

Evaluation of thermophysical properties of heterocyclic and polycyclic compounds for in situ  
upgrading applications

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Trabajo de Grado para Optar al Título de Magíster en Ingeniería Química

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**List of Symbols****Roman letters** $a(T)$  – Attractive parameter of mixing rule $a_{ii}(T)$  – Peng-Robinson attractive parameter $a_{nm}, b_{nm}, c_{nm}$  – Group interaction parameter  
in modified UNIFAC $A_R, B_R, C_R, D_R, B_T, C_T, E_T, b_o, b_1, b_2, b_3$  –  
TRIDEN parameters $b$  – Repulsive parameter of mixing rule $b_{ii}, b_{ij}, b_{jj}$  – Co-volume parameters $c$  – Mixture rule for volume translation $c_i$  – Volume translation parameter for  
component  $i$  $G^E$  – Excess Gibbs Energy $g^{E,R}$  – Excess residual Gibbs Energy $H^E$  – Excess Enthalpy $L_i, M_i, N_i$  –  $\alpha$  parameters $M$  – Real solution property $M^E$  – Excess property $M^{id}$  – Ideal solution property $p$  – Pressure $p_i$  – Internal pressure $p_{i,i}$  – Internal pressure of substance  $i$  $p_i^E$  – Excess internal pressure $p_0$  – Reference pressure $P_{c,i}$  – Critical pressure of substance  $i$  $Q_k$  – Relative Van der Waals Surface  
parameter of the subgroup  $k$  $R$  – Universal gas constant $S^E$  – Excess entropy $T$  – Temperature $T_{c,i}$  – Critical temperature of substance  $i$  $T_{r,i}$  – Reduce temperature of substance  $i$  $U$  – Internal energy $v$  – Molar volume $V^E$  – Excess molar volume $V_i^o$  – Experimental volume of  $i$  $x_i$  – Molar composition of  $i$ **Greek letters** $\alpha(T)$  – Temperature-dependent function of $a_{ii}(T)$  $\alpha_p$  – Thermal expansion coefficient $\alpha_p^E$  – Excess thermal expansion coefficient

$\alpha_{p,i}$  – Thermal expansion coefficient of  $i$

$\gamma_i$  – Activity coefficient of component  $i$

$\gamma_i^C$  – Combinatorial component of the activity coefficient of  $i$

$\gamma_i^R$  – Residual component of the activity coefficient of  $i$

$\Gamma_k$  – Group activity coefficient

$\Gamma_k^{(i)}$  – Residual contribution from molecule  $i$

$\theta_m$  – Superficial Area

$\kappa_T$  – Isothermal compressibility

$\kappa_T^E$  – Excess isothermal compressibility

$\kappa_{T,i}$  – Isothermal compressibility of  $i$

$v_k^{(i)}$  – Number of  $k$  structural groups inside  $i$

$\rho$  – Density

$\rho_0$  – Density at reference pressure

$\phi_i$  – Volume fraction of  $i$

$\psi_i$  – Compressibility fraction

$\psi_{nm}$  – UNIFAC parameter

## Resumen

**Título:** Evaluación de propiedades termofísicas de compuestos heterocíclicos y policíclicos para aplicaciones de *in situ* upgrading\*

**Autor:** Dayra Lisseth Riaño Núñez\*\*

**Palabras Clave:** Densidad, Propiedades termofísicas, Heterocompuestos, Alta presión, TRIDEN; VTPR, *in situ* upgrading.

**Descripción:** En los últimos 20 años se ha observado un aumento del 50% en la producción del crudo pesado, en el cual la presencia de heterocompuestos reduce su calidad. Un proceso de recobro mejorado, *in situ* upgrading, ayuda a la remoción de este tipo de compuestos antes que el crudo sea llevado a la refinería. La industria del petróleo se enfrenta al reto de la predicción de propiedades termofísicas, como lo es la densidad, la cual tiene alta relevancia. De esta manera, la obtención de datos exactos de presión-densidad-temperatura es fundamental. Adicionalmente, información de nivel molecular se puede obtener del análisis de densidad a alta presión. Por otro lado, el crudo pesado tiene un contenido alto de asfaltenos y resinas, en cuyas estructuras se pueden encontrar anillos aromáticos con alquilados, naftenos y heteroátomos (nitrógeno, azufre y oxígeno).

Los datos de presión-densidad-temperatura fueron obtenidos para soluciones en ciclohexanos de compuestos heterocíclicos y policíclicos distribuidos en tres grupos: aromáticos (Fenantreno y 2,6-Dietilnaftaleno), órgano-sulfurados (dibenzotiofeno) y órgano-nitrogenados (9-etilcarbazol y quinolina) a posibles condiciones del proceso *in situ* upgrading (373.15-473.15K y 2-40 MPa). Para los experimentos fueron usados un densímetro Anton Paar DMA 4200 M con una bomba manual hidráulica NovaSwiss. Con los datos de densidad fueron estimadas las propiedades termofísicas de compresibilidad isotérmica, expansibilidad isobárica y presión interna con la correlación TRIDEN. TRIDEN se ajusta correctamente a las densidades de las soluciones de interés, con desviaciones absolutas AAD promedio menores al 1%. Luego, las mezclas de las muestras modelo fueron medidas y analizadas con las propiedades en exceso. Para correlacionar el volumen en exceso se utilizó Redlich-Kister. Finalmente, la ecuación de estado VTPR obtuvo desviaciones AAD menores al 2% para todas las mediciones de densidad analizadas.

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\* Trabajo de Grado

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### Abstract

**Title:** Evaluation of thermophysical properties of heterocyclic and polycyclic compounds for in situ upgrading applications\*

**Author(s):** Dayra Lisseth Riaño Núñez<sup>1</sup>

**Key Words:** Density, Thermophysical properties, Heterocompounds, High pressure, TRIDEN; VTPR, in situ upgrading.

**Description:** A 50% increase in Colombian heavy oil production has been observed in the last 20 years. For such type of oil, the presence of hetero compounds reduces the quality of its products. *In situ* upgrading as an EOR aids the removal of hetero compounds before the crude goes to the refinery. A key stage of any process is its characterization. Specifically, the petroleum industry faces the challenge of predicting accurate thermophysical properties. One of the properties with high industrial relevance is density. Therefore, accurate pressure-density-temperature measurements are fundamental. Moreover, molecular-level information can be obtained from density high-pressure analysis. On the other hand, heavy crude oil has a higher asphaltene and resin content. Aromatic centers with attached alkyls, naphthene, and heteroatoms (nitrogen, sulfur, and oxygen) are present in their molecular structure.

Pressure-Density-Temperature data was obtained for dissolutions in cyclohexane of heterocyclic and polycyclic compounds, distributed in 3 groups: aromatics (Phenanthrene, 2,6-Diethylnaphthalene), organo-sulfur compounds (Dibenzothiophene) and organo-nitrogen compounds (9-Ethylcarbazole and Quinoline) at plausible *in situ* upgrading conditions (373.15-473.15 K and 2-40 MPa). The experiments are based on a U-tube vibrating densimeter Anton Paar DMA 4200 M. A NovaSwiss hydraulic manual pump helped as a pressure generator. With density data, thermophysical properties of isothermal compressibility  $\kappa_T$ , isobaric expansivity  $\alpha_p$ , and internal pressure  $p_i$  were calculated using TRIDEN. As a result of the TRIDEN adjustment, we got an average absolute deviation-AAD of less than 1 %, showing that this model fits the solutions of interest. Then, mixtures of the model families were measured and analyzed with excess properties. Redlich-Kister was used to correlate the excess volume. Finally, an improved equation of state VTPR showed an AAD of less than 2% for all analyzed density data.

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\* Degree Work

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## Introduction

In the past two decades, the Colombian petroleum industry has witnessed a remarkable 50% surge in the production of heavy crude oil (ENI, 2019). This noteworthy growth, however, brings with it a set of challenges in the handling of heavy crude oil due to its high viscosity, low API gravity ( $^{\circ}\text{API} < 22.3^{\circ}$ ), and elevated heteroatom content, such as sulfur exceeding 0.5% w/w. Notably, at room temperature, heavy crude oil exhibits a viscosity of more than  $10^3$  centipoises (cP), posing significant challenges in its transportation from the wellhead to the refinery via pipelines (Martínez-Palou et al., 2011). The presence of hetero compounds in such oils not only degrades the quality of their end products but also demands substantial efforts for their removal within the petroleum industry (Cheshkova et al., 2019).

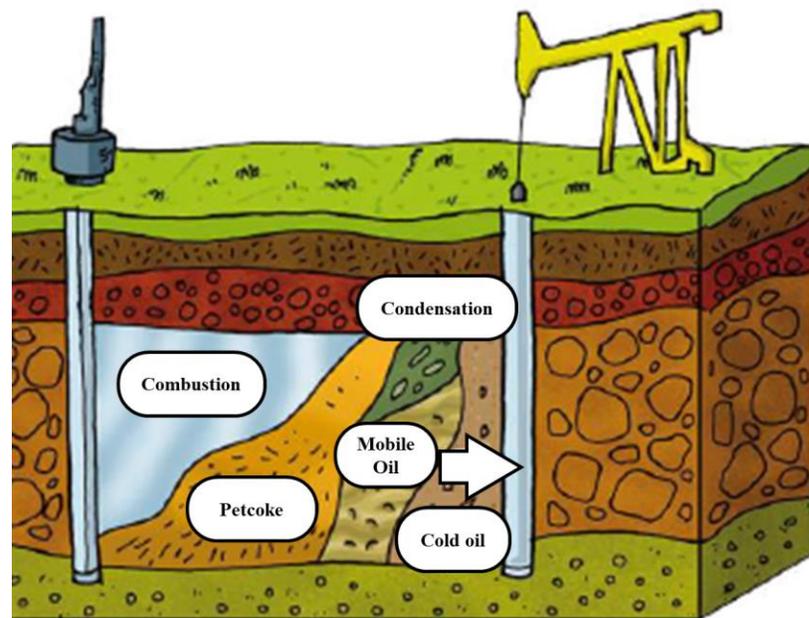
As the petroleum industry faces the challenge of improving the extraction and refining of heavy crude oil, one often sought-after solution is the implementation of Enhanced Oil Recovery (EOR) methods. EOR, considered a secondary extraction method, is designed to maximize the recovery of crude oil. Among the most prominent EOR techniques, In Situ Combustion stands out. This method involves controlled combustion of a portion of the well, generating gases that reduce the viscosity of the crude oil, as shown in Figure 1 (Perkins, 2018). However, In Situ Combustion can lead to unwanted complications, including polymerization reactions, aromatic ring condensation, and the formation of undesirable compounds. To address these issues, the use of catalysts and the injection of hydrogen donors have been proposed, and when combining In Situ Combustion with catalysts downhole, it is referred to as *in situ* upgrading (Weissman, 1997) (Schacht-Hernández et al., 2019). Catalysts, typically composed of Ni-Mo or Co-Mo, facilitate hydrogenation reactions similar to those found in hydrotreatment and FCC processes in refineries

where the reactions break carbon bonds with impurities like sulfur, nitrogen, oxygen, and metals, thus enhancing the overall value of the crude oil extracted from the well (Weissman, 1997).

It's important to note that *in situ* upgrading operates under conditions akin to those found in oil well extraction. For instance, in wells such as Chichimene, temperatures and pressures can reach up to 150°C and 40 MPa respectively. Additionally, given the considerable distance between the production well and the combustion front, the mobilized heavy crude oil passes through the catalyst bed at reservoir temperature and pressure (García Navas et al., 2018).

### Figure 1

#### *In situ combustion process*



*Note.* Adapted from *El petróleo y su mundo* (p.32), por (Ecopetrol S.A., 2014).

Characterizing crude oil in Enhanced Oil Recovery (EOR) processes is essential for efficient extraction from the well and subsequent transportation to the refinery. However, the Oil & Gas industry faces challenges in accurately predicting phase behavior, thermophysical properties, and transport properties. These properties are crucial for designing, operating,

controlling, and optimizing processes across various industries (Amorim et al., 2007a; Privat & Jaubert, 2012; Zambrano et al., 2018). Undoubtedly, density ranks among the most significant properties, alongside viscosity. Precise measurements of density as functions of pressure, composition, and temperature enable the estimation of other thermophysical properties and even transport properties. Density data serves as a foundation for developing correlations and equations of state (EOS) to determine key properties, including phase equilibrium, enthalpy, entropy and heat capacity, among others (Amorim et al., 2007a; Ihmels & Gmehling, 2001). Furthermore, high-pressure analysis of thermophysical properties lead to descriptions at molecular level of phenomena such as intermolecular forces of the compounds in the mixture (Dávila et al., 2011). To obtain accurate pressure-density-temperature data, a well-known methodology involves using a U-tube digital densimeter (Atilhan & Aparicio, 2013). This apparatus could give an accurate density measurement until the sixth figure, and modern technology could reach high pressures and high temperatures.

Another important thermodynamic area to investigate are excess properties. As mentioned before, heavy and extra-heavy crude oil have a lower API and a higher viscosity which make it difficult to transport and refine. Its transport throughout pipelines becomes a challenge because of the low mobility and the possibility of paraffin and asphaltene deposition. Many choose to reduce oil viscosity with its dilution with light substances. The addition of solvents, lighter crude oil, naphtha, or other liquid hydrocarbons in small amounts facilitates its transportation. This process has numerous issues: solvent separation, asphaltene, and paraffin instability, and changes in ideal volume due to mixing processes (Martínez-Palou et al., 2011; Santos et al., 2014). Petroleum components have different physical properties, their mixtures have excess volumes that could be either positive or negative. Significantly, it is critical to know the true volume of the mixtures since

the difference in volumes could represent thousands of barrels, therefore an economic impact (Shanshool et al., 2011).

Equations of state (EOS) are mathematical correlations that describe the pressure-volume-temperature (PVT) behavior of fluids. Along with empirical correlations and thermodynamic definitions, EOS can estimate the thermophysical properties of compounds and mixtures (Gmehling et al., 2012). In this context, Peng-Robinson (PR) and Soave-Redlich-Kwong, two of the most common Cubic EOS models, are used for studying hydrocarbon mixtures due to their simplicity, broad applicability, and accurate description of nonpolar substances. However, polar substances, often found in crude oil as hetero compounds, exhibit significant deviations of the values expected from experimental data. For this reason, in order to enhance the accuracy of density and liquid-liquid equilibrium estimation, volume translation is employed within EOS within predictive equations of state, such as VTPR or PSKR, offering improvements in the descriptions of crude oil phase behavior (Privat & Jaubert, 2012).

This work investigates model molecules of three important families inside polyaromatics and heterocompounds: aromatic, nitrogen and sulfur compounds. The density of the model dissolution and its mixtures were measured between 373.15 to 473 K and from 2 MPa to 40 MPa. The ppT data was correlated with TRIDEN while the excess volume with Redlich-Kister. The existence of a deviation from the ideal behavior of mixtures was evaluated. Finally, the Volume translated Peng Robinson (VTPR) was used to predict the density of each system.

## 1. Aims and Objectives

### 1.1 Research aim

To investigate thermophysical properties base on pressure-density-temperature behavior of model molecules at *in situ* upgrading conditions

### 1.2 Research objectives

- Estimate p- $\rho$ -T behavior of dissolutions in cyclohexane of model molecules (phenanthrene, 2,6-diethylnaphthalene, dibenzothiophene, quinoline, and 9-ethylcarbazole) and its binary and ternary mixtures
- Determine whether deviations from ideal behavior are present
- Predict thermophysical properties from VTPR EOS and estimate its deviation from experimental data

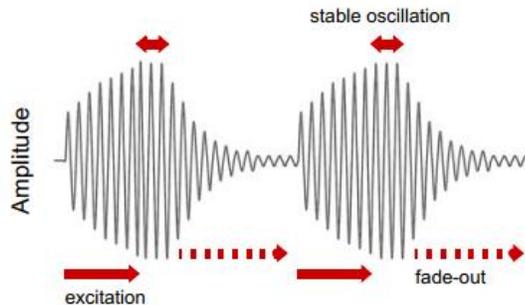
## 2. Equipment Installation and Adjustment

### 2.1 General description

Pressure-density-temperature measurements were performed using the Anton Paar DMA 4200 M, a high temperature and pressure U-tube densimeter. This equipment uses Anton Paar's innovative 'Pulse Excitation Method' consisting in exciting the U-tube until it stabilizes at its characteristic frequency after which the tube is allowed to oscillate freely (fade-out). This novel method represents an enhancement over the traditional oscillation method offering more precise density measurements, improved viscosity correction, and enhanced repeatability (Anton Paar, 2020).

#### Figure 2.

*Pulse excitation method oscillation*



*Note.* Taken from *Reference Guide DMA 4200 M Density Meter*, (Anton Paar, 2020)

Hence, the densimeter determines the density values of fluids based on the oscillation period of the substance within the U-tube. The relationship between density and periodic time is due to the changes in mass that happen to the liquid inside the tube at constant volume (Rechberger et al., 2019). This principle is similar to the one stated by the analysis of harmonic oscillators on Hooke's law, in which the frequency of the oscillator depends on the mass suspended on it. The density's value can be estimated with the equation:

$$\rho = A\tau^2 + B \quad (1)$$

Where  $A$  and  $B$  are constants that could be determined with measurements of well-known fluids with densities within the full operating range.

These U-tube densimeters are widely used in industry, academia, and different laboratories within a high variety of liquids. Simple fluids like solvents and alcohols alongside ionic fluids, crude oil, and alternative fuels could be measured (Outcalt, 2018). Density data as a function of pressure and temperature are substantial in the thermophysical characterization of liquids. It allows us to obtain isobaric expansivity and isothermal compressibility. Combined with the speed of sound and the isobaric heat capacity measurements, we could estimate the isentropic compressibility and isochoric molar heat capacity. And last, but not least, ppT measurements could be compared with the predictions of molecular-based Equations of State (Sanmamed et al., 2009).

Anton Paar's DMA 4200 M was acquired based on its technical specification shown in Table 1. This model has a Hastelloy C276 U-tube, an alloy material made of nickel-molybdenum-chromium and tungsten addition that is resistant to strong acids and bases. Table 1 includes the specifications given by Anton Paar for the equipment. The cell can reach the desired temperature, up to 200°C, with an integrated Peltier system. Precision and accuracy data are determined under ambient pressure and ideal conditions. It is expected that it changes according to operating differences.

The densimeter can achieve measurements under high-pressure conditions. To pressurize the system, it is necessary to use a pressure generator. In this case, a Nova Swiss 565.0275 hand pump, which has a non-rotating spindle that can go up to 2000 bar. On the other hand, to measure and control the pressure during the experimental procedure it was used a piezoresistive 2-wire

pressure transmitter Keller PA-21Y with a range of 0 to 8000 bar, typical accuracy of  $\pm 0.25\%$  full scale, and stability of  $\pm 0.3\%$  FS. The piece is integrated into the tubing throughout a tee SITEC 627.1610. Then, to assure pressure measurements, a certified ACHCROFT analog manometer was used. By direct comparison, a difference of 2.2% at ambient temperature led us to make a pressure sensor adjustment between the signal output (4 to 20 mA) and the needed pressure (up to 400 bar).

**Table 1.**

*DMA4200 M manufacturer specifications*

**Figure 3.**

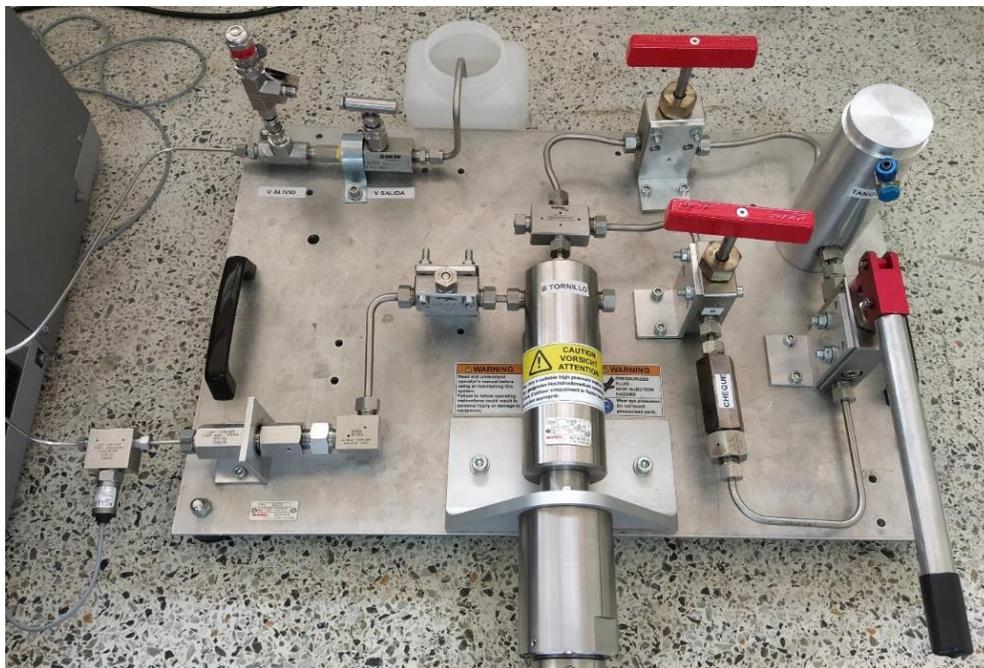
*Densimeter DMA 4200 M*



<b>Density</b> ( $\text{g}\cdot\text{cm}^{-3}$ )	
Measuring range	0 to 3
Repeatability	0.00005
Reproducibility	0.0001
Accuracy	0.0002
<b>Temperature</b> (K)	
Range	263.15 to 473.15
Accuracy	0.03
<b>Pressure</b>	
Range	0 to 500 bar
Sensor	4-20 mA

Furthermore, the connections between the densimeter and the pump use SITEC high-pressure 1/8" stainless steel tubing with an internal diameter of 1 mm. As a complement, it also has numerous fittings: a 1/4 "elbow SITEC 720.1532, a SITEC 720.2301 reducer from 1/4" to 1/8", unions, nuts and plugs. All SITEC pieces are made of AISI 316 and can resist up to 4000 bar.



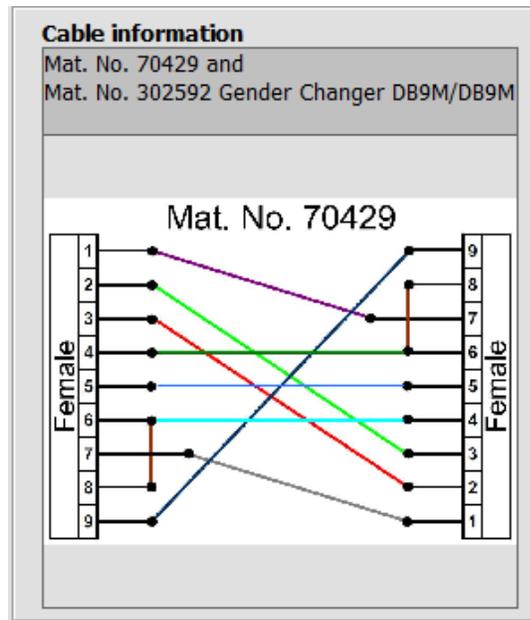
**Figure 5***NovaSwiss pump and connections***Figure 6***Measuring system*

To perform reliable data acquisition, measuring and cleaning steps were established. Air bubbles inside the U-tube can change the oscillation period, therefore density data. Hence, liquid degasification before entering the system could help prevent bubbles from entering the measuring cell. In this case, an ultrasonic bath Elma was used during a 10-minute cycle. Acoustic waves lead to the formation of vacuum bubbles, then the liquid's dissolved gas is transferred to them. During the sonification, bubbles coalesce, and when the pulse is interrupted, they raise to the surface(Hielscher Ultrasound Technology, 2013).

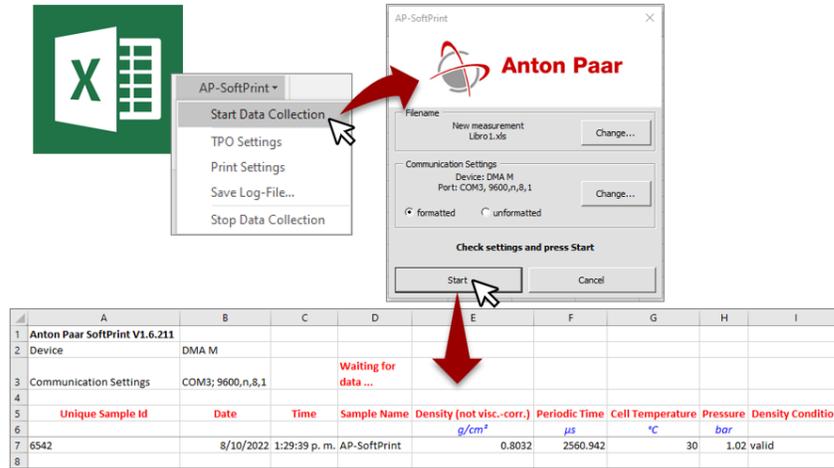
To perform the measurements, the tank is filled with the fluid of study, and with the help of the spindle is entered into the system. The pump valves are closed and with the exit needle valve open, the fluid exits the system. It is important to do this procedure at least 3 times to assure liquid in all the tubing. Additionally, it must be gentle, to avoid the forming of gas bubbles. Then, after closing all the valves, the pressure is set manually with the spindle and the temperature is programmed on the DMA4200 M interface. The measurements are performed on the ultrafast precision mode, recommended by the manufacturer for high-pressure measurements. This precision class has a temperature stability of  $<0.1$  °C for 10 s and density stability of  $<0.00005$  g·cm<sup>-3</sup> for 60 s. After the stabilization of the conditions, the data is acquired with the button START and is shown on the manufacturer's software.

## **2.2 Data acquisition**

Anton Paar's AP-SoftPrint 1.2.0 software allows the collection of density measurements on an Excel sheet. It is an add-in that requires an RS-232 cable connection as indicated in Figure 7. To connect to the computer, it needs an RS-232 to USB cable.

**Figure 7***RS-232 Cable connection*

The Add-In was installed in Excel, the option “AP-SoftPrint” can be found on the Add-ins tab. To open the software we have to click on the “Start Data Collection” option, as shown in the next figure. Then, we can select the desired folder and filename and click “Start”. The format will appear on the Sheet and each time a measurement is performed, the desired data will occupy a new row.

**Figure 8***Steps for data collection*

### 2.3 Calibration

As mentioned before, the densimeter can measure density through a relationship between this value and the periodic time of the U-tube cell. In this way, an adjustment should be performed to determine the coefficients of the characteristic equation of the DMA 4200 M. The equipment follows a second-degree polynomial which determines the values of density according to temperature and pressure:

$$\rho [kg \cdot m^{-3}] = \sum_{k=0}^1 \sum_{i=0}^2 \sum_{j=0}^2 (-1)^{1-k} \cdot a_{ijk} \cdot T[{}^{\circ}C]^i \cdot p[bar]^j \cdot \tau[\mu s]^{2k} \text{ for } (i + j \leq 2) \quad (2)$$

Data from well-known substances is necessary to find the equation parameters. In this way, we can perform measurements of the periodic time at different pressures and temperatures and use them with reference values to find the constants. Taking into account that the substance of interest is cyclohexane (0.5-0.8 g·cm<sup>-3</sup>), the standard liquids selected to cover all the working range (373.15 K to 473.15 K and pressures from 2 bar to 400 bar) were n-Hexane, n-Heptane, and water. As shown in Figure 9, the cyclohexane density line at maximum and minimum temperatures stays

between the reagents reference data. The reagents had purity values above 99%, as shown in the table.

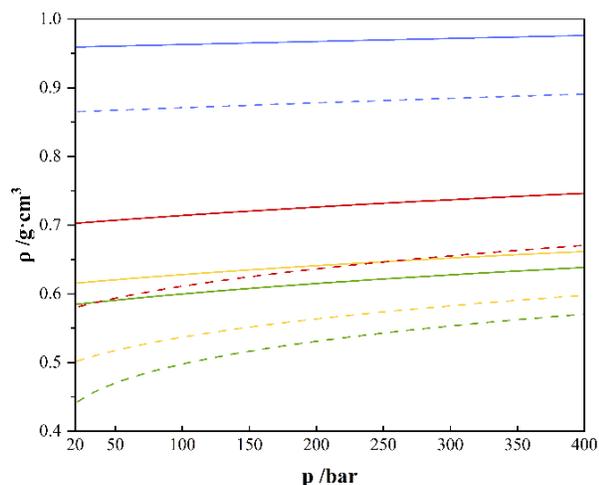
**Table 2.**

*Calibration and verification reagents*

Reagent	Manufacturer	Figure 9
n-Hexane	Merck>99.5%	<i>Cyclohexane (yellow), n-Heptane (red), n-Hexane (green), and water (blue) densities at 373.15 K (—) and 473.15 (- - -)</i>
n-Heptane	ITW Reagents>99%	
Cyclohexane	ITW Reagents>99.5%	

Water

Milli-Q water  
(18M $\Omega$ ·cm at 25 °C)



To perform measurements on the needed range of temperature and pressure, a Wide Range adjustment was performed with the help of the manufacturer's Excel tool: Wide Range Adjustment Tool for DMA 4200 M, software version 1.0.0. The tool finds the selected coefficients according to the given data using the least-square method. The deviation was estimated using the absolute average deviation of density. Theoretical density data is available in the NIST webbook (National Institute of Standards and Technology (NIST), 2021). The data adjustment used 112 points with densities between 0.4622-0.9762 g·cm<sup>-3</sup>, obtaining an average deviation of 4.89x10<sup>-4</sup> g·cm<sup>-3</sup>.

$$\%AAD = \frac{100}{n} \sum_{i=1}^n \left| \frac{\rho_{NIST} - \rho_{Estimated}}{\rho_{NIST}} \right| \quad (3)$$

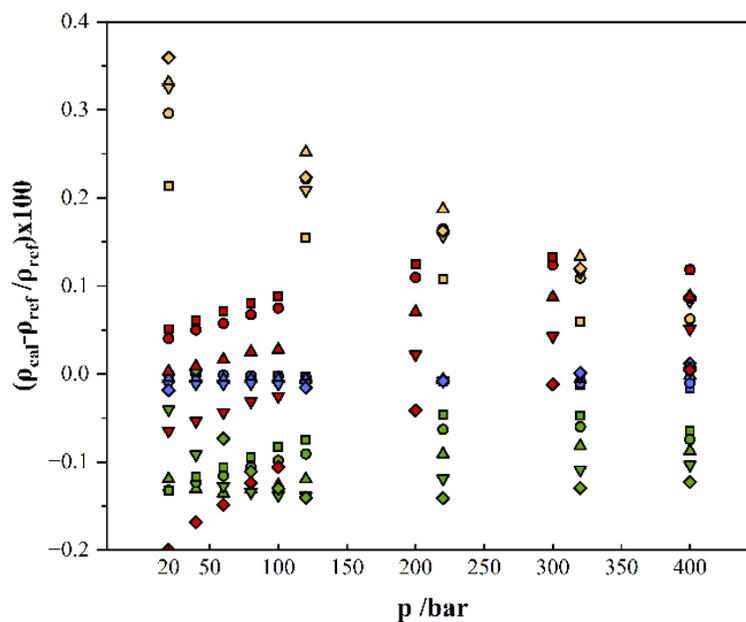
**Table 3.**

*Calibration coefficients from second-degree polynomial*

$a_{000}$	5.59158	$a_{001}$	$9.82862 \times 10^{-7}$
$a_{100}$	$-4.83082 \times 10^{-5}$	$a_{101}$	$-3.06581 \times 10^{-4}$
$a_{010}$	$2.65825 \times 10^{-6}$	$a_{011}$	$7.74854 \times 10^{-8}$
$a_{110}$	0	$a_{200}$	$-1.09663 \times 10^{-7}$
$a_{201}$	$-1.06780 \times 10^{-7}$	$a_{020}$	$-2.06316 \times 10^{-8}$
$a_{021}$	$-1.71676 \times 10^{-8}$	<b>AAD</b>	0.084%

**Figure 10**

*Density deviations percentages between experimental adjusted data and NIST webbook of water (blue), n-Hexane (green), n-Heptane (yellow), and cyclohexane (red) at different pressures and temperatures ( $\square$ ) 373.15 K ( $\circ$ ) 398.15 K ( $\triangle$ ) 423.15 K ( $\nabla$ ) 448.15 K ( $\diamond$ )*



Cyclohexane measurements verified the calibration coefficients. The red dots in Figure 10 show the results obtained, with a maximum deviation of -0.2%. High temperature and low pressure

have a higher deviation from reference data, with 473 K showing the higher values, this could happen because it's the higher limit of the temperature of the Peltier system

### 3. Experimental data

#### 3.1. Cyclohexane

**Table 4.**

*Experimental densities ( $\rho$ ) of Cyclohexane at different temperatures and pressures.*

	$\rho$ /g·cm <sup>3</sup> at T/K								
<b>p /bar</b>	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	0.70226	0.68923	0.67587	0.66201	0.64769	0.63269	0.61675	0.59976	0.58121
40	0.70521	0.69252	0.67952	0.66620	0.65245	0.63814	0.62311	0.60731	0.59042
60	0.70805	0.69568	0.68306	0.67014	0.65687	0.64319	0.62888	0.61403	0.59839
80	0.71078	0.69867	0.68639	0.67383	0.66103	0.64783	0.63418	0.62013	0.60539
100	0.71344	0.70158	0.68958	0.67735	0.66498	0.65219	0.63909	0.62563	0.61170
200	0.72546	0.71466	0.70380	0.69286	0.68186	0.67074	0.65949	0.64815	0.63662
300	0.73603	0.72595	0.71591	0.70587	0.69582	0.68575	0.67562	0.66550	0.65532
400	0.74550	0.73602	0.72657	0.71719	0.70784	0.69849	0.68914	0.67983	0.67056

#### 3.2. Model families

##### 3.2.1 Aromatic model

**Table 5.**

*Experimental densities ( $\rho$ ) of aromatics model mixture with Phenanthrene (1.5% w/w) and 2,6-Diethylnaphthalene (1.5% w/w) at different temperatures and pressures.*

	$\rho$ /g·cm <sup>3</sup> a T/K								
<b>p /bar</b>	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	0.70876	0.69588	0.68269	0.66912	0.65500	0.64022	0.62466	0.60812	0.59014
40	0.71162	0.69910	0.68628	0.67315	0.65958	0.64548	0.63079	0.61524	0.59886
60	0.71442	0.70218	0.68969	0.67697	0.66390	0.65035	0.63636	0.62176	0.60641
80	0.71711	0.70512	0.69298	0.68061	0.66792	0.65490	0.64149	0.62760	0.61312
100	0.71971	0.70799	0.69610	0.68410	0.67177	0.65917	0.64624	0.63298	0.61923
200	0.73153	0.72081	0.71005	0.69927	0.68831	0.67730	0.66618	0.65491	0.64348

		$\rho / \text{g} \cdot \text{cm}^3 \text{ a T/K}$							
<b>p /bar</b>	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
300	0.74191	0.73193	0.72195	0.71203	0.70204	0.69204	0.68200	0.67193	0.66181
400	0.75127	0.74184	0.73247	0.72316	0.71386	0.70456	0.69531	0.68605	0.67680

**Table 6.**

*Experimental densities ( $\rho$ ) of aromatics model mixture with Phenanthrene (1% w/w) and 2,6-Diethylnaphthalene (2% w/w) at different temperatures and pressures.*

		$\rho / \text{g} \cdot \text{cm}^3 \text{ a T/K}$							
<b>p /bar</b>	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	0.70779	0.69494	0.68179	0.66822	0.65426	0.63947	0.62390	0.60733	0.58931
40	0.71066	0.69816	0.68537	0.67221	0.65889	0.64478	0.63000	0.61455	0.59802
60	0.71344	0.70123	0.68879	0.67605	0.66319	0.64964	0.63563	0.62101	0.60564
80	0.71612	0.70417	0.69206	0.67966	0.66720	0.65417	0.64075	0.62684	0.61239
100	0.71870	0.70701	0.69516	0.68312	0.67103	0.65845	0.64556	0.63224	0.61859
200	0.73051	0.71978	0.70906	0.69825	0.68762	0.67662	0.66551	0.65425	0.64285
300	0.74087	0.73088	0.72094	0.71097	0.70129	0.69135	0.68135	0.67131	0.66120
400	0.75020	0.74077	0.73144	0.72210	0.71304	0.70384	0.69465	0.68547	0.67622

**Table 7.**

*Experimental densities ( $\rho$ ) of aromatics model mixture with Phenanthrene (2% w/w) and 2,6-Diethylnaphthalene (1 % w/w) at different temperatures and pressures.*

		$\rho / \text{g} \cdot \text{cm}^3 \text{ a T/K}$							
<b>p /bar</b>	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	0.70901	0.69615	0.68297	0.66940	0.65529	0.64049	0.62487	0.60824	0.59039
40	0.71189	0.69935	0.68654	0.67343	0.65984	0.64579	0.63101	0.61554	0.59908
60	0.71466	0.70243	0.68997	0.67725	0.66413	0.65066	0.63658	0.62198	0.60664
80	0.71734	0.70538	0.69323	0.68091	0.66821	0.65517	0.64173	0.62781	0.61338
100	0.71997	0.70825	0.69640	0.68437	0.67205	0.65945	0.64649	0.63323	0.61951
200	0.73174	0.72104	0.71028	0.69951	0.68859	0.67754	0.66643	0.65513	0.64374
300	0.74212	0.73212	0.72217	0.71223	0.70227	0.69227	0.68225	0.67219	0.66206
400	0.75143	0.74204	0.73267	0.72337	0.71405	0.70479	0.69553	0.68631	0.67705

### 3.2.2 Nitrogen model

**Table 8.**

*Experimental densities ( $\rho$ ) of nitrogen model mixture with Quinoline (0.7% w/w) and 9-Ethylcarbazole (0.3 % w/w) at different temperatures and pressures.*

$\rho / \text{g} \cdot \text{cm}^3 \text{ a T/K}$									
<b>p /bar</b>	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	0.70455	0.69161	0.67825	0.66449	0.65019	0.63520	0.61942	0.60245	0.58414
40	0.70750	0.69488	0.68190	0.66861	0.65490	0.64066	0.62567	0.61000	0.59318
60	0.71033	0.69802	0.68540	0.67254	0.65933	0.64561	0.63143	0.61660	0.60111
80	0.71306	0.70100	0.68872	0.67619	0.66342	0.65025	0.63669	0.62263	0.60801
100	0.71573	0.70392	0.69192	0.67973	0.66732	0.65464	0.64158	0.62811	0.61421
200	0.72772	0.71690	0.70605	0.69515	0.68415	0.67310	0.66183	0.65052	0.63901
300	0.73825	0.72818	0.71815	0.70811	0.69806	0.68802	0.67789	0.66777	0.65760
400	0.74771	0.73823	0.72878	0.71939	0.71004	0.70071	0.69136	0.68203	0.67274

**Table 9.**

*Experimental densities ( $\rho$ ) of nitrogen model mixture with Quinoline (0.5% w/w) and 9-Ethylcarbazole (0.5 % w/w) at different temperatures and pressures.*

$\rho / \text{g} \cdot \text{cm}^3 \text{ a T/K}$									
<b>p /bar</b>	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	0.70447	0.69146	0.67812	0.66419	0.64983	0.63479	0.61880	0.60176	0.58328
40	0.70738	0.69474	0.68179	0.66832	0.65456	0.64024	0.62525	0.60933	0.59245
60	0.71021	0.69787	0.68528	0.67228	0.65898	0.64523	0.63096	0.61600	0.60040
80	0.71295	0.70086	0.68854	0.67596	0.66312	0.64989	0.63626	0.62208	0.60735
100	0.71559	0.70375	0.69177	0.67952	0.66704	0.65428	0.64114	0.62760	0.61368
200	0.72757	0.71677	0.70590	0.69496	0.68394	0.67281	0.66156	0.65010	0.63855
300	0.73809	0.72805	0.71799	0.70793	0.69788	0.68776	0.67764	0.66745	0.65724
400	0.74757	0.73809	0.72862	0.71919	0.70987	0.70047	0.69115	0.68179	0.67247

**Table 10.**

*Experimental densities ( $\rho$ ) of nitrogen model mixture with Quinoline (0.3% w/w) and 9-Ethylcarbazole (0.7 % w/w) at different temperatures and pressures*

		$\rho$ /g·cm <sup>3</sup> a T/K								
<b>p /bar</b>	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15	
20	0.70462	0.69166	0.67835	0.66458	0.65035	0.63537	0.61962	0.60270	0.58439	
40	0.70754	0.69494	0.68200	0.66871	0.65504	0.64074	0.62587	0.61018	0.59343	
60	0.71037	0.69805	0.68548	0.67260	0.65943	0.64573	0.63162	0.61680	0.60122	
80	0.71309	0.70105	0.68879	0.67630	0.66351	0.65037	0.63685	0.62278	0.60812	
100	0.71574	0.70395	0.69198	0.67981	0.66743	0.65470	0.64173	0.62830	0.61442	
200	0.72773	0.71694	0.70611	0.69521	0.68423	0.67319	0.66200	0.65061	0.63914	
300	0.73824	0.72820	0.71816	0.70815	0.69813	0.68809	0.67800	0.66788	0.65773	
400	0.74767	0.73817	0.72878	0.71939	0.71007	0.70076	0.69146	0.68215	0.67287	

### 3.2.3 Sulfur model

**Table 11.**

*Experimental densities ( $\rho$ ) of sulfur model mixture with Dibenzothiophene (1% w/w) at different temperatures and pressures.*

		$\rho$ /g·cm <sup>3</sup> a T/K								
<b>p /bar</b>	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15	
20	0.70529	0.69232	0.67899	0.66525	0.65092	0.63597	0.62017	0.60324	0.58504	
40	0.70822	0.69559	0.68263	0.66937	0.65565	0.64138	0.62647	0.61072	0.59397	
60	0.71107	0.69872	0.68613	0.67328	0.66004	0.64633	0.63216	0.61737	0.60183	
80	0.71379	0.70172	0.68943	0.67699	0.66416	0.65099	0.63737	0.62334	0.60868	
100	0.71643	0.70462	0.69265	0.68051	0.66806	0.65528	0.64227	0.62886	0.61495	
200	0.72842	0.71760	0.70677	0.69588	0.68487	0.67376	0.66251	0.65115	0.63966	
300	0.73896	0.72888	0.71884	0.70882	0.69875	0.68868	0.67856	0.66843	0.65824	
400	0.74843	0.73893	0.72951	0.72011	0.71071	0.70138	0.69204	0.68269	0.67339	

**Table 12.**

*Experimental densities ( $\rho$ ) of sulfur model mixture with Dibenzothiophene (2.2% w/w) at different temperatures and pressures.*

p /bar	$\rho$ /g·cm <sup>3</sup> a T/K								
	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	0.70877	0.69586	0.68261	0.66894	0.65471	0.63987	0.62421	0.60744	0.58930
40	0.71168	0.69908	0.68622	0.67303	0.65936	0.64519	0.63038	0.61481	0.59820
60	0.71446	0.70216	0.68963	0.67686	0.66369	0.65008	0.63599	0.62131	0.60586
80	0.71715	0.70514	0.69293	0.68051	0.66776	0.65469	0.64116	0.62723	0.61262
100	0.71973	0.70801	0.69607	0.68400	0.67161	0.65900	0.64601	0.63267	0.61879
200	0.73162	0.72085	0.71007	0.69923	0.68828	0.67722	0.66604	0.65475	0.64327
300	0.74203	0.73200	0.72204	0.71203	0.70201	0.69198	0.68193	0.67185	0.66170
400	0.75138	0.74191	0.73255	0.72317	0.71385	0.70453	0.69526	0.68605	0.67679

**Table 13.**

*Experimental densities ( $\rho$ ) of sulfur model mixture with Dibenzothiophene (3.7% w/w) at different temperatures and pressures.*

p /bar	$\rho$ /g·cm <sup>3</sup> a T/K								
	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	0.71315	0.70027	0.68707	0.67347	0.65948	0.64472	0.62918	0.61272	0.59480
40	0.71600	0.70345	0.69063	0.67749	0.66405	0.64994	0.63530	0.61987	0.60344
60	0.71877	0.70651	0.69404	0.68130	0.66834	0.65484	0.64082	0.62620	0.61090
80	0.72145	0.70948	0.69728	0.68490	0.67234	0.65933	0.64592	0.63204	0.61758
100	0.72404	0.71233	0.70040	0.68836	0.67621	0.66358	0.65070	0.63741	0.62362
200	0.73578	0.72506	0.71427	0.70344	0.69269	0.68168	0.67050	0.65921	0.64775
300	0.74615	0.73614	0.72614	0.71616	0.70635	0.69633	0.68630	0.67618	0.66606
400	0.75547	0.74602	0.73661	0.72725	0.71813	0.70884	0.69956	0.69031	0.68102

