Supporting Information

# "Specific Solvation Interactions of $CO_2$ on Acetate and Trifluoroacetate Imidazolium Based Ionic Liquids at High Pressures"

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## Results and Discussion

The results of the application of the thermodynamic consistency test to the binary systems containing ionic liquid is presented in Table 1. In this Table, *NP* is the number of data points, *T* is the temperature, $k_{12}$, $\alpha_{12}$, $g_{12}$-$g_{22}$ and $g_{21}$-$g_{11}$ are the interaction parameters of the model, where *1* stands for the $CO_2$ and *2* for the ionic liquid. This Table is divided in sections for each system studied. The $CO_2$ + [$C_4$mim][Ac] system determined by Shifflet et al.[1] was also investigated.

## Thermodynamic Modeling and Consistency

Valderrama and Álvarez[2] developed a thermodynamic consistency test for systems with incomplete *PTxy* data, cataloging them as thermodynamic consistent (TC), thermodynamic inconsistent (TI) or not full consistent (NFC). The authors analyzed the difficulties normally found when modeling this type of mixtures and proposed a methodology to analyze the experimental data, concluding about their thermodynamic consistency or inconsistency. Recently, Álvarez and Aznar[3,4] applied an extension of this approach to several supercritical fluid + IL systems using a method based on the Gibbs-Duhem equation, on the fundamental phase equilibrium equation, and on the Peng-Robinson equation of state [5], with the Wong-Sandler mixing rule[6] using the UNIQUAC model[7] for the activity coefficient. The NRTL (three adjustable parameters) and UNIQUAC (two adjustable parameters) models produce similar fit results, nonetheless the NRTL model is preferable when the data present a statistical quirk, caused by inaccurate measurements, as shown in Álvarez and Aznar publication.[3] Therefore, the NRTL model was selected in the present work.

Similar to Van Ness-Byer-Gibbs test modeling procedure[8], a thermodynamic model is used to accurately fit the experimental data and thereafter, apply the consistency test. The experimental data fit requires the calculation of several model parameters, using an optimized objective function. Although

the consistency test is model dependent, good fitting does not guarantee that the data are consistent, since the proposed area test, consequent from the Gibbs–Duhem equation, must also be fulfilled.

As described previously[9], the test uses the Gibbs-Duhem equation expressed in the integral form, where the left-hand side is denoted as $AP$ and the right-hand side as $A\phi$, as it follows:

$$A_p = \int \frac{1}{Py_2} dp \tag{1}$$

$$A_\varphi = \int \frac{(1-y_2)}{y_2(Z-1)} \frac{d\varphi_1}{\varphi_1} + \int \frac{1}{(Z-1)} \frac{d\varphi_2}{\varphi_2} \tag{2}$$

The values for $A_P$ are obtained with experimental $Py_2$ data, and the values for $A_\phi$ are obtained with calculated values of $Z$, $\phi_i$ and $y_2$. The subscripts 1 and 2 denote $CO_2$ and ionic liquid compounds, respectively. The individual percent area deviation, $\%\Delta A_i$, is given as:

$$\% \Delta A_i = 100\left[ (A_\varphi - A_P)/A_P \right]_i \tag{3}$$

where the subscript $i$ refer to the $i^{th}$ data point. The quality of the correlation was analyzed through the relative deviations in the calculated pressure in the gas phase for each point $i$, defined as:

$$\% \Delta p_i = 100\,(p_i^{cal} - p_i^{\exp})/p_i^{\exp} \tag{4}$$

The method implies the minimization of the deviations of Eqs. 3 and 4 setting as the objective function, $OF$, for the consistency test the minimization of the deviations in VLE data and the individual percent area deviation.

$$OF = \sum_{i=1}^{N-1} \left[ \frac{A_P - A_\varphi}{\sigma_A} \right]_i^2 + \sum_{i=1}^{N} \left[ \frac{p^{cal} - p^{\exp}}{\sigma_P} \right]_i^2 + \sum_{i=1}^{N} \left[ \frac{y_{fluid}^{cal} - 1}{\sigma_y} \right]_i^2 \tag{5}$$

where $N$ is the number of data points, $p$ is the pressure, $y_{fluid}$ is the vapor mole fraction of the supercritical fluid for data point $i$, the superscripts "exp" and "cal" refers to the experimental and calculated values respectively, and $\sigma_A$, $\sigma_P$ and $\sigma_y$ are the standard deviations of those quantities. The experimental uncertainties in the pressure data were used for $\sigma_P$, the value $10^{-4}$ for $\sigma_y$ and the value of

