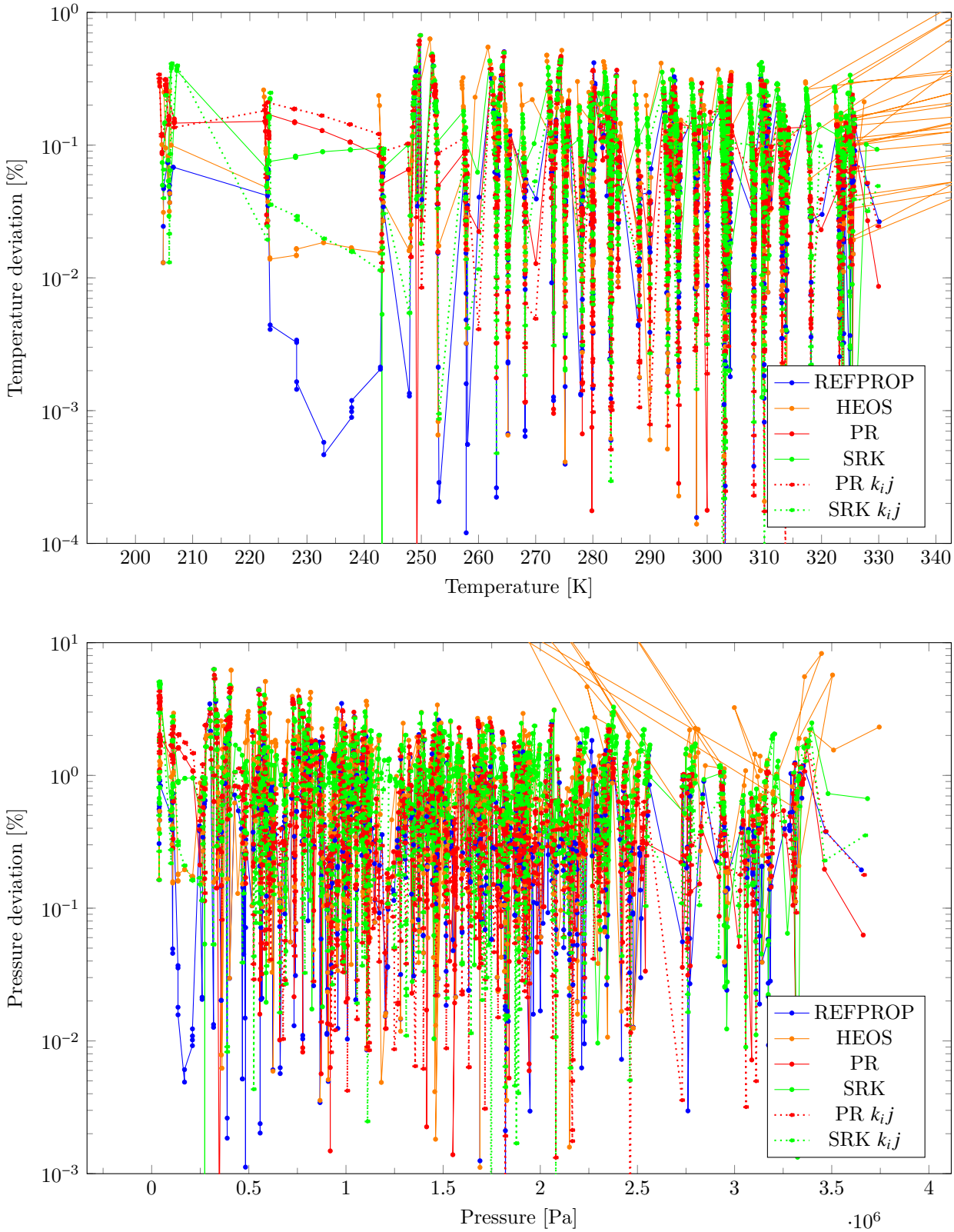
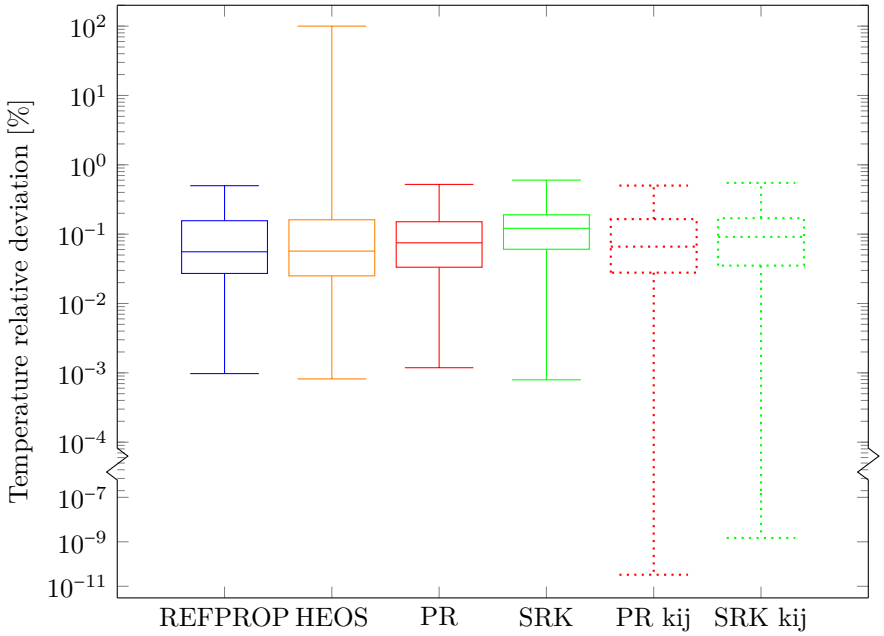