### 3.3. Mixtures

#### 3.3.1 Aromatic + Sulfur (AS)

**Table 14.**

*Experimental densities ( $\rho$ ) of the binary mixture of aromatics+sulfur model at different temperatures and pressures.*

		$\rho / \text{g} \cdot \text{cm}^3$						
$p / \text{bar}$	20	40	60	80	100	200	300	400
$x_A$	$T/^\circ\text{C} = 100$							
0.05	0.71312	0.71601	0.71878	0.72146	0.72406	0.73583	0.74619	0.75554
0.20	0.71249	0.71535	0.71815	0.72081	0.7234	0.73516	0.74552	0.75484
0.35	0.71183	0.71471	0.7175	0.72018	0.72278	0.73458	0.74493	0.75431
0.50	0.71133	0.71423	0.71699	0.71968	0.72229	0.73409	0.7444	0.75381
0.65	0.71060	0.71349	0.71627	0.71895	0.72155	0.73336	0.74374	0.7531
0.80	0.71004	0.71292	0.71571	0.7184	0.72101	0.7328	0.74322	0.75257
0.95	0.7094	0.71229	0.71508	0.71776	0.72038	0.73218	0.74259	0.75196
	$T/^\circ\text{C} = 112.5$							
0.05	0.70026	0.70347	0.70656	0.70950	0.71234	0.72511	0.73618	0.74607
0.20	0.69964	0.70281	0.70589	0.70884	0.71167	0.72444	0.73548	0.74540
0.35	0.69895	0.70215	0.70524	0.70819	0.71105	0.72381	0.73494	0.74486
0.50	0.69848	0.70168	0.70475	0.70770	0.71056	0.72334	0.73445	0.74435
0.65	0.69773	0.70094	0.70402	0.70700	0.70985	0.72262	0.73372	0.74366
0.80	0.69718	0.70041	0.70346	0.70642	0.70928	0.72207	0.73318	0.74313
0.95	0.69654	0.69974	0.70283	0.70579	0.70866	0.72147	0.73258	0.74253
	$T/^\circ\text{C} = 125$							
0.05	0.68710	0.69065	0.69405	0.69731	0.70046	0.71434	0.7262	0.73672
0.20	0.68644	0.69000	0.69340	0.69664	0.6998	0.71366	0.72553	0.73600
0.35	0.68578	0.68936	0.69278	0.69602	0.69918	0.7131	0.72499	0.73550
0.50	0.68531	0.68888	0.69226	0.69553	0.69868	0.71258	0.72444	0.73499
0.65	0.68455	0.68812	0.69155	0.69482	0.69796	0.71188	0.72378	0.73430
0.80	0.68399	0.68756	0.69099	0.69426	0.69739	0.71132	0.72322	0.73375
0.95	0.68334	0.68695	0.69036	0.69363	0.69676	0.71068	0.72254	0.73312
	$T/^\circ\text{C} = 137.5$							
0.05	0.67349	0.67753	0.68132	0.68497	0.68841	0.70347	0.71623	0.72735
0.20	0.67282	0.67684	0.68066	0.68426	0.68773	0.70281	0.71554	0.72666
0.35	0.67220	0.67623	0.68004	0.68366	0.68712	0.70225	0.71498	0.72614
0.50	0.67171	0.67575	0.67956	0.68315	0.68657	0.70175	0.71452	0.72565
0.65	0.67097	0.67502	0.67884	0.68245	0.68590	0.70104	0.71382	0.72494

$\rho / \text{g} \cdot \text{cm}^3$								
p /bar	20	40	60	80	100	200	300	400
0.80	0.67040	0.67446	0.67827	0.68188	0.68536	0.70050	0.71329	0.72443
0.95	0.66975	0.67377	0.67761	0.68123	0.68470	0.69984	0.71262	0.72380
<b>T/°C = 150</b>								
0.05	0.65932	0.66393	0.66821	0.67223	0.67604	0.69255	0.70621	0.71800
0.20	0.65874	0.66329	0.66761	0.67163	0.67545	0.69191	0.70558	0.71738
0.35	0.65805	0.66265	0.66693	0.67095	0.67478	0.6913	0.70497	0.71680
0.50	0.65760	0.66217	0.66644	0.67049	0.67432	0.69082	0.70451	0.71631
0.65	0.65684	0.66143	0.66571	0.66974	0.67355	0.69010	0.70382	0.71562
0.80	0.65629	0.66086	0.66515	0.66918	0.67301	0.68957	0.70325	0.71510
0.95	0.65566	0.66023	0.66453	0.66858	0.67243	0.68895	0.70265	0.71448
<b>T/°C = 162.5</b>								
0.05	0.64459	0.64981	0.65466	0.65918	0.66344	0.68149	0.69613	0.70869
0.20	0.64401	0.64922	0.65406	0.65857	0.66283	0.68089	0.69555	0.70808
0.35	0.64330	0.64855	0.65339	0.65791	0.66213	0.68026	0.69492	0.70750
0.50	0.64280	0.64807	0.65293	0.65748	0.66172	0.67978	0.69445	0.70702
0.65	0.64207	0.64733	0.65218	0.65674	0.66100	0.67909	0.6938	0.70634
0.80	0.64156	0.64679	0.65164	0.65614	0.66042	0.67851	0.69324	0.70581
0.95	0.64086	0.64616	0.65101	0.65553	0.65980	0.67791	0.69263	0.70519
<b>T/°C = 175</b>								
0.05	0.62909	0.63514	0.64065	0.64573	0.65051	0.67031	0.68610	0.69940
0.20	0.62844	0.63449	0.64002	0.64515	0.64990	0.66971	0.68550	0.69879
0.35	0.62777	0.63380	0.63935	0.64445	0.64925	0.66907	0.68487	0.69821
0.50	0.62726	0.63335	0.63891	0.64401	0.64879	0.66864	0.68443	0.69774
0.65	0.62655	0.63262	0.63816	0.64328	0.6481	0.66790	0.68372	0.69705
0.80	0.62597	0.63210	0.63764	0.64275	0.64752	0.66742	0.68323	0.69653
0.95	0.62533	0.63142	0.63699	0.64209	0.64693	0.66676	0.68256	0.6959
<b>T/°C = 187.5</b>								
0.05	0.61250	0.61963	0.62605	0.63179	0.63718	0.65898	0.67596	0.69012
0.20	0.61183	0.61904	0.62547	0.63125	0.63662	0.65843	0.67538	0.68951
0.35	0.61122	0.61839	0.62477	0.63057	0.63596	0.65777	0.67478	0.68893
0.50	0.61073	0.61791	0.62431	0.63010	0.63553	0.65733	0.67431	0.68847
0.65	0.60994	0.61711	0.62357	0.62936	0.63477	0.6566	0.67363	0.68779
0.80	0.60939	0.61659	0.62300	0.62886	0.63424	0.65611	0.6731	0.68724
0.95	0.60871	0.61592	0.62239	0.62821	0.63363	0.65546	0.67246	0.68663
<b>T/°C = 200</b>								

p /bar	$\rho / \text{g} \cdot \text{cm}^3$							
	20	40	60	80	100	200	300	400
0.05	0.59468	0.60325	0.61074	0.61735	0.62343	0.64758	0.66585	0.68084
0.20	0.59395	0.60264	0.61013	0.61683	0.62289	0.64699	0.66526	0.68021
0.35	0.59322	0.60191	0.60942	0.61613	0.62218	0.64637	0.66463	0.67962
0.50	0.59283	0.6015	0.60901	0.61567	0.62178	0.64591	0.66420	0.67920
0.65	0.59212	0.60078	0.60828	0.61497	0.62101	0.64524	0.66354	0.67851
0.80	0.59153	0.60018	0.60767	0.61443	0.62050	0.64470	0.66296	0.67796
0.95	0.59082	0.59948	0.60703	0.61375	0.61981	0.64406	0.66236	0.67734

### 3.3.2 Aromatic+Nitrogen (AN)

**Table 15.**

*Experimental densities ( $\rho$ ) of the binary mixture of aromatics+nitrogen model at different temperatures and pressures.*

p /bar	$\rho / \text{g} \cdot \text{cm}^3$							
	20	40	60	80	100	200	300	400
<b>x<sub>A</sub></b>	<b>T/°C = 100</b>							
0.05	0.70497	0.70791	0.71074	0.71344	0.71609	0.72805	0.73856	0.74803
0.20	0.70564	0.70857	0.71139	0.71410	0.71675	0.72868	0.73917	0.74862
0.35	0.70628	0.70920	0.71201	0.71473	0.71736	0.72926	0.73969	0.74913
0.50	0.70693	0.70985	0.71265	0.71536	0.71799	0.72986	0.74031	0.74971
0.65	0.70767	0.71055	0.71336	0.71607	0.71869	0.73051	0.74097	0.75037
0.80	0.70832	0.71119	0.71401	0.71670	0.71932	0.73111	0.74154	0.75093
0.95	0.70898	0.71189	0.71467	0.71735	0.71993	0.73176	0.74216	0.75152
	<b>T/°C = 112.5</b>							
0.05	0.69199	0.69527	0.69840	0.70138	0.70429	0.71727	0.72852	0.73854
0.20	0.69269	0.69595	0.69907	0.70206	0.70495	0.71789	0.72912	0.73913
0.35	0.69336	0.69660	0.69972	0.70272	0.70559	0.71851	0.72970	0.73969
0.50	0.69402	0.69727	0.70035	0.70334	0.70623	0.71908	0.73026	0.74025
0.65	0.69477	0.69799	0.70110	0.70407	0.70693	0.71979	0.73095	0.74092
0.80	0.69544	0.69865	0.70174	0.70471	0.70756	0.72040	0.73155	0.74148
0.95	0.69613	0.69933	0.70240	0.70539	0.70825	0.72102	0.73216	0.74208
	<b>T/°C = 125</b>							
0.05	0.67867	0.68232	0.68580	0.68911	0.69231	0.70642	0.71848	0.72909

p /bar	$\rho / \text{g} \cdot \text{cm}^3$							
	20	40	60	80	100	200	300	400
0.20	0.67940	0.68303	0.68651	0.68980	0.69297	0.70706	0.71911	0.72975
0.35	0.68009	0.68370	0.68717	0.69049	0.69367	0.70769	0.71969	0.73031
0.50	0.68076	0.68439	0.68782	0.69114	0.69428	0.70829	0.72028	0.73086
0.65	0.68153	0.68517	0.68859	0.69191	0.69506	0.70903	0.72100	0.73156
0.80	0.68222	0.68583	0.68925	0.69253	0.69570	0.70962	0.72157	0.73209
0.95	0.68295	0.68654	0.68996	0.69325	0.69639	0.71030	0.72221	0.73275
<b>T/°C = 137.5</b>								
0.05	0.66493	0.66905	0.67295	0.67663	0.68018	0.69553	0.70847	0.71972
0.20	0.66570	0.66979	0.67369	0.67736	0.68088	0.69621	0.70911	0.72036
0.35	0.66644	0.67050	0.67439	0.67808	0.68159	0.69685	0.70971	0.72092
0.50	0.66711	0.67121	0.67505	0.67872	0.68221	0.69748	0.71031	0.72153
0.65	0.66792	0.67199	0.67584	0.67946	0.68297	0.69818	0.71100	0.72219
0.80	0.66856	0.67265	0.67650	0.68014	0.68360	0.69879	0.71159	0.72276
0.95	0.66934	0.67338	0.67722	0.68084	0.68431	0.69946	0.71222	0.72338
<b>T/°C = 150</b>								
0.05	0.65069	0.65536	0.65975	0.66387	0.66778	0.68456	0.69844	0.71039
0.20	0.65146	0.65612	0.66048	0.66457	0.66848	0.68521	0.69907	0.71098
0.35	0.65219	0.65684	0.66120	0.66527	0.66917	0.68585	0.69968	0.71158
0.50	0.65292	0.65755	0.66191	0.66598	0.66984	0.68651	0.70028	0.71218
0.65	0.65370	0.65834	0.66266	0.66673	0.67060	0.68721	0.70098	0.71286
0.80	0.65448	0.65907	0.66337	0.66746	0.67134	0.68789	0.70161	0.71346
0.95	0.65522	0.65979	0.66409	0.66818	0.67200	0.68853	0.70226	0.71406
<b>T/°C = 162.5</b>								
0.05	0.63573	0.64116	0.64610	0.65073	0.65509	0.67344	0.68835	0.70104
0.20	0.63652	0.64188	0.64687	0.65148	0.65583	0.67414	0.68902	0.70166
0.35	0.63729	0.64263	0.64759	0.65216	0.65647	0.67481	0.68959	0.70226
0.50	0.63804	0.64338	0.64830	0.65288	0.65718	0.67544	0.69025	0.70286
0.65	0.63887	0.64418	0.64908	0.65364	0.65796	0.67617	0.69089	0.70353
0.80	0.63963	0.64494	0.64981	0.65441	0.65871	0.67681	0.69157	0.70418
0.95	0.64041	0.64567	0.65055	0.65508	0.65934	0.67751	0.69224	0.70478
<b>T/°C = 175</b>								
0.05	0.61994	0.62624	0.63194	0.63715	0.64202	0.66220	0.67823	0.69172
0.20	0.62073	0.62704	0.63268	0.63791	0.64281	0.66292	0.67889	0.69235

$\rho / \text{g} \cdot \text{cm}^3$								
p /bar	20	40	60	80	100	200	300	400
0.35	0.62161	0.62780	0.63343	0.63869	0.64353	0.66360	0.67952	0.69294
0.50	0.62239	0.62858	0.63418	0.63939	0.64425	0.66426	0.68015	0.69356
0.65	0.62321	0.62934	0.63503	0.64021	0.64500	0.66497	0.68086	0.69424
0.80	0.62410	0.63022	0.63581	0.64095	0.64576	0.66569	0.68154	0.69489
0.95	0.62487	0.63098	0.63654	0.64171	0.64648	0.66635	0.68217	0.69550
<b>T/°C = 187.5</b>								
0.05	0.60304	0.61052	0.61712	0.62308	0.62863	0.65087	0.66810	0.68240
0.20	0.60402	0.61138	0.61795	0.62390	0.62938	0.65156	0.66876	0.68303
0.35	0.60483	0.61219	0.61870	0.62463	0.63010	0.65226	0.66941	0.68365
0.50	0.60564	0.61298	0.61947	0.62542	0.63089	0.65293	0.67004	0.68427
0.65	0.60648	0.61383	0.62032	0.62622	0.63165	0.65368	0.67077	0.68498
0.80	0.60746	0.61466	0.62111	0.62702	0.63244	0.65438	0.67147	0.68561
0.95	0.60827	0.61553	0.62194	0.62781	0.63320	0.65511	0.67213	0.68627
<b>T/°C = 200</b>								
0.05	0.58482	0.59375	0.60153	0.60844	0.61479	0.63938	0.65792	0.67307
0.20	0.58572	0.59465	0.60243	0.60934	0.61557	0.64011	0.65863	0.67375
0.35	0.58654	0.59548	0.60323	0.61004	0.61630	0.64080	0.65929	0.67436
0.50	0.58752	0.59640	0.60409	0.61087	0.61709	0.64149	0.65991	0.67500
0.65	0.58849	0.59729	0.60498	0.61175	0.61790	0.64225	0.66065	0.67569
0.80	0.58946	0.59814	0.60573	0.61251	0.61866	0.64295	0.66132	0.67633
0.95	0.59034	0.59905	0.60658	0.61331	0.61938	0.64369	0.66200	0.67701

### 3.3.3 Nitrogen+Sulfur (NS)

**Table 16.**

*Experimental densities ( $\rho$ ) of the binary mixture of nitrogen+sulfur model at different temperatures and pressures.*

$\rho / (\text{g} \cdot \text{cm}^{-3})$								
p /bar	20	40	60	80	100	200	300	400
<b>T/°C = 100</b>								
$x_A$								
0.05	0.71297	0.71584	0.71862	0.72130	0.72390	0.73570	0.74606	0.75542
0.20	0.71161	0.71449	0.71729	0.71996	0.72258	0.73439	0.74478	0.75414
0.35	0.71010	0.71300	0.71581	0.71848	0.72110	0.73297	0.74338	0.75278

$\rho / (\text{g}\cdot\text{cm}^{-3})$								
$p / \text{bar}$	20	40	60	80	100	200	300	400
0.50	0.70897	0.71189	0.71470	0.71741	0.72001	0.73185	0.74233	0.75173
0.65	0.70755	0.71046	0.71326	0.71597	0.71860	0.73050	0.74098	0.75038
0.80	0.70643	0.70936	0.71219	0.71489	0.71753	0.72945	0.73995	0.74936
0.95	0.70524	0.70815	0.71098	0.71372	0.71635	0.72831	0.73886	0.74831
<b>T/°C = 112.5</b>								
0.05	0.70009	0.70329	0.70635	0.70932	0.71215	0.72493	0.73602	0.74594
0.20	0.69874	0.70194	0.70502	0.70797	0.71083	0.72364	0.73477	0.74471
0.35	0.69717	0.70040	0.70351	0.70649	0.70933	0.72218	0.73336	0.74330
0.50	0.69605	0.69929	0.70237	0.70534	0.70824	0.72109	0.73229	0.74225
0.65	0.69459	0.69783	0.70091	0.70392	0.70681	0.71970	0.73091	0.74091
0.80	0.69351	0.69674	0.69988	0.70286	0.70575	0.71868	0.72988	0.73989
0.95	0.69226	0.69550	0.69865	0.70166	0.70456	0.71754	0.72878	0.73883
<b>T/°C = 125</b>								
0.05	0.68688	0.69045	0.69385	0.69712	0.70025	0.71416	0.72603	0.73653
0.20	0.68558	0.68915	0.69255	0.69582	0.69896	0.71288	0.72479	0.73531
0.35	0.68396	0.68753	0.69099	0.69426	0.69741	0.71140	0.72331	0.73389
0.50	0.68279	0.68642	0.68986	0.69315	0.69629	0.71030	0.72228	0.73285
0.65	0.68130	0.68494	0.68837	0.69169	0.69488	0.70891	0.72089	0.73148
0.80	0.68021	0.68387	0.68734	0.69065	0.69383	0.70790	0.71992	0.73050
0.95	0.67892	0.68257	0.68605	0.68938	0.69259	0.70666	0.71871	0.72939
<b>T/°C = 137.5</b>								
0.05	0.67329	0.67731	0.68113	0.68474	0.68820	0.70330	0.71605	0.72719
0.20	0.67190	0.67595	0.67976	0.68338	0.68686	0.70201	0.71475	0.72586
0.35	0.67030	0.67435	0.67823	0.68188	0.68535	0.70055	0.71335	0.72456
0.50	0.66916	0.67322	0.67706	0.68072	0.68422	0.69942	0.71229	0.72348
0.65	0.66766	0.67171	0.67559	0.67925	0.68275	0.69804	0.71086	0.72213
0.80	0.66654	0.67065	0.67450	0.67818	0.68169	0.69701	0.70989	0.72113
0.95	0.66518	0.66930	0.67318	0.67688	0.68038	0.69576	0.70868	0.71997
<b>T/°C = 150</b>								
0.05	0.65918	0.66374	0.66801	0.67205	0.67587	0.69239	0.70606	0.71785
0.20	0.65772	0.66232	0.66660	0.67062	0.67445	0.69105	0.70476	0.71658
0.35	0.65613	0.66077	0.66508	0.66911	0.67299	0.68957	0.70334	0.71519
0.50	0.65492	0.65956	0.66388	0.66798	0.67185	0.68845	0.70226	0.71410
0.65	0.65340	0.65802	0.66239	0.66649	0.67035	0.68704	0.70085	0.71277

$\rho / (\text{g}\cdot\text{cm}^{-3})$								
p /bar	20	40	60	80	100	200	300	400
0.80	0.65227	0.65692	0.66129	0.66536	0.66927	0.68600	0.69985	0.71177
0.95	0.65090	0.65558	0.65998	0.66408	0.66797	0.68477	0.69864	0.71063
<b>T/°C = 162.5</b>								
0.05	0.64438	0.64965	0.65448	0.65903	0.66329	0.68133	0.69601	0.70856
0.20	0.64295	0.64821	0.65310	0.65762	0.66190	0.68001	0.69472	0.70728
0.35	0.64135	0.64659	0.65150	0.65603	0.66034	0.67854	0.69330	0.70589
0.50	0.64004	0.64538	0.65032	0.65489	0.65919	0.67738	0.69218	0.70479
0.65	0.63847	0.64384	0.64877	0.65334	0.65767	0.67596	0.69079	0.70340
0.80	0.63737	0.64271	0.64763	0.65227	0.65662	0.67489	0.68976	0.70243
0.95	0.63599	0.64138	0.64634	0.65097	0.65529	0.67371	0.68861	0.70130
<b>T/°C = 175</b>								
0.05	0.62887	0.63495	0.64047	0.64555	0.65034	0.67017	0.68595	0.69926
0.20	0.62735	0.63344	0.63902	0.64416	0.64895	0.66884	0.68467	0.69795
0.35	0.62564	0.63179	0.63743	0.64259	0.64735	0.66731	0.68320	0.69658
0.50	0.62440	0.63055	0.63618	0.64134	0.64620	0.66618	0.68208	0.69549
0.65	0.62285	0.62903	0.63468	0.63986	0.64472	0.66476	0.68071	0.69411
0.80	0.62154	0.62781	0.63351	0.63874	0.64363	0.66372	0.67967	0.69309
0.95	0.62025	0.62649	0.63218	0.63729	0.64225	0.66243	0.67842	0.69191
<b>T/°C = 187.5</b>								
0.05	0.61228	0.61947	0.62585	0.63164	0.63702	0.65884	0.67582	0.68996
0.20	0.61076	0.61797	0.62443	0.63022	0.63561	0.65752	0.67457	0.68872
0.35	0.60894	0.61622	0.62267	0.62859	0.63397	0.65601	0.67309	0.68729
0.50	0.60765	0.61498	0.62146	0.62740	0.63284	0.65484	0.67195	0.68617
0.65	0.60596	0.61337	0.61991	0.62585	0.63128	0.65340	0.67054	0.68477
0.80	0.60483	0.61221	0.61876	0.62471	0.63019	0.65233	0.66954	0.68380
0.95	0.60337	0.61075	0.61731	0.62333	0.62884	0.65108	0.66827	0.68260
<b>T/°C = 200</b>								
0.05	0.59437	0.60301	0.61053	0.61721	0.62326	0.64740	0.66569	0.68067
0.20	0.59279	0.60145	0.60898	0.61572	0.62181	0.64605	0.66437	0.67936
0.35	0.59094	0.59974	0.60731	0.61408	0.62023	0.64451	0.66295	0.67795
0.50	0.58968	0.59840	0.60605	0.61284	0.61897	0.64337	0.66179	0.67686
0.65	0.58773	0.59675	0.60444	0.61122	0.61744	0.64192	0.66041	0.67549
0.80	0.58653	0.59554	0.60328	0.61014	0.61637	0.64091	0.65939	0.67450
0.95	0.58504	0.59402	0.60183	0.60873	0.61494	0.63956	0.65815	0.67328

## 3.3.4 Aromatic+Nitrogen+Sulfur (ANS)

Table 17.

Experimental densities ( $\rho$ ) of the ternary mixture of aromatics+nitrogen+sulfur model at different temperatures and pressures.

p /bar		$\rho$ /g·cm <sup>3</sup>													
20		40		60		80		100		200		300		400	
X <sub>A</sub>	X <sub>N</sub>	T/°C = 100													
0.125	0.125	0.71165	0.71454	0.71730	0.71999	0.72260	0.73437	0.74473	0.75405						
0.125	0.375	0.70960	0.71250	0.71530	0.71801	0.72062	0.73246	0.74289	0.75226						
0.125	0.750	0.70633	0.70923	0.71206	0.71478	0.71744	0.72933	0.73982	0.74927						
0.250	0.50	0.70790	0.71081	0.71362	0.71632	0.71893	0.73081	0.74125	0.75065						
0.375	0.250	0.70955	0.71244	0.71526	0.71794	0.72055	0.73236	0.74279	0.75214						
0.500	0.375	0.70812	0.71099	0.71380	0.71648	0.71911	0.73098	0.74141	0.75082						
0.750	0.125	0.70911	0.71200	0.71478	0.71747	0.72010	0.73193	0.74233	0.75171						
		T/°C = 112.5													
0.125	0.125	0.69877	0.70196	0.70507	0.70801	0.71086	0.72361	0.73472	0.74463						
0.125	0.375	0.69670	0.69993	0.70302	0.70600	0.70886	0.72171	0.73286	0.74282						
0.125	0.750	0.69337	0.69664	0.69977	0.70275	0.70564	0.71856	0.72979	0.73978						
0.250	0.50	0.69499	0.69820	0.70134	0.70430	0.70719	0.72003	0.73124	0.74119						
0.375	0.250	0.69667	0.69987	0.70296	0.70593	0.70879	0.72160	0.73276	0.74269						
0.500	0.375	0.69519	0.69842	0.70150	0.70449	0.70736	0.72022	0.73138	0.74135						
0.750	0.125	0.69625	0.69947	0.70256	0.70550	0.70835	0.72119	0.73234	0.74224						
		T/°C = 125													
0.125	0.125	0.68556	0.68912	0.69254	0.69581	0.69894	0.71284	0.72470	0.73521						
0.125	0.375	0.68347	0.68705	0.69051	0.69381	0.69695	0.71094	0.72289	0.73343						
0.125	0.750	0.68010	0.68373	0.68719	0.69051	0.69368	0.70773	0.71977	0.73038						
0.250	0.50	0.68172	0.68534	0.68880	0.69206	0.69525	0.70926	0.72120	0.73181						
0.375	0.250	0.68343	0.68706	0.69048	0.69374	0.69692	0.71086	0.72279	0.73332						
0.500	0.375	0.68196	0.68556	0.68899	0.69229	0.69545	0.70943	0.72140	0.73196						
0.750	0.125	0.68305	0.68664	0.69007	0.69334	0.69649	0.71042	0.72235	0.73285						
		T/°C = 137.5													
0.125	0.125	0.67193	0.67598	0.67980	0.68343	0.68685	0.70200	0.71470	0.72585						
0.125	0.375	0.66985	0.67392	0.67773	0.68138	0.68484	0.70007	0.71288	0.72407						
0.125	0.750	0.66643	0.67052	0.67439	0.67805	0.68153	0.69687	0.70976	0.72101						

p /bar		$\rho / \text{g} \cdot \text{cm}^3$							
		20	40	60	80	100	200	300	400
0.250	0.50	0.66808	0.67216	0.67602	0.67967	0.68315	0.69840	0.71125	0.72244
0.375	0.250	0.66983	0.67388	0.67770	0.68134	0.68484	0.70001	0.71279	0.72396
0.500	0.375	0.66836	0.67241	0.67624	0.67989	0.68338	0.69859	0.71143	0.72261
0.750	0.125	0.66942	0.67346	0.67727	0.68090	0.68441	0.69958	0.71236	0.72352
<b>T/°C = 150</b>									
0.125	0.125	0.65785	0.66241	0.66670	0.67073	0.67454	0.69108	0.70476	0.71654
0.125	0.375	0.65567	0.66029	0.66458	0.66863	0.67246	0.68910	0.70287	0.71472
0.125	0.750	0.65215	0.65683	0.66119	0.66525	0.66918	0.68586	0.69970	0.71166
0.250	0.50	0.65388	0.65848	0.66282	0.66690	0.67075	0.68744	0.70121	0.71307
0.375	0.250	0.65564	0.66025	0.66456	0.66863	0.67248	0.68906	0.70278	0.71465
0.500	0.375	0.65416	0.65875	0.66310	0.66718	0.67104	0.68765	0.70141	0.71328
0.750	0.125	0.65529	0.65989	0.66422	0.66828	0.67211	0.68869	0.70241	0.71423
<b>T/°C = 162.5</b>									
0.125	0.125	0.64305	0.64830	0.65319	0.65770	0.66196	0.68004	0.69473	0.70724
0.125	0.375	0.64081	0.64612	0.65097	0.65557	0.65988	0.67803	0.69281	0.70539
0.125	0.750	0.63726	0.64260	0.64755	0.65213	0.65644	0.67477	0.68963	0.70230
0.250	0.50	0.63898	0.64433	0.64925	0.65383	0.65812	0.67637	0.69115	0.70378
0.375	0.250	0.64084	0.64611	0.65099	0.65557	0.65984	0.67800	0.69273	0.70532
0.500	0.375	0.63929	0.64461	0.64948	0.65414	0.65841	0.67661	0.69138	0.70396
0.750	0.125	0.64051	0.64581	0.65067	0.65520	0.65951	0.67763	0.69235	0.70492
<b>T/°C = 175</b>									
0.125	0.125	0.62749	0.63360	0.63913	0.64425	0.64900	0.66889	0.68471	0.69797
0.125	0.375	0.62518	0.63132	0.63694	0.64207	0.64692	0.66686	0.68269	0.69607
0.125	0.750	0.62149	0.62774	0.63341	0.63858	0.64346	0.66356	0.67953	0.69298
0.250	0.50	0.62334	0.62953	0.63515	0.64031	0.64516	0.66518	0.68106	0.69447
0.375	0.250	0.62522	0.63137	0.63694	0.64209	0.64690	0.66681	0.68267	0.69603
0.500	0.375	0.62369	0.62983	0.63546	0.64062	0.64546	0.66540	0.68128	0.69467
0.750	0.125	0.62496	0.63107	0.63661	0.64176	0.64662	0.66648	0.68230	0.69564
<b>T/°C = 187.5</b>									
0.125	0.125	0.61089	0.61808	0.62452	0.63038	0.63573	0.65759	0.67460	0.68875
0.125	0.375	0.60853	0.61578	0.62224	0.62812	0.63356	0.65553	0.67256	0.68675
0.125	0.750	0.60465	0.61210	0.61863	0.62461	0.63005	0.65222	0.66939	0.68367
0.250	0.50	0.60664	0.61395	0.62046	0.62631	0.63177	0.65385	0.67096	0.68518
0.375	0.250	0.60854	0.61583	0.62227	0.62812	0.63354	0.65550	0.67256	0.68673
0.500	0.375	0.60699	0.61428	0.62075	0.62667	0.63208	0.65408	0.67117	0.68535

p /bar		$\rho$ /g·cm <sup>3</sup>							
		20	40	60	80	100	200	300	400
0.750	0.125	0.60832	0.61553	0.62203	0.62782	0.63324	0.65519	0.67223	0.68637
<b>T/°C = 200</b>									
0.125	0.125	0.59299	0.60164	0.60912	0.61587	0.62196	0.64614	0.66446	0.67943
0.125	0.375	0.59060	0.59929	0.60688	0.61360	0.61986	0.64411	0.66249	0.67748
0.125	0.750	0.58643	0.59542	0.60316	0.60999	0.61619	0.64073	0.65923	0.67435
0.250	0.50	0.58850	0.59735	0.60497	0.61179	0.61802	0.64241	0.66084	0.67590
0.375	0.250	0.59051	0.59928	0.60692	0.61366	0.61977	0.64405	0.66245	0.67747
0.500	0.375	0.58894	0.59771	0.60534	0.61210	0.61832	0.64266	0.66103	0.67605
0.750	0.125	0.59037	0.59913	0.60667	0.61339	0.61947	0.64376	0.66211	0.67710

## 4. Model Dissolutions

### 4.1 General description

#### 4.1.1 Asphaltene composition

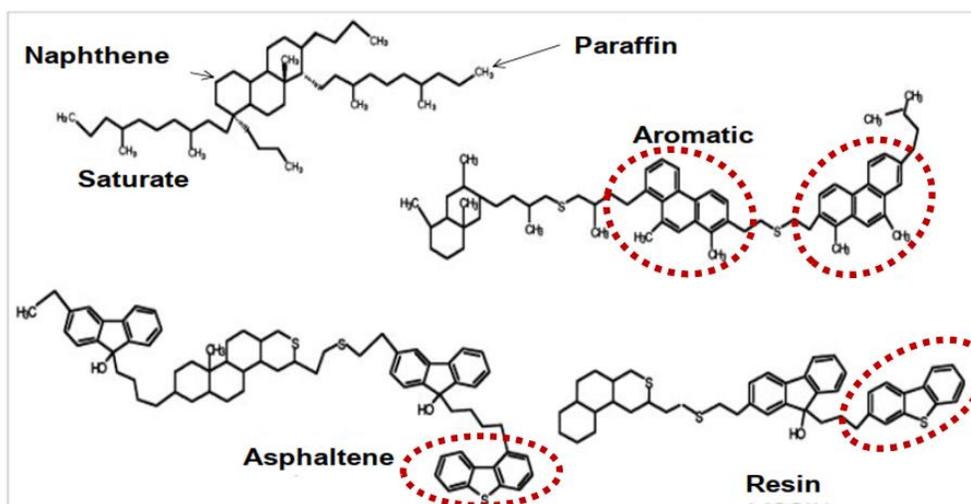
Crude oil composition has been a subject of interest throughout the years. It is a mixture of different compounds which can be as simple as methane or as big as substances with more than 300 carbon atoms (Jones, 2006). Therefore, when looking into a sample, researchers focus on finding the families of the molecules, the ones with bigger proportions or well-known substances. In the case of heavy crude oil, it has a lower hydrogen/carbon (H/C) relationship and a wider content of asphaltenes and resins. The H/C ratio could be 2.0-2.3 for high oils, while it can go as low as 1.4 in heavy crude oils. Aromatics generally have a ratio of less than 1, for example, phenanthrene is a three-cycle common aromatic and has a ratio of 0.714 (Strausz & Lown, 2003). These last two are known for an atom skeleton form with an aromatic center and adjoined tails of alkyls and naphthenes, heteroatoms (nitrogen, sulfur, and oxygen), and metallic compounds (Cheshkova et al., 2019; Moreno-Arciniegas et al., 2009). Sulfur and nitrogen heterocompounds can be found inside rings of cyclic, mainly aromatic molecules. Sulfur compounds are mainly present in a series of alkyl-thiophenes, alkyl-benzothiophenes, and alkyl-dibenzothiophenes, while

nitrogen is present in alkyl-carbazole, alkyl-pyridines, and alkyl-quinolines. Oxygen prefers groups of carboxylic acid groups, ketones, esters, and ethers, rather than in rings (Strausz & Lown, 2003).

Sergun et al. (2014) studied the composition of asphaltene in US heavy crude oil. They found polyaromatic compounds (PAHs), mostly with atoms of naphthalene, phenanthrene, and their C<sub>1</sub>-C<sub>4</sub> derivatives. C<sub>1</sub>-C<sub>3</sub> alkyl-carbazole and benzocarbazole for nitrogen compounds while for sulfur they found primarily Dibenzothiophene, benzothiophene, and their alkyl derivatives. A similar study was made with Russian heavy crude oil by Cheshkova et al., (2019). For sulfur compounds, dibenzothiophene and its alkyl derivatives were found as for nitrogen compounds quinoline, benzo quinoline, and their derivatives. Nevertheless, crude oil content is influenced by its well of origin, papers could be a guide for composition of Colombian heavy crude oil. For instance, in the Putumayo Basin, an FT-ICR MS analysis showed compounds generally associated with carbazole or indole derivatives in a study with samples of 30 wells (Orrego-Ruiz et al., 2020).

### Figure 11

*Heavy crude oil structure from analysis SARA*

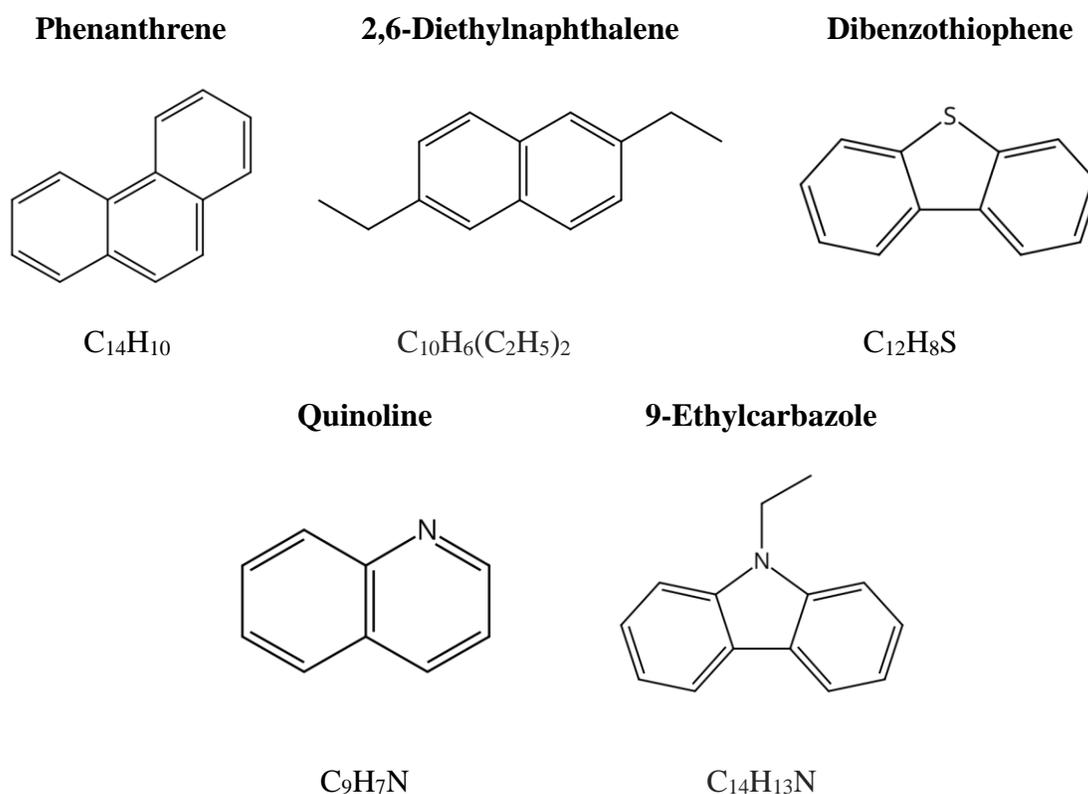


*Note: Adjusted from Strausz & Lown, 2003.*

Notably, nitrogen and sulfur are present in cyclic compounds of quinoline, carbazole, and dibenzothiophene with their derivatives, while aromatics are present as polycyclic molecules. Therefore, the model molecules selected for each family are dibenzothiophene (DBT) for sulfur compounds, quinoline (QUI) and 9-ethyl carbazole (EC) for nitrogen, and phenanthrene (PHE) with 2,6-diethylnaphthalene (DEN) for aromatics. As the carrier liquid is selected cyclohexane, as it had shown higher conversion in hydrodesulfurization of dibenzothiophene than other solvents (Wang et al., 2021).

**Figure 12**

*Model molecules for heavy crude oil*



#### ***4.1.2 Thermophysical properties and TRIDEN correlation***

Thermophysical properties have a fundamental role in chemical process development. Hence, density, viscosity, compressibility, and other properties of clear and accurate data results

in an adequate design, synthesis, analysis, and operation of extraction, production, and transport processes.

Undoubtedly, density plays an important part in the industry, it is defined as the mass occupied by a volume, nevertheless, it is associated with the API gravity of crude oil. Thus, density data acquisition and understanding are indispensable in the petroleum industry. Furthermore, density is the reciprocal of the specific volume, so it is easy to obtain the molar volume to analyze PVT behavior from a pressure-density-temperature thermodynamic study, with an easier experimental setup. Studies based on density experimental data look into not only the data behavior as a function of temperature, pressure, and concentration but also the PVT thermodynamic model that adjusts the data. Moreover, density is essential for empirical models that estimate thermophysical and transport properties such as viscosity, thermal conductivity, and many others (Assael et al., 1996).

Temperature and pressure in liquids lead to a variation in volume, hence properties like isothermal compressibility  $\kappa_T$  and isobaric thermal expansivity (or volume expansivity)  $\alpha_p$  are used for the study of liquids (Gmehling et al., 2012). These properties are dependent on temperature, an increase in temperature equals an increase in molecular energy and intermolecular spaces. On the contrary, an increase in pressure causes a reduction in intermolecular spaces that limits its capacity to be expanded or compressed and origins a diminution in both properties (Guerrero-Zárate et al., 2019). Furthermore,  $\kappa_T$  y  $\alpha_p$  are positive for liquids except for water, with negative expansivity values between 0°C -4°C (Smith et al., 2018). On the other hand, internal pressure is related to intermolecular forces, so it describes the macroscopic behavior of the substances generated by attraction and repulsion forces, that generate pressure inside the fluid (Guerrero-Amaya, 2012).

$$\alpha_p = \frac{1}{V} \left( \frac{\partial V}{\partial T} \right)_p = -\frac{1}{\rho} \left( \frac{\partial \rho}{\partial T} \right)_p \quad (4)$$

$$\kappa_T = -\frac{1}{V} \left( \frac{\partial V}{\partial p} \right)_T = \frac{1}{\rho} \left( \frac{\partial \rho}{\partial p} \right)_T \quad (5)$$

$$p_i = \left( \frac{\partial U}{\partial V} \right)_T = T \frac{\alpha_p}{\kappa_T} - p \quad (6)$$

Overall, with density experimental data we can estimate volume expansivity, isothermal compressibility, and internal pressure using a correlation that entangles the changes in density with temperature and pressure as independent variables. TRIDEN or tridimensional density is a group of equations developed by Ihmels & Gmehling, (2001) to describe the density behavior of liquids until the critical point. This correlation is composed of two important equations: a modified Tait correlation used for the density of liquids and a modified Rackett equation used for saturated liquids. Using a reference pressure of  $p_0$ , TRIDEN, a ten-parameter correlation is:

$$\text{Modified Tait: } \rho(T, p) = \frac{\rho_0}{1 - C_T \ln \frac{B_T(T) + p}{B_T(T) + p_0}} \quad (7)$$

$$B_T(T) = b_0 + b_1 \frac{T}{E_T} + b_2 \left( \frac{T}{E_T} \right)^2 + b_3 \left( \frac{T}{E_T} \right)^3 \quad (8)$$

$$\text{Modified Rackett } \rho_0 = \frac{A_R}{B_R \left[ 1 + \left( 1 - \frac{T}{C_R} \right)^{D_R} \right]} \quad (9)$$

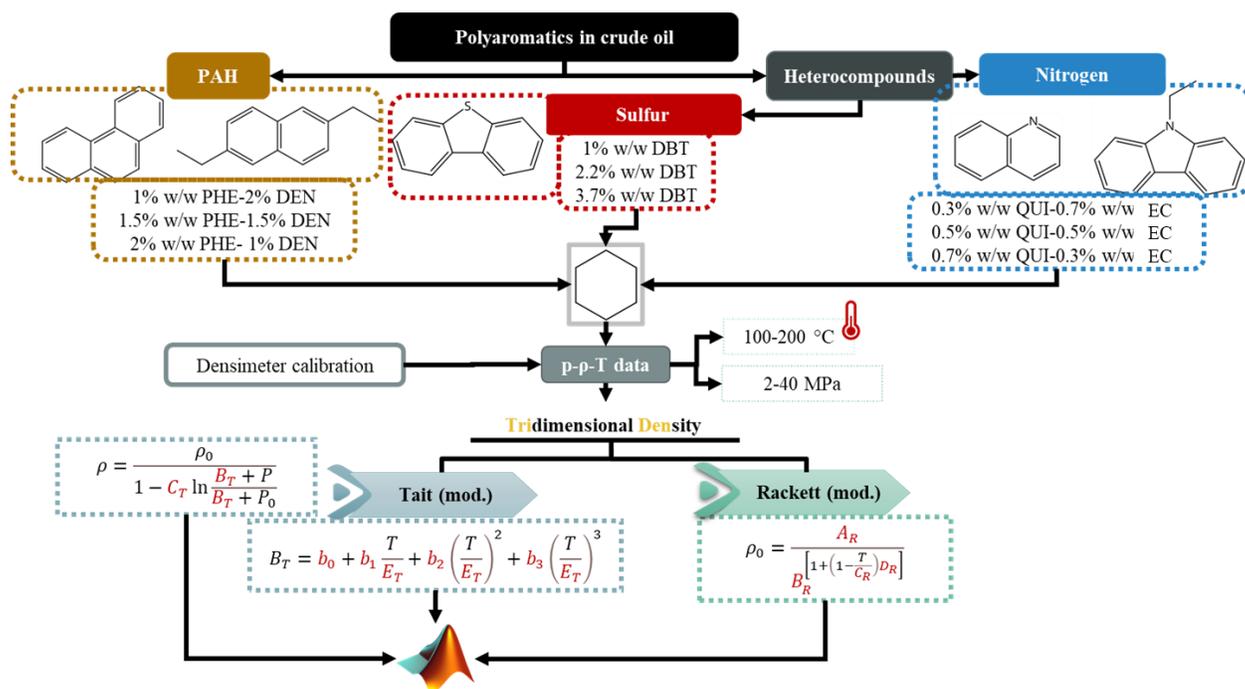
TRIDEN, Tait, Rackett and its modification have been used to correlate p- $\rho$ -T U-tube experimental data for hydrocarbons, crude oil, and cyclohexane. Dávila et al., (2011) used TRIDEN for cyclohexane measure in temperatures of 278.15-378.15 K and pressures up to 60 MPa, with an average deviation of 0.0109 %. In the same way, Antón et al., (2017) used it to estimate isothermal compressibility, isobaric thermal expansivity, and internal pressure of thiophenes. Moreover, Malta et al., (2020) with Tait correlation got a maximum deviation of

0.11% while studying synthetic mixtures of light crude oil at temperatures of 323-398 K and pressures from 1 MPa to 70 MPa. Likewise, a maximum deviation of 0.18% was obtained by Zambrano et al., (2018), with the analysis of Ecuadorian heavy crude oil between 288.69-373.13 K and pressures up to 140 MPa. Additionally, with the same experimental method, Zhou et al., (2010) estimated a root-mean-square error (RMSE) of  $0.34 \text{ kg}\cdot\text{m}^{-3}$  for cyclohexane in temperatures of 293.15-313.15 K and pressures up to 40 MPa, while Amorim et al., (2007a, 2007b), studied it at 318.15-413.15 K and up to 62 MPa with an RMSE of  $0.42 \text{ kg}\cdot\text{m}^{-3}$ . On the other hand, with a high-pressure pycnometer, a modified Rackett has been used to estimate the density of benzene, cyclohexane, n-. hexane and its liquid saturated mixtures between 298.15-473.15 K (Beg et al., 1993, 1994, 1995).