$A_P$ for $\sigma_A$. The minimization method was performed using a genetic algorithm code, implemented and fully explained in Alvarez et al..[10] The difference between experimental and calculated values was calculated as the average percent deviation, expressed in absolute form, as follows:

$$\%|\Delta p| = \frac{100}{N}\sum_{i=1}^{N}\left[|p_i^{cal} - p_i^{\exp}|/p_i^{\exp}\right] \quad (6)$$

The data set is considered consistent when the individual area deviation, $\%\Delta A_i$, is within acceptable defined deviations. The difference between experimental and calculated individual area is calculated as the average percent deviation, expressed in absolute form, as follows:

$$\%|\Delta A| = \frac{100}{N}\left[|A_\varphi - A_P|/A_P\right] \quad (7)$$

The isopleths, for the $CO_2$ + [$C_4$mim][Ac] system and for the $CO_2$+ [$C_4$mim][TFA] system, were interpolated with the method proposed by Álvarez and Aznar[4] and the results are reported in supporting information.

The isopleths were interpolated with the method proposed by Álvarez and Aznar[4] and the results are shown in Table 2, for the $CO_2$ + [$C_4$mim][Ac] system and for the $CO_2$+ [$C_4$mim][TFA] system, respectively.

Detailed results are shown in Tables 3 through 6. The tables are divided in two parts, the upper part shows the original data set, while the lower part shows the remaining data after removing some experimental points, that have been found to be thermodynamically inconsistent. Tables 3 and 5, show detailed results for the $CO_2$ + [$C_4$mim][Ac] systems at 323.1 and 348.1 K from Shifflet et al..[1] In Table 3 some data present deviations out the established limit for *%ΔAi* (bold and italic type). Nonetheless, deviations within the established limits are obtained by eliminating those points.

The data for the $CO_2$ + [C4mim][Ac] system at 348.1 K from Shifflet et al.[1] presented in Table 5 presents deviations out the established limit for the values of *%Δpi* and thereafter, the test could not be applied. In addition, the data from this work, at the same temperature, was correlated with confidence,

showing that the present data are more reliable. In Table 6, detailed results for the system $CO_2$ + [$C_4$mim][Ac] at 348 K show that, for the upper part, some data have deviations outside the established limits, in the final values of $\%\Delta A_i$ (bold and italic type), while for the lower part, when two points from the original data set are eliminated (the two with the highest area deviation, highlighted in the upper part), the deviations for the remaining eight points are within the defined limits of −20% to +20%. Therefore, while the original set with nine data points is not fully consistent the new set with the remaining eight points is thermodynamically consistent.

The same procedure is applied for the data in Table 7 where detailed results for the system $CO_2$ + [$C_4$mim][TFA] at 298 K are presented. The original data are not fully consistent, but after removing one data point, the remaining eight points are within the defined limits of −20% to +20%, which are thermodynamically consistent.

The results obtained for the $CO_2$ + [$C_4$mim][Ac] system denote greater deviations for the $x_1$>0.5 isopleths, while the system $CO_2$ + [$C_4$mim][TFA] present greater deviations for the $x_1$>0.65 isopleths leading to not fully consistent isotherms.

