

Vapor-liquid equilibrium data for the carbon dioxide and oxygen (CO₂ + O₂) system at the temperatures 218, 233, 253, 273, 288 and 298 K and pressures up to 14 MPa

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Abstract

Accurate thermophysical data for the CO₂-rich mixtures relevant for carbon capture, transport and storage (CCS) are essential for the development of the accurate equations of state (EOS) and models needed for the design and operation of the processes within CCS. Vapor-liquid equilibrium measurements for the binary system CO₂+O₂ are reported at 218, 233, 253, 273, 288 and 298 K, with estimated standard uncertainties of maximum 8 mK in temperature, maximum 3 kPa in pressure, and maximum 0.0031 in the mole fractions of the phases in the mixture critical regions, and 0.0005 in the mole fractions outside the critical regions. These measurements are compared with existing data. Although some data exists, there are little trustworthy literature data around critical conditions, and the measurements in the present work indicate a need to revise the parameters of existing models. The data in the present work has significantly less scatter than most of the literature data, and range from the vapor pressure of pure CO₂ to close to the mixture critical point pressure at all six temperatures. With the measurements in the present work, the data situation for the CO₂+O₂ system is significantly improved, forming the basis to develop better equations of state for the system. A scaling law model is fitted to the critical region data of each isotherm, and high accuracy estimates for the critical composition and pressure are found. The Peng-Robinson EOS with the alpha correction by Mathias and Copeman, the mixing rules by Wong and Sandler, and the NRTL excess Gibbs energy model is fitted to the data in the present work, with a maximum absolute average deviation of 0.01 in mole fraction.

Keywords:

vapor-liquid equilibrium, experimental measurements, carbon dioxide, oxygen, CO₂ capture and storage

1. Introduction

In the present study, vapor-liquid equilibrium (VLE) measurements for the CO₂+O₂ system are presented. It follows Westman et al. [1], which investigated the VLE of the CO₂+N₂ system. The need for new data for these systems and the other mixtures relevant for carbon capture, transport and storage (CCS) has been discussed for instance in the recently reported comprehensive literature studies by [2, 3, 4, 5]. Calculations using existing equations of state (EOS) [3, 6] show that even small amounts of impurities in CO₂-rich mixtures can significantly affect the behavior of the fluid [5, 7]. As an example, the maximum pressure at which a mixture of CO₂ and 5% O₂ can be in the two-phase region, the cricondenbar, will increase to approximately 8.4 MPa compared to the critical pressure of CO₂, 7.3773 MPa. Even with the recent progress of molecular modeling, empirical equations of state still provide the most accurate description of thermodynamic properties of such systems. Accurate data are required in order to develop such accurate models needed for the design and operation of various processes

within CCS. In the development and fitting of the highly flexible and potentially accurate multi-parameter equation of state EOS-CG for CCS mixtures, the development of the model for the CO₂+O₂ system suffered from the lack of high quality data [3, 4]. For instance, some of the seemingly most accurate available vapor-liquid equilibrium data for the CO₂+O₂ system were not consistent with the vapor pressure of pure CO₂ [3, 4], indicating an error in the measured pressure, temperature or composition of these data. The objective of the measurements in the present work was to reconcile the inconsistencies and cover gaps in the available literature data, including states close to critical conditions and temperatures above 273.15 K, where little data of sufficient quality existed.

The work presented here was part of a project called CO₂Mix. As described by Løvseth et al. [7], the CO₂Mix project aimed at performing accurate vapor-liquid equilibrium, speed of sound and density measurements of CO₂-rich mixtures at conditions relevant for transport and conditioning in CCS [5, 8]. As part of this project, a setup has been specifically designed and constructed in order to perform highly accurate phase equilibria measurements on CO₂-rich mixtures under relevant conditions for CCS. This setup has been described in detail in [9, 1]. The experimental appara-

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tus was validated by the VLE measurements on the CO₂+N₂ system performed by Westman et al. [1], as data of high quality were available for this system.

In the present paper, VLE measurements for the CO₂+O₂ system are reported for six isotherms at 218.15, 233.14, 253.15, 273.15, 288.14 and 298.14 K, spanning the region from close to the triple point temperature to close to the critical temperature of pure CO₂. The pressure ranges from 0.56 to 14.4 MPa. Comparison with existing data and EOSs are provided. Furthermore, an EOS is fitted to the data, with the possibility for use over the whole temperature range of the experimental data.

Special care has been taken to present the results and analysis in accordance with the IUPAC Guidelines for reporting of phase equilibrium measurements given in the work by Chirico et al. [10]. In particular, a thorough estimation of the standard uncertainties, as specified in the ISO Guide for the Estimation of Uncertainty in Measurement, commonly referred to as “GUM” [11], has been performed.

In the following the experimental setup and procedures are described in Section 2, the uncertainty analysis in Section 3. Results will be presented, discussed and analyzed in Sections 4 and 5, including fitting of EOS parameters before conclusions are drawn in Section 6. The detailed experimental data for liquid, vapor and supercritical states are tabulated in Appendix A.

2. Experimental apparatus

2.1. Description of setup

The apparatus used for the VLE measurements in the present work was described in [1]. Therefore, only a short summary of the experimental setup will be given here. A diagram of the cell and apparatus is shown in Fig. 1.

As described in [1], the measurements were performed using an isothermal analytical method with a variable-volume cell. This type of methodology has been described in, for example, [12].

According to Gibbs’ phase rule, for a system of two components with two coexisting phases, only two intensive variables can be varied freely. In the experiments in the present work, the temperature and pressure were the independent variables. The equilibrium cell, kept at constant temperature using a thermostatic bath, was filled with both CO₂ and O₂ until both liquid and vapor phases were present. A stirrer was used to mix the content to a stabilization of the temperature and pressure at their equilibrium values. The liquid and vapor phase CO₂ mole fractions at VLE were then the dependent variables. The temperature and pressure were measured. After stopping the stirrer, and waiting for the phases to settle according to density, samples of both the liquid and vapor phases were withdrawn from the cell to determine the VLE phase compositions. The samples were withdrawn using RolsiTM electromagnetic samplers (Armines patent [13]. Pneumatic version of the RolsiTM sampler described in [14]), one with the capillary inlet placed in the top of the vapor

phase, and one placed in the liquid phase. Several samples were taken of both phases. The samples were analyzed using a gas chromatograph (GC) with helium as the carrier gas, calibrated against gravimetrically prepared calibration gas mixtures. To prevent a decrease in the cell pressure due to the removal of mass from the cell, a plate bellows placed inside the cell was expanded to decrease the cell volume when samples were withdrawn. The bellows could be expanded approximately 1 cm³. The equilibrium cell consisted of a transparent sapphire cylinder placed between two titanium flanges, the internal cell volume being approximately 100 cm³.

2.2. Calibration

The calibration of the temperature and pressure sensors performed in [1] was used in the present work. The calibration was performed in-house. The temperature sensors were calibrated against fixed point cells according to the International Temperature Scale of 1990 (ITS-90). The pressure sensors were calibrated against a recently calibrated dead weight tester. Details concerning the estimated temperature and pressure measurement uncertainties are given in Section 3.2 below, and discussed in detail in [1].

The GC was calibrated against calibration gas mixtures prepared in-house using our custom built apparatus for gravimetric preparation of mixtures. Details about the calibration gas mixtures and the calibration can be found in Section 3.3 below. The manufacturer’s specification of the purities of these samples are given in Table 1. No additional analysis of the specified purities was performed.

2.3. Experimental procedures

2.3.1. General

The experimental procedures were quite similar to those of [1]. The complete procedure will be given here:

Before starting a VLE experiment, the whole circuit in connection with the VLE cell was evacuated, using the vacuum pump. The evacuation included the gas lines to the cell from the gas cylinders of pure CO₂ and O₂, and all lines transporting the gases into the cell.

The CO₂ pump and O₂ impurity pump and lines were first evacuated once, and then flushed with the respective gases to dilute any remaining impurities in the lines and pumps. This evacuation and flushing were repeated 5 times for each pump. After the final evacuation, the gases were filled onto their respective lines and pumps, and maintained at a pressure of at least 0.5 MPa to prevent contamination of the gases. After the flushing of the gas lines and pumps, the cell was flushed with CO₂, and evacuated. As with the pumps, the flushing and evacuation were repeated 5 times.

Following the flushing, and with the thermostatic bath kept at the desired temperature, CO₂ was injected until the volume fraction of liquid CO₂ was approximately 25% of the cell. The stirrer then ran until the measured pressure and temperature had stabilized. After the stirrer had been turned

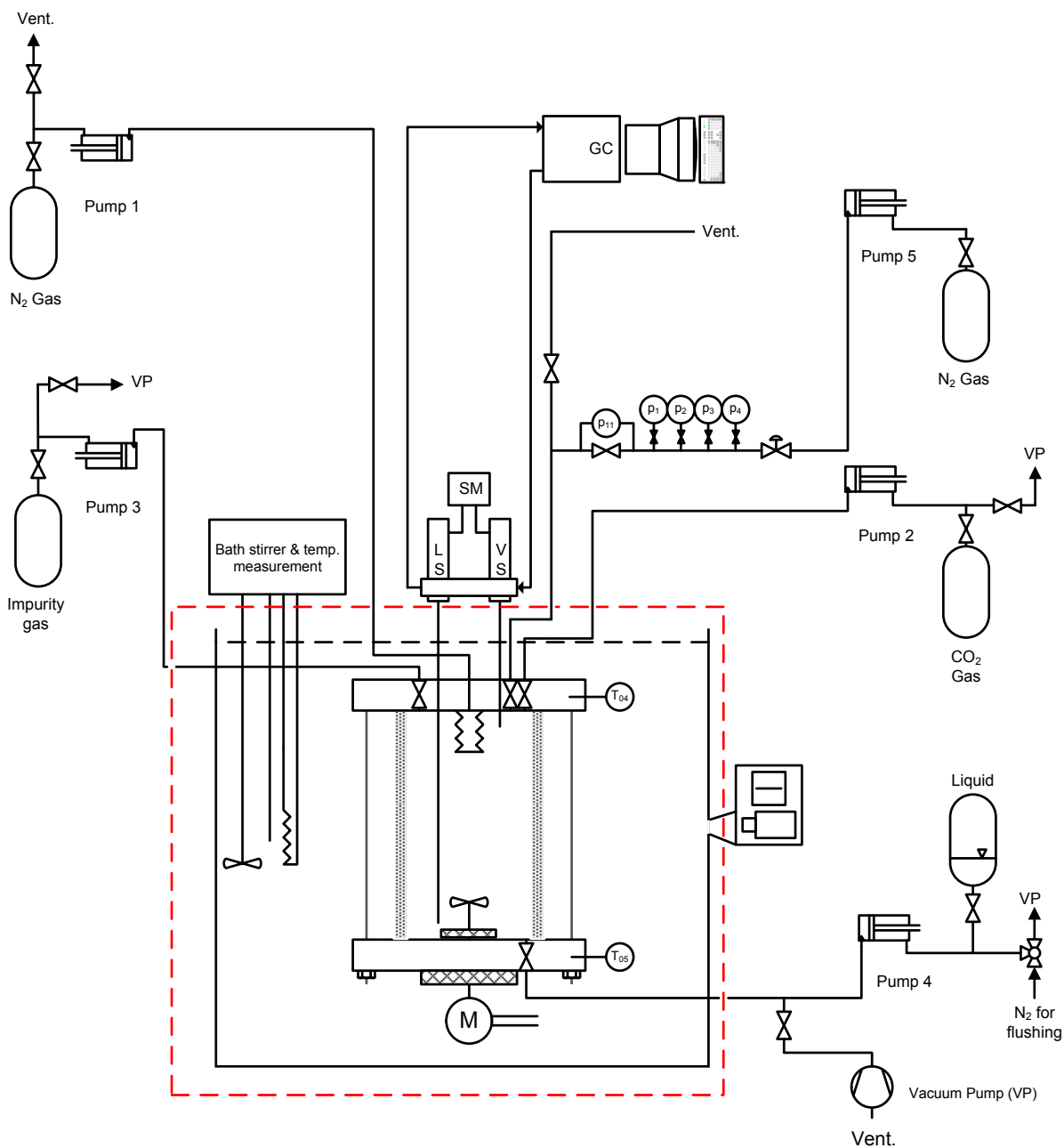


Fig. 1. Figure modified from [1]: Principal diagram of cell and ancillary apparatus. LS,VS: Liquid and vapor phase Rolsi™ samplers, respectively. SM: Rolsi™ controller. M: Gear for rotating permanent magnet below cell, which rotates stirrer inside cell. Gear connected to electric motor outside bath. T_{04} : Top flange SPRT. T_{05} : Bottom flange SPRT.

off, the vapor pressure of CO₂ was measured. If the measured vapor pressure were within the combined uncertainty of the Span-Wagner EOS [6] and our measurements, the purity of the CO₂ in the cell, and the accuracy of the current temperature and pressure measurements, were deemed to be sufficient.

After the CO₂ vapor pressure measurements, the stirrer was started and O₂ was filled onto the cell to increase the pressure. As part of the process of adjusting the pressure to the desired level, the volume fraction of liquid phase in the cell was adjusted to allow for as large as possible vapor samples, either by injecting more CO₂ or venting out some of the vapor or liquid phase. Based on VLE calculations using EOS-CG [3] for the CO₂+O₂ mixture, at constant temperature, as the pressure increased from the vapor pressure of CO₂ up to the critical pressure of the mixture, the difference between the densities of the liquid and vapor phases decreased: the density of the liquid phase decreased and that of the vapor phase increased, and ultimately approached the same value at the critical point. Taking this behavior into account, and considering the limitations of the stirrer size on the minimum liquid level, the liquid volume fraction was adjusted to around 25% for the VLE measurements at the lowest pressures at each temperature, and was gradually increased to around 50% for the measurements in the critical region.

When the pressure and temperature measurements had been stable for at least 20 min, the stirrer was turned off, and the vapor and liquid phases were left to settle before sampling started. The time allowed for settlement of the phases ranged from 30 min to 3 hours, depending on the proximity to the mixture critical pressure. At pressures between the CO₂ vapor pressure and the turning point in the vapor phase composition, the difference in densities of the liquid and vapor phase was quite large, and for these measurements we waited around 30 min for the phases to settle before sampling started. At pressures above the turning point in vapor phase composition, the settling time was increased to 1 hour.

When the pressure was increased to the point where it was observed that running the stirrer caused the phase boundary to disappear, the settling time was increased to 3 hours. At these pressures approaching the critical point, the small density difference of the phases necessitated these longer settling times. During the settling time, the borescope was used to take a picture of the cell content every 30 min. Immediately after the stirrer was turned off, both phases were cloudy white. After 2 hours, the phases were less cloudy, and it was not possible to see a difference in the opacity during

the last of these three hours.

During the settling period, the borescope was withdrawn from the thermostatic bath immediately after use to prevent unintended heat transfer from the surroundings into the bath fluid. At the end of the settling period, the borescope was put in for a very short time to confirm the existence of a liquid and vapor phase, and a visual measurement of the volume occupied by the phases was performed.

After the settling period, first the liquid and then the vapor phase was sampled. Nominally, 7 samples were taken from each phase. Upon sampling, the bellows was expanded to compensate for the pressure drop. A sample was withdrawn from the cell every 25 min. For some of the series of liquid and vapor samples at a certain temperature and pressure, we were not able to take as much as 7 samples, as we reached the maximum expansion limit of the bellows.

The same methodology as in [1] was applied to determine the sample size necessary to flush the Rolsi™ capillaries. The first sample from each phase was discarded as a flushing sample.

The pressure sensor readings were logged every second, and ratios of the temperature sensors were logged approximately every 20 seconds. The temperature and pressure measurements in the stable period before the first sample and until the last sample formed the data set for a VLE point measurement series. The treatment of these data sets is described in Section 3.4.

2.3.2. Critical region

At the temperatures 218.15, 233.14, 253.15 and 273.15 K, a special procedure was employed to perform measurements close to the critical point of the mixture at each temperature. In each of these measurement series at constant temperature and pressure, the removal of mass from the cell through the sampling lowered the equilibrium pressure for the following measurement series. This allowed for very small pressure steps compared to the general procedure described earlier, where CO₂ or O₂ was filled onto or removed from the cell using the pumps or the venting valve.

The procedure was as follows: The cell pressure was first increased to as close to the critical pressure as possible, while keeping the liquid volume fraction close to 50%. As mentioned earlier, the close proximity to the critical point was established by observing at which pressure the phases became indistinguishable when the stirrer was running. In addition, at this point the injection of very small amounts of either CO₂ or O₂ caused very large changes to the liquid phase volume

Table 1
Chemical samples used.

Chemical name	CASRN	Source	Initial mole fraction purity	Purification method	Final mole fraction purity	Analysis method
Carbon dioxide ^a	124-38-9	Yara Praxair/AGA	0.99999	None	0.99999	None
Oxygen ^b	7782-44-7	Yara Praxair	0.999999	None	0.999999	None
Helium ^c	7440-59-7	AGA	0.999999	None	0.999999	None

^a Maximum specified impurity content by volume was less than 2 ppm H₂O, 1 ppm O₂, 5 ppm N₂, 1 ppm hydrocarbons C_nH_m and 1 ppm H₂.

^b Maximum specified impurity content by volume was less than 0.5 ppm H₂O, 1 ppm N₂, 0.5 ppm Ar, 0.02 ppm methane CH₄, 0.1 ppm CO₂ and 0.2 ppm CO. Manufacturer's specification states that total impurity level was not above 1 ppm. ^c GC carrier gas.

fraction, as could be expected when the cell content was very close to the mixture critical point, but still in the two-phase region.

With the cell content in this state, at a pressure slightly below the critical pressure and with a liquid volume fraction of approximately 50%, the bellows was expanded slightly to increase the cell pressure. If the cell content was sufficiently close to the critical pressure before this pressure increase, the cell content would move out of the two-phase region into the supercritical region. With the stirrer running, this transition out of the two-phase region seemed to be discernible by the disappearance of a swirling motion of the cell content. At this state, it was not possible to observe any qualitative difference in the appearance of the cell content when the stirrer was running, compared to when it was stopped.

The bellows was then used to keep the cell pressure stable, and the stirrer was run for between 30 min and 2 hours, and then stopped. Given the possibility that the cell content could still be in the two-phase region, without any liquid-vapor phase boundary visible using the borescope, the cell content was allowed to settle for 2-3 hours.

Then, samples were withdrawn from the liquid and vapor phase, following the sampling procedure described earlier. After the sampling was finished, the stirrer was started, and the bellows was compressed by lowering the pressure on the bellows circuit. For the critical region measurements for the four temperatures mentioned earlier, the decrease in pressure brought the cell content back into the two-phase region, visible by the swirling motion of the cell content, and the separation of the content into a liquid and vapor phase when the stirrer was stopped.

With the bellows keeping the cell pressure constant at this new lowered pressure, the process of stirring and settling was repeated, and samples were withdrawn from both phases.

This procedure of starting at a pressure slightly into the supercritical region, and using the bellows to keep the pressure stable while samples were taken, and then repeating this at a lowered pressure using the bellows, allowed us to perform several VLE measurements very close to the critical point of the mixture. For each of the temperatures 218.15, 233.14, 253.15 and 273.15 K, this resulted in 2-3 VLE measurements very close to the critical point, and 1 pressure-temperature-composition state point in the supercritical region. Details concerning these measurements are presented in Sections 4 and 5.

3. Uncertainty analysis

3.1. Definitions

The terms and definitions in the “GUM” [11] is used in the uncertainty analysis. The uncertainties are evaluated as standard uncertainties, with symbol $u(y)$, where y is the estimate of the measurand Y . The propagation of the standard uncertainties in input quantities X_i into a final calculated value Y is described by the combined standard uncertainty, with symbol $u_c(y)$.

3.2. Pressure and temperature

A thorough analysis of the uncertainty of the pressure and temperature measurements was performed in [1], where VLE measurements of the CO_2+N_2 system were performed. The same methodology was used for the measurements in the present work, the only difference being that the density used in the hydrostatic pressure calculations was calculated using EOS-CG for CO_2+O_2 instead of CO_2+N_2 . Only the resulting uncertainty estimates are given here. The details of the uncertainty analysis methodology can be found in [1].

The uncertainty components contributing to the standard uncertainty for the measured pressure p at VLE are summarized in Table 2, and the resulting standard uncertainties in the pressure measurements are shown in Fig. 2. Similarly, Table 3 and Fig. 3 show the contributors to and the resulting standard uncertainty in the measured temperatures T .

As seen from Fig. 2, the standard uncertainty in the pressure was estimated to be below 0.05% of the measured pressure except at the lowest pressure. Similarly, as seen from Tables 7 and 8 and Fig. 3, the standard uncertainty in the temperature was estimated to be below 8 mK, and the variation in temperature had been less than 5 mK.

Table 2

Summary of standard uncertainty components for pressure measurements, cf. Westman et al. [1].

Symbol	Description and unit	u
Hydrostatic pressure p_{hs}		
$u(\rho_1)$	EOS-CG ^a vapor density of CO ₂ +O ₂ (kg m ⁻³)	$1 \cdot 10^{-2} \cdot \rho_1$
$u(\rho_2)$	Same as $u(\rho_1)$ (kg m ⁻³)	$1 \cdot 10^{-2} \cdot \rho_2$
$u(\rho_{4,1})$	SW ^b density at 313.15 K (kg m ⁻³)	$3 \cdot 10^{-4} \cdot \rho_{4,1}$
$u(\rho_{4,2})$	Same as $u(\rho_1)$ (kg m ⁻³)	$1 \cdot 10^{-2} \cdot \rho_{4,2}$
$u(\text{CAD})$	(m)	0
$u_c(h_1)$	(m)	0.0048
$u(h_{liq})$	(m)	0.0048
$u(h_{liq,1})$	Borescope h_{liq} (m)	0.0048
$u(h_{liq,2})$	Variation in h_{liq} (m)	0
$u(h_2)$	Bath liquid level variation (m)	0.006
$u_c(h_3)$	(m)	0.006
$u(h_4)$	Same as $u(\text{CAD})$ (m)	0
$u(g_1)$	Local g (m s ⁻²)	$2 \cdot 10^{-7}$
Differential pressure p_{11}		
$u(p_{11,1})$	Ambient temperature (MPa)	0
$u(p_{11,2})$	Line pressure zero (MPa)	0
$u(p_{11,3})$	Line pressure span (MPa)	$4.9 \cdot 10^{-5} \text{ MPa}^{-1} \cdot p_i \cdot p_{11}$
$u(p_{11,4})$	Mounting (MPa)	0
$u(p_{11,5})$	Vibration (MPa)	$2.8 \cdot 10^{-5}$
$u(p_{11,6})$	Power supply (MPa)	0
$u(p_{11,7})$	A/D conversion (MPa)	$2.4 \cdot 10^{-4}$
Pressure sensors p_i		
$u(p_1)$	1 MPa sensor (MPa)	$2.24 \cdot 10^{-4}$
$u(p_2)$	3 MPa sensor (MPa)	$2.33 \cdot 10^{-4}$
$u(p_3)$	10 MPa sensor (MPa)	$7.64 \cdot 10^{-4}$
$u(p_4)$	20 MPa sensor (MPa)	$1.965 \cdot 10^{-3}$

^a Gernert and Span [3] and Gernert [4] ^b Span and Wagner [6]

Table 3

Summary of standard uncertainty components for temperature measurements, cf. Westman et al. [1].

Symbol	Unit	u
$u(W_b)$	(-)	$0.35 \cdot 10^{-6}$
$u(R_{ref})$	(Ω)	$8.5 \cdot 10^{-6}$
$u(T_{H_2O})$	(mK)	0.51
$u(T_{Hg})$	(mK)	1.43
$u(T_{Ga})$	(mK)	0.85
$u(R_{H_2O}(T_{04}))$	(Ω)	$3.94 \cdot 10^{-5}$
$u(R_{H_2O}(T_{05}))$	(Ω)	$2.57 \cdot 10^{-5}$
$u(R_{Hg}(T_{04}))$	(Ω)	$2.29 \cdot 10^{-5}$
$u(R_{Hg}(T_{05}))$	(Ω)	$1.84 \cdot 10^{-5}$
$u(R_{Ga}(T_{04}))$	(Ω)	$2.69 \cdot 10^{-5}$
$u(R_{Ga}(T_{05}))$	(Ω)	$2.37 \cdot 10^{-5}$
$u(W_{Hg}(T_{04}))$	(-)	$6.2 \cdot 10^{-6}$
$u(W_{Hg}(T_{05}))$	(-)	$6.1 \cdot 10^{-6}$
$u(W_{Ga}(T_{04}))$	(-)	$4.5 \cdot 10^{-6}$
$u(W_{Ga}(T_{05}))$	(-)	$4.3 \cdot 10^{-6}$

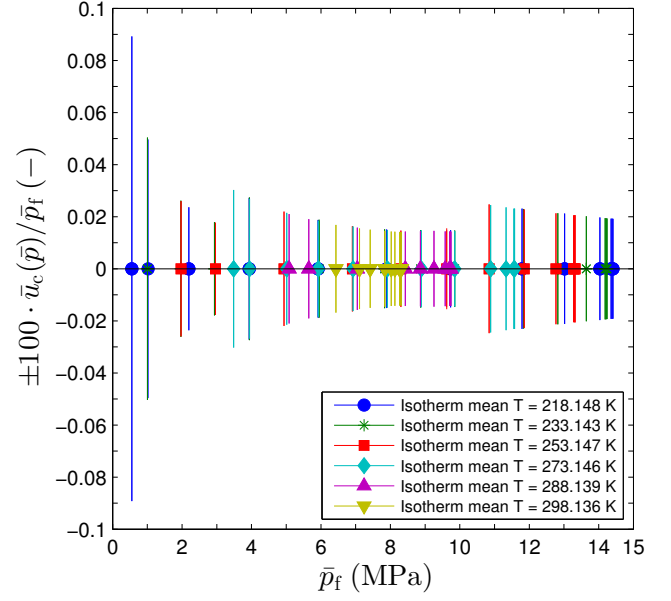


Fig. 2. Pressure standard uncertainty relative to the measured pressure for the VLE measurements performed, expressed as $100 \cdot \tilde{u}_c(\bar{p})/\bar{p}_f$. Measured pressure \bar{p}_f . Standard uncertainty $\tilde{u}_c(\bar{p})$.

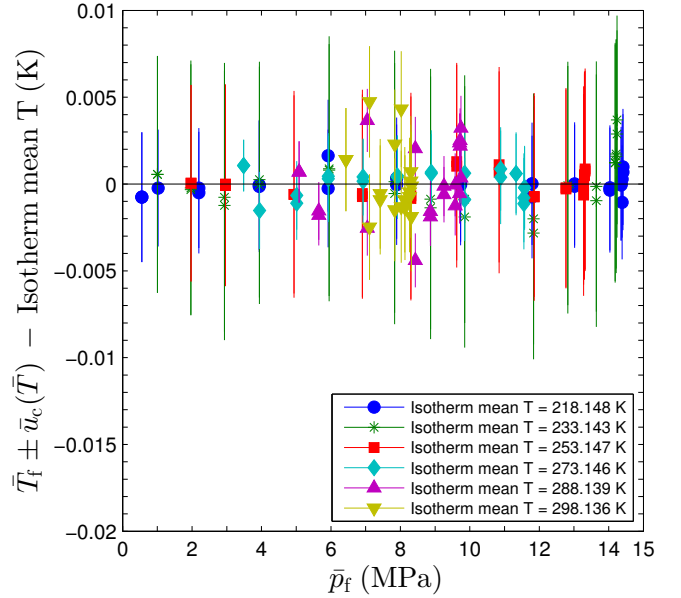


Fig. 3. Temperature deviations for each VLE measurement from isotherm mean temperature, and temperature standard uncertainty, expressed together as $\bar{T}_f \pm \tilde{u}_c(\bar{T}) - \text{isotherm mean temperature}$, versus VLE experiment pressure \bar{p}_f . VLE experiment mean temperature \bar{T}_f . Temperature standard uncertainty $\tilde{u}_c(\bar{T})$.

Table 4

Molar masses of atomic elements and compounds with uncertainties [16, 17].

Component i	M_i	$u(M_i)$	Unit
C ^a	0.0120108	0.0000003	kg mol ⁻¹
O ^a	0.01599938	0.0000007	kg mol ⁻¹
O ^b	0.01599940	0.00000035	kg mol ⁻¹
CO ₂	0.0440096	0.0000003	kg mol ⁻¹
O ₂	0.03199880	0.00000070	kg mol ⁻¹
CO ₂ +imp	0.0440094		kg mol ⁻¹
O ₂ +imp	0.03199880		kg mol ⁻¹
CO ₂ ,eff	0.0440097		kg mol ⁻¹
O ₂ ,eff	0.03199881		kg mol ⁻¹

^a In CO₂ molecule ^b In O₂ molecule

3.3. Composition

The VLE phase composition analysis and uncertainty estimation were performed in the same manner as in [1], with the methodology applied to CO₂+O₂ samples instead of CO₂+N₂. A summary will be provided here, with reference to [1] for further details.

The composition analysis was performed using the same GC as in [1], with its calibration performed using gravimetrically prepared gas mixtures using a custom-built rig in our laboratories [15].

For the measurement method utilized in the present work, it could be stated that the composition uncertainty stemmed from a range of sources, including the impurities of the gases used to prepare the calibration mixtures, the uncertainty in the molar masses, inaccuracies in the weighed masses, adsorption, repeatability / uncertainties of the sampling and GC analysis, and finally the consistency between the GC calibration function and data. The analysis of these contributing factors are given below.

3.3.1. Source gas composition and molar mass

The composition and the corresponding uncertainty of a gravimetrically prepared gas mixture are results of both the purity and the molar mass of the source gases used for the mixture. According to [16, 17], the molar masses of monoatomic carbon C, monoatomic oxygen O in commercial tank gas CO₂ and monoatomic oxygen O in commercial tank gas O₂ generally lie within ranges of width 0.6, 0.15, and 0.7 mg mol⁻¹, respectively. Based on this, the molar masses of CO₂ and O₂, M_{CO_2} and M_{O_2} respectively, were calculated with the corresponding uncertainty estimates shown in Table 4.

The minimum certified purities of the CO₂ and O₂ source gases used to prepare the calibration gas mixtures are given in Table 1, together with the manufacturers' specifications of the maximum content of certain impurities. Since the source gases were not entirely pure, estimates for the molar masses of the source gases, M_{CO_2+imp} and M_{O_2+imp} , should account for the impurities present, following the procedure used in [1].

M_{CO_2+imp} and M_{O_2+imp} were calculated based on the impurity specifications stated in Table 1. The molar mass of each impurity was calculated using data from Wieser et al.

[17], assuming methane CH₄ for the hydrocarbon impurity fraction. The molar masses of the source gases, M_{CO_2+imp} and M_{O_2+imp} , together with the effective molar masses of the source gases excluding the impurities, $M_{CO_2,eff}$ and $M_{O_2,eff}$, are shown in Table 4.

3.3.2. Gravimetric preparation

The methodology of gravimetric preparation of the calibration gas mixtures and the uncertainty estimation given in [1, 15] was used in the present work. To summarize the determination of the final composition of the gas mixtures, the mass of each source gas including impurities in the gravimetrically prepared gas mixture, m_{i+imp} , was converted into moles of the primary components CO₂ and O₂ excluding impurities, n_i , as

$$n_i = m_{i+imp}/M_{i,eff}, \quad (1)$$

with the mole fraction of CO₂ in the gravimetrically prepared gas mixture expressed as

$$y_{CO_2,cal} = \frac{n_{CO_2}}{n_{CO_2} + n_{O_2}}. \quad (2)$$

Six CO₂+O₂ calibration gas mixtures were made, spanning in CO₂ mole fractions $y_{CO_2,cal}$ from 0.13 to 0.95. An overview of the mixtures is given in Table 5.

3.3.3. Composition calibration procedure and estimated composition uncertainty

The calibration of the GC was performed as described in Appendix A.3.1 in [1], with the measures described to prevent adsorption of the gas onto the contact surfaces. In short, each calibration gas was filled onto the VLE cell after thorough evacuation and flushing with the calibration gas at 0.5 MPa, keeping the impurity pump, gas lines and cell at 313 K to ensure that the calibration gas was kept in a uniform supercritical state. Samples of varying sizes were withdrawn from the cell at different pressures between 5 and 10 MPa. These samples formed the calibration basis for the composition analysis, establishing a relation between the CO₂ mole fractions of the calibration gas mixtures and the GC detector response.

The uncertainty contribution from the calibration mixture uncertainty reaching the GC could be estimated as

$$u_c(y_{CO_2,cal}) = \sqrt{u^2(y_{CO_2,cal}, m) + u^2(y_{CO_2,cal}, M_{eff}) + u^2(y_{CO_2,cal}, ads.)}, \quad (3)$$

Table 5

CO₂+O₂ calibration gas mixtures: CO₂ mole fractions and corresponding standard uncertainties.

$y_{CO_2,cal}$	$u(y_{CO_2,cal}, m)$	$u(y_{CO_2,cal}, M_{eff})$	$u(y_{CO_2,cal}, ads.)$	$u_c(y_{CO_2,cal})$
0.131144	$2.7 \cdot 10^{-6}$	$17.4 \cdot 10^{-6}$	$1.4 \cdot 10^{-6}$	$17.6 \cdot 10^{-6}$
0.303027	$2.1 \cdot 10^{-6}$	$11.2 \cdot 10^{-6}$	$3.3 \cdot 10^{-6}$	$11.9 \cdot 10^{-6}$
0.549780	$2.6 \cdot 10^{-6}$	$5.4 \cdot 10^{-6}$	$5.9 \cdot 10^{-6}$	$8.4 \cdot 10^{-6}$
0.686269	$1.4 \cdot 10^{-6}$	$4.9 \cdot 10^{-6}$	$7.3 \cdot 10^{-6}$	$8.9 \cdot 10^{-6}$
0.898418	$5.1 \cdot 10^{-6}$	$7.4 \cdot 10^{-6}$	$9.7 \cdot 10^{-6}$	$13.2 \cdot 10^{-6}$
0.945826	$2.4 \cdot 10^{-6}$	$8.2 \cdot 10^{-6}$	$10.1 \cdot 10^{-6}$	$13.3 \cdot 10^{-6}$

where $u(y_{\text{CO}_2,\text{cal}}, m)$ and $u(y_{\text{CO}_2,\text{cal}}, M_{\text{eff}})$ are the contributing uncertainties stemming from the uncertainties in the masses of CO_2 and O_2 in the gas mixture and the uncertainties in the effective molar masses, respectively. These terms are described in detail in Appendix A.3 of [1]. The last term in Eq. (3), $u(y_{\text{CO}_2,\text{cal}}, \text{ads.})$, is the contributing uncertainty from adsorption, and was estimated assuming that CO_2 is adsorbed at a higher degree than O_2 , in the same way as in [1]. The uncertainty estimates used in Eq. (3) are given in Table 5.

As seen in Table 5, the uncertainty contribution from the molar mass of O_2 caused $u(y_{\text{CO}_2,\text{cal}}, M_{\text{eff}})$ to dominate the combined standard uncertainty of the CO_2 mole fraction $u_c(y_{\text{CO}_2,\text{cal}})$ for the gas mixtures with the highest O_2 -content. For the mixtures with the highest CO_2 -content, the uncertainty contribution from the adsorption of CO_2 was the dominating factor. The uncertainty contribution from the adsorption was for all the mixtures of the same order as the two other contributing factors, and as in [1], the uncertainty of the CO_2 mole fractions of the calibration gases, $u_c(y_{\text{CO}_2,\text{cal}})$, would have to be orders of magnitude larger to be of significance for the final uncertainty in the VLE composition data. As the discussion in the following section will show, the reason for this was that the main contributor to this final uncertainty was the calibration function error.

3.3.4. GC integration and calibration function

The GC column, method and detector used for CO_2+N_2 samples in [1] were utilized on CO_2+O_2 samples in the present work, with helium as the GC carrier gas. This setup gave just as good separation of the CO_2 and O_2 peaks in the GC chromatogram as in [1] for CO_2 and N_2 . The areas under the CO_2 and O_2 peaks in the chromatogram, denoted A_{CO_2} and A_{O_2} , were obtained for each sample by numerical integration. The GC thermal conductivity detector (TCD) response was nonlinear with respect to the number of moles of CO_2 and O_2 passing through the detector. The following model, consisting of both linear and nonlinear terms, described adequately the relation between moles of each component in the sample to the area of each component:

$$\hat{n}_{\text{CO}_2} \cdot k = A_{\text{CO}_2} + (A_{\text{CO}_2})^{c_1} + (A_{\text{CO}_2})^{c_2}, \quad (4)$$

$$\hat{n}_{\text{O}_2} \cdot k = c_3 \cdot (A_{\text{O}_2} + (A_{\text{O}_2})^{c_4} + (A_{\text{O}_2})^{c_5}), \quad (5)$$

$$\hat{y}_{\text{CO}_2,\text{cal}} = \frac{\hat{n}_{\text{CO}_2}}{\hat{n}_{\text{CO}_2} + \hat{n}_{\text{O}_2}}, \quad (6)$$

where $\hat{y}_{\text{CO}_2,\text{cal}}$ is the estimator of the CO_2 mole fraction of a calibration gas mixture sample given the areas for that sample, and k is an unknown factor relating the areas to the number of moles.

The parameters c_i for $i = 1$ through 5 were fitted by performing a weighted least squares minimization of the objective function S described by Eq. (A.32) in [1]. The mean values of the estimator, $\hat{y}_{\text{CO}_2,\text{cal}}$, calculated for each of the $n = 62$ series, with each series consisting of 6-9 valid samples, were fitted against the calibration mixture mole fractions,

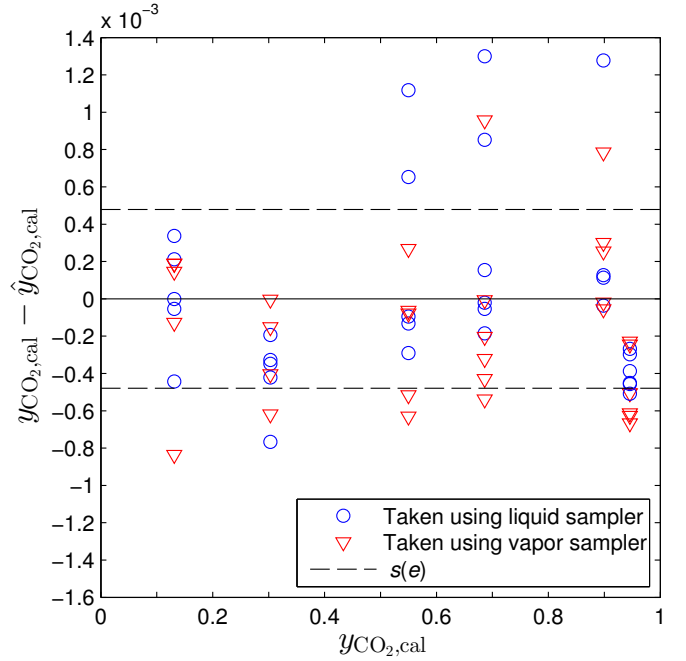


Fig. 4. Composition calibration: Error between actual compositions in Table 5 and composition model in Eq. (6), given as $y_{\text{CO}_2,\text{cal}} - \hat{y}_{\text{CO}_2,\text{cal}}$ versus $y_{\text{CO}_2,\text{cal}}$. Composition analysis uncertainty $u(x_{\text{CO}_2}) = u(y_{\text{CO}_2}) = s(e)$ from Table 6.

$y_{\text{CO}_2,\text{cal}}$, which resulted in the parameter estimates found in Table 6. As shown in Fig. 4, the errors between the calibration gas CO_2 mole fractions and the model predictions, $e = y_{\text{CO}_2,\text{cal}} - \hat{y}_{\text{CO}_2,\text{cal}}$, were randomly scattered around zero over the composition range $y_{\text{CO}_2,\text{cal}}$, which indicated an appropriate model structure. The sample standard deviation of the errors, $s(e)$, are also given in Table 6. This model was used to convert the areas resulting from the analysis of a composition sample taken during a VLE experiment into a CO_2 mole fraction.

For the same reasons as described in [1], it was assumed that the standard uncertainty of the CO_2 mole fraction of samples taken during VLE measurements, $u(x_{\text{CO}_2}) = u(y_{\text{CO}_2})$, was estimated by $s(e)$, which was 25-60 times larger than the standard uncertainties in the mole fractions of the calibration mixtures, $y_{\text{CO}_2,\text{cal}}$. It must be emphasized that this estimate only accounts for the uncertainty caused by the composition analysis of the samples. All other reasons that could cause the sample to not represent the actual VLE composition are not accounted for in this estimate, and these contributors could only be minimized by the measures described in Section 2.3 and in [1].