## 4.2 Experimental

**Figure 13**

*Methodology for density measurements and analysis of model dissolutions*



### 4.2.1 Measurements

Pressure-density-temperature measurements were made in 9 isotherms from 373.15-473.15 K between eight pressure points from 2-40 MPa, with 72 experimental points per mixture. First, cyclohexane measurements in the same conditions were performed. Specifically, pure cyclohexane is a well-known substance, that could be used to check the accuracy of the measurements and as a reference point for the density of the dissolutions (Sommer et al., 2011). The selection of three possible compositions of model dissolutions for each family (aromatic, sulfur, and nitrogen compounds) was made based on the composition of heteroatoms in heavy crude oil. **Table 18** shows the composition for each molecule, the rest is pure cyclohexane.

**Table 18**

*Model dissolution composition*

<b>Model dissolution</b>	<b>Model molecules composition (%w/w)</b>
<b>Aromatics</b>	Phenanthrene (2 %), 2,6- Diethylnaphthalene (1 %)
	Phenanthrene (1.5 %), 2,6- Diethylnaphthalene (1.5 %)
	Phenanthrene (1 %), 2,6- Diethylnaphthalene (2 %)
<b>Nitrogen compounds</b>	Quinoline (0.3 %), 9-ethylcarbazole (0.7 %)
	Quinoline (0.5 %), 9- ethylcarbazole (0.5 %)
	Quinoline (0.7 %), 9- ethylcarbazole (0.3 %)
<b>Sulfur compounds</b>	Dibenzithiophene (3.7 %)
	Dibenzithiophene (2.2 %)
	Dibenzithiophene (1 %)

#### 4.2.2 TRIDEN adjustment

The fitting of the ten parameters of TRIDEN equation was made using MATLAB with a non-linear least squares method and a Levenberg-Maquadt algorithm. The deviation from the experimental data was calculated with the average absolute deviation (AAD):

$$\%AAD = \frac{100}{n} \sum_{i=1}^n \left| \frac{\rho_{experimental} - \rho_{TRIDEN}}{\rho_{Experimental}} \right| \quad (10)$$

The derivatives of TRIDEN's density with temperature and pressure were calculated and replaced in equations (4), (5) and (6) to estimate isothermal compressibility, isobaric thermal expansivity, and internal pressure.

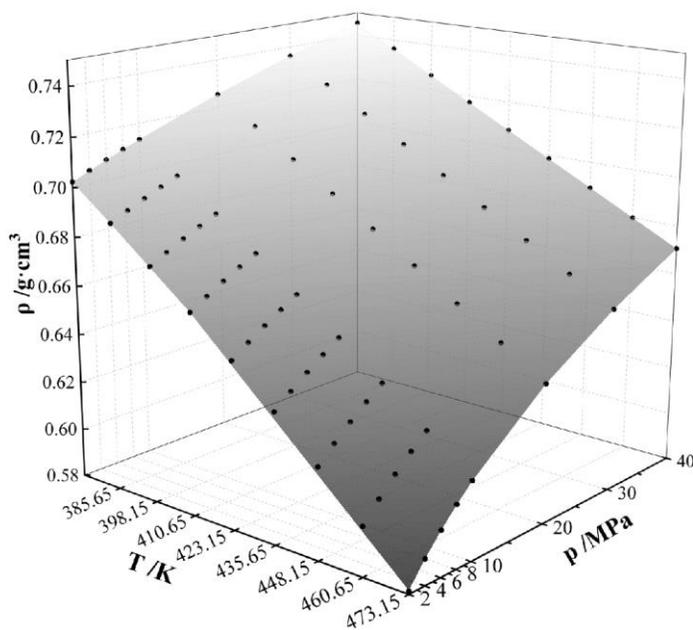
## 4.3 Results

### 4.3.1. Cyclohexane

Density measurements and its TRIDEN estimation are shown in figures 14 and 15 with a 2D and a 3D image. Also, the parameters of the correlation are compiled in Table 19. TRIDEN density estimations have good agreement with experimental data of cyclohexane, resulting in an AAD of 0.0097% and a root mean square error (RMSE) equal to  $8.3 \times 10^{-5} \text{ g} \cdot \text{cm}^{-3}$ .

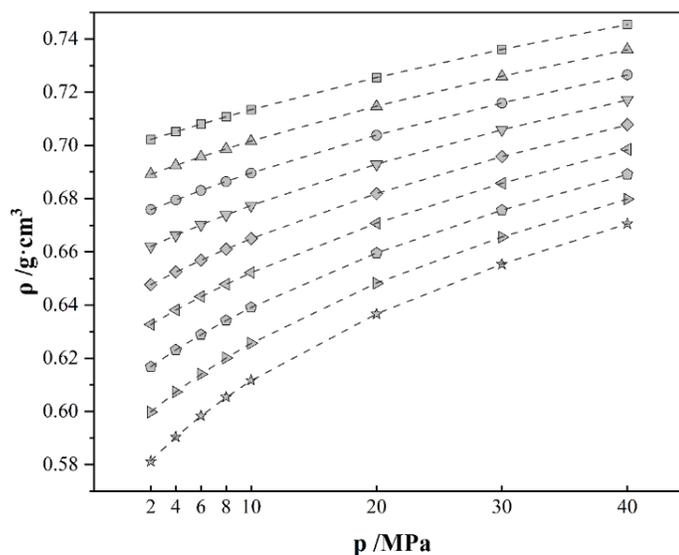
#### Figure 14

*Cyclohexane's density ( $\rho$ ) 3D as a function of temperature and pressure. Experimental data: (●)  
TRIDEN model Surface*



**Figure 15.**

Cyclohexane's density ( $\rho$ ) 2D as a function of temperature and pressure. Experimental data: (●) 373.15 K (△) 385.65 K (○) 398.15 K (▽) 410.65 K (◇) 423.15 K (<) 435.65 K (◇) 448.15 K (▷) 460.65 K (☆) 473.15 K. (---) TRIDEN estimation.

**Table 19.**

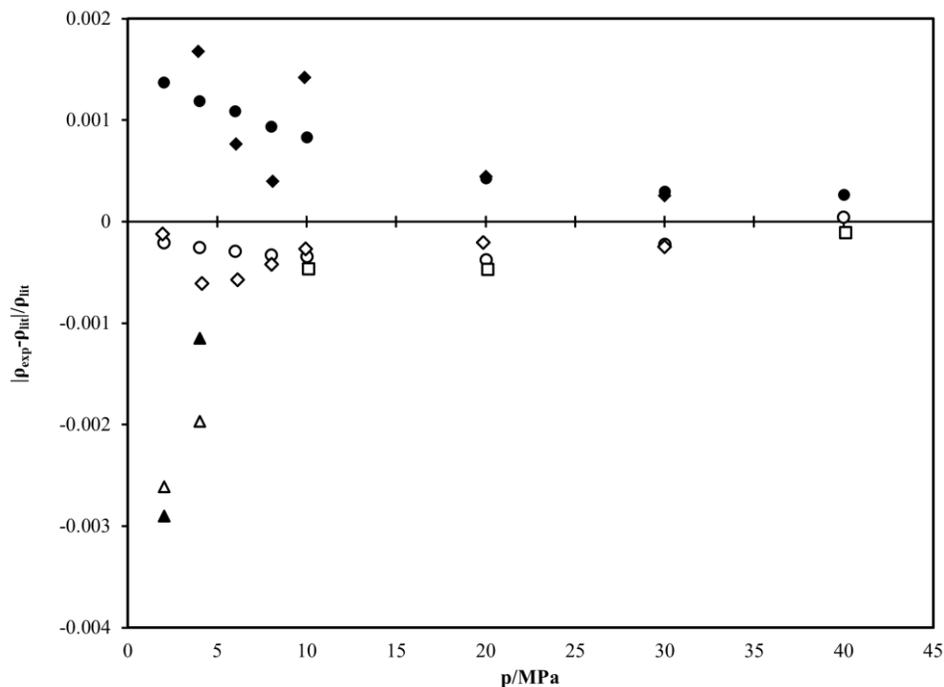
TRIDEN coefficients for cyclohexane

$A_R$ ( $g \cdot cm^{-3}$ )	$B_R$	$C_R$ (K)	$D_R$	$E_T$ (K)	$C_T$	$b_0$ (MPa)	$b_1$ (MPa)	$b_2$ (MPa)	$b_3$ (MPa)	AAD (%)
0.190	0.433	522	0.460	74.2	0.0868	304	-77.3	4.83	0.0049	<b>0.00973</b>

Density experimental data behavior is normal to typical tendencies, as the temperature increases the internal energy increases, and the molecules need more intermolecular space leading to a decrease in density. On the other hand, the molecules come close to each other with an increase in pressure causing a higher density. Cyclohexane has a linear density behavior, although it shows a slight curvature on the isotherms at higher temperatures.

**Figure 16**

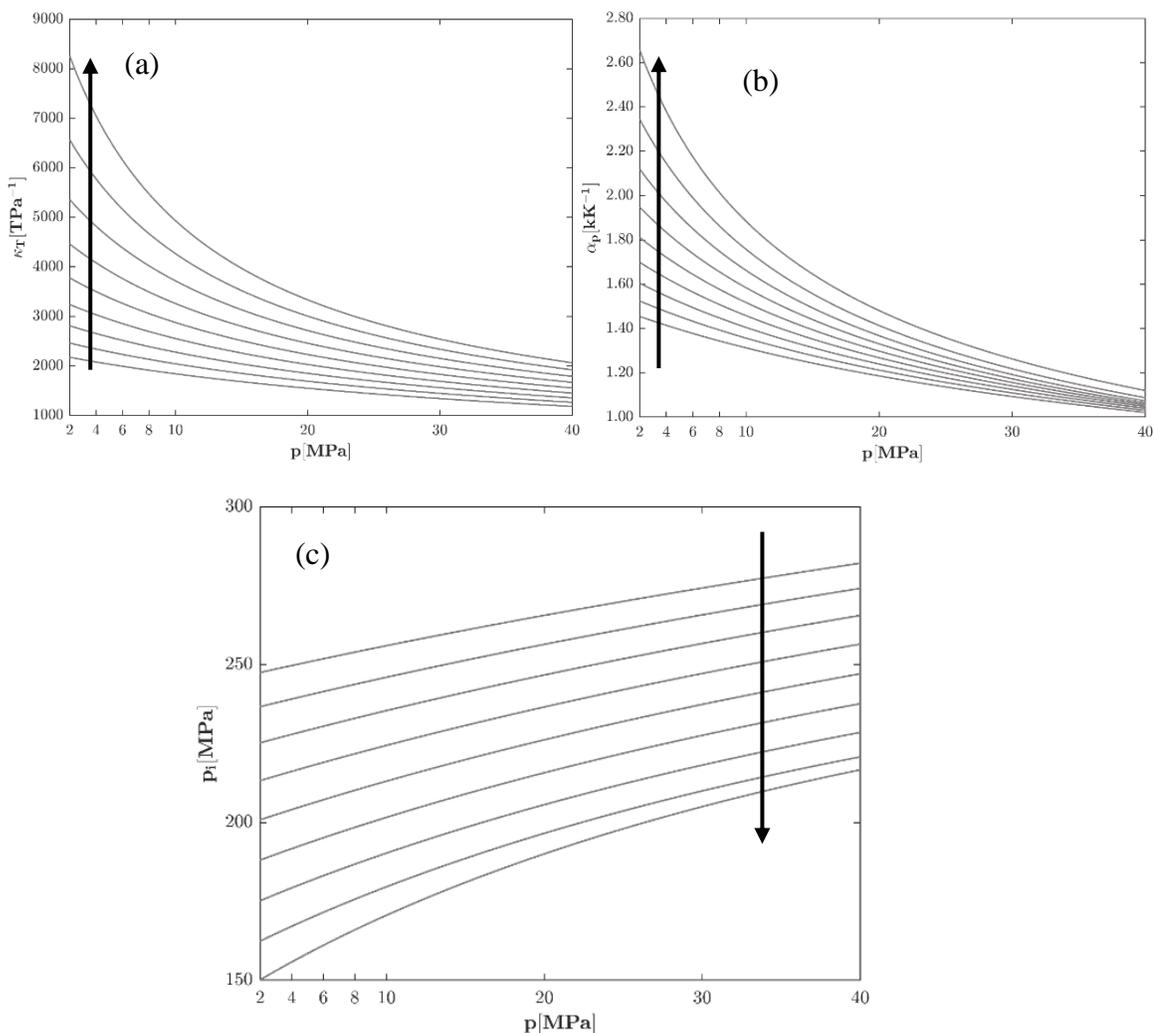
Cyclohexane's density density deviation from literature, black symbols represent data at 473.15K and empty ones data at 373.15 K ( $\circ$ ) (National Institute of Standards and Technology (NIST), 2021) ( $\diamond$ ) (Sommer et al., 2011) ( $\Delta$ ) (Dortmund Data Bank, n.d.) ( $\square$ ) (Shchemelev et al., 2021)



Numerous authors have studied cyclohexane in its liquid state with p- $\rho$ -T data in conditions up to 548 K and up to 100 MPa (Y. Zhou et al., 2014), however, a limited number of papers have experimental data with the same conditions studied by this work. Nevertheless, the NIST database has density data of all 72 experimental points and in literature we could be found data at temperatures of 373.15 K and 473.15 K. This work's experimental data has good agreement with the NIST database (National Institute of Standards and Technology (NIST), 2021) with an average absolute deviation AAD of 0.031% on the whole range of temperature and pressure. Therefore, in the figure are the deviations of experimental data at 373.15 K and 473.15 K.

**Figure 17**

Estimated isobaric expansivity (a), isothermal compressibility (b), and internal pressure (c) of cyclohexane as a function of temperature and pressure. Arrows show the increase in temperature.



With TRIDEN coefficients and the thermodynamic definition presented in equations (4), (5) and (6) **¡Error! No se encuentra el origen de la referencia.**, isothermal compressibility, isobaric expansivity, and internal pressure were estimated. As expected,  $\alpha_p$  and  $\kappa_T$  properties decrease with pressure and increase with temperature. Amorim et al. (2007b) estimated  $\alpha_p$  and  $\kappa_T$  up to 65 MPa and 413.15 K. TRIDEN estimation has the same

range of results of their work, with a compressibility from 1400-2800 TPa<sup>-1</sup> and an expansivity from 1-1.6 kK<sup>-1</sup> at similar conditions.

### 4.3.2. Model dissolutions

Density measurements for all model dissolutions of Table 18 are presented in 3.

Experimental data

**Table 20.**

*TRIDEN coefficients for model dissolutions*

	$A_R$ (g·cm <sup>-3</sup> )	$B_R$	$C_R$ (K)	$D_R$	$E_T$ (K)	$C_T$	$b_0$ (MPa)	$b_1$ (MPa)	$b_2$ (MPa)	$b_3$ (MPa)	AAD (%)
<b>1% DBT</b>	0.187	0.429	525	0.454	73.9	0.0869	306	-77.7	4.90	-0.00168	<b>0.00950</b>
<b>2.2% DBT</b>	0.194	0.436	524	0.462	75.2	0.0864	303	-76.4	4.48	0.0366	<b>0.00795</b>
<b>3.7% DBT</b>	0.214	0.457	520	0.498	74.3	0.0864	309	-77.2	4.55	0.0300	<b>0.00980</b>
<b>1%PHE</b>	0.226	0.469	514	0.523	58.2	0.0866	387	-92.7	7.17	-0.183	<b>0.00970</b>
<b>1.5% PHE</b>	0.189	0.431	527	0.456	75.4	0.0867	302	-76.1	4.41	0.043	<b>0.00820</b>
<b>2% PHE</b>	0.205	0.448	522	0.485	56.4	0.0865	397	-93.9	7.28	-0.191	<b>0.00820</b>
<b>0.3% QUI</b>	0.197	0.440	522	0.472	73.0	0.0867	310	-78.5	5.04	-0.0144	<b>0.00830</b>
<b>0.5% QUI</b>	0.178	0.419	526	0.436	75.5	0.0866	301	-76.1	4.37	0.0496	<b>0.00940</b>
<b>0.7% QUI</b>	0.188	0.430	524	0.456	74.2	0.08671	305	-77.4	4.83	0.00488	<b>0.00910</b>

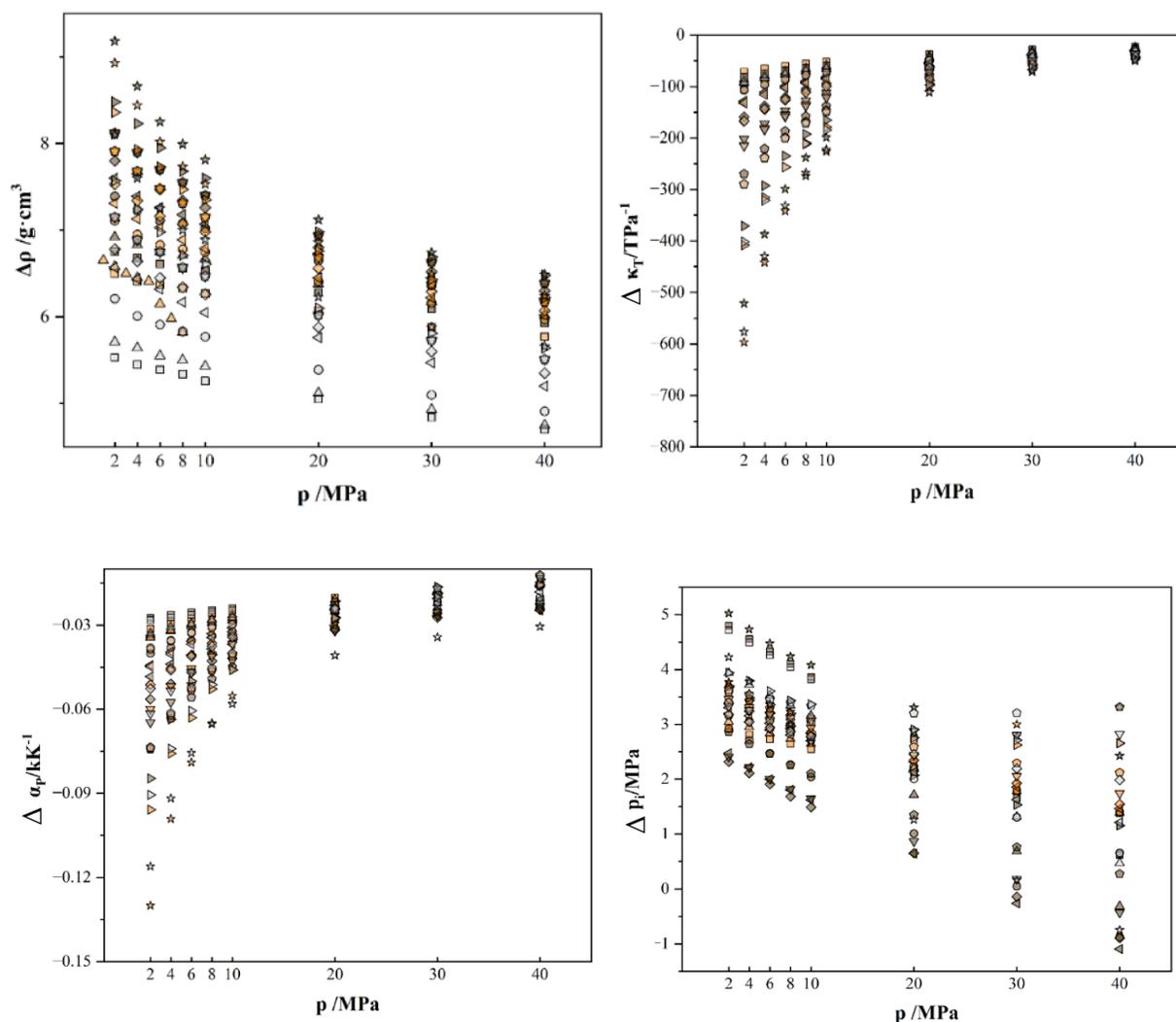
$$p_{ref} = 2 \text{ MPa}$$

With the MATLAB code found in **Appendix A: MATLAB TRIDEN code**, all coefficients for TRIDEN were estimated. For all data the average deviation AAD is less than 0.01%, showing a good agreement of this correlation with the experimental data.

#### 4.3.2.1 Aromatic model

**Figure 18**

A deviation compared with pure cyclohexane as a function of temperature and pressure a) Experimental density ( $\rho$ ) b) Estimated isobaric expansivity c) Estimated isothermal compressibility d) Estimated internal pressure of 1% PHE (gray), 1.5% PHE (yellow) and 2% PHE (brown). ( $\square$ ) 373.15 K ( $\triangle$ ) 385.65 K ( $\circ$ ) 398.15 K ( $\nabla$ ) 410.65 K ( $\diamond$ ) 423.15 K ( $\triangleleft$ ) 435.65 K ( $\triangleright$ ) 448.15 K ( $\triangleright$ ) 460.65 K ( $\star$ ) 473.15 K.



The figures above show how much the thermophysical properties of each three of the aromatic models deviate from pure cyclohexane data. Density has a behavior according to

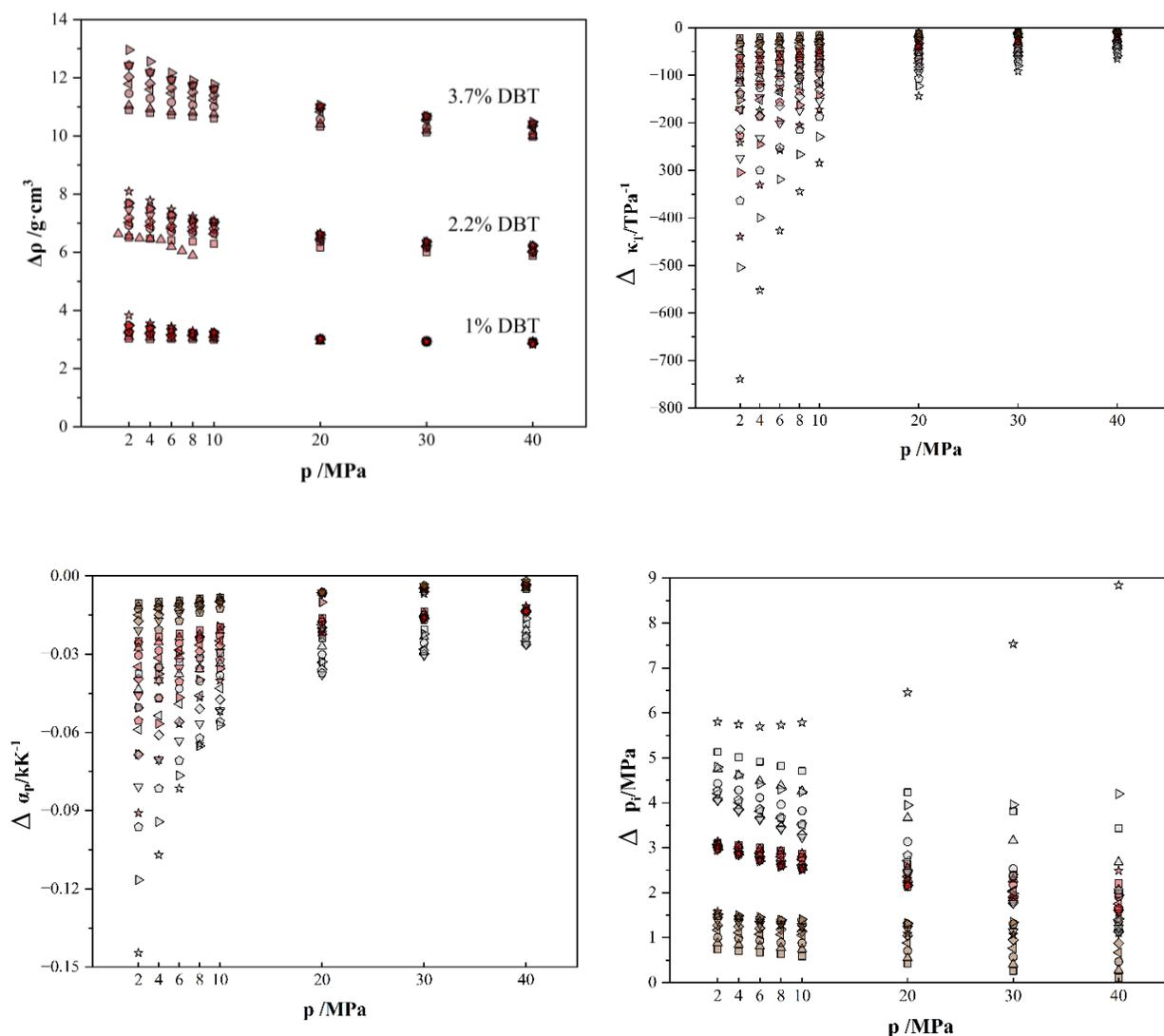
phenanthrene content, at higher composition, higher density. This result is interesting because phenanthrene has a lower molecular weight ( $178.23 \text{ g}\cdot\text{mol}^{-1}$ ) than 2,6-Diethylnaphthalene ( $184.28 \text{ g}\cdot\text{mol}^{-1}$ ), showing the interaction between the molecules of this substances and cyclohexane has an influence in the mixture, even at low concentrations. Therefore, cyclohexane seems to have more attraction with 2,6-Diethylnaphthalene, possibly due to its alkyl ramifications; with a higher concentration of this molecule, higher average molecular weight but lower density. Additionally, the difference increases with temperature and reduces with pressure. On the other hand, the expansivity and compressibility of the mixtures reduce with the molecules compared with pure cyclohexane.

#### *4.3.2.2 Sulfur model*

As expected, the density of sulfur model mixtures increases with the increase of dibenzothiophene composition, usually the increase of DBT molar composition in alkanes, increases the mixture density (De Oliveira et al., 2011). Similarly to the aromatic model, the deviation decreases with pressure. The negative deviation of expansivity and compressibility is higher at lower composition, and lower pressure, with higher composition is more difficult for mixtures to be compressed or expanded. On the other hand, internal pressure is higher with 1% DBT.

**Figure 19**

*S* deviation compared with pure cyclohexane as a function of temperature and pressure a) Experimental density ( $\rho$ ) b) Estimated isobaric expansivity c) Estimated isothermal compressibility d) Estimated internal pressure of 1% DBT (gray), 2.2% DBT (red) and 3.7% DBT (brown). ( $\square$ ) 373.15 K ( $\triangle$ ) 385.65 K ( $\circ$ ) 398.15 K ( $\nabla$ ) 410.65 K ( $\diamond$ ) 423.15 K ( $\triangleleft$ ) 435.65 K ( $\triangleleft$ ) 448.15 K ( $\triangleright$ ) 460.65 K ( $\star$ ) 473.15 K

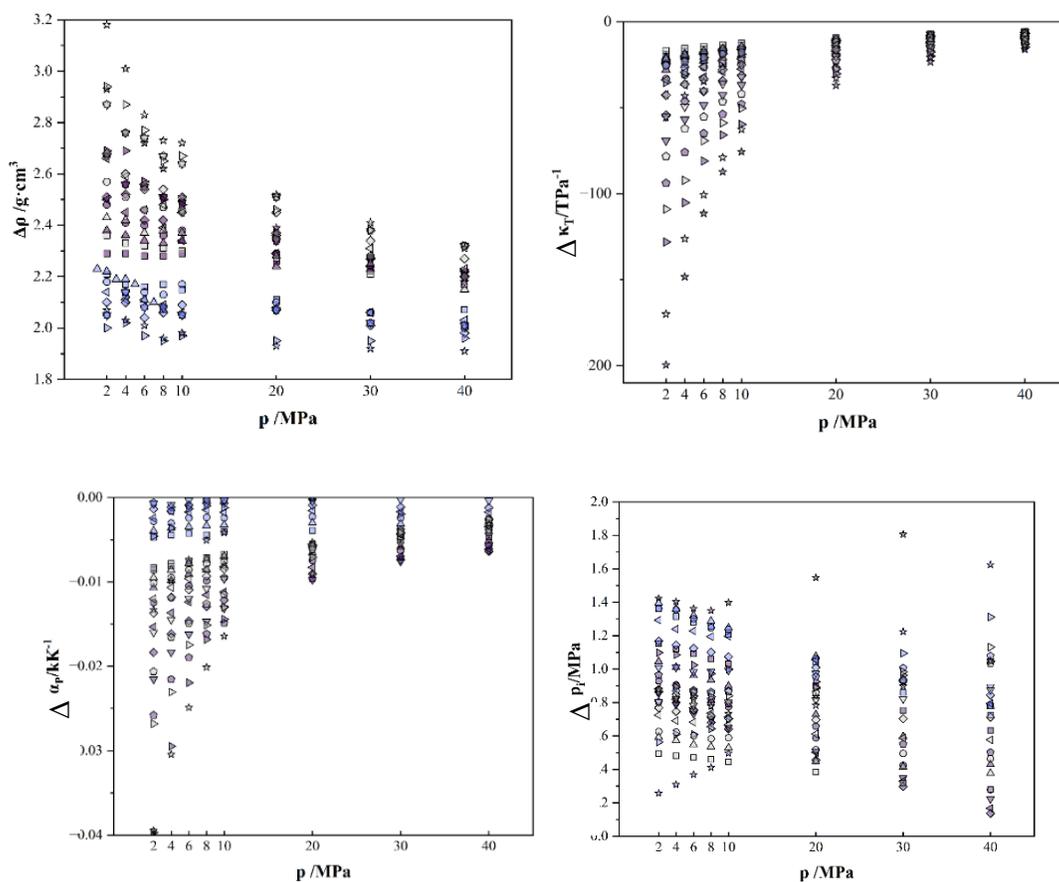


#### 4.3.2.3. Nitrogen model

In this case, density is higher with less quinoline in the mixture which can be attributed to the interaction between quinoline and cyclohexane and resulting in a negative excess volume at low compositions (Nath et al., 1978). In particular, the lower density has equal w/w composition of quinoline and 9-ethylcarbazole, which could imply the influence of the intermolecular forces between the compounds.

**Figure 20**

*N* deviation compared with pure cyclohexane as a function of temperature and pressure a) Experimental density ( $\rho$ ) b) Estimated isobaric expansivity c) Estimated isothermal compressibility d) Estimated internal pressure of 0.3% QUI (gray), 0.5% QUI (blue) and 07% QUI (purple). ( $\square$ ) 373.15 K ( $\Delta$ ) 385.65 K ( $\circ$ ) 398.15 K ( $\nabla$ ) 410.65 K ( $\diamond$ ) 423.15 K ( $\triangleleft$ ) 435.65 K ( $\diamond$ ) 448.15 K ( $\triangleright$ ) 460.65 K ( $\star$ ) 473.15 K.



## 5. Mixtures

### 5.1 General description

#### 5.1.1. Excess properties

Excess properties allow us to analyze the thermodynamic properties of liquid mixtures, as they establish the real solution deviations from the ideal solution. Furthermore, an analysis in a wide range of temperatures and pressures helps to understand the molecular interactions and structural changes during the mixture process (Guerrero et al., 2015; Smith et al., 2018). Additionally, properties like excess volume and excess enthalpy are involved in the analysis of the dependence of temperature and pressure within the liquid-liquid equilibrium. (Segura & Wisniak, 1997).

With an extensive molar property (V, U, H, S, G, etc), named M,  $M^E$  is the excess property as:

$$M^E \equiv M - M^{id} \quad (11)$$

$M^{id}$  is the property of the ideal solution evaluated at the same temperature, pressure, and composition. The next table contains some excess properties definitions.

**Table 21**

*Excess thermophysical properties*

Excess property	Equation
Excess molar volume	$V^E = V - \sum_i x_i V_i^o \quad (12)$
Excess expansivity	$\alpha_p^E = \alpha_p - \sum_i \phi_i \alpha_{p,i} \quad (13)$
	$\phi_i = \frac{x_i V_i^o}{\sum_i x_i V_i^o} \quad (14)$

Excess property	Equation
Excess Isothermal Compressibility	$\kappa_T^E = \kappa_T - \sum_i \phi_i \kappa_{T,i}$ (15)
Excess Internal pressure	$p_i^E = p_i - \sum_i \psi_i p_{i,i}$ (16)
	$\psi_i = \frac{x_i \kappa_{T,i} V_i^o}{\sum_i x_i \kappa_{T,i} V_i^o}$ (17)

More precisely, experimental data from a high-resolution densimeter allows us to estimate excess molar volume, excess expansivity, excess compressibility, and excess internal pressure, but not the excess Gibbs energy, excess enthalpy, nor excess entropy. (Guerrero-Amaya, 2012)

### 5.1.2. Redlich Kister

Excess properties behavior is generally studied with the expansion of the Redlich Kister polynomial. With the use of temperature and pressure-dependent parameters, Redlich Kister gives a better  $V^E$  fitting in a wide range (Beg et al., 1994; Guerrero et al., 2013).

$$M^E = x(1-x) \sum_{i=0}^n a_i(T,p)(2x-1)^{i-1} \quad (18)$$

Redlich Kister has been used to study different cyclohexane mixtures. Amorim et al., (2007b) used a first-degree polynomial to estimate density data from the mixture of cyclohexane + n-hexadecane between 318.15-416.15 K and up to 62 MPa with an RMSD of  $.0.64 \text{ kg}\cdot\text{m}^{-3}$ . Then, they got a  $0.43 \text{ kg}\cdot\text{m}^{-3}$  improvement with a second-degree equation. Also, Zhou et al., (2010) measured a mixture of dimethyl carbonate and cyclohexane within 293.15 K-313.15 K and 0.1 MPa-40 MPa with a maximum  $V^E$  RMSD of  $0.022 \text{ cm}^3\cdot\text{mol}^{-1}$  with a fifth-degree equation. On the other hand, Beg et al., (1994, 1995) found a better fitting for the excess volume of the mixture of

cyclohexane + benzene with an AAD of 1.38%, than cyclohexane + hexane with deviations higher than 10%. At ambient pressure at 293.15 to 333.15 K, (Zeqiraj et al., 2023) found standard deviation  $\sigma$  less than  $0.007 \text{ cm}^3 \cdot \text{mol}^{-1}$  in binary mixtures of cyclohexane with benzene, toluene, ethylbenzene, o-xylene, m-xylene, and p-xylene. Finally, Martínez-Reina & Amado-González, (2012) studied mixtures of cyclohexane with benzene, heptane, and toluene at ambient pressure and temperatures between 298.15-308.15 K. with a fourth-degree polynomial obtaining standard deviations  $\sigma$  of less than  $0.009 \text{ cm}^3 \cdot \text{mol}^{-1}$ .

## 5.2 Experimental

### 5.2.1. Measurements

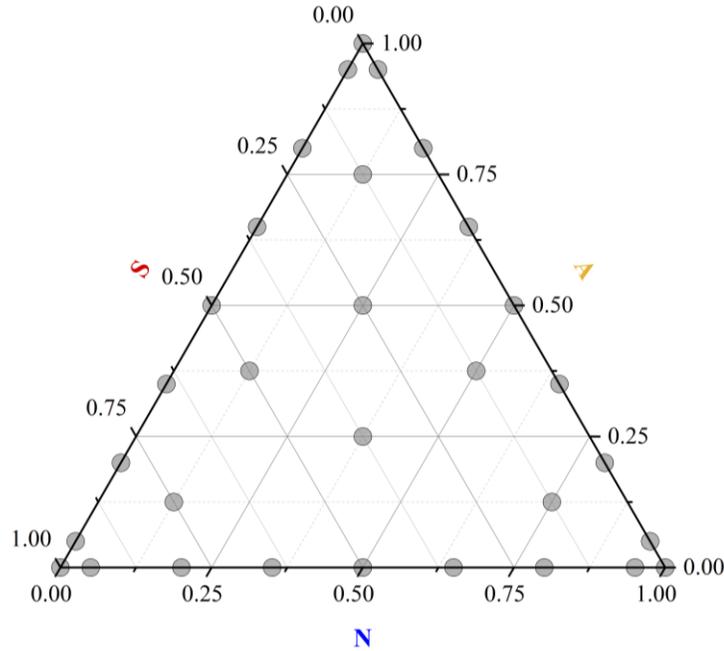
To study the mixture between aromatic, nitrogen, and sulfur compounds a composition from each family was selected from the previous chapter. The next table has the composition used for each molecule for the model. Then, Figure 21 shows all the molar fractions measured of the ternary mixtures of AS, AN, NS, and the ternary mixture ANS.

**Table 22.**

Model dissolution composition selected for mixtures.

Model dissolution	Model molecules composition (%w/w)
<b>Aromatics (A)</b>	Phenanthrene (2 %), 2,6- Diethylnaphthalene (1 %)
<b>Nitrogen compounds (N)</b>	Quinoline (0.5 %), 9- ethylcarbazole (0.5 %)
<b>Sulfur compounds (S)</b>	Dibenzithiophene (3.7 %)

For each of the binary mixtures, the density is adjusted with the TRIDEN correlation, with the procedure in 4.2

**Figure 21***Mixture ternary points***5.2.2. Excess properties**

Equations (12) to (17) are used to estimate the excess properties of each mixture.

**5.2.3. Redlich Kister Adjustment**

To fit these mixtures a fourth-degree polynomial was used according to equations (19) and (20) and adjusted with a generalized reduced gradient method. The terms  $T_0$  and  $p_0$  correspond to the reference conditions. In this case,  $T_0$  is 373.15 K and  $p_0$  is 2 MPa. To adjust the 20 parameters for each mixture, the standard deviation is used according to equation (20), where  $n$  is the total of data and  $r$  is the number of parameters used.

$$V^E(\text{cm}^3 \text{mol}^{-1}) = x_i(1 - x_i)(a_0(T, p) + a_1(T, p)(2x_i - 1)^{-1} + a_2(T, p)(2x_i - 1)^2 + a_3(T, p)(2x_i - 1)^3 + a_4(T, p)(2x_i - 1)^4) \quad (19)$$

$$a_0(T, p)(\text{cm}^3 \text{mol}^{-1}) = a_{i0} + a_{i1}(p - p_0) + a_{i2}(T - T_0) + a_{i3}(p - p_0)(T - T_0) \quad (20)$$

$$\sigma(V^E) = \sqrt{\frac{\sum_i (V_i^{E \text{ Exp}} - V_i^{E \text{ Cal}})^2}{n-r}} \quad (21)$$

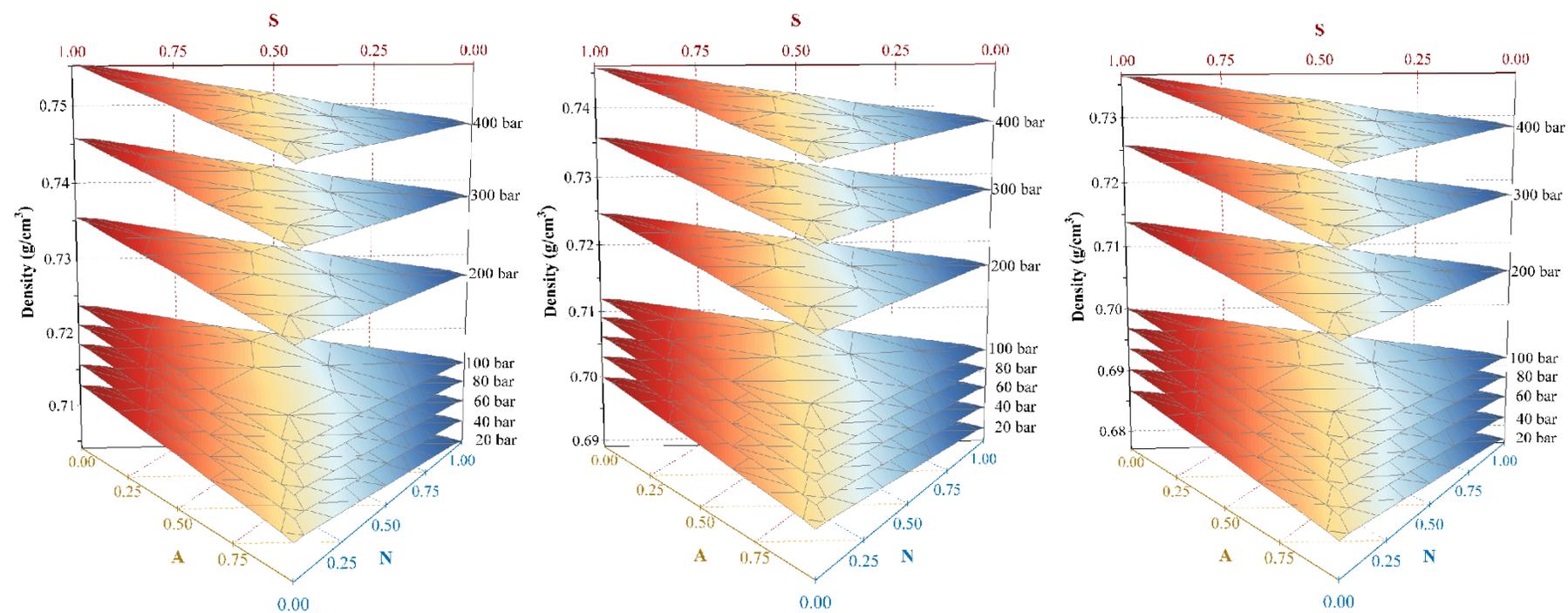
### 5.3 Results

#### 5.3.1. Density Ternary graphs

**¡Error! No se encuentra el origen de la referencia.¡Error! No se encuentra el origen de la referencia.¡Error! No se encuentra el origen de la referencia.** contains all the 2232 points measured. They showed the expected behavior of density, higher with compression and reduced with heating. In general, a higher content of S is higher the density, while it reduces with higher N content.

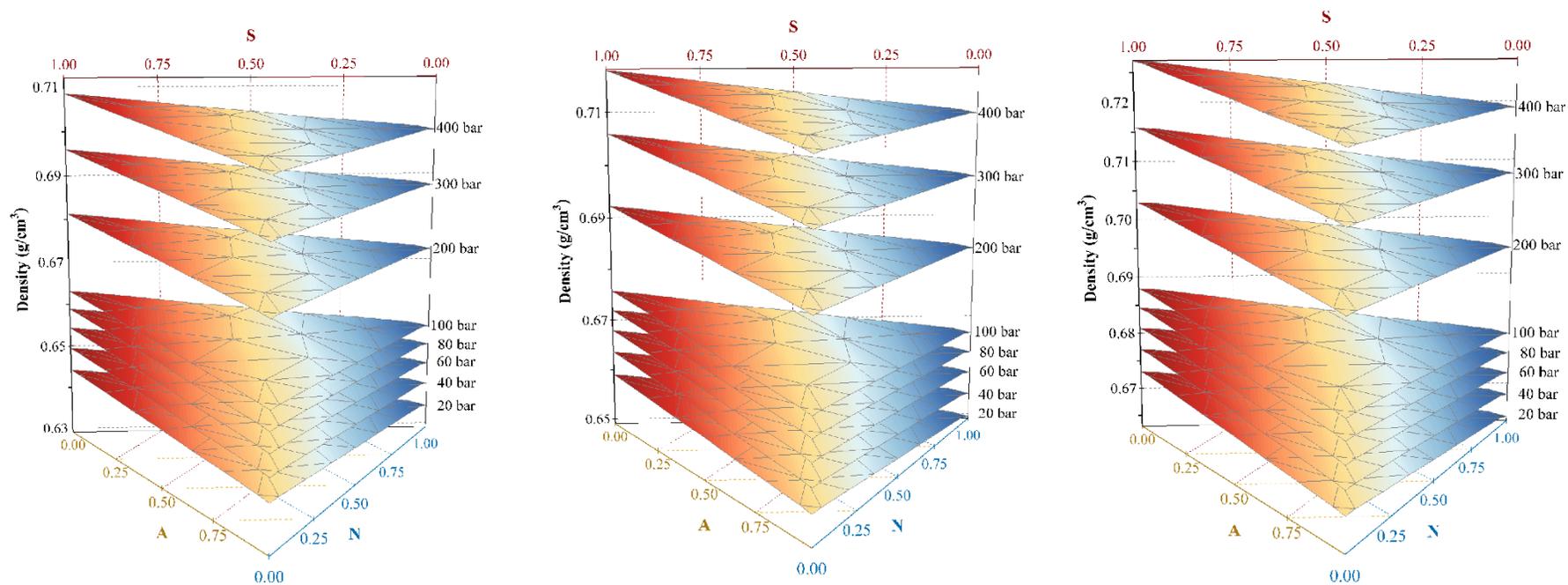
**Figure 22.**

Experimental density ( $\rho$ ) as function of Temperature and Pressure of ternary mixtures ANS at 373.15 K (left), 385.65 K. (middle) 398.15 K (right).