## Literature Cited


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**Table 1.** Results of the consistency test for all the experimental data.

| Reference | NP | $T$ /K | $k_{ij}$ | $\alpha_{12}$ | $g_{12}$-$g_{22}$ kJ /kmol | $g_{21}$-$g_{11}$ kJ/kmol | $\lvert\Delta p\rvert$ % | $\lvert\Delta A\rvert$ % | Result |
|---|---|---|---|---|---|---|---|---|---|
| $CO_2$ + [$C_4$mim][Ac] | | | | | | | | | |
| [1] | 5 | 283.10 | 1.0000 | 0.2000 | -11249.9893 | -1933.5936 | 25.3 | 19.7 | - |
| | 9 | 298.10 | -0.3274 | 0.2341 | -28123.0098 | 6021.4521 | 12.2 | 13.8 | NFC |
| | 9 | 323.10 | 1.0000 | 0.3171 | -11198.7109 | 3059.0808 | 10.4 | 14.6 | NFC |
| | 9 | 348.10 | 1.0000 | 0.3531 | -9138.5596 | 24552.2227 | 14.1 | 17.2 | - |
| [This work] | 6 | 313.10 | -0.3284 | 0.2397 | -40690.6016 | 17402.3555 | 1.6 | 19.7 | NFC |
| | 9 | 323.09 | -0.3667 | 0.2469 | -50782.2500 | -1592.4650 | 1.5 | 23.5 | NFC |
| | 8 | 333.00 | -0.4688 | 0.2635 | -50449.5625 | -1625.9657 | 1.0 | 13.1 | NFC |
| | 8 | 343.00 | -0.4912 | 0.2876 | -49008.6250 | -1777.7466 | 1.5 | 15.2 | NFC |
| | 8 | 348.00 | 0.5083 | 0.3660 | -39224.0273 | -3483.0093 | 6.3 | 17.8 | NFC |
| | 8 | 352.98 | -0.6875 | 0.2017 | -88945.3125 | -5754.0894 | 1.9 | 15.7 | NFC |
| $CO_2$ + [$C_4$mim][TFA] | | | | | | | | | |
| [This work] | 7 | 294.00 | 0.2188 | 0.2002 | 33310.5703 | -3054.2261 | 3.2 | 11.1 | NFC |
| | 7 | 298.00 | 0.2188 | 0.2000 | 34271.8711 | -2903.0513 | 3.1 | 14.6 | NFC |
| | 7 | 303.00 | 0.2188 | 0.2000 | 35683.6055 | -2633.8701 | 3.1 | 19.0 | NFC |
| | 7 | 313.00 | 0.2192 | 0.2000 | 37582.4805 | -2372.4836 | 3.5 | 30.8 | NFC |
| | 7 | 323.00 | 0.2120 | 0.2000 | 39737.5508 | -2080.5359 | 3.7 | 90.1 | NFC |
| | 6 | 333.00 | 0.9596 | 0.2462 | 89950.1328 | 52675.3438 | 16.5 | 11.5 | NFC |
| | 6 | 343.00 | 0.2020 | 0.2018 | 42681.1992 | -1757.8231 | 5.6 | 47.4 | NFC |
| | 6 | 348.00 | 0.1959 | 0.2001 | 44655.1328 | -1552.4625 | 5.5 | 57.8 | NFC |
| | 6 | 353.00 | 0.1973 | 0.2018 | 44912.1094 | -1494.4839 | 5.6 | 71.6 | NFC |
| | 6 | 363.00 | 0.1759 | 0.2036 | 45757.1133 | -1367.4760 | 9.9 | 10.2 | NFC |

**Table 2.** Interpolated VLE data for the system supercritical $CO_2$ (1) + [$C_4$mim][Ac] (2) and $CO_2$ (1) + [$C_4$mim][TFA] (2).

| $CO_2$ (1) + [$C_4$mim][Ac] (2) | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| $x_1$ T(K) | 0.201 | 0.251 | 0.300 | 0.351 | 0.402 | 0.450 | 0.500 | 0.55 | 0.6 |
| 313.10 | - | 0.496 | 1.403 | 2.593 | 4.108 | 5.731 | - | - | 67.371 |
| 323.09 | 0.228 | 0.845 | 1.908 | 3.383 | 5.213 | 7.403 | 13.515 | 34.649 | 75.526 |
| 333.00 | 0.380 | 1.245 | 2.502 | 4.247 | 6.509 | 9.527 | 18.058 | 41.557 | - |
| 343.00 | 0.617 | 1.705 | 3.195 | 5.243 | 8.038 | 12.142 | 22.900 | 47.955 | - |
| 348.00 | 0.779 | 1.956 | 3.576 | 5.799 | 8.892 | 13.627 | 25.417 | 50.946 | - |
| 352.98 | 0.975 | 2.220 | 3.980 | 6.400 | 9.806 | 15.224 | 27.988 | 53.863 | - |