3.3.5. Total uncertainty in liquid and vapor phase mole fractions x_{CO_2} and y_{CO_2}

For a given VLE measurement, the uncertainty of T and p contributed to additional uncertainty in the composition, giving the following total standard uncertainty of the com-

position:

$$u_{\text{tot}}(z_{\text{CO}_2}) = \sqrt{u^2(z_{\text{CO}_2}) + \left(u_c(\bar{T}) \cdot \frac{\partial z_{\text{CO}_2}}{\partial T}\right)^2 + \left(u_c(\bar{p}) \cdot \frac{\partial z_{\text{CO}_2}}{\partial p}\right)^2} \quad (7)$$

where z_{CO_2} was equal to either x_{CO_2} or y_{CO_2} , and the temperature and pressure uncertainties $u_c(\bar{T})$ and $u_c(\bar{p})$ are described in Section 3.4 and in [1]. Similar to [1], the derivatives in Eq. (7) were, in general, calculated numerically from the PR-MC-WS-NRTL Case 2 EOS fitted to our data. Details about this EOS are explained in Section 5.4.2. For the VLE measurements in the critical region used to fit the scaling law in Section 5.3, the derivatives with respect to pressure, $\partial z_{\text{CO}_2}/\partial p$, were calculated analytically from the fitted scaling law in Eq. (13), as this gave better estimates for the derivatives than the PR-MC-WS-NRTL Case 2 EOS in this region. Details concerning the scaling law are given in Section 5.3.

3.4. Data reduction

As described in Section 2.3, the drop in cell pressure after each composition sample was compensated using the bellows to decrease the cell volume. For the VLE measurements in this work, the cell pressure was in most cases back at its original value after around 1-3 min, and for a few of the measurements after around 5 min. After the cell pressure was back to its stable value, it remained stable for the remaining 20-24 min until the next sample was withdrawn.

In each series of either consecutive liquid or vapor phase composition samples, x_{CO_2} or y_{CO_2} , at a nominal temperature and pressure, it was assumed that each composition sample represented the equilibrium composition at the temperature and pressure just before the sample was withdrawn from the cell. These temperature and pressure values, denoted \bar{T} and \bar{p} , respectively, were assumed to be represented by the temperature and pressure measurements averaged over the last 75% of the time period between the previous and the current composition sample. As in [1], the bellows was able to stabilize the cell pressure sufficiently fast after each sample withdrawal, and it was not possible to see any systematic trends in the temperature or pressure during these time periods. It was also not possible to see any temperature variations caused by the removal of mass from the cell in the composition sampling.

Table 6

Fitted parameters of the $\bar{y}_{\text{CO}_2, \text{cal}}$ model and standard uncertainty of composition analysis $u(x_{\text{CO}_2}) = u(y_{\text{CO}_2})$.

Variable	Value
c_1	0.899 902
c_2	1.154 287
c_3	1.270 181
c_4	1.155 333
c_5	0.914 593
$u(x_{\text{CO}_2}) = u(y_{\text{CO}_2}) = s(e)$	$4.7894 \cdot 10^{-4}$
n	62

For each of these series of samples, the arithmetic mean values of the temperature, pressure, liquid and vapor phase compositions were calculated, denoted as \bar{T}_f , \bar{p}_f , \bar{x}_{CO_2} and \bar{y}_{CO_2} , respectively. The subscript f is used to differentiate between the temperature and pressure values associated with each composition sample x_{CO_2} or y_{CO_2} , and of those associated with the average compositions \bar{x}_{CO_2} or \bar{y}_{CO_2} .

Details about the methodology for describing and calculating the propagation of the uncertainty in the measured variables T , p , x_{CO_2} and y_{CO_2} into resulting estimates associated with each composition sample are given in [1], and the symbols used are summarized in Table A.1 together with the data for the individual composition samples.

The propagation of uncertainty from the data of an individual sample, \bar{T} , \bar{p} , x_{CO_2} or y_{CO_2} , into the mean values for a series of samples, \bar{T}_f , \bar{p}_f , \bar{x}_{CO_2} or \bar{y}_{CO_2} , is defined by:

$$u_c(\bar{T}_f) = \sqrt{s^2(\bar{T}_f) + \bar{u}_c(\bar{T})^2}, \quad (8)$$

$$u_c(\bar{p}_f) = \sqrt{s^2(\bar{p}_f) + \bar{u}_c(\bar{p})^2}, \quad (9)$$

$$u_c(\bar{x}_{\text{CO}_2}) = \sqrt{s^2(\bar{x}_{\text{CO}_2}) + \bar{u}_{\text{tot}}(x_{\text{CO}_2})^2}, \quad (10)$$

$$u_c(\bar{y}_{\text{CO}_2}) = \sqrt{s^2(\bar{y}_{\text{CO}_2}) + \bar{u}_{\text{tot}}(y_{\text{CO}_2})^2}, \quad (11)$$

where $\bar{u}_c(\bar{T})$, $\bar{u}_c(\bar{p})$, $\bar{u}_{\text{tot}}(x_{\text{CO}_2})$ and $\bar{u}_{\text{tot}}(y_{\text{CO}_2})$ are calculated as the means of $u_c(\bar{T})$, $u_c(\bar{p})$, $u_{\text{tot}}(x_{\text{CO}_2})$ and $u_{\text{tot}}(y_{\text{CO}_2})$ in each series, respectively. The sample standard deviations of the mean $s(\bar{z})$ were calculated according to the standard formula:

$$s(\bar{z}) = \frac{1}{\sqrt{n}} \sqrt{\sum_{i=1}^n \frac{(z_i - \bar{z})^2}{n-1}}, \quad (12)$$

where $\bar{z} = \bar{T}_f$, \bar{p}_f , \bar{x}_{CO_2} or \bar{y}_{CO_2} .

4. Results

VLE measurements at the average temperatures 218.15, 233.14, 253.15, 273.15, 288.14 and 298.14 K were conducted, spanning from close to the triple point temperature (216.59 K) to close to the critical temperature of CO_2 (304.13 K), and covered pressures from the vapor pressure of CO_2 up to close to the critical point at each temperature.

The temperature \bar{T} , pressure \bar{p} and mole fractions for the liquid phase x_{CO_2} and the vapor phase y_{CO_2} for each individual sample are given in Tables A.2 and A.3, together

with their uncertainty estimates. The composition derivatives with respect to pressure, $\partial x_{\text{CO}_2}/\partial p$ and $\partial y_{\text{CO}_2}/\partial p$, and the total standard uncertainties in the composition of the samples, $u_{\text{tot}}(x_{\text{CO}_2})$ and $u_{\text{tot}}(y_{\text{CO}_2})$, which were calculated using the scaling law in Section 5.3, are identified in Tables A.2 and A.3 using the marker symbol ⁺.

The data for each series of samples are given at mean temperature \bar{T}_f , mean pressure \bar{p}_f and mean mole fractions for the liquid phase \bar{x}_{CO_2} and the vapor phase \bar{y}_{CO_2} in Tables 7 and 8. These averaged data are plotted with the uncertainties in composition and pressure in Figs. 5a to 5f. The relative volatilities based on the measured data are plotted in Figs. B.1a to B.1f. The means of the total standard uncertainties of the mole fractions, $\bar{u}_{\text{tot}}(x_{\text{CO}_2})$ and $\bar{u}_{\text{tot}}(y_{\text{CO}_2})$, and the final standard uncertainties of the mole fractions, $u_c(\bar{x}_{\text{CO}_2})$ and $u_c(\bar{y}_{\text{CO}_2})$, which were calculated using the scaling law in Section 5.3, are identified in Tables 7 and 8 using the marker symbol ⁺.

As discussed in Section 2.3.2, a special procedure was used to obtain VLE measurements close to the critical point at the temperatures 218.15, 233.14, 253.15 and 273.15 K. Four pressure-temperature-composition state points in the supercritical region were obtained, consisting of 4 pairs of composition sample series taken using both the liquid and vapor phase samplers. The individual sample data are given in Table A.4, and the average values for each series can be found in Table 9. The VLE points obtained using this procedure are identified in Tables A.2, A.3, 7 and 8. These VLE and supercritical measurements will be discussed in detail in Section 5.3.

5. Analysis and discussion

5.1. Summary and analysis of uncertainty estimates

With reference to Table 7, the maximum and average sample standard deviation of the liquid phase mole fractions, $s(\bar{x}_{\text{CO}_2})$, were $1.3 \cdot 10^{-4}$ and $1.2 \cdot 10^{-5}$, respectively. Similarly, for the vapor phase mole fractions in Table 8, the maximum and average $s(\bar{y}_{\text{CO}_2})$ were respectively $1.2 \cdot 10^{-4}$ and $2.5 \cdot 10^{-5}$. Some of the vapor phase points at the lowest pressures at each temperature showed increase in these standard deviations, as could be expected by the high VLE composition sensitivity to pressure changes. Also, there seemed to be a slight increase in the standard deviations for some of the VLE points at the highest pressures. Inspecting the composition sample data for these points in Tables A.2 and A.3, the liquid and vapor phase mole fractions were respectively increasing and decreasing slightly throughout the series. This could imply that VLE had not been achieved completely or more likely, that the separation of the phases was incomplete, even though the settling times had been increased significantly for these measurements at close proximity to the critical point, as described in Section 2.3. It can be noted that the observed variations did not exceed the estimated uncertainty of the composition analysis, $4.8 \cdot 10^{-4}$ from Table 6.

However, if the cause for the variations was incomplete settling, there is a possibility that the actual VLE compositions are outside the values covered by the composition analysis uncertainty.

The mean standard uncertainty in the phase mole fractions caused by the composition analysis and the temperature and pressure uncertainties described in Section 3.3.5, $\bar{u}_{\text{tot}}(z_{\text{CO}_2})$ where $z_{\text{CO}_2} = x_{\text{CO}_2}$ or y_{CO_2} , increased as a function of pressure at each temperature. At pressures close to the critical points, where the scaling law was used to estimate the VLE composition sensitivity to pressure, $\partial z_{\text{CO}_2}/\partial p$, $\bar{u}_{\text{tot}}(z_{\text{CO}_2})$ was $3.1 \cdot 10^{-3}$ at its maximum. For the series outside the critical region, $\bar{u}_{\text{tot}}(z_{\text{CO}_2})$ was close to the composition analysis uncertainty, $4.8 \cdot 10^{-4}$, as the uncertainties in pressure and temperature did not contribute significantly.

The final standard uncertainty of the mole fractions, $u_c(\bar{z}_{\text{CO}_2})$, combining $s(\bar{z}_{\text{CO}_2})$ and $\bar{u}_{\text{tot}}(z_{\text{CO}_2})$ described above, was maximum $3.1 \cdot 10^{-3}$ for the series in the critical region, and approximately $5 \cdot 10^{-4}$ for the series outside the critical region.

As can be seen in Tables A.2 and A.3, the combined standard uncertainty of the measured temperatures, $u_c(\bar{T})$, was below 8 mK for all samples, and around 4 mK on average. The combined standard uncertainty of the measured pressures, $u_c(\bar{p})$, ranged from 0.5 kPa at the lowest measured pressure 0.56 MPa (0.09%) to 3 kPa at the highest measured pressure 14.4 MPa (0.02%).

5.2. Comparison with literature data

The literature data reviews in [2, 3, 4, 5] provided in total five works reporting isothermal analytic VLE measurements [18, 20, 19, 25, 26] and two works reporting synthetic VLE measurements [21, 22]. The work by [26] from 2009 contained isothermal VLE measurements at 240.9 K, and apart from this the other works were from 1972 or earlier. In addition, two works reporting synthetic VLE measurements were found, one from 1903 [23] and the other from 2014 [24]. A summary of these literature data is given in Table 10.

Literature data at temperatures comparable to our measurements [18, 20, 19, 22, 23, 21, 24] are plotted together with our data in Figs. 5a to 5f.

At 218.15 K, the bubble point data by Zenner and Dana [18] were in very good agreement with our measurements, while their dew point data showed increasing deviations with our data as the pressure increased. Our three dew and bubble point pairs at the highest pressures close to the critical point cover a region previously not measured.

The data by Zenner and Dana [18] at 232.88 K were at a slightly lower temperature than our data at 233.14 K, but the data should be comparable as the temperature sensitivity of the VLE compositions are relatively low at these temperatures (cf. Tables A.2 and A.3). Like at 218.15 K, the bubble points by Zenner and Dana [18] were in good agreement with our data. However, their dew point data showed much more scatter than our data, and only about half of their data points agreed well with our data. Our three VLE data

Table 7

Liquid phase: Experimental VLE data for CO₂ (1) + O₂ (2) at mean temperature \bar{T}_f , mean pressure \bar{p}_f , and mean liquid phase mole fraction \bar{x}_{CO_2} ^a.

ID	Data			Temperature			Pressure			Composition			
	\bar{T}_f (K)	\bar{p}_f (MPa)	\bar{x}_{CO_2} (-)	$s(\bar{T}_f)$ (K)	$\bar{u}_c(\bar{T})$ (K)	$u_c(\bar{T}_f)$ (K)	$s(\bar{p}_f)$ (MPa)	$\bar{u}_c(\bar{p})$ (MPa)	$u_c(\bar{p}_f)$ (MPa)	$s(\bar{x}_{\text{CO}_2})$ (-)	$\bar{u}_{\text{tot}}(x_{\text{CO}_2})$ (-)	$u_c(\bar{x}_{\text{CO}_2})$ (-)	$x_{\text{CO}_2,\text{calc}}$ (-)
P1	218.147	0.5546 ^b	0.99999	7.3e-5	3.7e-3	3.7e-3	1.1e-6	4.9e-4	4.9e-4				
L1	218.148	2.1957	0.96687	2.0e-4	3.5e-3	3.5e-3	9.5e-6	5.2e-4	5.2e-4	4.8e-6	4.8e-4	4.8e-4	0.96887
L2	218.148	3.9362	0.92958	7.8e-5	3.7e-3	3.7e-3	1.9e-5	1.1e-3	1.1e-3	3.8e-6	4.8e-4	4.8e-4	0.93250
L3	218.148	5.9189	0.88226	4.3e-4	3.4e-3	3.4e-3	6.8e-6	1.1e-3	1.1e-3	3.5e-6	4.8e-4	4.8e-4	0.88563
L4	218.149	7.8935	0.82832	1.7e-4	3.5e-3	3.5e-3	5.0e-6	1.2e-3	1.2e-3	4.8e-6	4.8e-4	4.8e-4	0.83104
L5	218.148	9.7335	0.76941	9.8e-5	3.4e-3	3.4e-3	5.5e-6	1.4e-3	1.4e-3	3.0e-6	4.8e-4	4.8e-4	0.76955
L6	218.148	11.7910	0.68723	1.3e-4	3.5e-3	3.5e-3	1.0e-5	2.7e-3	2.7e-3	5.3e-6	5.0e-4	5.0e-4	0.67972
L7	218.148	13.0212	0.61994	1.4e-4	3.5e-3	3.5e-3	1.3e-5	2.8e-3	2.8e-3	7.2e-6	5.2e-4	5.2e-4	0.60470
L8	218.148	14.0358	0.53329	1.6e-4	3.6e-3	3.6e-3	2.0e-5	2.8e-3	2.8e-3	2.5e-5	6.0e-4 ⁺	6.0e-4 ⁺	0.51002
L9*	218.148	14.3563	0.47535	1.2e-4	3.3e-3	3.3e-3	1.3e-5	2.8e-3	2.8e-3	5.0e-6	9.8e-4 ⁺	9.8e-4 ⁺	0.45826
L10*	218.148	14.3873	0.46440	1.2e-4	3.4e-3	3.4e-3	1.7e-5	2.8e-3	2.8e-3	5.4e-6	1.3e-3 ⁺	1.3e-3 ⁺	0.45116
L11*	218.149	14.4111	0.45232	2.1e-4	3.3e-3	3.3e-3	1.6e-5	2.8e-3	2.8e-3	2.4e-5	1.9e-3 ⁺	1.9e-3 ⁺	0.44512
P2	233.143	1.0048 ^c	0.99999	7.4e-5	6.8e-3	6.8e-3	1.1e-5	5.1e-4	5.1e-4				
L13	233.142	1.9677	0.98023	1.1e-4	7.2e-3	7.2e-3	8.4e-6	5.1e-4	5.1e-4	8.9e-5	4.8e-4	4.9e-4	0.98262
L14	233.141	2.9345	0.96020	5.5e-5	7.8e-3	7.8e-3	2.3e-5	5.3e-4	5.3e-4	4.4e-6	4.8e-4	4.8e-4	0.96410
L15	233.143	3.9408	0.93829	2.3e-4	6.8e-3	6.8e-3	4.4e-5	1.1e-3	1.1e-3	4.6e-6	4.8e-4	4.8e-4	0.94358
L16	233.143	5.9477	0.89067	2.6e-4	7.3e-3	7.3e-3	7.2e-6	1.1e-3	1.1e-3	3.0e-6	4.8e-4	4.8e-4	0.89803
L17	233.143	7.8334	0.84017	2.0e-4	7.5e-3	7.5e-3	9.7e-6	1.2e-3	1.2e-3	3.5e-6	4.8e-4	4.8e-4	0.84775
L18	233.142	8.8724	0.80939	6.0e-4	7.5e-3	7.5e-3	9.4e-6	1.3e-3	1.3e-3	1.8e-5	4.8e-4	4.8e-4	0.81577
L19	233.142	9.8514	0.77736	3.3e-4	7.1e-3	7.1e-3	1.1e-5	1.4e-3	1.4e-3	8.9e-6	4.8e-4	4.8e-4	0.78187
L20	233.140	11.8341	0.69897	1.5e-4	7.3e-3	7.3e-3	8.8e-6	2.7e-3	2.7e-3	4.8e-6	5.0e-4	5.0e-4	0.69628
L21	233.142	12.8248	0.64711	1.2e-4	6.9e-3	6.9e-3	8.7e-6	2.7e-3	2.7e-3	7.7e-6	5.1e-4	5.1e-4	0.63897
L22	233.142	13.6445	0.58762	5.2e-4	7.2e-3	7.2e-3	9.3e-6	2.8e-3	2.8e-3	7.4e-6	5.4e-4 ⁺	5.4e-4 ⁺	0.57569
L23*	233.144	14.1868	0.51081	7.8e-5	6.9e-3	6.9e-3	1.0e-5	2.8e-3	2.8e-3	3.2e-6	9.7e-4 ⁺	9.7e-4 ⁺	0.51244
L24*	233.144	14.2158	0.50044	9.6e-5	6.7e-3	6.7e-3	1.7e-5	2.8e-3	2.8e-3	4.4e-6	1.3e-3 ⁺	1.3e-3 ⁺	0.50771
L25*	233.146	14.2407	0.48640	2.5e-4	6.0e-3	6.0e-3	1.1e-5	2.8e-3	2.8e-3	4.3e-6	2.4e-3 ⁺	2.4e-3 ⁺	0.50339
P3	253.147	1.9699 ^d	0.99999	1.5e-5	5.7e-3	5.7e-3	5.5e-6	5.1e-4	5.1e-4				
L27	253.146	2.9632	0.97899	1.3e-4	5.8e-3	5.8e-3	2.9e-5	5.2e-4	5.2e-4	1.3e-5	4.8e-4	4.8e-4	0.98167
L28	253.146	4.9365	0.93518	1.2e-4	6.0e-3	6.0e-3	9.4e-5	1.1e-3	1.1e-3	2.6e-6	4.8e-4	4.8e-4	0.94105
L29	253.146	6.9081	0.88640	1.9e-4	6.0e-3	6.0e-3	4.4e-5	1.1e-3	1.1e-3	9.5e-6	4.8e-4	4.8e-4	0.89327
L30	253.146	8.3058	0.84783	1.4e-4	5.9e-3	5.9e-3	1.3e-5	1.2e-3	1.2e-3	5.2e-6	4.8e-4	4.8e-4	0.85331
L31	253.148	9.6226	0.80640	1.3e-4	5.7e-3	5.7e-3	3.9e-4	1.5e-3	1.5e-3	8.4e-6	4.8e-4	4.8e-4	0.80906
L32	253.147	10.8463	0.76222	1.4e-4	5.8e-3	5.8e-3	4.3e-5	2.7e-3	2.7e-3	7.7e-6	4.9e-4	4.9e-4	0.75948
L33	253.146	11.8557	0.71747	9.3e-5	6.0e-3	6.0e-3	2.5e-5	2.7e-3	2.7e-3	8.3e-6	5.0e-4	5.0e-4	0.70866
L34	253.146	12.7678	0.66173	8.9e-5	5.7e-3	5.7e-3	3.6e-5	2.7e-3	2.7e-3	6.6e-6	5.2e-4 ⁺	5.2e-4 ⁺	0.64728
L35*	253.146	13.2762	0.59988	1.2e-4	5.7e-3	5.7e-3	1.7e-5	2.7e-3	2.7e-3	8.6e-6	8.8e-4 ⁺	8.8e-4 ⁺	0.59446
L36*	253.147	13.3024	0.59165	1.1e-4	5.8e-3	5.8e-3	1.8e-5	2.7e-3	2.7e-3	1.7e-5	1.1e-3 ⁺	1.1e-3 ⁺	0.59060
L37*	253.147	13.3201	0.58371	1.2e-4	5.8e-3	5.8e-3	5.7e-5	2.7e-3	2.7e-3	1.6e-5	1.6e-3 ⁺	1.6e-3 ⁺	0.58784
P4	273.147	3.4848 ^e	0.99999	2.4e-5	1.5e-3	1.5e-3	9.9e-7	1.1e-3	1.1e-3				
L39	273.145	5.0161	0.96558	8.5e-5	2.0e-3	2.0e-3	2.2e-5	1.1e-3	1.1e-3	3.0e-6	4.8e-4	4.8e-4	0.96828
L40	273.146	5.9255	0.94385	1.6e-4	2.5e-3	2.5e-3	2.7e-5	1.1e-3	1.1e-3	3.1e-6	4.8e-4	4.8e-4	0.94709
L41	273.146	6.9258	0.91829	6.8e-5	2.4e-3	2.4e-3	3.7e-5	1.1e-3	1.1e-3	2.7e-6	4.8e-4	4.8e-4	0.92127
L42	273.146	7.9107	0.89110	1.2e-4	2.4e-3	2.4e-3	2.9e-5	1.2e-3	1.2e-3	6.6e-6	4.8e-4	4.8e-4	0.89260
L43	273.146	8.8894	0.86113	9.3e-5	2.4e-3	2.4e-3	6.1e-5	1.3e-3	1.3e-3	1.4e-5	4.8e-4	4.8e-4	0.85979
L44	273.145	9.8537	0.82710	1.8e-4	2.4e-3	2.4e-3	1.5e-4	1.4e-3	1.4e-3	6.3e-6	4.8e-4	4.8e-4	0.82128
L45	273.147	10.8864	0.78003	6.0e-5	2.4e-3	2.4e-3	1.6e-5	2.7e-3	2.7e-3	6.8e-5	5.1e-4	5.1e-4	0.76737
L46	273.146	11.3314	0.74899	8.2e-5	2.3e-3	2.3e-3	1.2e-4	2.7e-3	2.7e-3	2.8e-5	5.4e-4 ⁺	5.4e-4 ⁺	0.73428
L47*	273.145	11.5579	0.71514	2.5e-4	2.6e-3	2.6e-3	1.5e-5	2.7e-3	2.7e-3	1.6e-5	1.1e-3 ⁺	1.1e-3 ⁺	0.70945
L48*	273.146	11.5779	0.70363	1.7e-4	2.3e-3	2.3e-3	6.6e-6	2.7e-3	2.7e-3	1.3e-4	3.0e-3 ⁺	3.0e-3 ⁺	0.70648
P5	288.139	5.0859 ^f	0.99999	2.8e-4	1.8e-3	1.8e-3	2.9e-6	1.1e-3	1.1e-3				
L50	288.137	5.6498	0.98649	9.1e-4	1.7e-3	2.0e-3	1.3e-5	1.1e-3	1.1e-3	2.0e-5	4.8e-4	4.8e-4	0.98744
L51	288.136	7.0494	0.95060	4.2e-4	1.6e-3	1.6e-3	7.5e-6	1.1e-3	1.1e-3	1.3e-6	4.8e-4	4.8e-4	0.95110
L52	288.134	8.4289	0.90854	6.8e-4	1.6e-3	1.7e-3	9.2e-6	1.2e-3	1.2e-3	1.8e-6	4.8e-4	4.8e-4	0.90541
L53	288.137	8.8666	0.89230	9.0e-4	1.7e-3	1.9e-3	1.7e-6	1.3e-3	1.3e-3	4.4e-6	4.8e-4	4.8e-4	0.88720
L54	288.138	9.2573	0.87508	1.7e-4	1.6e-3	1.6e-3	1.1e-5	1.3e-3	1.3e-3	6.1e-6	4.8e-4	4.8e-4	0.86795
L55	288.139	9.5784	0.85590	9.8e-4	1.8e-3	2.1e-3	1.0e-5	1.4e-3	1.4e-3	5.2e-6	4.9e-4 ⁺	4.9e-4 ⁺	0.84786
L56	288.138	9.7066	0.84282	1.2e-3	1.7e-3	2.1e-3	2.6e-5	1.4e-3	1.4e-3	5.2e-6	5.2e-4 ⁺	5.2e-4 ⁺	0.83726
L57	288.141	9.7231	0.84006	4.2e-5	1.8e-3	1.8e-3	1.3e-5	1.4e-3	1.4e-3	3.5e-6	5.5e-4 ⁺	5.5e-4 ⁺	0.83565
L58	288.139	9.7447	0.83495	1.5e-3	1.9e-3	2.4e-3	8.7e-6	1.4e-3	1.4e-3	2.6e-5	6.6e-4 ⁺	6.6e-4 ⁺	0.83343
P6	298.137	6.4328 ^g	0.99999	1.1e-4	3.0e-3	3.0e-3	8.6e-6	1.1e-3	1.1e-3				
L59	298.133	7.1110	0.98137	6.6e-4	3.0e-3	3.1e-3	6.5e-6	1.1e-3	1.1e-3	1.1e-6	4.8e-4	4.8e-4	0.98158
L60	298.135	7.4191	0.97218	5.0e-4	3.1e-3	3.2e-3	5.0e-6	1.1e-3	1.1e-3	7.0e-7	4.8e-4	4.8e-4	0.97195
L61	298.134	7.8403	0.95809	1.0e-3	3.0e-3	3.1e-3	1.1e-4	1.1e-3	1.2e-3	2.3e-6	4.8e-4	4.8e-4	0.95692
L62	298.135	8.0258	0.95087	1.4e-3	3.2e-3	3.5e-3	7.7e-6	1.1e-3	1.1e-3	2.7e-6	4.8e-4	4.8e-4	0.94920
L63	298.135	8.1284	0.94625	2.6e-4	3.0e-3	3.0e-3	9.6e-6	1.2e-3	1.2e-3	1.0e-6	4.8e-4	4.8e-4	0.94443
L64	298.135	8.2648	0.93815	2.3e-4	3.2e-3	3.2e-3	9.7e-6	1.2e-3	1.2e-3	1.5e-6	4.9e-4 ⁺	4.9e-4 ⁺	0.93709
L65	298.136	8.3019	0.93439	5.1e-4	3.3e-3	3.3e-3	1.0e-5	1.2e-3	1.2e-3	5.2e-6	5.1e-4 ⁺	5.1e-4 ⁺	0.93474
L66	298.134	8.3180	0.93085	4.1e-4	3.1e-3	3.2e-3	4.5e-6	1.2e-3	1.2e-3	2.8e-5	7.2e-4 ⁺	7.2e-4 ⁺	0.93363

^a Sample standard deviation of the mean of the temperatures $s(\bar{T}_f)$, mean of the standard systematic uncertainty of the temperatures $\bar{u}_c(\bar{T})$, total standard uncertainty of the temperature $u_c(\bar{T}_f)$, sample standard deviation of the mean of the pressures $s(\bar{p}_f)$, mean of the standard systematic uncertainty of the pressures $\bar{u}_c(\bar{p})$, total standard uncertainty of the pressure $u_c(\bar{p}_f)$, sample standard deviation of the mean of the mole fractions $s(\bar{x}_{\text{CO}_2})$, mean of the total standard uncertainty of the mole fractions $\bar{u}_{\text{tot}}(x_{\text{CO}_2})$, final standard uncertainty of the mole fraction $u_c(\bar{x}_{\text{CO}_2})$, PR-MC-WS-NRTL Case 2 EOS calculated mole fraction $x_{\text{CO}_2,\text{calc}}(\bar{T}_f, \bar{p}_f)$ ^b Span-Wagner CO₂ vapor pressure is 0.5539 ± 0.0002 MPa.

^c Span-Wagner CO₂ vapor pressure is 1.0042 ± 0.0003 MPa. ^d Span-Wagner CO₂ vapor pressure is 1.9694 ± 0.0006 MPa. ^e Span-Wagner CO₂ vapor pressure is 3.4849 ± 0.0010 MPa. ^f Span-Wagner CO₂ vapor pressure is 5.0859 ± 0.0015 MPa. ^g Span-Wagner CO₂ vapor pressure is 6.4324 ± 0.0019 MPa. ^h Measured together with the supercritical data in Table 9 using the procedure in Section 2.3.2. ⁺ The derivatives $\partial x_{\text{CO}_2} / \partial p$ used in Eq. (7) to obtain $\bar{u}_{\text{tot}}(x_{\text{CO}_2})$ were calculated using the scaling law in Eq. (13) with the parameters in Table 11 instead of the PR-MC-WS-NRTL Case 2 fitted EOS. See Table A.2 for the values of the derivatives, and Section 5.3 for details.

Table 8

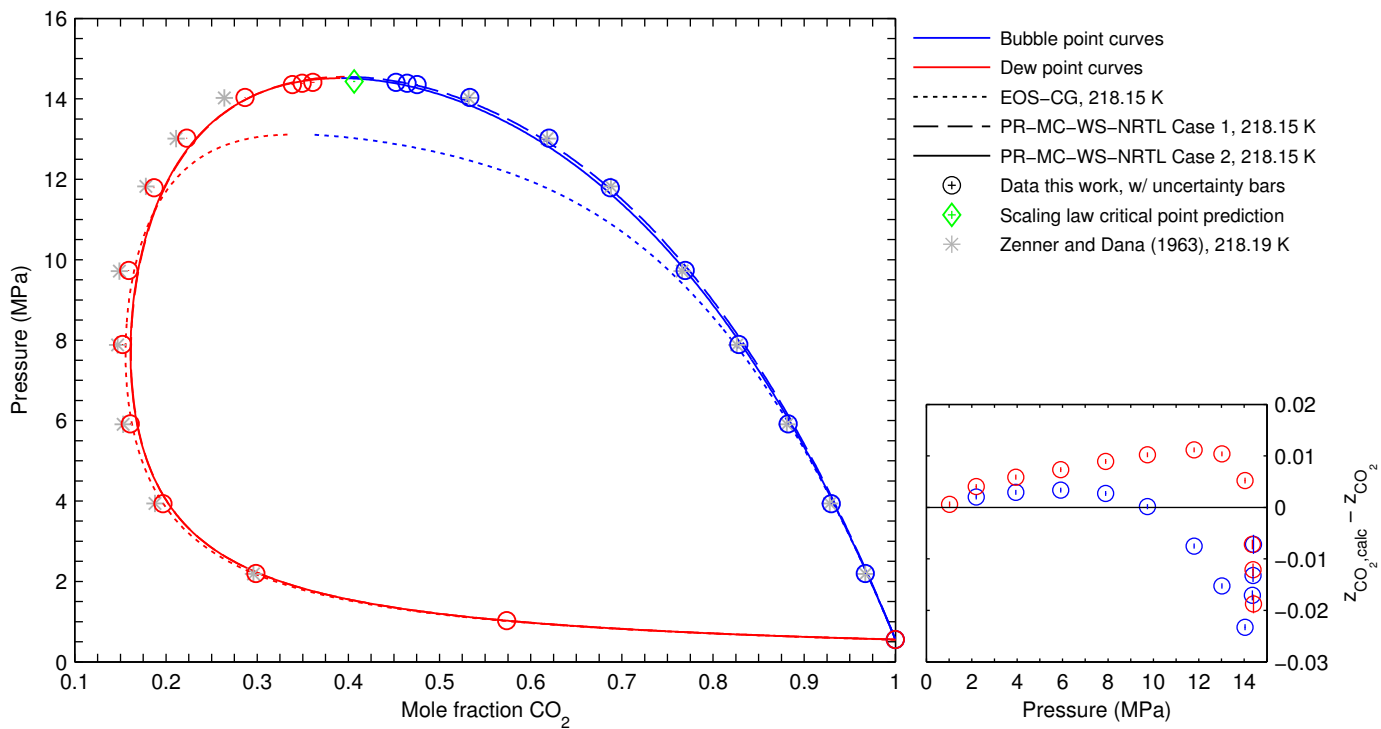
Vapor phase: Experimental VLE data for CO₂ (1) + O₂ (2) at mean temperature \bar{T}_f , mean pressure \bar{p}_f , and mean vapor phase mole fraction \bar{y}_{CO_2} ^a.