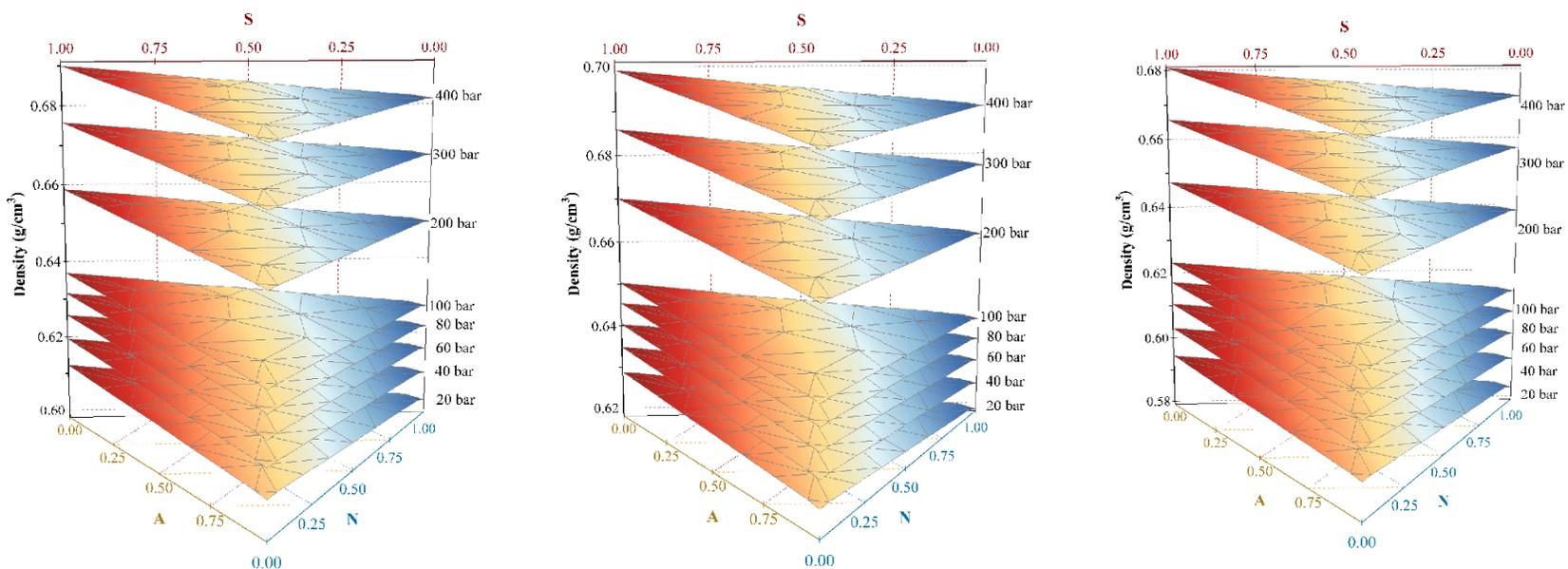
**Figure 23.**

Experimental density ( $\rho$ ) as function of Temperature and Pressure of ternary mixtures ANS at 410.65 K (left), 423.15 K. (middle) 435.65 K (right).



**Figure 24.**

Experimental density ( $\rho$ ) as function of Temperature and Pressure of ternary mixtures ANS at 448.15 K (left), 460.65 K. (middle) 473.15 K (right)



### 5.3.2. TRIDEN

**Table 23, Table 24, Table 25** have all TRIDEN parameters and their average absolute deviation. All the mixtures have a good agreement with the TRIDEN correlation, with an AAD of less than 0.01%. The AS mixture has the lowest deviation of all mixtures, with an average of 0.0086 % of AAD.

**Table 23.**

*TRIDEN coefficients for AS mixture*

$x_A$	$A_R$ ( $g \cdot cm^{-3}$ )	$B_R$	$C_R$ (K)	$D_R$	$E_T$ (K)	$C_T$	$b_0$ (MPa)	$b_1$ (MPa)	$b_2$ (MPa)	$b_3$ (MPa)	AAD (%)
<b>0.05</b>	0.182	0.422	530	0.440	76.6	0.0865	299	-75.0	4.12	0.0715	<b>0.00824</b>
<b>0.20</b>	0.195	0.437	526	0.464	74.7	0.0863	306	-76.8	4.52	0.0329	<b>0.00890</b>
<b>0.35</b>	0.188	0.429	528	0.451	76.0	0.0866	301	-75.6	4.30	0.0521	<b>0.00860</b>
<b>0.50</b>	0.185	0.426	529	0.447	76.5	0.0866	299	-75.0	4.16	0.0696	<b>0.00887</b>
<b>0.65</b>	0.180	0.421	530	0.440	77.5	0.0867	295	-74.0	3.87	0.0951	<b>0.00833</b>
<b>0.80</b>	0.189	0.431	527	0.455	76.3	0.0866	299	-75.3	4.23	0.0599	<b>0.00855</b>
<b>0.95</b>	0.197	0.439	525	0.469	74.5	0.0866	306	-77.1	4.71	0.0142	<b>0.00877</b>

$p_{ref} = 2$  MPa

**Table 24.**

*TRIDEN coefficients for AN mixture*

$x_A$	$A_R$ ( $g \cdot cm^{-3}$ )	$B_R$	$C_R$ (K)	$D_R$	$E_T$ (K)	$C_T$	$b_0$ (MPa)	$b_1$ (MPa)	$b_2$ (MPa)	$b_3$ (MPa)	AAD (%)
<b>0.05</b>	0.192	0.435	523	0.463	73.3	0.0867	308	-78.3	5.01	-0.0125	<b>0.00950</b>
<b>0.20</b>	0.193	0.435	523	0.464	71.6	0.0867	315	-79.9	5.37	-0.0451	<b>0.00964</b>

$x_A$	$A_R$ ( $g \cdot cm^{-3}$ )	$B_R$	$C_R$ (K)	$D_R$	$E_T$ (K)	$C_T$	$b_0$ (MPa)	$b_1$ (MPa)	$b_2$ (MPa)	$b_3$ (MPa)	AAD (%)
<b>0.35</b>	0.189	0.431	525	0.455	72.8	0.0866	310	-78.5	5.08	-0.0203	<b>0.00895</b>
<b>0.50</b>	0.188	0.431	526	0.455	74.1	0.0865	306	-77.3	4.77	0.0087	<b>0.00956</b>
<b>0.65</b>	0.177	0.418	529	0.434	77.1	0.0865	295	-74.5	4.08	0.0744	<b>0.00958</b>
<b>0.80</b>	0.198	0.441	524	0.471	73.0	0.0866	311	-78.5	5.00	-0.0116	<b>0.00880</b>
<b>0.95</b>	0.210	0.453	520	0.496	54.9	0.0866	406	-95.3	7.44	-0.1998	<b>0.00839</b>

$$p_{ref} = 2 \text{ MPa}$$

**Table 25.**

*TRIDEN coefficients for NS mixture*

$x_N$	$A_R$ ( $g \cdot cm^{-3}$ )	$B_R$	$C_R$ (K)	$D_R$	$E_T$ (K)	$C_T$	$b_0$ (MPa)	$b_1$ (MPa)	$b_2$ (MPa)	$b_3$ (MPa)	AAD (%)
<b>0.05</b>	0.195	0.437	526	0.464	75.4	0.0864	303	-76.1	4.43	0.0405	<b>0.00868</b>
<b>0.20</b>	0.211	0.453	520	0.495	57.6	0.0864	390	-93.2	7.27	-0.1898	<b>0.00801</b>
<b>0.35</b>	0.190	0.432	526	0.456	74.5	0.0864	306	-77.1	4.67	0.0193	<b>0.00923</b>
<b>0.50</b>	0.185	0.427	527	0.449	76.0	0.0866	300	-75.6	4.32	0.0519	<b>0.00911</b>
<b>0.65</b>	0.198	0.440	522	0.471	72.9	0.0865	310	-78.6	5.12	-0.0238	<b>0.00971</b>
<b>0.80</b>	0.183	0.425	526	0.445	74.6	0.0865	303	-76.9	4.72	0.0139	<b>0.00962</b>
<b>0.95</b>	0.196	0.439	522	0.471	72.0	0.0869	313	-79.4	5.29	-0.0388	<b>0.00938</b>

$$p_{ref} = 2 \text{ MPa}$$

### 5.3.3. Excess properties

#### 5.3.3.1. Excess Volume $V^E$

##### 5.3.3.1.1. Aromatic + Sulfur (AS)

**Table 26.**

*Excess volume ( $V^E$ ) of the binary mixture of aromatics + sulfur model at different temperatures and pressures.*

$V^E / \text{cm}^3 \cdot \text{mol}^{-1}$								
p /bar	20	40	60	80	100	200	300	400
<b>x<sub>A</sub></b>	<b>T/°C = 100</b>							
0.05	-0.033	-0.038	-0.037	-0.035	-0.035	-0.043	-0.041	-0.044
0.20	-0.029	-0.031	-0.031	-0.029	-0.030	-0.030	-0.031	-0.032
0.35	-0.020	-0.022	-0.024	-0.025	-0.027	-0.035	-0.039	-0.043
0.50	-0.041	-0.044	-0.044	-0.043	-0.045	-0.049	-0.053	-0.056
0.65	-0.021	-0.022	-0.023	-0.024	-0.026	-0.034	-0.039	-0.042
0.80	-0.029	-0.033	-0.031	-0.036	-0.036	-0.045	-0.049	-0.053
0.95	-0.028	-0.030	-0.030	-0.031	-0.034	-0.043	-0.049	-0.054
	<b>T/°C = 112.5</b>							
0.05	-0.038	-0.041	-0.040	-0.037	-0.038	-0.040	-0.040	-0.043
0.20	-0.035	-0.033	-0.032	-0.032	-0.029	-0.029	-0.028	-0.028
0.35	-0.024	-0.027	-0.026	-0.027	-0.024	-0.034	-0.034	-0.038
0.50	-0.051	-0.048	-0.049	-0.050	-0.046	-0.051	-0.052	-0.052
0.65	-0.026	-0.031	-0.028	-0.030	-0.029	-0.032	-0.035	-0.038
0.80	-0.035	-0.039	-0.035	-0.035	-0.036	-0.042	-0.047	-0.047
0.95	-0.029	-0.032	-0.031	-0.034	-0.032	-0.042	-0.043	-0.044
	<b>T/°C = 125</b>							
0.05	-0.039	-0.041	-0.038	-0.036	-0.039	-0.039	-0.041	-0.041
0.20	-0.032	-0.033	-0.031	-0.028	-0.031	-0.028	-0.025	-0.025
0.35	-0.024	-0.030	-0.028	-0.026	-0.026	-0.030	-0.031	-0.035
0.50	-0.051	-0.053	-0.052	-0.048	-0.051	-0.048	-0.048	-0.049
0.65	-0.026	-0.030	-0.028	-0.029	-0.024	-0.030	-0.031	-0.034
0.80	-0.038	-0.038	-0.038	-0.038	-0.034	-0.039	-0.039	-0.040
0.95	-0.030	-0.037	-0.031	-0.033	-0.033	-0.032	-0.033	-0.034
	<b>T/°C = 137.5</b>							
0.05	-0.039	-0.039	-0.034	-0.030	-0.030	-0.033	-0.032	-0.037
0.20	-0.030	-0.027	-0.030	-0.021	-0.024	-0.021	-0.023	-0.021
0.35	-0.023	-0.027	-0.024	-0.022	-0.019	-0.024	-0.025	-0.029
0.50	-0.052	-0.049	-0.051	-0.043	-0.046	-0.041	-0.046	-0.045
0.65	-0.027	-0.030	-0.030	-0.025	-0.024	-0.022	-0.027	-0.027

$V^E / \text{cm}^3 \cdot \text{mol}^{-1}$								
p /bar	20	40	60	80	100	200	300	400
0.80	-0.037	-0.041	-0.037	-0.032	-0.033	-0.032	-0.036	-0.037
0.95	-0.035	-0.031	-0.034	-0.027	-0.029	-0.026	-0.029	-0.030
<b>T/°C = 150</b>								
0.05	-0.029	-0.033	-0.025	-0.028	-0.022	-0.022	-0.021	-0.023
0.20	-0.029	-0.027	-0.028	-0.027	-0.022	-0.017	-0.014	-0.013
0.35	-0.020	-0.028	-0.019	-0.018	-0.016	-0.018	-0.015	-0.021
0.50	-0.051	-0.049	-0.051	-0.047	-0.043	-0.038	-0.037	-0.039
0.65	-0.024	-0.030	-0.026	-0.023	-0.023	-0.019	-0.020	-0.025
0.80	-0.041	-0.040	-0.041	-0.033	-0.033	-0.032	-0.032	-0.034
0.95	-0.034	-0.036	-0.037	-0.030	-0.033	-0.025	-0.026	-0.027
<b>T/°C = 162.5</b>								
0.05	-0.015	-0.016	-0.008	-0.015	-0.015	-0.005	-0.006	-0.012
0.20	-0.021	-0.018	-0.014	-0.019	-0.018	-0.009	-0.007	-0.008
0.35	-0.015	-0.015	-0.009	-0.013	-0.010	-0.010	-0.009	-0.012
0.50	-0.050	-0.043	-0.041	-0.041	-0.041	-0.035	-0.035	-0.036
0.65	-0.027	-0.024	-0.016	-0.021	-0.016	-0.019	-0.022	-0.023
0.80	-0.044	-0.038	-0.033	-0.031	-0.031	-0.028	-0.032	-0.034
0.95	-0.035	-0.035	-0.029	-0.029	-0.027	-0.027	-0.028	-0.029
<b>T/°C = 175</b>								
0.05	-0.010	-0.010	-0.003	0.000	-0.002	0.001	0.001	-0.001
0.20	-0.013	-0.011	-0.009	-0.011	-0.012	-0.008	-0.005	0.001
0.35	-0.009	0.001	-0.002	0.001	-0.008	-0.001	-0.002	-0.005
0.50	-0.046	-0.042	-0.037	-0.039	-0.040	-0.032	-0.034	-0.032
0.65	-0.027	-0.022	-0.018	-0.014	-0.022	-0.012	-0.015	-0.020
0.80	-0.047	-0.048	-0.042	-0.037	-0.035	-0.031	-0.034	-0.034
0.95	-0.047	-0.042	-0.044	-0.039	-0.041	-0.028	-0.030	-0.033
<b>T/°C = 187.5</b>								
0.05	-0.002	0.008	-0.005	0.006	0.008	0.007	0.005	0.003
0.20	-0.009	-0.003	-0.018	-0.009	-0.004	-0.007	-0.001	0.001
0.35	-0.004	0.000	-0.002	0.003	0.009	0.003	0.001	-0.001
0.50	-0.048	-0.038	-0.050	-0.039	-0.031	-0.034	-0.029	-0.030
0.65	-0.025	-0.014	-0.021	-0.010	-0.012	-0.012	-0.011	-0.018
0.80	-0.047	-0.038	-0.040	-0.040	-0.028	-0.033	-0.028	-0.030
0.95	-0.042	-0.039	-0.044	-0.037	-0.030	-0.027	-0.024	-0.028

$V^E / \text{cm}^3 \cdot \text{mol}^{-1}$								
p /bar	20	40	60	80	100	200	300	400
$T/^\circ\text{C} = 200$								
0.05	-0.025	-0.009	-0.012	0.000	-0.006	-0.004	0.000	-0.003
0.20	-0.016	-0.019	-0.019	-0.018	-0.015	-0.009	-0.001	0.003
0.35	-0.011	0.000	-0.003	-0.002	-0.003	-0.003	0.004	-0.002
0.50	-0.069	-0.062	-0.059	-0.054	-0.045	-0.036	-0.029	-0.026
0.65	-0.054	-0.039	-0.035	-0.029	-0.022	-0.016	-0.011	-0.011
0.80	-0.078	-0.053	-0.046	-0.044	-0.040	-0.027	-0.019	-0.018
0.95	-0.066	-0.046	-0.044	-0.032	-0.026	-0.021	-0.016	-0.016

### 5.3.3.1.2 Aromatic + Nitrogen (AN)

**Table 27.**

*Excess volume ( $V^E$ ) of the binary mixture of aromatics + nitrogen model at different temperatures and pressures.*

$V^E / \text{cm}^3 \cdot \text{mol}^{-1}$								
p /bar	20	40	60	80	100	200	300	400
$T/^\circ\text{C} = 100$								
$x_A$								
0.05	-0.046	-0.048	-0.049	-0.043	-0.045	-0.042	-0.043	-0.042
0.20	-0.043	-0.046	-0.045	-0.043	-0.045	-0.043	-0.045	-0.043
0.35	-0.033	-0.035	-0.036	-0.036	-0.036	-0.033	-0.034	-0.034
0.50	-0.028	-0.029	-0.029	-0.031	-0.030	-0.033	-0.033	-0.033
0.65	-0.035	-0.035	-0.037	-0.036	-0.038	-0.043	-0.045	-0.046
0.80	-0.029	-0.029	-0.032	-0.033	-0.034	-0.037	-0.041	-0.043
0.95	-0.035	-0.038	-0.037	-0.035	-0.037	-0.038	-0.040	-0.041
$T/^\circ\text{C} = 112.5$								
0.05	-0.055	-0.055	-0.054	-0.052	-0.050	-0.047	-0.044	-0.042
0.20	-0.051	-0.052	-0.052	-0.052	-0.050	-0.046	-0.045	-0.042
0.35	-0.048	-0.044	-0.044	-0.045	-0.042	-0.041	-0.039	-0.036
0.50	-0.039	-0.039	-0.035	-0.036	-0.035	-0.035	-0.034	-0.032
0.65	-0.048	-0.049	-0.046	-0.046	-0.045	-0.046	-0.045	-0.044
0.80	-0.037	-0.037	-0.037	-0.036	-0.036	-0.039	-0.039	-0.036
0.95	-0.038	-0.039	-0.036	-0.039	-0.038	-0.041	-0.040	-0.038
$T/^\circ\text{C} = 125$								

$V^E / \text{cm}^3 \cdot \text{mol}^{-1}$								
<b>p /bar</b>	<b>20</b>	<b>40</b>	<b>60</b>	<b>80</b>	<b>100</b>	<b>200</b>	<b>300</b>	<b>400</b>
0.05	-0.065	-0.063	-0.062	-0.058	-0.058	-0.053	-0.046	-0.042
0.20	-0.061	-0.061	-0.064	-0.059	-0.057	-0.051	-0.045	-0.045
0.35	-0.058	-0.057	-0.055	-0.054	-0.050	-0.044	-0.038	-0.036
0.50	-0.044	-0.045	-0.044	-0.044	-0.039	-0.035	-0.032	-0.029
0.65	-0.052	-0.054	-0.053	-0.052	-0.050	-0.045	-0.042	-0.040
0.80	-0.042	-0.043	-0.040	-0.039	-0.039	-0.034	-0.035	-0.031
0.95	-0.036	-0.038	-0.039	-0.040	-0.034	-0.035	-0.039	-0.037
<b>T/°C = 137.5</b>								
0.05	-0.087	-0.086	-0.077	-0.075	-0.075	-0.060	-0.054	-0.050
0.20	-0.079	-0.077	-0.073	-0.070	-0.065	-0.055	-0.053	-0.045
0.35	-0.075	-0.070	-0.062	-0.060	-0.059	-0.046	-0.043	-0.037
0.50	-0.055	-0.057	-0.051	-0.049	-0.047	-0.037	-0.034	-0.030
0.65	-0.061	-0.063	-0.061	-0.052	-0.054	-0.045	-0.043	-0.038
0.80	-0.046	-0.048	-0.049	-0.041	-0.040	-0.033	-0.034	-0.032
0.95	-0.035	-0.036	-0.040	-0.034	-0.033	-0.032	-0.036	-0.036
<b>T/°C = 150</b>								
0.05	-0.112	-0.100	-0.098	-0.095	-0.091	-0.070	-0.060	-0.050
0.20	-0.101	-0.096	-0.091	-0.085	-0.080	-0.064	-0.054	-0.046
0.35	-0.090	-0.082	-0.081	-0.071	-0.069	-0.055	-0.046	-0.038
0.50	-0.070	-0.065	-0.067	-0.056	-0.055	-0.041	-0.034	-0.030
0.65	-0.068	-0.071	-0.067	-0.059	-0.060	-0.049	-0.044	-0.041
0.80	-0.060	-0.056	-0.055	-0.048	-0.051	-0.041	-0.035	-0.035
0.95	-0.042	-0.044	-0.042	-0.039	-0.039	-0.038	-0.036	-0.037
<b>T/°C = 162.5</b>								
0.05	-0.137	-0.128	-0.117	-0.111	-0.103	-0.077	-0.065	-0.057
0.20	-0.125	-0.111	-0.112	-0.104	-0.096	-0.070	-0.062	-0.051
0.35	-0.110	-0.098	-0.095	-0.085	-0.077	-0.062	-0.051	-0.044
0.50	-0.088	-0.075	-0.072	-0.068	-0.061	-0.050	-0.041	-0.033
0.65	-0.078	-0.069	-0.067	-0.061	-0.063	-0.052	-0.043	-0.039
0.80	-0.065	-0.059	-0.051	-0.053	-0.053	-0.042	-0.037	-0.037
0.95	-0.051	-0.042	-0.040	-0.039	-0.039	-0.037	-0.036	-0.035
<b>T/°C = 175</b>								
0.05	-0.186	-0.157	-0.150	-0.132	-0.130	-0.086	-0.072	-0.060
0.20	-0.163	-0.146	-0.131	-0.121	-0.116	-0.081	-0.066	-0.053

$V^E / \text{cm}^3 \cdot \text{mol}^{-1}$								
p /bar	20	40	60	80	100	200	300	400
0.35	-0.144	-0.119	-0.113	-0.105	-0.101	-0.067	-0.055	-0.045
0.50	-0.120	-0.099	-0.088	-0.083	-0.081	-0.055	-0.046	-0.035
0.65	-0.102	-0.082	-0.083	-0.079	-0.070	-0.055	-0.046	-0.043
0.80	-0.087	-0.075	-0.073	-0.066	-0.063	-0.049	-0.045	-0.042
0.95	-0.069	-0.062	-0.053	-0.053	-0.046	-0.033	-0.033	-0.035
$T/^\circ\text{C} = 187.5$								
0.05	-0.222	-0.202	-0.183	-0.158	-0.141	-0.104	-0.077	-0.067
0.20	-0.209	-0.182	-0.165	-0.144	-0.128	-0.093	-0.072	-0.061
0.35	-0.165	-0.151	-0.136	-0.122	-0.108	-0.080	-0.056	-0.052
0.50	-0.131	-0.121	-0.110	-0.097	-0.091	-0.066	-0.048	-0.043
0.65	-0.108	-0.097	-0.095	-0.084	-0.070	-0.066	-0.048	-0.045
0.80	-0.100	-0.082	-0.074	-0.073	-0.064	-0.054	-0.044	-0.043
0.95	-0.071	-0.061	-0.055	-0.056	-0.043	-0.042	-0.033	-0.033
$T/^\circ\text{C} = 200$								
0.05	-0.287	-0.238	-0.205	-0.182	-0.170	-0.116	-0.086	-0.073
0.20	-0.261	-0.213	-0.193	-0.173	-0.151	-0.110	-0.082	-0.068
0.35	-0.205	-0.171	-0.148	-0.135	-0.125	-0.089	-0.069	-0.053
0.50	-0.181	-0.155	-0.131	-0.112	-0.101	-0.070	-0.049	-0.040
0.65	-0.158	-0.126	-0.127	-0.108	-0.089	-0.071	-0.052	-0.044
0.80	-0.127	-0.101	-0.087	-0.070	-0.070	-0.049	-0.040	-0.033
0.95	-0.081	-0.067	-0.061	-0.055	-0.040	-0.043	-0.035	-0.035

### 5.3.3.1.3 Nitrogen + Sulfur (NS)

**Table 28.**

*Excess volume ( $V^E$ ) of the binary mixture of nitrogen + sulfur model at different temperatures and pressures.*

$V^E / \text{cm}^3 \cdot \text{mol}^{-1}$								
p /bar	20	40	60	80	100	200	300	400
$x_A$	$T/^\circ\text{C} = 100$							
0.05	-0.044	-0.047	-0.048	-0.045	-0.046	-0.050	-0.051	-0.053
0.20	-0.042	-0.043	-0.044	-0.038	-0.039	-0.040	-0.037	-0.034

$V^E / \text{cm}^3 \cdot \text{mol}^{-1}$								
<b>p /bar</b>	<b>20</b>	<b>40</b>	<b>60</b>	<b>80</b>	<b>100</b>	<b>200</b>	<b>300</b>	<b>400</b>
0.35	0.003	-0.001	-0.003	0.002	0.000	-0.007	-0.009	-0.010
0.50	-0.026	-0.031	-0.031	-0.028	-0.029	-0.030	-0.031	-0.032
0.65	-0.004	-0.007	-0.008	-0.006	-0.005	-0.008	-0.010	-0.008
0.80	-0.037	-0.041	-0.041	-0.036	-0.038	-0.038	-0.038	-0.035
0.95	-0.057	-0.055	-0.057	-0.056	-0.054	-0.053	-0.057	-0.055
<b>T/°C = 112.5</b>								
0.05	-0.047	-0.048	-0.047	-0.046	-0.043	-0.048	-0.047	-0.049
0.20	-0.042	-0.042	-0.041	-0.039	-0.038	-0.038	-0.036	-0.038
0.35	-0.001	-0.002	-0.002	-0.003	-0.004	-0.003	-0.008	-0.009
0.50	-0.035	-0.036	-0.032	-0.034	-0.033	-0.031	-0.031	-0.033
0.65	-0.009	-0.010	-0.006	-0.009	-0.007	-0.006	-0.007	-0.007
0.80	-0.055	-0.051	-0.051	-0.050	-0.047	-0.044	-0.040	-0.037
0.95	-0.063	-0.060	-0.062	-0.062	-0.060	-0.057	-0.056	-0.054
<b>T/°C = 125</b>								
0.05	-0.044	-0.048	-0.046	-0.047	-0.048	-0.048	-0.048	-0.047
0.20	-0.041	-0.041	-0.036	-0.040	-0.038	-0.039	-0.039	-0.041
0.35	-0.005	-0.006	-0.007	-0.003	-0.007	-0.007	-0.007	-0.008
0.50	-0.040	-0.040	-0.042	-0.037	-0.037	-0.035	-0.030	-0.030
0.65	-0.014	-0.017	-0.011	-0.013	-0.014	-0.009	-0.005	-0.004
0.80	-0.061	-0.062	-0.061	-0.060	-0.057	-0.049	-0.044	-0.040
0.95	-0.073	-0.071	-0.071	-0.068	-0.068	-0.059	-0.057	-0.055
<b>T/°C = 137.5</b>								
0.05	-0.044	-0.044	-0.045	-0.040	-0.038	-0.041	-0.039	-0.043
0.20	-0.042	-0.043	-0.039	-0.036	-0.036	-0.038	-0.036	-0.037
0.35	-0.006	-0.005	-0.007	-0.006	-0.005	-0.004	-0.006	-0.008
0.50	-0.050	-0.051	-0.043	-0.041	-0.039	-0.033	-0.031	-0.032
0.65	-0.027	-0.024	-0.021	-0.020	-0.019	-0.010	-0.007	-0.008
0.80	-0.083	-0.080	-0.073	-0.073	-0.068	-0.056	-0.050	-0.045
0.95	-0.091	-0.095	-0.082	-0.083	-0.074	-0.067	-0.060	-0.059
<b>T/°C = 150</b>								
0.05	-0.047	-0.047	-0.037	-0.043	-0.040	-0.034	-0.033	-0.032
0.20	-0.040	-0.046	-0.040	-0.040	-0.037	-0.032	-0.032	-0.032
0.35	-0.010	-0.014	-0.010	-0.006	-0.003	-0.002	-0.001	0.001
0.50	-0.057	-0.059	-0.048	-0.051	-0.044	-0.034	-0.031	-0.024

$V^E / \text{cm}^3 \cdot \text{mol}^{-1}$								
p /bar	20	40	60	80	100	200	300	400
0.65	-0.039	-0.031	-0.031	-0.033	-0.022	-0.014	-0.009	-0.004
0.80	-0.100	-0.090	-0.089	-0.081	-0.075	-0.060	-0.051	-0.042
0.95	-0.118	-0.106	-0.106	-0.096	-0.088	-0.075	-0.062	-0.058
<b>T/°C = 162.5</b>								
0.05	-0.035	-0.040	-0.024	-0.032	-0.032	-0.022	-0.022	-0.023
0.20	-0.042	-0.041	-0.036	-0.036	-0.035	-0.021	-0.019	-0.018
0.35	-0.012	-0.006	-0.002	-0.003	-0.005	0.004	0.007	0.005
0.50	-0.065	-0.063	-0.054	-0.051	-0.046	-0.030	-0.025	-0.023
0.65	-0.050	-0.046	-0.040	-0.036	-0.031	-0.015	-0.008	0.001
0.80	-0.122	-0.112	-0.101	-0.097	-0.088	-0.065	-0.054	-0.043
0.95	-0.147	-0.137	-0.126	-0.120	-0.104	-0.083	-0.072	-0.060
<b>T/°C = 175</b>								
0.05	-0.029	-0.029	-0.030	-0.022	-0.024	-0.021	-0.015	-0.012
0.20	-0.048	-0.039	-0.037	-0.033	-0.034	-0.023	-0.015	-0.008
0.35	-0.017	-0.010	-0.007	-0.003	0.002	0.009	0.012	0.012
0.50	-0.086	-0.067	-0.062	-0.054	-0.054	-0.031	-0.026	-0.019
0.65	-0.076	-0.059	-0.052	-0.042	-0.040	-0.017	-0.005	0.006
0.80	-0.152	-0.127	-0.127	-0.112	-0.104	-0.076	-0.057	-0.042
0.95	-0.198	-0.163	-0.152	-0.134	-0.130	-0.087	-0.073	-0.061
<b>T/°C = 187.5</b>								
0.05	-0.031	-0.026	-0.031	-0.026	-0.017	-0.015	-0.012	-0.010
0.20	-0.056	-0.043	-0.050	-0.036	-0.029	-0.015	-0.006	-0.004
0.35	-0.019	-0.016	-0.009	-0.009	-0.001	0.004	0.013	0.013
0.50	-0.098	-0.087	-0.079	-0.067	-0.056	-0.034	-0.022	-0.018
0.65	-0.090	-0.073	-0.071	-0.058	-0.048	-0.022	-0.005	0.002
0.80	-0.189	-0.175	-0.156	-0.138	-0.124	-0.088	-0.064	-0.051
0.95	-0.241	-0.208	-0.184	-0.164	-0.148	-0.102	-0.078	-0.071
<b>T/°C = 200</b>								
0.05	-0.043	-0.028	-0.029	-0.032	-0.024	-0.022	-0.015	-0.018
0.20	-0.072	-0.054	-0.041	-0.043	-0.036	-0.030	-0.020	-0.019
0.35	-0.049	-0.036	-0.018	-0.017	-0.012	0.003	0.004	0.010
0.50	-0.156	-0.114	-0.097	-0.087	-0.077	-0.045	-0.027	-0.021
0.65	-0.120	-0.096	-0.086	-0.068	-0.055	-0.032	-0.015	-0.004
0.80	-0.246	-0.204	-0.188	-0.167	-0.154	-0.105	-0.076	-0.058
0.95	-0.294	-0.251	-0.214	-0.192	-0.166	-0.110	-0.088	-0.073

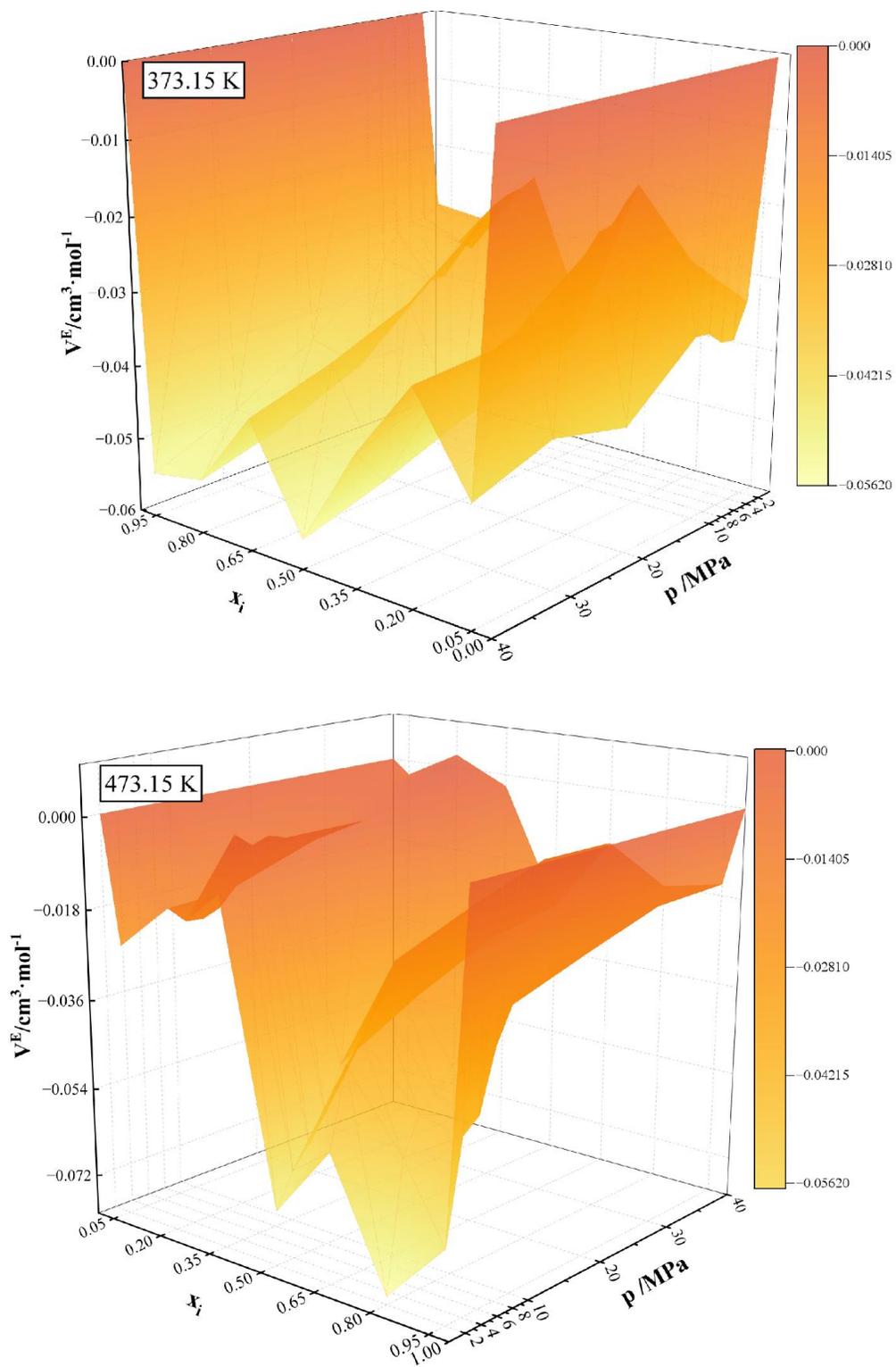
The graphics containig the excess volume for each of the three binary mixtures are shown in Figure 25, Figure 26, and Figure 27. Subsequently, the excess isothermal compressibilities for the mixtures are in Figure 28, Figure 29, and Figure 30 The excess volume expansivities are in

Figure **31**, Figure 32, and Figure 33. Finally, the excess internal pressures of the binary mixtures are in

Figure 34, Figure 35, andFigure 36.