| $CO_2$ (1) + [$C_4$mim][TFA] (2) | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| $x_1$ $T$ /K | 0.225 | 0.300 | 0.401 | 0.502 | 0.601 | 0.650 | 0.679 | |
| 294.00 | 1.001 | 1.579 | 2.445 | 3.527 | 8.239 | 27.010 | 44.006 | |
| 298.00 | 1.139 | 1.771 | 2.723 | 3.956 | 10.406 | 29.326 | 46.545 | |
| 303.00 | 1.321 | 2.025 | 3.100 | 4.538 | 13.151 | 32.175 | 49.717 | |
| 313.00 | 1.709 | 2.586 | 3.940 | 5.856 | 18.452 | 37.715 | 56.063 | |
| 323.00 | 2.131 | 3.216 | 4.881 | 7.382 | 22.733 | 43.047 | 62.409 | |
| 333.00 | 2.588 | 3.915 | 5.906 | 9.117 | 28.216 | 48.169 | - | |
| 343.00 | 3.080 | 4.682 | 6.999 | 11.057 | 32.537 | 53.083 | - | |
| 348.00 | 3.338 | 5.092 | 7.566 | 12.102 | 34.400 | 55.462 | - | |
| 353.00 | 3.606 | 5.519 | 8.143 | 13.195 | 36.498 | 57.788 | - | |
| 363.00 | 4.166 | 6.425 | 9.320 | 15.521 | 42.004 | 62.284 | - | |

**Table 3.** Detailed results for $CO_2$ + [$C_4$mim][Ac] at 323.1 K from [1].

| $A_p \cdot 10^7$ | $A_\phi \cdot 10^7$ | $\%\Delta A_i$ | $p^{exp}$ | $p^{cal}$ | $\%\Delta p$ | $y_1^{cal}$ | $y_2^{cal}$ | $x_1$ |
|---|---|---|---|---|---|---|---|---|
| (9 data points) $k_{ij}$ = 1.0000, $\alpha_{12}$ = 0.3171, ($g_{12}$-$g_{22}$) = -11198.7109, ($g_{21}$-$g_{11}$) = 3059.0808, \|ΔP\| (%) = 10.4 | | | | | | | | |
| 0.0593 | 0.0957 | ***61.50*** | ***0.010*** | ***0.003*** | ***-69.16*** | ***0.9999803*** | ***0.0000197*** | ***0.108*** |
| 0.146 | 0.172 | 17.40 | 0.050 | 0.050 | -0.01 | 0.9999992 | 0.0000008 | 0.176 |
| 1.22 | 1.16 | -5.00 | 0.100 | 0.113 | 12.71 | 0.9999997 | 0.0000003 | 0.204 |
| 1.54 | 1.38 | -10.10 | 0.400 | 0.420 | 5.23 | 0.9999999 | 0.0000001 | 0.263 |
| 1.78 | 1.75 | -1.91 | 0.700 | 0.697 | -0.48 | 1.0000000 | 0.0000000 | 0.292 |
| 2.07 | 2.07 | 0.10 | 1.000 | 0.987 | -1.27 | 1.0000000 | 0.0000000 | 0.315 |
| 1.54 | 1.68 | 8.72 | 1.300 | 1.284 | -1.25 | 1.0000000 | 0.0000000 | 0.334 |
| 4.56 | 5.13 | ***12.50*** | 1.500 | 1.499 | -0.01 | 1.0000000 | 0.0000000 | 0.346 |
| - | - | - | ***1.999*** | ***2.074*** | ***3.75*** | ***1.0000000*** | ***0.0000000*** | ***0.373*** |
| (7 data points) $k_{ij}$ = 1.0000, $\alpha_{12}$ = 0.3244, ($g_{12}$-$g_{22}$) = -11206.7412, ($g_{21}$-$g_{11}$) = 2763.3943, \|ΔP\| (%) =3.4 | | | | | | | | |
| 0.144 | 0.172 | 20.00 | 0.050 | 0.047 | -6.28 | 0.9999992 | 0.0000008 | 0.176 |
| 1.23 | 1.19 | -3.17 | 0.100 | 0.108 | 7.63 | 0.9999997 | 0.0000003 | 0.204 |
| 1.58 | 1.44 | -8.80 | 0.400 | 0.411 | 2.99 | 0.9999999 | 0.0000001 | 0.263 |
| 1.85 | 1.83 | -0.69 | 0.700 | 0.687 | -1.89 | 1.0000000 | 0.0000000 | 0.292 |
| 2.16 | 2.18 | 1.19 | 1.000 | 0.978 | -2.24 | 1.0000000 | 0.0000000 | 0.315 |
| 1.61 | 1.77 | 9.80 | 1.300 | 1.275 | -1.94 | 1.0000000 | 0.0000000 | 0.334 |
| - | - | - | 1.500 | 1.491 | -0.56 | 1.0000000 | 0.0000000 | 0.346 |