ID	Data			Temperature			Pressure			Composition			
	\bar{T}_f (K)	\bar{p}_f (MPa)	\bar{y}_{CO_2} (-)	$s(\bar{T}_f)$ (K)	$\bar{u}_c(\bar{T})$ (K)	$u_c(\bar{T}_f)$ (K)	$s(\bar{p}_f)$ (MPa)	$\bar{u}_c(\bar{p})$ (MPa)	$u_c(\bar{p}_f)$ (MPa)	$s(\bar{y}_{\text{CO}_2})$ (-)	$\bar{u}_{\text{tot}}(\bar{y}_{\text{CO}_2})$ (-)	$u_c(\bar{y}_{\text{CO}_2})$ (-)	$y_{\text{CO}_2,\text{calc}}$ (-)
P1	218.147	0.5546 ^b	0.99999	7.3e-5	3.7e-3	3.7e-3	1.1e-6	4.9e-4	4.9e-4				
V1	218.148	1.0237	0.57354	6.1e-5	3.4e-3	3.4e-3	3.6e-5	5.1e-4	5.1e-4	1.0e-4	5.5e-4	5.6e-4	0.57416
V2	218.148	2.1957	0.29849	2.0e-4	3.5e-3	3.5e-3	1.6e-5	5.2e-4	5.2e-4	5.0e-5	4.8e-4	4.9e-4	0.30252
V3	218.148	3.9362	0.19663	4.8e-5	3.8e-3	3.8e-3	1.1e-5	1.1e-3	1.1e-3	4.2e-5	4.8e-4	4.8e-4	0.20251
V4	218.150	5.9189	0.16093	7.3e-5	3.2e-3	3.2e-3	4.7e-6	1.1e-3	1.1e-3	1.4e-5	4.8e-4	4.8e-4	0.16826
V5	218.148	7.8935	0.15229	2.4e-4	3.5e-3	3.5e-3	5.9e-6	1.2e-3	1.2e-3	1.1e-5	4.8e-4	4.8e-4	0.16120
V6	218.148	9.7335	0.15918	1.1e-4	3.5e-3	3.5e-3	8.1e-6	1.4e-3	1.4e-3	7.2e-6	4.8e-4	4.8e-4	0.16940
V7	218.147	11.7910	0.18681	1.7e-4	3.5e-3	3.5e-3	1.1e-5	2.7e-3	2.7e-3	5.6e-6	4.8e-4	4.8e-4	0.19797
V8	218.148	13.0211	0.22283	1.4e-4	3.5e-3	3.5e-3	1.6e-5	2.8e-3	2.8e-3	8.8e-6	4.9e-4	4.9e-4	0.23321
V9	218.148	14.0359	0.28665	2.0e-4	3.6e-3	3.6e-3	2.2e-5	2.8e-3	2.8e-3	3.8e-5	5.7e-4 ⁺	5.7e-4 ⁺	0.29187
V10*	218.148	14.3563	0.33855	4.8e-5	3.2e-3	3.2e-3	9.5e-6	2.8e-3	2.8e-3	1.7e-5	9.4e-4 ⁺	9.4e-4 ⁺	0.33136
V11*	218.147	14.3873	0.34936	2.0e-4	3.3e-3	3.3e-3	7.4e-6	2.8e-3	2.8e-3	2.0e-5	1.2e-3 ⁺	1.2e-3 ⁺	0.33726
V12*	218.149	14.4111	0.36111	1.9e-4	3.3e-3	3.3e-3	1.5e-5	2.8e-3	2.8e-3	7.5e-5	1.8e-3 ⁺	1.8e-3 ⁺	0.34237
P2	233.143	1.0048 ^c	0.99999	7.4e-5	6.8e-3	6.8e-3	1.1e-5	5.1e-4	5.1e-4				
V14	233.142	1.9677	0.56397	1.5e-4	7.3e-3	7.3e-3	2.3e-6	5.1e-4	5.1e-4	1.2e-4	5.1e-4	5.3e-4	0.56621
V15	233.142	2.9346	0.41117	2.1e-4	7.7e-3	7.7e-3	1.3e-5	5.2e-4	5.3e-4	3.3e-5	4.9e-4	4.9e-4	0.41571
V16	233.143	3.9408	0.33185	3.1e-4	6.8e-3	6.8e-3	2.5e-5	1.1e-3	1.1e-3	1.4e-5	4.9e-4	4.9e-4	0.33997
V17	233.143	5.9475	0.26280	7.5e-5	7.6e-3	7.6e-3	9.5e-5	1.1e-3	1.1e-3	4.7e-6	4.8e-4	4.8e-4	0.27331
V18	233.142	7.8335	0.24021	2.3e-4	7.5e-3	7.5e-3	3.5e-6	1.2e-3	1.2e-3	2.0e-5	4.8e-4	4.8e-4	0.25240
V19	233.141	8.8724	0.23715	3.2e-4	7.6e-3	7.6e-3	4.4e-6	1.3e-3	1.3e-3	2.2e-5	4.8e-4	4.8e-4	0.25033
V20	233.141	9.8514	0.23940	1.1e-4	7.5e-3	7.5e-3	7.7e-6	1.4e-3	1.4e-3	5.4e-6	4.8e-4	4.8e-4	0.25343
V21	233.141	11.8341	0.26143	1.6e-4	7.2e-3	7.2e-3	9.4e-6	2.7e-3	2.7e-3	1.0e-5	4.8e-4	4.8e-4	0.27633
V22	233.142	12.8248	0.28657	2.0e-4	7.2e-3	7.2e-3	1.1e-5	2.7e-3	2.7e-3	1.3e-5	4.9e-4	4.9e-4	0.30036
V23	233.142	13.6445	0.32548	1.6e-4	7.3e-3	7.3e-3	7.4e-6	2.7e-3	2.7e-3	1.5e-5	5.2e-4 ⁺	5.2e-4 ⁺	0.33416
V24*	233.144	14.1868	0.39244	2.0e-4	6.8e-3	6.8e-3	1.5e-5	2.8e-3	2.8e-3	2.8e-5	9.4e-4 ⁺	9.4e-4 ⁺	0.37661
V25*	233.144	14.2158	0.40299	3.9e-4	6.6e-3	6.6e-3	7.2e-6	2.8e-3	2.8e-3	2.7e-5	1.3e-3 ⁺	1.3e-3 ⁺	0.38020
V26*	233.145	14.2407	0.41751	1.2e-4	6.0e-3	6.0e-3	1.1e-5	2.8e-3	2.8e-3	1.1e-5	2.4e-3 ⁺	2.4e-3 ⁺	0.38354
P3	253.147	1.9699 ^d	0.99999	1.5e-5	5.7e-3	5.7e-3	5.5e-6	5.1e-4	5.1e-4				
V28	253.147	2.9631	0.72731	8.7e-5	5.7e-3	5.7e-3	6.3e-5	5.3e-4	5.3e-4	9.5e-6	5.0e-4	5.0e-4	0.73135
V29	253.146	4.9363	0.51051	7.5e-5	5.7e-3	5.7e-3	1.5e-5	1.1e-3	1.1e-3	2.2e-5	4.9e-4	4.9e-4	0.51935
V30	253.146	6.9080	0.42654	1.6e-4	5.9e-3	5.9e-3	9.4e-6	1.1e-3	1.1e-3	2.7e-5	4.8e-4	4.8e-4	0.43955
V31	253.146	8.3057	0.39990	1.8e-4	5.9e-3	5.9e-3	1.1e-5	1.2e-3	1.2e-3	1.1e-5	4.8e-4	4.8e-4	0.41507
V32	253.148	9.6222	0.39110	6.1e-5	5.8e-3	5.8e-3	2.2e-5	1.4e-3	1.4e-3	8.6e-5	4.8e-4	4.9e-4	0.40751
V33	253.148	10.8461	0.39517	2.1e-4	5.6e-3	5.6e-3	2.3e-4	2.7e-3	2.7e-3	1.5e-5	4.8e-4	4.8e-4	0.41263
V34	253.146	11.8558	0.41081	6.8e-5	5.8e-3	5.8e-3	4.8e-5	2.7e-3	2.7e-3	1.2e-5	4.9e-4	4.9e-4	0.42773
V35	253.146	12.7677	0.44495	1.4e-4	5.7e-3	5.7e-3	8.4e-6	2.7e-3	2.7e-3	5.7e-6	5.2e-4 ⁺	5.2e-4 ⁺	0.45666
V36*	253.146	13.2762	0.50132	3.5e-4	5.8e-3	5.8e-3	4.2e-5	2.7e-3	2.7e-3	1.6e-5	8.6e-4 ⁺	8.6e-4 ⁺	0.49109
V37*	253.147	13.3023	0.50988	1.2e-4	6.0e-3	6.0e-3	2.2e-5	2.7e-3	2.7e-3	6.0e-5	1.1e-3 ⁺	1.1e-3 ⁺	0.49401
V38*	253.147	13.3200	0.51743	5.8e-5	5.8e-3	5.8e-3	6.6e-6	2.7e-3	2.7e-3	1.1e-5	1.6e-3 ⁺	1.6e-3 ⁺	0.49612
P4	273.147	3.4848 ^e	0.99999	2.4e-5	1.5e-3	1.5e-3	9.9e-7	1.1e-3	1.1e-3				
V40	273.144	3.9433	0.91844	1.3e-4	2.2e-3	2.2e-3	1.7e-5	1.1e-3	1.1e-3	1.1e-4	5.1e-4	5.2e-4	0.92150
V41	273.145	5.0162	0.78625	2.1e-4	2.1e-3	2.1e-3	4.9e-5	1.1e-3	1.1e-3	3.6e-5	4.9e-4	4.9e-4	0.79225
V42	273.146	5.9256	0.71346	6.1e-5	2.5e-3	2.5e-3	2.5e-5	1.1e-3	1.1e-3	1.2e-5	4.9e-4	4.9e-4	0.72173
V43	273.146	6.9259	0.65904	8.1e-5	2.2e-3	2.2e-3	5.2e-5	1.1e-3	1.1e-3	1.2e-5	4.8e-4	4.8e-4	0.66945
V44	273.146	7.9107	0.62377	2.4e-4	2.3e-3	2.3e-3	5.1e-5	1.2e-3	1.2e-3	1.1e-5	4.8e-4	4.8e-4	0.63597
V45	273.146	8.8896	0.60275	9.9e-5	2.3e-3	2.3e-3	8.9e-5	1.3e-3	1.3e-3	1.0e-5	4.8e-4	4.8e-4	0.61637
V46	273.146	9.8539	0.59503	1.5e-4	2.5e-3	2.5e-3	2.0e-5	1.4e-3	1.4e-3	5.3e-6	4.8e-4	4.8e-4	0.60925
V47	273.146	10.8864	0.60684	1.7e-4	2.7e-3	2.7e-3	1.8e-5	2.7e-3	2.7e-3	7.8e-6	4.8e-4	4.8e-4	0.61857
V48	273.146	11.3312	0.62764	9.4e-5	2.4e-3	2.4e-3	1.7e-5	2.7e-3	2.7e-3	2.6e-5	5.3e-4 ⁺	5.4e-4 ⁺	0.63335
V49*	273.145	11.5578	0.66096	2.5e-5	2.6e-3	2.6e-3	2.3e-5	2.7e-3	2.7e-3	1.8e-5	1.1e-3 ⁺	1.1e-3 ⁺	0.64900
V50*	273.146	11.5780	0.67276	1.3e-4	2.4e-3	2.4e-3	1.5e-5	2.7e-3	2.7e-3	9.9e-5	3.1e-3 ⁺	3.1e-3 ⁺	0.65119
P5	288.139	5.0859 ^f	0.99999	2.8e-4	1.8e-3	1.8e-3	2.9e-6	1.1e-3	1.1e-3				
V52	288.137	5.6498	0.94168	8.5e-4	1.7e-3	1.9e-3	3.5e-6	1.1e-3	1.1e-3	2.6e-5	4.9e-4	4.9e-4	0.94516
V53	288.142	7.0493	0.84273	2.1e-5	1.8e-3	1.8e-3	6.8e-6	1.1e-3	1.1e-3	3.7e-5	4.8e-4	4.8e-4	0.84963
V54	288.141	8.4289	0.79080	1.3e-3	1.8e-3	2.3e-3	1.4e-5	1.2e-3	1.2e-3	2.4e-5	4.8e-4	4.8e-4	0.79918
V55	288.137	8.8666	0.78344	5.1e-4	1.8e-3	1.8e-3	2.3e-5	1.3e-3	1.3e-3	1.7e-6	4.8e-4	4.8e-4	0.79132
V56	288.139	9.2573	0.78234	5.5e-4	1.7e-3	1.8e-3	8.7e-6	1.3e-3	1.3e-3	1.2e-6	4.8e-4	4.8e-4	0.78870
V57	288.138	9.5784	0.78942	4.3e-4	1.7e-3	1.8e-3	1.2e-5	1.4e-3	1.4e-3	2.8e-6	4.9e-4 ⁺	4.9e-4 ⁺	0.79159
V58	288.141	9.7066	0.79944	1.1e-4	1.7e-3	1.7e-3	2.0e-5	1.4e-3	1.4e-3	8.5e-6	5.1e-4 ⁺	5.1e-4 ⁺	0.79558
V59	288.141	9.7232	0.80207	4.1e-4	1.9e-3	1.9e-3	1.0e-5	1.4e-3	1.4e-3	9.5e-6	5.3e-4 ⁺	5.3e-4 ⁺	0.79633
V60	288.142	9.7447	0.80674	2.9e-5	1.9e-3	1.9e-3	3.9e-6	1.4e-3	1.4e-3	7.8e-5	6.4e-4 ⁺	6.5e-4 ⁺	0.79746
P6	298.137	6.4328 ^g	0.99999	1.1e-4	3.0e-3	3.0e-3	8.6e-6	1.1e-3	1.1e-3				
V61	298.141	7.1110	0.95624	4.8e-5	3.2e-3	3.2e-3	2.8e-6	1.1e-3	1.1e-3	1.3e-5	4.8e-4	4.8e-4	0.95967
V62	298.135	7.4191	0.94072	7.8e-4	3.2e-3	3.3e-3	4.1e-6	1.1e-3	1.1e-3	2.7e-6	4.8e-4	4.8e-4	0.94483
V63	298.138	7.8392	0.92467	1.4e-3	3.1e-3	3.4e-3	1.4e-4	1.1e-3	1.1e-3	1.1e-5	4.8e-4	4.8e-4	0.92886
V64	298.140	8.0258	0.91978	3.9e-5	3.3e-3	3.3e-3	3.9e-6	1.1e-3	1.1e-3	8.6e-6	4.8e-4	4.8e-4	0.92365
V65	298.135	8.1339	0.91818	3.6e-4	3.0e-3	3.0e-3	6.7e-6	1.2e-3	1.2e-3	1.0e-5	4.8e-4	4.8e-4	0.92129
V66	298.135	8.2648	0.91898	7.1e-4	3.1e-3	3.2e-3	3.8e-6	1.2e-3	1.2e-3	9.2e-7	4.8e-4 ⁺	4.8e-4 ⁺	0.91966
V67	298.137	8.3019	0.92108	4.4e-4	3.2e-3	3.2e-3	9.0e-6	1.2e-3	1.2e-3	6.4e-6	4.9e-4 ⁺	4.9e-4 ⁺	0.91960
V68	298.136	8.3180	0.92389	1.0e-3	3.1e-3	3.3e-3	6.0e-6	1.2e-3	1.2e-3	1.0e-5	6.9e-4 ⁺	6.9e-4 ⁺	0.91965

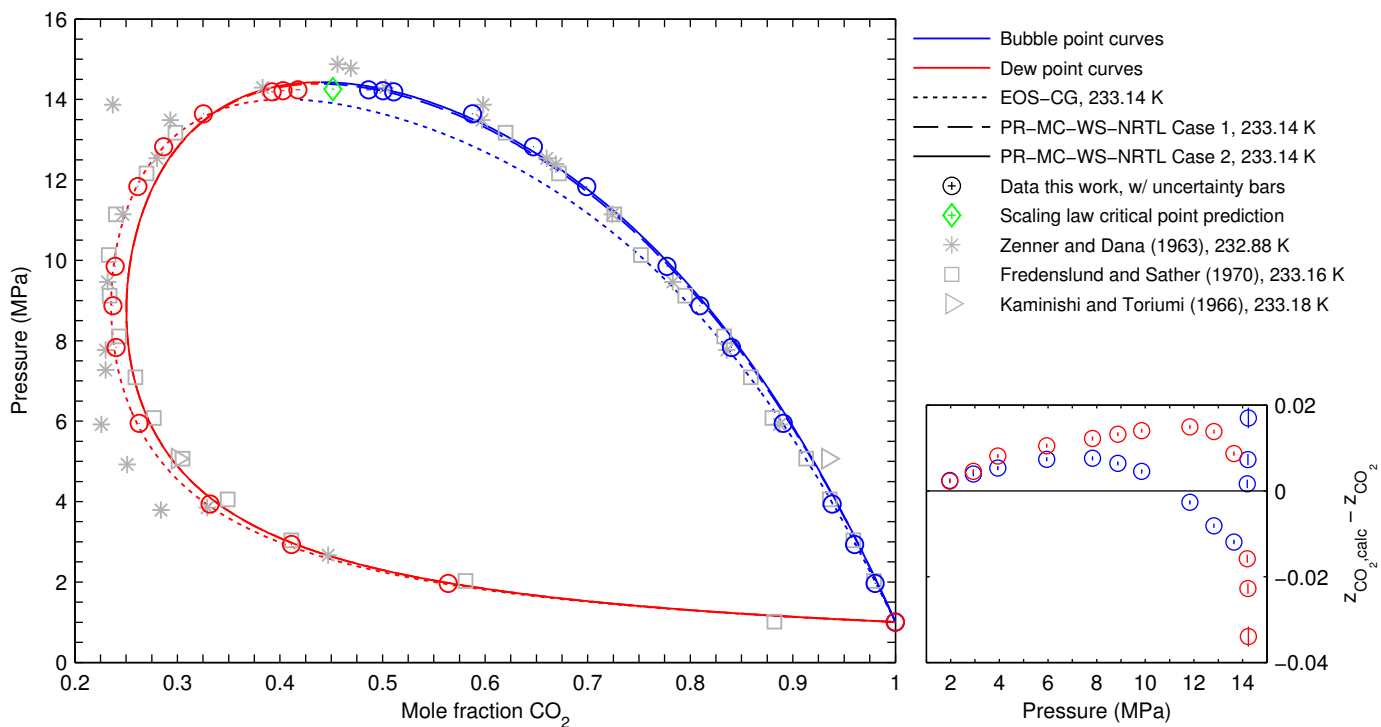
^a Sample standard deviation of the mean of the temperatures $s(\bar{T}_f)$, mean of the standard systematic uncertainty of the temperatures $\bar{u}_c(\bar{T})$, total standard uncertainty of the temperature $u_c(\bar{T}_f)$, sample standard deviation of the mean of the pressures $s(\bar{p}_f)$, mean of the standard systematic uncertainty of the pressures $\bar{u}_c(\bar{p})$, total standard uncertainty of the pressure $u_c(\bar{p}_f)$, sample standard deviation of the mean of the mole fractions $s(\bar{y}_{\text{CO}_2})$, mean of the total standard uncertainty of the mole fractions $\bar{u}_{\text{tot}}(\bar{y}_{\text{CO}_2})$, final standard uncertainty of the mole fraction $u_c(\bar{y}_{\text{CO}_2})$, PR-MC-WS-NRTL Case 2 EOS calculated mole fraction $y_{\text{CO}_2,\text{calc}}(\bar{T}_f, \bar{p}_f)$ ^b Span-Wagner CO₂ vapor pressure is 0.5539 ± 0.0002 MPa.

^c Span-Wagner CO₂ vapor pressure is 1.0042 ± 0.0003 MPa. ^d Span-Wagner CO₂ vapor pressure is 1.9694 ± 0.0006 MPa. ^e Span-Wagner CO₂ vapor pressure is 3.4849 ± 0.0010 MPa.

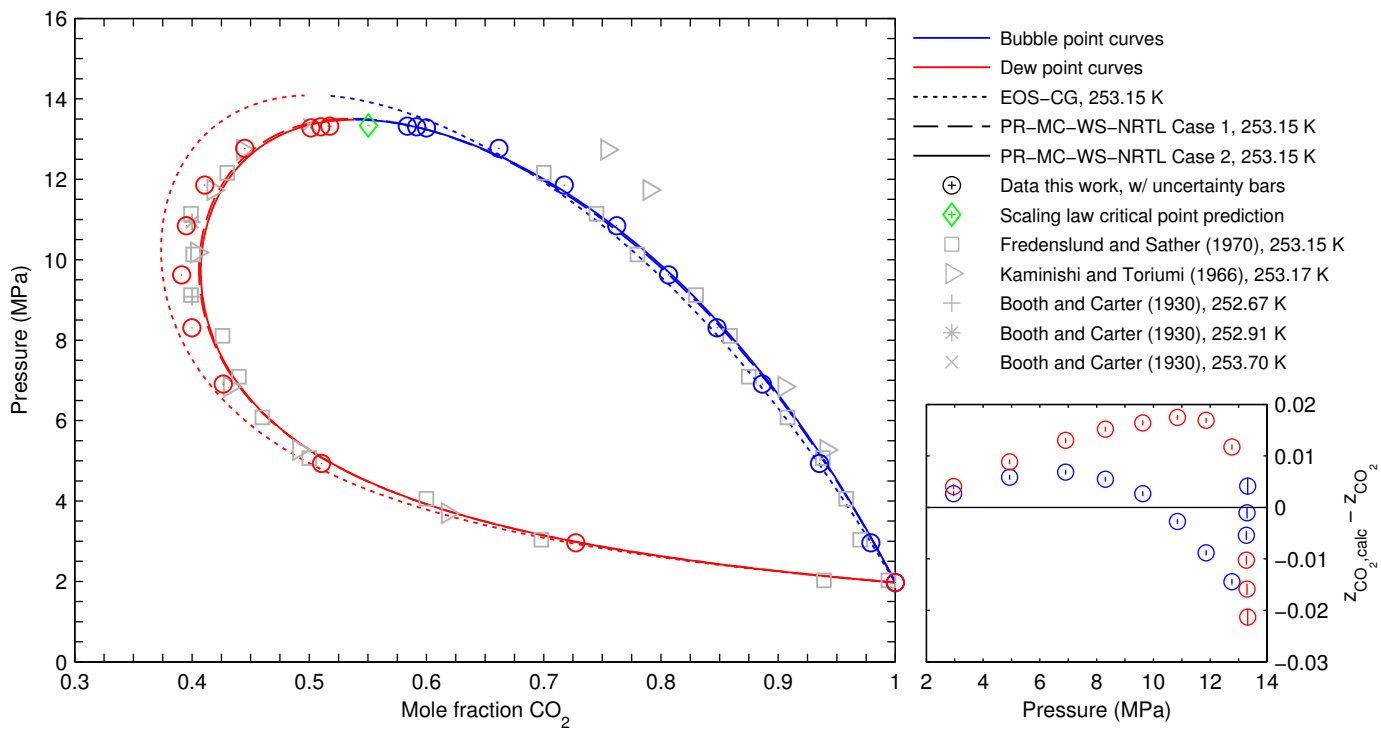
^f Span-Wagner CO₂ vapor pressure is 5.0859 ± 0.0015 MPa. ^g Span-Wagner CO₂ vapor pressure is 6.4324 ± 0.0019 MPa. ^h Measured together with the supercritical data in Table 9 using the procedure



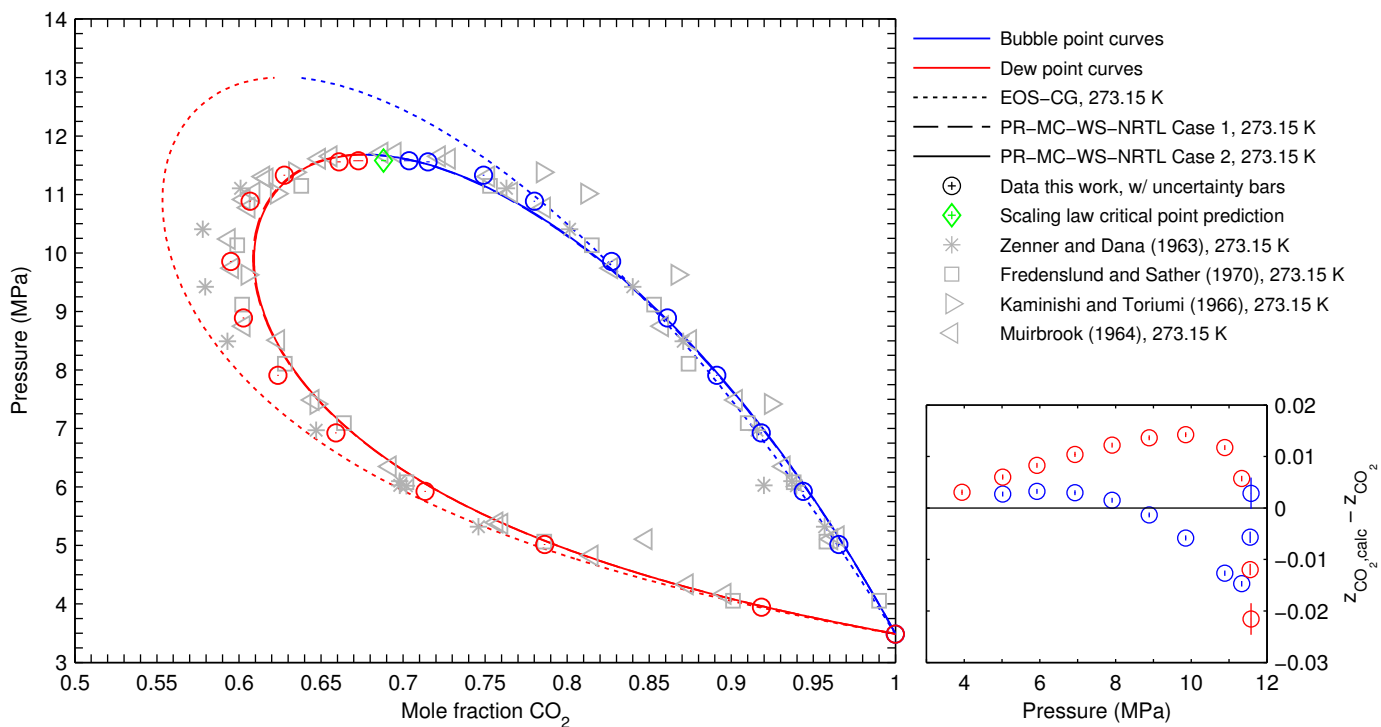
(a) Mean temperature of measurements in present work 218.148 K. VLE data from literature [18].



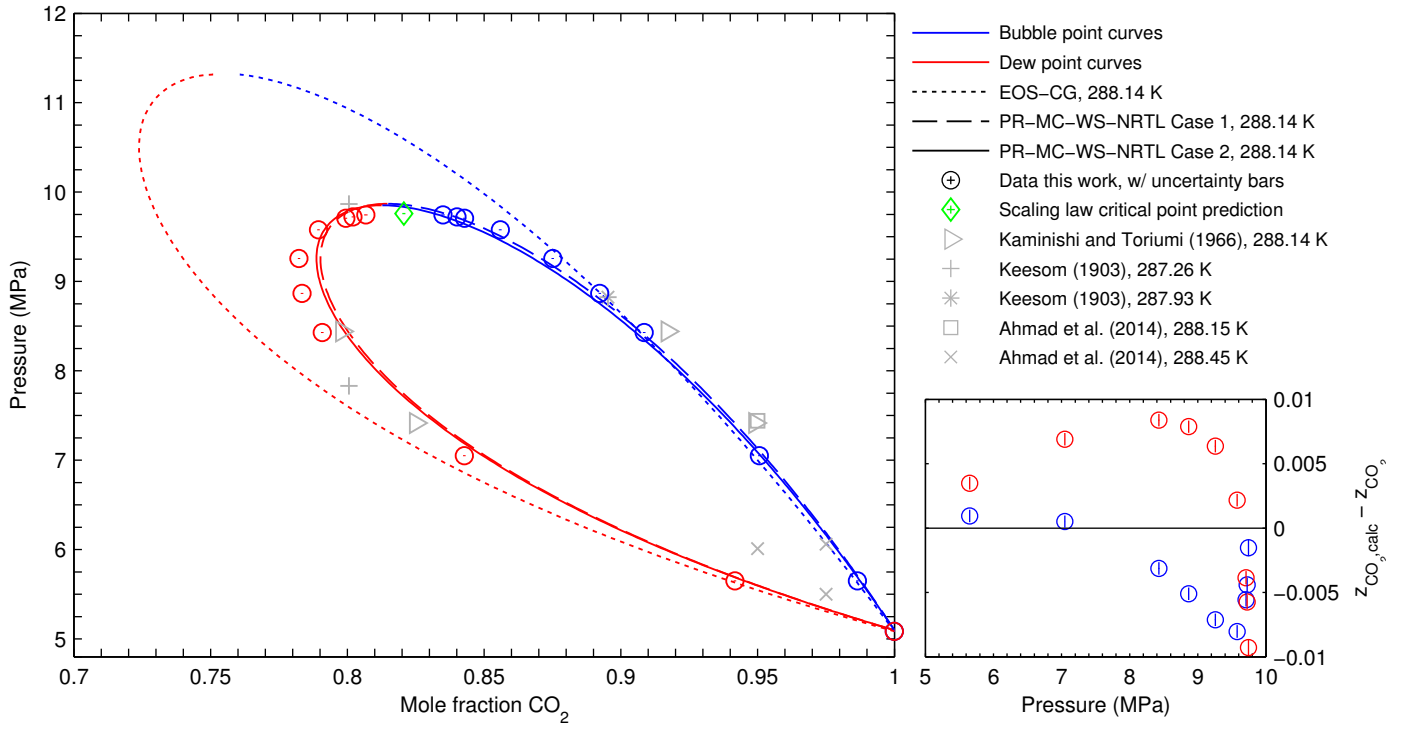
(b) Mean temperature of measurements in present work 233.143 K. VLE data from literature [18, 19, 20].



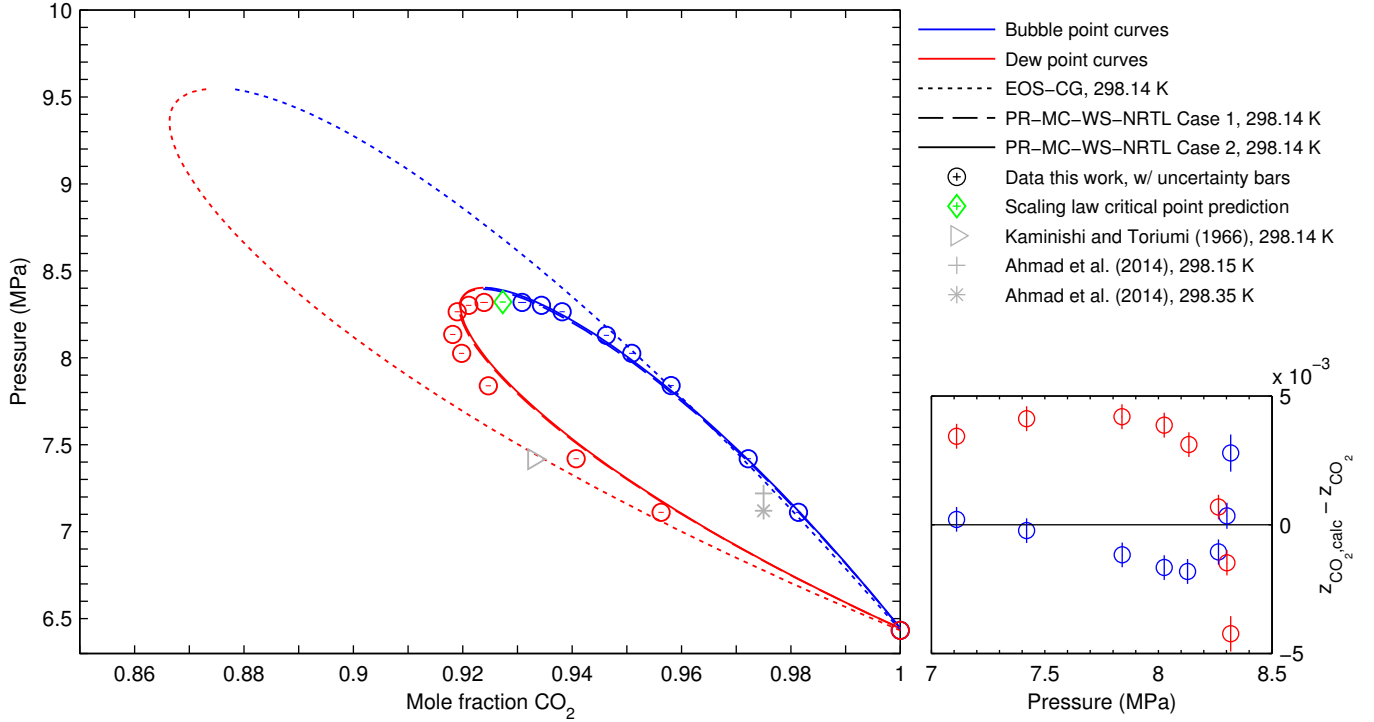
(c) Mean temperature of measurements in present work 253.147 K. VLE data from literature [19, 20, 21].



(d) Mean temperature of measurements in present work 273.146 K. VLE data from literature [18, 19, 20, 22].



(e) Mean temperature of measurements in present work 288.139 K. VLE data from literature [20, 23, 24].



(f) Mean temperature of measurements in present work 298.136 K. VLE data from literature [20, 24].

Fig. 5. Left: Pressure-composition diagram based on EOS calculations at the different mean temperatures, VLE data from literature, and VLE measurements with estimated uncertainties from present work: \bar{x}_{CO_2} , \bar{y}_{CO_2} , \bar{p}_f , $u_c(\bar{x}_{\text{CO}_2})$, $u_c(\bar{y}_{\text{CO}_2})$ and $u_c(\bar{p}_f)$ from Tables 7 and 8. Please note that the uncertainty bars are very small compared to the scale of the plots. Critical point estimation and its uncertainties are from Section 5.3. Right: Plot of deviation between PR-MC-WS-NRTL Case 2 $z_{\text{CO}_2,\text{calc}}$ and VLE measurements from present work z_{CO_2} , where z_{CO_2} is equal to either x_{CO_2} or y_{CO_2} .

Table 9

Composition data at supercritical states for the liquid and vapor samplers for CO₂ (1) + O₂ (2) at mean temperature \bar{T}_f , mean pressure \bar{p}_f , and mean mole fraction \bar{z}_{CO_2} ^a.

ID	Data			Temperature			Pressure			Composition	
	\bar{T}_f (K)	\bar{p}_f (MPa)	\bar{z}_{CO_2} (-)	$s(\bar{T}_f)$ (K)	$\bar{u}_c(\bar{T})$ (K)	$u_c(\bar{T}_f)$ (K)	$s(\bar{p}_f)$ (MPa)	$\bar{u}_c(\bar{p})$ (MPa)	$u_c(\bar{p}_f)$ (MPa)	$s(\bar{z}_{\text{CO}_2})$ (-)	$u_c(\bar{z}_{\text{CO}_2})$ (-)
L12	218.148	14.4390	0.39450	2.1e-4	3.4e-3	3.4e-3	1.2e-5	2.8e-3	2.8e-3	4.3e-6	4.8e-4
V13	218.147	14.4390	0.39472	1.4e-4	3.4e-3	3.4e-3	6.2e-6	2.8e-3	2.8e-3	9.0e-6	4.8e-4
L26	233.142	14.2617	0.44465	2.5e-4	7.4e-3	7.4e-3	1.3e-5	2.8e-3	2.8e-3	1.1e-5	4.8e-4
V27	233.142	14.2617	0.44445	7.7e-5	7.5e-3	7.5e-3	1.3e-5	2.8e-3	2.8e-3	9.3e-6	4.8e-4
L38	253.147	13.3560	0.55468	6.3e-5	5.9e-3	5.9e-3	3.5e-5	2.7e-3	2.7e-3	1.9e-5	4.8e-4
V39	253.148	13.3561	0.55470	3.3e-5	5.6e-3	5.6e-3	1.3e-4	2.7e-3	2.7e-3	1.3e-5	4.8e-4
L49	273.146	11.5976	0.68191	4.5e-4	2.6e-3	2.6e-3	9.5e-5	2.7e-3	2.7e-3	1.9e-5	4.8e-4
V51	273.145	11.5975	0.68219	1.2e-4	2.5e-3	2.5e-3	1.4e-5	2.7e-3	2.7e-3	5.5e-6	4.8e-4

^a Samples taken using liquid sampler given with ID L, samples taken using vapor sampler given with ID V. Sample standard deviation of the mean of the temperatures $s(\bar{T}_f)$, mean of the standard systematic uncertainty of the temperatures $\bar{u}_c(\bar{T})$, total standard uncertainty of the temperature $u_c(\bar{T}_f)$, sample standard deviation of the mean of the pressures $s(\bar{p}_f)$, mean of the standard systematic uncertainty of the pressures $\bar{u}_c(\bar{p})$, total standard uncertainty of the pressure $u_c(\bar{p}_f)$, sample standard deviation of the mean of the mole fractions $s(\bar{z}_{\text{CO}_2})$. Standard uncertainty in mean of the mole fractions $u_c(\bar{z}_{\text{CO}_2}) = \sqrt{s^2(\bar{z}_{\text{CO}_2}) + \bar{u}^2(\bar{z}_{\text{CO}_2})}$, where $\bar{u}(\bar{z}_{\text{CO}_2})$ is the mean of $u(\bar{z}_{\text{CO}_2})$ for the corresponding series in Table A.4.

Table 10

Available isothermal (ISOT) and synthetic (SYN) VLE literature data and the temperature, pressure and composition ranges.

Authors	Year	Type	T (K)	p (MPa)	Composition CO ₂	No. of points
Zenner and Dana [18]	1963	ISOT	218.19, 232.88, 273.15	2.2-14.9	0.147-0.967	58
Kaminishi and Toriumi [20]	1966	ISOT	233.18, 253.17, 273.15, 288.14, 293.14, 298.14	3.7-12.7	0.300-0.949	30
Fredenslund and Sather [19]	1970	ISOT	223.16, 233.16, 243.16, 253.15, 263.15, 273.15, 283.15	1.0-13.2	0.180-0.994	143
Fredenslund et al. [25]	1972	ISOT	223.76	0.9-14.2	0.186-0.996	21
Engberg et al. [26]	2009	ISOT	240.9	1.9-7.2	0.301-0.986	20
Muirbrook [22]	1964	ISOT	273.15	4.2-11.7	0.594-0.965	33
Keesom [23]	1903	SYN	283.21-296.38	6.7-10.4	0.8006, 0.8953	36
Booth and Carter [21]	1930	SYN	212.76-259.91	3.6-14.3	0.2, 0.3, 0.4, 0.5	34 ^a
Ahmad et al. [24]	2014	SYN	277.35-298.35	4.1-8.1	0.9493, 0.9506, 0.9745, 0.9751	22

^a The authors did not report VLE data directly, only the observed phases present at different pressure-temperature states at constant total composition. VLE data points approximated as mean of state variables where difference in temperature or pressure was small across a liquid to vapor-liquid or vapor to vapor-liquid transition.

pairs in the critical region seemed to agree with their data at 14.3 MPa. Their data points at approximately 14.85 MPa did not agree with our critical point prediction (See Section 5.3 below). However, Zenner and Dana [18] indicated in their work that these two points were outside the two-phase region. The data by Fredenslund and Sather [19] agreed reasonably well with our data, except at lower pressures where the deviations between their dew point data and ours were somewhat larger. The two data points by Kaminishi and Toriumi [20] were not directly comparable with our data in terms of pressure, but their bubble point seemed to be slightly off in composition compared to our neighboring data points at 3.9 and 6.0 MPa.

At 253.15 K, the bubble point data by Fredenslund and Sather [19] agreed well with our data, while their dew point data did not agree that well, and their data showed more scatter than ours. The bubble point data by Kaminishi and Toriumi [20] showed large deviations from our data at high pressures, whereas their dew point data seemed to agree better. Although at slightly different temperatures than our data, the data by Booth and Carter [21] agreed well with our data at lower pressures, and very well with our data in the critical region.

At 273.15 K, the data by Zenner and Dana [18] showed a similar deviation pattern to our data as at 233.14 K: Their bubble points agreed well with our data, while their dew points did not agree very well with ours. The data by Fredenslund and Sather [19] agreed reasonably well with our

data. The authors suggested that their bubble and dew points at 11.2 MPa might be erroneous, caused by entrainment. Our bubble and dew points neighboring these points were at respectively higher and lower CO₂ mole fractions, which indicated that this might be correct. Similarly to the data at 253.15 K, the bubble points by Kaminishi and Toriumi [20] did not agree very well with our data, while the dew points agreed better. The data by Muirbrook [22] agreed very well with our data, also in the critical region.

At 288.14 K, we found few literature data points to compare our measurements with. The four data points by Kaminishi and Toriumi [20] agreed better in terms of composition than at the lower temperatures. The data by Keesom [23], although at different temperatures than our data, agreed reasonably well with ours. Of the recent data by Ahmad et al. [24], the dew point data did not match our data very well. The reason for this could have been that the temperature uncertainty in the data by [24] was stated as 1 K, which was very high for measurements at these temperatures when considering the composition temperature derivatives given in Tables A.2 and A.3. The data situation at this temperature was improved considerably by the addition of our data.

At 298.14 K, the only data we were able to find in the literature was the dew point by Kaminishi and Toriumi [20], and the data by Ahmad et al. [24]. The data point by [20] deviated in composition from our data by approximately the same amount as the data by the same authors at 288.14 K. The bubble point by [24] seemed to agree well with our data,

while the dew point at a slightly higher temperature did not match well with our data. Similarly to at 288.14 K, the data situation was improved with our data.

In general, the agreement between our data and literature data varied significantly, also from one temperature to another by the same author. This highlighted the inconsistencies in the literature data noted in [3, 4, 5]. Compared with the existing literature data, the data in the present work described the VLE at the six measured temperatures with considerably less scatter, and included several measurements in the critical region at each temperature, thus forming a good basis for modeling the system. In addition, the VLE measurements at 288.14 and 298.14 K constituted the only complete isotherms at temperatures above 273.15 K.

5.3. Critical point estimation

The procedure for estimating the critical point in terms of pressure and composition for a binary mixture at a certain temperature utilizing scaling laws from statistical mechanics [27, 28, 29] was described for the use on CO₂+N₂ mixtures in [1]. The same procedure was used for estimating the critical points in the present work, the only exception being the estimation of the uncertainty in the critical composition, which is discussed below. The critical point for a binary mixture in terms of pressure and temperature is dependent on the composition. For a given temperature, the composition, if any, where the critical point is attained, is denoted the critical composition, with symbol $z_{\text{CO}_2,c}$, and the corresponding critical pressure, with symbol p_c , is identified as the point of maximum pressure in closed isothermal pressure-composition phase envelopes for a binary mixture, as seen in Figs. 5a to 5f.

Like in [1], the following scaling law was applied [30, 31]:

$$z_{\text{CO}_2} = \hat{z}_{\text{CO}_2,c} + \left(\lambda_1 - \epsilon \frac{\lambda_2}{2} \right) (\hat{p}_c - p) - \epsilon \frac{\mu}{2} (\hat{p}_c - p)^\beta, \quad (13)$$

where

$$\epsilon = \begin{cases} 1 & \text{for bubble points,} \\ -1 & \text{for dew points,} \end{cases}$$

and z_{CO_2} was the bubble point ($z_{\text{CO}_2} = x_{\text{CO}_2}$) or dew point ($z_{\text{CO}_2} = y_{\text{CO}_2}$) CO₂ mole fraction at pressure p . Keeping β fixed at 0.325 [32], the critical composition $z_{\text{CO}_2,c}$ and pressure p_c and the parameters λ_1 , λ_2 and μ were fitted at each isotherm average temperature using the VLE data identified in Table 11. The regression was performed using the ordinary unweighted least squares method, giving the estimators $\hat{z}_{\text{CO}_2,c}$, \hat{p}_c , $\hat{\lambda}_1$, $\hat{\lambda}_2$ and $\hat{\mu}$ shown in Table 11.

The uncertainties in the estimated critical composition and pressure, respectively $u(\hat{z}_{\text{CO}_2,c})$ and $u(\hat{p}_c)$, were estimated according to Eqs. (16) and (17) in [1]. These estimates were based on the uncertainties in the composition and pressure of the VLE data used in the fitting, and the standard errors of regression of the critical composition and pressure, $S_E(\hat{z}_{\text{CO}_2,c})$ and $S_E(\hat{p}_c)$, respectively. The estimates for the uncertainty in

the composition of the VLE data used in the fitting, $u_c(\bar{x}_{\text{CO}_2})$ and $u_c(\bar{y}_{\text{CO}_2})$, were calculated based on values for the composition derivatives with respect to pressure, $\partial z_{\text{CO}_2} / \partial p$, derived from Eq. (13). The values that were calculated using the scaling law are given in Tables A.2, A.3, 7 and 8, indicated with the marker symbol ⁺.

The estimated critical compositions and pressures with their corresponding uncertainties are given in Table 11, and are plotted together with the critical region VLE data and the supercritical state points from Table 9 in Fig. 6.

The standard errors of regression were very low compared to the corresponding uncertainties in the compositions and pressures in the VLE data used for each regression at all temperatures.

Attempts to increase or decrease the number of VLE points used to fit the parameters, compared to the sets of points stated in Table 11, did not result in changes in the critical compositions and pressures that were larger than the uncertainties in these fitted parameters. However, this was only valid if the VLE points closest to the mixture critical points were included in the fit. If fewer of these VLE points were included in the fit, the deviations in the estimated critical compositions and pressures from the estimates given in Table 11 became more pronounced. Two examples are given. First, if the eight VLE points identified as L6-9 and V7-10 in Tables 7 and 8 were used to fit the scaling law at 218.15 K, the estimated critical composition and pressure were respectively 0.4057 and 14.421 MPa. In this data set, the four VLE points closest to the mixture critical point were not included. The estimated critical composition did not change significantly, considering the uncertainty given in Table 11, $u(\hat{z}_{\text{CO}_2,c}) = 0.00115$. However, the estimated critical pressure decreased with 0.014 MPa. Second, if the data set contained the eight VLE points identified as L5-8 and V6-9 were used for the fit, the estimated critical composition and pressure were respectively 0.4052 and 14.346 MPa. In this data set, the six VLE points closest to the mixture critical point were not included. The estimated critical composition decreased slightly more compared to the estimate given in Table 11. Also, the estimated critical pressure decreased with 0.089 MPa.

The supercritical state point pairs at each temperature in Table 9 showed a small difference in composition. As indicated in Section 2.3.2, there was always a possibility that the content of the cell was in the two-phase region during these measurements, but sufficiently close to the critical point such that critical opalescence (see e.g. Ref. [33]) caused the cell phases to become indiscernible. However, the differences in composition shown in Table 9 were below the estimated uncertainty in the composition analysis, $4.8 \cdot 10^{-4}$. Hence, on this basis, it was not possible to conclude that this difference suggested an actual difference in composition, caused by the presence of two phases. In addition, as Fig. 6 shows, the supercritical state points at 218.15, 233.14, 253.15 and 273.15 K were all at higher pressures than the predicted critical pressures, which supported the assumption that these supercritical measurements were indeed outside the two-phase

region.

Based on this discussion, it was assumed that the estimates for the critical points were reasonable, and that the VLE measurements in the critical region also were reasonable, within their corresponding uncertainty estimates and their aforementioned limitations.