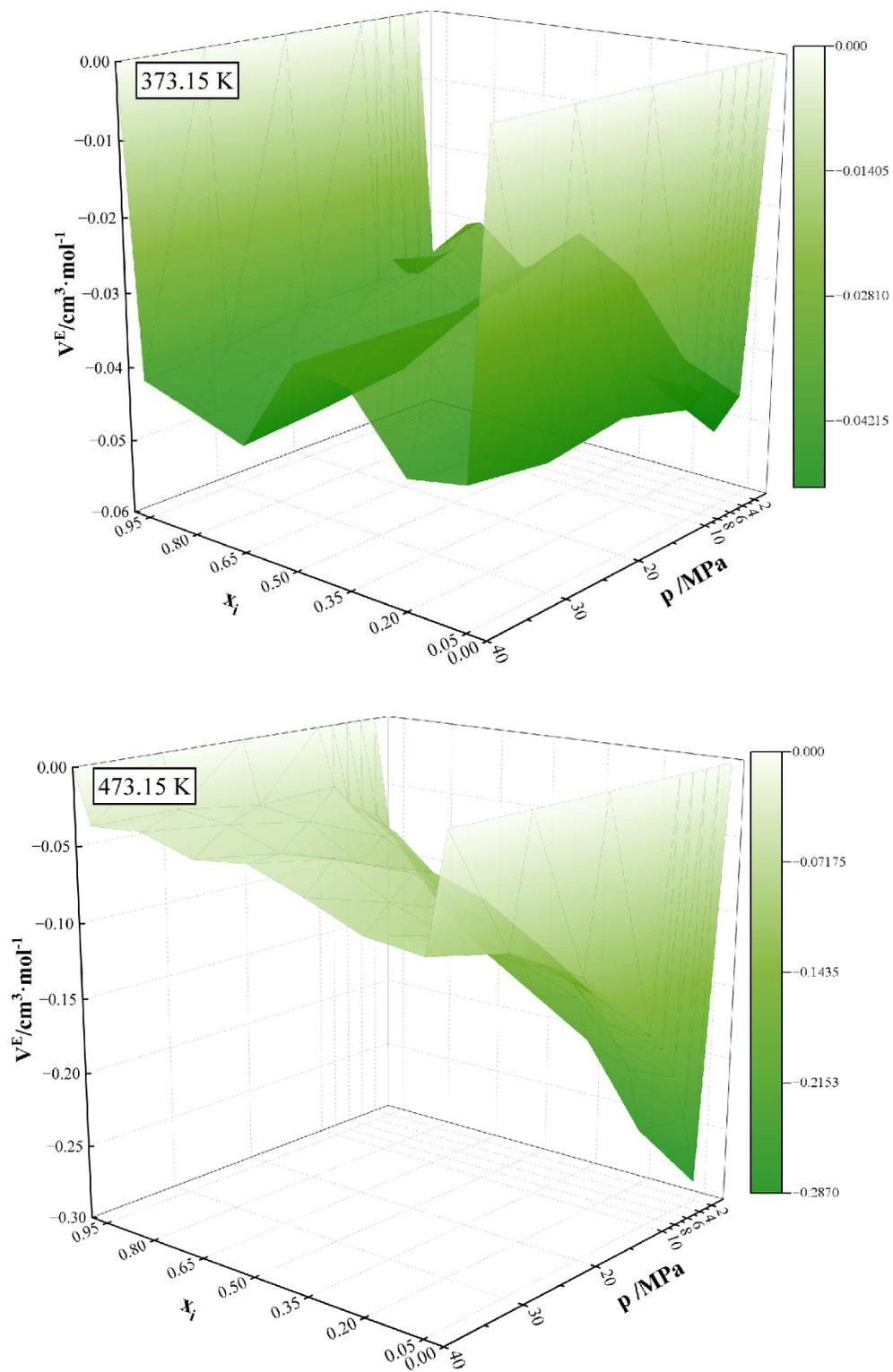
**Figure 25**

*Excess volume ( $V^E$ ) of AS as a function of temperature and pressure*



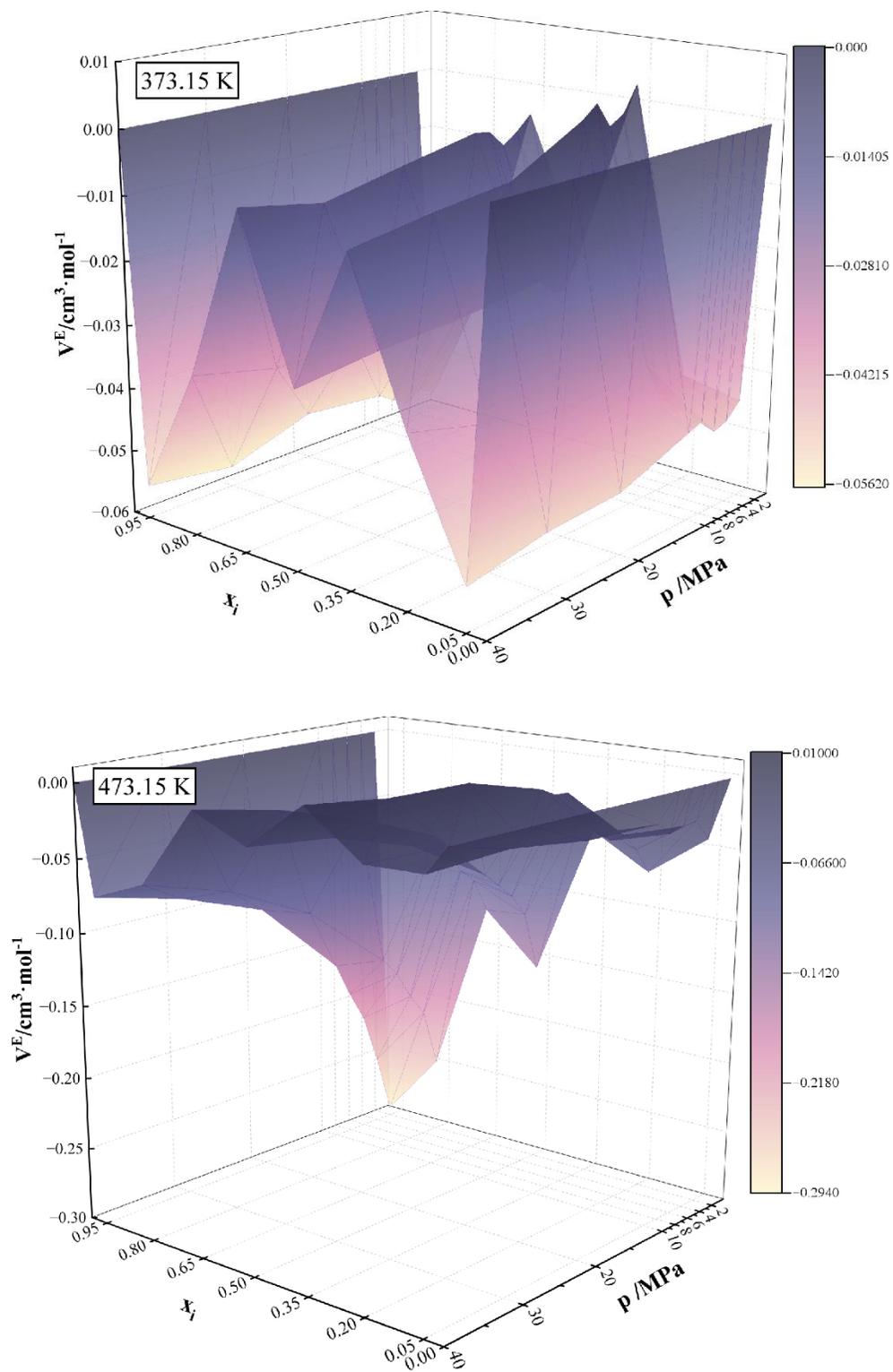
**Figure 26**

*Excess volume ( $V^E$ ) of AN as a function of temperature and pressure*



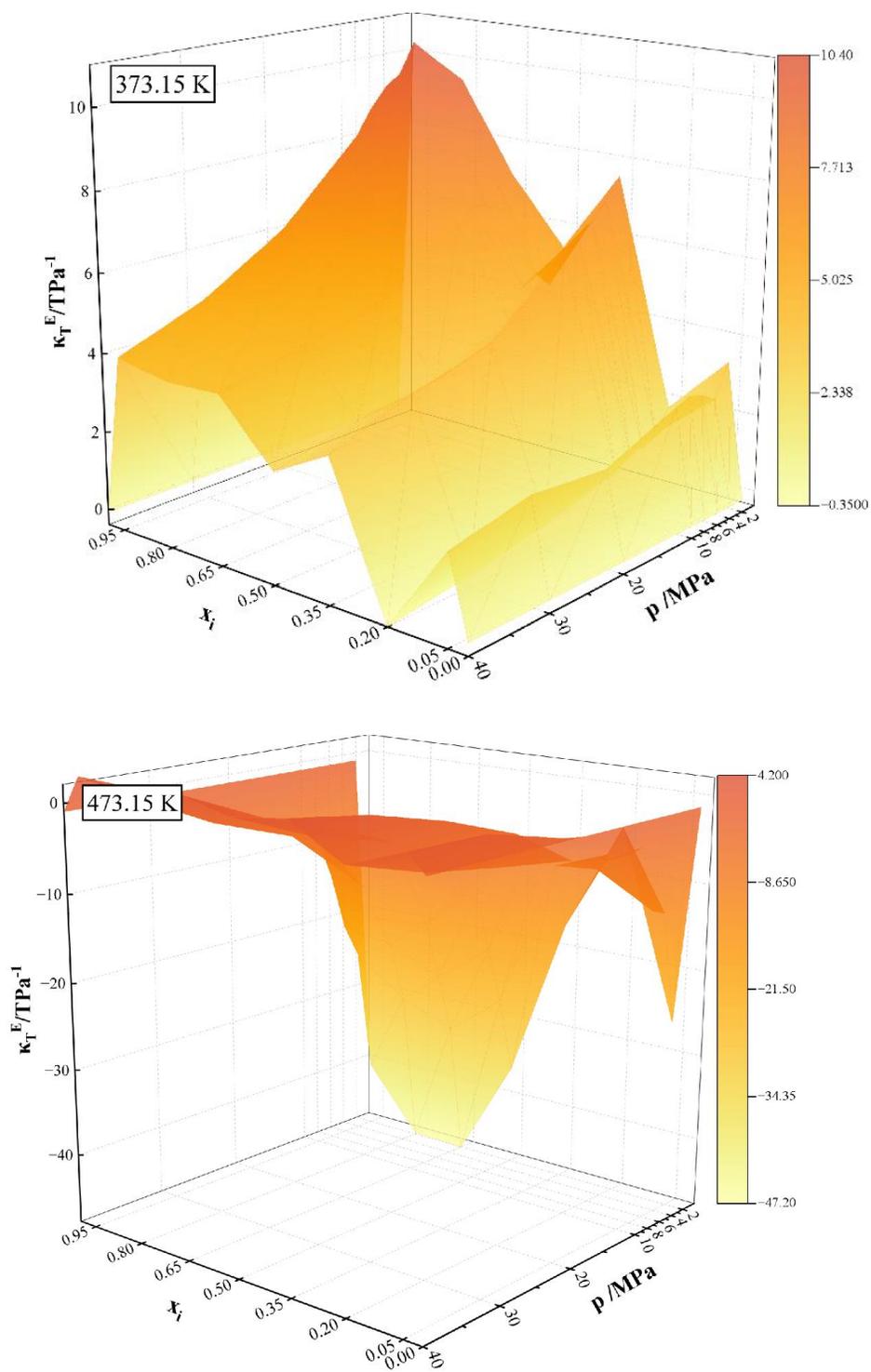
**Figure 27**

*Excess volume ( $V^E$ ) of NS as a function of temperature and pressure*



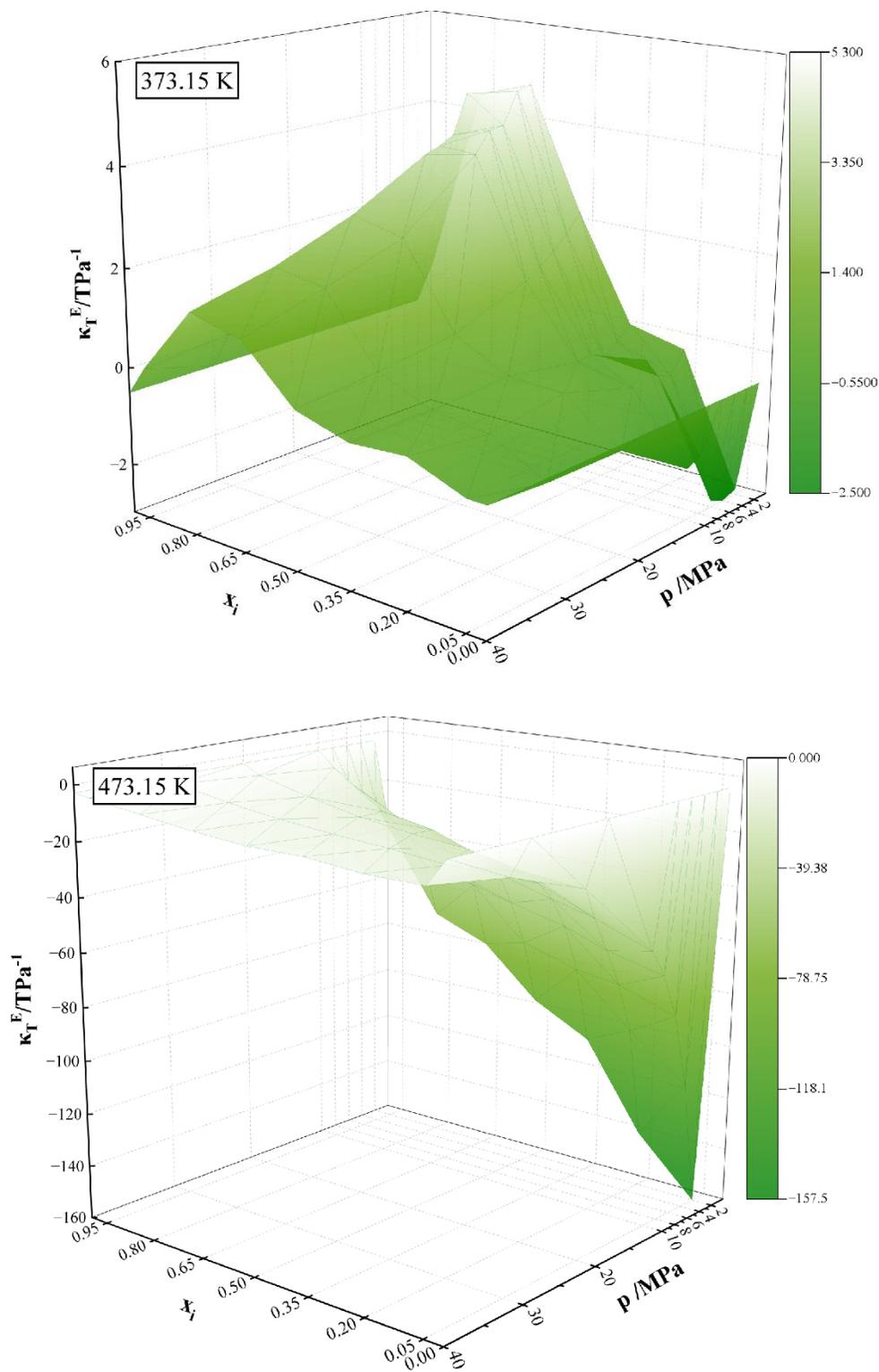
5.3.3.2. Excess Isothermal Compressibility  $\kappa_T^E$ **Figure 28**

Excess isothermal compressibility ( $\kappa_T^E$ ) of AS as a function of temperature and pressure



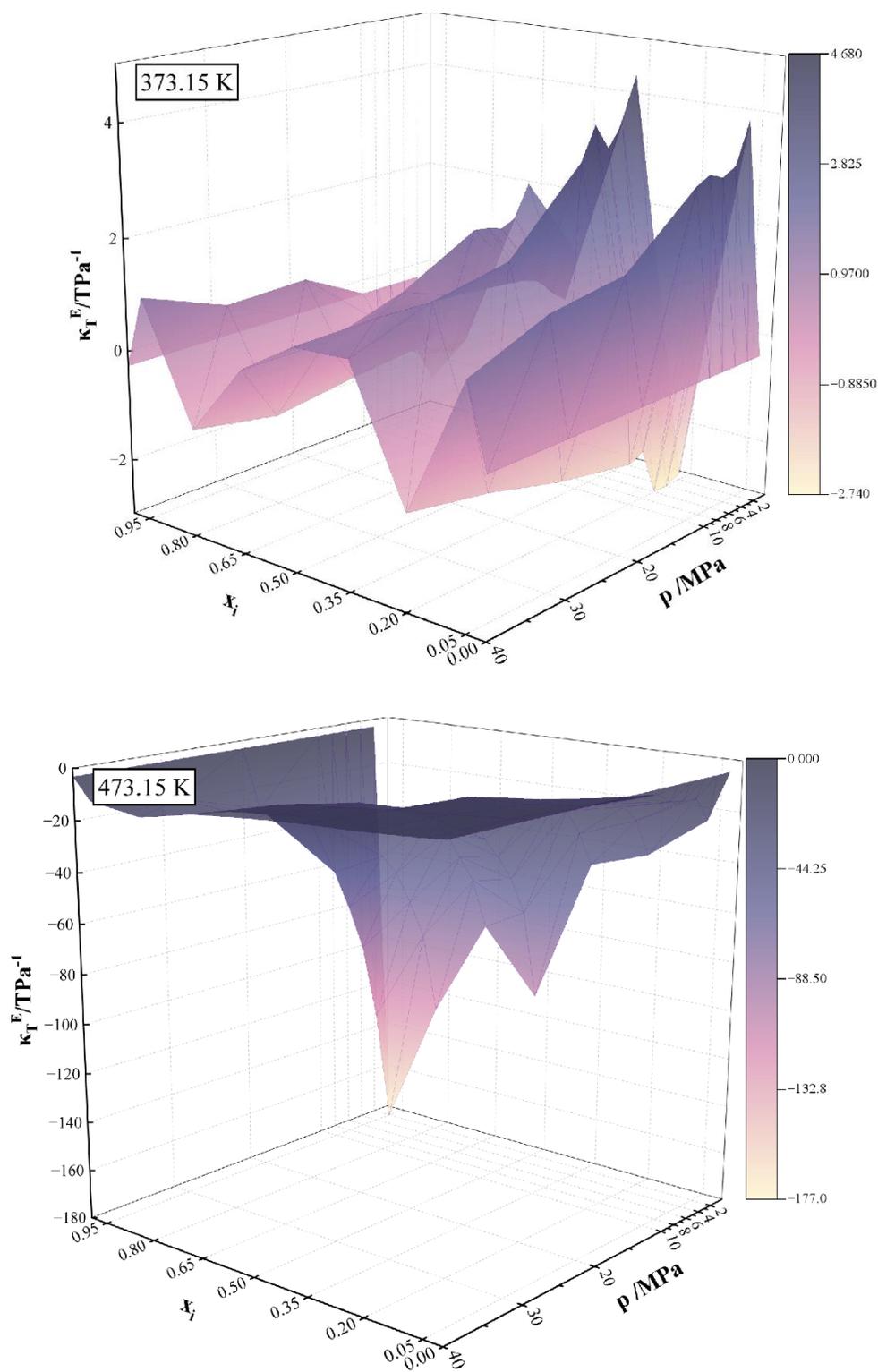
**Figure 29**

*Excess isothermal compressibility ( $\kappa_T^E$ ) of AN as a function of temperature and pressure*



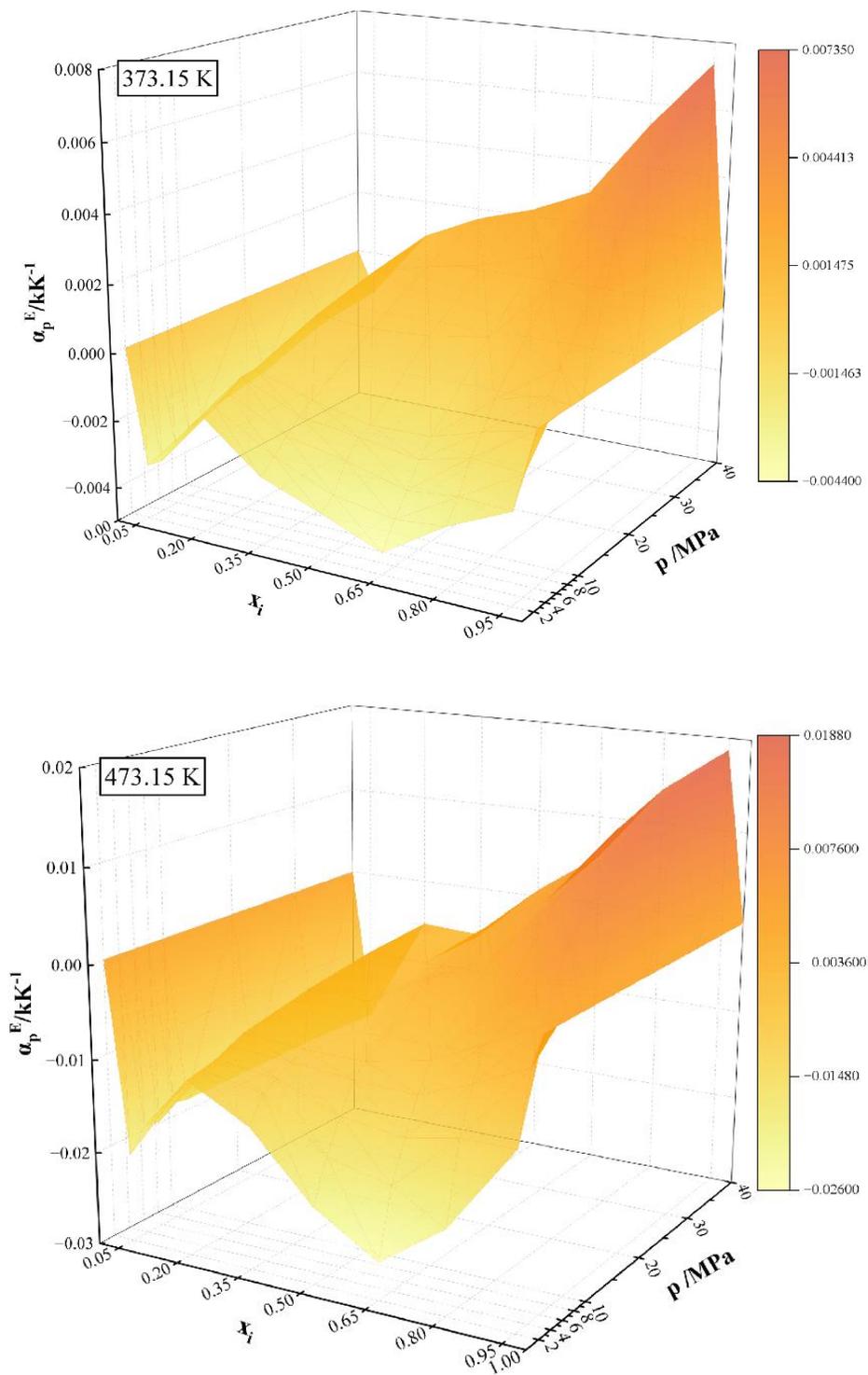
**Figure 30**

*Excess isothermal compressibility ( $\kappa_T^E$ ) of NS as a function of temperature and pressure*



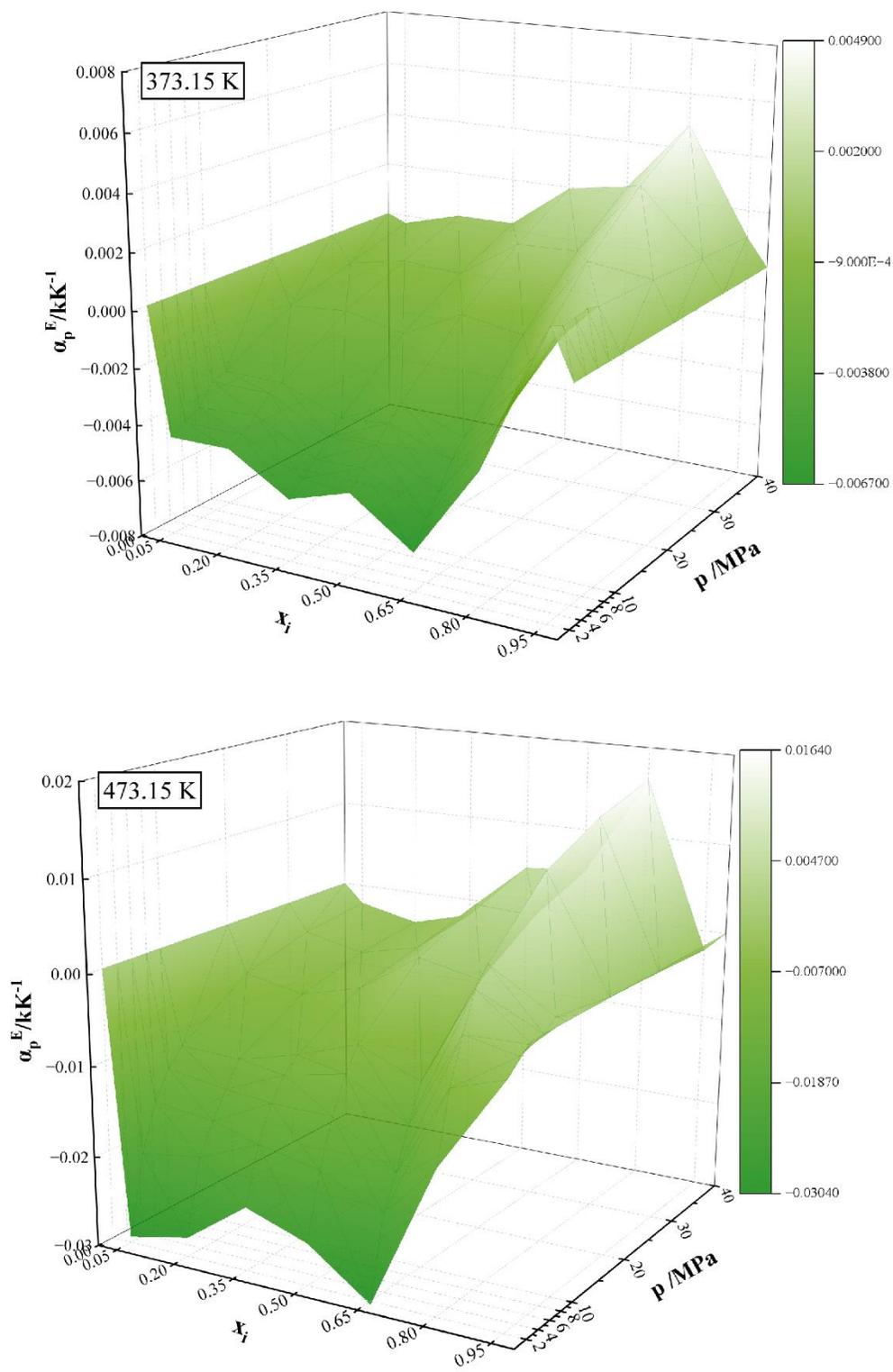
5.3.3.3. Excess Volume Expansivity  $a_p^E$ **Figure 31**

Excess volume expansivity ( $a_p^E$ ) of AS as a function of temperature and pressure



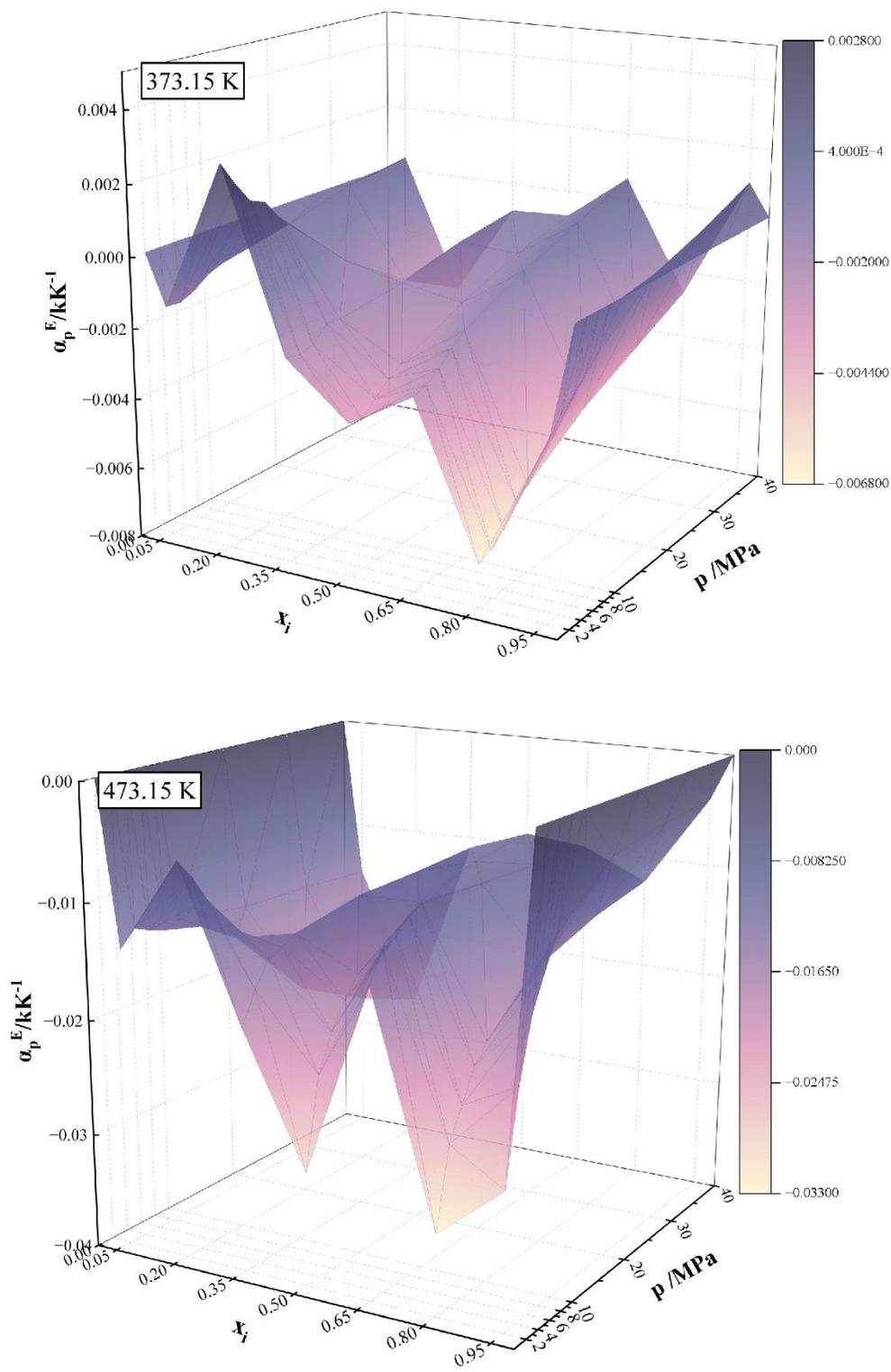
**Figure 32**

*Excess volume expansivity ( $\alpha_p^E$ ) of AN as a function of temperature and pressure*



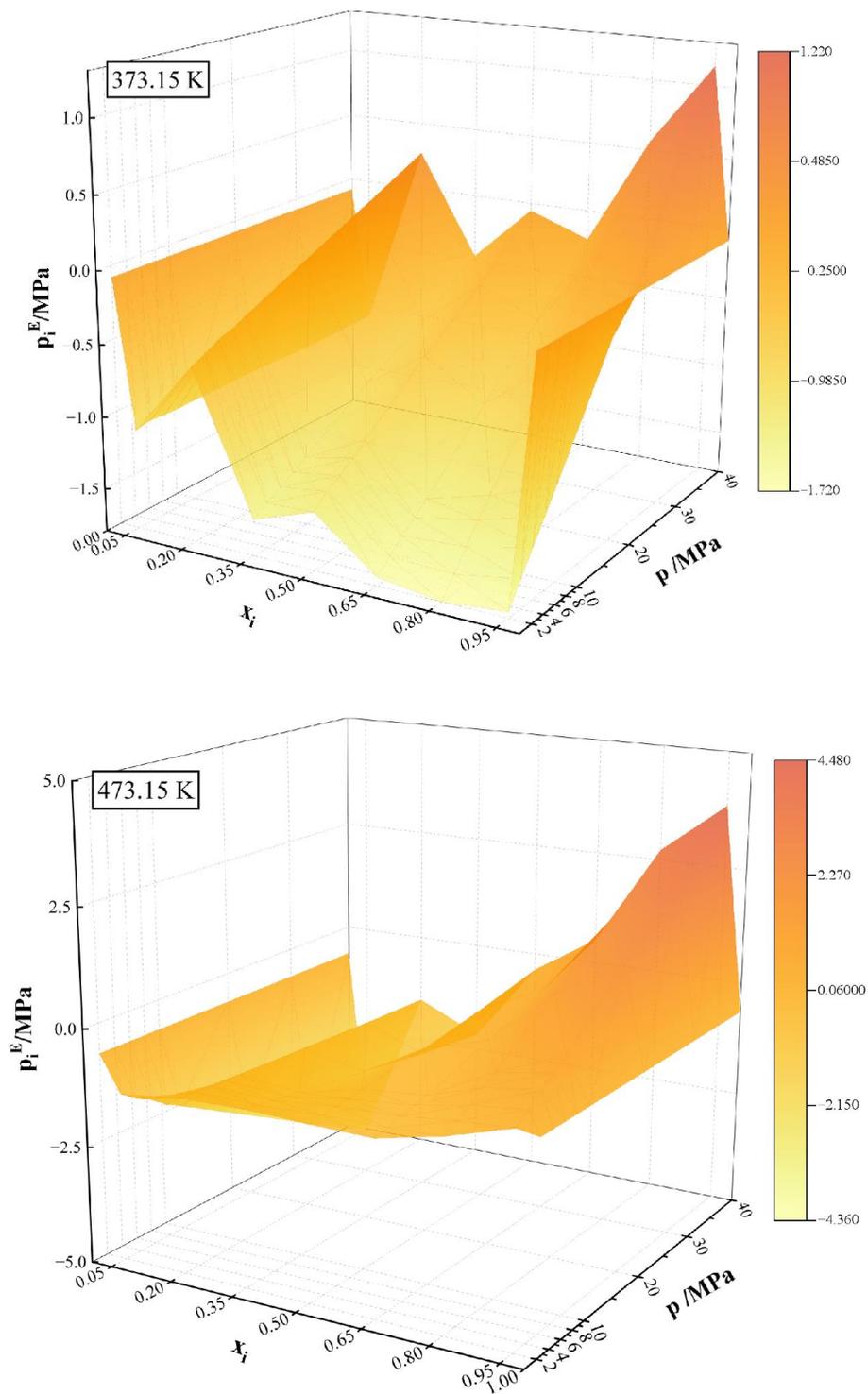
**Figure 33 .**

*Excess volume expansivity ( $\alpha_p^E$ ) of NS as a function of temperature and pressure*



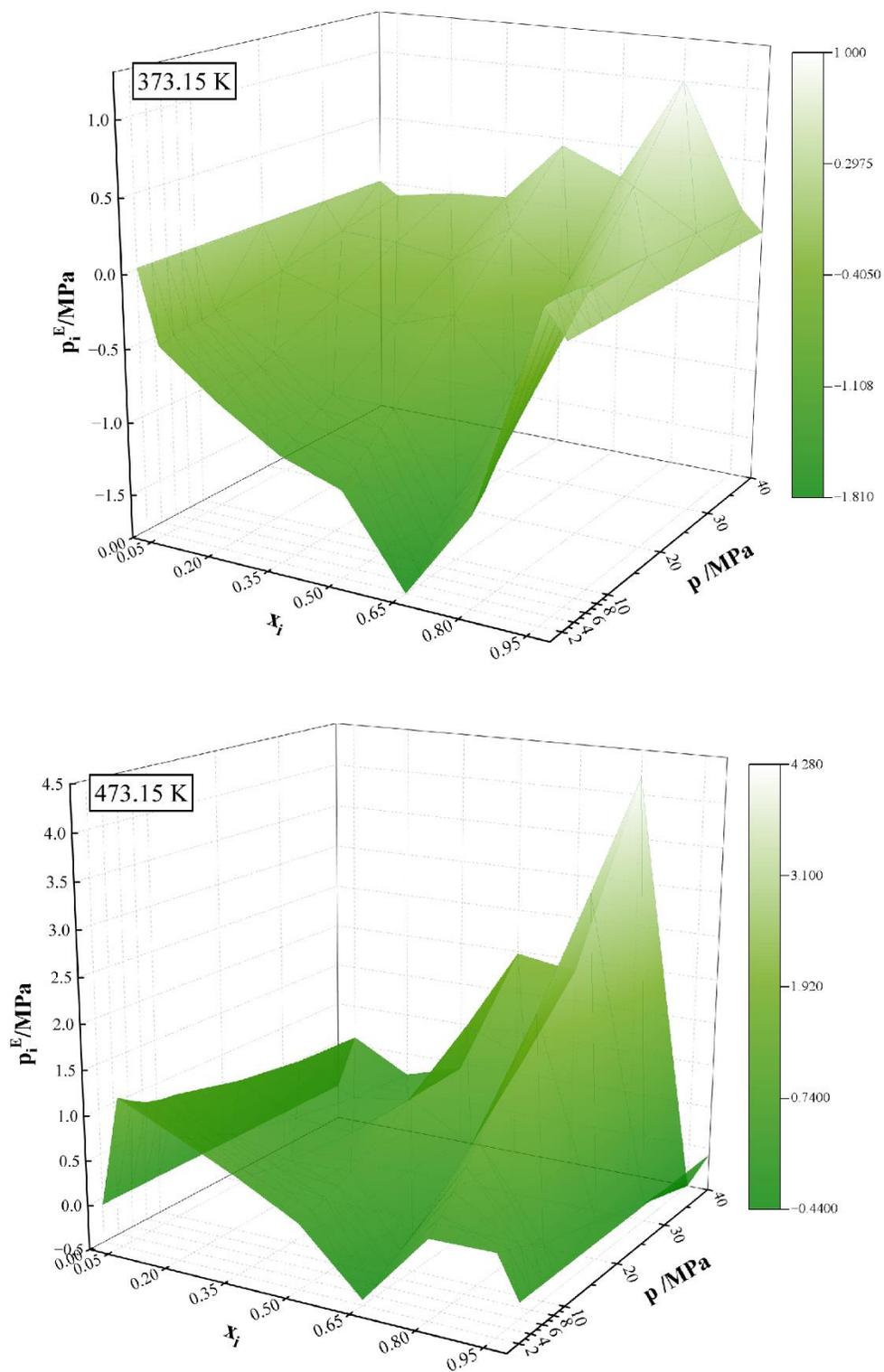
5.3.3.4. Excess Internal Pressure  $p_i^E$ **Figure 34**

Excess internal pressure ( $p_i^E$ ) of AS as a function of temperature and pressure



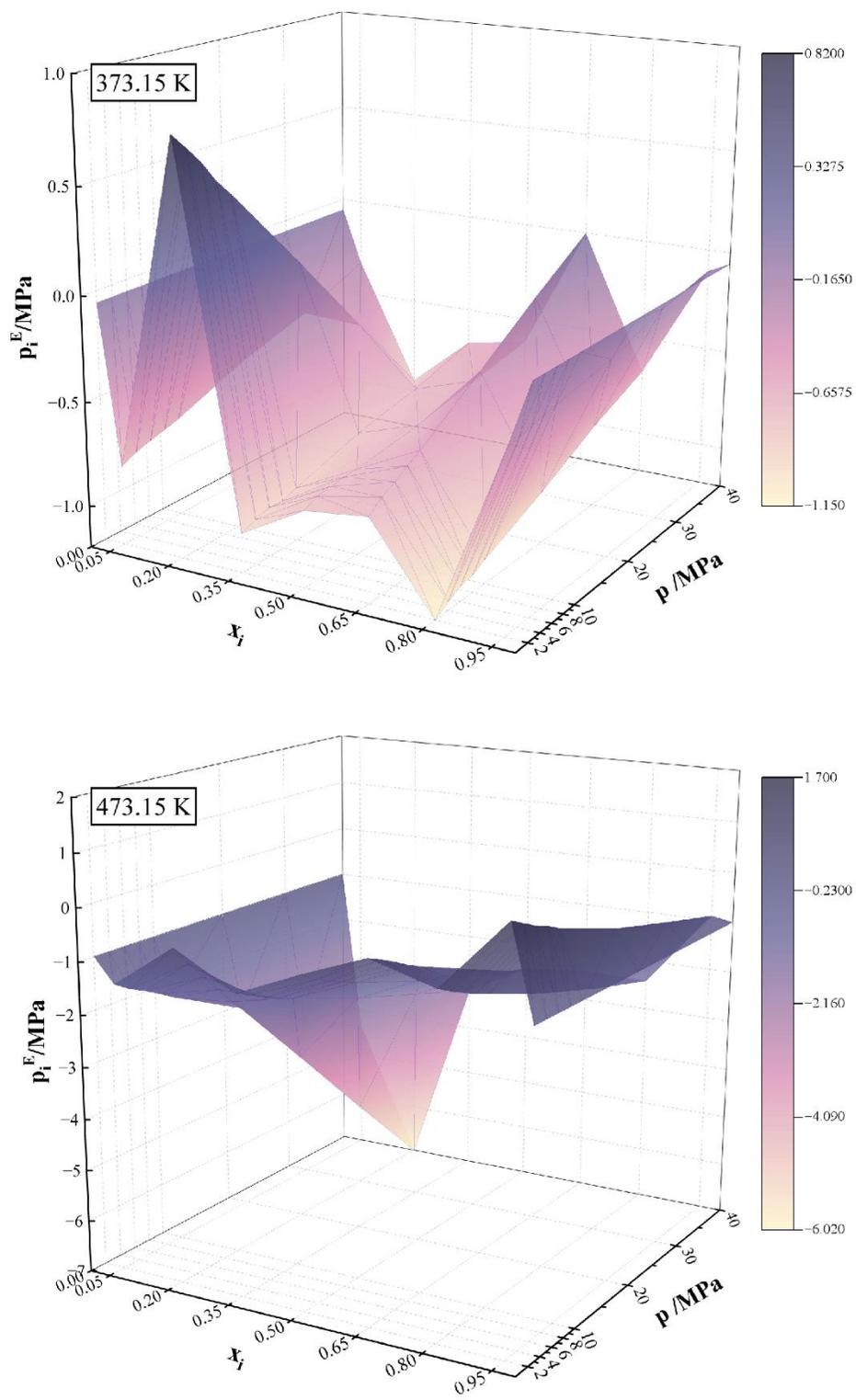
**Figure 35**

Excess internal pressure ( $p_i^E$ ) of AN as a function of temperature and pressure



**Figure 36**

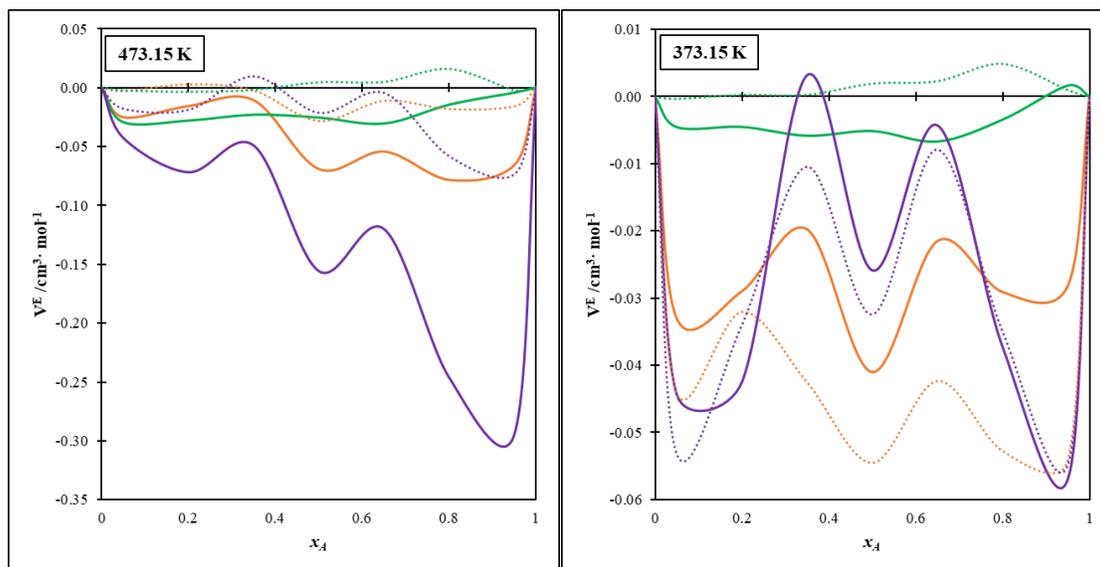
*Excess internal pressure ( $p_i^E$ ) of NS as a function of temperature and pressure*



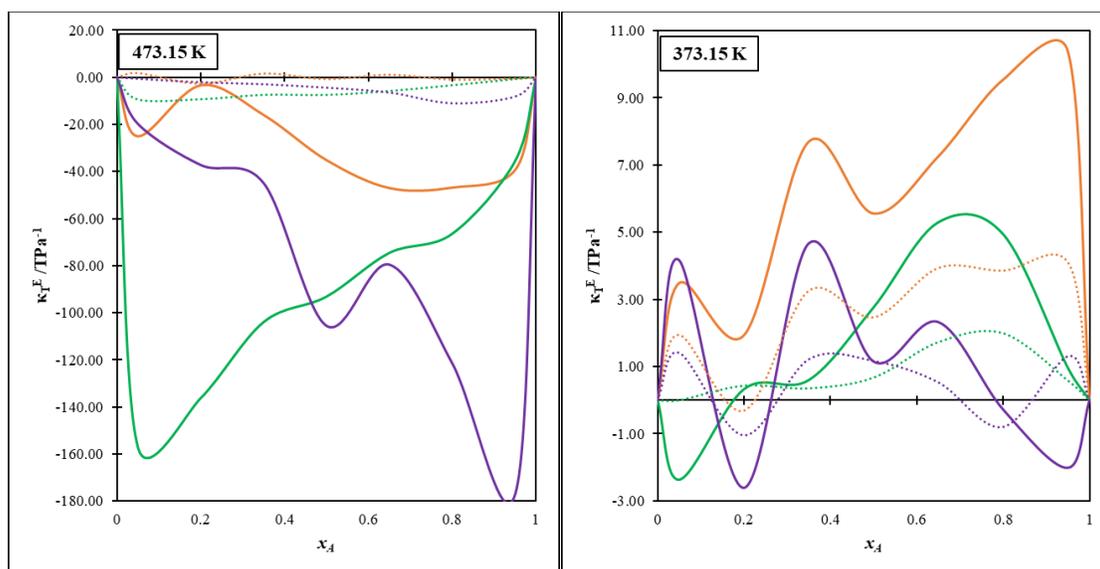
## 5.3.3.3. Comparison of binary mixtures

**Figure 37**

Excess volume ( $V^E$ ) of AS (orange), AN (green), and NS (purple) as a function of composition. (---) at 40 MPa. (—) at 2 MPa.

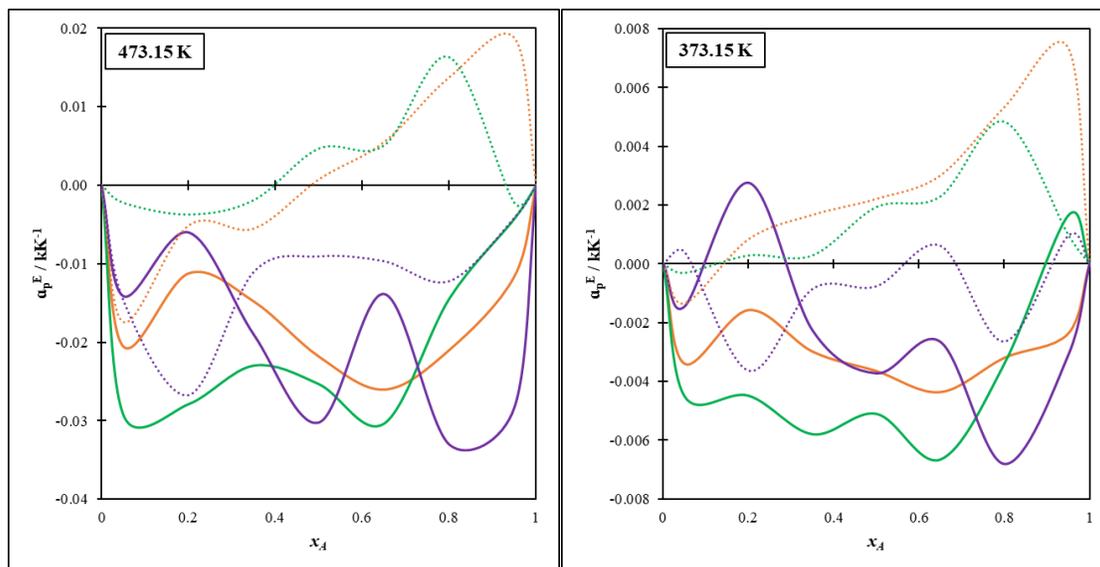
**Figure 38 .**

Excess isothermal compressibility ( $\kappa_T^E$ ) of AS (orange), AN (green), and NS (purple) as a function of composition. (---) at 40 MPa. (—) at 2 MPa

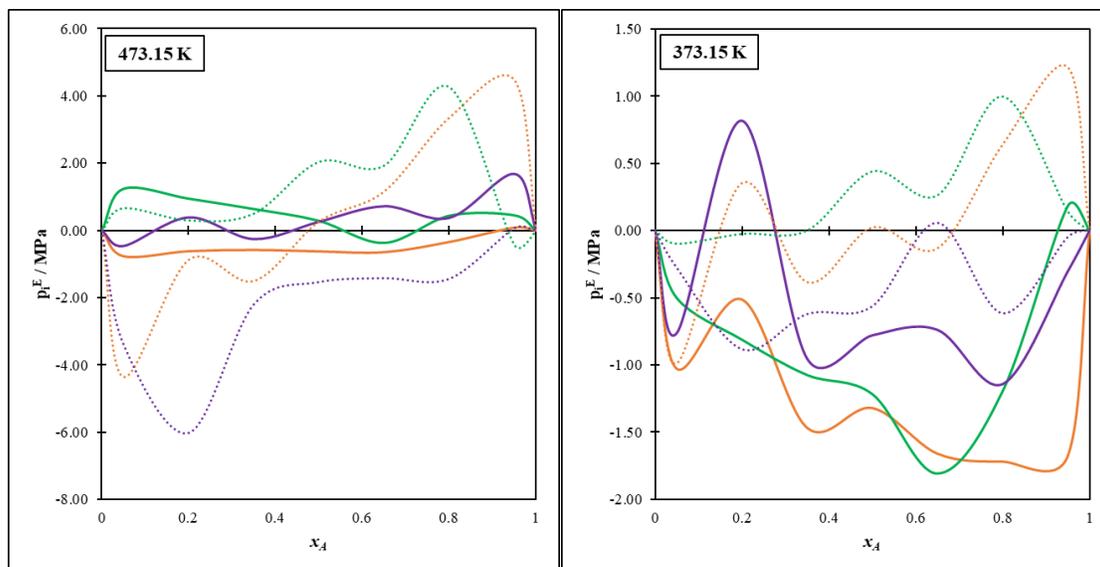


**Figure 39 .**

Excess volume expansivity ( $a_p^E$ ) of AS (orange), AN (green), and NS (purple) as a function of composition. ( - - - ) at 40 MPa. (—) at 2 MPa.

**Figure 40**

Excess internal pressure ( $p_i^E$ ) of AS (orange), AN (green), and NS (purple) as a function of composition. ( - - - ) at 40 MPa. (—) at 2 MPa.



Usually, excess properties of liquid mixtures show a monomodal symmetrical or skewed curve or with an *s* shape. However, in this work, as the mixtures are from model compounds the excess properties differ from the common shapes. It is evident the interactions between the molecules of the studied families, where all the binary mixtures have a deviation from the ideal solution.

The values of the excess volumes vary from negative to positive. Positive values indicate that the interactions between the molecules in the mixture are weaker than the interactions in pure liquids. While negative values indicate stronger interactions like dipole-dipole or hydrogen bonds between the molecules in the mixture (Khorami et al., 2017; Zeqiraj et al., 2023). In general, excess volumes became more negative with higher temperatures. The molecule's interactions increase with more kinetic energy, therefore a higher absolute excess value. Aromatic and nitrogen mixtures are the closest to the ideal behavior, hence the lesser interaction between the molecules, while Nitrogen and Sulfur mixtures have a higher absolute excess volume. This could happen because the nitrogen model contains two polar molecules that are more familiar to the polar dibenzothiophene than the less polar and non-polar aromatics.