**Table 4.** Detailed results for $CO_2$ + [$C_4$mim][Ac] at 323.09 K from this work.

| Ap | Aϕ | %ΔAi | $p^{exp}$ | $p^{cal}$ | %ΔP | $y_1^{cal}$ | $y_2^{cal}$ | $x_1$ |
|---|---|---|---|---|---|---|---|---|
| (9 data points) kij = 1.0000, α12 = 0.3171, (g12-g22) = -11198.7109, (g21-g11) = 3059.0808, \|ΔP\| (%) = 10.4 | | | | | | | | |
| 6.81E+13 | 6.87E+13 | 0.95 | 0.228 | 0.233 | 2.14 | 1.000000 | 0.0000000 | 0.201 |
| 7.48E+13 | 7.15E+13 | -4.35 | 0.845 | 0.873 | 3.31 | 1.000000 | 0.0000000 | 0.251 |
| 4.01E+13 | 3.96E+13 | -1.25 | 1.908 | 1.920 | 0.61 | 1.000000 | 0.0000000 | 0.300 |
| 1.09E+13 | 1.11E+13 | 2.16 | 3.383 | 3.401 | 0.54 | 1.000000 | 0.0000000 | 0.351 |
| 1.30E+12 | 1.42E+12 | 8.64 | 5.213 | 5.316 | 1.97 | 1.000000 | 0.0000000 | 0.402 |
| 7.09E+10 | 6.11E+10 | -13.80 | 7.403 | 7.793 | 5.27 | 1.000000 | 0.0000000 | 0.450 |
| 9.10E+05 | 3.41E+05 | ***-62.60*** | 13.515 | 14.234 | 5.32 | 0.999999 | 0.0000009 | 0.500 |
| 6.21E+03 | 6.21E+03 | 0.00 | ***34.649*** | ***32.819*** | ***-5.28*** | ***0.999897*** | ***0.0001027*** | ***0.550*** |
| - | - | - | ***75.526*** | ***66.592*** | ***-11.83*** | ***0.999418*** | ***0.0005825*** | ***0.599*** |
| (7 data points) $k_{ij}$ = -0.8433, $\alpha_{12}$ = 0.2261, ($g_{12}$-$g_{22}$) = -55755.3516, ($g_{21}$-$g_{11}$) = -552.6208, \|ΔP\| (%) = 4.0 | | | | | | | | |
| 2.97E+14 | 3.15E+14 | 6.20 | 0.228 | 0.223 | -2.14 | 1.0000000 | 0.0000000 | 0.201 |
| 2.57E+14 | 2.51E+14 | -2.55 | 0.845 | 0.882 | 4.37 | 1.0000000 | 0.0000000 | 0.251 |
| 8.45E+13 | 8.28E+13 | -2.02 | 1.908 | 1.969 | 3.20 | 1.0000000 | 0.0000000 | 0.300 |
| 1.14E+13 | 1.13E+13 | -1.47 | 3.383 | 3.482 | 2.93 | 1.0000000 | 0.0000000 | 0.351 |
| 5.61E+11 | 5.71E+11 | 1.77 | 5.213 | 5.374 | 3.09 | 1.0000000 | 0.0000000 | 0.402 |
| 9.56E+09 | 8.77E+09 | -8.28 | 7.403 | 7.717 | 4.24 | 1.0000000 | 0.0000000 | 0.450 |
| - | - | - | 13.515 | 14.605 | 8.06 | 0.9998809 | 0.0001191 | 0.500 |