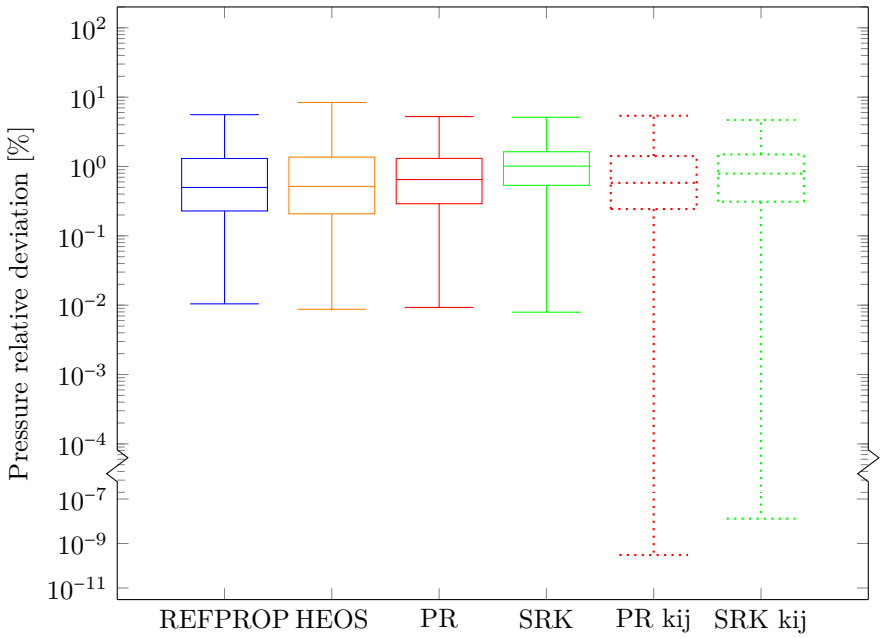