In the same way, the other properties have positive and negative results. Excess isothermal compressibility is negative at high temperatures and positive at the lowest. On the other hand, excess volume expansivity has negative values at lower pressure while positive at 40 MPa. Finally, the excess internal pressure shows for some mixtures an *s*-like behavior.

#### **5.3.4. Redlich Kister**

For the binary mixtures, Redlich-Kister has a standard deviation of less than  $0.015 \text{ cm}^3 \cdot \text{mol}^{-1}$ . In particular the mixture between aromatics and sulfur compounds have the better fitting of the fourth degree polynomial.

**Table 29.***Redlich-Kister coefficients for AS mixture*

$i$	$a_{i0}$	$a_{i1}$	$a_{i2}$	$a_{i3}$	$\sigma$ ( $\text{cm}^3\cdot\text{mol}^{-1}$ )
0	-0.152	-0.001469	0.000246	0.000038	
1	-0.013	-0.000603	-0.000758	0.000015	
2	0.352	0.000362	-0.001287	-0.000017	0.0075
3	0.170	-0.006076	-0.005639	0.000112	
4	-1.331	-0.007614	0.004701	0.000243	

**Table 30.***Redlich-Kister coefficients for AN mixture*

$i$	$a_{i0}$	$a_{i1}$	$a_{i2}$	$a_{i3}$	$\sigma$ ( $\text{cm}^3\cdot\text{mol}^{-1}$ )
0	-0.091	-0.001300	-0.004521	0.000126	
1	-0.024	-0.000706	0.000530	-0.000006	
2	-0.016	-0.000390	-0.000091	-0.000005	0.0126
3	-0.009	0.003607	0.018839	-0.000451	
4	-0.648	-0.009350	-0.027588	0.000774	

**Table 31.***Redlich-Kister coefficients for NS mixture*

$i$	$a_{i0}$	$a_{i1}$	$a_{i2}$	$a_{i3}$	$\sigma$ ( $\text{cm}^3\cdot\text{mol}^{-1}$ )
0	-0.035	-0.001925	-0.002800	0.000113	
1	0.000	0.000958	-0.000706	0.000012	
2	0.231	0.006609	0.002090	-0.000185	0.0138
3	0.221	-0.007008	-0.025734	0.000545	
4	-1.616	-0.017444	-0.026298	0.001055	

## 6. Volume Translated Peng-Robinson (VTPR)

## 6.1 General description

Since 1873, with Van der Waals's first cubic EoS (Equations of state), scientists have continuously developed thermodynamic models that could describe every phase of fluids and mixtures in chemical processes. Although activity-coefficient models  $g^E$  have higher popularity, Equations of State have advantages in describing supercritical behavior and thermophysical properties like density, enthalpies, and heat capacities (Schmid & Gmehling, 2010).

The mixture of different compounds should include the mixing rules within the equations of state, to incorporate the influence of composition inside pressure-volume-temperature behavior. However, the first mixing rules, known as Van der Waals mixing rules, are limited to describing simple mixtures, with the same nature and non-polar compounds (Poling et al., 2001; Sandler, 2006; Schmid & Gmehling, 2010).

Therefore, to study non-ideal solutions such as organic polar mixtures,  $G^E$  mixing rules were developed. They are also known as “Excess free energy mixing rules,” these rules establish that the compositional effect is better described by excess properties, linking EoS’s fugacity coefficient with  $g^E$  model activity coefficient. Hence, these mixing rules lead to the combination of EoS and activity-coefficient models that result in a better mixture description. Overall, they are recommended for liquid mixtures of polar compounds at high-pressure conditions (Poling et al., 2001; Sandler, 2006).

In this way, Holderbaum & Gmehling, (1991) developed the Predictive- Soave-Redlich-Kwong (PSRK) as a “Group Contribution Equation of State” (GCEoS) based on Soave-Redlich-Kwong with UNIFAC. PSRK is used as a predictive thermodynamic model in process design due to its accurate estimation of Vapor-Liquid- Equilibrium (VLE). Nevertheless, it has the limitations of SRK and UNIFAC: On one hand, SRK has poor reliability of liquid density and UNIFAC’s

poor description of asymmetrical systems, infinite dilution activity coefficient, and enthalpy of mixing (Gmehling et al., 2012).

To improve the weaknesses of PSRK estimations, Ahlers & Gmehling, (2001) developed a new GCEoS, Volume translated Peng Robinson (VTPR). VTPR uses Peng Robinson as EoS and Modified (Dortmund) UNIFAC as a group contribution model. This model includes the concept of volume translation, an empirical correction that replaces the molar volume with its linear translation, to obtain a better fit of experimental data (Assael et al., 1996; Poling et al., 2001). In this case, VTPR uses Pénéoux et al., (1982) volume translation, proposed to improve non-polar description of SRK. This modification is represented by the  $c$  parameter, dependent on composition and fluid properties. Therefore, the VTPR equation is:

$$P = \frac{RT}{(V + c - b)} - \frac{a(T)}{(V + c) \cdot (V + c + b) + b \cdot (V + c - b)} \quad (22)$$

Where the  $c$  parameter is established by equation (23), in which  $c_i$  could be estimated with the experimental data with equation (24) or with the critical properties in equation (25).

$$c = \sum_i x_i c_i \quad (23) \quad c_i = V_{PR,i} - V_{exp,i} (a T_{r,i} = 0.7) \quad (24)$$

$$c_i = -0.252 \frac{R \cdot T_c}{P_c} (1.5448 Z_c - 0.4024) \quad (25)$$

Then, to establish the attraction parameter  $a(T)$ , Chen et al., (2002)  $G^E$  mixing rules are used with the equation:

$$a(T) = b \left( \sum_i x_i \frac{a_{ii}(T)}{b_{ii}} + \frac{g^{E,R}}{-0.53087} \right) \quad (26)$$

The molecule attraction parameter  $a_{ii}(T)$  and the covolume parameter  $b_{ii}$  are dependent on the critical properties of the compounds with the original Peng Robinson equations:

$$\alpha_{ii}(T) = 0.45724 \frac{R^2 T_{c,i}^2}{P_{c,i}} * \alpha_i(T) \quad (27)$$

$$b_{ii} = 0.0778 \frac{RT_{c,i}}{P_{c,i}} \quad (28)$$

On the other hand, the original attraction parameter  $\alpha_i(T)$  is replaced with the function by Twu et al., (1995):

$$\alpha_i(T) = T_{r,i}^{N_i(M_i-1)} e^{[L_i*(1-T_{r,i}^{N_i M_i})]} \quad (29)$$

The parameters  $L_i$ ,  $M_i$ , and  $N_i$  are usually estimated from the adjustment with pure component vapor pressures or liquid heat capacities at low temperatures (Schmid et al., 2014). Recently, an investigation of these parameters for pure compounds proposed correlations based on the experimental acentric factor  $\omega$  (Piña-Martinez et al., 2022).

Moreover, with the quadratic mixing rule, which allows a better description of asymmetric systems, the  $b$  parameter is estimated with:

$$b = \sum_i \sum_j x_i x_j b_{ij} \quad (30) \quad b_{ij}^{3/4} = \frac{(b_{ii}^{3/4} + b_{jj}^{3/4})}{2} \quad (31)$$

Furthermore, to determine the residual part of excess Gibbs free energy  $g^{E,R}$  it is necessary to estimate the residual activity coefficient  $\ln \gamma_i^R$  with modified UNIFAC:

$$g^{E,R} = RT \sum_i x_i \ln \gamma_i^R \quad (32)$$

Modified UNIFAC is based on classic UNIFAC. UNIFAC is a group contribution method that predicts activity coefficients from its molecules' functional groups. The characteristic data of every part of the molecules are estimated using experimental data and can be found in the literature. Overall, the activity coefficient for the substance  $i$   $\ln \gamma_i$  is analyzed in two parts: the first one is the

combinatorial  $\ln\gamma_i^C$ , it represents the contributions of the difference in molecular size. The second is the residual part  $\ln\gamma_i^R$  which focuses on the molecular interactions (Poling et al., 2001; Sandler, 2006).

$$\ln\gamma_i = \ln\gamma_i^C + \ln\gamma_i^R \quad (33)$$

To solve the equation of state, we only need the residual component and its equations. Inside this model,  $i$  and  $j$  are going to represent the substances, while  $k$  represents the functional group.

In particular, the residual component has two terms:  $\ln\Gamma_k$  represents the effect of the interaction between compounds, on the other hand, the contribution of the interaction inside each molecule is given by  $\ln\Gamma_k^{(i)}$ .

$$\ln\gamma_i^R = \sum_k v_k^{(i)} (\ln\Gamma_k - \ln\Gamma_k^{(i)}) \quad (34)$$

$v_k^{(i)}$  is the quantity of the  $k$  functional group inside the substance  $i$ . Furthermore, the activity coefficient of each functional group can be estimated with the equation:

$$\ln\Gamma_k = Q_k \left\{ 1 - \ln \left( \sum_m \theta_m \psi_{mk} \right) - \sum_m \frac{\theta_m \psi_{km}}{\sum_n \theta_n \psi_{nm}} \right\} \quad (35)$$

The last equation has the term  $\psi_{mk}$ , which represents the contributions of the interactions between functional groups.

$$\theta_m = \frac{Q_m X_m}{\sum_n Q_n X_n} \quad (36) \quad X_m = \frac{\sum_j v_n^{(j)} x_j}{\sum_j \sum_n v_n^{(j)} x_j} \quad (37) \quad \psi_{nm} = e^{-\frac{a_{nm}}{T}} \quad (38)$$

Afterward, the development of Modified UNIFAC (Dortmund) improved UNIFAC's estimations. Mod. UNIFAC implements additional groups, different values of  $Q_k$  and  $R_k$ , and a

better prediction of asymmetric systems behavior. It uses a temperature-dependent interaction group parameter  $\Psi_{nm}$  that allows a better description of the molecules (Guerrero-Amaya, 2012).

$$\Psi_{nm} = e^{-\frac{a_{nm}+b_{nm}T+c_{nm}T^2}{T}} \quad (39)$$

VTPR model is also known for improving the result of liquid densities, prediction of VLE for symmetric and asymmetric systems, and Solid-Liquid equilibrium for alkanes, esters, and aromatics. In addition, it can be applied to find azeotropic points, the design of separation columns, solvent selection, flash point prediction, and many others (Schmid & Gmehling, 2010). Although the database of the parameters is often updated, this model has the disadvantage of using literature-based parameters that could leave some molecules behind.

Cubic equations of state are the first option in the oil and gas industry. Especially, SRK and the PR EoS are the to-go choice modeling processes at high-pressure conditions. Nevertheless, petroleum fluids contain numerous compounds in which the EoS must involve the interactions of the molecules. Therefore, it is recommended to use predictive cubic EoS, like PPR78, PSRK, or VTPR, to simulate the phase behavior of crude oils and natural gases (Privat & Jaubert, 2012). There are different investigations with similar thermodynamic models with good results in the oil and gas industry. Nourozieh et al., (2015) used P eneloux volume translation in PR, with Van der Waals mixing rules, and they obtained a deviation of 3.2 kg·m<sup>-3</sup> in mixtures of Athabasca bitumen/propane from in situ upgrading EOR. On the other hand, with experiments of cyclohexane with a U-tube densimeter between 318.15-413.15 K and up to 62 MPa, Amorim et al., (2007b) got an improvement with a volume translation of PR with an RMSD of 0.6 kg·m<sup>-3</sup>, while Peng Robinson estimated the data with an RMSD of 47.3 kg·m<sup>-3</sup>

## 6.2. Experimental

To evaluate VTPR's predictions in the molecules and mixtures from this work, seven systems were selected.

**Table 32.**

Systems for VTPR prediction

Model dissolution	Model molecules composition (%w/w)
<b>Aromatics (A)</b>	Phenanthrene PHE (2 %), 2,6- Diethylnaphthalene DEN (1 %)
<b>Nitrogen compounds (N)</b>	Quinoline QUI (0.5 %), 9- Ethyl carbazole EC (0.5 %)
<b>Sulfur compounds (S)</b>	Dibenzothiophene DBT (3.7 %)
<b>Aromatics + Sulfur (AS)</b>	$X_A=0.5$
<b>Aromatics + Nitrogen (AN)</b>	$X_A=0.5$
<b>Nitrogen + Sulfur (NS)</b>	$X_N=0.5$
<b>Aromatics + Nitrogen+ Sulfur (ANS)</b>	$X_A=0.375$ $X_N=0.250$

For each system the parameters  $b$  and  $c$  are estimated, while for  $a(T)$  the temperature dependence must be considered.

### 6.2.1. Attraction parameter $a(T)$

Although, the literature has the critical properties of a significant number of compounds (Poling et al., 2001), for uncommon molecules, like 9-Ethylcarbazole and 2,6-Diethylnaphthalene, the only way to use these properties is with an estimation. One of the most famous estimation methods is Joback, Marrero-Morejon & Pardillo-Fontdevilá (1999) use Joback as a Group Contribution (GC) estimation and proposed an improvement of this method with a Group Interaction Contribution GIC. GIC allows us to consider the interactions of the groups inside the molecule. The next table contains the literature critical properties and the estimation

with GC and GIC. Then, Table 34 shows the equation used in these methods and their corresponding parameters.

**Table 33.**

*Critical properties of the molecules*

	DBT	CHX	PHE	DEN	QUI	EC
$T_c$ [K]	897.0 <sup>a</sup>	553.5 <sup>a</sup>	869.0 <sup>a</sup>	796.0 <sup>b</sup>	782.0 <sup>a</sup>	929.8 <sup>b</sup>
$P_c$ [MPa]	3.86 <sup>a</sup>	4.07 <sup>a</sup>	2.87 <sup>a</sup>	2.52 <sup>c</sup>	4.50 <sup>a</sup>	2.6986 <sup>c</sup>
$V_c$ [cm <sup>3</sup> /mol]	515.6 <sup>a</sup>	308.0 <sup>a</sup>	554.0 <sup>a</sup>	636.9 <sup>c</sup>	402.0 <sup>a</sup>	637.7 <sup>c</sup>
$z_c$	0.267	0.273	0.220	0.243	0.278	0.223
$M$ [g/mol]	184.26	84.16	178.23	184.28	129.16	195.25

Notes. *a.*Data taken from (Poling et al., 2001) *b.* GIC and *c.* GC estimated from (Marrero-Morejon & Pardillo-Fontdevilá, 1999)

**Table 34.**

*GC and GIC equations and parameters*

Property	Unit	Equation	GC		GIC	
			<i>a</i>	<i>b</i>	<i>a</i>	<i>b</i>
Normal boiling point	K	$T_b = M^a \Sigma + b$	-0.366	149.84	-0.404	156
Critical temperature	K	$T_c = Tb / (a + b \Sigma - \Sigma^2)$	0.5881	-0.9305	0.5851	-0.9286
Critical pressure	bar	$P_c = [a + b \cdot n_A \Sigma - \Sigma]^2$	0.1218	0.4609	0.1285	-0.0059
Critical volume	cm <sup>3</sup> mol <sup>-1</sup>	$V_c = a + \Sigma$	26.3	-	25.1	-

Notes. Equations and data taken from (Marrero-Morejon & Pardillo-Fontdevilá, 1999) where  $\Sigma$  is the sum of the products each simple group (or interaction) appears in the molecule and contributions,  $M$  is molecular weight and  $n_A$  is the total number of atoms in the molecule.

To continue with equation (27), the alpha parameter must be estimated. If we look into equation (29) we need parameters L, M, and N for each molecule. These values could be estimated

with the vapor pressure; however, Twu has been studied since the 90's. Bell et al., (2018) estimated the parameters for 2500 molecules.

**Table 35.**

*Parameters for Twu's attraction parameter*

	L	M	N
DBT	0.5540	0.8215	1.4120
CHX	0.5906	0.8165	0.9814
PHE	0.4960	0.8306	1.6367
DEN	0.4643	0.8527	2.1161
QUI	0.7262	0.8379	1.0649
EC	2.1715	0.9984	0.4152

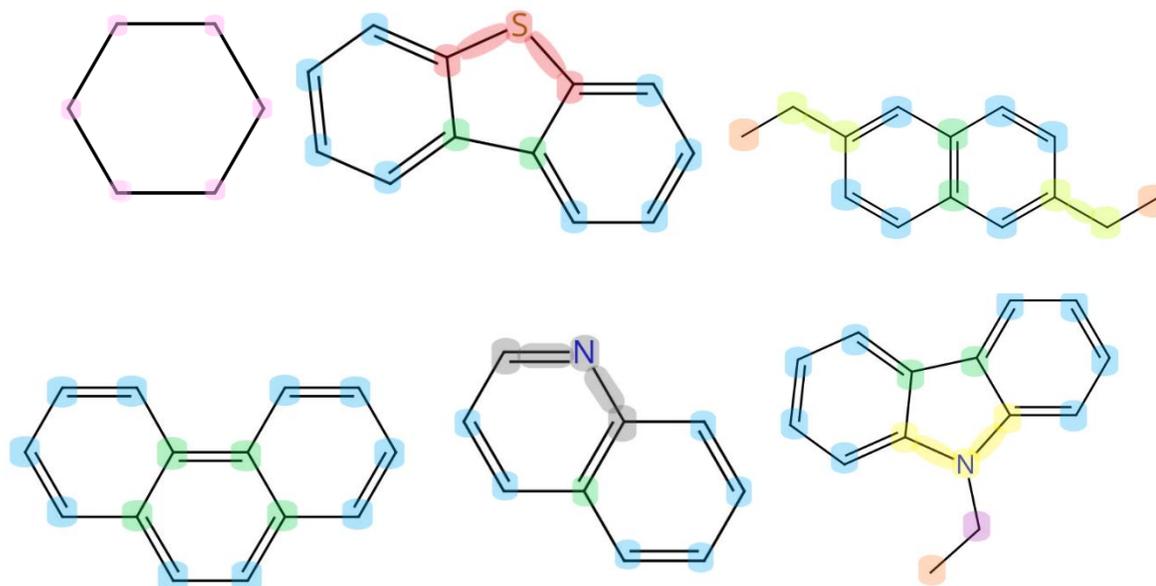
### 6.2.2. Mod. UNIFAC

First, to use mod. UNIFAC we must split up the six molecules into groups and subgroups and look for interaction values in the Dortmund database (DDBST, n.d.) The next table and subsequent figure show each subgroup and group that contains the molecules.

**Table 36.**

*Functional groups and  $Q_k$  values*

Group	Subgroup	CHX	DBT	PHE	DEN	QUI	EC	$Q_k$
CH <sub>2</sub>	CH <sub>3</sub>	-	-	-	2	-	1	1.0608
	CH <sub>2</sub>	-	-	-	-	-	1	0.7081
ACH	ACH	-	8	10	6	6	8	0.4321
	AC	-	2	4	2	1	2	0.2113
ACCH <sub>2</sub>	ACCH <sub>2</sub>	-	-	-	2	-	-	0.7962
Pyridine	AC <sub>2</sub> HN	-	-	-	-	1	-	0.6330
	AC <sub>2</sub> N	-	-	-	-	-	1	0.3530
Cy-CH <sub>2</sub>	Cy-CH <sub>2</sub>	6	-	-	-	-	-	0.8635
ACS	AC <sub>2</sub> S	-	1	-	-	-	-	0.7800

**Figure 41***Mod. UNIFAC functional groups*

Furthermore, for the estimation of the interaction parameter, the values of  $a_{ij}$ ,  $b_{ij}$  and  $c_{ij}$  are used with equation (39). These values are shown in tables **Table 37**, **Table 38**, and **Table 39**.

**Table 37** *$a_{ij}$  group interaction parameter*

$a_{ij}$	CH <sub>3</sub>	CH <sub>2</sub>	ACH	AC	ACCH <sub>2</sub>	AC <sub>2</sub> HN	AC <sub>2</sub> N	Cy-CH <sub>2</sub>	AC <sub>2</sub> S
CH <sub>3</sub>	-	-	114.2	114.2	7.339	1802.3	1802.3	-117.1	24.432
CH <sub>2</sub>	-	-	114.2	114.2	7.339	1802.3	1802.3	-117.1	24.432
ACH	16.07	16.07	-	-	139.2	-1553.9	-1553.9	134.6	1412
AC	16.07	16.07	-	-	139.2	-1553.9	-1553.9	134.6	1412
ACCH <sub>2</sub>	47.2	47.2	-45.33	-45.33	-	135.3	135.3	-107.1	1000.8
AC <sub>2</sub> HN	-436.15	-436.15	1810.8	1810.8	1698.1	-	-	268.23	-674
AC <sub>2</sub> N	-436.15	-436.15	1810.8	1810.8	1698.1	-	-	268.23	-674
Cy-CH <sub>2</sub>	170.9	170.9	-2.619	-2.619	191.5	-5894.1	-5894.1	-	313.43
AC <sub>2</sub> S	-16.034	-16.034	-660.25	-660.25	-139.78	4998.6	4998.6	-30.564	-

**Table 38.***b<sub>ij</sub> group interaction parameter*

<i>b<sub>ij</sub></i>	CH <sub>3</sub>	CH <sub>2</sub>	ACH	AC	ACCH <sub>2</sub>	AC <sub>2</sub> HN	AC <sub>2</sub> N	Cy-CH <sub>2</sub>	AC <sub>2</sub> S
CH <sub>3</sub>	-	-	0.0933	0.0933	-0.4538	-17.171	-17.171	0.5481	0.2915
CH <sub>2</sub>	-	-	0.0933	0.0933	-0.4538	-17.171	-17.171	0.5481	0.2915
ACH	-0.2998	-0.2998	-	-	-0.65	0.1615	0.1615	-1.231	-3.9917
AC	-0.2998	-0.2998	-	-	-0.65	0.1615	0.1615	-1.231	-3.9917
ACCH <sub>2</sub>	0.3575	0.3575	0.4223	0.4223	-	-2.369	-2.369	0.2564	-2.5149
AC <sub>2</sub> HN	3.4225	3.4225	-5.7594	-5.7594	-9.8887	-	-	-1.4137	1.8854
AC <sub>2</sub> N	3.4225	3.4225	-5.7594	-5.7594	-9.8887	-	-	-1.4137	1.8854
Cy-CH <sub>2</sub>	-0.8062	-0.8062	1.094	1.094	-0.5561	13.088	13.088	-	0.0911
AC <sub>2</sub> S	-0.5337	-0.5337	1.4602	1.4602	0.1146	1.1962	1.1962	-0.2455	-

**Table 39.***c<sub>ij</sub> group interaction parameter*

<i>c<sub>ij</sub></i>	CH <sub>3</sub>	CH <sub>2</sub>	ACH	AC	ACCH <sub>2</sub>	AC <sub>2</sub> HN	AC <sub>2</sub> N	Cy-CH <sub>2</sub>	AC <sub>2</sub> S
CH <sub>3</sub>	-	-	-	-	-	0.036	0.036	-0.00098	-
CH <sub>2</sub>	-	-	-	-	-	0.036	0.036	-0.00098	-
ACH	-	-	-	-	-	0.0082	0.0082	0.00149	-
AC	-	-	-	-	-	0.0082	0.0082	0.00149	-
ACCH <sub>2</sub>	-	-	-	-	-	0.0039	0.0039	-	-
AC <sub>2</sub> HN	-0.0087	-0.0087	0.0023	0.0023	0.0153	-	-	-	-
AC <sub>2</sub> N	-0.0087	-0.0087	0.0023	0.0023	0.0153	-	-	-	-
Cy-CH <sub>2</sub>	0.00129	0.00129	-0.00156	-0.00156	0	-	-	-	-
AC <sub>2</sub> S	-	-	-	-	-	-	-	-	-

**6.2.3. Covolume parameter *b***

To estimate this parameter for each system, the equations (28), (30), and (31) were used with the critical properties given by Table 33.

#### **6.2.4. Volume translation parameter $c$**

In this work, the translation parameter is calculated with two methods. In this way, we can compare the results of the estimation using only the critical properties (equation (24)) or the estimation with the measured data.

Finally, to evaluate the accuracy of the model estimation compared with the experimental data, the absolute average deviation is used.

### **6.3. Results**

Table 40 contains the results of the parameters  $b$  and  $c$  with the two equations mentioned to calculate  $c$  and its deviation from the experimental data. In general, the estimation of  $c$  with the equation improves the similarities with the experimental data for all the systems. Overall, the estimations are under a 2% AAD deviation from the data, nevertheless, the equation brings that value down to less than 1%. The VTPR prediction is shown in the figures below.

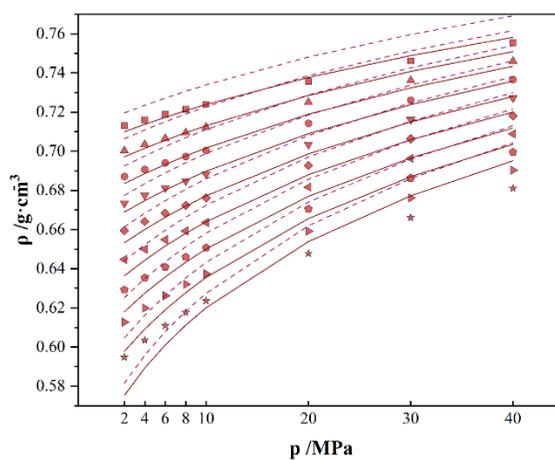
In the results of the systems, VTPR shows a better fitting at lower temperatures and lower pressures, with a better accuracy between 2-10 MPa. In particular, temperature-independent volume translations, like Penéloux, have good liquid density predictions at low reduced temperatures. Despite this, density could be overestimated with reduced temperatures higher than 0.7 and some authors use temperature-dependent volume translation (Abudour et al., 2012). However, until now those parameters have led to a negative isochoric heat capacity. In this way, it is recommended temperature-independent covolume and volume translation parameters to maintain the consistency of the estimations (Privat & Jaubert, 2023).

**Table 40.** *VTPR results**VTPR results*

Sample	<i>b</i>	With critical properties		With experimental data	
		<i>c</i>	AAD (%)	<i>c</i>	AAD (%)
S	88.947	-5.315	1.508	-6.932	0.806
A	89.405	-4.783	1.551	-6.434	0.824
N	89.063	-5.236	1.027	-5.941	0.857
AS	89.174	-5.050	1.502	-6.634	0.818
AN	89.235	-5.009	1.248	-6.154	0.852
NS	89.002	-5.276	1.234	-6.154	0.852
ANS	89.145	-5.095	1.379	-6.478	0.830

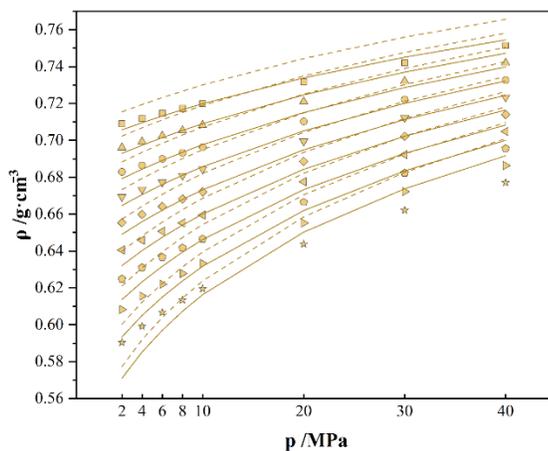
**Figure 42**

Density ( $\rho$ ) of *S* as a function of temperature and pressure. Experimental data: (●) 373.15 K (△) 385.65 K (○) 398.15 K (▽) 410.65 K (◇) 423.15 K (◁) 435.65 K (◊) 448.15 K (▷) 460.65 K (☆) 473.15 K. (---) VTPR with *c* estimated from critical properties. (—) VTPR with *c* estimated from experimental data

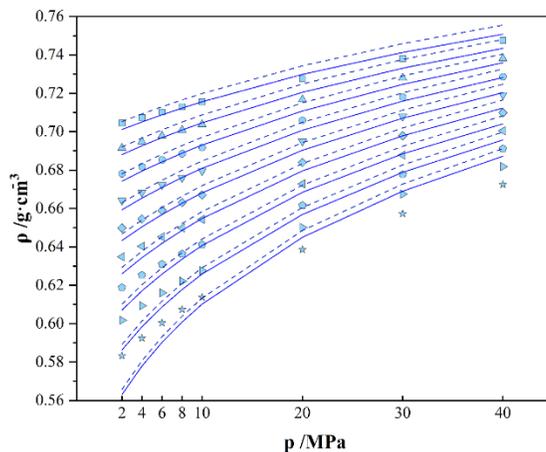


**Figure 43**

Density ( $\rho$ ) of A as a function of temperature and pressure. Experimental data: (●) 373.15 K ( $\Delta$ ) 385.65 K ( $\circ$ ) 398.15 K ( $\nabla$ ) 410.65 K ( $\diamond$ ) 423.15 K ( $\triangleleft$ ) 435.65 K ( $\triangleright$ ) 448.15 K ( $\triangleright$ ) 460.65 K ( $\star$ ) 473.15 K. (---) VTPR with  $c$  estimated from critical properties. (—) VTPR with  $c$  estimated from experimental data.

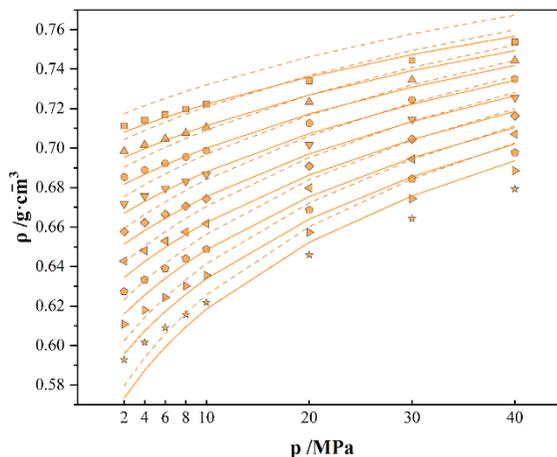
**Figure 44**

Density ( $\rho$ ) of N as a function of temperature and pressure. Experimental data: (●) 373.15 K ( $\Delta$ ) 385.65 K ( $\circ$ ) 398.15 K ( $\nabla$ ) 410.65 K ( $\diamond$ ) 423.15 K ( $\triangleleft$ ) 435.65 K ( $\triangleright$ ) 448.15 K ( $\triangleright$ ) 460.65 K ( $\star$ ) 473.15 K. (---) VTPR with  $c$  estimated from critical properties. (—) VTPR with  $c$  estimated from experimental data.

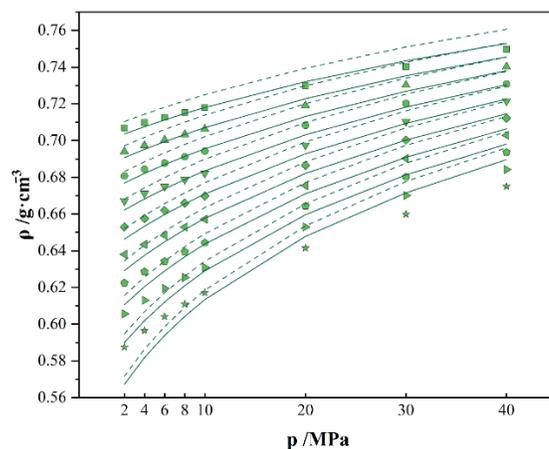


**Figure 45**

Density ( $\rho$ ) of AS as a function of temperature and pressure. Experimental data: (●) 373.15 K ( $\Delta$ ) 385.65 K ( $\circ$ ) 398.15 K ( $\nabla$ ) 410.65 K ( $\diamond$ ) 423.15 K ( $\triangleleft$ ) 435.65 K ( $\square$ ) 448.15 K ( $\triangleright$ ) 460.65 K ( $\star$ ) 473.15 K. (---) VTPR with  $c$  estimated from critical properties. (—) VTPR with  $c$  estimated from experimental data

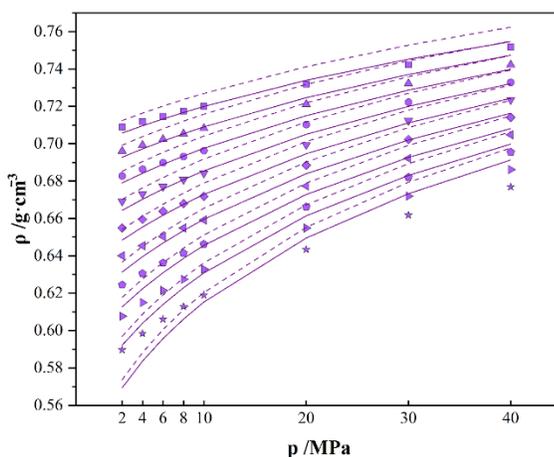
**Figure 46**

Density ( $\rho$ ) of AN as a function of temperature and pressure. Experimental data: (●) 373.15 K ( $\Delta$ ) 385.65 K ( $\circ$ ) 398.15 K ( $\nabla$ ) 410.65 K ( $\diamond$ ) 423.15 K ( $\triangleleft$ ) 435.65 K ( $\square$ ) 448.15 K ( $\triangleright$ ) 460.65 K ( $\star$ ) 473.15 K. (---) VTPR with  $c$  estimated from critical properties. (—) VTPR with  $c$  estimated from experimental data

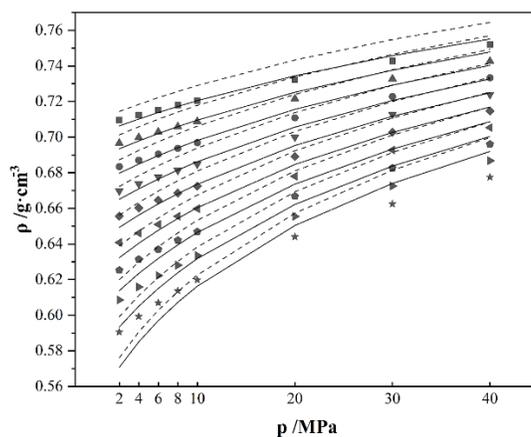


**Figure 47**

Density ( $\rho$ ) of NS as a function of temperature and pressure. Experimental data: (●) 373.15 K (△) 385.65 K (○) 398.15 K (▽) 410.65 K (◇) 423.15 K (◁) 435.65 K (◊) 448.15 K (▷) 460.65 K (☆) 473.15 K. (---) VTPR with  $c$  estimated from critical properties. (—) VTPR with  $c$  estimated from experimental data

**Figure 48**

Density ( $\rho$ ) of ANS as a function of temperature and pressure. Experimental data: (●) 373.15 K (△) 385.65 K (○) 398.15 K (▽) 410.65 K (◇) 423.15 K (◁) 435.65 K (◊) 448.15 K (▷) 460.65 K (☆) 473.15 K. (---) VTPR with  $c$  estimated from critical properties. (—) VTPR with  $c$  estimated from experimental data



## 7. Conclusions

The density of the selected model compounds for aromatic, sulfur and nitrogen compounds and their mixtures has the expected behavior. At higher temperatures the density decreases, while at higher pressure the density increases. All  $p\rho T$  measurements were adjusted with TRIDEN, a correlation that combines Tait's and Racket's models. An average absolute deviation AAD of less than 0.01% was obtained, proving the good fitting of this model with cyclohexane and its dissolutions.

On the other hand, the excess volume of the binary mixtures shows an evident interaction between these families of molecules. Remarkably, sulfur and nitrogen compounds have the strongest molecule interaction, possibly due to their polarity. Furthermore, Redlich Kister present and adjustment with standard deviations of less than  $0.015 \text{ cm}^3 \cdot \text{mol}^{-1}$

Finally, Volume Translated Peng Robinson or VTPR estimated density data for all the systems studied with an AAD of less than 2%. Notably, it obtains better results with the use of the experimental data to estimate the volume translation parameter  $c$ .

## 8. Recomendaciones

- To perform the measurements and analysis with crude oil or its dissolutions in cyclohexane.
- To analyze the results with other EOS

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## Appendix

## Appendix A: MATLAB TRIDEN code

```

format long
p0=2;%Reference pressure
[xData, yData, zData] = prepareSurfaceData( t, p, ro );
ft = fitype( '(AR/(BR^(1+((1-t/CR)^DR)))/(1-CT*log((b0+b1*(t/ET)+b2*(t/ET)^2+b3*(t/ET)^3+p)/(b0+b1*(t/ET)+b2*(t/ET)^2+b3*(t/ET)^3+2)))', 'independent', {'t', 'p'}, 'dependent', 'rho' );
opts = fitoptions( 'Method', 'NonlinearLeastSquares' );
opts.Algorithm = 'Levenberg-Marquardt';
opts.Display = 'off';
opts.MaxFunEvals = 6000;
%Start point= [AR BR CR CT DR ET b0 b1 b2 b3]
opts.StartPoint = [0.022477 0.16007 532.92326 0.09142 0.21153 96.91 169.20366 11.8645 -29.14744 4.2399];%n-Hexano tesis Guerrero Amaya
% Fit model to data.
[fitresult, gof] = fit( [xData, yData], zData, ft, opts );
%Save obtained coefficients for estimations
coeffTRIDEN=coeffvalues(fitresult);

fprintf('TRIDEN coefficients:')

AR=coeffTRIDEN(1)
BR=coeffTRIDEN(2)
CR=coeffTRIDEN(3)
DR=coeffTRIDEN(5)
b0=coeffTRIDEN(7)
b1=coeffTRIDEN(8)
b2=coeffTRIDEN(9)
b3=coeffTRIDEN(10)
CT=coeffTRIDEN(4)
ET=coeffTRIDEN(6)

% Deviation analysis-DCRM and AAD
% Temperature and pressure data
ti=[373.15 385.65 398.15 410.65 423.15 435.65 448.15 460.65 473.15];
pj=[2 4 6 8 10 20 30 40];
devs=0
sumsdev=0;%for finding deviations
for i=1:numel(ti)
    t_i=ti(i);

```

```
for j=1: numel(pj)
    p_j=pj(j);
    ro_j=ro(i,j);

    ro0(i,j)=AR/(BR^(1+(1-t_i/CR)^DR));%Rackett's equation
    BT(i,j)=b0+b1*(t_i/ET)+b2*(t_i/ET)^2+b3*(t_i/ET)^3;
    roTRIDEN(i,j)=ro0(i,j)/(1-CT*log((BT(i,j)+p_j)/(BT(i,j)+p0)));%estimation with
    TRIDEN parameters
    dev(i,j)=(ro_j-roTRIDEN(i,j))/ro_j;
    devs=devs+dev(i,j);
    sdev(i,j)=dev(i,j)^2;
    sumsdev=sumsdev+sdev(i,j);
    DCRM=100*((1/numel(ro))*sumsdev)^(1/2);
```

**Appendix B: Estimations of isothermal compressibility, isobaric expansivity, and internal pressure**

**B.1. Cyclohexane**

**Table 41.**

*Estimation of isothermal compressibility ( $\kappa_T$ ) of Cyclohexane at different temperatures and pressures*

<b>p /bar</b>	<b><math>\kappa_T</math> /TPa at T/K</b>								
	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	2175.5	2463.4	2811.4	3242.6	3780.1	4466.1	5365.3	6574.9	8270.7
40	2080.9	2341.9	2656.0	3035.6	3502.2	4084.1	4824.1	5781.9	7050.9
60	1994.3	2232.7	2515.8	2854.5	3264.4	3764.9	4386.9	5163.1	6156.4
80	1915.0	2134.1	2391.0	2695.6	3057.9	3494.2	4024.0	4669.8	5472.6
100	1841.7	2043.9	2278.9	2554.6	2877.4	3261.4	3721.2	4269.7	4932.0
200	1549.9	1691.2	1850.2	2029.3	2231.5	2459.6	2717.0	3007.0	3334.5
300	1340.6	1446.4	1562.2	1689.7	1830.0	1983.7	2153.3	2338.2	2541.5
400	1183.3	1265.5	1354.5	1450.8	1555.1	1667.9	1790.0	1921.9	2063.5

**Table 42.**

*Estimation of volume expansivity ( $\alpha_p$ ) of Cyclohexane at different temperatures and pressures*

<b>p /bar</b>	<b><math>\alpha_p</math> /Kk<sup>-1</sup> at T/K</b>								
	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	1.453	1.523	1.604	1.700	1.812	1.949	2.121	2.343	2.651
40	1.413	1.475	1.547	1.628	1.723	1.835	1.972	2.145	2.376
60	1.376	1.432	1.494	1.564	1.645	1.739	1.851	1.988	2.170
80	1.343	1.392	1.447	1.508	1.577	1.656	1.749	1.861	2.010
100	1.311	1.356	1.405	1.458	1.517	1.584	1.663	1.757	1.881
200	1.185	1.212	1.239	1.268	1.298	1.331	1.368	1.413	1.481
300	1.093	1.109	1.125	1.141	1.157	1.173	1.192	1.218	1.264
400	1.021	1.031	1.040	1.048	1.056	1.063	1.073	1.089	1.122

**Table 43.***Estimation of internal pressure ( $p_i$ ) of Cyclohexane at different temperatures and pressures*

<b>p /bar</b>	<b><math>p_i</math> /MPa at T/K</b>								
	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	247.2	236.5	225.2	213.3	200.9	188.1	175.1	162.2	149.6
40	249.4	238.9	227.8	216.2	204.1	191.7	179.2	166.9	155.4
60	251.5	241.3	230.4	219.1	207.2	195.2	183.1	171.4	160.8
80	253.6	243.6	233.0	221.8	210.2	198.5	186.7	175.6	165.8
100	255.7	245.8	235.4	224.4	213.2	201.6	190.2	179.5	170.4
200	265.3	256.3	246.7	236.6	226.2	215.7	205.6	196.5	190.1
300	274.1	265.7	256.7	247.3	237.5	227.6	218.1	210.0	205.3
400	282.1	274.2	265.7	256.7	247.2	237.7	228.6	220.9	217.3

**B.2. Aromatic model****Table 44.***Estimation of isothermal compressibility ( $\kappa_T$ ) of aromatics model mixture with Phenanthrene (1% w/w) and 2,6-Diethylnaphtalene (2% w/w) at different temperatures and pressures.*

<b>p /bar</b>	<b><math>\kappa_T</math> /TPa at T/K</b>								
	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	2094.0	2371.9	2706.4	3114.3	3621.0	4263.9	5095.1	6203.8	7749.5
40	2006.1	2259.2	2560.5	2924.4	3364.3	3911.8	4603.1	5489.3	6663.8
60	1925.1	2157.0	2430.6	2755.9	3143.2	3617.7	4200.0	4928.1	5857.4
80	1850.8	2064.7	2313.3	2606.2	2952.4	3366.2	3866.0	4477.2	5234.5
100	1782.2	1979.9	2208.4	2473.0	2783.0	3149.2	3582.9	4104.3	4732.9
200	1506.4	1646.1	1802.0	1976.1	2171.2	2391.4	2639.3	2919.1	3235.2
300	1307.3	1412.1	1526.5	1651.8	1787.6	1937.3	2101.5	2281.0	2479.2
400	1156.3	1238.5	1326.7	1421.9	1523.8	1633.5	1752.2	1879.9	2019.5

**Table 45.**

*Estimation of volume expansivity ( $\alpha_p$ ) of aromatics model mixture with Phenanthrene (1% w/w) and 2,6-Diethylnaphtalene (2% w/w) at different temperatures and pressures.*

		$\alpha_p$ /Kk <sup>-1</sup> at T/K								
p /bar		373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20		1.425	1.490	1.564	1.651	1.756	1.884	2.046	2.261	2.566
40		1.387	1.444	1.508	1.584	1.672	1.777	1.909	2.078	2.312
60		1.351	1.401	1.459	1.524	1.598	1.687	1.795	1.932	2.120
80		1.318	1.363	1.413	1.470	1.534	1.609	1.699	1.813	1.969
100		1.287	1.328	1.372	1.422	1.477	1.542	1.618	1.714	1.846
200		1.163	1.187	1.212	1.238	1.267	1.299	1.336	1.385	1.459
300		1.071	1.085	1.099	1.114	1.129	1.146	1.167	1.196	1.248
400		1.000	1.008	1.016	1.023	1.031	1.040	1.051	1.070	1.108

**Table 46.**

*Estimation of internal pressure ( $p_i$ ) of aromatics model mixture with Phenanthrene (1% w/w) and 2,6-Diethylnaphtalene (2% w/w) at different temperatures and pressures.*