**Table 5.** Detailed results for $CO_2$ + [$C_4$mim][Ac] at 348.1 K from [1].

| $A_p$ | $A_\phi$ | $\%\Delta A_i$ | $p^{exp}$ | $p^{cal}$ | $\%\Delta P$ | $y_1^{cal}$ | $y_2^{cal}$ | $x_1$ |
|---|---|---|---|---|---|---|---|---|
| (9 data points) $k_{ij}$ = 1.0000, $\alpha_{12}$ = 0.3531, ($g_{12}$-$g_{22}$) = -9138.5596, ($g_{21}$-$g_{11}$) = 24552.2227, \|ΔP\| (%) = 14.2 | | | | | | | | |
| | | | 0.0104 | 0.0097 | -6.69 | 0.9999002 | 0.0000998 | 0.063 |
| | | | 0.0505 | 0.0555 | 9.98 | 0.9999855 | 0.0000145 | 0.129 |
| | | | 0.1 | 0.1185 | 18.50 | 0.9999941 | 0.0000059 | 0.161 |
| | | | 0.4002 | 0.4206 | 5.10 | 0.9999988 | 0.0000012 | 0.226 |
| | | | 0.6994 | 0.6489 | -7.21 | 0.9999993 | 0.0000007 | 0.253 |
| | | | 1.0003 | 0.8572 | -14.30 | 0.9999995 | 0.0000005 | 0.272 |
| | | | 1.2994 | 1.0532 | -18.95 | 0.9999996 | 0.0000004 | 0.287 |
| | | | 1.4997 | 1.1549 | -22.99 | 0.9999997 | 0.0000003 | 0.294 |
| | | | 1.9993 | 1.5237 | -23.79 | 0.9999998 | 0.0000002 | 0.316 |

**Table 6.** Detailed results for $CO_2$ + [$C_4$mim][Ac] at 348.0 K from this work.

| $A_p$ | $A_\phi$ | $\%\Delta A_i$ | $p^{exp}$ | $p^{cal}$ | $\%\Delta P$ | $y_1^{cal}$ | $y_2^{cal}$ | $x_1$ |
|---|---|---|---|---|---|---|---|---|
| (8 data points) $k_{ij}$ = 0.5083, $\alpha_{12}$= 0.3660, ($g_{12}$-$g_{22}$) = -39224.0273, ($g_{21}$-$g_{11}$) = -3483.0093, \|ΔP\|(%) = 6.3 | | | | | | | | |
| 1.59E+11 | 1.58E+11 | -1.08 | 0.779 | 0.779 | 0.00 | 1.0000000 | 0.0000000 | 0.201 |
| 1.86E+11 | 1.86E+11 | -0.11 | 1.956 | 1.939 | -0.89 | 1.0000000 | 0.0000000 | 0.251 |
| 1.70E+11 | 1.72E+11 | 1.03 | 3.576 | 3.547 | -0.81 | 1.0000000 | 0.0000000 | 0.300 |
| 1.05E+11 | 1.06E+11 | 0.14 | 5.799 | 5.800 | 0.01 | 1.0000000 | 0.0000000 | 0.351 |
| 3.47E+10 | 3.20E+10 | -7.81 | 8.893 | 8.983 | 1.02 | 1.0000000 | 0.0000000 | 0.402 |
| 2.97E+09 | 1.54E+09 | ***-48.10*** | 13.627 | 13.804 | 1.30 | 1.0000000 | 0.0000000 | 0.450 |
| 2.52E+07 | 8.47E+06 | ***-66.30*** | ***25.417*** | ***22.318*** | ***-12.19*** | ***1.0000000*** | ***0.0000000*** | ***0.500*** |
| - | - | - | ***50.946*** | ***33.341*** | ***-34.56*** | ***0.9999991*** | ***0.0000009*** | ***0.550*** |
| (6 data points) $k_{ij}$ = 0.7969, $\alpha_{12}$= 0.4229, ($g_{12}$-$g_{22}$) = -32920.5625, ($g_{21}$-$g_{11}$) = -3534.8833, \|ΔP\|(%) = 1.2 | | | | | | | | |
| 2.76E+10 | 2.68E+10 | -2.81 | 0.779 | 0.789 | 1.29 | 1.0000000 | 0.0000000 | 0.201 |
| 4.10E+10 | 4.08E+10 | -0.61 | 1.956 | 1.930 | -1.33 | 1.0000000 | 0.0000000 | 0.251 |
| 5.34E+10 | 5.44E+10 | 1.89 | 3.576 | 3.515 | -1.72 | 1.0000000 | 0.0000000 | 0.300 |
| 5.26E+10 | 5.40E+10 | 2.49 | 5.799 | 5.754 | -0.77 | 1.0000000 | 0.0000000 | 0.351 |
| 3.03E+10 | 2.85E+10 | -5.94 | 8.893 | 8.955 | 0.70 | 1.0000000 | 0.0000000 | 0.402 |
| - | - | - | 13.627 | 13.800 | 1.27 | 1.0000000 | 0.0000000 | 0.450 |