Figure 258: Dependence on the temperature and pressure for the binary mixture R125-R32

Mixture R125-R134A.



(a) Temperature deviation



(b) Pressure deviation

Figure 259: Relative deviation to experimental saturation data for mixtures based on R125 and R134A

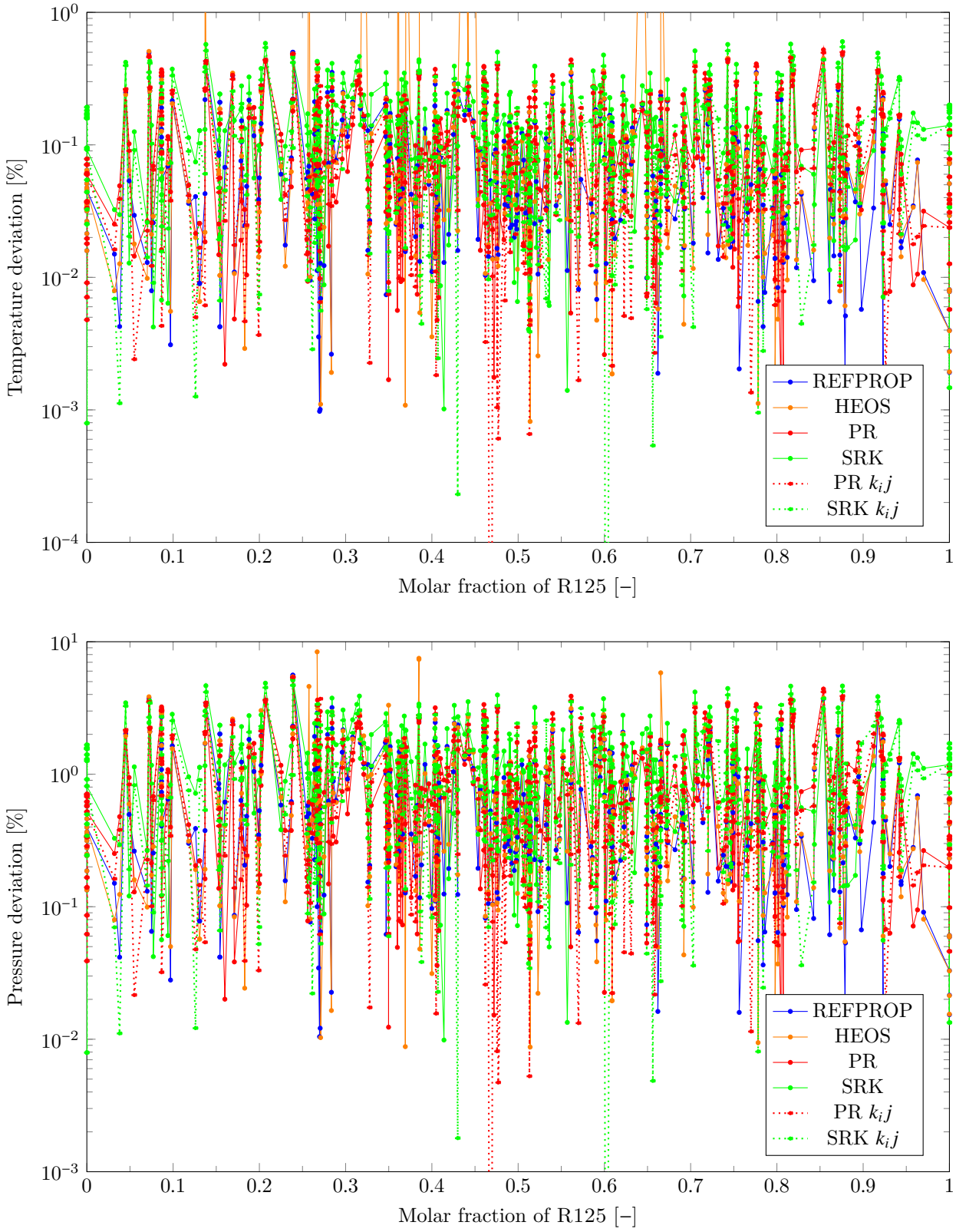


Figure 260: Dependence on the molar fraction for the binary mixture R125-R134A

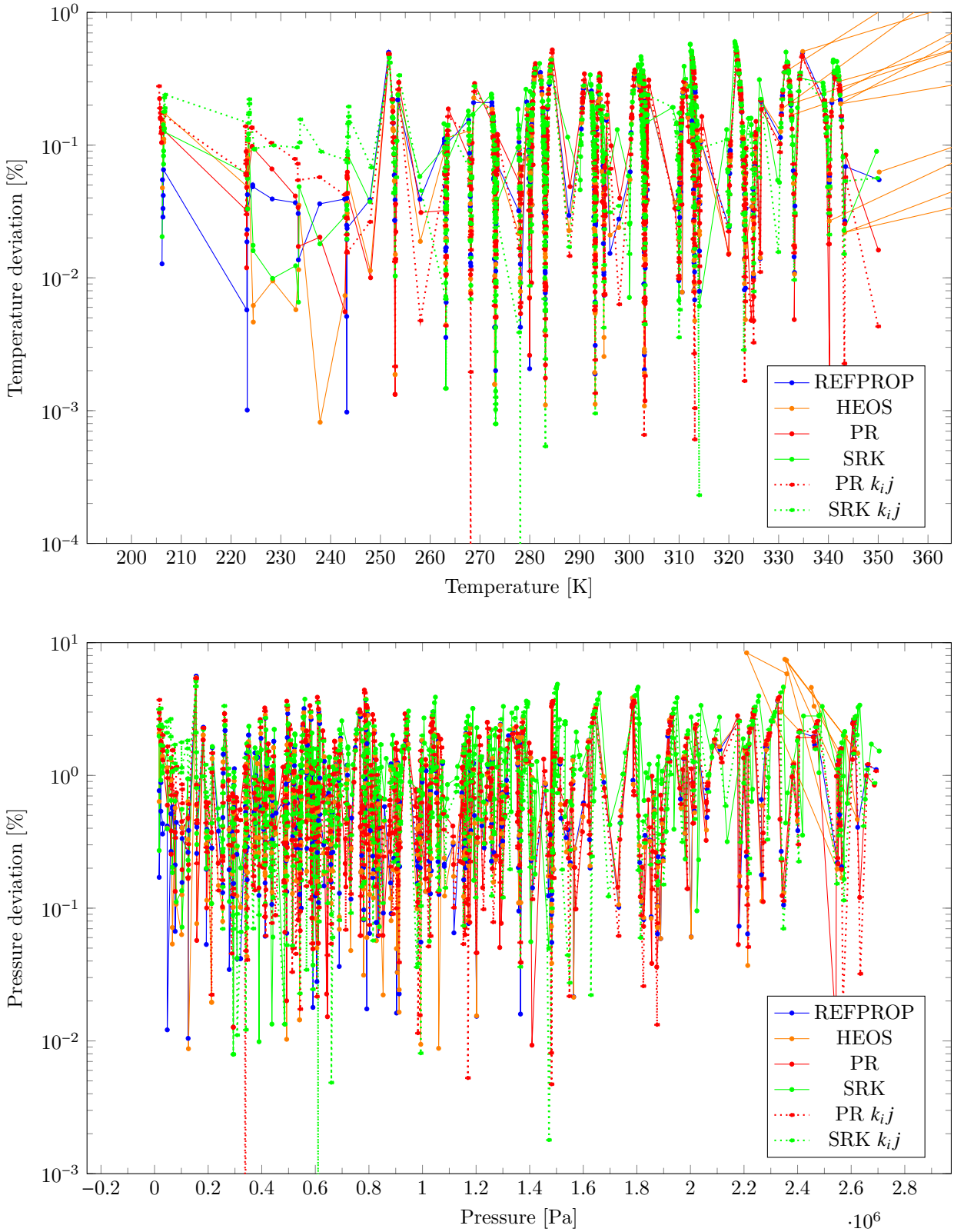
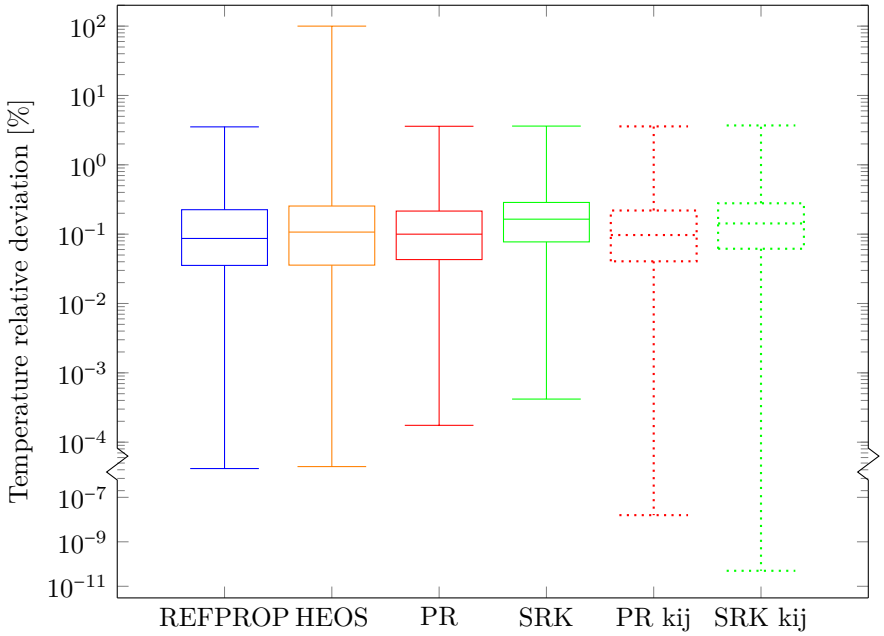
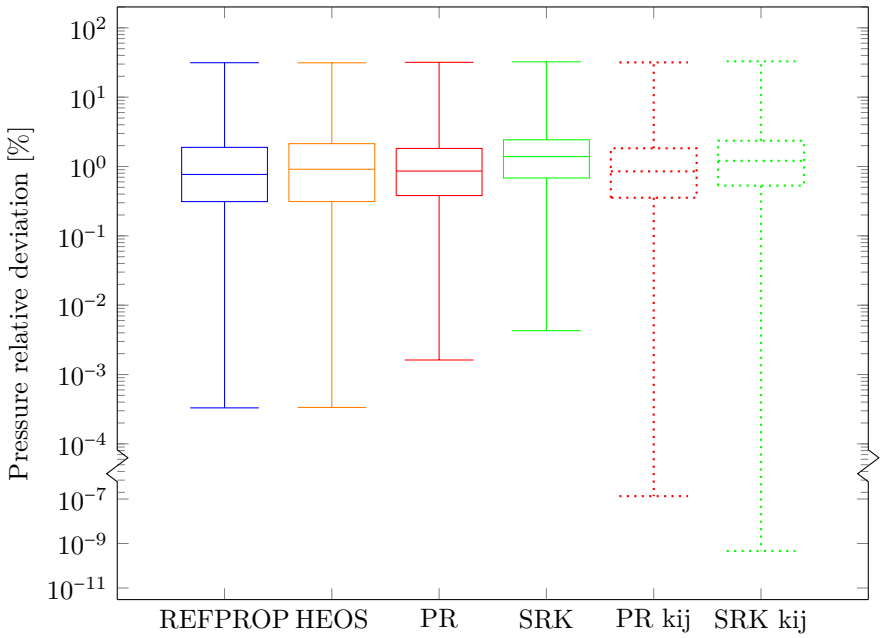