		$p_i$ /MPa at T/K								
p /bar		373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20		252.0	240.2	228.1	215.7	203.2	190.5	178.0	165.9	154.7
40		253.9	242.4	230.6	218.4	206.2	193.9	181.8	170.4	160.2
60		255.8	244.5	232.9	221.1	209.2	197.2	185.5	174.6	165.3
80		257.7	246.6	235.2	223.6	211.9	200.3	189.0	178.5	170.0
100		259.5	248.6	237.4	226.1	214.6	203.3	192.3	182.3	174.5
200		268.1	258.0	247.7	237.3	226.9	216.6	206.9	198.6	193.4
300		275.7	266.4	256.8	247.0	237.3	227.8	218.9	211.6	208.1
400		282.7	273.9	264.9	255.6	246.3	237.3	228.8	222.1	219.7

**Table 47.**

*Estimation of isothermal compressibility ( $\kappa_T$ ) of aromatics model mixture with Phenanthrene (1.5% w/w) and 2,6-Diethylnaphtalene (1.5% w/w) at different temperatures and pressures.*

		$\kappa_T$ /TPa at T/K								
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<b>p /bar</b>	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	2104.1	2377.4	2706.1	3110.2	3612.6	4251.5	5075.5	6166.7	7674.2
40	2015.3	2263.6	2560.6	2919.9	3357.5	3903.1	4586.1	5466.4	6609.2
60	1933.8	2161.5	2431.2	2752.5	3137.8	3609.7	4187.7	4906.5	5814.9
80	1859.0	2069.0	2313.8	2603.5	2947.2	3358.9	3855.3	4460.0	5199.1
100	1789.8	1983.8	2208.6	2470.5	2778.4	3142.2	3574.8	4090.7	4705.5
200	1512.2	1649.0	1802.5	1974.8	2169.6	2388.7	2635.3	2912.1	3223.7
300	1312.1	1414.6	1527.1	1650.9	1786.8	1935.8	2099.5	2277.6	2472.3
400	1160.3	1240.7	1327.6	1421.5	1523.2	1633.1	1750.9	1878.5	2015.2

**Table 48.**

*Estimation of volume expansivity ( $\alpha_p$ ) of aromatics model mixture with Phenanthrene (1.5% w/w) and 2,6-Diethylnaphtalene (1.5% w/w) at different temperatures and pressures*

<b><math>\alpha_p</math> /Kk<sup>-1</sup> at T/K</b>									
<b>p /bar</b>	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	1.421	1.489	1.566	1.655	1.761	1.889	2.047	2.248	2.521
40	1.384	1.443	1.511	1.588	1.677	1.783	1.910	2.069	2.277
60	1.349	1.402	1.462	1.529	1.604	1.693	1.798	1.925	2.091
80	1.316	1.364	1.417	1.475	1.541	1.615	1.703	1.808	1.945
100	1.287	1.330	1.376	1.427	1.484	1.548	1.621	1.711	1.826
200	1.165	1.191	1.218	1.245	1.274	1.306	1.342	1.386	1.451
300	1.075	1.091	1.107	1.122	1.137	1.154	1.173	1.200	1.245
400	1.006	1.015	1.024	1.032	1.040	1.048	1.058	1.075	1.110

**Table 49.**

*Estimation of internal pressure ( $p_i$ ) of aromatics model mixture with Phenanthrene (1.5% w/w) and 2,6-Diethylnaphtalene (1.5% w/w) at different temperatures and pressures.*

<b><math>p_i</math> /MPa at T/K</b>									
<b>p /bar</b>	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	250.1	239.5	228.4	216.6	204.3	191.6	178.7	165.9	153.4
40	252.2	241.9	230.9	219.4	207.4	195.0	182.6	170.4	159.0
60	254.2	244.1	233.4	222.1	210.4	198.4	186.4	174.7	164.2
80	256.3	246.3	235.8	224.7	213.2	201.5	189.9	178.8	169.0

100	258.2	248.5	238.1	227.3	216.0	204.6	193.3	182.6	173.6
200	267.4	258.5	248.9	238.9	228.6	218.2	208.2	199.3	193.0
300	275.8	267.5	258.5	249.1	239.4	229.7	220.4	212.7	208.3
400	283.5	275.6	267.1	258.1	248.8	239.4	230.7	223.6	220.6

**Table 50.**

*Estimation of isothermal compressibility ( $\kappa_T$ ) of aromatics model mixture with Phenanthrene (2% w/w) and 2,6-Diethylnaphthalene (1% w/w) at different temperatures and pressures.*

$\kappa_T$ /TPa at T/K									
p /bar	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	2093.8	2371.0	2704.2	3110.7	3613.6	4250.8	5075.7	6173.0	7694.1
40	2005.3	2258.7	2559.3	2919.9	3359.5	3900.3	4585.3	5460.8	6621.2
60	1924.3	2156.3	2429.0	2752.1	3139.5	3606.4	4186.4	4906.4	5824.8
80	1850.0	2063.4	2312.2	2602.2	2946.4	3356.4	3852.5	4458.3	5204.9
100	1781.3	1978.3	2205.5	2469.3	2777.8	3140.1	3571.6	4085.3	4709.6
200	1505.8	1645.0	1800.2	1973.5	2167.8	2386.3	2631.2	2909.4	3223.1
300	1306.6	1411.2	1525.2	1649.7	1785.1	1933.6	2096.0	2273.9	2470.6
400	1155.7	1237.4	1325.5	1420.0	1521.6	1630.5	1748.1	1875.1	2013.1

**Table 51.**

*Estimation of volume expansivity ( $\alpha_p$ ) of aromatics model mixture with Phenanthrene (2% w/w) and 2,6-Diethylnaphthalene (1% w/w) at different temperatures and pressures.*

$\alpha_p$ /Kk <sup>-1</sup> at T/K									
p /bar	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	1.425	1.491	1.566	1.655	1.760	1.887	2.047	2.253	2.535
40	1.386	1.445	1.511	1.587	1.677	1.782	1.911	2.071	2.284
60	1.350	1.402	1.461	1.528	1.604	1.692	1.798	1.928	2.095
80	1.317	1.364	1.416	1.474	1.540	1.615	1.703	1.810	1.945
100	1.287	1.329	1.375	1.426	1.483	1.548	1.622	1.711	1.823
200	1.162	1.188	1.215	1.243	1.274	1.307	1.343	1.386	1.440
300	1.071	1.087	1.103	1.120	1.138	1.156	1.175	1.198	1.230
400	0.999	1.010	1.020	1.030	1.040	1.050	1.061	1.073	1.091

**Table 52.**

*Estimation of internal pressure ( $p_i$ ) of aromatics model mixture with Phenanthrene (2% w/w) and 2,6-Diethylnaphthalene (1% w/w) at different temperatures and pressures.*

		$p_i$ /MPa at T/K							
$p$ /bar	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	251.9	240.4	228.6	216.5	204.1	191.4	178.7	166.1	153.9
40	253.9	242.7	231.1	219.2	207.2	195.0	182.7	170.7	159.2
60	255.8	244.8	233.5	222.0	210.2	198.4	186.5	175.0	164.2
80	257.7	246.9	235.9	224.6	213.1	201.6	190.1	179.0	168.8
100	259.5	249.0	238.2	227.1	215.9	204.7	193.6	182.9	173.1
200	268.0	258.5	248.7	238.7	228.7	218.6	208.8	199.4	191.4
300	275.7	267.0	258.0	248.9	239.6	230.4	221.3	212.7	205.5
400	282.7	274.7	266.4	257.9	249.2	240.5	231.9	223.6	216.5

### B.3. Nitrogen model

**Table 53.**

*Estimation of isothermal compressibility ( $\kappa_T$ ) of nitrogen model mixture with Quinoline (0.3% w/w) and 9-Ethylcarbazole (0.7 % w/w) at different temperatures and pressures.*

		$\kappa_T$ /TPa at T/K							
$p$ /bar	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	2152.8	2435.4	2778.3	3200.1	3725.8	4397.0	5271.4	6446.8	8071.1
40	2059.9	2316.7	2625.2	2998.9	3455.9	4027.3	4748.2	5676.7	6902.5
60	1974.8	2210.0	2489.4	2822.3	3224.0	3716.4	4321.9	5082.1	6044.9
80	1896.9	2113.2	2366.9	2666.5	3023.5	3451.6	3970.3	4604.0	5385.2
100	1824.9	2024.7	2256.4	2527.2	2846.1	3224.6	3673.2	4210.0	4856.4
200	1537.4	1677.7	1835.1	2012.1	2211.9	2436.2	2689.9	2976.8	3297.5
300	1331.2	1435.8	1551.2	1677.4	1816.3	1968.2	2135.8	2318.2	2518.1
400	1175.5	1257.5	1345.9	1441.6	1545.0	1656.7	1777.2	1907.2	2047.4

**Table 54.**

*Estimation of volume expansivity ( $\alpha_p$ ) of nitrogen model mixture with Quinoline (0.3% w/w) and 9-Ethylcarbazole (0.7 % w/w) at different temperatures and pressures.*

		$\alpha_p$ /Kk <sup>-1</sup> at T/K								
<b>p /bar</b>		373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20		1.444	1.513	1.592	1.684	1.794	1.928	2.095	2.313	2.611
40		1.405	1.465	1.535	1.614	1.706	1.817	1.951	2.120	2.346
60		1.369	1.423	1.484	1.552	1.630	1.722	1.832	1.968	2.148
80		1.335	1.384	1.437	1.497	1.564	1.641	1.733	1.845	1.993
100		1.304	1.348	1.395	1.447	1.505	1.571	1.648	1.741	1.866
200		1.179	1.205	1.232	1.260	1.289	1.321	1.358	1.405	1.475
300		1.087	1.103	1.119	1.134	1.149	1.165	1.185	1.213	1.262
400		1.017	1.026	1.034	1.042	1.049	1.057	1.067	1.085	1.122

**Table 55.**

*Estimation of internal pressure ( $p_i$ ) of nitrogen model mixture with Quinoline (0.3% w/w) and 9-Ethylcarbazole (0.7 % w/w) at different temperatures and pressures.*

		$p_i$ /MPa at T/K								
<b>p /bar</b>		373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20		248.3	237.5	226.1	214.1	201.7	189.0	176.1	163.3	151.1
40		250.5	239.9	228.7	217.0	204.9	192.5	180.1	168.0	156.8
60		252.6	242.3	231.3	219.8	208.0	195.9	183.9	172.4	162.2
80		254.7	244.5	233.8	222.5	210.9	199.2	187.6	176.6	167.1
100		256.7	246.7	236.2	225.1	213.8	202.3	191.0	180.5	171.8
200		266.2	257.0	247.3	237.1	226.7	216.2	206.2	197.4	191.6
300		274.8	266.3	257.2	247.6	237.7	227.9	218.7	211.0	207.1
400		282.7	274.7	266.0	256.8	247.4	237.9	229.1	222.0	219.4

**Table 56.**

*Estimation of isothermal compressibility ( $\kappa_T$ ) of nitrogen model mixture with Quinoline (0.5% w/w) and 9-Ethylcarbazole (0.5 % w/w) at different temperatures and pressures.*

		$\kappa_T$ /TPa at T/K								
<b>p /bar</b>		373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20		2156.7	2442.7	2789.8	3218.4	3755.6	4441.0	5339.8	6539.6	8215.0
40		2063.7	2323.2	2635.2	3015.6	3480.6	4061.2	4797.3	5751.6	7007.8
60		1978.3	2215.5	2498.0	2835.8	3245.6	3745.9	4364.7	5142.3	6121.8
80		1899.6	2118.2	2374.9	2679.2	3041.4	3477.3	4005.4	4651.3	5445.9
100		1827.8	2029.1	2263.6	2538.5	2862.4	3245.4	3704.3	4250.8	4907.4
200		1539.1	1680.5	1839.5	2018.5	2220.9	2448.5	2705.4	2996.0	3321.2
300		1332.4	1437.7	1553.8	1681.5	1821.8	1976.2	2145.2	2329.7	2531.9
400		1176.1	1258.4	1347.8	1444.7	1548.8	1662.1	1783.5	1915.2	2056.4

**Table 57.**

*Estimation of volume expansivity ( $\alpha_p$ ) of nitrogen model mixture with Quinoline (0.5% w/w) and 9-Ethylcarbazole (0.5 % w/w) at different temperatures and pressures.*

		$\alpha_p$ /Kk <sup>-1</sup> at T/K								
<b>p /bar</b>		373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20		1.448	1.520	1.602	1.697	1.811	1.948	2.120	2.339	2.637
40		1.408	1.472	1.543	1.626	1.721	1.834	1.970	2.142	2.366
60		1.372	1.428	1.492	1.563	1.644	1.738	1.850	1.987	2.163
80		1.338	1.389	1.445	1.507	1.577	1.656	1.748	1.860	2.005
100		1.307	1.353	1.402	1.457	1.517	1.584	1.662	1.755	1.877
200		1.181	1.209	1.237	1.267	1.297	1.330	1.368	1.414	1.481
300		1.089	1.106	1.123	1.139	1.155	1.173	1.193	1.220	1.266
400		1.017	1.028	1.038	1.046	1.054	1.063	1.073	1.090	1.125

**Table 58.**

*Estimation of internal pressure ( $p_i$ ) of nitrogen model mixture with Quinoline (0.5% w/w) and 9-Ethylcarbazole (0.5 % w/w) at different temperatures and pressures.*

		$p_i$ /MPa at T/K							
<b>p /bar</b>	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	248.5	237.9	226.6	214.6	202.0	189.1	175.9	162.7	149.9
40	250.7	240.3	229.2	217.4	205.3	192.7	180.1	167.5	155.7
60	252.8	242.6	231.7	220.3	208.4	196.2	183.9	172.0	161.2
80	254.9	244.9	234.2	223.0	211.3	199.5	187.6	176.2	166.2
100	256.9	247.1	236.6	225.6	214.2	202.6	191.1	180.2	170.9
200	266.4	257.4	247.8	237.7	227.2	216.7	206.5	197.4	190.9
300	274.9	266.6	257.7	248.2	238.4	228.5	219.1	211.1	206.5
400	282.8	275.0	266.5	257.5	248.1	238.6	229.6	222.2	218.9

**Table 59.**

*Estimation of isothermal compressibility ( $\kappa_T$ ) of nitrogen model mixture with Quinoline (0.7% w/w) and 9-Ethylcarbazole (0.3 % w/w) at different temperatures and pressures.*

		$\kappa_T$ /TPa at T/K							
<b>p /bar</b>	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	2158.8	2441.9	2786.0	3208.8	3737.4	4411.1	5287.0	6465.9	8100.7
40	2065.4	2322.8	2632.7	3006.2	3465.8	4034.8	4762.0	5689.7	6924.6
60	1979.8	2215.7	2495.1	2828.3	3231.2	3724.6	4331.6	5093.9	6055.8
80	1901.5	2118.4	2372.4	2672.9	3030.0	3458.2	3977.6	4610.9	5393.6
100	1829.3	2029.2	2261.1	2533.0	2852.4	3229.3	3679.3	4219.3	4869.3
200	1540.6	1680.9	1838.3	2015.7	2215.3	2439.7	2694.6	2979.6	3301.7
300	1333.5	1438.2	1553.1	1679.8	1818.5	1970.7	2138.1	2320.6	2520.7
400	1177.4	1259.0	1347.6	1443.3	1546.6	1658.1	1778.8	1909.0	2049.5

**Table 60.**

*Estimation of volume expansivity ( $\alpha_p$ ) of nitrogen model mixture with Quinoline (0.7% w/w) and 9-Ethylcarbazole (0.3 % w/w) at different temperatures and pressures*

		$\alpha_p / \text{Kk}^{-1}$ at T/K								
<b>p /bar</b>		373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20		1.444	1.514	1.594	1.688	1.799	1.933	2.100	2.317	2.611
40		1.405	1.467	1.537	1.617	1.711	1.820	1.956	2.122	2.345
60		1.369	1.424	1.485	1.555	1.634	1.727	1.836	1.971	2.145
80		1.335	1.385	1.439	1.500	1.568	1.645	1.736	1.846	1.990
100		1.305	1.349	1.397	1.450	1.509	1.575	1.651	1.744	1.864
200		1.180	1.206	1.234	1.263	1.293	1.325	1.361	1.406	1.472
300		1.088	1.104	1.120	1.136	1.152	1.169	1.188	1.214	1.258
400		1.017	1.027	1.036	1.045	1.052	1.060	1.070	1.086	1.119

**Table 61.**

*Estimation of internal pressure ( $p_i$ ) of nitrogen model mixture with Quinoline (0.7% w/w) and 9-Ethylcarbazole (0.3 % w/w) at different temperatures and pressures.*

		$p_i / \text{MPa}$ at T/K								
<b>p /bar</b>		373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20		247.7	237.1	225.8	214.0	201.6	188.9	176.0	163.0	150.5
40		249.8	239.5	228.5	216.9	204.9	192.6	180.0	167.8	156.3
60		252.0	241.8	231.0	219.7	208.0	196.0	183.9	172.2	161.6
80		254.1	244.1	233.5	222.4	211.0	199.3	187.6	176.4	166.6
100		256.1	246.4	236.0	225.1	213.9	202.4	191.1	180.4	171.2
200		265.7	256.8	247.2	237.2	226.9	216.5	206.4	197.4	190.9
300		274.4	266.1	257.2	247.8	238.2	228.4	219.1	211.0	206.2
400		282.4	274.6	266.2	257.2	248.0	238.6	229.6	222.1	218.3

#### B.4. Sulfur model

**Table 62.**

*Estimation of isothermal compressibility ( $\kappa_T$ ) of sulfur model mixture with Dibenzothiophene (1% w/w) at different temperatures and pressures.*

		$\kappa_T$ /TPa at T/K								
<b>p /bar</b>		373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20		2153.8	2435.5	2777.0	3196.7	3720.8	4386.2	5256.0	6423.0	8029.2
40		2060.9	2317.1	2624.1	2996.7	3451.2	4018.7	4736.1	5661.4	6876.6
60		1975.5	2210.1	2488.0	2820.3	3220.7	3710.2	4313.9	5067.4	6022.7
80		1898.1	2113.6	2366.7	2664.0	3019.5	3445.8	3964.1	4592.8	5369.8
100		1826.3	2025.2	2256.1	2525.8	2844.3	3221.1	3668.2	4202.7	4847.7
200		1539.0	1679.1	1835.6	2012.1	2210.9	2435.3	2689.1	2974.4	3294.7
300		1332.5	1437.4	1552.2	1678.1	1816.5	1968.5	2135.4	2317.7	2517.9
400		1177.0	1258.7	1347.1	1442.6	1545.9	1657.4	1777.7	1908.0	2048.2

**Table 63.**

*Estimation of volume expansivity ( $\alpha_p$ ) of sulfur model mixture with Dibenzothiophene (1% w/w) at different temperatures and pressures.*

		$\alpha_p$ /Kk <sup>-1</sup> at T/K								
<b>p /bar</b>		373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20		1.442	1.512	1.592	1.685	1.795	1.928	2.095	2.310	2.600
40		1.403	1.465	1.535	1.615	1.708	1.818	1.951	2.119	2.338
60		1.367	1.422	1.483	1.553	1.632	1.724	1.834	1.967	2.141
80		1.334	1.383	1.438	1.498	1.566	1.643	1.735	1.844	1.987
100		1.303	1.347	1.396	1.448	1.508	1.574	1.650	1.742	1.861
200		1.178	1.205	1.233	1.262	1.292	1.324	1.361	1.406	1.471
300		1.087	1.104	1.120	1.136	1.152	1.169	1.188	1.215	1.258
400		1.016	1.027	1.036	1.045	1.053	1.061	1.071	1.087	1.118

**Table 64.**

*Estimation of internal pressure ( $p_i$ ) of sulfur model mixture with Dibenzothiophene (1% w/w) at different temperatures and pressures.*

		$p_i$ /MPa at T/K								
$p$ /bar		373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20		247.9	237.4	226.2	214.4	202.2	189.5	176.6	163.7	151.2
40		250.1	239.8	228.8	217.3	205.4	193.1	180.7	168.4	156.9
60		252.2	242.1	231.4	220.1	208.5	196.5	184.5	172.8	162.2
80		254.2	244.4	233.8	222.9	211.4	199.8	188.1	177.0	167.1
100		256.3	246.6	236.3	225.5	214.3	202.9	191.6	180.9	171.7
200		265.7	256.9	247.4	237.5	227.3	216.9	206.9	197.8	191.2
300		274.3	266.1	257.3	248.0	238.4	228.7	219.4	211.4	206.4
400		282.2	274.5	266.2	257.3	248.1	238.8	229.9	222.4	218.4

**Table 65.**

*Estimation of isothermal compressibility ( $\kappa_T$ ) of sulfur model mixture with Dibenzothiophene (2.2% w/w) at different temperatures and pressures.*

		$\kappa_T$ /TPa at T/K								
$p$ /bar		373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20		2112.1	2387.4	2721.3	3131.4	3644.0	4294.4	5138.4	6270.4	7831.4
40		2021.9	2273.3	2573.2	2937.1	3383.6	3937.6	4636.7	5536.7	6720.0
60		1939.6	2170.0	2442.3	2767.5	3160.2	3639.2	4229.9	4966.6	5898.9
80		1864.4	2075.6	2323.8	2616.5	2965.1	3383.4	3890.2	4506.9	5267.2
100		1794.9	1989.8	2216.6	2482.1	2794.1	3163.1	3602.9	4128.4	4760.3
200		1514.9	1652.6	1807.6	1981.3	2177.4	2398.9	2648.9	2930.2	3246.5
300		1313.5	1416.6	1529.8	1654.4	1791.7	1942.4	2107.1	2288.0	2485.0
400		1161.1	1241.9	1329.1	1423.9	1526.0	1636.9	1756.1	1884.2	2022.5

**Table 66.**

*Estimation of volume expansivity ( $\alpha_p$ ) of sulfur model mixture with Dibenzothiophene (2.2% w/w) at different temperatures and pressures.*

		$\alpha_p$ /Kk <sup>-1</sup> at T/K							
<b>p /bar</b>	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	1.428	1.496	1.574	1.665	1.773	1.903	2.065	2.275	2.560
40	1.389	1.450	1.518	1.596	1.687	1.795	1.925	2.089	2.305
60	1.354	1.408	1.468	1.536	1.613	1.703	1.810	1.942	2.113
80	1.322	1.370	1.423	1.482	1.548	1.624	1.713	1.821	1.963
100	1.292	1.335	1.382	1.434	1.491	1.555	1.630	1.721	1.841
200	1.169	1.195	1.222	1.249	1.279	1.310	1.346	1.391	1.457
300	1.079	1.095	1.110	1.125	1.141	1.157	1.175	1.202	1.248
400	1.009	1.019	1.027	1.035	1.042	1.049	1.059	1.075	1.110

**Table 67.**

*Estimation of internal pressure ( $p_i$ ) of sulfur model mixture with Dibenzothiophene (2.2% w/w) at different temperatures and pressures.*

		$p_i$ /MPa at T/K							
<b>p /bar</b>	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	250.3	239.6	228.3	216.3	203.9	191.1	178.1	165.1	152.7
40	252.4	242.0	230.9	219.2	207.0	194.6	182.1	169.8	158.3
60	254.5	244.3	233.4	221.9	210.0	197.9	185.8	174.1	163.5
80	256.5	246.5	235.8	224.6	213.0	201.1	189.4	178.2	168.4
100	258.5	248.7	238.2	227.2	215.8	204.2	192.8	182.0	173.0
200	268.0	258.9	249.1	239.0	228.5	217.9	207.7	198.7	192.4
300	276.5	268.0	258.9	249.3	239.4	229.4	220.0	212.0	207.6
400	284.3	276.3	267.6	258.4	248.9	239.3	230.2	222.9	219.8

**Table 68.**

*Estimation of isothermal compressibility ( $\kappa_T$ ) of sulfur model mixture with Dibenzothiophene (3.7% w/w) at different temperatures and pressures.*

		$\kappa_T$ /TPa at T/K								
<b>p /bar</b>		373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20		2076.6	2346.4	2671.0	3070.1	3565.8	4191.7	5001.3	6070.5	7531.4
40		1989.9	2235.8	2529.2	2883.3	3317.0	3852.3	4524.2	5382.0	6498.7
60		1909.9	2135.5	2401.2	2719.0	3100.1	3563.5	4134.7	4844.0	5729.5
80		1836.4	2043.7	2286.8	2572.7	2913.1	3319.9	3809.2	4403.3	5127.7
100		1768.8	1960.4	2183.2	2442.3	2747.0	3107.8	3533.7	4040.0	4647.3
200		1496.5	1631.9	1784.4	1955.5	2148.2	2365.1	2610.4	2884.5	3190.8
300		1299.2	1400.9	1513.1	1636.3	1770.9	1919.0	2081.4	2258.4	2449.2
400		1149.7	1229.5	1316.1	1409.9	1510.5	1619.6	1737.2	1863.1	1997.6

**Table 69.**

*Estimation of volume expansivity ( $\alpha_p$ ) of sulfur model mixture with Dibenzothiophene (3.7% w/w) at different temperatures and pressures.*

		$\alpha_p$ /Kk <sup>-1</sup> at T/K								
<b>p /bar</b>		373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20		1.415	1.480	1.554	1.641	1.744	1.868	2.024	2.227	2.506
40		1.378	1.435	1.500	1.574	1.662	1.765	1.891	2.051	2.269
60		1.343	1.394	1.451	1.515	1.589	1.675	1.780	1.912	2.089
80		1.311	1.357	1.407	1.463	1.526	1.599	1.687	1.796	1.945
100		1.282	1.322	1.367	1.415	1.470	1.533	1.607	1.699	1.829
200		1.161	1.185	1.209	1.235	1.263	1.293	1.330	1.380	1.460
300		1.072	1.086	1.099	1.113	1.127	1.142	1.163	1.196	1.257
400		1.003	1.010	1.017	1.023	1.029	1.037	1.049	1.072	1.124

**Table 70.**

*Estimation of internal pressure ( $p_i$ ) of sulfur model mixture with Dibenzothiophene (3.7% w/w) at different temperatures and pressures.*

	$p_i$ /MPa at T/K								
<b>p /bar</b>	373.15	385.65	398.15	410.65	423.15	435.65	448.15	460.65	473.15
20	252.3	241.3	229.6	217.5	204.9	192.2	179.4	167.0	155.4
40	254.4	243.5	232.1	220.2	208.0	195.5	183.3	171.5	161.2
60	256.4	245.8	234.6	222.9	210.9	198.8	186.9	175.8	166.5
80	258.4	248.0	236.9	225.4	213.7	201.9	190.4	179.9	171.5
100	260.4	250.1	239.2	227.9	216.4	204.9	193.8	183.8	176.2
200	269.6	260.0	249.8	239.3	228.7	218.2	208.4	200.5	196.6
300	277.9	268.9	259.3	249.3	239.2	229.4	220.5	214.0	212.8
400	285.5	276.9	267.7	258.1	248.4	238.9	230.6	225.1	226.1

**Appendix C: Estimations of Excess properties for Mixtures: Excess Isothermal  
Compressibility, Excess Isobaric Expansivity, and Excess Internal pressure**

**C.1. Aromatics + Sulfur (AS)**

**Table 71**

*Estimation of excess volume expansivity ( $\alpha_p^E$ ) of AS at different temperatures and pressures.*

p /bar	$\alpha_p^E / \text{kK}^{-1}$							
	20	40	60	80	100	200	300	400
<b>x<sub>A</sub></b>	<b>T/°C = 100</b>							
0.05	-0.003	-0.003	-0.003	-0.003	-0.003	-0.002	-0.002	-0.001
0.20	-0.002	-0.002	-0.001	-0.001	-0.001	0.000	0.000	0.001
0.35	-0.003	-0.003	-0.002	-0.002	-0.002	0.000	0.001	0.002
0.50	-0.004	-0.003	-0.003	-0.002	-0.002	0.000	0.001	0.002
0.65	-0.004	-0.004	-0.003	-0.002	-0.002	0.000	0.002	0.003
0.80	-0.003	-0.003	-0.002	-0.001	0.000	0.002	0.004	0.005
0.95	-0.002	-0.002	-0.001	0.000	0.001	0.004	0.006	0.007
	<b>T/°C = 112.5</b>							
0.05	-0.001	-0.001	-0.001	0.000	0.000	0.000	0.001	0.001
0.20	-0.001	0.000	0.000	0.000	0.001	0.001	0.002	0.002
0.35	-0.001	-0.001	0.000	0.000	0.001	0.001	0.003	0.003
0.50	-0.002	-0.002	-0.001	-0.001	0.000	0.001	0.002	0.003
0.65	-0.002	-0.002	-0.001	-0.001	0.000	0.002	0.003	0.004
0.80	-0.002	-0.002	-0.001	0.000	0.001	0.002	0.004	0.005
0.95	-0.001	-0.001	0.000	0.000	0.001	0.003	0.005	0.007
	<b>T/°C = 125</b>							
0.05	0.001	0.002	0.002	0.002	0.002	0.003	0.003	0.004
0.20	0.001	0.001	0.001	0.002	0.002	0.002	0.003	0.003
0.35	0.001	0.001	0.001	0.002	0.002	0.003	0.004	0.004
0.50	0.000	0.000	0.001	0.001	0.001	0.002	0.003	0.004
0.65	0.000	0.000	0.001	0.001	0.002	0.003	0.003	0.004
0.80	-0.001	0.000	0.000	0.001	0.001	0.003	0.004	0.004
0.95	-0.001	-0.001	0.000	0.001	0.001	0.003	0.004	0.005
	<b>T/°C = 137.5</b>							
0.05	0.004	0.004	0.004	0.005	0.005	0.005	0.006	0.006
0.20	0.002	0.003	0.002	0.003	0.003	0.004	0.004	0.004

$\alpha_p^E / \text{kK}^{-1}$								
p /bar	20	40	60	80	100	200	300	400
0.35	0.003	0.003	0.003	0.004	0.004	0.004	0.005	0.005
0.50	0.001	0.001	0.002	0.002	0.003	0.003	0.003	0.004
0.65	0.001	0.002	0.002	0.002	0.003	0.003	0.003	0.004
0.80	0.000	0.000	0.001	0.002	0.002	0.003	0.003	0.003
0.95	-0.001	0.000	0.000	0.001	0.001	0.002	0.003	0.003
<b>T/°C = 150</b>								
0.05	0.006	0.006	0.006	0.006	0.007	0.007	0.008	0.008
0.20	0.003	0.003	0.003	0.003	0.004	0.004	0.004	0.004
0.35	0.004	0.003	0.004	0.005	0.005	0.005	0.005	0.005
0.50	0.002	0.002	0.003	0.003	0.003	0.003	0.003	0.003
0.65	0.003	0.002	0.003	0.003	0.003	0.003	0.003	0.003
0.80	0.001	0.001	0.001	0.001	0.002	0.002	0.002	0.002
0.95	0.000	0.000	0.000	0.001	0.000	0.001	0.001	0.001
<b>T/°C = 162.5</b>								
0.05	0.007	0.007	0.008	0.007	0.007	0.008	0.008	0.008
0.20	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004
0.35	0.004	0.005	0.005	0.005	0.005	0.005	0.005	0.005
0.50	0.003	0.002	0.003	0.003	0.003	0.003	0.003	0.003
0.65	0.002	0.003	0.003	0.003	0.003	0.002	0.002	0.002
0.80	0.000	0.001	0.001	0.001	0.001	0.001	0.000	0.000
0.95	0.000	0.000	0.000	0.000	0.000	0.000	-0.001	-0.001
<b>T/°C = 175</b>								
0.05	0.005	0.005	0.006	0.006	0.006	0.007	0.007	0.007
0.20	0.003	0.003	0.003	0.003	0.003	0.003	0.003	0.004
0.35	0.003	0.004	0.004	0.004	0.004	0.004	0.004	0.004
0.50	0.000	0.001	0.001	0.001	0.001	0.002	0.002	0.002
0.65	0.000	0.000	0.001	0.001	0.001	0.002	0.001	0.001
0.80	-0.002	-0.002	-0.001	-0.001	0.000	0.000	0.000	0.000
0.95	-0.002	-0.001	-0.002	-0.001	-0.001	-0.001	-0.001	-0.001
<b>T/°C = 187.5</b>								
0.05	-0.001	0.000	-0.001	0.000	0.001	0.000	0.000	0.000
0.20	-0.001	0.000	-0.001	0.000	0.000	0.000	0.001	0.001
0.35	-0.002	-0.001	-0.001	0.000	0.001	0.001	0.001	0.001
0.50	-0.005	-0.004	-0.004	-0.002	-0.002	0.000	0.001	0.001
0.65	-0.007	-0.004	-0.004	-0.002	-0.002	0.000	0.001	0.002

$\alpha_p^E / \text{kK}^{-1}$								
p /bar	20	40	60	80	100	200	300	400
0.80	-0.007	-0.004	-0.003	-0.003	-0.001	0.001	0.002	0.003
0.95	-0.004	-0.002	-0.002	-0.001	0.000	0.002	0.003	0.003
<b>T/°C = 200</b>								
0.05	-0.0205	-0.0181	-0.0184	-0.0170	-0.0174	-0.0174	-0.0172	-0.0175
0.20	-0.0112	-0.0108	-0.0103	-0.0096	-0.0088	-0.0071	-0.0059	-0.0051
0.35	-0.0148	-0.0120	-0.0111	-0.0101	-0.0094	-0.0073	-0.0059	-0.0055
0.50	-0.0218	-0.0173	-0.0138	-0.0107	-0.0095	-0.0037	-0.0009	0.0007
0.65	-0.0260	-0.0189	-0.0147	-0.0110	-0.0082	-0.0007	0.0031	0.0055
0.80	-0.0209	-0.0126	-0.0079	-0.0046	-0.0016	0.0067	0.0111	0.0138
0.95	-0.0115	-0.0044	-0.0008	0.0031	0.0060	0.0128	0.0165	0.0188

**Table 72.**

*Estimation of excess isothermal compressibility ( $\kappa_T^E$ ) of AS at different temperatures and pressures.*

$\kappa_T^E / \text{TPa}^{-1}$								
p /bar	20	40	60	80	100	200	300	400
<b>T/°C = 100</b>								
$x_A$								
0.05	3.496	2.677	2.917	3.043	2.908	2.139	2.350	1.937
0.20	1.942	1.375	1.136	1.288	0.844	0.339	-0.040	-0.321
0.35	7.708	7.179	6.764	6.471	6.085	4.485	3.956	3.250
0.50	5.568	4.675	5.053	4.874	4.124	3.216	2.922	2.459
0.65	7.268	7.010	6.662	6.632	6.287	4.923	4.391	3.931
0.80	9.554	8.640	8.439	7.702	7.539	5.463	4.537	3.851
0.95	10.383	9.601	9.338	8.848	8.197	6.182	4.911	4.098
<b>T/°C = 112.5</b>								
0.05	1.491	1.293	1.144	1.976	1.901	1.688	1.948	1.731
0.20	-0.182	0.148	-0.139	0.026	0.264	-0.445	-0.404	-0.660
0.35	5.072	4.621	4.587	4.429	4.719	3.283	3.087	2.547
0.50	1.896	1.464	1.594	2.218	2.166	1.923	1.554	1.573
0.65	3.549	2.716	3.153	3.264	3.372	3.204	3.074	2.851
0.80	4.829	3.814	4.496	4.475	4.440	3.324	2.590	2.450
0.95	5.765	4.994	5.080	4.483	4.652	3.107	2.802	2.513
<b>T/°C = 125</b>								

p /bar	$\kappa_T^E / \text{TPa}^{-1}$							
	20	40	60	80	100	200	300	400
0.05	-0.535	-0.280	0.461	0.792	0.537	1.039	1.334	1.322
0.20	-0.880	-1.242	-0.959	-0.764	-1.385	-1.185	-1.077	-1.238
0.35	2.569	1.792	2.169	2.557	2.629	2.109	2.037	1.672
0.50	-1.500	-1.513	-0.285	-0.142	0.271	0.289	0.800	0.686
0.65	0.028	-0.261	0.465	0.514	1.656	1.612	1.773	1.905
0.80	0.754	0.743	1.134	0.874	1.939	1.285	1.317	1.338
0.95	1.201	-0.158	1.090	0.826	1.261	1.325	1.326	1.198
<b>T/°C = 137.5</b>								
0.05	-3.149	-2.520	-1.224	-0.479	0.159	0.625	0.985	0.836
0.20	-2.311	-1.662	-2.410	-0.840	-1.563	-1.268	-1.907	-1.665
0.35	0.037	-0.393	0.376	1.046	1.697	1.332	1.370	1.182
0.50	-3.794	-3.621	-3.279	-1.157	-0.596	0.105	-0.178	0.181
0.65	-3.271	-3.083	-2.560	-0.940	-0.221	1.162	1.078	1.712
0.80	-2.246	-2.617	-1.572	-0.125	-0.240	0.616	0.187	0.449
0.95	-3.294	-2.005	-2.329	-0.664	-0.777	0.273	0.196	0.406
<b>T/°C = 150</b>								
0.05	-4.783	-4.492	-2.446	-2.330	-0.415	0.502	1.088	1.194
0.20	-3.262	-2.745	-3.168	-3.072	-1.795	-1.591	-1.475	-1.546
0.35	-2.381	-3.558	-1.187	-0.291	0.547	0.750	1.473	1.194
0.50	-6.119	-5.564	-3.595	-3.206	-2.227	-0.789	0.160	0.267
0.65	-4.797	-5.327	-3.754	-2.307	-1.155	0.907	1.548	1.651
0.80	-4.847	-4.212	-3.466	-1.625	-0.981	-0.082	0.377	0.358
0.95	-4.975	-4.890	-4.679	-2.452	-2.739	-0.094	0.042	0.245
<b>T/°C = 162.5</b>								
0.05	-7.246	-5.792	-2.786	-3.685	-3.128	0.631	1.235	0.953
0.20	-4.143	-2.803	-2.003	-3.259	-2.983	-1.912	-1.915	-1.939
0.35	-4.718	-3.651	-1.547	-1.966	-0.347	0.762	1.456	1.194
0.50	-7.343	-7.245	-3.673	-4.274	-2.520	-0.210	0.345	0.357
0.65	-7.931	-5.397	-2.178	-2.908	-0.815	0.835	1.455	1.830
0.80	-7.433	-4.296	-2.528	-1.285	-1.012	0.508	0.524	0.550
0.95	-5.910	-4.797	-2.209	-2.013	-0.892	-0.220	0.114	0.373
<b>T/°C = 175</b>								
0.05	-12.374	-9.194	-5.961	-3.897	-3.546	-0.181	0.619	0.970
0.20	-3.064	-1.930	-1.842	-2.881	-3.186	-2.540	-2.529	-2.068
0.35	-8.214	-2.540	-2.425	-1.073	-2.334	0.870	1.342	1.103

$\kappa_T^E / \text{TPa}^{-1}$								
p /bar	20	40	60	80	100	200	300	400
0.50	-10.977	-7.568	-6.449	-4.801	-4.146	-1.017	0.205	0.381
0.65	-12.528	-7.746	-4.610	-2.303	-3.236	2.008	2.501	2.158
0.80	-10.145	-8.281	-5.698	-3.405	-2.203	0.217	0.582	0.621
0.95	-10.111	-6.137	-6.240	-3.505	-3.525	0.832	1.037	0.790
<b>T/°C = 187.5</b>								
0.05	-14.401	-7.099	-10.852	-4.251	-2.664	-0.303	0.366	0.867
0.20	-1.579	-0.572	-7.152	-3.352	-2.361	-3.645	-2.782	-2.494
0.35	-11.503	-6.464	-6.276	-2.728	-0.589	0.753	1.111	1.287
0.50	-15.477	-12.431	-12.114	-6.164	-5.672	-1.293	0.101	0.323
0.65	-17.450	-9.151	-9.691	-4.283	-3.031	0.716	2.231	2.130
0.80	-15.703	-9.534	-7.936	-7.504	-2.737	-1.525	0.349	0.561
0.95	-13.041	-9.061	-8.550	-5.763	-2.945	0.231	1.467	0.973
<b>T/°C = 200</b>								
0.05	-25.065	-11.856	-11.154	-3.680	-4.101	-0.472	1.817	1.748
0.20	-3.424	-6.156	-7.528	-6.853	-5.759	-4.509	-3.087	-2.577
0.35	-16.018	-8.500	-7.396	-4.982	-3.732	-0.536	1.863	1.511
0.50	-35.203	-26.066	-19.220	-12.245	-11.953	-3.740	-1.408	-0.730
0.65	-47.041	-30.965	-23.862	-16.765	-11.569	-3.344	-0.250	1.040
0.80	-46.847	-28.529	-21.019	-17.441	-13.026	-5.040	-1.752	-0.917
0.95	-39.271	-24.091	-20.059	-13.056	-8.004	-3.334	-0.958	-0.501

**Table 73.**

*Estimation of excess internal pressure ( $p_i^E$ ) of AS at different temperatures and pressures.*

$p_i^E / \text{MPa}$								
p /bar	20	40	60	80	100	200	300	400
<b>T/°C = 100</b>								
<b>x<sub>A</sub></b>								
0.05	-1.028	-1.007	-1.015	-1.016	-1.011	-0.999	-1.010	-0.990
0.20	-0.512	-0.462	-0.407	-0.374	-0.325	-0.098	0.124	0.354
0.35	-1.467	-1.407	-1.349	-1.295	-1.243	-0.945	-0.689	-0.384
0.50	-1.320	-1.231	-1.176	-1.107	-1.032	-0.672	-0.359	0.024
0.65	-1.660	-1.578	-1.494	-1.422	-1.348	-0.933	-0.543	-0.132
0.80	-1.720	-1.593	-1.469	-1.343	-1.230	-0.604	0.016	0.641
0.95	-1.678	-1.522	-1.372	-1.224	-1.075	-0.315	0.447	1.218

$p^E$ /MPa								
$p$ /bar	20	40	60	80	100	200	300	400
<b>T/°C = 112.5</b>								
0.05	-0.334	-0.311	-0.283	-0.289	-0.278	-0.190	-0.133	-0.058
0.20	-0.077	-0.040	0.017	0.054	0.090	0.347	0.565	0.822
0.35	-0.708	-0.651	-0.594	-0.548	-0.500	-0.227	0.045	0.320
0.50	-0.531	-0.466	-0.410	-0.369	-0.310	-0.021	0.279	0.560
0.65	-0.723	-0.651	-0.593	-0.532	-0.478	-0.184	0.115	0.425
0.80	-0.828	-0.713	-0.640	-0.547	-0.459	0.018	0.501	0.982
0.95	-0.824	-0.704	-0.590	-0.469	-0.360	0.228	0.808	1.395
<b>T/°C = 125</b>								
0.05	0.248	0.272	0.291	0.326	0.366	0.512	0.643	0.804
0.20	0.239	0.293	0.336	0.384	0.450	0.694	0.943	1.199
0.35	-0.097	-0.039	0.008	0.049	0.104	0.366	0.612	0.871
0.50	0.067	0.111	0.134	0.184	0.222	0.453	0.656	0.902
0.65	-0.024	0.018	0.053	0.098	0.118	0.325	0.519	0.713
0.80	-0.193	-0.128	-0.070	0.004	0.042	0.381	0.703	1.027
0.95	-0.221	-0.119	-0.062	0.021	0.077	0.468	0.837	1.246
<b>T/°C = 137.5</b>								
0.05	0.690	0.739	0.769	0.825	0.855	1.062	1.287	1.506
0.20	0.460	0.506	0.569	0.602	0.667	0.921	1.203	1.466
0.35	0.346	0.397	0.436	0.475	0.513	0.748	0.970	1.207
0.50	0.445	0.482	0.512	0.512	0.524	0.694	0.866	1.010
0.65	0.422	0.448	0.465	0.461	0.467	0.541	0.640	0.696
0.80	0.194	0.240	0.263	0.269	0.311	0.460	0.649	0.804
0.95	0.144	0.169	0.215	0.225	0.266	0.430	0.625	0.806
<b>T/°C = 150</b>								
0.05	0.929	0.997	1.042	1.102	1.123	1.396	1.652	1.908
0.20	0.549	0.595	0.663	0.719	0.745	1.004	1.271	1.543
0.35	0.583	0.644	0.667	0.695	0.718	0.916	1.090	1.288
0.50	0.612	0.634	0.636	0.655	0.655	0.725	0.798	0.873
0.65	0.603	0.618	0.606	0.587	0.559	0.524	0.495	0.457
0.80	0.351	0.360	0.357	0.338	0.329	0.339	0.339	0.364
0.95	0.288	0.294	0.296	0.268	0.272	0.219	0.204	0.191
<b>T/°C = 162.5</b>								
0.05	1.035	1.089	1.122	1.198	1.259	1.498	1.757	2.040
0.20	0.555	0.593	0.630	0.696	0.748	0.997	1.260	1.524

p /bar	$p^E$ /MPa							
	20	40	60	80	100	200	300	400
0.35	0.670	0.700	0.710	0.752	0.758	0.907	1.031	1.193
0.50	0.598	0.613	0.595	0.623	0.609	0.610	0.614	0.650
0.65	0.593	0.563	0.520	0.526	0.487	0.371	0.252	0.137
0.80	0.351	0.304	0.272	0.243	0.226	0.118	0.023	-0.060
0.95	0.272	0.238	0.185	0.158	0.114	-0.044	-0.212	-0.372
<b>T/°C = 175</b>								
0.05	0.889	0.908	0.938	0.965	1.009	1.182	1.361	1.548
0.20	0.387	0.411	0.459	0.520	0.564	0.796	1.034	1.275
0.35	0.566	0.539	0.563	0.573	0.609	0.667	0.739	0.845
0.50	0.421	0.405	0.413	0.401	0.407	0.396	0.382	0.397
0.65	0.401	0.353	0.319	0.286	0.290	0.121	0.006	-0.082
0.80	0.187	0.168	0.142	0.110	0.090	-0.004	-0.086	-0.152
0.95	0.192	0.134	0.113	0.053	0.045	-0.175	-0.346	-0.484
<b>T/°C = 187.5</b>								
0.05	0.320	0.272	0.304	0.224	0.202	0.087	-0.020	-0.128
0.20	0.008	0.041	0.128	0.122	0.145	0.320	0.469	0.631
0.35	0.186	0.163	0.173	0.145	0.134	0.107	0.095	0.086
0.50	0.026	0.029	0.055	0.033	0.056	0.095	0.147	0.236
0.65	-0.037	-0.066	-0.026	-0.048	-0.040	-0.010	0.035	0.113
0.80	-0.069	-0.058	-0.022	0.034	0.039	0.246	0.426	0.645
0.95	0.073	0.082	0.128	0.154	0.175	0.309	0.450	0.649
<b>T/°C = 200</b>								
0.05	-0.772	-1.013	-1.189	-1.431	-1.605	-2.542	-3.484	-4.356
0.20	-0.622	-0.625	-0.631	-0.649	-0.670	-0.750	-0.824	-0.872
0.35	-0.585	-0.645	-0.690	-0.747	-0.805	-1.048	-1.307	-1.502
0.50	-0.629	-0.594	-0.561	-0.551	-0.491	-0.289	-0.037	0.269
0.65	-0.652	-0.585	-0.502	-0.433	-0.368	0.113	0.623	1.164
0.80	-0.346	-0.190	-0.019	0.183	0.355	1.329	2.314	3.362
0.95	0.081	0.285	0.523	0.732	0.927	2.105	3.273	4.477