5.4. Model fitting

5.4.1. Introduction

In [1], the model for the CO₂+N₂ system in the equation of state called EOS-CG [3, 4] was fitted to the VLE data measured in [1]. The highly flexible structure of the GERG-2008 EOS [34], developed for natural gas mixtures, was used by Gernert and Span [3] to develop EOS-CG, which was fitted to data for the mixtures of some of the components expected in captured CO₂ in CCS processes [3]. The model and parameters used for the CO₂+N₂ system in EOS-CG were almost unchanged compared to that used in the GERG-2008 [3]. The EOS-CG model for the CO₂+O₂ system was an improvement compared to that of the GERG-2008 model. However, as noted in [3, 4], some restrictions on the number of fitting parameters and number of terms utilized in EOS-CG were set due to the inferior data situation. The quality of the description of the CO₂+O₂ system by EOS-CG was reduced accordingly.

The EOS-CG model calculations are plotted in Figs. 5a to 5f. The deviations between the model and the new data of this work were significant. The VLE data provided in the present work considerably improved the data situation for the CO₂+O₂ system, and can be used together with the other available literature data for VLE and properties such as density and speed of sound, to improve the model description of the system.

In this work, the parameters of the Peng-Robinson (PR) cubic EOS [35] with the alpha correction by Mathias and Copeman [36] (MC), the mixing rules by Wong and Sandler [37] (WS), and the NRTL [38] excess Gibbs energy model were fitted. This combination of EOS, alpha correction, mixing rule, and excess Gibbs energy model, designated here as PR-MC-WS-NRTL, has been used to fit VLE data of binary systems containing one supercritical component in our previous work [1] (CO₂+N₂) and in the work of Coquelet et al. [39] (CO₂+Ar).

The data in Tables 7 and 8 formed the basis for the model fitting. Similar to [1], the fitting was performed using orthogonal distance regression (ODR) [40], which consisted in our case of minimizing an objective function with weighting of the minimum deviation between data and model predictions in both composition \bar{x}_{CO_2} and \bar{y}_{CO_2} , and in pressure \bar{p}_f , at a fixed temperature. The objective function can be stated as

$$S^2 = \frac{1}{n - n_p} \sum_i \left(\frac{p_{i,\text{calc}} - \bar{p}_{i,f}}{u_c(\bar{p}_{i,f})} \right)^2 + \frac{1}{n - n_p} \sum_i \left(\frac{z_{i,\text{CO}_2,\text{calc}} - \bar{z}_{i,\text{CO}_2}}{u(z_{\text{CO}_2})} \right)^2, \quad (14)$$

where \bar{z}_{CO_2} is equal to either \bar{x}_{CO_2} or \bar{y}_{CO_2} , n is the total number of experimental data points, n_p is the number of parameters adjusted in the model fit and $u(z_{\text{CO}_2})$ is the composition uncertainty caused by the analysis given in Table 6. In addition to S , two other statistics were used to quantify the agreement between model and data: the absolute average deviation (AAD) and the bias (BIAS), whose formulas are given in Table 12.

5.4.2. Peng-Robinson EOS

The formulas and corresponding nomenclature used in the present work for the MC alpha correction [36], the WS mixing rules [37] and the NRTL [38] excess Gibbs energy model were given in [1] and are not reproduced here. The critical temperature and pressure used in the EOS phase equilibrium calculations for $i = \text{CO}_2$ or O_2 are given in Table 13, together with the parameters $c_{1,i}$, $c_{2,i}$ and $c_{3,i}$ used in the MC alpha correction.

The parameters of the PR-MC-WS-NRTL EOS consist of the Wong-Sandler binary interaction parameters, k_{ij} , the binary interaction parameters of the NRTL model, τ_{ij} , and the non-randomness parameters of the NRTL model, α_{ij} .

Like in [1], the following restrictions were put on the parameters:

$$\begin{aligned} k_{ij} &= k_{ji}, & k_{ii} &= 0, \\ \alpha_{ij} &= \alpha_{ji}, & \alpha_{ii} &= 0, \\ \tau_{ij} &\neq \tau_{ji}, & \tau_{ii} &= 0. \end{aligned} \quad (15)$$

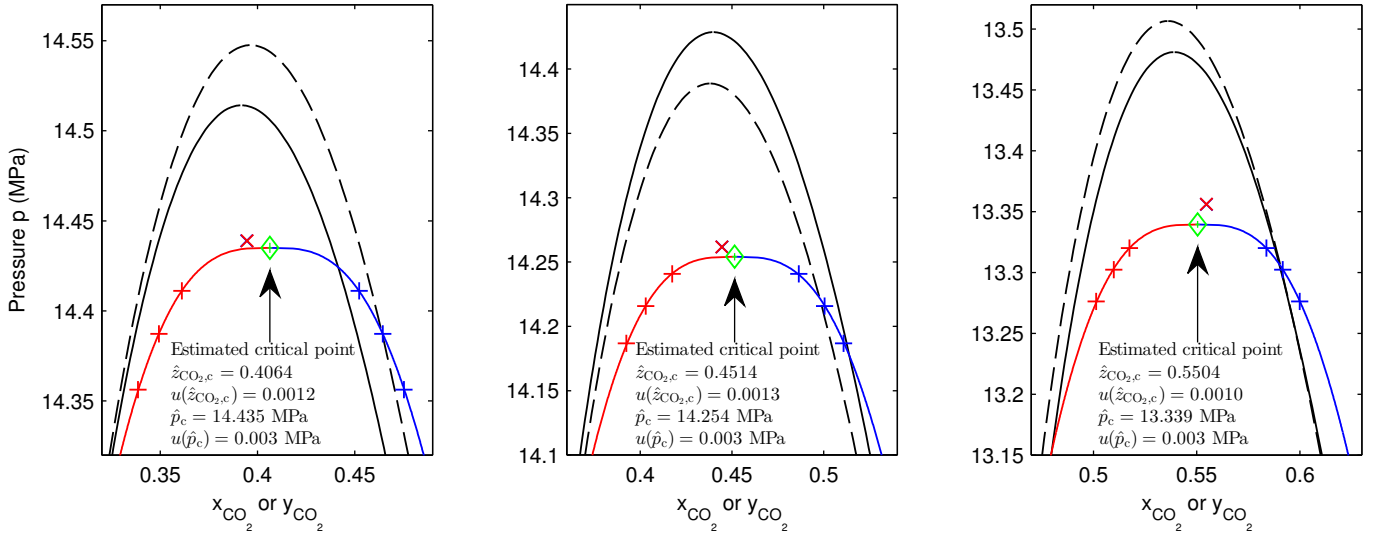
Furthermore, a constant value for $\alpha_{12} = \alpha_{21} = 0.3$ was assumed (cf. [1, 39]), based on the suggestions by Renon and Prausnitz [38] for a system of two non-polar components such as the CO₂+O₂ system. This leaves $n_p = 3$ adjustable parameters in the PR-MC-WS-NRTL model: k_{12} , τ_{12} and τ_{21} . These parameters were assumed to be temperature dependent, to obtain the best possible fit of the data. It was therefore of interest to fit the parameters to data at different temperatures, and try to determine a model for the temperature dependence of the parameters, enabling the use of the EOS over the whole temperature range of the data.

The parameters of the model were fitted to the data at each of the average temperatures 218.15, 233.14, 253.15, 273.15, 288.14 and 298.14 K. The fitted parameters for each temperature are given in Table 12 and plotted in Figs. 7a and 7b, denoted as Case 1. For the temperatures where there were several measurements close to the critical point, only the measurements at the highest pressure were included in the fit, in order to avoid a too strong emphasis on this region. An overview of the points that were excluded are given in Table 12.

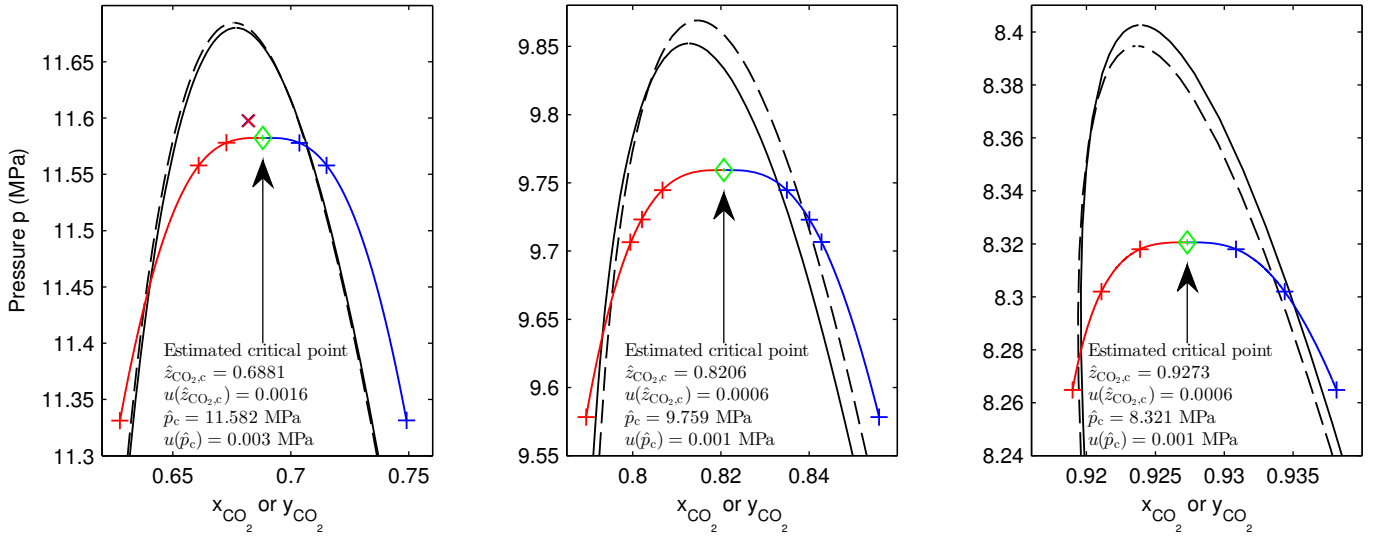
With reference to Fig. 7a, the temperature dependencies of τ_{12} and τ_{21} could be approximately described by the function given in [41]:

$$\tau_{12}(T) = a_{\tau_{12}} + b_{\tau_{12}} \cdot \left| (T - T_{c,\text{CO}_2}) / T_{c,\text{CO}_2} \right|^{c_{\tau_{12}}}, \quad (16)$$

$$\tau_{21}(T) = a_{\tau_{21}} + b_{\tau_{21}} \cdot \left| (T - T_{c,\text{CO}_2}) / T_{c,\text{CO}_2} \right|^{c_{\tau_{21}}}. \quad (17)$$



(a) 218.15 K. The figure shows only 6 of the 8 VLE points used for fitting the scaling law. (b) 233.14 K. The figure shows only 6 of the 8 VLE points used for fitting the scaling law. (c) 253.15 K. The figure shows only 6 of the 8 VLE points used for fitting the scaling law.



(d) 273.15 K.

(e) 288.14 K.

(f) 298.14 K.

- + Liquid phase measurements used for fitting scaling law
- + Vapor phase measurements used for fitting scaling law
- × Supercritical measurements taken using liquid phase sampler
- × Supercritical measurements taken using vapor phase sampler

- Scaling law bubble point curve
- Scaling law dew point curve
- - - PR-MC-WS-NRTL Case 1
- PR-MC-WS-NRTL Case 2

Fig. 6. Comparison of the predictions of the pressure-composition phase behavior in the critical region by three different models: PR-MC-WS-NRTL Case 1 and Case 2 EOSs, and the scaling law model in Eq. (13). Please note that the scales of the graphs are very different from each other. Please refer to Table 11 for an overview of the VLE points used to fit the scaling law and the parameters at the different temperatures. Supercritical measurements are shown in Table 9.

Table 11

Parameters of the scaling law in Eq. (13) fitted to critical region data from this work at six different average temperatures.

T (K)	Used points ^a	n_p (-)	$\hat{\lambda}_1$ (MPa ⁻¹)	$\hat{\lambda}_2$ (MPa ⁻¹)	$\hat{\mu}$ (MPa ^{-β)}	$\hat{z}_{\text{CO}_2,c}$ (-)	\hat{p}_c (MPa)	$S_E(\hat{z}_{\text{CO}_2,c})$ (-)	$u(\hat{z}_{\text{CO}_2,c})$ (-)	$S_E(\hat{p}_c)$ (MPa)	$u(\hat{p}_c)$ (MPa)
218.148	L8-11, V9-12	8	$8.8655 \cdot 10^{-3}$	$-5.6184 \cdot 10^{-2}$	-0.30221	0.4064	14.435	$7.3 \cdot 10^{-5}$	0.00115	$3.6 \cdot 10^{-4}$	0.0028
233.143	L22-25, V23-26	8	$8.3022 \cdot 10^{-3}$	$-4.3134 \cdot 10^{-2}$	-0.27699	0.4514	14.254	$2.1 \cdot 10^{-4}$	0.00130	$6.3 \cdot 10^{-4}$	0.0028
253.147	L34-37, V35-38	8	$5.0483 \cdot 10^{-3}$	$-3.5444 \cdot 10^{-2}$	-0.23569	0.5504	13.339	$1.1 \cdot 10^{-4}$	0.00104	$6.3 \cdot 10^{-4}$	0.0028
273.146	L46-48, V48-50	6	$8.5843 \cdot 10^{-4}$	$-3.0614 \cdot 10^{-2}$	-0.17810	0.6881	11.582	$7.0 \cdot 10^{-5}$	0.00156	$1.3 \cdot 10^{-4}$	0.0027
288.139	L55-58, V57-60	8	$1.1095 \cdot 10^{-2}$	$-1.8503 \cdot 10^{-2}$	-0.11004	0.8206	9.759	$5.7 \cdot 10^{-5}$	0.00055	$5.1 \cdot 10^{-4}$	0.0015
298.136	L64-66, V66-68	6	$2.2534 \cdot 10^{-2}$	$-5.7951 \cdot 10^{-3}$	-0.048162	0.9273	8.321	$5.6 \cdot 10^{-6}$	0.00056	$2.5 \cdot 10^{-5}$	0.0012

^a Data from Tables 7 and 8, identified with the given IDs.**Table 12**Optimal parameters k_{12} , τ_{12} and τ_{21} for the PR-MC-WS-NRTL model, fitted against data from the present work. Objective function S^c and absolute average deviation AAD^d and bias BIAS^e.

T (K)	Case 1 ^a						Case 2 ^b						Both cases
	k_{12}	τ_{12}	τ_{21}	S	AAD (%)	BIAS (%)	k_{12}	τ_{12}	τ_{21}	S	AAD (%)	BIAS (%)	Excluded points
218.148	0.306378	1.271116	0.362629	16.98	0.74	-0.26	0.3065	1.2536	0.3510	18.75	0.77	-0.02	L9-10, V10-11
233.143	0.308267	1.351550	0.161755	22.38	0.94	-0.34	0.3095	1.3578	0.1698	23.02	0.97	-0.45	L23-24, V24-25
253.147	0.315030	1.507658	-0.093799	24.48	0.96	-0.30	0.3135	1.5281	-0.0806	24.91	0.99	-0.47	L35-36, V36-37
273.146	0.317778	1.753552	-0.350178	20.70	0.80	-0.17	0.3175	1.7628	-0.3453	20.74	0.81	-0.22	L47, V49
288.139	0.322426	2.067354	-0.529082	11.90	0.44	-0.09	0.3205	2.0384	-0.5598	12.81	0.50	0.10	
298.136	0.320166	2.370883	-0.735367	5.89	0.22	-0.03	0.3225	2.3813	-0.7190	5.97	0.21	-0.07	

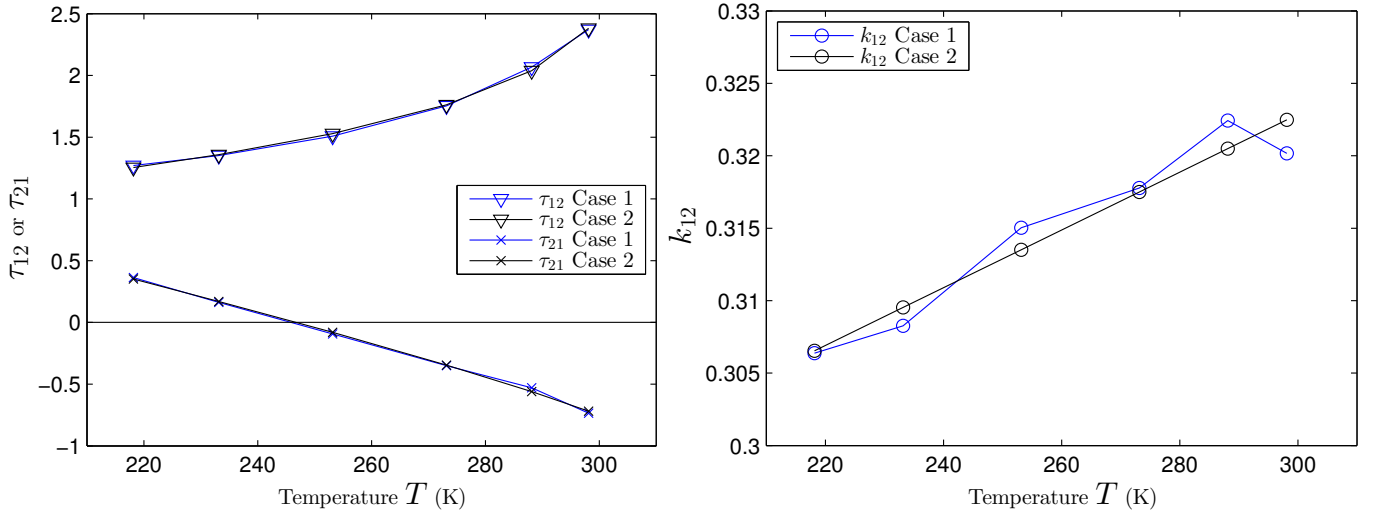
^a $k_{12} = k_{21}$ varies freely, $\alpha = 0.3$ ^b $\alpha = 0.3$, τ_{12} , τ_{21} and $k_{12} = k_{21}$ calculated from Eqs. (16), (17) and (18) respectively using $a_{\tau_{12}} = 3.87841$, $b_{\tau_{12}} = -3.42853$, $c_{\tau_{12}} = 0.211545$, $a_{\tau_{21}} = -0.839864$, $b_{\tau_{21}} = 3.53709$, $c_{\tau_{21}} = 0.862063$, $a_{k_{12}} = 0.323688$, $b_{k_{12}} = 0.0606321$ and $T_{c,\text{CO}_2} = 304.19$ K from Table 13.^c Number of parameters fitted $n_p = 3$. ^d $\text{AAD} = (100/n) \sum_i |z_{i,\text{CO}_2} - z_{i,\text{CO}_2,\text{calc}}|$ ^e $\text{BIAS} = (100/n) \sum_i (z_{i,\text{CO}_2} - z_{i,\text{CO}_2,\text{calc}})$ (a) Optimal values for τ_{12} and τ_{21} for the different temperature data sets in Table 12. (b) Optimal values for k_{12} for the different temperature data sets in Table 12.**Fig. 7.** Optimal values for τ_{12} , τ_{21} and k_{12} for the different temperature data sets in Table 12.

Table 13

Critical properties^a and Mathias-Copeman coefficients^b used in PR-MC-WS-NRTL EOS for CO₂ and O₂.

<i>i</i>	<i>T_{c,i}</i> (K)	<i>p_{c,i}</i> (MPa)	<i>c_{1,i}</i>	<i>c_{2,i}</i>	<i>c_{3,i}</i>
CO ₂	304.19	7.381	0.7050	-0.3185	1.9012
O ₂	154.58	5.043	0.4133	-0.0190	0.0944

^a From Chiavone-Filho et al. [42]. Slightly different from the values used in [6] and [43]: $T_{c,CO_2} = 304.1282$ K, $p_{c,CO_2} = 7.3773$ MPa, $T_{c,O_2} = 154.581$ K, $p_{c,O_2} = 5.043$ MPa. ^b From Chiavone-Filho et al. [42].

Similarly, with reference to Fig. 7b, the temperature dependency of k_{12} was assumed to be described by a simple linear relationship:

$$k_{12}(T) = a_{k_{12}} + b_{k_{12}} \cdot (T - T_{c,CO_2}) / T_{c,CO_2}. \quad (18)$$

With T_{c,CO_2} given in Table 13, the parameters $a_{\tau_{ij}}$, $b_{\tau_{ij}}$, $c_{\tau_{ij}}$, $a_{k_{12}}$ and $b_{k_{12}}$ in Eqs. (16), (17) and (18) were fitted using ordinary unweighted least squares to the optimal Case 1 parameters in Table 12. The fitted parameters of these equations and the calculated values of τ_{12} , τ_{21} , and k_{12} are given in the same table, denoted as Case 2. These calculated Case 2 EOS parameters are plotted in Figs. 7a and 7b with the optimal Case 1 parameters.

The VLE predictions of the PR-MC-WS-NRTL model using both the Case 1 and 2 parameters are shown in Figs. 5a to 5f together with the data from this work and literature. In addition, the deviations between the Case 2 calculated mole fractions and the experimental values are plotted in these figures. The objective function value, absolute average deviation and bias for both cases are given in Table 12.

With reference to Figs. 5a to 5f, the description of our measurements by the Case 2 model was very close to that of the Case 1 model, and this was reflected with only a minor increase in the values for S and AAD, as seen in Table 12. Therefore, for simplicity, only the Case 2 model will now be discussed. First, the model will be compared with our data, and, second, with the literature data in Table 10.

With reference to our measurement data, three aspects of the Case 2 model could be observed. First, except in the critical region, the vapor CO₂ compositions were slightly overestimated by the model, as seen in Figs. 5a to 5f. In fact, the deviations in composition were in general the largest for the vapor phase, as seen from the pressure-composition deviation plots in these figures. With reference to Table 12, the largest absolute average deviation (AAD), including both liquid and vapor measurements, was 0.01 in mole fraction, which was approximately 3 times larger than the maximum final standard uncertainty of the mole fractions, $u_c(\bar{z}_{CO_2})$, $3.1 \cdot 10^{-3}$. Second, the match between the Case 2 model critical points and those estimated by the scaling law in Section 5.3, was quite good, as seen in Figs. 6a to 6f. The critical pressures estimated by the PR-MC-WS-NRTL Case 2 model were approximately 1% higher than the pressures predicted by the scaling law, and the differences in critical compositions were less than 0.015. Third, as seen in the pressure-composition deviation plots in Figs. 5a to 5f, for each of the isotherms the deviation in composition seemed to develop in a similar

manner as a function of pressure, with no apparent scatter. If there had been any apparent scatter, there would have been reason to suspect that the composition samples of the series that deviated from the pattern did not represent the composition at VLE. To be precise, the absence of scatter indicated that the samples represented the VLE composition, however not necessarily that the measured mole fractions for these samples were correct.

As the PR-MC-WS-NRTL Case 2 model was fitted against our data only, it was of interest to compare the model with the literature data in Table 10, and especially the data at other temperatures than those we measured. Table 14 shows the AAD and BIAS for the different VLE literature data in Table 10. Since the AAD and BIAS were calculated as the difference between experimental and calculated mole fractions, the values will in general be higher if a data set contained data in the critical region. The data sets that contained critical region data with proximity to the critical point comparable to our data are identified in Table 14. The AAD for these data sets were comparable to or higher than the AAD for our data at similar temperatures. The same was valid for the literature data sets in general, with a maximum AAD of 0.025 in mole fraction.

The synthetic VLE data sets in Tables 10 and 14 are plotted in a pressure-temperature phase diagram in Fig. 8, together with the PR-MC-WS-NRTL Case 2 VLE calculations at constant compositions. As seen from this figure, the data by Booth and Carter [21] and Ahmad et al. [24] deviated more from the model than the data by Keesom [23].

As it was not possible to find any literature data at temperatures above 298 K (see Table 10), it was difficult to determine how well the PR-MC-WS-NRTL Case 2 model extrapolates up to the critical temperature of CO₂ at 304.19 K.

It has been established that the PR-MC-WS-NRTL Case 2 model provides a fairly accurate description of the VLE for the CO₂+O₂ system given by our data from the temperatures 218 to 298 K, with an AAD of maximum 0.01 in mole fraction and an apparently good description of the critical locus. The most significant shortcoming of the model was the description of the vapor phase compositions, where the deviations were at their largest. With respect to the ability of the model to describe the literature data, the AAD were comparable or somewhat higher considering the lack of critical region data for most of the literature data sets.

6. Conclusions

This work reports accurate vapor-liquid equilibrium (VLE) data for the CO₂+O₂ binary system, at the temperatures 218.15, 233.14, 253.15, 273.15, 288.14 and 298.14 K.

The data measured in this study cover a large range of VLE liquid and vapor phase compositions, spanning CO₂ mole fractions from approximately 0.45 to 0.987 in the liquid phase, and from 0.15 to 0.956 in the vapor phase. The measured CO₂ vapor pressures at the six temperatures are consistent with the values calculated from the Span-Wagner EOS, considering the uncertainty in both the measured pressures and

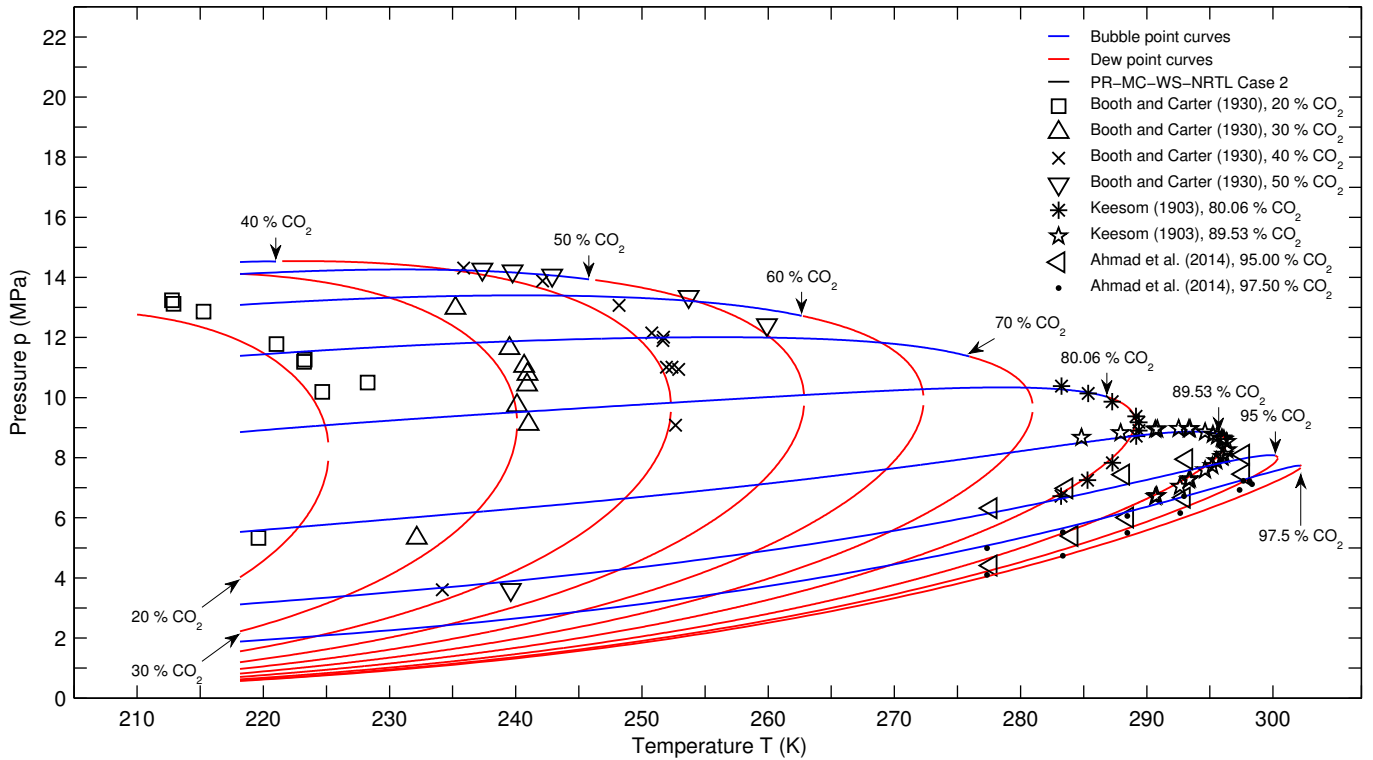


Fig. 8. Pressure-temperature phase diagram at constant compositions based on the PR-MC-WS-NRTL Case 2 model, and synthetic VLE data from literature [21, 23, 24].

that of the EOS. The agreement between our data and literature data varies significantly, also from one temperature to another by the same author. This highlights the inconsistencies in the literature data noted in [3, 4, 5]. As in [1], it was possible to perform very stable measurements close to the mixture critical point at each temperature, and these data formed the basis for the fitting of a scaling law, resulting in estimates for the critical points with low uncertainties. These critical point estimates were slightly lower in pressure than supercritical state point measurements performed at each temperature, which showed the consistency of the critical point estimates.

The Peng-Robinson (PR) cubic EOS [35] with the alpha correction by Mathias and Copeman [36] (MC), the mixing rules by Wong and Sandler [37] (WS), and the NRTL [38] excess Gibbs energy model was fitted to the data in the present work. Based on the parameters sets at each of the six temperatures, expressions for the temperature dependencies of the parameters were developed, resulting in an EOS that can be utilized for VLE calculations over the temperature range from 218 to 298 K and possibly be extrapolated to the critical temperature of CO_2 at 304.19 K. This model described our data quite accurately, and absolute average deviation of our data compared to this model was maximum 0.01 in mole fraction, and maximum 0.025 for the literature data. Additionally, the model matched well with the critical locus given by the scaling law predictions. The critical points calculated

by the PR-MC-WS-NRTL model differed from the scaling law prediction by being approximately 1% higher in pressure, and differed in critical compositions with less than 0.015.

The data measured in the present work showed significantly less scatter than the data found in literature, and included measurements close to the mixture critical points for all six temperatures. This data set significantly improves the data situation for the CO_2+O_2 system. It can be used to enhance highly flexible multi-parameter equations of state such as EOS-CG [3, 4], which should be able to describe other thermodynamic properties of the system more accurately than the PR-MC-WS-NRTL model fit provided in the present work.

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Table 14
AAD and BIAS for the literature data in Table 10, calculated^a using the PR-MC-WS-NRTL Case 2 model.

Authors	Type	$T^b, z_{CO_2}^c$ (K), (-)	AAD (%)	BIAS (%)	n^d
Zenner and Dana [18]	ISOT	218.19	1.29	-0.76	16
		232.88	2.36	-1.70	22 [§]
		273.15	1.49	-1.29	18
Kaminishi and Toriumi [20]	ISOT	233.18	1.02	1.02	2
		253.17	2.46	1.46	10
		273.15	2.16	1.89	8
		288.14	0.73	0.31	4
		293.14	0.82	0.13	5
Fredenslund and Sather [19]	ISOT	298.14	1.19	-1.19	1
		223.16	0.83	-0.79	26
		233.16	1.50	-0.93	25
		243.16	1.06	-0.99	22
		253.15	0.92	-0.57	22
		263.15	0.65	-0.13	20
		273.15	0.63	-0.30	16
Fredenslund et al. [25]	ISOT	283.15	1.27	-0.76	12
		223.76	1.79	1.24	21 [§]
Engberg et al. [26]	ISOT	240.9	1.08	-1.08	20
Muirbrook [22]	ISOT	273.15	1.10	0.06	31 [§]
Keesom [23]	SYN	0.8006	2.00	-1.77	10 [§]
		0.8953	0.74	-0.40	26 [§]
Booth and Carter [21]	SYN	0.2	1.67	-1.31	9
		0.3	1.27	-0.73	8
		0.4	1.56	-1.05	11 [§]
		0.5	2.04	1.20	6 [§]
Ahmad et al. [24]	SYN	0.9493 ^e	2.38	2.38	5 [§]
		0.9506 ^f	0.90	0.90	5 [§]
		0.9745 ^e	1.01	1.01	6 [§]
		0.9751 ^f	0.22	-0.20	6 [§]

^a CO₂ mole fractions at VLE calculated at the temperature and pressure given in the literature data. ^b Temperature T if type is ISOT. ^c z_{CO_2} CO₂ mole fraction if type is SYN. ^d Number of temperature and pressure points that were in the VLE region according to the PR-MC-WS-NRTL Case 2 model. ^e Dew points. ^f Bubble points. [§] Data set contains critical region data.

List of symbols

g_L	local acceleration of gravity. See Appendix A.1 in [1]. (m s^{-2})	T_{Ga}	ITS-90 temperature at gallium melting point. See Appendix A.2 in [1]. (K)
h_i	$i = 1, 2, 3, 4$, liq. Distance used in p_{hs} calculation. See Appendix A.1 in [1]. (m)	$T_{\text{H}_2\text{O}}$	ITS-90 temperature at water triple point. See Appendix A.2 in [1]. (K)
k_{ij}	WS binary interaction parameter between components i and j in Eq. (25) in [1]. (–)	T_{Hg}	ITS-90 temperature at mercury triple point. See Appendix A.2 in [1]. (K)
M	molar mass (kg mol^{-1})	$u(z)$	standard uncertainty of variable z
p	pressure at VLE (MPa)	$u_c(z)$	combined standard uncertainty of variable z
p_c	estimated critical pressure, defined in Section 5.3 (MPa)	$u_{\text{tot}}(z)$	total standard uncertainty of variable $z = x_{\text{CO}_2}$ or y_{CO_2} , from Eq. (7). (–)
p_i	absolute pressure of sensor i , where $i = 1, 2, 3, 4$. See Appendix A.1 in [1]. (MPa)	W	ITS-90 ratio $R/R_{\text{H}_2\text{O}}$. See Appendix A.2 in [1]. (–)
p_{hs}	hydrostatic pressure. See Appendix A.1 in [1]. (MPa)	W_b	thermometry bridge ratio R/R_{ref} . See Appendix A.2 in [1]. (–)
p_{11}	differential pressure. See Appendix A.1 in [1]. (MPa)	x_{CO_2}	liquid phase CO_2 mole fraction at VLE in Table A.2 (–)
\bar{p}	pressure at VLE: mean pressure before one composition sample in Tables A.2 and A.3 (MPa)	\bar{x}_{CO_2}	liquid phase CO_2 mole fraction at VLE: mean mole fraction a series of composition samples in Table 7 (–)
\bar{p}_f	pressure at VLE: mean of the pressures \bar{p} for a series of composition samples in Tables 7 and 8 (MPa)	$x_{\text{CO}_2, \text{calc}}$	liquid phase CO_2 mole fraction at VLE, calculated from the PR-MC-WS-NRTL Case 2 model. See Section 5.4.2. (–)
R	resistance of SPRT at a temperature. See Appendix A.2 in [1]. (Ω)	y_{CO_2}	vapor phase CO_2 mole fraction at VLE in Table A.3 (–)
R	universal gas constant = $8.3145 \text{ J K}^{-1} \text{ mol}^{-1}$	\bar{y}_{CO_2}	vapor phase CO_2 mole fraction at VLE: mean mole fraction a series of composition samples in Table 8 (–)
R_{Ga}	resistance of SPRT at T_{Ga} . See Appendix A.2 in [1]. (Ω)	$y_{\text{CO}_2, \text{calc}}$	vapor phase CO_2 mole fraction at VLE, calculated from the PR-MC-WS-NRTL Case 2 model. See Section 5.4.2. (–)
$R_{\text{H}_2\text{O}}$	resistance of SPRT at $T_{\text{H}_2\text{O}}$. See Appendix A.2 in [1]. (Ω)	z_{CO_2}	liquid or vapor phase CO_2 mole fraction (–)
R_{Hg}	resistance of SPRT at T_{Hg} . See Appendix A.2 in [1]. (Ω)	$z_{\text{CO}_2, c}$	estimated critical composition in terms of CO_2 mole fraction, defined in Section 5.3 (–)
R_{ref}	resistance of reference normal. See Appendix A.2 in [1]. (Ω)		
$s(z)$	sample standard deviation of variable z	<i>Greek letters</i>	
$s(\bar{z})$	sample standard deviation of the mean of variable z	α_{ij}	NRTL non-randomness parameter for binary interaction between components i and j in Eq. (26) in [1].
S	model fitting objective function to be minimized (–)	β	universal critical exponent of scaling law in Eq. (13)
S_E	standard error of regression. See Section 5.3.	$\lambda_1, \lambda_2, \mu$	parameters of scaling law in Eq. (13).
T_{04}	ITS-90 temperature of top flange SPRT (K)	ρ	density (kg m^{-3})
T_{05}	ITS-90 temperature of bottom flange SPRT (K)	ρ_i	density in the four different regions $i = 1, 2, 3, 4$ used for calculation of p_{hs} . See Appendix A.1 in [1]. (kg m^{-3})
T	ITS-90 temperature at VLE (K)	$\rho_{4,1}$	density of pure CO_2 in Region 4 used for calculation of p_{hs} . See Appendix A.1 in [1]. (kg m^{-3})
\bar{T}	ITS-90 temperature at VLE: mean temperature before one composition sample in Tables A.2 and A.3 (K)	$\rho_{4,2}$	density of fluid in Region 4 used for calculation of p_{hs} . See Appendix A.1 in [1]. (kg m^{-3})
\bar{T}_f	ITS-90 temperature at VLE: mean of the temperatures \bar{T} for a series of composition samples in Tables 7 and 8 (K)		

τ_{ij} NRTL parameter for binary interaction between components i and j in Eq. (26) in [1]. (–)

Subscripts

c critical state

Superscripts

– arithmetic mean

Abbreviations

AAD absolute average deviation. See Section 5.4.1 and Table 12.

BIAS bias. See Section 5.4.1 and Table 12.

CAD computer-aided design

CCS carbon capture, transport and storage

EOS equation of state

EOS-CG equation of state for combustion gases and combustion gas like mixtures [3, 4]

GC gas chromatograph

GUM ISO Guide for the Estimation of Uncertainty in Measurement [11]

ITS-90 International Temperature Scale of 1990 [44]

MC Mathias-Copeman alpha correction [36]

NRTL non-random two-liquid excess Gibbs energy model [38]

ODR orthogonal distance regression

PR Peng-Robinson EOS [35]

PR-MC- PR EOS with MC alpha correction and WS

WS-NRTL mixing rule with the NRTL excess Gibbs energy model

SPRT standard platinum resistance thermometer

SW Span-Wagner EOS for CO₂ [6]

TCD thermal conductivity detector in GC

VLE vapor-liquid equilibrium

WS Wong-Sandler mixing rule [37]

Appendix A. Detailed experimental data

Detailed VLE data for the liquid phase samples are given in Table A.2, and for the vapor phase samples in Table A.3. Each row in the tables corresponds to one composition sample. A series of samples taken at the same VLE experiment is identified by the same ID.

For ease of reading, a summary of the symbols used in the tables will be given in Table A.1. The descriptions can also be found in the [list of symbols](#).

Table A.1
Summary of symbols used in Tables A.2 and A.3.

Symbol	Description
ID	Identifier for a series of samples. L, V and P corresponds to liquid, vapor and CO ₂ vapor pressure series, respectively. Marker * means that the series was measured using procedure in Section 2.3.2.
\bar{T}	Mean temperature before the sample is withdrawn from the cell. See Section 3.4.
\bar{p}	Mean pressure before the sample is withdrawn from the cell. See Section 3.4.
x_{CO_2}	Liquid phase CO ₂ mole fraction of the sample.
y_{CO_2}	Vapor phase CO ₂ mole fraction of the sample.
$s(\bar{T})$	Sample standard deviation of the measured temperatures used to calculate \bar{T} . See Eq. (7) in [1].
$s(\bar{T})$	Standard random uncertainty of \bar{T} , considering the autocorrelation of the measurements of T . See Eq. (6) in [1].
$\bar{u}(T)$	Standard systematic uncertainty of \bar{T} . See Section 3.5 in [1].
$u_c(\bar{T})$	Combined standard uncertainty of \bar{T} . Calculated as $\sqrt{s^2(\bar{T}) + \bar{u}^2(T)}$.
$s(p)$	Sample standard deviation of the measured pressures used to calculate \bar{p} . See Eq. (7) in [1].
$s(\bar{p})$	Standard random uncertainty of \bar{p} , considering the autocorrelation of the measurements of p . See Eq. (6) in [1].
$\bar{u}(p)$	Standard systematic uncertainty of \bar{p} . See Section 3.5 in [1].
$u_c(\bar{p})$	Combined standard uncertainty of \bar{p} . Calculated as $\sqrt{s^2(\bar{p}) + \bar{u}^2(p)}$.
$u(z_{\text{CO}_2})^a$	Standard uncertainty of a sample from composition analysis alone. See Section 3.3 and Table 6.
$u_{\text{tot}}(z_{\text{CO}_2})^a$	Total standard uncertainty of a sample, caused by additional contribution from the uncertainty in temperature and pressure. See Eq. (7). Marker + means that the derivative $\partial z_{\text{CO}_2} / \partial p$ used in Eq. (7) was calculated using the scaling law in Eq. (13) with the parameters in Table 11 instead of the PR-MC-WS-NRTL Case 2 fitted EOS.
$z_{\text{CO}_2, \text{calc}}^a$	VLE CO ₂ mole fraction at (\bar{T}, \bar{p}) , calculated using the PR-MC-WS-NRTL Case 2 fitted EOS. See Section 5.4.2.
$\partial z_{\text{CO}_2} / \partial T^a$	Partial derivative of phase composition at VLE with respect to temperature, calculated using the PR-MC-WS-NRTL Case 2 fitted EOS. Used in Eq. (7).
$\partial z_{\text{CO}_2} / \partial p^a$	Partial derivative of phase composition at VLE with respect to pressure. Used in Eq. (7). Marker + means that the derivative was calculated using the scaling law in Eq. (13) with the parameters in Table 11 instead of the PR-MC-WS-NRTL Case 2 fitted EOS.