Figure 261: Dependence on the temperature and pressure for the binary mixture R125-R134A

Mixture R134A-R32.



(a) Temperature deviation



(b) Pressure deviation

Figure 262: Relative deviation to experimental saturation data for mixtures based on R134A and R32

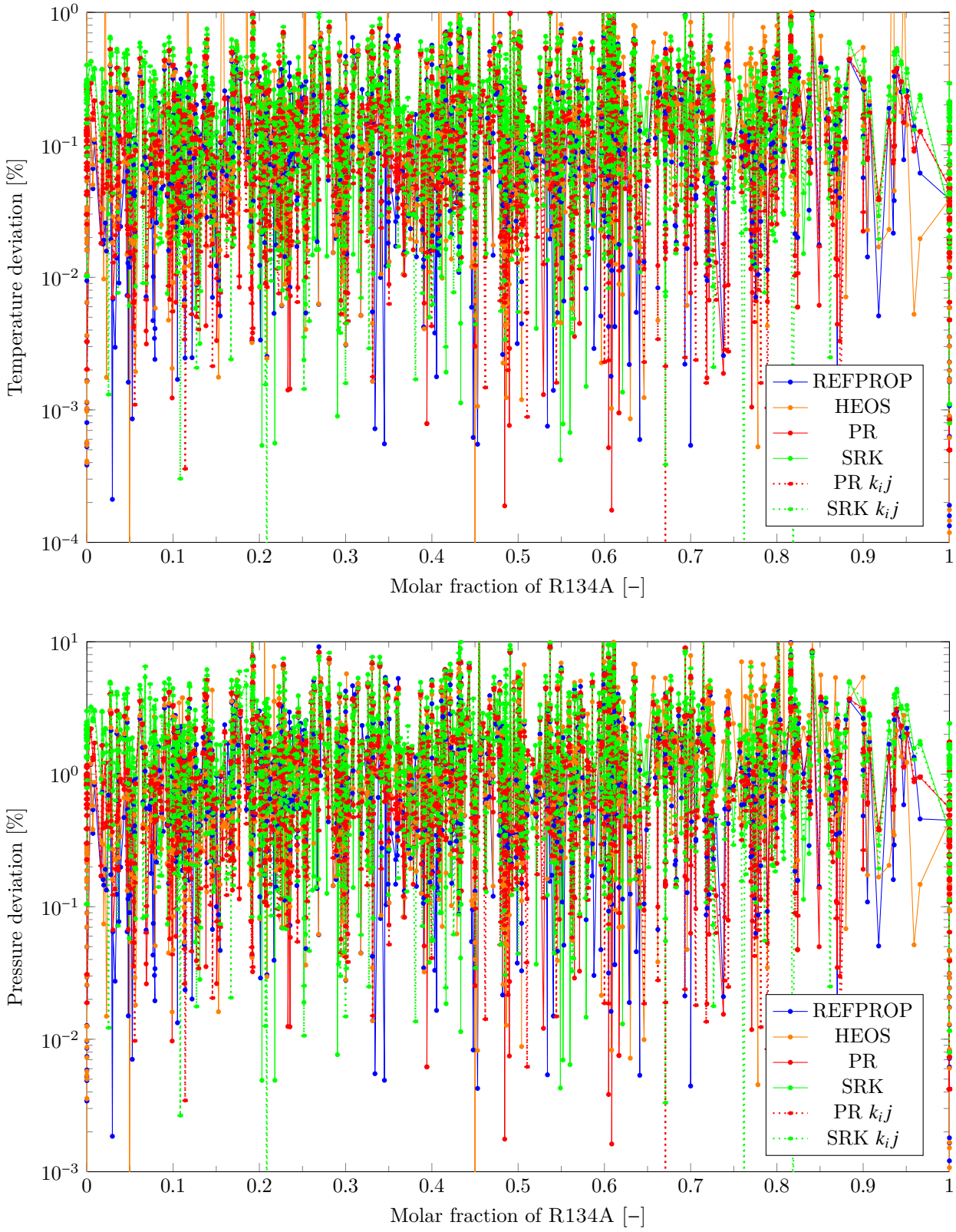


Figure 263: Dependence on the molar fraction for the binary mixture R134A-R32

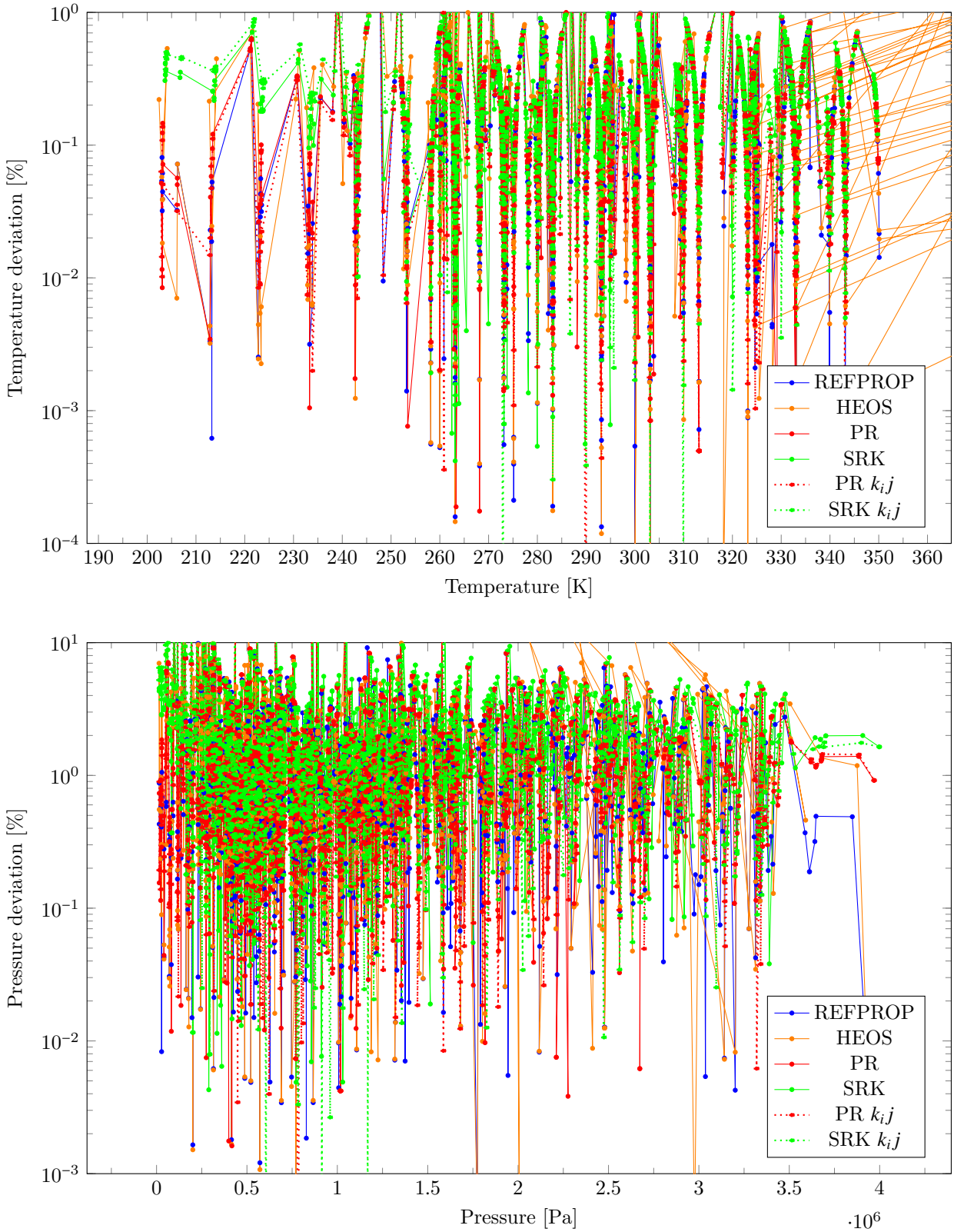
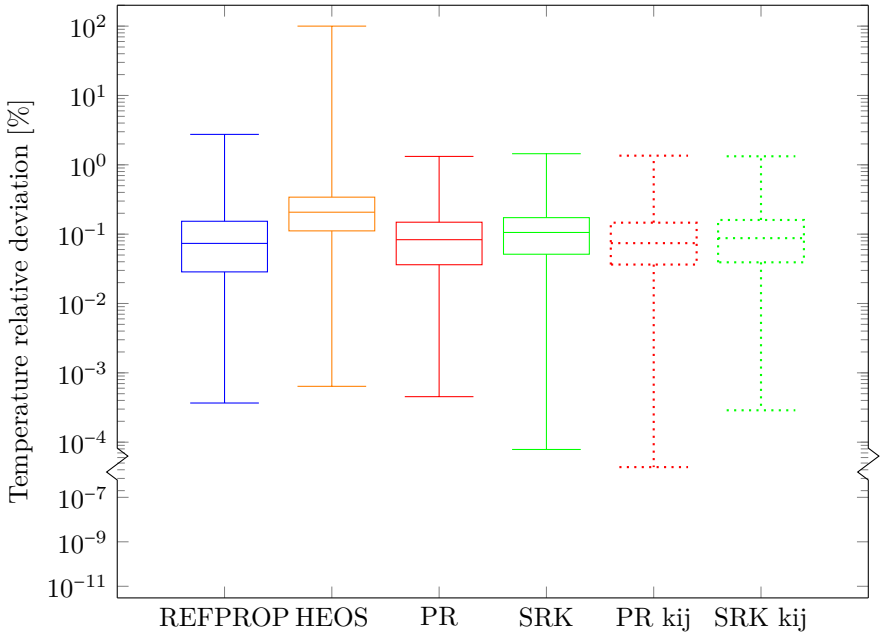