**Table 7.** Detailed results for $CO_2$ + [$C_4$mim][TFA] at 298 K from this work.

| $A_p$ | $A_\phi$ | $\%\Delta A_i$ | $p^{exp}$ | $p^{cal}$ | $\%\Delta P$ | $y_1^{cal}$ | $y_2^{cal}$ | $x_1$ |
|---|---|---|---|---|---|---|---|---|
| (7 data points) $k_{ij}$ = 0.2188, $\alpha_{12}$ = 0.2000, ($g_{12}$-$g_{22}$) = 34271.8711, ($g_{21}$-$g_{11}$) = -2903.0513, \|ΔP\| (%) = 3.1 | | | | | | | | |
| 3.08E+07 | 3.03E+07 | -1.52 | 1.140 | 1.112 | -2.4 | 1.0000000 | 0.0000000 | 0.225 |
| 2.94E+07 | 3.40E+07 | 15.6 | 1.771 | 1.718 | -3.0 | 1.0000000 | 0.0000000 | 0.300 |
| 1.72E+07 | 2.07E+07 | 20.6 | 2.723 | 2.814 | 3.3 | 1.0000000 | 0.0000000 | 0.401 |
| 2.11E+07 | 1.84E+07 | -12.8 | ***3.956*** | ***4.386*** | ***10.9*** | ***1.0000000*** | ***0.0000000*** | ***0.502*** |
| 2.20E+04 | 2.42E+04 | 10.3 | 10.406 | 10.274 | -1.3 | 0.9999431 | 0.0000569 | 0.601 |
| 9.81E+03 | 1.24E+04 | ***26.5*** | 29.326 | 29.156 | -0.6 | 0.9999461 | 0.0000539 | 0.650 |
| - | - | - | ***46.545*** | ***46.501*** | ***-0.1*** | ***0.9999577*** | ***0.0000423*** | ***0.679*** |
| (5 data points) $k_{ij}$ = 0.2236, $\alpha_{12}$ = 0.2059, ($g_{12}$-$g_{22}$) = 34037.5859, ($g_{21}$-$g_{11}$) = -2354.5664, \|ΔP\| (%) = 6.2 | | | | | | | | |
| 3.04E+07 | 2.87E+07 | -5.55 | 1.140 | 1.226 | 7.58 | 1.0000000 | 0.0000000 | 0.225 |
| 2.76E+07 | 3.04E+07 | 10.10 | 1.771 | 1.862 | 5.18 | 1.0000000 | 0.0000000 | 0.300 |
| 7.39E+07 | 7.18E+07 | -2.93 | 2.723 | 2.985 | 9.61 | 1.0000000 | 0.0000000 | 0.401 |
| 2.30E+04 | 2.29E+04 | -0.35 | 10.406 | 11.321 | 8.79 | 0.9999449 | 0.0000551 | 0.601 |
| - | - | - | 29.326 | 29.329 | 0.01 | 0.9999501 | 0.0000499 | 0.650 |