^a z_{CO_2} equal to either x_{CO_2} or y_{CO_2} .

Table A.2

Liquid phase: Experimental VLE data for CO₂ + O₂ at mean temperature \bar{T} , mean pressure \bar{p} , and sample liquid phase mole fraction x_{CO_2} .

ID	Data			Temperature				Pressure				Composition			Composition derivatives	
	\bar{T} (K)	\bar{p} (MPa)	x_{CO_2} (-)	$s(T)$ (K)	$s(\bar{T})$ (K)	$\bar{u}(T)$ (K)	$u_c(\bar{T})$ (K)	$s(p)$ (MPa)	$s(\bar{p})$ (MPa)	$\bar{u}(p)$ (MPa)	$u_c(\bar{p})$ (MPa)	$u(x_{\text{CO}_2})$ (-)	$u_{\text{tot}}(x_{\text{CO}_2})$ (-)	$x_{\text{CO}_2, \text{calc}}$ (-)	$\partial x_{\text{CO}_2} / \partial T$ (K ⁻¹)	$\partial x_{\text{CO}_2} / \partial p$ (MPa ⁻¹)
P1	218.147	0.5546	0.99999	4.7e-4	7.3e-5	3.7e-3	3.7e-3	1.3e-5	1.1e-6	4.9e-4	4.9e-4					
L1	218.147	2.1957	0.96687	5.1e-4	1.1e-4	3.5e-3	3.6e-3	2.5e-5	6.0e-6	5.2e-4	5.2e-4	4.8e-4	4.8e-4	0.96887	0.00057	-0.01984
	218.147	2.1957	0.96688	8.8e-4	1.9e-4	3.5e-3	3.5e-3	3.2e-5	1.1e-5	5.2e-4	5.2e-4	4.8e-4	4.8e-4	0.96887	0.00057	-0.01984
	218.148	2.1957	0.96687	8.8e-4	3.3e-4	3.6e-3	3.6e-3	4.8e-5	1.6e-5	5.2e-4	5.2e-4	4.8e-4	4.8e-4	0.96887	0.00057	-0.01984
	218.148	2.1957	0.96688	5.3e-4	5.9e-5	3.4e-3	3.4e-3	2.8e-5	3.8e-6	5.2e-4	5.2e-4	4.8e-4	4.8e-4	0.96888	0.00057	-0.01984
	218.148	2.1958	0.96686	4.9e-4	1.4e-4	3.5e-3	3.5e-3	7.5e-5	1.6e-5	5.2e-4	5.2e-4	4.8e-4	4.8e-4	0.96887	0.00057	-0.01984
L2	218.148	3.9363	0.92960	8.9e-4	1.1e-4	3.7e-3	3.7e-3	1.4e-4	5.6e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.93249	0.00073	-0.02205
	218.148	3.9363	0.92958	7.0e-4	8.4e-5	3.7e-3	3.7e-3	7.8e-5	6.9e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.93249	0.00073	-0.02205
	218.148	3.9362	0.92957	7.5e-4	1.4e-4	3.8e-3	3.8e-3	1.5e-4	5.7e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.93250	0.00073	-0.02205
	218.148	3.9362	0.92958	7.6e-4	1.3e-4	3.9e-3	3.9e-3	1.1e-4	3.8e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.93250	0.00073	-0.02205
	218.148	3.9362	0.92957	6.6e-4	1.0e-4	3.7e-3	3.7e-3	5.3e-5	6.3e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.93250	0.00073	-0.02205
	218.148	3.9363	0.92958	7.6e-4	9.5e-5	3.7e-3	3.7e-3	7.6e-5	2.2e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.93249	0.00073	-0.02205
L3	218.147	5.9189	0.88227	7.6e-4	1.2e-4	3.6e-3	3.6e-3	1.2e-4	1.3e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.88563	0.00091	-0.02541
	218.147	5.9190	0.88226	8.2e-4	8.2e-5	3.7e-3	3.7e-3	2.5e-4	1.5e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.88562	0.00091	-0.02541
	218.147	5.9189	0.88227	2.0e-3	4.0e-4	3.4e-3	3.4e-3	1.2e-4	7.7e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.88562	0.00091	-0.02541
	218.149	5.9189	0.88225	1.3e-3	3.4e-4	3.1e-3	3.2e-3	2.0e-4	2.9e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.88563	0.00091	-0.02541
	218.149	5.9189	0.88226	9.5e-4	1.5e-4	3.2e-3	3.2e-3	1.4e-4	1.1e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.88563	0.00091	-0.02541
	218.149	5.9189	0.88226	1.0e-3	2.0e-4	3.2e-3	3.2e-3	1.1e-4	1.1e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.88563	0.00091	-0.02541
L4	218.148	7.8935	0.82833	3.9e-4	3.6e-5	3.4e-3	3.4e-3	1.1e-4	5.3e-6	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.83104	0.00110	-0.03021
	218.149	7.8935	0.82831	1.4e-3	2.4e-4	3.5e-3	3.5e-3	1.1e-4	3.2e-6	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.83104	0.00110	-0.03021
	218.148	7.8935	0.82831	7.6e-4	8.0e-5	3.5e-3	3.5e-3	1.1e-4	4.1e-6	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.83104	0.00110	-0.03021
	218.149	7.8935	0.82832	6.7e-4	6.7e-5	3.5e-3	3.5e-3	1.2e-4	6.3e-6	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.83104	0.00110	-0.03021
	218.148	7.8935	0.82834	7.4e-4	8.0e-5	3.5e-3	3.5e-3	1.0e-4	3.7e-6	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.83104	0.00110	-0.03021
L5	218.149	9.7335	0.76940	5.3e-4	1.0e-4	3.5e-3	3.5e-3	1.6e-4	6.8e-6	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.76955	0.00130	-0.03720
	218.148	9.7335	0.76941	4.6e-4	5.3e-5	3.4e-3	3.4e-3	1.2e-4	4.3e-6	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.76955	0.00130	-0.03720
	218.148	9.7335	0.76941	5.0e-4	7.2e-5	3.5e-3	3.5e-3	1.4e-4	8.9e-6	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.76955	0.00130	-0.03720
	218.148	9.7335	0.76941	9.1e-4	1.3e-4	3.4e-3	3.4e-3	1.3e-4	1.0e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.76955	0.00130	-0.03720
	218.148	9.7335	0.76942	8.4e-4	9.5e-5	3.5e-3	3.5e-3	1.6e-4	7.5e-6	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.76955	0.00130	-0.03720
	218.148	9.7335	0.76941	6.6e-4	8.0e-5	3.4e-3	3.4e-3	1.2e-4	1.5e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.76955	0.00130	-0.03720
L6	218.148	11.7910	0.68723	5.4e-4	5.9e-5	3.5e-3	3.5e-3	2.1e-4	1.7e-5	2.7e-3	2.7e-3	4.8e-4	5.0e-4	0.67972	0.00157	-0.05216
	218.148	11.7909	0.68722	8.5e-4	1.1e-4	3.5e-3	3.5e-3	2.5e-4	1.6e-5	2.7e-3	2.7e-3	4.8e-4	5.0e-4	0.67972	0.00157	-0.05216
	218.148	11.7910	0.68721	7.3e-4	1.2e-4	3.6e-3	3.6e-3	1.8e-4	6.9e-6	2.7e-3	2.7e-3	4.8e-4	5.0e-4	0.67972	0.00157	-0.05216
	218.148	11.7910	0.68723	6.4e-4	8.1e-5	3.6e-3	3.6e-3	2.0e-4	8.7e-6	2.7e-3	2.7e-3	4.8e-4	5.0e-4	0.67972	0.00157	-0.05216
	218.149	11.7909	0.68725	5.2e-4	1.0e-4	3.5e-3	3.5e-3	2.2e-4	1.2e-5	2.7e-3	2.7e-3	4.8e-4	5.0e-4	0.67972	0.00157	-0.05215
	218.148	11.7910	0.68722	5.0e-4	5.5e-5	3.5e-3	3.5e-3	2.0e-4	9.7e-6	2.7e-3	2.7e-3	4.8e-4	5.0e-4	0.67972	0.00157	-0.05216
L7	218.148	13.0211	0.61991	1.1e-3	1.7e-4	3.7e-3	3.7e-3	2.4e-4	1.1e-5	2.8e-3	2.8e-3	4.8e-4	5.2e-4	0.60471	0.00188	-0.07268
	218.149	13.0212	0.61993	6.7e-4	1.8e-4	3.4e-3	3.4e-3	2.1e-4	1.7e-5	2.8e-3	2.8e-3	4.8e-4	5.2e-4	0.60470	0.00188	-0.07268
	218.148	13.0212	0.61995	8.7e-4	2.7e-4	3.5e-3	3.5e-3	2.3e-4	1.5e-5	2.8e-3	2.8e-3	4.8e-4	5.2e-4	0.60470	0.00188	-0.07268
	218.148	13.0212	0.61994	9.8e-4	2.2e-4	3.5e-3	3.5e-3	2.0e-4	1.1e-5	2.8e-3	2.8e-3	4.8e-4	5.2e-4	0.60470	0.00188	-0.07268
	218.148	13.0211	0.61995	8.5e-4	1.1e-4	3.5e-3	3.5e-3	2.4e-4	2.4e-5	2.8e-3	2.8e-3	4.8e-4	5.2e-4	0.60471	0.00188	-0.07268
	218.148	13.0211	0.61996	6.4e-4	1.4e-4	3.6e-3	3.6e-3	2.1e-4	2.6e-5	2.8e-3	2.8e-3	4.8e-4	5.2e-4	0.60471	0.00188	-0.07268
L8	218.148	14.0359	0.53319	9.6e-4	1.0e-4	3.5e-3	3.5e-3	2.5e-4	2.1e-5	2.8e-3	2.8e-3	4.8e-4	6.0e-4 ⁺	0.51002	0.00276	-0.12824 ⁺
	218.149	14.0359	0.53324	8.0e-4	1.5e-4	3.6e-3	3.6e-3	2.1e-4	2.5e-5	2.8e-3	2.8e-3	4.8e-4	6.0e-4 ⁺	0.51001	0.00276	-0.12825 ⁺
	218.148	14.0358	0.53335	1.2e-3	4.7e-4	3.6e-3	3.6e-3	2.6e-4	1.4e-5	2.8e-3	2.8e-3	4.8e-4	6.0e-4 ⁺	0.51003	0.00276	-0.12823 ⁺
	218.147	14.0359	0.53333	1.4e-3	3.8e-4	3.7e-3	3.7e-3	2.4e-4	2.8e-5	2.8e-3	2.8e-3	4.8e-4	6.0e-4 ⁺	0.51002	0.00276	-0.12824 ⁺
	218.148	14.0358	0.53331	8.8e-4	9.0e-5	3.5e-3	3.6e-3	2.4e-4	3.0e-5	2.8e-3	2.8e-3	4.8e-4	6.0e-4 ⁺	0.51002	0.00276	-0.12823 ⁺
	218.148	14.0358	0.53333	1.1e-3	2.7e-4	3.6e-3	3.6e-3	2.3e-4	3.4e-5	2.8e-3	2.8e-3	4.8e-4	6.0e-4 ⁺	0.51003	0.00276	-0.12823 ⁺

L9*	218.148	14.3563	0.47535	6.4e-4	9.8e-5	3.4e-3	3.4e-3	2.9e-4	2.0e-5	2.8e-3	2.8e-3	4.8e-4	9.8e-4 ⁺	0.45827	0.00403	-0.30998 ⁺
	218.148	14.3563	0.47536	5.4e-4	8.8e-5	3.4e-3	3.4e-3	3.0e-4	2.1e-5	2.8e-3	2.8e-3	4.8e-4	9.8e-4 ⁺	0.45827	0.00403	-0.31001 ⁺
	218.148	14.3563	0.47533	6.1e-4	4.0e-5	3.2e-3	3.2e-3	2.7e-4	1.8e-5	2.8e-3	2.8e-3	4.8e-4	9.8e-4 ⁺	0.45826	0.00403	-0.31002 ⁺
	218.148	14.3564	0.47536	1.0e-3	1.4e-4	3.2e-3	3.2e-3	2.4e-4	2.9e-5	2.8e-3	2.8e-3	4.8e-4	9.8e-4 ⁺	0.45825	0.00403	-0.31013 ⁺
L10*	218.148	14.3563	0.47536	6.1e-4	2.0e-4	3.2e-3	3.2e-3	1.2e-4	4.6e-6	2.8e-3	2.8e-3	4.8e-4	9.8e-4 ⁺	0.45827	0.00403	-0.30996 ⁺
	218.149	14.3873	0.46438	6.3e-4	2.2e-4	3.4e-3	3.4e-3	2.6e-4	2.4e-5	2.8e-3	2.8e-3	4.8e-4	1.3e-3 ⁺	0.45116	0.00435	-0.41964 ⁺
	218.149	14.3873	0.46441	7.0e-4	1.8e-4	3.3e-3	3.3e-3	2.4e-4	1.8e-5	2.8e-3	2.8e-3	4.8e-4	1.3e-3 ⁺	0.45117	0.00435	-0.41955 ⁺
	218.149	14.3873	0.46440	6.3e-4	1.2e-4	3.2e-3	3.3e-3	2.0e-4	8.1e-6	2.8e-3	2.8e-3	4.8e-4	1.3e-3 ⁺	0.45116	0.00435	-0.41961 ⁺
	218.149	14.3873	0.46441	6.4e-4	8.4e-5	3.4e-3	3.4e-3	2.9e-4	2.5e-5	2.8e-3	2.8e-3	4.8e-4	1.3e-3 ⁺	0.45117	0.00435	-0.41946 ⁺
	218.148	14.3874	0.46438	6.2e-4	8.0e-5	3.5e-3	3.5e-3	2.2e-4	1.4e-5	2.8e-3	2.8e-3	4.8e-4	1.3e-3 ⁺	0.45114	0.00435	-0.42010 ⁺
L11*	218.148	14.3873	0.46440	6.2e-4	6.2e-5	3.4e-3	3.4e-3	2.8e-4	3.8e-5	2.8e-3	2.8e-3	4.8e-4	1.3e-3 ⁺	0.45117	0.00435	-0.41953 ⁺
	218.148	14.4110	0.45222	1.5e-3	3.6e-4	3.4e-3	3.4e-3	3.0e-4	3.6e-5	2.8e-3	2.8e-3	4.8e-4	1.9e-3 ⁺	0.44514	0.00467	-0.64579 ⁺
	218.149	14.4111	0.45231	8.6e-4	1.3e-4	3.4e-3	3.4e-3	2.6e-4	1.3e-5	2.8e-3	2.8e-3	4.8e-4	1.9e-3 ⁺	0.44512	0.00467	-0.64692 ⁺
	218.149	14.4111	0.45231	8.3e-4	1.3e-4	3.4e-3	3.4e-3	2.7e-4	3.1e-5	2.8e-3	2.8e-3	4.8e-4	1.9e-3 ⁺	0.44511	0.00467	-0.64770 ⁺
	218.149	14.4111	0.45233	8.9e-4	1.3e-4	3.3e-3	3.3e-3	2.4e-4	1.6e-5	2.8e-3	2.8e-3	4.8e-4	1.9e-3 ⁺	0.44513	0.00467	-0.64630 ⁺
	218.149	14.4111	0.45235	7.8e-4	1.1e-4	3.3e-3	3.3e-3	2.4e-4	1.3e-5	2.8e-3	2.8e-3	4.8e-4	1.9e-3 ⁺	0.44512	0.00467	-0.64703 ⁺
218.149	14.4111	0.45240	6.8e-4	1.0e-4	3.3e-3	3.3e-3	2.8e-4	1.9e-5	2.8e-3	2.8e-3	4.8e-4	1.9e-3 ⁺	0.44512	0.00467	-0.64703 ⁺	
P2	233.143	1.0048	0.99999	9.7e-4	7.4e-5	6.8e-3	6.8e-3	4.3e-5	1.1e-5	5.1e-4	5.1e-4					
L13	233.143	1.9677	0.98003	9.0e-4	1.5e-4	7.3e-3	7.3e-3	4.3e-5	7.6e-6	5.1e-4	5.1e-4	4.8e-4	4.8e-4	0.98262	0.00070	-0.01860
	233.142	1.9677	0.98022	7.6e-4	1.3e-4	7.0e-3	7.0e-3	4.9e-5	1.1e-5	5.1e-4	5.1e-4	4.8e-4	4.8e-4	0.98262	0.00070	-0.01860
	233.142	1.9677	0.98046	9.1e-4	1.0e-4	7.2e-3	7.2e-3	2.4e-5	5.6e-6	5.1e-4	5.1e-4	4.8e-4	4.8e-4	0.98262	0.00070	-0.01860
L14	233.142	1.9677	0.98020	1.1e-3	1.9e-4	7.4e-3	7.4e-3	2.8e-5	7.7e-6	5.1e-4	5.1e-4	4.8e-4	4.8e-4	0.98262	0.00070	-0.01860
	233.141	2.9346	0.96022	1.0e-3	1.5e-4	7.6e-3	7.6e-3	1.1e-4	4.7e-5	5.3e-4	5.3e-4	4.8e-4	4.8e-4	0.96410	0.00075	-0.01973
	233.141	2.9345	0.96022	1.1e-3	1.9e-4	7.9e-3	7.9e-3	2.0e-4	7.4e-5	5.3e-4	5.3e-4	4.8e-4	4.8e-4	0.96410	0.00075	-0.01973
	233.141	2.9345	0.96019	7.0e-4	6.9e-5	7.6e-3	7.6e-3	4.4e-5	1.5e-5	5.2e-4	5.2e-4	4.8e-4	4.8e-4	0.96410	0.00075	-0.01973
	233.141	2.9345	0.96019	8.7e-4	9.4e-5	8.1e-3	8.1e-3	1.2e-4	1.8e-5	5.3e-4	5.3e-4	4.8e-4	4.8e-4	0.96410	0.00075	-0.01973
	233.141	2.9345	0.96021	9.6e-4	3.2e-4	7.7e-3	7.7e-3	2.9e-5	2.1e-6	5.2e-4	5.2e-4	4.8e-4	4.8e-4	0.96410	0.00075	-0.01973
L15	233.141	2.9346	0.96020	1.0e-3	1.1e-4	7.7e-3	7.7e-3	6.1e-5	8.5e-6	5.3e-4	5.3e-4	4.8e-4	4.8e-4	0.96409	0.00075	-0.01973
	233.143	3.9407	0.93831	1.5e-3	2.1e-4	6.7e-3	6.7e-3	7.3e-4	8.4e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94358	0.00079	-0.02108
	233.143	3.9407	0.93830	1.3e-3	4.1e-4	6.6e-3	6.6e-3	5.8e-4	8.9e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94358	0.00079	-0.02108
	233.142	3.9409	0.93829	1.1e-3	1.6e-4	6.9e-3	6.9e-3	6.5e-4	9.5e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94358	0.00079	-0.02108
	233.143	3.9409	0.93829	1.2e-3	2.5e-4	6.8e-3	6.8e-3	6.1e-4	8.2e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94358	0.00079	-0.02108
	233.142	3.9406	0.93828	9.4e-4	1.4e-4	6.8e-3	6.8e-3	7.2e-4	8.4e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94358	0.00079	-0.02108
L16	233.142	3.9408	0.93829	1.2e-3	1.3e-4	7.2e-3	7.2e-3	6.3e-4	1.1e-4	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94358	0.00079	-0.02108
	233.142	5.9478	0.89066	1.1e-3	3.1e-4	7.0e-3	7.1e-3	1.2e-4	1.3e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.89802	0.00087	-0.02451
	233.143	5.9477	0.89066	7.8e-4	2.1e-4	7.0e-3	7.1e-3	1.3e-4	1.6e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.89803	0.00087	-0.02451
	233.143	5.9477	0.89068	1.3e-3	2.9e-4	7.2e-3	7.2e-3	7.8e-5	5.9e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.89803	0.00087	-0.02451
	233.144	5.9478	0.89068	7.8e-4	1.1e-4	7.2e-3	7.2e-3	1.1e-4	1.5e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.89803	0.00087	-0.02451
	233.144	5.9477	0.89068	9.9e-4	1.5e-4	7.8e-3	7.8e-3	1.0e-4	1.6e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.89803	0.00087	-0.02451
L17	233.144	5.9477	0.89066	7.6e-4	1.0e-4	7.2e-3	7.2e-3	1.2e-4	1.0e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.89803	0.00087	-0.02451
	233.143	7.8334	0.84019	1.2e-3	3.2e-4	7.7e-3	7.7e-3	2.1e-4	1.5e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.84775	0.00094	-0.02911
	233.142	7.8335	0.84017	1.1e-3	3.3e-4	7.5e-3	7.6e-3	2.6e-4	3.0e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.84775	0.00094	-0.02911
	233.143	7.8334	0.84017	8.3e-4	8.3e-5	7.7e-3	7.7e-3	2.3e-4	1.3e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.84775	0.00094	-0.02911
	233.144	7.8334	0.84018	1.4e-3	4.3e-4	7.5e-3	7.5e-3	1.9e-4	1.4e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.84775	0.00094	-0.02911
	233.143	7.8334	0.84018	1.6e-3	6.5e-4	7.5e-3	7.5e-3	2.3e-4	1.9e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.84775	0.00094	-0.02911
L18	233.142	7.8334	0.84017	7.8e-4	2.0e-4	7.3e-3	7.3e-3	2.1e-4	2.2e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.84775	0.00094	-0.02911
	233.142	7.8335	0.84016	9.9e-4	9.6e-5	7.5e-3	7.5e-3	1.6e-4	8.7e-6	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.84775	0.00094	-0.02911
	233.141	8.8724	0.80941	2.0e-3	6.3e-4	7.3e-3	7.4e-3	2.2e-4	9.3e-6	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.81577	0.00096	-0.03259
	233.143	8.8724	0.80934	1.6e-3	3.0e-4	7.2e-3	7.2e-3	2.0e-4	1.1e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.81577	0.00096	-0.03259
	233.141	8.8724	0.80940	1.8e-3	2.9e-4	7.9e-3	7.9e-3	1.4e-4	8.0e-6	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.81577	0.00096	-0.03259
	233.141	8.8724	0.80941	1.2e-3	1.6e-4	7.6e-3	7.6e-3	1.6e-4	1.4e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.81577	0.00096	-0.03259
L19	233.142	9.8513	0.77736	1.6e-3	4.9e-4	7.1e-3	7.1e-3	2.0e-4	2.2e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.78187	0.00098	-0.03685
	233.143	9.8514	0.77735	1.1e-3	2.0e-4	7.1e-3	7.2e-3	2.5e-4	2.8e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.78187	0.00098	-0.03686
	233.141	9.8514	0.77734	1.2e-3	1.9e-4	7.0e-3	7.0e-3	1.4e-4	6.7e-6	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.78187	0.00098	-0.03685

	233.141	9.8514	0.77738	9.7e-4	1.9e-4	7.2e-3	7.2e-3	1.4e-4	4.6e-6	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.78187	0.00098	-0.03686
L20	233.140	11.8341	0.69898	1.1e-3	1.2e-4	7.3e-3	7.3e-3	3.7e-4	9.9e-6	2.7e-3	2.7e-3	4.8e-4	5.0e-4	0.69628	0.00098	-0.05132
	233.140	11.8342	0.69897	7.0e-4	6.2e-5	7.7e-3	7.7e-3	3.6e-4	1.7e-5	2.7e-3	2.7e-3	4.8e-4	5.0e-4	0.69628	0.00098	-0.05132
	233.140	11.8342	0.69895	1.1e-3	2.4e-4	7.2e-3	7.2e-3	2.2e-4	1.5e-5	2.7e-3	2.7e-3	4.8e-4	5.0e-4	0.69628	0.00098	-0.05132
	233.139	11.8342	0.69897	1.3e-3	4.3e-4	7.2e-3	7.3e-3	2.2e-4	2.0e-5	2.7e-3	2.7e-3	4.8e-4	5.0e-4	0.69628	0.00098	-0.05132
	233.140	11.8341	0.69897	1.9e-3	4.3e-4	6.8e-3	6.8e-3	2.7e-4	5.7e-5	2.7e-3	2.7e-3	4.8e-4	5.0e-4	0.69628	0.00098	-0.05132
L21	233.143	12.8248	0.64712	7.4e-4	1.2e-4	7.0e-3	7.0e-3	2.4e-4	1.5e-5	2.7e-3	2.7e-3	4.8e-4	5.1e-4	0.63897	0.00093	-0.06595
	233.142	12.8248	0.64708	9.1e-4	8.9e-5	6.7e-3	6.7e-3	2.6e-4	1.5e-5	2.7e-3	2.7e-3	4.8e-4	5.1e-4	0.63897	0.00093	-0.06594
	233.143	12.8248	0.64712	1.3e-3	3.9e-4	7.1e-3	7.1e-3	2.3e-4	1.4e-5	2.7e-3	2.7e-3	4.8e-4	5.1e-4	0.63897	0.00093	-0.06594
	233.142	12.8248	0.64711	6.1e-4	3.2e-5	6.6e-3	6.6e-3	1.9e-4	1.1e-5	2.7e-3	2.7e-3	4.8e-4	5.1e-4	0.63897	0.00093	-0.06595
	233.143	12.8248	0.64711	1.0e-3	1.9e-4	7.0e-3	7.0e-3	1.8e-4	2.2e-5	2.7e-3	2.7e-3	4.8e-4	5.1e-4	0.63897	0.00093	-0.06591
L22	233.141	13.6445	0.58764	1.7e-3	6.8e-4	7.2e-3	7.2e-3	2.5e-4	2.0e-5	2.7e-3	2.7e-3	4.8e-4	5.4e-4 ⁺	0.57569	0.00070	-0.09273 ⁺
	233.143	13.6445	0.58764	8.5e-4	1.2e-4	7.4e-3	7.4e-3	2.8e-4	1.9e-5	2.8e-3	2.8e-3	4.8e-4	5.4e-4 ⁺	0.57569	0.00070	-0.09273 ⁺
	233.144	13.6445	0.58761	1.5e-3	3.0e-4	7.1e-3	7.2e-3	2.6e-4	2.7e-5	2.8e-3	2.8e-3	4.8e-4	5.4e-4 ⁺	0.57569	0.00070	-0.09273 ⁺
	233.143	13.6445	0.58760	5.8e-4	4.1e-5	6.8e-3	6.8e-3	2.5e-4	9.0e-6	2.8e-3	2.8e-3	4.8e-4	5.4e-4 ⁺	0.57569	0.00070	-0.09273 ⁺
	233.143	13.6445	0.58759	6.2e-4	1.5e-4	7.3e-3	7.3e-3	2.7e-4	2.1e-5	2.8e-3	2.8e-3	4.8e-4	5.4e-4 ⁺	0.57569	0.00070	-0.09273 ⁺
	233.141	13.6444	0.58762	2.0e-3	5.3e-4	7.4e-3	7.4e-3	2.1e-4	9.9e-6	2.7e-3	2.7e-3	4.8e-4	5.4e-4 ⁺	0.57569	0.00070	-0.09273 ⁺
L23*	233.144	14.1868	0.51082	7.6e-4	1.1e-4	6.9e-3	6.9e-3	2.4e-4	1.7e-5	2.8e-3	2.8e-3	4.8e-4	9.7e-4 ⁺	0.51244	-0.00036	-0.30787 ⁺
	233.144	14.1868	0.51081	7.7e-4	1.4e-4	6.8e-3	6.8e-3	1.8e-4	1.1e-5	2.8e-3	2.8e-3	4.8e-4	9.7e-4 ⁺	0.51244	-0.00036	-0.30779 ⁺
	233.144	14.1868	0.51081	4.8e-4	6.8e-5	6.9e-3	6.9e-3	2.6e-4	3.4e-5	2.8e-3	2.8e-3	4.8e-4	9.8e-4 ⁺	0.51244	-0.00036	-0.30788 ⁺
	233.144	14.1868	0.51080	6.3e-4	1.9e-4	7.1e-3	7.1e-3	3.1e-4	2.1e-5	2.8e-3	2.8e-3	4.8e-4	9.8e-4 ⁺	0.51244	-0.00036	-0.30788 ⁺
	233.144	14.1867	0.51082	5.1e-4	4.5e-5	6.9e-3	6.9e-3	2.7e-4	1.8e-5	2.8e-3	2.8e-3	4.8e-4	9.7e-4 ⁺	0.51245	-0.00035	-0.30771 ⁺
	233.144	14.1868	0.51080	6.8e-4	6.3e-5	6.8e-3	6.8e-3	3.1e-4	1.8e-5	2.8e-3	2.8e-3	4.8e-4	9.8e-4 ⁺	0.51244	-0.00036	-0.30783 ⁺
L24*	233.144	14.2158	0.50043	6.1e-4	9.8e-5	7.0e-3	7.0e-3	2.6e-4	2.5e-5	2.8e-3	2.8e-3	4.8e-4	1.3e-3 ⁺	0.50770	-0.00054	-0.43666 ⁺
	233.144	14.2158	0.50045	6.6e-4	1.6e-4	6.4e-3	6.4e-3	2.5e-4	2.0e-5	2.8e-3	2.8e-3	4.8e-4	1.3e-3 ⁺	0.50771	-0.00054	-0.43628 ⁺
	233.144	14.2158	0.50044	6.9e-4	1.6e-4	6.9e-3	6.9e-3	2.9e-4	4.4e-5	2.8e-3	2.8e-3	4.8e-4	1.3e-3 ⁺	0.50770	-0.00054	-0.43663 ⁺
	233.144	14.2157	0.50043	6.3e-4	9.8e-5	6.8e-3	6.8e-3	2.7e-4	2.0e-5	2.8e-3	2.8e-3	4.8e-4	1.3e-3 ⁺	0.50772	-0.00054	-0.43584 ⁺
	233.144	14.2158	0.50044	6.2e-4	1.5e-4	6.7e-3	6.7e-3	2.2e-4	1.8e-5	2.8e-3	2.8e-3	4.8e-4	1.3e-3 ⁺	0.50771	-0.00054	-0.43625 ⁺
	233.144	14.2158	0.50045	4.7e-4	7.7e-5	6.7e-3	6.7e-3	1.9e-4	1.4e-5	2.8e-3	2.8e-3	4.8e-4	1.3e-3 ⁺	0.50771	-0.00054	-0.43619 ⁺
L25*	233.146	14.2408	0.48640	1.4e-3	4.7e-4	5.9e-3	5.9e-3	2.2e-4	1.7e-5	2.8e-3	2.8e-3	4.8e-4	2.4e-3 ⁺	0.50338	-0.00074	-0.85676 ⁺
	233.146	14.2408	0.48639	7.9e-4	1.2e-4	6.1e-3	6.1e-3	2.5e-4	2.8e-5	2.8e-3	2.8e-3	4.8e-4	2.4e-3 ⁺	0.50338	-0.00074	-0.85715 ⁺
	233.146	14.2407	0.48640	6.2e-4	1.0e-4	6.0e-3	6.0e-3	2.4e-4	1.2e-5	2.8e-3	2.8e-3	4.8e-4	2.4e-3 ⁺	0.50339	-0.00074	-0.85446 ⁺
	233.146	14.2407	0.48642	8.2e-4	3.0e-4	6.0e-3	6.0e-3	1.6e-4	1.3e-5	2.8e-3	2.8e-3	4.8e-4	2.4e-3 ⁺	0.50339	-0.00074	-0.85608 ⁺
	233.146	14.2407	0.48642	9.3e-4	1.8e-4	6.0e-3	6.0e-3	2.3e-4	1.7e-5	2.8e-3	2.8e-3	4.8e-4	2.4e-3 ⁺	0.50339	-0.00074	-0.85516 ⁺
	233.148	14.2407	0.48640	1.4e-3	6.2e-4	6.0e-3	6.0e-3	1.8e-4	8.4e-6	2.8e-3	2.8e-3	4.8e-4	2.4e-3 ⁺	0.50339	-0.00074	-0.85451 ⁺
P3	253.147	1.9699	0.99999	8.5e-4	1.5e-5	5.7e-3	5.7e-3	3.7e-5	5.5e-6	5.1e-4	5.1e-4					
L27	253.146	2.9632	0.97897	8.9e-4	1.7e-4	5.9e-3	5.9e-3	4.1e-5	7.5e-6	5.2e-4	5.2e-4	4.8e-4	4.8e-4	0.98168	0.00111	-0.01913
	253.147	2.9633	0.97902	9.6e-4	2.2e-4	5.8e-3	5.8e-3	1.1e-4	4.4e-5	5.2e-4	5.2e-4	4.8e-4	4.8e-4	0.98167	0.00111	-0.01913
	253.146	2.9633	0.97901	8.1e-4	1.1e-4	5.8e-3	5.8e-3	2.8e-5	3.5e-6	5.2e-4	5.2e-4	4.8e-4	4.8e-4	0.98167	0.00111	-0.01913
	253.147	2.9632	0.97897	8.2e-4	1.1e-4	5.7e-3	5.7e-3	3.6e-5	6.0e-6	5.2e-4	5.2e-4	4.8e-4	4.8e-4	0.98167	0.00111	-0.01913
L28	253.146	4.9363	0.93518	9.3e-4	2.0e-4	6.0e-3	6.0e-3	1.4e-4	5.1e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94105	0.00114	-0.02220
	253.146	4.9367	0.93519	9.4e-4	1.7e-4	6.3e-3	6.3e-3	8.1e-5	2.4e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94104	0.00114	-0.02220
	253.146	4.9364	0.93519	1.1e-3	1.5e-4	6.1e-3	6.1e-3	6.4e-5	7.1e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94105	0.00114	-0.02220
	253.146	4.9363	0.93518	9.1e-4	1.0e-4	5.3e-3	5.3e-3	1.7e-4	6.1e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94105	0.00114	-0.02220
	253.146	4.9368	0.93518	1.1e-3	2.7e-4	6.1e-3	6.1e-3	7.7e-5	2.4e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94104	0.00114	-0.02220
L29	253.146	6.9082	0.88642	7.2e-4	8.5e-5	5.9e-3	5.9e-3	2.1e-4	6.5e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.89326	0.00113	-0.02653
	253.146	6.9080	0.88638	1.3e-3	3.5e-4	6.0e-3	6.0e-3	2.1e-4	7.8e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.89327	0.00113	-0.02653
	253.147	6.9080	0.88643	9.1e-4	2.1e-4	5.8e-3	5.8e-3	1.1e-4	1.2e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.89327	0.00113	-0.02653
	253.146	6.9080	0.88640	1.1e-3	1.2e-4	6.2e-3	6.2e-3	8.7e-5	2.3e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.89327	0.00113	-0.02653
	253.146	6.9080	0.88639	5.4e-4	7.5e-5	6.1e-3	6.1e-3	2.2e-4	8.8e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.89327	0.00113	-0.02653
L30	253.146	8.3058	0.84781	8.0e-4	1.2e-4	6.1e-3	6.1e-3	1.8e-4	5.1e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.85331	0.00109	-0.03088
	253.146	8.3057	0.84783	1.4e-3	1.9e-4	5.7e-3	5.7e-3	2.5e-4	7.7e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.85331	0.00109	-0.03088
	253.145	8.3057	0.84784	9.0e-4	1.7e-4	5.9e-3	5.9e-3	1.2e-4	3.1e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.85331	0.00109	-0.03088
	253.146	8.3058	0.84783	1.1e-3	2.8e-4	6.1e-3	6.1e-3	1.4e-4	1.7e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.85331	0.00109	-0.03088