## C.2. Aromatics + Nitrogen (AN)

**Table 74.***Estimation of excess volume expansivity ( $a_p^E$ ) of AN at different temperatures and pressures.*

		$a_p^E / \text{kK}^{-1}$							
p /bar		20	40	60	80	100	200	300	400
<b>x<sub>A</sub></b>		<b>T/°C = 100</b>							
0.05		-0.005	-0.004	-0.004	-0.003	-0.003	-0.002	-0.001	0.000
0.20		-0.004	-0.004	-0.004	-0.003	-0.003	-0.002	-0.001	0.000
0.35		-0.006	-0.005	-0.005	-0.004	-0.004	-0.002	-0.001	0.000
0.50		-0.005	-0.005	-0.004	-0.003	-0.003	-0.001	0.001	0.002
0.65		-0.007	-0.006	-0.005	-0.004	-0.004	-0.001	0.001	0.002
0.80		-0.003	-0.003	-0.002	-0.001	-0.001	0.002	0.003	0.005
0.95		0.002	0.001	0.001	0.002	0.001	0.001	0.001	0.001
		<b>T/°C = 112.5</b>							
0.05		-0.007	-0.006	-0.005	-0.005	-0.005	-0.003	-0.002	-0.001
0.20		-0.006	-0.006	-0.005	-0.005	-0.004	-0.002	-0.001	0.000
0.35		-0.007	-0.006	-0.005	-0.005	-0.004	-0.002	-0.001	0.000
0.50		-0.006	-0.005	-0.004	-0.004	-0.003	-0.001	0.000	0.001
0.65		-0.006	-0.005	-0.004	-0.004	-0.003	-0.001	0.001	0.002
0.80		-0.004	-0.003	-0.002	-0.002	-0.001	0.001	0.003	0.004
0.95		0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001
		<b>T/°C = 125</b>							
0.05		-0.009	-0.008	-0.007	-0.006	-0.006	-0.004	-0.002	-0.001
0.20		-0.008	-0.007	-0.007	-0.006	-0.005	-0.003	-0.002	-0.001
0.35		-0.008	-0.007	-0.006	-0.005	-0.005	-0.003	-0.001	0.000
0.50		-0.006	-0.005	-0.005	-0.004	-0.003	-0.001	0.000	0.001
0.65		-0.005	-0.004	-0.004	-0.003	-0.002	0.000	0.001	0.002
0.80		-0.004	-0.003	-0.002	-0.002	-0.001	0.000	0.001	0.002
0.95		0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.001
		<b>T/°C = 137.5</b>							
0.05		-0.012	-0.011	-0.009	-0.008	-0.008	-0.005	-0.003	-0.002
0.20		-0.010	-0.009	-0.008	-0.007	-0.007	-0.004	-0.002	-0.001
0.35		-0.009	-0.008	-0.007	-0.006	-0.005	-0.003	-0.002	-0.001
0.50		-0.006	-0.006	-0.005	-0.004	-0.004	-0.002	-0.001	0.000
0.65		-0.004	-0.004	-0.003	-0.002	-0.002	0.000	0.000	0.001
0.80		-0.004	-0.004	-0.003	-0.002	-0.002	-0.001	0.000	0.000

$\alpha_p^E / \text{kK}^{-1}$								
p /bar	20	40	60	80	100	200	300	400
0.95	-0.001	-0.001	-0.001	0.000	0.000	0.000	0.001	0.001
<b>T/°C = 150</b>								
0.05	-0.015	-0.013	-0.011	-0.010	-0.010	-0.006	-0.004	-0.002
0.20	-0.013	-0.011	-0.010	-0.009	-0.008	-0.005	-0.003	-0.001
0.35	-0.010	-0.009	-0.008	-0.007	-0.006	-0.004	-0.002	-0.001
0.50	-0.008	-0.007	-0.006	-0.005	-0.005	-0.003	-0.002	-0.001
0.65	-0.004	-0.004	-0.003	-0.002	-0.002	-0.001	0.000	0.000
0.80	-0.004	-0.004	-0.004	-0.003	-0.003	-0.002	-0.002	-0.002
0.95	-0.002	-0.002	-0.002	-0.001	-0.001	0.000	0.001	0.001
<b>T/°C = 162.5</b>								
0.05	-0.018	-0.016	-0.013	-0.012	-0.011	-0.006	-0.004	-0.003
0.20	-0.016	-0.013	-0.012	-0.011	-0.009	-0.005	-0.003	-0.002
0.35	-0.012	-0.010	-0.009	-0.007	-0.006	-0.004	-0.003	-0.002
0.50	-0.009	-0.008	-0.007	-0.006	-0.005	-0.004	-0.003	-0.002
0.65	-0.005	-0.004	-0.004	-0.003	-0.003	-0.002	-0.001	-0.001
0.80	-0.005	-0.004	-0.004	-0.004	-0.004	-0.003	-0.003	-0.003
0.95	-0.004	-0.002	-0.002	-0.001	-0.001	0.000	0.001	0.001
<b>T/°C = 175</b>								
0.05	-0.023	-0.018	-0.016	-0.013	-0.012	-0.006	-0.004	-0.003
0.20	-0.020	-0.016	-0.014	-0.012	-0.011	-0.006	-0.004	-0.002
0.35	-0.015	-0.012	-0.010	-0.009	-0.008	-0.004	-0.003	-0.002
0.50	-0.013	-0.010	-0.009	-0.008	-0.007	-0.004	-0.003	-0.003
0.65	-0.009	-0.006	-0.006	-0.005	-0.005	-0.003	-0.002	-0.002
0.80	-0.007	-0.006	-0.005	-0.005	-0.004	-0.003	-0.003	-0.003
0.95	-0.006	-0.004	-0.003	-0.002	-0.002	0.000	0.001	0.001
<b>T/°C = 187.5</b>								
0.05	-0.026	-0.021	-0.017	-0.014	-0.012	-0.006	-0.004	-0.003
0.20	-0.024	-0.019	-0.016	-0.013	-0.011	-0.006	-0.004	-0.003
0.35	-0.018	-0.015	-0.012	-0.010	-0.009	-0.005	-0.003	-0.003
0.50	-0.016	-0.013	-0.011	-0.009	-0.008	-0.004	-0.002	-0.001
0.65	-0.014	-0.011	-0.010	-0.008	-0.006	-0.004	-0.002	-0.001
0.80	-0.010	-0.007	-0.005	-0.004	-0.003	0.000	0.001	0.001
0.95	-0.005	-0.004	-0.003	-0.003	-0.001	-0.001	0.000	0.000
<b>T/°C = 200</b>								

p /bar	$\alpha_p^E / \text{kK}^{-1}$							
	20	40	60	80	100	200	300	400
0.05	-0.0293	-0.0207	-0.0156	-0.0125	-0.0106	-0.0054	-0.0032	-0.0022
0.20	-0.0279	-0.0197	-0.0164	-0.0136	-0.0110	-0.0067	-0.0047	-0.0037
0.35	-0.0230	-0.0169	-0.0132	-0.0108	-0.0093	-0.0050	-0.0031	-0.0019
0.50	-0.0254	-0.0183	-0.0133	-0.0094	-0.0069	-0.0005	0.0028	0.0047
0.65	-0.0304	-0.0215	-0.0180	-0.0136	-0.0097	-0.0019	0.0025	0.0051
0.80	-0.0144	-0.0070	-0.0022	0.0017	0.0037	0.0107	0.0142	0.0164
0.95	-0.0042	-0.0026	-0.0021	-0.0017	-0.0006	-0.0017	-0.0019	-0.0022

**Table 75.**

*Estimation of excess isothermal compressibility ( $\kappa_T^E$ ) of AN at different temperatures and pressures.*

p /bar	$\kappa_T^E / \text{TPa}^{-1}$							
	20	40	60	80	100	200	300	400
$x_A$	<b>T/°C = 100</b>							
0.05	-2.379	-2.489	-2.361	-1.289	-1.419	-0.408	-0.375	0.002
0.20	0.318	-0.122	-0.030	0.421	-0.046	0.425	0.233	0.436
0.35	0.589	0.331	0.091	0.251	0.213	0.473	0.376	0.357
0.50	2.756	2.390	2.104	1.863	1.655	1.052	0.832	0.673
0.65	5.293	5.219	4.563	4.529	4.102	2.774	2.221	1.731
0.80	4.936	5.018	4.187	4.019	3.908	3.029	2.405	1.993
0.95	0.948	0.531	0.736	0.994	0.960	0.933	0.753	0.587
	<b>T/°C = 112.5</b>							
0.05	-5.559	-5.181	-4.488	-3.820	-3.751	-2.210	-1.151	-0.658
0.20	-3.045	-2.941	-2.623	-2.551	-2.328	-1.174	-0.763	-0.433
0.35	-3.703	-2.884	-2.653	-2.820	-2.408	-1.776	-1.145	-0.752
0.50	-1.605	-1.866	-1.029	-1.081	-1.117	-0.877	-0.836	-0.659
0.65	0.532	0.273	0.543	0.475	0.716	0.345	0.233	0.200
0.80	0.232	0.362	0.524	0.586	0.743	0.656	0.562	0.896
0.95	0.503	0.585	1.126	0.653	0.828	0.808	0.756	0.998
	<b>T/°C = 125</b>							
0.05	-10.325	-8.763	-8.088	-7.093	-6.389	-4.280	-2.557	-1.551
0.20	-7.733	-6.578	-7.118	-5.841	-4.989	-3.163	-2.125	-1.731
0.35	-8.926	-7.598	-7.043	-6.577	-5.688	-3.966	-2.480	-2.131
0.50	-5.556	-5.504	-4.797	-5.060	-3.641	-2.824	-2.262	-1.821

p /bar	$\kappa_T^E / \text{TPa}^{-1}$							
	20	40	60	80	100	200	300	400
0.65	-3.619	-4.069	-3.478	-3.355	-2.745	-1.947	-1.503	-1.162
0.80	-4.160	-4.273	-3.286	-2.959	-2.559	-1.292	-1.090	-0.439
0.95	0.390	-0.067	0.226	-0.104	1.089	0.906	0.488	0.773
<b>T/°C = 137.5</b>								
0.05	-18.555	-16.750	-13.532	-12.203	-11.540	-6.240	-4.194	-2.917
0.20	-15.517	-13.636	-11.986	-10.866	-9.241	-5.546	-4.118	-2.847
0.35	-15.948	-13.676	-11.352	-10.671	-9.710	-5.598	-4.139	-3.056
0.50	-11.064	-10.728	-8.697	-7.954	-7.020	-4.737	-3.609	-2.859
0.65	-8.807	-8.454	-7.682	-5.431	-5.635	-3.420	-2.760	-2.058
0.80	-7.735	-7.771	-7.029	-5.256	-4.505	-2.290	-2.028	-1.362
0.95	-0.861	-0.928	-1.415	0.057	0.312	0.619	0.451	0.641
<b>T/°C = 150</b>								
0.05	-29.906	-24.313	-21.360	-19.178	-17.297	-9.434	-6.009	-3.756
0.20	-25.604	-21.991	-19.316	-16.250	-14.514	-8.470	-5.601	-3.719
0.35	-23.763	-19.906	-18.029	-14.824	-13.481	-8.113	-5.568	-3.884
0.50	-17.242	-15.259	-14.561	-11.287	-10.350	-6.385	-4.517	-3.614
0.65	-12.248	-12.610	-10.651	-8.267	-8.019	-4.744	-3.428	-2.723
0.80	-12.231	-10.937	-9.242	-7.143	-7.461	-3.641	-2.016	-1.544
0.95	-3.501	-3.374	-2.734	-1.962	-1.675	-0.442	-0.055	0.237
<b>T/°C = 162.5</b>								
0.05	-44.376	-37.465	-31.302	-27.086	-23.327	-11.965	-7.861	-5.597
0.20	-38.496	-30.718	-28.588	-24.503	-21.085	-11.057	-7.791	-5.407
0.35	-34.389	-27.614	-24.703	-20.285	-16.906	-10.211	-6.695	-5.140
0.50	-25.288	-19.800	-17.364	-15.473	-12.519	-8.056	-5.763	-4.253
0.65	-17.801	-13.623	-11.910	-9.764	-9.722	-5.895	-3.616	-2.823
0.80	-15.263	-11.811	-8.554	-8.763	-7.623	-3.445	-2.016	-1.763
0.95	-8.439	-5.184	-3.730	-3.025	-2.354	-1.071	-0.657	-0.147
<b>T/°C = 175</b>								
0.05	-71.435	-53.976	-46.094	-37.319	-33.649	-15.082	-9.780	-6.648
0.20	-60.222	-47.903	-39.166	-32.610	-29.350	-14.419	-9.286	-6.483
0.35	-52.938	-38.897	-33.252	-28.807	-25.452	-12.165	-7.760	-5.554
0.50	-40.832	-29.901	-23.756	-20.881	-19.029	-9.218	-6.483	-4.648
0.65	-27.857	-17.957	-17.665	-14.971	-11.932	-5.871	-3.925	-3.169
0.80	-24.786	-17.825	-15.183	-11.259	-9.875	-4.011	-2.310	-1.753

$\kappa_T^E / \text{TPa}^{-1}$								
p /bar	20	40	60	80	100	200	300	400
0.95	-18.907	-13.694	-9.826	-8.427	-5.989	-1.258	-0.568	-0.533
<b>T/°C = 187.5</b>								
0.05	-101.225	-80.288	-65.189	-50.589	-41.794	-20.589	-11.652	-8.312
0.20	-92.741	-70.164	-57.056	-45.078	-36.427	-18.223	-11.443	-8.003
0.35	-71.911	-57.446	-45.415	-36.759	-29.859	-15.353	-8.658	-6.760
0.50	-52.666	-42.138	-34.320	-27.443	-23.619	-12.223	-7.448	-5.646
0.65	-37.717	-28.723	-24.690	-19.620	-13.970	-9.303	-5.060	-4.015
0.80	-36.273	-23.822	-17.988	-16.342	-11.492	-5.552	-2.790	-1.914
0.95	-25.523	-18.289	-13.579	-12.386	-7.098	-3.993	-1.260	-0.760
<b>T/°C = 200</b>								
0.05	-157.095	-109.756	-81.742	-64.832	-54.207	-24.665	-13.777	-9.316
0.20	-136.325	-93.702	-74.329	-59.718	-46.171	-22.600	-13.379	-9.228
0.35	-104.036	-74.596	-56.294	-44.521	-37.304	-18.034	-11.312	-7.383
0.50	-93.207	-68.341	-51.222	-38.701	-31.641	-16.001	-9.791	-7.410
0.65	-74.624	-49.434	-44.129	-33.489	-23.994	-13.055	-7.827	-5.772
0.80	-66.479	-44.785	-32.638	-23.227	-20.132	-8.719	-5.109	-3.360
0.95	-35.476	-23.779	-17.509	-12.680	-6.003	-3.631	-1.390	-0.782

**Table 76.**

*Estimation of excess internal pressure ( $p_i^E$ ) of AN at different temperatures and pressures.*

$p_i^E / \text{MPa}$								
p /bar	20	40	60	80	100	200	300	400
<b>T/°C = 100</b>								
$x_A$								
0.05	-0.503	-0.468	-0.446	-0.448	-0.418	-0.324	-0.204	-0.096
0.20	-0.813	-0.760	-0.720	-0.691	-0.638	-0.445	-0.231	-0.023
0.35	-1.076	-1.014	-0.954	-0.902	-0.847	-0.571	-0.296	0.002
0.50	-1.218	-1.123	-1.036	-0.951	-0.863	-0.435	0.000	0.441
0.65	-1.808	-1.713	-1.595	-1.490	-1.386	-0.851	-0.300	0.264
0.80	-1.196	-1.096	-0.961	-0.849	-0.744	-0.178	0.404	0.997
0.95	0.182	0.192	0.187	0.182	0.158	0.156	0.143	0.143
<b>T/°C = 112.5</b>								
0.05	-0.479	-0.457	-0.440	-0.427	-0.391	-0.304	-0.216	-0.114
0.20	-0.666	-0.628	-0.592	-0.548	-0.505	-0.330	-0.135	0.066
0.35	-0.694	-0.656	-0.606	-0.544	-0.501	-0.261	-0.024	0.227

$p^E$ /MPa								
$p$ /bar	20	40	60	80	100	200	300	400
0.50	-0.725	-0.647	-0.596	-0.520	-0.442	-0.110	0.252	0.617
0.65	-0.978	-0.893	-0.807	-0.719	-0.642	-0.207	0.238	0.687
0.80	-0.600	-0.521	-0.438	-0.351	-0.276	0.146	0.587	1.002
0.95	0.043	0.041	0.031	0.050	0.045	0.035	0.059	0.053
<b>T/°C = 125</b>								
0.05	-0.405	-0.402	-0.382	-0.352	-0.345	-0.249	-0.166	-0.077
0.20	-0.506	-0.486	-0.435	-0.400	-0.383	-0.204	-0.017	0.193
0.35	-0.362	-0.341	-0.299	-0.240	-0.213	-0.015	0.173	0.410
0.50	-0.360	-0.303	-0.265	-0.185	-0.167	0.106	0.380	0.660
0.65	-0.365	-0.284	-0.235	-0.151	-0.107	0.216	0.547	0.878
0.80	-0.184	-0.121	-0.083	-0.025	0.020	0.273	0.549	0.808
0.95	-0.043	-0.027	-0.030	-0.008	-0.027	0.011	0.054	0.089
<b>T/°C = 137.5</b>								
0.05	-0.247	-0.235	-0.249	-0.234	-0.213	-0.179	-0.100	-0.011
0.20	-0.284	-0.264	-0.244	-0.213	-0.195	-0.058	0.106	0.286
0.35	-0.056	-0.043	-0.030	0.011	0.034	0.146	0.297	0.458
0.50	-0.075	-0.030	-0.025	0.010	0.032	0.197	0.367	0.557
0.65	0.067	0.109	0.142	0.149	0.200	0.377	0.582	0.786
0.80	0.052	0.088	0.104	0.105	0.113	0.186	0.300	0.391
0.95	-0.075	-0.059	-0.039	-0.053	-0.043	0.009	0.074	0.131
<b>T/°C = 150</b>								
0.05	-0.064	-0.081	-0.082	-0.074	-0.062	-0.050	-0.002	0.062
0.20	-0.086	-0.077	-0.062	-0.060	-0.032	0.061	0.192	0.323
0.35	0.150	0.153	0.167	0.160	0.180	0.235	0.327	0.425
0.50	0.089	0.102	0.122	0.109	0.117	0.173	0.243	0.341
0.65	0.250	0.284	0.287	0.279	0.299	0.345	0.420	0.509
0.80	0.175	0.164	0.137	0.111	0.114	0.003	-0.081	-0.139
0.95	-0.060	-0.041	-0.026	-0.012	-0.006	0.050	0.136	0.207
<b>T/°C = 162.5</b>								
0.05	0.145	0.142	0.127	0.122	0.117	0.079	0.126	0.195
0.20	0.112	0.096	0.131	0.138	0.144	0.176	0.287	0.397
0.35	0.315	0.291	0.302	0.284	0.265	0.285	0.295	0.368
0.50	0.170	0.147	0.141	0.140	0.114	0.105	0.114	0.133

$p_i^E$ /MPa								
$p$ /bar	20	40	60	80	100	200	300	400
0.65	0.293	0.265	0.253	0.241	0.247	0.215	0.163	0.175
0.80	0.181	0.128	0.070	0.059	0.017	-0.208	-0.396	-0.544
0.95	0.010	0.001	0.009	0.027	0.030	0.121	0.201	0.280
<b>T/°C = 175</b>								
0.05	0.453	0.389	0.384	0.346	0.352	0.240	0.259	0.303
0.20	0.361	0.331	0.315	0.300	0.324	0.274	0.319	0.404
0.35	0.488	0.414	0.399	0.397	0.392	0.289	0.258	0.271
0.50	0.244	0.188	0.159	0.152	0.162	0.074	0.065	0.087
0.65	0.196	0.126	0.151	0.132	0.112	0.023	-0.004	-0.005
0.80	0.209	0.138	0.099	0.039	0.011	-0.207	-0.381	-0.521
0.95	0.156	0.140	0.135	0.146	0.145	0.144	0.194	0.269
<b>T/°C = 187.5</b>								
0.05	0.773	0.737	0.706	0.640	0.627	0.500	0.441	0.460
0.20	0.665	0.594	0.565	0.516	0.484	0.380	0.357	0.377
0.35	0.587	0.542	0.494	0.456	0.427	0.334	0.272	0.283
0.50	0.234	0.220	0.214	0.216	0.232	0.278	0.371	0.521
0.65	-0.048	-0.050	-0.037	-0.028	-0.033	0.089	0.206	0.387
0.80	0.248	0.210	0.214	0.254	0.253	0.356	0.485	0.633
0.95	0.294	0.265	0.239	0.245	0.204	0.170	0.111	0.092
<b>T/°C = 200</b>								
0.05	1.246	1.136	1.051	1.009	0.991	0.807	0.703	0.669
0.20	0.952	0.843	0.786	0.745	0.672	0.483	0.368	0.305
0.35	0.644	0.597	0.553	0.515	0.506	0.448	0.468	0.507
0.50	0.292	0.345	0.397	0.447	0.527	0.968	1.474	2.045
0.65	-0.368	-0.312	-0.187	-0.101	-0.028	0.569	1.224	1.936
0.80	0.443	0.595	0.766	0.947	1.148	2.147	3.195	4.265
0.95	0.455	0.399	0.337	0.280	0.191	-0.004	-0.225	-0.428

### C.3. Nitrogen + Sulfur (NS)

**Table 77.***Estimation of excess volume expansivity ( $a_p^E$ ) of NS at different temperatures and pressures.*

		$a_p^E / \text{kK}^{-1}$							
p /bar		20	40	60	80	100	200	300	400
<b>x<sub>A</sub></b>		<b>T/°C = 100</b>							
0.05		-0.001	-0.001	-0.001	-0.001	-0.001	0.000	0.000	0.000
0.20		0.003	0.002	0.001	0.001	0.001	-0.001	-0.003	-0.004
0.35		-0.002	-0.002	-0.002	-0.002	-0.002	-0.002	-0.001	-0.001
0.50		-0.004	-0.004	-0.003	-0.003	-0.003	-0.002	-0.001	-0.001
0.65		-0.003	-0.003	-0.002	-0.002	-0.002	-0.001	0.000	0.001
0.80		-0.007	-0.007	-0.006	-0.006	-0.006	-0.004	-0.003	-0.003
0.95		-0.003	-0.003	-0.002	-0.002	-0.002	0.000	0.000	0.001
		<b>T/°C = 112.5</b>							
0.05		0.000	0.000	0.000	0.001	0.001	0.001	0.002	0.002
0.20		0.002	0.002	0.001	0.001	0.001	0.000	-0.001	-0.002
0.35		-0.002	-0.002	-0.001	-0.001	-0.001	0.000	0.000	0.000
0.50		-0.004	-0.003	-0.003	-0.003	-0.002	-0.001	0.000	0.000
0.65		-0.004	-0.003	-0.003	-0.003	-0.002	-0.001	0.000	0.001
0.80		-0.008	-0.007	-0.007	-0.006	-0.006	-0.004	-0.003	-0.002
0.95		-0.005	-0.005	-0.004	-0.004	-0.003	-0.002	-0.001	0.000
		<b>T/°C = 125</b>							
0.05		0.001	0.001	0.002	0.002	0.002	0.003	0.003	0.004
0.20		0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001
0.35		-0.001	-0.001	-0.001	0.000	0.000	0.001	0.001	0.002
0.50		-0.004	-0.003	-0.003	-0.002	-0.002	0.000	0.001	0.001
0.65		-0.005	-0.004	-0.003	-0.003	-0.003	-0.001	0.000	0.001
0.80		-0.008	-0.008	-0.007	-0.007	-0.006	-0.004	-0.002	-0.001
0.95		-0.008	-0.007	-0.006	-0.006	-0.005	-0.003	-0.001	0.000
		<b>T/°C = 137.5</b>							
0.05		0.002	0.003	0.003	0.004	0.004	0.005	0.005	0.005
0.20		0.000	0.000	0.001	0.001	0.002	0.002	0.003	0.003
0.35		-0.001	0.000	0.000	0.000	0.001	0.002	0.002	0.003
0.50		-0.004	-0.003	-0.002	-0.002	-0.001	0.001	0.001	0.002
0.65		-0.006	-0.005	-0.005	-0.004	-0.003	-0.001	0.001	0.001
0.80		-0.010	-0.009	-0.007	-0.007	-0.006	-0.003	-0.002	-0.001

$\alpha_p^E / \text{kK}^{-1}$								
p /bar	20	40	60	80	100	200	300	400
0.95	-0.011	-0.010	-0.009	-0.008	-0.007	-0.004	-0.002	-0.001
<b>T/°C = 150</b>								
0.05	0.003	0.003	0.004	0.004	0.005	0.006	0.006	0.007
0.20	-0.001	0.000	0.001	0.001	0.002	0.004	0.005	0.006
0.35	-0.001	-0.001	0.000	0.001	0.001	0.003	0.003	0.004
0.50	-0.005	-0.004	-0.003	-0.002	-0.001	0.001	0.002	0.003
0.65	-0.008	-0.006	-0.006	-0.005	-0.004	-0.001	0.001	0.002
0.80	-0.012	-0.010	-0.009	-0.007	-0.006	-0.003	-0.001	0.000
0.95	-0.015	-0.013	-0.011	-0.010	-0.008	-0.005	-0.002	-0.001
<b>T/°C = 162.5</b>								
0.05	0.003	0.003	0.005	0.005	0.005	0.006	0.007	0.007
0.20	-0.002	-0.001	0.001	0.002	0.002	0.006	0.007	0.008
0.35	-0.002	-0.001	0.000	0.001	0.001	0.003	0.004	0.004
0.50	-0.006	-0.005	-0.003	-0.002	-0.002	0.001	0.002	0.003
0.65	-0.009	-0.008	-0.006	-0.005	-0.004	-0.001	0.000	0.002
0.80	-0.014	-0.012	-0.010	-0.008	-0.007	-0.003	-0.001	0.000
0.95	-0.019	-0.016	-0.014	-0.012	-0.010	-0.005	-0.003	-0.001
<b>T/°C = 175</b>								
0.05	0.002	0.003	0.003	0.004	0.004	0.005	0.005	0.005
0.20	-0.003	-0.001	0.000	0.001	0.002	0.005	0.006	0.007
0.35	-0.004	-0.002	-0.001	0.000	0.000	0.002	0.003	0.004
0.50	-0.010	-0.007	-0.005	-0.004	-0.003	0.000	0.002	0.002
0.65	-0.012	-0.009	-0.008	-0.006	-0.005	-0.002	0.000	0.001
0.80	-0.018	-0.013	-0.012	-0.010	-0.009	-0.004	-0.002	-0.001
0.95	-0.024	-0.018	-0.015	-0.012	-0.011	-0.005	-0.003	-0.001
<b>T/°C = 187.5</b>								
0.05	-0.002	-0.001	-0.002	-0.001	0.000	0.000	0.000	0.000
0.20	-0.004	-0.003	-0.003	-0.002	-0.002	-0.001	-0.001	-0.001
0.35	-0.007	-0.006	-0.005	-0.004	-0.003	-0.002	-0.001	0.000
0.50	-0.015	-0.012	-0.010	-0.008	-0.006	-0.003	-0.001	-0.001
0.65	-0.013	-0.010	-0.009	-0.007	-0.006	-0.004	-0.003	-0.002
0.80	-0.023	-0.019	-0.016	-0.014	-0.012	-0.007	-0.005	-0.004
0.95	-0.027	-0.021	-0.016	-0.013	-0.011	-0.006	-0.003	-0.002
<b>T/°C = 200</b>								

$\alpha_p^E / \text{kK}^{-1}$								
p /bar	20	40	60	80	100	200	300	400
0.05	-0.0141	-0.0127	-0.0133	-0.0137	-0.0132	-0.0141	-0.0142	-0.0146
0.20	-0.0060	-0.0077	-0.0099	-0.0125	-0.0141	-0.0208	-0.0242	-0.0267
0.35	-0.0190	-0.0163	-0.0142	-0.0136	-0.0129	-0.0116	-0.0114	-0.0110
0.50	-0.0302	-0.0225	-0.0194	-0.0173	-0.0156	-0.0115	-0.0098	-0.0090
0.65	-0.0138	-0.0113	-0.0107	-0.0095	-0.0089	-0.0092	-0.0094	-0.0096
0.80	-0.0330	-0.0262	-0.0236	-0.0209	-0.0194	-0.0151	-0.0132	-0.0122
0.95	-0.0282	-0.0205	-0.0153	-0.0124	-0.0098	-0.0055	-0.0046	-0.0041

**Table 78.**

*Estimation of excess isothermal compressibility ( $\kappa_T^E$ ) of NS at different temperatures and pressures.*

$\kappa_T^E / \text{TPa}^{-1}$								
p /bar	20	40	60	80	100	200	300	400
<b>x<sub>A</sub></b>	<b>T/°C = 100</b>							
0.05	4.171	3.433	3.296	3.412	3.279	2.161	1.961	1.403
0.20	-2.612	-2.727	-2.710	-1.843	-1.966	-1.704	-1.314	-1.045
0.35	4.670	3.866	3.471	3.953	3.351	1.966	1.693	1.208
0.50	1.155	0.374	0.592	0.888	1.000	1.144	1.191	1.161
0.65	2.330	1.745	1.615	1.699	1.736	0.981	0.520	0.525
0.80	-0.278	-0.903	-1.021	-0.474	-0.705	-0.868	-1.082	-0.798
0.95	-2.016	-1.438	-1.225	-0.793	-0.474	0.777	0.724	1.300
	<b>T/°C = 112.5</b>							
0.05	2.660	2.505	2.494	2.626	2.791	1.737	1.705	1.272
0.20	-0.467	-0.299	-0.360	0.154	0.128	0.087	0.234	-0.034
0.35	3.612	3.252	2.910	2.796	2.604	2.024	1.251	0.992
0.50	-1.478	-1.722	-0.573	-0.766	-0.631	0.162	0.558	0.657
0.65	0.178	0.008	0.683	0.070	-0.074	0.188	-0.046	-0.301
0.80	-4.082	-3.376	-3.271	-3.234	-2.888	-2.367	-1.782	-1.613
0.95	-5.359	-4.022	-3.809	-3.372	-2.932	-1.012	0.000	0.585
	<b>T/°C = 125</b>							
0.05	1.901	1.195	1.600	1.092	1.137	0.692	0.666	0.777
0.20	0.851	0.719	1.639	0.910	0.905	0.751	0.545	0.213
0.35	1.954	1.748	1.501	1.784	1.362	0.876	0.814	0.563

p /bar	$\kappa_T^E / \text{TPa}^{-1}$							
	20	40	60	80	100	200	300	400
0.50	-5.010	-4.257	-4.003	-2.940	-2.637	-1.256	-0.275	-0.003
0.65	-2.817	-3.263	-1.958	-2.429	-2.602	-1.772	-1.199	-1.030
0.80	-7.424	-7.175	-6.792	-6.733	-6.098	-4.587	-3.613	-2.900
0.95	-10.592	-8.972	-7.940	-6.956	-6.422	-2.678	-1.314	-0.448
<b>T/°C = 137.5</b>								
0.05	-0.816	-0.580	-0.811	0.252	0.537	0.223	0.230	-0.061
0.20	-0.873	-0.744	0.059	0.600	0.536	0.178	0.270	0.207
0.35	-0.623	-0.381	-0.875	-0.837	-0.140	-0.119	-0.362	-0.510
0.50	-10.721	-9.446	-7.028	-6.243	-4.995	-2.286	-1.465	-0.997
0.65	-9.482	-7.823	-6.890	-6.413	-5.589	-3.552	-2.603	-2.508
0.80	-15.206	-13.703	-11.145	-11.038	-9.699	-6.718	-5.095	-4.425
0.95	-19.513	-18.142	-13.905	-13.207	-10.164	-5.600	-2.647	-1.627
<b>T/°C = 150</b>								
0.05	-5.026	-3.849	-1.666	-2.751	-1.538	-0.503	-0.177	0.083
0.20	-3.749	-4.538	-2.557	-2.130	-1.558	-0.794	-0.633	-0.401
0.35	-4.530	-4.950	-3.631	-2.301	-1.706	-0.992	-0.753	-0.374
0.50	-17.208	-15.569	-11.670	-11.029	-8.930	-4.214	-2.579	-1.073
0.65	-16.734	-13.379	-12.277	-11.740	-8.990	-6.048	-4.420	-3.362
0.80	-24.230	-19.718	-18.292	-15.638	-13.886	-9.151	-6.971	-5.250
0.95	-33.273	-27.086	-24.092	-19.693	-16.415	-8.856	-4.531	-2.720
<b>T/°C = 162.5</b>								
0.05	-6.921	-7.647	-3.030	-4.562	-3.969	-1.232	-0.952	-0.700
0.20	-12.087	-10.434	-8.420	-7.701	-7.026	-2.835	-2.185	-1.786
0.35	-10.621	-7.552	-5.737	-5.290	-5.375	-2.406	-1.597	-1.545
0.50	-26.359	-22.864	-18.222	-15.599	-13.258	-5.959	-3.450	-2.219
0.65	-26.074	-22.649	-19.032	-16.824	-14.528	-8.575	-6.392	-4.561
0.80	-36.702	-30.657	-25.853	-23.196	-20.078	-11.783	-9.064	-7.029
0.95	-51.479	-42.823	-35.514	-30.650	-24.425	-12.652	-7.505	-4.421
<b>T/°C = 175</b>								
0.05	-11.290	-9.455	-8.539	-5.608	-5.359	-3.216	-1.599	-1.068
0.20	-23.640	-17.619	-15.681	-13.232	-12.421	-7.052	-4.667	-3.048
0.35	-18.413	-13.121	-11.569	-9.410	-7.077	-3.564	-2.696	-2.281
0.50	-43.408	-30.870	-26.195	-21.310	-19.463	-8.337	-5.313	-3.247
0.65	-44.219	-33.501	-28.846	-23.267	-21.560	-11.164	-7.659	-5.505

$\kappa_T^E / \text{TPa}^{-1}$								
p /bar	20	40	60	80	100	200	300	400
0.80	-55.972	-41.952	-38.766	-32.386	-28.613	-16.235	-11.163	-8.249
0.95	-83.566	-61.119	-50.927	-40.128	-35.788	-15.454	-8.893	-5.394
<b>T/°C = 187.5</b>								
0.05	-14.232	-11.105	-12.267	-7.950	-5.255	-2.854	-1.800	-0.954
0.20	-34.922	-26.219	-26.307	-18.436	-15.006	-8.133	-5.271	-4.155
0.35	-24.627	-20.153	-16.126	-14.277	-9.908	-6.416	-3.772	-3.130
0.50	-61.200	-47.921	-39.056	-31.037	-25.050	-11.239	-6.175	-4.128
0.65	-58.225	-44.745	-39.668	-31.703	-25.766	-13.626	-8.600	-6.412
0.80	-81.833	-66.574	-54.242	-43.995	-36.525	-20.186	-13.344	-10.115
0.95	-120.876	-90.357	-70.942	-57.167	-46.654	-20.667	-11.115	-7.458
<b>T/°C = 200</b>								
0.05	-19.749	-9.956	-9.716	-8.766	-4.886	-2.985	-0.807	-0.666
0.20	-37.254	-21.984	-15.245	-12.826	-9.477	-5.562	-2.755	-2.117
0.35	-44.932	-30.711	-20.170	-16.750	-13.015	-5.942	-4.528	-2.947
0.50	-105.480	-67.618	-51.756	-41.082	-32.444	-13.749	-6.950	-4.395
0.65	-79.528	-57.939	-46.387	-34.786	-27.591	-14.687	-9.178	-6.421
0.80	-121.505	-86.248	-69.787	-55.514	-46.953	-23.784	-15.168	-10.929
0.95	-176.774	-127.433	-94.367	-74.587	-57.615	-23.669	-13.502	-8.101

**Table 79.**

*Estimation of excess internal pressure ( $p_i^E$ ) of NS at different temperatures and pressures.*

$p_i^E / \text{MPa}$								
p /bar	20	40	60	80	100	200	300	400
<b>T/°C = 100</b>								
$x_A$								
0.05	-0.764	-0.727	-0.705	-0.686	-0.664	-0.523	-0.419	-0.278
0.20	0.817	0.738	0.653	0.547	0.466	0.023	-0.435	-0.884
0.35	-0.954	-0.927	-0.906	-0.912	-0.885	-0.784	-0.718	-0.622
0.50	-0.781	-0.750	-0.740	-0.732	-0.729	-0.687	-0.621	-0.564
0.65	-0.740	-0.688	-0.654	-0.616	-0.577	-0.364	-0.147	0.055
0.80	-1.143	-1.102	-1.070	-1.059	-1.027	-0.894	-0.741	-0.616
0.95	-0.304	-0.292	-0.278	-0.265	-0.252	-0.200	-0.104	-0.050
<b>T/°C = 112.5</b>								
0.05	-0.318	-0.279	-0.245	-0.215	-0.188	0.011	0.182	0.379
0.20	0.339	0.289	0.247	0.184	0.140	-0.089	-0.324	-0.544

$p_i^E$ /MPa								
$p$ /bar	20	40	60	80	100	200	300	400
0.35	-0.645	-0.615	-0.581	-0.557	-0.539	-0.402	-0.251	-0.113
0.50	-0.429	-0.401	-0.402	-0.383	-0.354	-0.279	-0.186	-0.092
0.65	-0.611	-0.564	-0.534	-0.470	-0.413	-0.190	0.058	0.322
0.80	-0.849	-0.829	-0.789	-0.754	-0.718	-0.550	-0.387	-0.194
0.95	-0.333	-0.337	-0.311	-0.289	-0.267	-0.204	-0.141	-0.052
<b>T/°C = 125</b>								
0.05	0.055	0.109	0.146	0.212	0.258	0.516	0.752	0.994
0.20	0.094	0.091	0.072	0.088	0.089	0.090	0.094	0.112
0.35	-0.347	-0.319	-0.275	-0.233	-0.198	0.004	0.182	0.397
0.50	-0.106	-0.081	-0.059	-0.029	-0.013	0.112	0.237	0.380
0.65	-0.448	-0.388	-0.356	-0.274	-0.216	0.055	0.320	0.612
0.80	-0.576	-0.532	-0.488	-0.422	-0.389	-0.168	0.051	0.276
0.95	-0.294	-0.288	-0.274	-0.235	-0.218	-0.167	-0.086	0.027
<b>T/°C = 137.5</b>								
0.05	0.386	0.443	0.510	0.562	0.617	0.925	1.235	1.553
0.20	0.050	0.098	0.132	0.177	0.227	0.477	0.717	0.959
0.35	-0.070	-0.025	0.035	0.092	0.122	0.371	0.626	0.904
0.50	0.211	0.235	0.241	0.280	0.299	0.434	0.615	0.795
0.65	-0.194	-0.157	-0.109	-0.046	-0.001	0.289	0.572	0.919
0.80	-0.248	-0.200	-0.190	-0.124	-0.088	0.154	0.406	0.698
0.95	-0.126	-0.104	-0.127	-0.092	-0.112	-0.041	0.023	0.142
<b>T/°C = 150</b>								
0.05	0.592	0.649	0.698	0.788	0.830	1.173	1.510	1.841
0.20	0.122	0.220	0.287	0.373	0.448	0.918	1.379	1.839
0.35	0.125	0.190	0.235	0.276	0.330	0.606	0.905	1.197
0.50	0.410	0.445	0.458	0.507	0.530	0.676	0.874	1.046
0.65	0.005	0.036	0.095	0.161	0.194	0.482	0.788	1.111
0.80	0.007	0.030	0.083	0.117	0.171	0.427	0.718	1.010
0.95	0.087	0.077	0.089	0.080	0.077	0.124	0.179	0.284
<b>T/°C = 162.5</b>								
0.05	0.682	0.773	0.799	0.896	0.964	1.270	1.618	1.961
0.20	0.358	0.469	0.574	0.689	0.807	1.347	1.940	2.536
0.35	0.288	0.320	0.370	0.425	0.493	0.776	1.091	1.420

$p_i^E$ /MPa								
$p$ /bar	20	40	60	80	100	200	300	400
0.50	0.558	0.597	0.623	0.655	0.685	0.822	1.021	1.233
0.65	0.215	0.265	0.303	0.348	0.394	0.638	0.931	1.217
0.80	0.234	0.260	0.293	0.350	0.395	0.611	0.919	1.235
0.95	0.367	0.357	0.348	0.348	0.320	0.330	0.384	0.461
<b>T/°C = 175</b>								
0.05	0.629	0.666	0.717	0.749	0.804	1.059	1.292	1.553
0.20	0.579	0.636	0.739	0.831	0.930	1.396	1.875	2.350
0.35	0.310	0.320	0.386	0.428	0.454	0.685	0.959	1.247
0.50	0.648	0.611	0.642	0.653	0.697	0.781	0.939	1.121
0.65	0.487	0.460	0.495	0.499	0.548	0.658	0.849	1.054
0.80	0.403	0.384	0.445	0.469	0.518	0.664	0.885	1.136
0.95	0.762	0.667	0.654	0.579	0.606	0.485	0.469	0.499
<b>T/°C = 187.5</b>								
0.05	0.264	0.260	0.280	0.238	0.222	0.185	0.156	0.122
0.20	0.649	0.613	0.630	0.558	0.529	0.428	0.345	0.271
0.35	0.132	0.130	0.133	0.142	0.119	0.185	0.244	0.335
0.50	0.530	0.507	0.491	0.469	0.455	0.389	0.389	0.431
0.65	0.614	0.581	0.575	0.533	0.497	0.400	0.346	0.327
0.80	0.488	0.456	0.435	0.401	0.385	0.347	0.388	0.472
0.95	1.169	1.071	1.001	0.947	0.901	0.663	0.503	0.434
<b>T/°C = 200</b>								
0.05	-0.470	-0.659	-0.800	-0.958	-1.133	-1.890	-2.656	-3.373
0.20	0.388	0.001	-0.352	-0.690	-1.034	-2.694	-4.369	-6.009
0.35	-0.263	-0.404	-0.550	-0.660	-0.773	-1.299	-1.741	-2.189
0.50	0.256	0.059	-0.064	-0.174	-0.296	-0.772	-1.184	-1.525
0.65	0.722	0.599	0.461	0.310	0.183	-0.382	-0.908	-1.409
0.80	0.373	0.225	0.096	-0.027	-0.134	-0.639	-1.065	-1.428
0.95	1.692	1.557	1.425	1.328	1.199	0.738	0.398	0.078