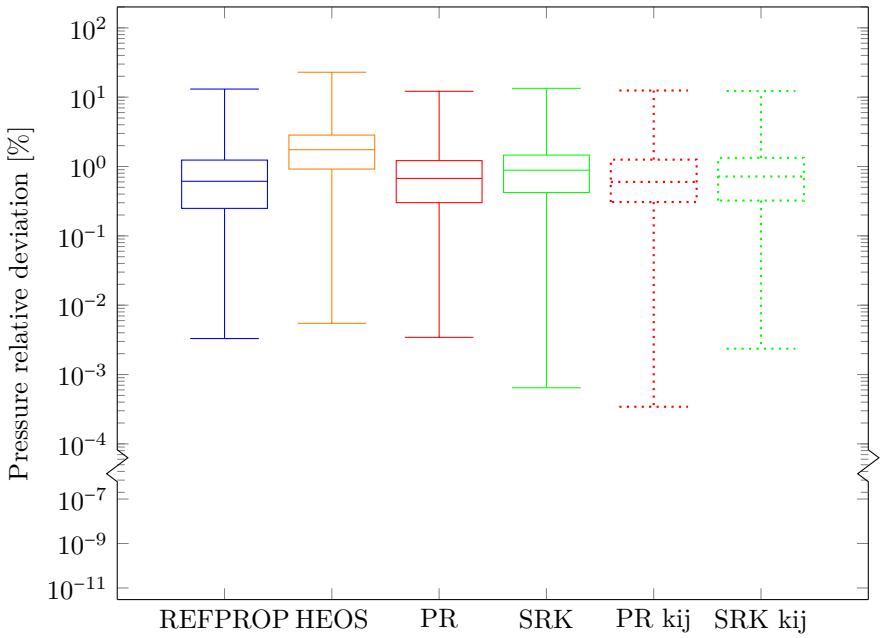
Figure 264: Dependence on the temperature and pressure for the binary mixture R134A-R32

2.4.2. Ternary mixture

Mixture R125-R32-R134A.