	253.146	8.3058	0.84783	5.9e-4	5.5e-5	5.9e-3	5.9e-3	1.7e-4	4.6e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.85331	0.00109	-0.03088
L31	253.148	9.6222	0.80638	7.4e-4	1.1e-4	5.7e-3	5.7e-3	6.8e-4	3.1e-4	1.4e-3	1.5e-3	4.8e-4	4.8e-4	0.80907	0.00098	-0.03670
	253.148	9.6241	0.80640	1.0e-3	1.8e-4	5.9e-3	5.9e-3	1.5e-3	7.0e-4	1.5e-3	1.7e-3	4.8e-4	4.8e-4	0.80900	0.00098	-0.03671
	253.148	9.6222	0.80643	6.4e-4	1.2e-4	5.9e-3	5.9e-3	1.0e-3	3.5e-4	1.4e-3	1.5e-3	4.8e-4	4.8e-4	0.80907	0.00098	-0.03670
	253.148	9.6222	0.80641	7.7e-4	1.2e-4	5.7e-3	5.7e-3	2.3e-4	2.9e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.80908	0.00098	-0.03670
	253.148	9.6221	0.80640	9.1e-4	9.0e-5	5.3e-3	5.3e-3	5.7e-4	1.6e-4	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.80908	0.00098	-0.03670
L32	253.147	10.8464	0.76222	6.3e-4	6.4e-5	6.1e-3	6.1e-3	2.5e-4	5.2e-5	2.7e-3	2.7e-3	4.8e-4	4.9e-4	0.75947	0.00076	-0.04501
	253.147	10.8462	0.76219	4.9e-4	7.3e-5	5.8e-3	5.8e-3	4.0e-4	5.5e-5	2.7e-3	2.7e-3	4.8e-4	4.9e-4	0.75948	0.00076	-0.04501
	253.147	10.8463	0.76223	6.1e-4	1.0e-4	6.0e-3	6.0e-3	3.2e-4	6.8e-5	2.7e-3	2.7e-3	4.8e-4	4.9e-4	0.75948	0.00076	-0.04501
	253.147	10.8463	0.76222	6.0e-4	7.8e-5	5.7e-3	5.7e-3	1.7e-4	3.7e-5	2.7e-3	2.7e-3	4.8e-4	4.9e-4	0.75947	0.00076	-0.04501
	253.148	10.8463	0.76221	9.9e-4	3.2e-4	5.6e-3	5.6e-3	3.4e-4	4.8e-5	2.7e-3	2.7e-3	4.8e-4	4.9e-4	0.75948	0.00076	-0.04501
L33	253.146	11.8557	0.71750	9.0e-4	1.0e-4	5.6e-3	5.6e-3	1.8e-4	3.1e-5	2.7e-3	2.7e-3	4.8e-4	5.0e-4	0.70865	0.00032	-0.05692
	253.146	11.8557	0.71745	1.1e-3	1.4e-4	5.9e-3	5.9e-3	3.3e-4	6.5e-5	2.7e-3	2.7e-3	4.8e-4	5.0e-4	0.70865	0.00032	-0.05692
	253.146	11.8557	0.71746	6.9e-4	5.8e-5	6.2e-3	6.2e-3	3.4e-4	4.2e-5	2.7e-3	2.7e-3	4.8e-4	5.0e-4	0.70865	0.00032	-0.05692
	253.146	11.8557	0.71749	1.0e-3	1.5e-4	6.1e-3	6.1e-3	3.8e-4	6.5e-5	2.7e-3	2.7e-3	4.8e-4	5.0e-4	0.70866	0.00032	-0.05693
	253.146	11.8556	0.71747	1.0e-3	2.3e-4	6.1e-3	6.1e-3	3.0e-4	5.9e-5	2.7e-3	2.7e-3	4.8e-4	5.0e-4	0.70866	0.00032	-0.05691
L34	253.146	12.7679	0.66172	8.2e-4	9.1e-5	5.7e-3	5.7e-3	5.0e-4	7.5e-5	2.7e-3	2.7e-3	4.8e-4	5.2e-4 ⁺	0.64727	-0.00094	-0.07864 ⁺
	253.146	12.7678	0.66174	7.6e-4	9.2e-5	5.8e-3	5.8e-3	4.0e-4	6.3e-5	2.7e-3	2.7e-3	4.8e-4	5.2e-4 ⁺	0.64728	-0.00094	-0.07863 ⁺
	253.146	12.7677	0.66172	6.3e-4	1.3e-4	5.9e-3	5.9e-3	2.7e-4	3.0e-5	2.7e-3	2.7e-3	4.8e-4	5.2e-4 ⁺	0.64729	-0.00094	-0.07863 ⁺
	253.146	12.7678	0.66174	7.5e-4	5.6e-5	5.6e-3	5.6e-3	3.4e-4	5.4e-5	2.7e-3	2.7e-3	4.8e-4	5.2e-4 ⁺	0.64728	-0.00094	-0.07863 ⁺
L35*	253.146	13.2763	0.59985	8.1e-4	1.1e-4	5.9e-3	5.9e-3	5.8e-4	6.2e-5	2.7e-3	2.7e-3	4.8e-4	8.8e-4 ⁺	0.59446	-0.00471	-0.26976 ⁺
	253.146	13.2762	0.59987	8.8e-4	1.1e-4	5.5e-3	5.5e-3	5.3e-4	7.8e-5	2.7e-3	2.7e-3	4.8e-4	8.8e-4 ⁺	0.59446	-0.00471	-0.26960 ⁺
	253.147	13.2762	0.59989	1.2e-3	4.1e-4	5.5e-3	5.6e-3	2.7e-4	4.8e-5	2.7e-3	2.7e-3	4.8e-4	8.8e-4 ⁺	0.59446	-0.00471	-0.26955 ⁺
	253.146	13.2763	0.59988	7.4e-4	1.5e-4	6.0e-3	6.0e-3	3.5e-4	5.6e-5	2.7e-3	2.7e-3	4.8e-4	8.8e-4 ⁺	0.59445	-0.00471	-0.26977 ⁺
	253.146	13.2762	0.59989	6.9e-4	9.9e-5	5.6e-3	5.6e-3	2.8e-4	6.5e-5	2.7e-3	2.7e-3	4.8e-4	8.8e-4 ⁺	0.59446	-0.00471	-0.26965 ⁺
L36*	253.147	13.3024	0.59159	9.4e-4	2.2e-4	5.8e-3	5.8e-3	5.8e-4	8.0e-5	2.7e-3	2.7e-3	4.8e-4	1.1e-3 ⁺	0.59060	-0.00531	-0.37659 ⁺
	253.147	13.3024	0.59163	5.8e-4	9.6e-5	6.1e-3	6.1e-3	4.6e-4	9.1e-5	2.7e-3	2.7e-3	4.8e-4	1.1e-3 ⁺	0.59060	-0.00531	-0.37660 ⁺
	253.147	13.3023	0.59166	4.8e-4	4.9e-5	5.7e-3	5.7e-3	5.2e-4	8.0e-5	2.7e-3	2.7e-3	4.8e-4	1.1e-3 ⁺	0.59060	-0.00531	-0.37652 ⁺
	253.147	13.3024	0.59167	7.7e-4	1.0e-4	5.8e-3	5.8e-3	5.2e-4	9.9e-5	2.7e-3	2.7e-3	4.8e-4	1.1e-3 ⁺	0.59059	-0.00531	-0.37699 ⁺
	253.147	13.3023	0.59169	9.0e-4	1.3e-4	5.7e-3	5.7e-3	3.3e-4	5.1e-5	2.7e-3	2.7e-3	4.8e-4	1.1e-3 ⁺	0.59060	-0.00531	-0.37628 ⁺
L37*	253.147	13.3199	0.58367	8.7e-4	2.5e-4	5.9e-3	5.9e-3	6.8e-4	1.6e-4	2.7e-3	2.8e-3	4.8e-4	1.6e-3 ⁺	0.58787	-0.00579	-0.56725 ⁺
	253.147	13.3202	0.58368	6.8e-4	1.2e-4	5.9e-3	5.9e-3	1.3e-4	2.9e-5	2.7e-3	2.7e-3	4.8e-4	1.6e-3 ⁺	0.58781	-0.00581	-0.57410 ⁺
	253.148	13.3200	0.58373	7.9e-4	8.7e-5	5.6e-3	5.6e-3	5.4e-4	8.5e-5	2.7e-3	2.7e-3	4.8e-4	1.6e-3 ⁺	0.58784	-0.00580	-0.57029 ⁺
	253.148	13.3201	0.58372	9.0e-4	2.4e-4	5.6e-3	5.6e-3	6.3e-4	6.6e-5	2.7e-3	2.7e-3	4.8e-4	1.6e-3 ⁺	0.58783	-0.00580	-0.57117 ⁺
	253.147	13.3200	0.58376	5.4e-4	6.6e-5	6.0e-3	6.0e-3	6.1e-4	1.3e-4	2.7e-3	2.7e-3	4.8e-4	1.6e-3 ⁺	0.58784	-0.00580	-0.57030 ⁺
P4	273.147	3.4848	0.99999	7.2e-4	2.4e-5	1.5e-3	1.5e-3	5.6e-5	9.9e-7	1.1e-3	1.1e-3					
L39	273.145	5.0161	0.96558	1.1e-3	3.5e-4	2.3e-3	2.4e-3	2.0e-4	8.9e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.96828	0.00183	-0.02227
	273.145	5.0162	0.96558	1.0e-3	1.7e-4	1.6e-3	1.6e-3	1.2e-4	3.1e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.96828	0.00183	-0.02227
	273.145	5.0161	0.96557	1.1e-3	1.1e-4	2.3e-3	2.3e-3	7.9e-5	1.9e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.96828	0.00183	-0.02227
	273.145	5.0161	0.96559	7.6e-4	6.9e-5	1.9e-3	1.9e-3	8.2e-5	1.3e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.96828	0.00183	-0.02227
	273.145	5.0160	0.96559	9.9e-4	2.2e-4	1.7e-3	1.7e-3	1.9e-4	7.5e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.96828	0.00183	-0.02227
	273.145	5.0160	0.96559	6.5e-4	6.0e-5	2.0e-3	2.0e-3	6.4e-5	5.5e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.96828	0.00183	-0.02227
L40	273.147	5.9255	0.94386	6.1e-4	6.9e-5	2.2e-3	2.2e-3	1.0e-4	1.3e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94709	0.00183	-0.02441
	273.146	5.9255	0.94385	5.8e-4	1.5e-4	2.9e-3	2.9e-3	9.8e-5	2.7e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94709	0.00183	-0.02441
	273.146	5.9256	0.94385	4.7e-4	6.1e-5	2.4e-3	2.4e-3	8.6e-5	1.7e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94708	0.00183	-0.02441
	273.146	5.9255	0.94384	6.0e-4	6.8e-5	2.7e-3	2.7e-3	1.3e-4	4.3e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94709	0.00183	-0.02441
	273.147	5.9255	0.94385	5.1e-4	1.2e-4	2.2e-3	2.2e-3	7.4e-5	1.3e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94709	0.00183	-0.02441
	273.146	5.9256	0.94385	8.1e-4	1.8e-4	2.6e-3	2.6e-3	7.3e-5	1.4e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94709	0.00183	-0.02441
L41	273.146	6.9257	0.91830	7.2e-4	2.0e-4	2.5e-3	2.5e-3	2.1e-4	5.1e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.92127	0.00180	-0.02733
	273.146	6.9258	0.91829	5.4e-4	1.2e-4	2.2e-3	2.2e-3	3.1e-4	8.2e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.92127	0.00180	-0.02733
	273.146	6.9258	0.91829	9.0e-4	1.0e-4	2.4e-3	2.4e-3	1.9e-4	3.8e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.92127	0.00180	-0.02733
	273.146	6.9259	0.91829	7.2e-4	5.8e-5	2.7e-3	2.7e-3	2.3e-4	4.0e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.92127	0.00180	-0.02733
	273.146	6.9258	0.91829	6.2e-4	4.3e-5	2.3e-3	2.3e-3	2.8e-4	2.8e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.92127	0.00180	-0.02733
L42	273.146	7.9106	0.89112	7.3e-4	1.4e-4	2.5e-3	2.5e-3	3.7e-4	7.1e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.89260	0.00171	-0.03108

	273.146	7.9108	0.89110	7.2e-4	1.7e-4	2.3e-3	2.3e-3	4.8e-4	1.5e-4	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.89259	0.00171	-0.03108
	273.146	7.9107	0.89111	5.5e-4	5.4e-5	2.3e-3	2.4e-3	2.7e-4	5.0e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.89260	0.00171	-0.03108
	273.146	7.9107	0.89109	9.4e-4	1.5e-4	2.7e-3	2.7e-3	2.6e-4	6.5e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.89259	0.00171	-0.03108
L43	273.147	7.9106	0.89108	5.8e-4	8.7e-5	2.1e-3	2.1e-3	2.3e-4	4.7e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.89260	0.00171	-0.03108
	273.147	8.8895	0.86116	6.7e-4	1.4e-4	2.5e-3	2.5e-3	7.1e-4	1.3e-4	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.85979	0.00153	-0.03628
	273.146	8.8895	0.86116	5.5e-4	8.2e-5	2.5e-3	2.5e-3	3.8e-4	1.0e-4	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.85979	0.00153	-0.03628
	273.147	8.8894	0.86112	5.7e-4	8.8e-5	2.1e-3	2.1e-3	3.2e-4	4.8e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.85979	0.00153	-0.03628
	273.146	8.8892	0.86110	7.1e-4	1.0e-4	2.5e-3	2.5e-3	6.1e-4	9.5e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.85980	0.00153	-0.03628
	273.146	8.8893	0.86110	6.7e-4	9.4e-5	2.4e-3	2.4e-3	4.4e-4	9.1e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.85979	0.00153	-0.03628
L44	273.145	9.8539	0.82709	8.6e-4	1.2e-4	2.3e-3	2.3e-3	6.3e-4	7.3e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.82127	0.00111	-0.04432
	273.145	9.8532	0.82712	9.8e-4	2.0e-4	2.1e-3	2.1e-3	2.2e-4	3.1e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.82130	0.00111	-0.04431
	273.144	9.8540	0.82711	1.4e-3	3.4e-4	2.7e-3	2.7e-3	4.7e-4	8.5e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.82126	0.00111	-0.04432
	273.145	9.8538	0.82710	7.6e-4	2.1e-4	2.5e-3	2.5e-3	3.2e-4	8.1e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.82127	0.00111	-0.04432
	273.145	9.8538	0.82709	8.3e-4	1.1e-4	2.3e-3	2.3e-3	1.8e-4	1.8e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.82128	0.00111	-0.04432
L45	273.147	10.8865	0.78023	6.5e-4	1.2e-4	2.5e-3	2.5e-3	2.9e-4	8.0e-5	2.7e-3	2.7e-3	4.8e-4	5.1e-4	0.76737	-0.00031	-0.06367
	273.146	10.8864	0.78016	4.3e-4	4.7e-5	2.5e-3	2.5e-3	2.4e-4	2.9e-5	2.7e-3	2.7e-3	4.8e-4	5.1e-4	0.76738	-0.00031	-0.06367
	273.147	10.8865	0.77987	4.6e-4	3.9e-5	2.2e-3	2.2e-3	2.3e-4	4.3e-5	2.7e-3	2.7e-3	4.8e-4	5.1e-4	0.76737	-0.00031	-0.06367
	273.147	10.8864	0.77996	6.7e-4	4.0e-5	2.6e-3	2.6e-3	2.1e-4	3.1e-5	2.7e-3	2.7e-3	4.8e-4	5.1e-4	0.76737	-0.00031	-0.06367
	273.147	10.8864	0.77995	4.6e-4	6.3e-5	2.3e-3	2.3e-3	2.7e-4	5.4e-5	2.7e-3	2.7e-3	4.8e-4	5.1e-4	0.76738	-0.00031	-0.06367
L46	273.147	11.3315	0.74889	6.2e-4	1.5e-4	2.2e-3	2.2e-3	4.5e-4	8.3e-5	2.7e-3	2.7e-3	4.8e-4	5.4e-4 ⁺	0.73427	-0.00275	-0.08975 ⁺
	273.146	11.3311	0.74904	5.2e-4	5.1e-5	2.4e-3	2.4e-3	1.4e-4	3.2e-5	2.7e-3	2.7e-3	4.8e-4	5.4e-4 ⁺	0.73431	-0.00274	-0.08967 ⁺
	273.146	11.3318	0.74903	6.0e-4	8.3e-5	2.0e-3	2.0e-3	1.5e-4	2.5e-5	2.7e-3	2.7e-3	4.8e-4	5.4e-4 ⁺	0.73425	-0.00275	-0.08981 ⁺
	273.146	11.3313	0.74900	9.2e-4	1.3e-4	2.4e-3	2.4e-3	2.4e-4	5.2e-5	2.7e-3	2.7e-3	4.8e-4	5.4e-4 ⁺	0.73429	-0.00274	-0.08971 ⁺
	273.146	11.3313	0.74901	6.2e-4	1.0e-4	2.4e-3	2.4e-3	2.8e-4	5.0e-5	2.7e-3	2.7e-3	4.8e-4	5.4e-4 ⁺	0.73429	-0.00274	-0.08971 ⁺
L47*	273.144	11.5579	0.71517	9.0e-4	7.4e-5	2.9e-3	2.9e-3	2.1e-4	3.4e-5	2.7e-3	2.7e-3	4.8e-4	1.1e-3 ⁺	0.70945	-0.00803	-0.36948 ⁺
	273.145	11.5579	0.71516	7.6e-4	1.0e-4	2.5e-3	2.5e-3	1.7e-4	5.1e-5	2.7e-3	2.7e-3	4.8e-4	1.1e-3 ⁺	0.70945	-0.00804	-0.36924 ⁺
	273.145	11.5579	0.71515	7.6e-4	2.3e-4	2.5e-3	2.6e-3	1.6e-4	2.9e-5	2.7e-3	2.7e-3	4.8e-4	1.1e-3 ⁺	0.70944	-0.00804	-0.36946 ⁺
	273.145	11.5578	0.71509	7.4e-4	9.1e-5	2.5e-3	2.5e-3	1.8e-4	5.2e-5	2.7e-3	2.7e-3	4.8e-4	1.1e-3 ⁺	0.70946	-0.00803	-0.36866 ⁺
	273.145	11.5579	0.71511	6.5e-4	6.7e-5	2.4e-3	2.4e-3	2.7e-4	4.2e-5	2.7e-3	2.7e-3	4.8e-4	1.1e-3 ⁺	0.70945	-0.00804	-0.36906 ⁺
L48*	273.145	11.5779	0.70323	6.9e-4	5.7e-5	2.4e-3	2.4e-3	3.3e-4	6.4e-5	2.7e-3	2.7e-3	4.8e-4	3.0e-3 ⁺	0.70648	-0.00928	-1.12188 ⁺
	273.146	11.5780	0.70342	7.0e-4	7.4e-5	2.5e-3	2.5e-3	1.7e-4	4.3e-5	2.7e-3	2.7e-3	4.8e-4	3.0e-3 ⁺	0.70648	-0.00928	-1.12681 ⁺
	273.146	11.5779	0.70374	6.1e-4	5.9e-5	2.2e-3	2.2e-3	1.0e-4	8.1e-6	2.7e-3	2.7e-3	4.8e-4	3.0e-3 ⁺	0.70647	-0.00928	-1.12323 ⁺
	273.146	11.5780	0.70385	5.7e-4	6.5e-5	2.1e-3	2.1e-3	1.8e-4	3.1e-5	2.7e-3	2.7e-3	4.8e-4	3.0e-3 ⁺	0.70647	-0.00928	-1.12771 ⁺
	273.145	11.5779	0.70392	7.7e-4	7.8e-5	2.5e-3	2.5e-3	2.4e-4	4.0e-5	2.7e-3	2.7e-3	4.8e-4	3.0e-3 ⁺	0.70648	-0.00928	-1.12423 ⁺
P5	288.139	5.0859	0.99999	6.9e-4	2.8e-4	1.8e-3	1.8e-3	5.7e-5	2.9e-6	1.1e-3	1.1e-3					
L50	288.135	5.6497	0.98646	5.5e-4	7.9e-5	1.6e-3	1.6e-3	7.8e-5	7.3e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.98744	0.00274	-0.02353
	288.139	5.6498	0.98646	1.2e-3	4.7e-4	1.8e-3	1.8e-3	1.1e-4	1.5e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.98745	0.00274	-0.02353
	288.135	5.6498	0.98646	4.6e-4	4.9e-5	1.7e-3	1.7e-3	8.2e-5	1.1e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.98743	0.00274	-0.02353
	288.138	5.6498	0.98654	2.1e-3	5.7e-4	1.6e-3	1.7e-3	7.5e-5	4.5e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.98744	0.00274	-0.02353
	288.138	5.6498	0.98654	1.1e-3	3.0e-4	1.8e-3	1.8e-3	8.0e-5	1.4e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.98744	0.00274	-0.02353
L51	288.137	7.0494	0.95060	1.0e-3	2.9e-4	1.5e-3	1.5e-3	1.3e-4	1.3e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.95110	0.00273	-0.02882
	288.137	7.0493	0.95060	7.4e-4	2.3e-4	1.5e-3	1.5e-3	1.5e-4	8.9e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.95110	0.00273	-0.02882
	288.138	7.0493	0.95060	1.0e-3	2.9e-4	1.7e-3	1.7e-3	1.4e-4	8.2e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.95110	0.00273	-0.02882
	288.136	7.0494	0.95060	3.8e-4	6.8e-5	1.6e-3	1.6e-3	9.8e-5	3.8e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.95110	0.00273	-0.02882
	288.135	7.0493	0.95060	8.5e-4	2.6e-4	1.6e-3	1.6e-3	1.1e-4	1.1e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.95110	0.00273	-0.02882
	288.135	7.0494	0.95059	7.6e-4	2.0e-4	1.5e-3	1.5e-3	1.1e-4	1.0e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.95110	0.00273	-0.02882
L52	288.136	8.4289	0.90854	1.9e-3	8.3e-4	1.5e-3	1.7e-3	2.3e-4	8.9e-6	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.90541	0.00234	-0.03878
	288.134	8.4290	0.90854	9.8e-4	1.3e-4	1.6e-3	1.6e-3	2.1e-4	1.0e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.90541	0.00234	-0.03878
	288.137	8.4289	0.90854	1.7e-3	5.5e-4	1.5e-3	1.6e-3	2.9e-4	1.9e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.90542	0.00234	-0.03878
	288.134	8.4289	0.90854	7.3e-4	9.6e-5	1.6e-3	1.6e-3	2.0e-4	1.4e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.90541	0.00234	-0.03878
	288.132	8.4289	0.90855	7.5e-4	7.4e-5	1.4e-3	1.4e-3	1.8e-4	8.2e-6	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.90540	0.00234	-0.03878
	288.134	8.4289	0.90855	8.8e-4	1.7e-4	1.5e-3	1.5e-3	1.8e-4	1.5e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.90541	0.00234	-0.03878
L53	288.136	8.8666	0.89229	1.4e-3	3.9e-4	1.7e-3	1.7e-3	1.4e-4	2.0e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.88720	0.00191	-0.04495
	288.139	8.8666	0.89230	7.3e-4	1.2e-4	1.7e-3	1.7e-3	1.2e-4	6.0e-6	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.88720	0.00191	-0.04495

L54	288.136	8.8666	0.89231	5.6e-4	7.4e-5	1.7e-3	1.7e-3	1.6e-4	1.4e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.88720	0.00191	-0.04495	
	288.139	9.2573	0.87507	5.9e-4	3.5e-5	1.5e-3	1.5e-3	1.8e-4	1.1e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.86795	0.00106	-0.05470	
	288.138	9.2573	0.87510	7.8e-4	2.4e-4	1.4e-3	1.4e-3	1.7e-4	6.7e-6	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.86795	0.00106	-0.05470	
	288.138	9.2573	0.87508	4.6e-4	3.3e-5	1.7e-3	1.7e-3	1.4e-4	5.5e-6	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.86795	0.00106	-0.05470	
	288.138	9.2573	0.87507	1.2e-3	2.6e-4	1.5e-3	1.5e-3	2.1e-4	2.2e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.86795	0.00106	-0.05470	
	288.138	9.2573	0.87507	9.9e-4	1.8e-4	1.7e-3	1.7e-3	1.5e-4	7.4e-6	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.86795	0.00106	-0.05470	
L55	288.138	9.2573	0.87506	5.3e-4	5.2e-5	1.7e-3	1.7e-3	1.7e-4	8.5e-6	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.86795	0.00106	-0.05470	
	288.137	9.5784	0.85588	5.7e-4	9.7e-5	1.7e-3	1.7e-3	1.2e-4	1.7e-5	1.4e-3	1.4e-3	4.8e-4	4.9e-4 ⁺	0.84787	-0.00098	-0.07705 ⁺	
	288.137	9.5784	0.85590	4.4e-4	7.6e-5	1.8e-3	1.8e-3	1.1e-4	4.8e-6	1.4e-3	1.4e-3	4.8e-4	4.9e-4 ⁺	0.84787	-0.00098	-0.07704 ⁺	
	288.140	9.5785	0.85591	1.4e-3	6.2e-4	1.8e-3	1.9e-3	1.2e-4	8.2e-6	1.4e-3	1.4e-3	4.8e-4	4.9e-4 ⁺	0.84786	-0.00099	-0.07705 ⁺	
	288.141	9.5784	0.85589	3.1e-4	3.2e-5	1.9e-3	1.9e-3	1.1e-4	5.1e-6	1.4e-3	1.4e-3	4.8e-4	4.9e-4 ⁺	0.84786	-0.00099	-0.07705 ⁺	
	L56	288.135	9.7067	0.84280	9.8e-4	2.0e-4	1.9e-3	1.9e-3	2.1e-4	3.1e-5	1.4e-3	1.4e-3	4.8e-4	5.2e-4 ⁺	0.83726	-0.00349	-0.15076 ⁺
288.135		9.7067	0.84282	5.6e-4	1.4e-4	1.6e-3	1.6e-3	1.9e-4	2.4e-5	1.4e-3	1.4e-3	4.8e-4	5.2e-4 ⁺	0.83726	-0.00349	-0.15074 ⁺	
288.136		9.7067	0.84282	6.0e-4	9.3e-5	1.5e-3	1.5e-3	1.6e-4	1.4e-5	1.4e-3	1.4e-3	4.8e-4	5.2e-4 ⁺	0.83726	-0.00349	-0.15075 ⁺	
288.140		9.7067	0.84283	1.8e-3	5.5e-4	1.8e-3	1.9e-3	1.5e-4	2.4e-5	1.4e-3	1.4e-3	4.8e-4	5.2e-4 ⁺	0.83725	-0.00351	-0.15070 ⁺	
288.141		9.7066	0.84282	3.0e-4	1.8e-5	1.8e-3	1.8e-3	1.4e-4	6.2e-6	1.4e-3	1.4e-3	4.8e-4	5.2e-4 ⁺	0.83725	-0.00351	-0.15056 ⁺	
288.141		9.7066	0.84284	3.9e-4	2.0e-5	1.7e-3	1.7e-3	1.3e-4	8.9e-6	1.4e-3	1.4e-3	4.8e-4	5.2e-4 ⁺	0.83726	-0.00351	-0.15053 ⁺	
L57	288.141	9.7231	0.84006	2.2e-4	2.0e-5	1.9e-3	1.9e-3	1.5e-4	1.2e-5	1.4e-3	1.4e-3	4.8e-4	5.5e-4 ⁺	0.83565	-0.00410	-0.18809 ⁺	
	288.141	9.7230	0.84007	2.8e-4	2.6e-5	1.8e-3	1.8e-3	1.3e-4	1.4e-5	1.4e-3	1.4e-3	4.8e-4	5.5e-4 ⁺	0.83565	-0.00410	-0.18797 ⁺	
	288.141	9.7230	0.84006	2.6e-4	2.3e-5	1.8e-3	1.8e-3	1.4e-4	8.7e-6	1.4e-3	1.4e-3	4.8e-4	5.5e-4 ⁺	0.83565	-0.00410	-0.18791 ⁺	
	288.141	9.7231	0.84005	1.5e-4	2.8e-5	1.9e-3	1.9e-3	1.2e-4	7.7e-6	1.4e-3	1.4e-3	4.8e-4	5.5e-4 ⁺	0.83565	-0.00410	-0.18803 ⁺	
	L58	288.134	9.7447	0.83482	6.9e-4	7.6e-5	1.5e-3	1.5e-3	2.0e-4	8.6e-6	1.4e-3	1.4e-3	4.8e-4	6.6e-4 ⁺	0.83345	-0.00503	-0.32930 ⁺
		288.135	9.7447	0.83498	4.8e-4	8.1e-5	1.6e-3	1.6e-3	1.9e-4	8.5e-6	1.4e-3	1.4e-3	4.8e-4	6.6e-4 ⁺	0.83345	-0.00503	-0.32919 ⁺
288.140		9.7447	0.83499	3.4e-3	1.4e-3	1.8e-3	2.3e-3	1.5e-4	7.1e-6	1.4e-3	1.4e-3	4.8e-4	6.6e-4 ⁺	0.83343	-0.00506	-0.32930 ⁺	
288.142		9.7447	0.83497	2.7e-4	6.2e-5	2.0e-3	2.0e-3	1.6e-4	9.3e-6	1.4e-3	1.4e-3	4.8e-4	6.6e-4 ⁺	0.83341	-0.00508	-0.32986 ⁺	
288.142		9.7447	0.83497	2.9e-4	3.5e-5	1.9e-3	1.9e-3	1.5e-4	1.7e-5	1.4e-3	1.4e-3	4.8e-4	6.6e-4 ⁺	0.83341	-0.00508	-0.32928 ⁺	
288.142		9.7447	0.83497	3.1e-4	5.7e-5	2.0e-3	2.0e-3	1.5e-4	8.1e-6	1.4e-3	1.4e-3	4.8e-4	6.6e-4 ⁺	0.83342	-0.00508	-0.32893 ⁺	
P6	298.137	6.4328	0.99999	7.5e-4	1.1e-4	3.0e-3	3.0e-3	9.4e-5	8.6e-6	1.1e-3	1.1e-3						
L59	298.134	7.1110	0.98138	1.6e-3	6.2e-4	3.0e-3	3.0e-3	1.0e-4	2.3e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.98158	0.00383	-0.02989	
	298.133	7.1110	0.98137	6.5e-4	7.8e-5	3.0e-3	3.0e-3	1.0e-4	1.1e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.98157	0.00383	-0.02989	
	298.132	7.1110	0.98137	6.5e-4	5.9e-5	3.0e-3	3.0e-3	9.0e-5	2.3e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.98157	0.00383	-0.02989	
	298.132	7.1111	0.98137	7.4e-4	2.4e-4	2.8e-3	2.9e-3	9.1e-5	1.1e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.98157	0.00383	-0.02989	
	298.133	7.1110	0.98137	6.9e-4	1.2e-4	3.1e-3	3.1e-3	9.1e-5	9.8e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.98158	0.00383	-0.02989	
	298.136	7.1110	0.98138	3.0e-3	1.3e-3	3.1e-3	3.4e-3	8.8e-5	1.2e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.98159	0.00383	-0.02989	
L60	298.135	7.4191	0.97218	8.7e-4	3.3e-4	3.2e-3	3.2e-3	1.1e-4	8.6e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.97195	0.00379	-0.03281	
	298.134	7.4191	0.97218	6.3e-4	1.0e-4	3.1e-3	3.1e-3	9.7e-5	1.2e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.97195	0.00379	-0.03281	
	298.135	7.4191	0.97218	6.1e-4	1.3e-4	3.0e-3	3.0e-3	1.0e-4	6.0e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.97195	0.00379	-0.03281	
	298.134	7.4191	0.97218	5.6e-4	5.0e-5	3.1e-3	3.1e-3	8.9e-5	8.4e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.97194	0.00379	-0.03281	
	298.137	7.4191	0.97218	4.9e-4	1.4e-4	3.2e-3	3.2e-3	9.0e-5	7.2e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.97196	0.00379	-0.03281	
	298.136	7.4191	0.97218	4.4e-4	3.8e-5	3.2e-3	3.2e-3	9.5e-5	1.3e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.97195	0.00379	-0.03281	
L61	298.139	7.8406	0.95810	1.7e-3	3.8e-4	3.0e-3	3.0e-3	7.1e-4	8.9e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.95692	0.00349	-0.03927	
	298.133	7.8403	0.95809	1.8e-3	4.6e-4	2.9e-3	3.0e-3	3.2e-4	9.0e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.95692	0.00349	-0.03925	
	298.134	7.8404	0.95809	7.5e-4	1.1e-4	2.9e-3	2.9e-3	1.2e-4	2.1e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.95692	0.00349	-0.03926	
	298.133	7.8402	0.95809	9.1e-4	2.2e-4	2.9e-3	2.9e-3	1.1e-4	1.7e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.95692	0.00349	-0.03925	
	298.133	7.8400	0.95810	8.7e-4	3.0e-4	3.0e-3	3.0e-3	1.3e-4	1.7e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.95693	0.00349	-0.03925	
	L62	298.132	8.0258	0.95086	4.7e-4	5.0e-5	3.1e-3	3.1e-3	1.3e-4	1.8e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94920	0.00310	-0.04439
298.132		8.0258	0.95086	8.1e-4	2.9e-4	3.1e-3	3.1e-3	1.3e-4	1.3e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94919	0.00310	-0.04439	
298.133		8.0258	0.95087	4.8e-4	4.9e-5	3.1e-3	3.1e-3	1.4e-4	1.0e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94920	0.00310	-0.04439	
298.133		8.0258	0.95087	8.2e-4	1.8e-4	3.2e-3	3.2e-3	1.2e-4	7.4e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94920	0.00310	-0.04439	
298.137		8.0258	0.95087	2.7e-3	1.2e-3	3.2e-3	3.5e-3	1.1e-4	9.9e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94921	0.00310	-0.04440	
298.140		8.0258	0.95088	2.0e-4	2.8e-5	3.4e-3	3.4e-3	1.2e-4	9.5e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94922	0.00310	-0.04442	
L63	298.136	8.1284	0.94625	6.0e-4	1.8e-4	3.0e-3	3.1e-3	1.3e-4	2.3e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.94443	0.00267	-0.04892	
	298.135	8.1284	0.94625	6.4e-4	8.4e-5	3.1e-3	3.1e-3	1.2e-4	2.2e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.94443	0.00267	-0.04892	
	298.135	8.1284	0.94625	5.5e-4	7.2e-5	3.1e-3	3.1e-3	1.4e-4	2.8e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.94443	0.00267	-0.04891	

	298.135	8.1285	0.94625	5.3e-4	4.4e-5	3.0e-3	3.0e-3	1.3e-4	2.1e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.94443	0.00267	-0.04891
	298.134	8.1285	0.94625	4.2e-4	3.5e-5	3.0e-3	3.0e-3	1.6e-4	2.5e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.94443	0.00267	-0.04891
	298.134	8.1284	0.94625	4.5e-4	8.3e-5	2.9e-3	2.9e-3	1.2e-4	2.0e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.94443	0.00267	-0.04891
L64	298.136	8.2648	0.93816	7.8e-4	2.3e-4	3.3e-3	3.3e-3	1.4e-4	3.2e-5	1.2e-3	1.2e-3	4.8e-4	4.9e-4 ⁺	0.93709	0.00133	-0.08034 ⁺
	298.136	8.2648	0.93815	7.9e-4	1.4e-4	3.1e-3	3.1e-3	1.5e-4	1.6e-5	1.2e-3	1.2e-3	4.8e-4	4.9e-4 ⁺	0.93709	0.00133	-0.08037 ⁺
	298.135	8.2648	0.93815	6.1e-4	4.5e-5	3.2e-3	3.2e-3	1.2e-4	2.5e-5	1.2e-3	1.2e-3	4.8e-4	4.9e-4 ⁺	0.93709	0.00133	-0.08037 ⁺
	298.135	8.2648	0.93815	5.5e-4	7.1e-5	3.1e-3	3.2e-3	1.2e-4	1.3e-5	1.2e-3	1.2e-3	4.8e-4	4.9e-4 ⁺	0.93709	0.00134	-0.08036 ⁺
	298.135	8.2648	0.93815	5.3e-4	8.3e-5	3.2e-3	3.2e-3	1.2e-4	2.0e-5	1.2e-3	1.2e-3	4.8e-4	4.9e-4 ⁺	0.93709	0.00133	-0.08036 ⁺
	298.135	8.2648	0.93816	5.2e-4	6.8e-5	3.1e-3	3.1e-3	1.1e-4	1.1e-5	1.2e-3	1.2e-3	4.8e-4	4.9e-4 ⁺	0.93709	0.00134	-0.08033 ⁺
L65	298.135	8.3020	0.93438	5.4e-4	5.1e-5	3.3e-3	3.3e-3	1.8e-4	2.7e-5	1.2e-3	1.2e-3	4.8e-4	5.1e-4 ⁺	0.93473	0.00051	-0.14060 ⁺
	298.135	8.3020	0.93439	3.9e-4	3.6e-5	3.3e-3	3.3e-3	1.4e-4	2.1e-5	1.2e-3	1.2e-3	4.8e-4	5.1e-4 ⁺	0.93473	0.00050	-0.14069 ⁺
	298.138	8.3019	0.93439	1.2e-3	3.0e-4	3.2e-3	3.2e-3	1.0e-4	1.3e-5	1.2e-3	1.2e-3	4.8e-4	5.1e-4 ⁺	0.93474	0.00050	-0.14043 ⁺
	298.138	8.3019	0.93438	5.1e-4	6.8e-5	3.2e-3	3.2e-3	1.4e-4	2.3e-5	1.2e-3	1.2e-3	4.8e-4	5.1e-4 ⁺	0.93474	0.00069	-0.14048 ⁺
	298.135	8.3019	0.93440	1.0e-3	3.8e-4	3.2e-3	3.2e-3	1.6e-4	4.3e-5	1.2e-3	1.2e-3	4.8e-4	5.1e-4 ⁺	0.93474	0.00051	-0.14053 ⁺
	298.136	8.3019	0.93441	2.0e-3	8.8e-4	3.2e-3	3.3e-3	1.4e-4	2.4e-5	1.2e-3	1.2e-3	4.8e-4	5.1e-4 ⁺	0.93474	0.00051	-0.14043 ⁺
L66	298.133	8.3180	0.93085	1.0e-3	3.0e-4	3.0e-3	3.0e-3	1.2e-4	7.7e-6	1.2e-3	1.2e-3	4.8e-4	7.2e-4 ⁺	0.93363	-0.00001	-0.46243 ⁺
	298.135	8.3180	0.93077	9.8e-4	1.2e-4	3.2e-3	3.2e-3	1.0e-4	1.2e-5	1.2e-3	1.2e-3	4.8e-4	7.2e-4 ⁺	0.93363	-0.00001	-0.46047 ⁺
	298.133	8.3180	0.93090	8.4e-4	6.1e-5	3.2e-3	3.2e-3	1.1e-4	1.1e-5	1.2e-3	1.2e-3	4.8e-4	7.2e-4 ⁺	0.93363	-0.00000	-0.46319 ⁺
	298.134	8.3180	0.93082	2.2e-3	8.8e-4	3.2e-3	3.3e-3	1.3e-4	1.4e-5	1.2e-3	1.2e-3	4.8e-4	7.2e-4 ⁺	0.93363	-0.00001	-0.46008 ⁺
	298.134	8.3180	0.93096	6.6e-4	1.4e-4	3.0e-3	3.0e-3	1.3e-4	1.5e-5	1.2e-3	1.2e-3	4.8e-4	7.2e-4 ⁺	0.93363	-0.00001	-0.46153 ⁺
	298.136	8.3180	0.93081	1.3e-3	4.7e-4	3.1e-3	3.1e-3	1.1e-4	9.9e-6	1.2e-3	1.2e-3	4.8e-4	7.2e-4 ⁺	0.93363	-0.00002	-0.46044 ⁺

Table A.3

Vapor phase: Experimental VLE data for CO₂ + O₂ at mean temperature \bar{T} , mean pressure \bar{p} , and sample vapor phase mole fraction y_{CO_2} .

ID	Data			Temperature				Pressure				Composition			Composition derivatives	
	\bar{T} (K)	\bar{p} (MPa)	y_{CO_2} (-)	$s(T)$ (K)	$s(\bar{T})$ (K)	$\bar{u}(T)$ (K)	$u_c(\bar{T})$ (K)	$s(p)$ (MPa)	$s(\bar{p})$ (MPa)	$\bar{u}(p)$ (MPa)	$u_c(\bar{p})$ (MPa)	$u(y_{\text{CO}_2})$ (-)	$u_{\text{tot}}(y_{\text{CO}_2})$ (-)	$y_{\text{CO}_2, \text{calc}}$ (-)	$\partial y_{\text{CO}_2} / \partial T$ (K ⁻¹)	$\partial y_{\text{CO}_2} / \partial p$ (MPa ⁻¹)
P1	218.147	0.5546	0.99999	4.7e-4	7.3e-5	3.7e-3	3.7e-3	1.3e-5	1.1e-6	4.9e-4	4.9e-4					
V1	218.148	1.0238	0.57407	8.9e-4	1.4e-4	3.4e-3	3.4e-3	2.3e-5	7.2e-6	5.1e-4	5.1e-4	4.8e-4	5.5e-4	0.57409	0.02295	-0.49749
	218.148	1.0238	0.57376	8.9e-4	1.2e-4	3.5e-3	3.5e-3	2.8e-5	1.1e-5	5.1e-4	5.1e-4	4.8e-4	5.5e-4	0.57411	0.02295	-0.49753
	218.148	1.0238	0.57373	1.1e-3	1.6e-4	3.4e-3	3.4e-3	3.1e-5	1.3e-5	5.1e-4	5.1e-4	4.8e-4	5.5e-4	0.57412	0.02295	-0.49755
	218.148	1.0237	0.57348	1.2e-3	1.8e-4	3.3e-3	3.3e-3	3.3e-5	1.4e-5	5.1e-4	5.1e-4	4.8e-4	5.5e-4	0.57413	0.02295	-0.49758
	218.148	1.0237	0.57340	1.0e-3	1.7e-4	3.4e-3	3.4e-3	2.6e-5	8.6e-6	5.1e-4	5.1e-4	4.8e-4	5.5e-4	0.57417	0.02295	-0.49764
	218.148	1.0236	0.57325	8.8e-4	1.1e-4	3.2e-3	3.2e-3	3.4e-5	1.5e-5	5.1e-4	5.1e-4	4.8e-4	5.5e-4	0.57419	0.02295	-0.49768
	218.148	1.0236	0.57344	1.4e-3	2.0e-4	3.4e-3	3.5e-3	3.1e-5	1.3e-5	5.1e-4	5.1e-4	4.8e-4	5.5e-4	0.57421	0.02295	-0.49772
	218.148	1.0236	0.57323	9.7e-4	1.9e-4	3.3e-3	3.3e-3	3.7e-5	1.6e-5	5.1e-4	5.1e-4	4.8e-4	5.5e-4	0.57423	0.02296	-0.49775
V2	218.148	2.1957	0.29873	4.7e-4	1.2e-4	3.5e-3	3.5e-3	3.3e-5	1.1e-5	5.2e-4	5.2e-4	4.8e-4	4.8e-4	0.30251	0.01191	-0.10668
	218.147	2.1957	0.29847	7.5e-4	1.6e-4	3.5e-3	3.5e-3	2.2e-5	2.3e-6	5.2e-4	5.2e-4	4.8e-4	4.8e-4	0.30251	0.01191	-0.10668
	218.148	2.1957	0.29849	4.4e-4	6.2e-5	3.4e-3	3.4e-3	3.3e-5	7.7e-6	5.2e-4	5.2e-4	4.8e-4	4.8e-4	0.30252	0.01191	-0.10668
	218.148	2.1957	0.29844	5.2e-4	1.0e-4	3.4e-3	3.4e-3	4.6e-5	1.7e-5	5.2e-4	5.2e-4	4.8e-4	4.8e-4	0.30252	0.01191	-0.10669
	218.148	2.1957	0.29842	4.2e-4	3.1e-5	3.4e-3	3.4e-3	7.5e-5	3.2e-5	5.2e-4	5.2e-4	4.8e-4	4.8e-4	0.30252	0.01191	-0.10669
	218.148	2.1956	0.29839	4.9e-4	5.9e-5	3.5e-3	3.5e-3	6.5e-5	3.0e-5	5.2e-4	5.2e-4	4.8e-4	4.8e-4	0.30253	0.01191	-0.10669
V3	218.148	3.9361	0.19677	7.6e-4	1.5e-4	3.9e-3	3.9e-3	5.3e-5	1.1e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.20251	0.00762	-0.02965
	218.148	3.9362	0.19668	9.3e-4	1.3e-4	3.7e-3	3.7e-3	5.2e-5	6.4e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.20251	0.00762	-0.02965
	218.148	3.9362	0.19662	1.1e-3	2.4e-4	3.6e-3	3.6e-3	6.3e-5	1.8e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.20251	0.00762	-0.02965
	218.148	3.9362	0.19656	1.1e-3	2.2e-4	3.8e-3	3.8e-3	6.0e-5	9.0e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.20251	0.00762	-0.02965
	218.148	3.9362	0.19654	8.8e-4	1.2e-4	3.8e-3	3.8e-3	5.2e-5	7.5e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.20251	0.00762	-0.02965
V4	218.150	5.9189	0.16098	6.2e-4	8.5e-5	3.2e-3	3.2e-3	8.2e-5	5.0e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.16825	0.00589	-0.00866
	218.150	5.9189	0.16093	8.8e-4	1.3e-4	3.3e-3	3.3e-3	1.1e-4	8.8e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.16826	0.00589	-0.00866
	218.150	5.9189	0.16094	5.3e-4	7.7e-5	3.2e-3	3.2e-3	8.9e-5	6.6e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.16826	0.00589	-0.00866
	218.150	5.9189	0.16091	8.6e-4	1.5e-4	3.2e-3	3.2e-3	8.1e-5	5.4e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.16826	0.00589	-0.00866
	218.150	5.9189	0.16089	8.0e-4	1.1e-4	3.2e-3	3.2e-3	8.6e-5	9.2e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.16825	0.00589	-0.00866
V5	218.148	7.8935	0.15232	6.1e-4	4.1e-5	3.5e-3	3.5e-3	1.0e-4	3.9e-6	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.16120	0.00510	0.00080
	218.148	7.8935	0.15231	6.7e-4	1.2e-4	3.4e-3	3.4e-3	1.0e-4	4.6e-6	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.16120	0.00510	0.00080
	218.148	7.8935	0.15230	7.9e-4	2.6e-4	3.4e-3	3.4e-3	9.1e-5	5.3e-6	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.16120	0.00510	0.00080
	218.147	7.8935	0.15227	7.6e-4	1.6e-4	3.4e-3	3.4e-3	9.5e-5	1.2e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.16120	0.00510	0.00080
	218.149	7.8935	0.15225	4.3e-4	6.0e-5	3.5e-3	3.5e-3	1.1e-4	2.3e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.16121	0.00510	0.00080
	218.148	7.8935	0.15227	5.5e-4	1.1e-4	3.5e-3	3.5e-3	1.0e-4	1.3e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.16120	0.00510	0.00080
V6	218.148	9.7335	0.15919	7.7e-4	2.3e-4	3.4e-3	3.4e-3	1.3e-4	7.8e-6	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.16940	0.00466	0.00826
	218.148	9.7336	0.15919	7.1e-4	1.2e-4	3.5e-3	3.5e-3	1.2e-4	1.0e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.16941	0.00466	0.00826
	218.148	9.7335	0.15917	6.4e-4	1.1e-4	3.5e-3	3.5e-3	1.2e-4	6.8e-6	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.16940	0.00466	0.00826
	218.148	9.7335	0.15919	7.5e-4	1.4e-4	3.5e-3	3.5e-3	1.3e-4	7.1e-6	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.16940	0.00466	0.00826
	218.148	9.7335	0.15916	5.7e-4	9.4e-5	3.5e-3	3.5e-3	1.3e-4	1.6e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.16940	0.00466	0.00826
V7	218.148	11.7910	0.18682	7.0e-4	6.4e-5	3.6e-3	3.6e-3	1.9e-4	1.1e-5	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.19797	0.00416	0.02109
	218.148	11.7910	0.18681	5.8e-4	6.6e-5	3.5e-3	3.5e-3	1.7e-4	2.0e-5	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.19797	0.00416	0.02109
	218.147	11.7910	0.18681	7.5e-4	1.5e-4	3.4e-3	3.4e-3	1.7e-4	8.4e-6	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.19797	0.00416	0.02109
	218.147	11.7910	0.18683	1.0e-3	1.1e-4	3.5e-3	3.5e-3	1.5e-4	1.9e-5	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.19796	0.00416	0.02109
	218.147	11.7910	0.18679	8.2e-4	1.0e-4	3.5e-3	3.5e-3	1.4e-4	9.0e-6	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.19797	0.00416	0.02109
	218.148	11.7910	0.18683	5.2e-4	6.8e-5	3.7e-3	3.7e-3	1.5e-4	6.5e-6	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.19797	0.00416	0.02109
	218.148	11.7910	0.18679	7.6e-4	2.0e-4	3.4e-3	3.4e-3	1.6e-4	2.5e-5	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.19797	0.00416	0.02109
V8	218.148	13.0212	0.22285	7.3e-4	1.7e-4	3.6e-3	3.6e-3	1.7e-4	1.7e-5	2.8e-3	2.8e-3	4.8e-4	4.9e-4	0.23322	0.00358	0.03885
	218.149	13.0211	0.22281	8.3e-4	2.8e-4	3.6e-3	3.6e-3	1.5e-4	6.3e-6	2.8e-3	2.8e-3	4.8e-4	4.9e-4	0.23322	0.00358	0.03886
	218.148	13.0211	0.22282	6.4e-4	8.2e-5	3.5e-3	3.5e-3	2.0e-4	2.9e-5	2.8e-3	2.8e-3	4.8e-4	4.9e-4	0.23321	0.00358	0.03885
	218.148	13.0211	0.22283	8.0e-4	1.6e-4	3.4e-3	3.4e-3	1.8e-4	8.3e-6	2.8e-3	2.8e-3	4.8e-4	4.9e-4	0.23321	0.00358	0.03885

V9	218.148	14.0360	0.28671	6.9e-4	1.1e-4	3.7e-3	3.7e-3	1.8e-4	2.1e-5	2.8e-3	2.8e-3	4.8e-4	5.7e-4+	0.29187	0.00229	0.11052+
	218.147	14.0359	0.28671	8.7e-4	1.0e-4	3.6e-3	3.6e-3	2.3e-4	1.7e-5	2.8e-3	2.8e-3	4.8e-4	5.7e-4+	0.29187	0.00229	0.11051+
	218.148	14.0359	0.28663	6.4e-4	8.3e-5	3.6e-3	3.6e-3	1.8e-4	1.2e-5	2.8e-3	2.8e-3	4.8e-4	5.7e-4+	0.29187	0.00229	0.11052+
V10*	218.148	14.0359	0.28655	7.1e-4	8.4e-5	3.5e-3	3.5e-3	1.9e-4	7.4e-6	2.8e-3	2.8e-3	4.8e-4	5.7e-4+	0.29186	0.00229	0.11050+
	218.148	14.3562	0.33858	6.8e-4	8.9e-5	3.2e-3	3.2e-3	2.4e-4	2.0e-5	2.8e-3	2.8e-3	4.8e-4	9.4e-4+	0.33135	0.00084	0.29213+
	218.148	14.3563	0.33861	7.3e-4	1.2e-4	3.1e-3	3.1e-3	1.8e-4	1.1e-5	2.8e-3	2.8e-3	4.8e-4	9.4e-4+	0.33136	0.00084	0.29221+
	218.148	14.3563	0.33855	7.6e-4	2.3e-4	3.2e-3	3.2e-3	1.8e-4	2.0e-5	2.8e-3	2.8e-3	4.8e-4	9.4e-4+	0.33136	0.00084	0.29218+
	218.148	14.3563	0.33850	7.5e-4	2.2e-4	3.2e-3	3.2e-3	1.8e-4	7.7e-6	2.8e-3	2.8e-3	4.8e-4	9.4e-4+	0.33136	0.00084	0.29216+
	218.148	14.3562	0.33858	5.2e-4	1.2e-4	3.1e-3	3.1e-3	1.7e-4	1.1e-5	2.8e-3	2.8e-3	4.8e-4	9.4e-4+	0.33135	0.00084	0.29204+
	218.148	14.3562	0.33853	5.7e-4	1.1e-4	3.1e-3	3.1e-3	2.0e-4	1.2e-5	2.8e-3	2.8e-3	4.8e-4	9.4e-4+	0.33136	0.00084	0.29215+
V11*	218.148	14.3563	0.33849	4.9e-4	8.5e-5	3.2e-3	3.2e-3	2.0e-4	1.6e-5	2.8e-3	2.8e-3	4.8e-4	9.4e-4+	0.33136	0.00084	0.29221+
	218.148	14.3873	0.34939	6.1e-4	8.4e-5	3.1e-3	3.1e-3	2.4e-4	1.7e-5	2.8e-3	2.8e-3	4.8e-4	1.2e-3+	0.33726	0.00050	0.40199+
	218.147	14.3873	0.34927	1.2e-3	2.6e-4	3.4e-3	3.4e-3	2.1e-4	8.8e-6	2.8e-3	2.8e-3	4.8e-4	1.2e-3+	0.33726	0.00050	0.40215+
	218.147	14.3873	0.34937	9.9e-4	1.3e-4	3.3e-3	3.3e-3	1.6e-4	9.6e-6	2.8e-3	2.8e-3	4.8e-4	1.2e-3+	0.33726	0.00050	0.40196+
	218.147	14.3873	0.34939	9.0e-4	2.3e-4	3.2e-3	3.2e-3	2.2e-4	1.1e-5	2.8e-3	2.8e-3	4.8e-4	1.2e-3+	0.33726	0.00050	0.40201+
	218.147	14.3873	0.34933	8.3e-4	8.0e-5	3.3e-3	3.3e-3	2.2e-4	3.3e-5	2.8e-3	2.8e-3	4.8e-4	1.2e-3+	0.33725	0.00050	0.40185+
	218.147	14.3873	0.34939	9.6e-4	2.4e-4	3.3e-3	3.3e-3	2.2e-4	3.1e-5	2.8e-3	2.8e-3	4.8e-4	1.2e-3+	0.33726	0.00050	0.40203+
V12*	218.149	14.4111	0.36118	6.4e-4	1.1e-4	3.4e-3	3.4e-3	2.0e-4	1.1e-5	2.8e-3	2.8e-3	4.8e-4	1.8e-3+	0.34236	0.00017	0.62899+
	218.148	14.4111	0.36122	1.0e-3	3.6e-4	3.2e-3	3.3e-3	2.1e-4	8.4e-6	2.8e-3	2.8e-3	4.8e-4	1.8e-3+	0.34236	0.00017	0.62908+
	218.149	14.4111	0.36122	9.2e-4	2.2e-4	3.4e-3	3.4e-3	1.6e-4	1.3e-5	2.8e-3	2.8e-3	4.8e-4	1.8e-3+	0.34237	0.00032	0.62982+
	218.150	14.4111	0.36115	9.3e-4	2.8e-4	3.4e-3	3.5e-3	1.8e-4	8.8e-6	2.8e-3	2.8e-3	4.8e-4	1.8e-3+	0.34237	0.00017	0.62952+
	218.149	14.4111	0.36117	1.1e-3	1.9e-4	3.3e-3	3.3e-3	1.9e-4	1.5e-5	2.8e-3	2.8e-3	4.8e-4	1.8e-3+	0.34236	0.00017	0.62884+
	218.149	14.4111	0.36113	1.0e-3	2.1e-4	3.3e-3	3.3e-3	1.8e-4	7.7e-6	2.8e-3	2.8e-3	4.8e-4	1.8e-3+	0.34236	0.00017	0.62915+
	218.150	14.4112	0.36067	9.1e-4	2.3e-4	3.3e-3	3.3e-3	1.7e-4	3.5e-6	2.8e-3	2.8e-3	4.8e-4	1.8e-3+	0.34239	0.00017	0.63082+
P2	233.143	1.0048	0.99999	9.7e-4	7.4e-5	6.8e-3	6.8e-3	4.3e-5	1.1e-5	5.1e-4	5.1e-4	4.8e-4	5.1e-4	0.56621	0.01852	-0.23333
V14	233.143	1.9677	0.56443	9.5e-4	1.6e-4	7.4e-3	7.4e-3	3.5e-5	1.2e-5	5.1e-4	5.1e-4	4.8e-4	5.1e-4	0.56621	0.01852	-0.23333
	233.143	1.9677	0.56407	1.1e-3	1.5e-4	7.1e-3	7.1e-3	2.2e-5	2.5e-6	5.1e-4	5.1e-4	4.8e-4	5.1e-4	0.56621	0.01852	-0.23333
	233.143	1.9677	0.56405	1.1e-3	2.1e-4	7.2e-3	7.2e-3	2.1e-5	2.1e-6	5.1e-4	5.1e-4	4.8e-4	5.1e-4	0.56621	0.01852	-0.23333
	233.142	1.9677	0.56395	1.1e-3	1.3e-4	7.2e-3	7.3e-3	2.0e-5	2.1e-6	5.1e-4	5.1e-4	4.8e-4	5.1e-4	0.56621	0.01852	-0.23333
	233.142	1.9677	0.56369	1.1e-3	1.7e-4	7.4e-3	7.4e-3	2.8e-5	7.9e-6	5.1e-4	5.1e-4	4.8e-4	5.1e-4	0.56620	0.01852	-0.23333
	233.142	1.9677	0.56362	1.1e-3	1.5e-4	7.7e-3	7.7e-3	2.0e-5	2.3e-6	5.1e-4	5.1e-4	4.8e-4	5.1e-4	0.56620	0.01852	-0.23333
V15	233.141	2.9346	0.41129	1.3e-3	3.2e-4	7.8e-3	7.8e-3	9.9e-5	4.3e-5	5.3e-4	5.3e-4	4.8e-4	4.9e-4	0.41569	0.01345	-0.10307
	233.141	2.9346	0.41115	1.3e-3	2.3e-4	7.4e-3	7.4e-3	2.6e-5	6.1e-6	5.2e-4	5.2e-4	4.8e-4	4.9e-4	0.41570	0.01345	-0.10308
	233.143	2.9345	0.41116	9.7e-4	1.2e-4	8.1e-3	8.1e-3	2.4e-5	2.7e-6	5.2e-4	5.2e-4	4.8e-4	4.9e-4	0.41572	0.01345	-0.10308
	233.142	2.9346	0.41126	6.0e-4	6.3e-5	7.5e-3	7.5e-3	2.5e-5	4.7e-6	5.2e-4	5.2e-4	4.8e-4	4.9e-4	0.41571	0.01345	-0.10308
	233.142	2.9345	0.41118	6.2e-4	5.4e-5	7.7e-3	7.7e-3	2.6e-5	6.3e-6	5.2e-4	5.2e-4	4.8e-4	4.9e-4	0.41571	0.01345	-0.10308
	233.142	2.9345	0.41106	1.2e-3	3.3e-4	8.0e-3	8.0e-3	2.5e-5	5.5e-6	5.2e-4	5.2e-4	4.8e-4	4.9e-4	0.41572	0.01345	-0.10308
	233.142	2.9345	0.41107	8.7e-4	9.6e-5	7.8e-3	7.8e-3	6.8e-5	1.6e-5	5.2e-4	5.3e-4	4.8e-4	4.9e-4	0.41571	0.01345	-0.10308
	233.141	3.9408	0.33186	1.8e-3	5.7e-4	6.8e-3	6.8e-3	3.0e-4	7.1e-5	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.33995	0.01079	-0.05441
V16	233.143	3.9407	0.33186	9.8e-4	1.1e-4	6.9e-3	6.9e-3	2.5e-4	5.8e-5	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.33996	0.01079	-0.05442
	233.143	3.9407	0.33179	1.0e-3	2.4e-4	6.6e-3	6.6e-3	6.7e-5	1.2e-5	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.33997	0.01079	-0.05442
	233.143	3.9409	0.33190	9.3e-4	1.1e-4	6.6e-3	6.6e-3	7.6e-5	2.7e-5	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.33996	0.01079	-0.05441
	233.144	3.9408	0.33184	8.5e-4	1.7e-4	6.8e-3	6.8e-3	6.0e-5	1.2e-5	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.33997	0.01079	-0.05442
	233.143	3.9408	0.33188	6.2e-4	1.2e-4	7.1e-3	7.1e-3	5.8e-5	1.1e-5	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.33997	0.01079	-0.05441
	233.144	5.9477	0.26280	9.3e-4	2.4e-4	8.0e-3	8.0e-3	8.7e-5	1.2e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.27331	0.00821	-0.01872
	233.143	5.9476	0.26279	7.5e-4	7.4e-5	7.4e-3	7.4e-3	2.9e-4	1.0e-4	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.27331	0.00821	-0.01872
	233.143	5.9475	0.26279	7.0e-4	1.2e-4	7.6e-3	7.6e-3	3.2e-4	1.3e-4	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.27331	0.00821	-0.01872
V17	233.143	5.9474	0.26282	6.5e-4	7.7e-5	7.4e-3	7.4e-3	4.3e-4	1.9e-4	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.27331	0.00821	-0.01872
	233.144	5.9472	0.26280	8.4e-4	2.7e-4	7.8e-3	7.8e-3	5.7e-4	2.7e-4	1.1e-3	1.2e-3	4.8e-4	4.8e-4	0.27332	0.00821	-0.01872
	233.141	7.8335	0.24023	2.1e-3	7.1e-4	7.6e-3	7.6e-3	1.5e-4	1.2e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.25239	0.00708	-0.00479
	233.142	7.8335	0.24025	1.3e-3	3.4e-4	7.5e-3	7.5e-3	1.5e-4	1.3e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.25240	0.00708	-0.00479
	233.142	7.8335	0.24023	8.7e-4	1.2e-4	7.8e-3	7.8e-3	1.3e-4	6.3e-6	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.25240	0.00708	-0.00479
	233.142	7.8334	0.24020	1.1e-3	1.8e-4	7.4e-3	7.4e-3	1.1e-4	7.2e-6	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.25240	0.00708	-0.00479
	233.142	7.8335	0.24014	1.0e-3	2.8e-4	7.4e-3	7.4e-3	1.2e-4	5.5e-6	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.25240	0.00708	-0.00479

V19	233.140	8.8724	0.23720	1.3e-3	1.9e-4	7.5e-3	7.5e-3	1.9e-4	9.2e-6	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.25032	0.00671	0.00070
	233.140	8.8724	0.23719	1.1e-3	2.7e-4	7.1e-3	7.1e-3	1.4e-4	1.4e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.25032	0.00671	0.00070
	233.141	8.8724	0.23720	1.0e-3	9.7e-5	7.8e-3	7.8e-3	1.2e-4	1.1e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.25033	0.00671	0.00070
	233.141	8.8724	0.23715	8.7e-4	1.6e-4	7.6e-3	7.6e-3	1.4e-4	9.4e-6	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.25033	0.00671	0.00070
	233.142	8.8724	0.23710	7.5e-4	1.1e-4	7.7e-3	7.7e-3	1.3e-4	8.5e-6	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.25034	0.00671	0.00070
V20	233.142	8.8724	0.23708	8.3e-4	1.0e-4	7.7e-3	7.7e-3	1.3e-4	4.4e-6	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.25034	0.00671	0.00070
	233.141	9.8514	0.23940	1.0e-3	1.4e-4	7.4e-3	7.4e-3	1.6e-4	1.0e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.25343	0.00645	0.00566
	233.140	9.8513	0.23942	1.5e-3	4.3e-4	7.4e-3	7.4e-3	2.1e-4	1.0e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.25342	0.00645	0.00566
	233.141	9.8514	0.23938	8.8e-4	1.1e-4	7.7e-3	7.7e-3	1.3e-4	4.6e-6	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.25343	0.00645	0.00566
	233.141	9.8514	0.23940	8.3e-4	8.5e-5	7.5e-3	7.5e-3	1.5e-4	1.0e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.25343	0.00645	0.00566
V21	233.140	9.8514	0.23941	9.6e-4	1.3e-4	7.7e-3	7.7e-3	1.5e-4	1.0e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.25343	0.00645	0.00566
	233.141	9.8513	0.23939	1.0e-3	1.2e-4	7.4e-3	7.4e-3	1.5e-4	7.2e-6	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.25343	0.00645	0.00566
	233.141	11.8342	0.26146	1.3e-3	2.0e-4	6.9e-3	7.0e-3	2.0e-4	1.0e-5	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.27633	0.00616	0.01869
	233.140	11.8341	0.26145	1.0e-3	2.8e-4	7.4e-3	7.4e-3	1.7e-4	9.8e-6	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.27633	0.00616	0.01869
	233.140	11.8341	0.26139	1.0e-3	6.9e-5	7.1e-3	7.1e-3	1.8e-4	1.8e-5	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.27633	0.00616	0.01869
V22	233.141	11.8341	0.26144	7.1e-4	8.4e-5	7.5e-3	7.5e-3	1.6e-4	6.1e-6	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.27633	0.00616	0.01869
	233.141	11.8341	0.26143	1.4e-3	1.9e-4	7.1e-3	7.1e-3	1.7e-4	9.4e-6	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.27633	0.00616	0.01869
	233.141	11.8341	0.26142	8.3e-4	1.5e-4	7.3e-3	7.3e-3	1.5e-4	8.6e-6	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.27633	0.00616	0.01869
	233.143	12.8248	0.28660	7.0e-4	6.5e-5	7.2e-3	7.2e-3	2.4e-4	1.7e-5	2.7e-3	2.7e-3	4.8e-4	4.9e-4	0.30037	0.00615	0.03119
	233.143	12.8248	0.28657	1.0e-3	2.1e-4	7.4e-3	7.4e-3	2.4e-4	1.2e-5	2.7e-3	2.7e-3	4.8e-4	4.9e-4	0.30036	0.00615	0.03120
V23	233.142	12.8248	0.28655	7.7e-4	1.4e-4	7.1e-3	7.1e-3	1.5e-4	1.9e-5	2.7e-3	2.7e-3	4.8e-4	4.9e-4	0.30036	0.00615	0.03119
	233.142	12.8248	0.28653	6.2e-4	9.3e-5	7.2e-3	7.2e-3	1.7e-4	7.8e-6	2.7e-3	2.7e-3	4.8e-4	4.9e-4	0.30036	0.00615	0.03118
	233.142	12.8248	0.28659	6.6e-4	6.0e-5	7.2e-3	7.2e-3	2.1e-4	1.3e-5	2.7e-3	2.7e-3	4.8e-4	4.9e-4	0.30036	0.00615	0.03119
	233.142	13.6445	0.32553	9.3e-4	1.2e-4	7.1e-3	7.1e-3	2.4e-4	1.5e-5	2.8e-3	2.8e-3	4.8e-4	5.2e-4 ⁺	0.33416	0.00638	0.07613 ⁺
	233.142	13.6445	0.32550	9.9e-4	1.7e-4	7.4e-3	7.4e-3	2.8e-4	2.5e-5	2.8e-3	2.8e-3	4.8e-4	5.2e-4 ⁺	0.33416	0.00638	0.07612 ⁺
V24*	233.141	13.6445	0.32544	8.7e-4	9.5e-5	7.4e-3	7.4e-3	1.8e-4	5.4e-6	2.7e-3	2.7e-3	4.8e-4	5.2e-4 ⁺	0.33415	0.00638	0.07613 ⁺
	233.142	13.6445	0.32546	1.1e-3	1.8e-4	7.3e-3	7.3e-3	1.6e-4	8.9e-6	2.7e-3	2.7e-3	4.8e-4	5.2e-4 ⁺	0.33416	0.00638	0.07613 ⁺
	233.141	13.6445	0.32551	1.0e-3	1.4e-4	7.3e-3	7.3e-3	1.5e-4	1.0e-5	2.7e-3	2.7e-3	4.8e-4	5.2e-4 ⁺	0.33416	0.00638	0.07613 ⁺
	233.142	13.6445	0.32545	1.0e-3	1.5e-4	7.1e-3	7.1e-3	1.9e-4	8.6e-6	2.7e-3	2.7e-3	4.8e-4	5.2e-4 ⁺	0.33416	0.00638	0.07613 ⁺
	233.144	14.1867	0.39251	5.9e-4	1.4e-4	6.8e-3	6.8e-3	2.1e-4	1.2e-5	2.8e-3	2.8e-3	4.8e-4	9.4e-4 ⁺	0.37661	0.00747	0.29114 ⁺
V25*	233.144	14.1867	0.39244	9.8e-4	1.4e-4	6.9e-3	6.9e-3	2.8e-4	1.3e-5	2.8e-3	2.8e-3	4.8e-4	9.4e-4 ⁺	0.37661	0.00747	0.29115 ⁺
	233.144	14.1867	0.39238	8.0e-4	1.5e-4	6.7e-3	6.7e-3	2.4e-4	1.5e-5	2.8e-3	2.8e-3	4.8e-4	9.4e-4 ⁺	0.37661	0.00747	0.29115 ⁺
	233.144	14.1868	0.39253	8.1e-4	1.5e-4	6.8e-3	6.8e-3	2.9e-4	2.9e-5	2.8e-3	2.8e-3	4.8e-4	9.4e-4 ⁺	0.37661	0.00747	0.29120 ⁺
	233.144	14.1868	0.39242	6.1e-4	1.1e-4	7.0e-3	7.0e-3	2.0e-4	1.3e-5	2.8e-3	2.8e-3	4.8e-4	9.4e-4 ⁺	0.37662	0.00747	0.29139 ⁺
	233.143	14.1868	0.39236	1.7e-3	6.0e-4	6.7e-3	6.8e-3	2.0e-4	1.2e-5	2.8e-3	2.8e-3	4.8e-4	9.4e-4 ⁺	0.37661	0.00747	0.29132 ⁺
V26*	233.144	14.2158	0.40310	5.5e-4	9.8e-5	6.7e-3	6.7e-3	2.0e-4	1.2e-5	2.8e-3	2.8e-3	4.8e-4	1.3e-3 ⁺	0.38020	0.00766	0.41949 ⁺
	233.145	14.2158	0.40303	1.0e-3	3.1e-4	6.7e-3	6.7e-3	2.0e-4	8.4e-6	2.8e-3	2.8e-3	4.8e-4	1.3e-3 ⁺	0.38021	0.00766	0.41962 ⁺
	233.145	14.2158	0.40299	8.5e-4	1.9e-4	6.5e-3	6.5e-3	1.6e-4	1.1e-5	2.8e-3	2.8e-3	4.8e-4	1.3e-3 ⁺	0.38021	0.00766	0.41970 ⁺
	233.144	14.2158	0.40298	7.8e-4	2.2e-4	6.7e-3	6.7e-3	2.2e-4	1.7e-5	2.8e-3	2.8e-3	4.8e-4	1.3e-3 ⁺	0.38021	0.00766	0.41959 ⁺
	233.143	14.2158	0.40290	1.9e-3	4.1e-4	6.5e-3	6.5e-3	2.3e-4	1.8e-5	2.8e-3	2.8e-3	4.8e-4	1.3e-3 ⁺	0.38019	0.00766	0.41959 ⁺
P3	233.145	14.2158	0.40296	4.9e-4	4.0e-5	6.4e-3	6.4e-3	2.2e-4	2.8e-5	2.8e-3	2.8e-3	4.8e-4	1.3e-3 ⁺	0.38021	0.00766	0.41986 ⁺
	233.145	14.2408	0.41751	6.7e-4	7.1e-5	6.0e-3	6.0e-3	2.0e-4	1.7e-5	2.8e-3	2.8e-3	4.8e-4	2.4e-3 ⁺	0.38355	0.00786	0.84058 ⁺
	233.146	14.2407	0.41756	6.6e-4	1.3e-4	5.9e-3	5.9e-3	2.0e-4	1.1e-5	2.8e-3	2.8e-3	4.8e-4	2.4e-3 ⁺	0.38354	0.00786	0.83931 ⁺
	233.146	14.2407	0.41751	5.2e-4	5.4e-5	6.0e-3	6.0e-3	1.8e-4	1.5e-5	2.8e-3	2.8e-3	4.8e-4	2.4e-3 ⁺	0.38354	0.00786	0.83833 ⁺
	233.145	14.2407	0.41752	5.5e-4	1.2e-4	6.0e-3	6.0e-3	2.2e-4	1.5e-5	2.8e-3	2.8e-3	4.8e-4	2.4e-3 ⁺	0.38353	0.00786	0.83708 ⁺
V28	233.145	14.2407	0.41750	4.7e-4	8.4e-5	5.9e-3	5.9e-3	1.8e-4	9.4e-6	2.8e-3	2.8e-3	4.8e-4	2.4e-3 ⁺	0.38354	0.00786	0.83851 ⁺
	233.145	14.2407	0.41747	6.6e-4	1.0e-4	6.1e-3	6.1e-3	1.5e-4	7.6e-6	2.8e-3	2.8e-3	4.8e-4	2.4e-3 ⁺	0.38354	0.00786	0.83871 ⁺
	253.147	2.9634	0.99999	8.5e-4	1.5e-5	5.7e-3	5.7e-3	3.7e-5	5.5e-6	5.1e-4	5.1e-4	5.0e-4	5.0e-4	0.73129	0.01824	-0.18197
	253.147	2.9630	0.72728	1.0e-3	1.4e-4	5.8e-3	5.8e-3	8.1e-5	1.3e-5	5.2e-4	5.2e-4	4.8e-4	5.0e-4	0.73136	0.01824	-0.18201
	253.146	2.9630	0.72729	7.9e-4	1.9e-4	5.4e-3	5.4e-3	1.6e-4	1.6e-4	5.2e-4	5.3e-4	4.8e-4	5.0e-4	0.73135	0.01824	-0.18201
V28	253.147	2.9630	0.72731	7.4e-4	7.6e-5	6.0e-3	6.0e-3	1.4e-4	5.5e-5	5.2e-4	5.3e-4	4.8e-4	5.0e-4	0.73135	0.01824	-0.18201
	253.147	2.9630	0.72735	5.8e-4	4.5e-5	5.6e-3	5.6e-3	1.3e-4	5.5e-5	5.2e-4	5.3e-4	4.8e-4	5.0e-4	0.73136	0.01824	-0.18201
	253.147	2.9630	0.72732	6.7e-4	1.1e-4	6.0e-3	6.0e-3	1.3e-4	5.6e-5	5.2e-4	5.3e-4	4.8e-4	5.0e-4	0.73136	0.01824	-0.18201
	253.146	2.9630	0.72730	9.2e-4	2.7e-4	5.7e-3	5.7e-3	1.3e-4	5.3e-5	5.2e-4	5.3e-4	4.8e-4	5.0e-4	0.73136	0.01824	-0.18202

V29	253.146	4.9363	0.51059	8.8e-4	8.5e-5	5.5e-3	5.5e-3	1.8e-4	6.2e-5	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.51935	0.01278	-0.06146
	253.146	4.9364	0.51053	1.2e-3	2.2e-4	5.8e-3	5.8e-3	9.5e-5	2.8e-5	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.51934	0.01278	-0.06146
	253.146	4.9363	0.51049	9.8e-4	1.9e-4	5.7e-3	5.7e-3	9.1e-5	1.7e-5	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.51935	0.01278	-0.06146
	253.146	4.9363	0.51047	1.2e-3	1.7e-4	5.7e-3	5.7e-3	9.7e-5	2.5e-5	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.51935	0.01278	-0.06146
	253.146	4.9363	0.51047	9.5e-4	1.4e-4	5.9e-3	5.9e-3	6.6e-5	9.7e-6	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.51934	0.01278	-0.06146
V30	253.146	6.9080	0.42662	9.8e-4	2.5e-4	5.7e-3	5.7e-3	1.4e-4	4.5e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.43955	0.01042	-0.02485
	253.146	6.9080	0.42662	1.1e-3	1.1e-4	6.0e-3	6.0e-3	1.6e-4	3.3e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.43955	0.01042	-0.02485
	253.146	6.9080	0.42651	1.2e-3	1.9e-4	6.0e-3	6.0e-3	1.2e-4	2.8e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.43955	0.01042	-0.02485
	253.145	6.9080	0.42650	1.3e-3	2.5e-4	5.9e-3	5.9e-3	1.6e-4	3.9e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.43954	0.01041	-0.02485
	253.146	6.9080	0.42648	1.2e-3	1.5e-4	5.4e-3	5.4e-3	1.1e-4	1.7e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.43955	0.01042	-0.02485
253.146	6.9080	0.42649	1.4e-3	1.3e-4	6.2e-3	6.2e-3	1.0e-4	1.9e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.43954	0.01042	-0.02485	
V31	253.146	8.3057	0.39991	1.2e-3	1.2e-4	5.7e-3	5.7e-3	1.2e-4	2.3e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.41508	0.00950	-0.01100
	253.145	8.3057	0.39991	1.1e-3	2.0e-4	5.8e-3	5.8e-3	1.2e-4	1.2e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.41507	0.00950	-0.01100
	253.146	8.3057	0.39990	8.8e-4	6.4e-5	6.1e-3	6.1e-3	1.5e-4	2.1e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.41507	0.00950	-0.01100
V32	253.146	8.3058	0.39986	1.1e-3	1.6e-4	5.8e-3	5.8e-3	1.6e-4	3.4e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.41507	0.00950	-0.01100
	253.147	9.6222	0.39145	5.6e-4	1.5e-4	5.9e-3	5.9e-3	3.2e-4	8.4e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.40750	0.00900	-0.00069
	253.148	9.6223	0.39124	6.4e-4	8.3e-5	5.7e-3	5.7e-3	2.7e-4	1.1e-4	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.40751	0.00900	-0.00069
	253.148	9.6222	0.39110	4.7e-4	3.8e-5	5.9e-3	5.9e-3	2.5e-4	3.9e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.40750	0.00900	-0.00069
	253.148	9.6222	0.39098	8.9e-4	1.1e-4	5.9e-3	5.9e-3	2.9e-4	1.0e-4	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.40751	0.00900	-0.00069
253.147	9.6223	0.39092	6.5e-4	1.7e-4	5.8e-3	5.8e-3	1.7e-4	3.4e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.40750	0.00900	-0.00069	
253.148	9.6222	0.39092	1.1e-3	3.1e-4	5.8e-3	5.8e-3	2.2e-4	7.3e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.40751	0.00900	-0.00069	
V33	253.148	10.8464	0.39521	5.7e-4	1.5e-4	5.3e-3	5.3e-3	3.3e-4	5.2e-5	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.41264	0.00882	0.00943
	253.148	10.8464	0.39516	1.1e-3	3.1e-4	5.4e-3	5.4e-3	2.1e-4	6.6e-5	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.41264	0.00882	0.00943
	253.148	10.8463	0.39515	6.2e-4	1.7e-4	5.7e-3	5.7e-3	2.6e-4	8.1e-5	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.41264	0.00882	0.00943
V34	253.147	10.8454	0.39516	3.1e-4	2.7e-5	6.0e-3	6.0e-3	1.1e-4	1.5e-5	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.41262	0.00882	0.00942
	253.146	11.8558	0.41082	1.1e-3	1.8e-4	6.0e-3	6.0e-3	3.2e-4	6.7e-5	2.7e-3	2.7e-3	4.8e-4	4.9e-4	0.42773	0.00903	0.02158
	253.146	11.8557	0.41078	1.0e-3	2.0e-4	5.8e-3	5.8e-3	3.9e-4	5.3e-5	2.7e-3	2.7e-3	4.8e-4	4.9e-4	0.42772	0.00903	0.02158
	253.146	11.8557	0.41085	8.0e-4	1.3e-4	5.6e-3	5.6e-3	1.2e-4	1.4e-5	2.7e-3	2.7e-3	4.8e-4	4.9e-4	0.42773	0.00903	0.02158
	253.146	11.8559	0.41080	1.1e-3	1.7e-4	5.6e-3	5.6e-3	2.9e-4	5.0e-5	2.7e-3	2.7e-3	4.8e-4	4.9e-4	0.42773	0.00903	0.02158
253.146	11.8558	0.41079	9.2e-4	2.4e-4	5.9e-3	5.9e-3	2.2e-4	3.9e-5	2.7e-3	2.7e-3	4.8e-4	4.9e-4	0.42773	0.00903	0.02158	
V35	253.146	12.7677	0.44494	5.3e-4	8.7e-5	5.9e-3	5.9e-3	2.9e-4	8.0e-5	2.7e-3	2.7e-3	4.8e-4	5.2e-4 ⁺	0.45666	0.01016	0.06853 ⁺
	253.146	12.7677	0.44495	7.1e-4	6.7e-5	5.8e-3	5.8e-3	2.2e-4	3.2e-5	2.7e-3	2.7e-3	4.8e-4	5.2e-4 ⁺	0.45666	0.01016	0.06853 ⁺
	253.146	12.7677	0.44496	1.1e-3	1.6e-4	5.5e-3	5.5e-3	3.7e-4	5.3e-5	2.7e-3	2.7e-3	4.8e-4	5.2e-4 ⁺	0.45667	0.01016	0.06853 ⁺
V36*	253.145	13.2761	0.50134	9.0e-4	1.7e-4	5.7e-3	5.7e-3	3.3e-4	6.1e-5	2.7e-3	2.7e-3	4.8e-4	8.6e-4 ⁺	0.49107	0.01389	0.25936 ⁺
	253.147	13.2763	0.50133	8.2e-4	1.4e-4	5.7e-3	5.7e-3	2.0e-4	2.5e-5	2.7e-3	2.7e-3	4.8e-4	8.6e-4 ⁺	0.49111	0.01389	0.25974 ⁺
	253.146	13.2762	0.50129	1.1e-3	1.1e-4	6.1e-3	6.1e-3	2.5e-4	3.9e-5	2.7e-3	2.7e-3	4.8e-4	8.6e-4 ⁺	0.49109	0.01389	0.25953 ⁺
V37*	253.147	13.3024	0.51003	6.4e-4	1.0e-4	6.1e-3	6.1e-3	3.2e-4	5.2e-5	2.7e-3	2.7e-3	4.8e-4	1.1e-3 ⁺	0.49401	0.01449	0.36676 ⁺
	253.147	13.3023	0.50991	6.3e-4	1.2e-4	6.1e-3	6.1e-3	2.6e-4	6.5e-5	2.7e-3	2.7e-3	4.8e-4	1.1e-3 ⁺	0.49401	0.01449	0.36640 ⁺
	253.147	13.3023	0.50980	5.4e-4	6.2e-5	5.8e-3	5.8e-3	3.2e-4	6.4e-5	2.7e-3	2.7e-3	4.8e-4	1.1e-3 ⁺	0.49400	0.01449	0.36611 ⁺
	253.147	13.3023	0.50977	6.5e-4	9.5e-5	6.0e-3	6.0e-3	3.2e-4	5.7e-5	2.7e-3	2.7e-3	4.8e-4	1.1e-3 ⁺	0.49401	0.01449	0.36622 ⁺
	V38*	253.147	13.3200	0.51746	7.7e-4	8.3e-5	5.9e-3	5.9e-3	6.4e-4	1.3e-4	2.7e-3	2.7e-3	4.8e-4	1.6e-3 ⁺	0.49613	0.01498
253.147		13.3200	0.51740	7.8e-4	6.8e-5	5.9e-3	5.9e-3	5.4e-4	9.5e-5	2.7e-3	2.7e-3	4.8e-4	1.6e-3 ⁺	0.49612	0.01498	0.56009 ⁺
253.147		13.3200	0.51744	8.5e-4	2.5e-4	5.4e-3	5.4e-3	6.6e-4	1.3e-4	2.7e-3	2.7e-3	4.8e-4	1.6e-3 ⁺	0.49612	0.01498	0.55985 ⁺
253.147		13.3200	0.51741	7.0e-4	8.0e-5	5.8e-3	5.8e-3	5.3e-4	9.0e-5	2.7e-3	2.7e-3	4.8e-4	1.6e-3 ⁺	0.49612	0.01498	0.55978 ⁺
253.147		13.3200	0.51742	6.8e-4	7.3e-5	5.9e-3	5.9e-3	6.4e-4	1.0e-4	2.7e-3	2.7e-3	4.8e-4	1.6e-3 ⁺	0.49612	0.01498	0.56033 ⁺
P4	273.147	3.4848	0.99999	7.2e-4	2.4e-5	1.5e-3	1.5e-3	5.6e-5	9.9e-7	1.1e-3	1.1e-3					
V40	273.145	3.9434	0.91884	1.0e-3	1.3e-4	2.3e-3	2.3e-3	7.1e-5	9.6e-6	1.1e-3	1.1e-3	4.8e-4	5.1e-4	0.92150	0.01688	-0.15393
	273.144	3.9433	0.91876	1.2e-3	1.8e-4	2.2e-3	2.2e-3	1.3e-4	4.6e-5	1.1e-3	1.1e-3	4.8e-4	5.1e-4	0.92150	0.01688	-0.15394
	273.144	3.9434	0.91829	1.5e-3	2.4e-4	2.2e-3	2.2e-3	6.8e-5	1.5e-5	1.1e-3	1.1e-3	4.8e-4	5.1e-4	0.92149	0.01688	-0.15393
	273.144	3.9433	0.91828	1.3e-3	1.8e-4	2.0e-3	2.0e-3	5.1e-5	4.7e-6	1.1e-3	1.1e-3	4.8e-4	5.1e-4	0.92149	0.01688	-0.15393
	273.144	3.9433	0.91824	1.4e-3	1.5e-4	2.6e-3	2.6e-3	6.4e-5	1.9e-5	1.1e-3	1.1e-3	4.8e-4	5.1e-4	0.92150	0.01688	-0.15394
273.144	3.9434	0.91825	9.4e-4	1.1e-4	2.1e-3	2.1e-3	8.8e-5	3.2e-5	1.1e-3	1.1e-3	4.8e-4	5.1e-4	0.92150	0.01688	-0.15393	
V41	273.144	5.0162	0.78639	1.3e-3	3.4e-4	2.4e-3	2.5e-3	1.3e-4	4.2e-5	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.79224	0.01471	-0.09350
	273.144	5.0162	0.78629	1.3e-3	1.3e-4	1.9e-3	1.9e-3	1.9e-4	8.2e-5	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.79224	0.01471	-0.09350