(a) Temperature deviation



(b) Pressure deviation

Figure 265: Relative deviation to experimental saturation data for mixtures based on R125, R32 and R134A

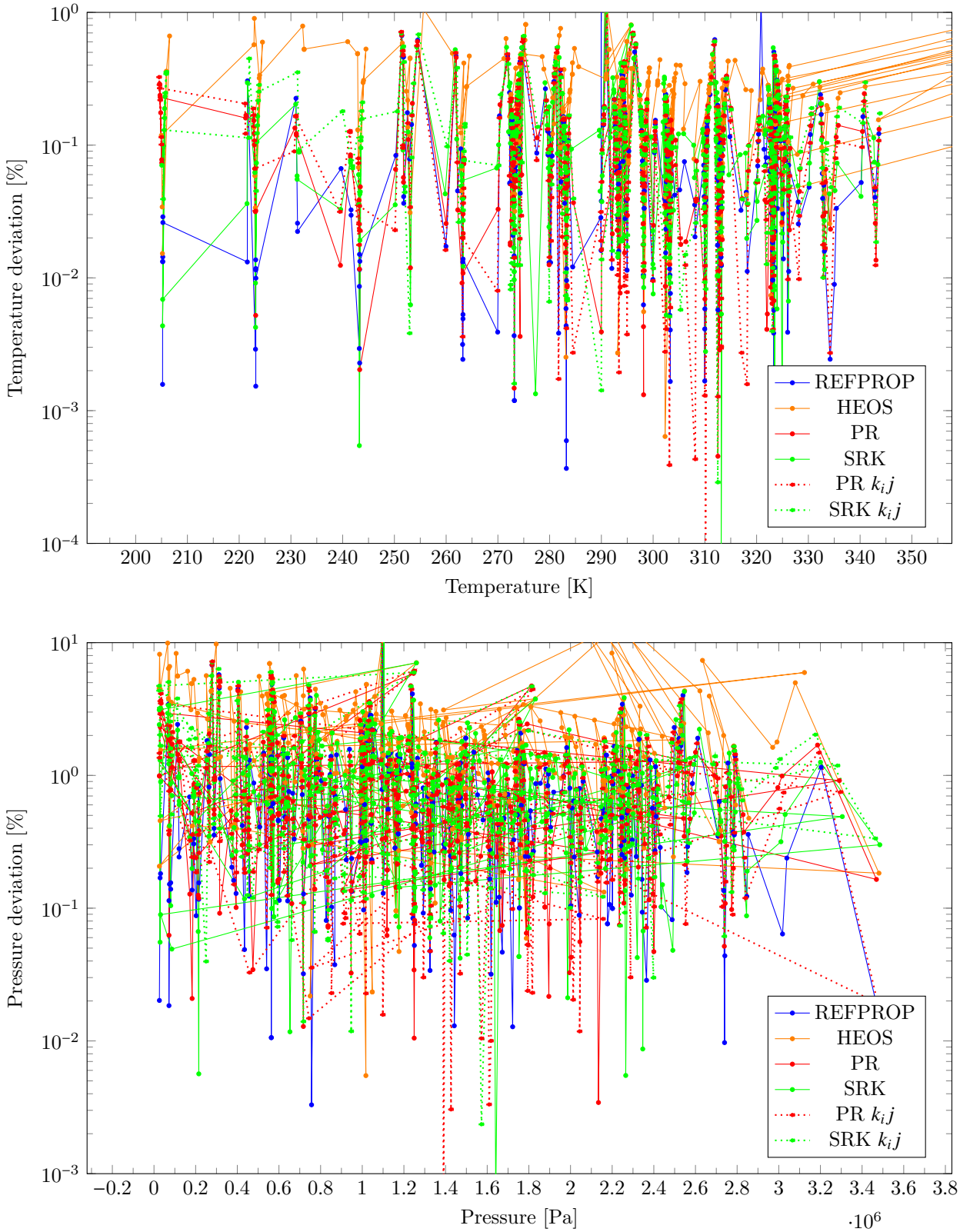


Figure 266: Dependence on the temperature and pressure for the ternary mixture R125-R32-R134A

3. References:

All the mixture VLE data comes from the sources: [?]

All the non cited sources are for the pure fluid data.

The support from NIST by providing access to the database of experimental data for pure refrigerants and mixture vapour-liquid equilibrium is gratefully acknowledged.