	273.145	5.0161	0.78627	1.0e-3	1.7e-4	1.9e-3	1.9e-3	6.6e-5	6.3e-6	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.79226	0.01471	-0.09351
	273.145	5.0162	0.78619	8.3e-4	1.3e-4	2.3e-3	2.3e-3	1.1e-4	3.0e-5	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.79225	0.01471	-0.09350
	273.145	5.0164	0.78620	9.1e-4	3.1e-4	2.1e-3	2.1e-3	1.8e-4	7.3e-5	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.79224	0.01471	-0.09350
	273.145	5.0160	0.78615	7.2e-4	1.6e-4	2.0e-3	2.0e-3	1.6e-4	4.7e-5	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.79227	0.01471	-0.09351
V42	273.146	5.9256	0.71350	8.1e-4	1.6e-4	2.6e-3	2.6e-3	1.0e-4	3.7e-5	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.72173	0.01340	-0.06380
	273.146	5.9255	0.71347	7.7e-4	1.1e-4	2.7e-3	2.7e-3	1.9e-4	6.7e-5	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.72173	0.01340	-0.06380
	273.146	5.9256	0.71345	4.9e-4	8.3e-5	2.5e-3	2.5e-3	9.3e-5	1.1e-5	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.72173	0.01340	-0.06379
	273.146	5.9256	0.71344	8.1e-4	2.2e-4	2.5e-3	2.5e-3	1.1e-4	3.4e-5	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.72172	0.01340	-0.06379
	273.146	5.9255	0.71343	6.7e-4	8.6e-5	2.1e-3	2.1e-3	9.6e-5	2.5e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.72174	0.01340	-0.06380
V43	273.146	6.9260	0.65908	5.8e-4	7.9e-5	2.2e-3	2.2e-3	1.1e-4	3.0e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.66945	0.01236	-0.04209
	273.146	6.9258	0.65903	5.6e-4	9.4e-5	2.2e-3	2.2e-3	3.2e-4	1.1e-4	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.66946	0.01236	-0.04209
	273.146	6.9260	0.65901	4.8e-4	4.5e-5	2.4e-3	2.4e-3	2.1e-4	8.9e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.66944	0.01236	-0.04208
	273.146	6.9259	0.65903	6.7e-4	7.1e-5	2.0e-3	2.0e-3	1.3e-4	4.2e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.66946	0.01236	-0.04209
	273.146	6.9257	0.65904	5.3e-4	5.1e-5	2.3e-3	2.3e-3	2.5e-4	8.3e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.66946	0.01236	-0.04209
V44	273.145	7.9107	0.62381	9.5e-4	2.7e-4	2.8e-3	2.8e-3	2.5e-4	5.8e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.63597	0.01165	-0.02656
	273.147	7.9107	0.62380	1.1e-3	3.5e-4	2.0e-3	2.1e-3	3.5e-4	8.7e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.63598	0.01165	-0.02656
	273.146	7.9106	0.62376	7.8e-4	1.2e-4	2.3e-3	2.3e-3	3.2e-4	7.0e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.63598	0.01165	-0.02657
	273.146	7.9106	0.62375	8.2e-4	2.5e-4	2.4e-3	2.4e-3	1.4e-4	3.8e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.63597	0.01165	-0.02657
	273.147	7.9109	0.62376	7.1e-4	8.0e-5	2.0e-3	2.0e-3	2.5e-4	9.6e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.63597	0.01165	-0.02656
V45	273.147	8.8895	0.60277	8.4e-4	1.3e-4	2.3e-3	2.3e-3	4.1e-4	8.4e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.61637	0.01123	-0.01370
	273.146	8.8898	0.60274	8.1e-4	2.8e-4	2.4e-3	2.5e-3	4.3e-4	6.6e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.61636	0.01123	-0.01370
	273.147	8.8896	0.60273	4.0e-4	5.2e-5	2.0e-3	2.0e-3	3.9e-4	5.0e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.61637	0.01123	-0.01370
	273.146	8.8894	0.60277	7.6e-4	2.9e-4	2.3e-3	2.3e-3	3.1e-4	6.1e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.61637	0.01123	-0.01370
V46	273.146	9.8539	0.59504	6.7e-4	4.7e-5	2.7e-3	2.7e-3	2.4e-4	7.9e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.60925	0.01118	-0.00068
	273.147	9.8539	0.59501	7.2e-4	1.2e-4	2.2e-3	2.2e-3	2.5e-4	4.3e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.60926	0.01118	-0.00068
	273.147	9.8539	0.59503	9.7e-4	2.9e-4	2.3e-3	2.4e-3	3.3e-4	4.4e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.60926	0.01118	-0.00068
	273.146	9.8538	0.59504	5.8e-4	6.7e-5	2.5e-3	2.5e-3	3.3e-4	6.3e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.60925	0.01118	-0.00069
	273.146	9.8539	0.59503	5.2e-4	3.7e-5	2.8e-3	2.8e-3	2.7e-4	9.4e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.60925	0.01118	-0.00068
	273.146	9.8539	0.59501	9.4e-4	1.6e-4	2.5e-3	2.5e-3	1.7e-4	3.6e-5	1.4e-3	1.4e-3	4.8e-4	4.8e-4	0.60925	0.01118	-0.00068
V47	273.146	10.8864	0.60682	6.3e-4	6.5e-5	2.8e-3	2.8e-3	2.8e-4	4.5e-5	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.61856	0.01222	0.02203
	273.147	10.8864	0.60684	5.5e-4	4.8e-5	2.5e-3	2.5e-3	1.9e-4	2.6e-5	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.61857	0.01222	0.02203
	273.147	10.8865	0.60686	1.1e-3	3.4e-4	2.4e-3	2.4e-3	3.4e-4	6.8e-5	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.61857	0.01222	0.02203
	273.146	10.8865	0.60683	8.5e-4	1.4e-4	3.0e-3	3.0e-3	2.2e-4	4.1e-5	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.61856	0.01222	0.02203
	273.146	10.8865	0.60685	8.8e-4	2.8e-4	2.8e-3	2.8e-3	2.7e-4	5.6e-5	2.7e-3	2.7e-3	4.8e-4	4.8e-4	0.61856	0.01222	0.02203
V48	273.146	11.3312	0.62771	6.2e-4	1.0e-4	2.6e-3	2.6e-3	2.5e-4	3.6e-5	2.7e-3	2.7e-3	4.8e-4	5.3e-4+	0.63335	0.01451	0.08798+
	273.147	11.3313	0.62763	5.5e-4	7.3e-5	2.4e-3	2.4e-3	2.9e-4	4.6e-5	2.7e-3	2.7e-3	4.8e-4	5.3e-4+	0.63336	0.01451	0.08799+
	273.146	11.3312	0.62768	6.8e-4	2.0e-4	2.3e-3	2.3e-3	2.9e-4	4.1e-5	2.7e-3	2.7e-3	4.8e-4	5.3e-4+	0.63335	0.01451	0.08798+
	273.146	11.3312	0.62760	5.3e-4	6.0e-5	2.3e-3	2.3e-3	2.7e-4	4.5e-5	2.7e-3	2.7e-3	4.8e-4	5.3e-4+	0.63335	0.01451	0.08798+
	273.146	11.3313	0.62757	5.6e-4	3.7e-5	2.5e-3	2.5e-3	2.8e-4	5.1e-5	2.7e-3	2.7e-3	4.8e-4	5.3e-4+	0.63335	0.01451	0.08799+
V49*	273.145	11.5578	0.66099	8.3e-4	1.2e-4	2.1e-3	2.1e-3	1.8e-4	4.5e-5	2.7e-3	2.7e-3	4.8e-4	1.1e-3+	0.64900	0.01974	0.36702+
	273.145	11.5579	0.66096	7.4e-4	7.1e-5	3.0e-3	3.0e-3	1.7e-4	2.4e-5	2.7e-3	2.7e-3	4.8e-4	1.1e-3+	0.64901	0.01974	0.36757+
	273.145	11.5578	0.66093	6.3e-4	9.9e-5	2.8e-3	2.8e-3	1.3e-4	1.9e-5	2.7e-3	2.7e-3	4.8e-4	1.1e-3+	0.64900	0.01973	0.36684+
V50*	273.146	11.5780	0.67303	6.5e-4	1.6e-4	2.5e-3	2.5e-3	2.3e-4	5.3e-5	2.7e-3	2.7e-3	4.8e-4	3.0e-3+	0.65120	0.02098	1.12607+
	273.146	11.5780	0.67294	6.9e-4	1.2e-4	2.1e-3	2.1e-3	2.0e-4	2.8e-5	2.7e-3	2.7e-3	4.8e-4	3.0e-3+	0.65119	0.02098	1.12668+
	273.145	11.5780	0.67271	6.1e-4	9.1e-5	2.4e-3	2.4e-3	2.4e-4	3.8e-5	2.7e-3	2.7e-3	4.8e-4	3.1e-3+	0.65119	0.02098	1.13799+
	273.146	11.5780	0.67255	4.5e-4	6.2e-5	2.4e-3	2.4e-3	2.2e-4	4.6e-5	2.7e-3	2.7e-3	4.8e-4	3.1e-3+	0.65119	0.02098	1.12707+
	273.145	11.5780	0.67255	1.0e-3	1.0e-4	2.7e-3	2.7e-3	1.9e-4	3.7e-5	2.7e-3	2.7e-3	4.8e-4	3.1e-3+	0.65119	0.02098	1.13580+
P5	288.139	5.0859	0.99999	6.9e-4	2.8e-4	1.8e-3	1.8e-3	5.7e-5	2.9e-6	1.1e-3	1.1e-3					
V52	288.138	5.6498	0.94180	8.1e-4	1.6e-4	1.6e-3	1.6e-3	6.9e-5	3.0e-6	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.94518	0.01309	-0.08892
	288.135	5.6498	0.94168	1.1e-3	3.1e-4	1.5e-3	1.5e-3	6.5e-5	3.1e-6	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.94514	0.01309	-0.08891
	288.139	5.6498	0.94167	2.0e-3	4.5e-4	1.7e-3	1.8e-3	8.5e-5	7.4e-6	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.94519	0.01309	-0.08892
	288.140	5.6498	0.94166	1.6e-3	3.1e-4	1.7e-3	1.8e-3	7.3e-5	6.9e-6	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.94519	0.01309	-0.08892
	288.136	5.6498	0.94163	6.0e-4	1.1e-4	1.7e-3	1.7e-3	7.1e-5	6.0e-6	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.94515	0.01309	-0.08892
	288.135	5.6498	0.94163	6.6e-4	1.2e-4	1.7e-3	1.7e-3	6.6e-5	5.9e-6	1.1e-3	1.1e-3	4.8e-4	4.9e-4	0.94513	0.01309	-0.08891

V53	288.143	7.0494	0.84287	3.7e-4	5.0e-5	1.8e-3	1.8e-3	1.1e-4	7.3e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.84963	0.01209	-0.05068
	288.142	7.0493	0.84275	3.7e-4	3.7e-5	1.8e-3	1.8e-3	8.7e-5	1.3e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.84963	0.01209	-0.05068
	288.142	7.0493	0.84271	3.9e-4	6.9e-5	1.9e-3	1.9e-3	9.2e-5	5.9e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.84963	0.01209	-0.05068
	288.142	7.0493	0.84268	4.0e-4	4.2e-5	1.8e-3	1.8e-3	1.3e-4	7.2e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.84963	0.01209	-0.05068
V54	288.142	7.0493	0.84267	3.4e-4	5.5e-5	1.9e-3	1.9e-3	1.0e-4	8.6e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.84963	0.01209	-0.05068
	288.134	8.4289	0.79087	6.2e-4	6.3e-5	1.6e-3	1.6e-3	1.6e-4	1.0e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.79910	0.01177	-0.02272
	288.142	8.4288	0.79084	4.1e-4	2.4e-5	1.9e-3	1.9e-3	4.7e-4	4.4e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.79920	0.01177	-0.02272
	288.142	8.4289	0.79082	2.8e-4	4.2e-5	1.9e-3	1.9e-3	1.7e-4	8.7e-6	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.79920	0.01177	-0.02272
	288.142	8.4289	0.79081	4.2e-4	4.5e-5	1.9e-3	1.9e-3	1.4e-4	1.8e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.79920	0.01177	-0.02272
	288.142	8.4289	0.79075	2.6e-4	4.1e-5	1.9e-3	1.9e-3	1.1e-4	1.3e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.79920	0.01177	-0.02272
V55	288.142	8.4289	0.79072	3.0e-4	3.4e-5	1.8e-3	1.8e-3	1.3e-4	6.5e-6	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.79920	0.01177	-0.02272
	288.136	8.8666	0.78344	4.5e-4	5.0e-5	1.7e-3	1.7e-3	1.7e-4	1.3e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.79131	0.01201	-0.01263
	288.138	8.8666	0.78345	6.2e-4	2.5e-4	1.8e-3	1.8e-3	1.5e-4	1.2e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.79134	0.01201	-0.01262
	288.138	8.8667	0.78344	1.1e-3	4.2e-4	1.8e-3	1.8e-3	1.9e-4	1.7e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.79133	0.01201	-0.01263
	288.138	8.8666	0.78345	9.5e-4	2.3e-4	1.8e-3	1.8e-3	1.6e-4	2.4e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.79133	0.01201	-0.01260
V56	288.136	8.8665	0.78344	9.7e-4	3.0e-4	1.7e-3	1.7e-3	1.2e-4	6.9e-6	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.79131	0.01201	-0.01261
	288.138	9.2573	0.78233	1.1e-3	4.1e-4	1.8e-3	1.8e-3	1.3e-4	3.3e-6	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.78869	0.01271	0.00527
	288.139	9.2574	0.78233	6.4e-4	2.1e-4	1.7e-3	1.7e-3	1.3e-4	6.4e-6	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.78871	0.01272	0.00012
	288.139	9.2573	0.78234	7.7e-4	1.7e-4	1.7e-3	1.7e-3	1.5e-4	1.6e-5	1.3e-3	1.3e-3	4.8e-4	4.8e-4	0.78870	0.01271	0.00308
V57	288.136	9.5784	0.78942	5.6e-4	7.2e-5	1.8e-3	1.8e-3	1.5e-4	1.2e-5	1.4e-3	1.4e-3	4.8e-4	4.9e-4+	0.79157	0.01465	0.05484+
	288.137	9.5783	0.78943	9.8e-4	3.4e-4	1.7e-3	1.7e-3	1.5e-4	1.7e-6	1.4e-3	1.4e-3	4.8e-4	4.9e-4+	0.79158	0.01465	0.05484+
	288.138	9.5783	0.78942	1.5e-3	3.2e-4	1.6e-3	1.7e-3	1.3e-4	1.4e-5	1.4e-3	1.4e-3	4.8e-4	4.9e-4+	0.79159	0.01465	0.05483+
	288.139	9.5784	0.78942	1.2e-3	2.8e-4	1.7e-3	1.7e-3	1.3e-4	1.5e-5	1.4e-3	1.4e-3	4.8e-4	4.9e-4+	0.79161	0.01465	0.05485+
	288.137	9.5784	0.78942	5.5e-4	4.6e-5	1.7e-3	1.7e-3	1.5e-4	1.2e-5	1.4e-3	1.4e-3	4.8e-4	4.9e-4+	0.79159	0.01465	0.05484+
V58	288.141	9.7065	0.79946	3.7e-4	3.9e-5	1.8e-3	1.8e-3	1.7e-4	1.1e-5	1.4e-3	1.4e-3	4.8e-4	5.1e-4+	0.79558	0.01713	0.12831+
	288.141	9.7065	0.79944	4.0e-4	6.1e-5	1.7e-3	1.7e-3	1.1e-4	1.3e-5	1.4e-3	1.4e-3	4.8e-4	5.1e-4+	0.79557	0.01713	0.12832+
	288.141	9.7065	0.79943	3.2e-4	3.3e-5	1.6e-3	1.6e-3	1.4e-4	1.3e-5	1.4e-3	1.4e-3	4.8e-4	5.1e-4+	0.79557	0.01713	0.12831+
	288.141	9.7066	0.79942	4.2e-4	2.1e-5	1.7e-3	1.7e-3	1.7e-4	1.6e-5	1.4e-3	1.4e-3	4.8e-4	5.1e-4+	0.79558	0.01713	0.12845+
V59	288.139	9.7232	0.80208	2.3e-3	1.0e-3	1.9e-3	2.2e-3	2.2e-4	3.1e-5	1.4e-3	1.4e-3	4.8e-4	5.3e-4+	0.79630	0.01771	0.16625+
	288.141	9.7232	0.80210	2.2e-4	4.1e-5	1.8e-3	1.8e-3	1.9e-4	1.2e-5	1.4e-3	1.4e-3	4.8e-4	5.3e-4+	0.79634	0.01772	0.16623+
	288.141	9.7232	0.80207	2.3e-4	3.3e-5	1.8e-3	1.8e-3	1.8e-4	1.6e-5	1.4e-3	1.4e-3	4.8e-4	5.3e-4+	0.79634	0.01772	0.16629+
	288.141	9.7232	0.80206	2.3e-4	2.2e-5	1.8e-3	1.8e-3	1.4e-4	9.4e-6	1.4e-3	1.4e-3	4.8e-4	5.3e-4+	0.79634	0.01772	0.16618+
	288.142	9.7232	0.80205	2.2e-4	2.3e-5	1.9e-3	1.9e-3	1.6e-4	1.2e-5	1.4e-3	1.4e-3	4.8e-4	5.3e-4+	0.79634	0.01772	0.16611+
V60	288.142	9.7447	0.80691	2.2e-4	2.6e-5	1.9e-3	1.9e-3	1.4e-4	7.9e-6	1.4e-3	1.4e-3	4.8e-4	6.4e-4+	0.79746	0.01869	0.30671+
	288.142	9.7447	0.80684	4.2e-4	3.8e-5	1.8e-3	1.8e-3	1.2e-4	5.8e-6	1.4e-3	1.4e-3	4.8e-4	6.4e-4+	0.79746	0.01869	0.30679+
	288.142	9.7447	0.80662	3.1e-4	5.1e-5	1.9e-3	1.9e-3	1.1e-4	6.0e-6	1.4e-3	1.4e-3	4.8e-4	6.4e-4+	0.79746	0.01869	0.30692+
	288.142	9.7447	0.80660	3.1e-4	2.2e-5	1.8e-3	1.8e-3	1.2e-4	5.1e-6	1.4e-3	1.4e-3	4.8e-4	6.4e-4+	0.79746	0.01869	0.30695+
P6	298.137	6.4328	0.99999	7.5e-4	1.1e-4	3.0e-3	3.0e-3	9.4e-5	8.6e-6	1.1e-3	1.1e-3					
V61	298.141	7.1110	0.95630	4.3e-4	6.0e-5	3.3e-3	3.3e-3	8.6e-5	8.5e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.95967	0.01018	-0.05191
	298.141	7.1110	0.95625	4.0e-4	3.3e-5	3.2e-3	3.2e-3	7.5e-5	4.3e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.95967	0.01018	-0.05191
	298.141	7.1110	0.95622	3.6e-4	7.8e-5	3.1e-3	3.1e-3	9.9e-5	1.6e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.95967	0.01018	-0.05191
	298.141	7.1110	0.95622	1.5e-4	7.1e-6	3.4e-3	3.4e-3	9.4e-5	1.2e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.95967	0.01018	-0.05191
	298.141	7.1110	0.95623	3.2e-4	2.0e-5	3.2e-3	3.2e-3	1.0e-4	1.0e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.95967	0.01018	-0.05191
	298.140	7.1110	0.95622	3.0e-4	3.1e-5	3.1e-3	3.1e-3	8.1e-5	6.1e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.95967	0.01018	-0.05191
V62	298.134	7.4191	0.94072	5.1e-4	4.5e-5	3.1e-3	3.1e-3	9.6e-5	8.2e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94482	0.01024	-0.04399
	298.134	7.4191	0.94071	5.0e-4	5.5e-5	3.0e-3	3.0e-3	8.7e-5	8.6e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94482	0.01024	-0.04399
	298.134	7.4191	0.94071	5.5e-4	1.2e-4	3.1e-3	3.2e-3	1.0e-4	1.1e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94482	0.01024	-0.04399
	298.138	7.4191	0.94073	1.6e-3	5.0e-4	3.2e-3	3.3e-3	1.1e-4	1.2e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94486	0.01024	-0.04399
	298.137	7.4191	0.94073	6.5e-4	1.9e-4	3.2e-3	3.2e-3	1.1e-4	1.1e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94485	0.01024	-0.04399
V63	298.136	7.4191	0.94072	4.7e-4	3.6e-5	3.2e-3	3.2e-3	8.6e-5	5.6e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.94484	0.01024	-0.04399
	298.134	7.8396	0.92471	7.6e-4	1.6e-4	3.0e-3	3.0e-3	1.1e-4	9.2e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.92880	0.01057	-0.03163
	298.134	7.8394	0.92468	6.3e-4	1.7e-4	3.0e-3	3.0e-3	1.3e-4	1.7e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.92881	0.01057	-0.03163
	298.139	7.8393	0.92465	2.5e-3	1.1e-3	3.1e-3	3.3e-3	1.3e-4	3.8e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.92887	0.01057	-0.03163
	298.141	7.8392	0.92464	2.2e-3	8.8e-4	3.2e-3	3.3e-3	3.7e-4	1.5e-4	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.92889	0.01057	-0.03163

	298.141	7.8390	0.92465	2.5e-4	3.6e-5	3.1e-3	3.1e-3	1.4e-4	1.9e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.92889	0.01057	-0.03164
	298.141	7.8387	0.92467	2.1e-4	3.6e-5	3.1e-3	3.1e-3	1.0e-4	1.1e-5	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.92890	0.01057	-0.03165
V64	298.140	8.0258	0.91981	2.5e-4	5.0e-5	3.3e-3	3.3e-3	1.1e-4	9.0e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.92365	0.01097	-0.02411
	298.140	8.0258	0.91979	2.2e-4	2.3e-5	3.3e-3	3.3e-3	1.1e-4	6.3e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.92365	0.01097	-0.02411
	298.140	8.0258	0.91977	2.4e-4	6.2e-5	3.4e-3	3.4e-3	1.0e-4	6.5e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.92365	0.01097	-0.02411
	298.140	8.0258	0.91977	2.2e-4	2.2e-5	3.4e-3	3.4e-3	1.1e-4	5.3e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.92365	0.01097	-0.02411
	298.140	8.0258	0.91976	3.0e-4	2.0e-5	3.3e-3	3.3e-3	1.1e-4	9.9e-6	1.1e-3	1.1e-3	4.8e-4	4.8e-4	0.92364	0.01097	-0.02411
V65	298.134	8.1339	0.91821	7.2e-4	1.1e-4	3.1e-3	3.1e-3	1.2e-4	1.4e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.92128	0.01144	-0.01802
	298.136	8.1339	0.91818	1.3e-3	5.5e-4	2.9e-3	2.9e-3	1.3e-4	2.3e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.92130	0.01144	-0.01801
	298.134	8.1339	0.91818	5.6e-4	8.4e-5	2.9e-3	2.9e-3	1.4e-4	1.4e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.92128	0.01144	-0.01802
	298.134	8.1339	0.91816	8.3e-4	3.3e-4	3.1e-3	3.1e-3	1.3e-4	1.7e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.92128	0.01144	-0.01802
	298.135	8.1339	0.91815	5.3e-4	1.1e-4	3.2e-3	3.2e-3	1.2e-4	1.0e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4	0.92129	0.01144	-0.01802
V66	298.134	8.2648	0.91898	9.6e-4	1.8e-4	3.2e-3	3.2e-3	1.2e-4	1.8e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4 ⁺	0.91965	0.01276	0.03529 ⁺
	298.136	8.2648	0.91898	5.7e-4	5.2e-5	3.2e-3	3.2e-3	1.3e-4	1.8e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4 ⁺	0.91967	0.01276	0.03530 ⁺
	298.137	8.2648	0.91898	5.6e-4	7.2e-5	3.0e-3	3.0e-3	1.0e-4	1.7e-5	1.2e-3	1.2e-3	4.8e-4	4.8e-4 ⁺	0.91968	0.01276	0.03529 ⁺
V67	298.136	8.3019	0.92107	3.8e-4	5.9e-5	3.2e-3	3.2e-3	1.1e-4	2.2e-5	1.2e-3	1.2e-3	4.8e-4	4.9e-4 ⁺	0.91959	0.01358	0.09541 ⁺
	298.137	8.3019	0.92108	5.5e-4	6.5e-5	3.2e-3	3.2e-3	1.6e-4	2.7e-5	1.2e-3	1.2e-3	4.8e-4	4.9e-4 ⁺	0.91961	0.01359	0.09540 ⁺
	298.138	8.3019	0.92110	1.2e-3	5.0e-4	3.1e-3	3.2e-3	1.8e-4	1.2e-5	1.2e-3	1.2e-3	4.8e-4	4.9e-4 ⁺	0.91962	0.01359	0.09535 ⁺
	298.136	8.3020	0.92109	1.3e-3	5.7e-4	3.2e-3	3.3e-3	1.2e-4	2.0e-5	1.2e-3	1.2e-3	4.8e-4	4.9e-4 ⁺	0.91959	0.01358	0.09552 ⁺
V68	298.135	8.3180	0.92391	6.3e-4	1.5e-4	3.1e-3	3.1e-3	1.0e-4	8.5e-6	1.2e-3	1.2e-3	4.8e-4	6.9e-4 ⁺	0.91964	0.01410	0.41623 ⁺
	298.134	8.3180	0.92389	6.2e-4	9.8e-5	3.0e-3	3.0e-3	9.5e-5	8.2e-6	1.2e-3	1.2e-3	4.8e-4	6.8e-4 ⁺	0.91963	0.01410	0.41573 ⁺
	298.134	8.3180	0.92391	6.1e-4	1.1e-4	3.0e-3	3.0e-3	1.2e-4	8.8e-6	1.2e-3	1.2e-3	4.8e-4	6.9e-4 ⁺	0.91962	0.01410	0.41580 ⁺
	298.134	8.3180	0.92389	7.6e-4	2.6e-4	3.0e-3	3.0e-3	1.0e-4	9.1e-6	1.2e-3	1.2e-3	4.8e-4	6.9e-4 ⁺	0.91963	0.01410	0.41859 ⁺
	298.138	8.3180	0.92389	2.7e-3	1.2e-3	3.2e-3	3.4e-3	1.2e-4	1.2e-5	1.2e-3	1.2e-3	4.8e-4	6.9e-4 ⁺	0.91967	0.01412	0.41944 ⁺
	298.140	8.3180	0.92384	2.5e-4	3.5e-5	3.3e-3	3.3e-3	1.1e-4	9.2e-6	1.2e-3	1.2e-3	4.8e-4	6.9e-4 ⁺	0.91971	0.01413	0.41870 ⁺

Table A.4

Composition data at supercritical states for the liquid and vapor Rolsi™ samplers for CO₂ + O₂ at mean temperature \bar{T} , mean pressure \bar{p} , and sample mole fraction z_{CO_2} .

ID	Data			Temperature				Pressure				Composition
	\bar{T} (K)	\bar{p} (MPa)	z_{CO_2} (-)	$s(T)$ (K)	$s(\bar{T})$ (K)	$\bar{u}(T)$ (K)	$u_c(\bar{T})$ (K)	$s(p)$ (MPa)	$s(\bar{p})$ (MPa)	$\bar{u}(p)$ (MPa)	$u_c(\bar{p})$ (MPa)	$u(z_{\text{CO}_2})$ (-)
L12	218.149	14.4390	0.39451	5.6e-4	7.1e-5	3.4e-3	3.4e-3	2.0e-4	9.7e-6	2.8e-3	2.8e-3	4.8e-4
	218.148	14.4390	0.39451	8.8e-4	1.0e-4	3.3e-3	3.3e-3	1.9e-4	1.4e-5	2.8e-3	2.8e-3	4.8e-4
	218.148	14.4390	0.39449	1.1e-3	1.6e-4	3.3e-3	3.3e-3	2.3e-4	1.7e-5	2.8e-3	2.8e-3	4.8e-4
	218.147	14.4390	0.39451	8.1e-4	1.3e-4	3.4e-3	3.4e-3	1.7e-4	1.5e-5	2.8e-3	2.8e-3	4.8e-4
V13	218.148	14.4390	0.39449	6.8e-4	9.7e-5	3.4e-3	3.5e-3	2.3e-4	3.2e-5	2.8e-3	2.8e-3	4.8e-4
	218.147	14.4390	0.39474	1.5e-3	2.9e-4	3.4e-3	3.4e-3	1.4e-4	1.3e-5	2.8e-3	2.8e-3	4.8e-4
	218.147	14.4390	0.39473	9.6e-4	1.1e-4	3.5e-3	3.5e-3	1.6e-4	8.7e-6	2.8e-3	2.8e-3	4.8e-4
	218.147	14.4390	0.39472	1.3e-3	1.3e-4	3.5e-3	3.5e-3	1.6e-4	1.9e-5	2.8e-3	2.8e-3	4.8e-4
L26	218.147	14.4390	0.39471	8.7e-4	8.9e-5	3.4e-3	3.4e-3	1.3e-4	9.4e-6	2.8e-3	2.8e-3	4.8e-4
	218.147	14.4390	0.39469	9.9e-4	1.7e-4	3.3e-3	3.3e-3	1.4e-4	8.8e-6	2.8e-3	2.8e-3	4.8e-4
	233.142	14.2617	0.44462	6.4e-4	1.7e-4	7.3e-3	7.3e-3	2.0e-4	9.3e-6	2.8e-3	2.8e-3	4.8e-4
	233.142	14.2617	0.44464	6.4e-4	9.2e-5	7.0e-3	7.0e-3	2.1e-4	1.4e-5	2.8e-3	2.8e-3	4.8e-4
V27	233.144	14.2617	0.44464	1.4e-3	5.3e-4	7.7e-3	7.7e-3	2.1e-4	2.1e-5	2.8e-3	2.8e-3	4.8e-4
	233.142	14.2617	0.44469	9.7e-4	3.3e-4	7.7e-3	7.7e-3	1.8e-4	1.5e-5	2.8e-3	2.8e-3	4.8e-4
	233.142	14.2618	0.44466	4.5e-4	6.9e-5	7.5e-3	7.5e-3	1.8e-4	1.2e-5	2.8e-3	2.8e-3	4.8e-4
	233.142	14.2617	0.44468	6.7e-4	8.1e-5	7.2e-3	7.2e-3	1.3e-4	9.4e-6	2.8e-3	2.8e-3	4.8e-4
L38	233.142	14.2618	0.44442	4.9e-4	7.1e-5	7.6e-3	7.6e-3	2.0e-4	2.3e-5	2.8e-3	2.8e-3	4.8e-4
	233.142	14.2617	0.44444	6.3e-4	5.8e-5	7.3e-3	7.3e-3	1.4e-4	9.6e-6	2.8e-3	2.8e-3	4.8e-4
	233.142	14.2618	0.44446	6.4e-4	1.4e-4	7.6e-3	7.6e-3	1.7e-4	1.1e-5	2.8e-3	2.8e-3	4.8e-4
	233.142	14.2617	0.44447	4.9e-4	5.1e-5	7.5e-3	7.5e-3	1.9e-4	1.3e-5	2.8e-3	2.8e-3	4.8e-4
V39	233.142	14.2617	0.44446	3.8e-4	3.2e-5	7.4e-3	7.4e-3	1.3e-4	1.7e-5	2.8e-3	2.8e-3	4.8e-4
	253.147	13.3559	0.55473	5.7e-4	6.2e-5	5.8e-3	5.8e-3	3.0e-4	4.6e-5	2.7e-3	2.7e-3	4.8e-4
	253.147	13.3560	0.55471	6.0e-4	8.6e-5	6.1e-3	6.1e-3	2.6e-4	6.9e-5	2.7e-3	2.7e-3	4.8e-4
	253.147	13.3561	0.55470	8.1e-4	2.2e-4	5.7e-3	5.7e-3	4.1e-4	8.9e-5	2.7e-3	2.7e-3	4.8e-4
L49	253.147	13.3560	0.55465	6.4e-4	1.2e-4	6.0e-3	6.0e-3	2.3e-4	3.1e-5	2.7e-3	2.7e-3	4.8e-4
	253.147	13.3560	0.55465	7.3e-4	1.4e-4	5.8e-3	5.8e-3	1.9e-4	2.1e-5	2.7e-3	2.7e-3	4.8e-4
	253.148	13.3561	0.55473	6.8e-4	7.1e-5	5.7e-3	5.7e-3	2.7e-4	5.6e-5	2.7e-3	2.7e-3	4.8e-4
	253.147	13.3559	0.55469	6.6e-4	1.1e-4	5.8e-3	5.8e-3	2.7e-4	4.7e-5	2.7e-3	2.7e-3	4.8e-4
V51	253.147	13.3564	0.55469	6.7e-4	1.9e-4	5.4e-3	5.4e-3	1.5e-4	3.6e-5	2.7e-3	2.7e-3	4.8e-4
	273.144	11.5979	0.68190	1.0e-3	2.1e-4	3.0e-3	3.0e-3	1.9e-4	6.7e-5	2.7e-3	2.7e-3	4.8e-4
	273.146	11.5975	0.68187	7.2e-4	1.2e-4	2.9e-3	2.9e-3	1.4e-4	2.5e-5	2.7e-3	2.7e-3	4.8e-4
	273.146	11.5975	0.68186	5.5e-4	7.4e-5	2.4e-3	2.4e-3	2.1e-4	3.6e-5	2.7e-3	2.7e-3	4.8e-4
L49	273.146	11.5974	0.68195	6.6e-4	9.8e-5	2.5e-3	2.5e-3	3.5e-4	6.9e-5	2.7e-3	2.7e-3	4.8e-4
	273.145	11.5975	0.68195	8.0e-4	1.3e-4	2.1e-3	2.2e-3	1.9e-4	3.0e-5	2.7e-3	2.7e-3	4.8e-4
	273.144	11.5974	0.68220	6.4e-4	6.0e-5	2.9e-3	2.9e-3	2.6e-4	3.9e-5	2.7e-3	2.7e-3	4.8e-4
	273.144	11.5975	0.68220	9.4e-4	6.6e-5	2.6e-3	2.6e-3	1.9e-4	3.7e-5	2.7e-3	2.7e-3	4.8e-4
	273.144	11.5975	0.68218	8.9e-4	1.9e-4	2.3e-3	2.3e-3	1.8e-4	4.0e-5	2.7e-3	2.7e-3	4.8e-4
	273.145	11.5975	0.68219	1.1e-3	2.8e-4	2.3e-3	2.3e-3	2.2e-4	3.9e-5	2.7e-3	2.7e-3	4.8e-4
L49	273.144	11.5975	0.68217	6.6e-4	4.0e-5	2.6e-3	2.6e-3	1.8e-4	4.8e-5	2.7e-3	2.7e-3	4.8e-4
	273.145	11.5975	0.68218	9.8e-4	1.1e-4	2.4e-3	2.5e-3	1.6e-4	5.2e-5	2.7e-3	2.7e-3	4.8e-4

^a Samples taken using liquid sampler given with ID L, samples taken using vapor sampler given with ID V

Appendix B. Additional plots

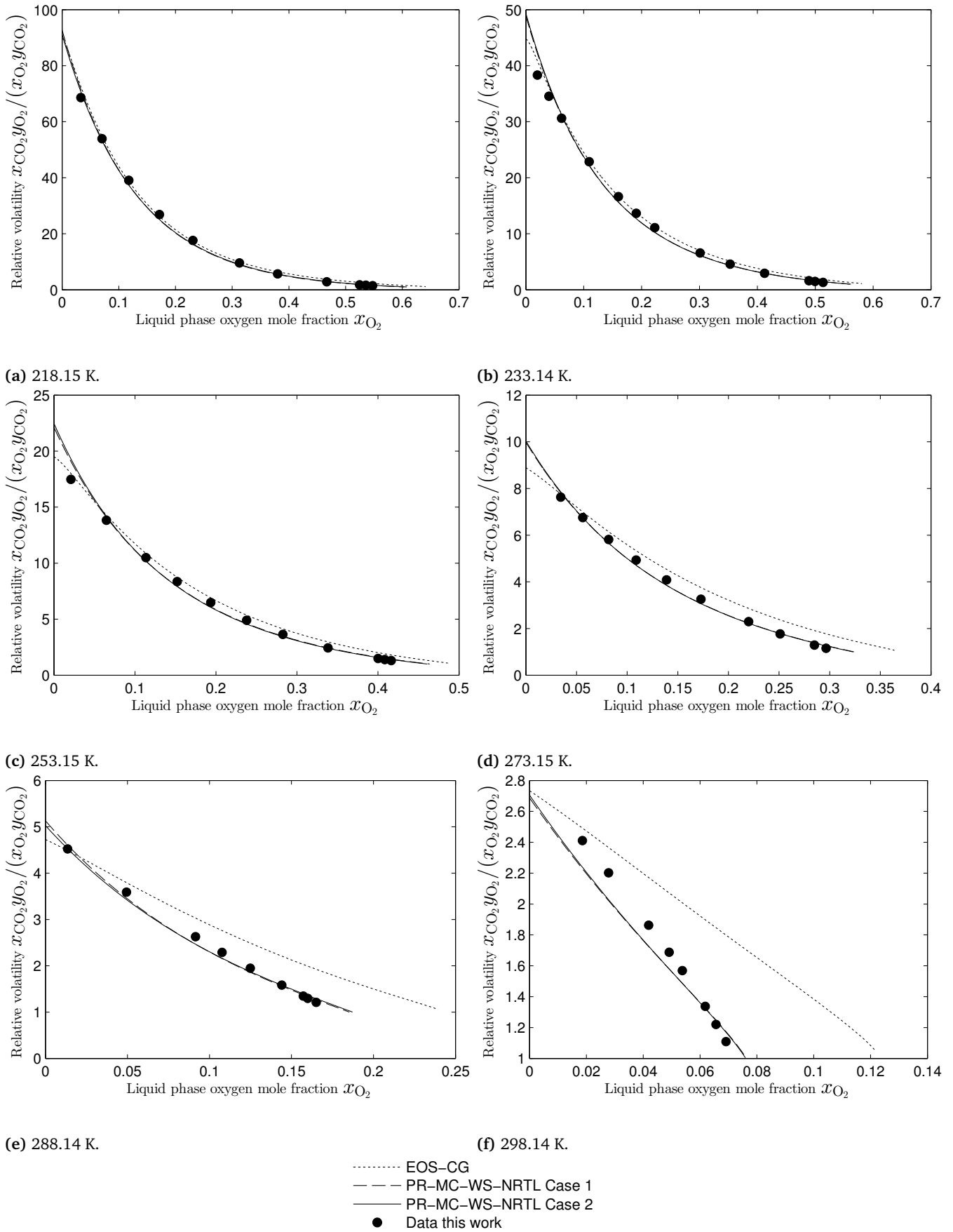


Fig. B.1. Measured relative volatilities compared with different models.

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