Extremely Low Vapor-Pressure Data as Access to PC-SAFT Parameter Estimation for Ionic Liquids and Modeling of Precursor Solubility in Ionic Liquids

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Table 51 The results of the temperature dependences of the frequency shift velocities $\Delta f/\Delta t$ and absolute vapor pressures $p_{sat}$ measured by the QCM for $[\text{C}m\text{im}]\text{[Anion]}$ and vaporization enthalpies $\Delta_{vap}^{\text{i}}H_m(T)$ derived from these data.\textsuperscript{a}

| Run | $T$ [K] | $\Delta f/\Delta t$ [Hz·s$^{-1}$] | $10^6 p_{sat}$ [Pa]$^c$ | $\text{T}^1$ [K]$^1$ | $R\cdot\ln(p_{sat}/p^o)$ | $\Delta_{vap}^{\text{i}}H_m(T)$ [kJ·mol$^{-1}$] |
|-----|--------|-------------------------------|-------------------|------------------|------------------|-----------------------------|
| 1   | 402.38 | 0.5565                        | 224               | 0.002485         | -165.6           | 119.4                      |
|     | 397.01 | 0.3460                        | 138               | 0.002519         | -169.6           | 119.7                      |
|     | 391.99 | 0.2175                        | 86                | 0.002551         | -173.5           | 120.1                      |
|     | 387.05 | 0.1368                        | 54                | 0.002584         | -177.4           | 120.4                      |
|     | 382.08 | 0.08485                       | 33                | 0.002617         | -181.5           | 120.7                      |
|     | 377.08 | 0.05128                       | 20                | 0.002652         | -185.7           | 121.1                      |
|     | 372.13 | 0.03085                       | 12                | 0.002687         | -190.0           | 121.4                      |
|     | 366.93 | 0.01789                       | 6.9               | 0.002725         | -194.6           | 121.7                      |
|     | 361.15 | 0.009668                      | 3.7               | 0.002769         | -199.7           | 122.1                      |
| 2   | 404.80 | 0.6923                        | 279               | 0.002470         | -163.8           | 119.2                      |
|     | 399.51 | 0.4326                        | 174               | 0.002503         | -167.7           | 119.5                      |
|     | 394.52 | 0.2751                        | 110               | 0.002535         | -171.5           | 119.9                      |
|     | 389.54 | 0.17339                       | 69                | 0.002567         | -175.4           | 120.2                      |
|     | 384.56 | 0.10793                       | 42                | 0.002600         | -179.4           | 120.6                      |
|     | 379.56 | 0.06557                       | 26                | 0.002635         | -183.6           | 120.9                      |
|     | 374.37 | 0.03894                       | 15                | 0.002671         | -188.0           | 121.2                      |
|     | 369.11 | 0.02260                       | 8.7               | 0.002709         | -192.6           | 121.6                      |
| 2 (1.088) | 429.36 | 0.4524                        | 175               | 0.002329         | -167.6           | 125.3                      |
|     | 424.38 | 0.3014                        | 116               | 0.002356         | -171.1           | 125.6                      |
|     | 419.40 | 0.2002                        | 76                | 0.002384         | -174.5           | 125.9                      |
|     | 414.42 | 0.1317                        | 50                | 0.002413         | -178.1           | 126.3                      |
|     | 409.43 | 0.08422                       | 32                | 0.002442         | -181.8           | 126.6                      |
|     | 404.43 | 0.05364                       | 20                | 0.002473         | -185.6           | 126.9                      |
|     | 399.44 | 0.03339                       | 12                | 0.002504         | -189.6           | 127.3                      |
|     | 394.45 | 0.02050                       | 7.6               | 0.002535         | -193.7           | 127.6                      |
|     | 431.88 | 0.5462                        | 211               | 0.002315         | -166.0           | 125.1                      |
|     | 426.92 | 0.3745                        | 144               | 0.002342         | -169.2           | 125.4                      |

\[\ln(p_{sat}/p^o) = - \frac{60184}{RT_0} - \frac{120594}{R} \frac{1}{T - T_0} - \frac{63}{R} \frac{T_0}{T - 1 - \ln \left( \frac{T}{T_0} \right)}, \ T_0 = 383.9 \text{ K}\]

\[\ln(p_{sat}/p^o) = - \frac{740841}{RT_0} - \frac{126379}{R} \frac{1}{T - T_0} - \frac{68}{R} \frac{T_0}{T - 1 - \ln \left( \frac{T}{T_0} \right)}, \ T_0 = 412.8 \text{ K}\]
\[ \ln(p_{\text{sat}}/p^\circ) = -\frac{75179}{RT_0} - \frac{133033}{R} \left( \frac{T}{T_0} - 1 \right) - \frac{68}{R} \left( \frac{T}{T_0} - 1 - \ln \left( \frac{T}{T_0} \right) \right) \] 
\[ T_0 = 422.3 \text{ K} \]

| Temperature (°C) | Pressure (atm) | Molarity (mol/L) | Conductivity (mS/cm) |
|------------------|----------------|------------------|----------------------|
| 421.93           | 0.2536         | 97               | 0.002370             |
| 416.94           | 0.1641         | 62               | 0.002398             |
| 411.95           | 0.1054         | 40               | 0.002427             |
| 406.96           | 0.06650        | 25               | 0.002457             |
| 401.56           | 0.04089        | 15               | 0.002490             |
| 396.36           | 0.02462        | 9.1              | 0.002523             |

\[ [\text{Cmim}][\text{CH}_3\text{SO}_3]\]
\[
\ln(p_{sat}^*/p_o) = -\frac{76440}{RT_0} - \frac{122267}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right) - \frac{62}{R} \left(\frac{T_0}{T} - 1 - \ln \left(\frac{T}{T_0}\right)\right), \quad T_0 = 431.6 \text{ K}
\]

|   |   |   |   |   |
|---|---|---|---|---|
| 1 |   |   |   |   |
| 454.31 | 0.6126 | 284 | 0.002201 | -163.6 | 120.9 |
| 449.35 | 0.4321 | 201 | 0.002225 | -166.5 | 121.2 |
| 444.32 | 0.2991 | 140 | 0.002251 | -169.5 | 121.5 |
| 439.34 | 0.2066 | 97 | 0.002276 | -172.5 | 121.8 |
| 434.35 | 0.1390 | 67 | 0.002302 | -175.7 | 122.1 |
| 429.35 | 0.0891 | 44 | 0.002329 | -179.1 | 122.4 |
| 424.38 | 0.0557 | 29 | 0.002356 | -182.5 | 122.7 |
| 419.38 | 0.0336 | 20 | 0.002384 | -185.9 | 123.0 |
| 414.38 | 0.0191 | 13 | 0.002413 | -189.2 | 123.3 |

\[
\ln(p_{sat}^*/p_o) = -\frac{78196}{RT_0} - \frac{129904}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right) - \frac{74}{R} \left(\frac{T_0}{T} - 1 - \ln \left(\frac{T}{T_0}\right)\right), \quad T_0 = 435.2 \text{ K}
\]

|   |   |   |   |   |
|---|---|---|---|---|
| 2 |   |   |   |   |
| 451.88 | 0.5682 | 245 | 0.002213 | -164.9 | 121.0 |
| 441.86 | 0.2748 | 117 | 0.002263 | -171.0 | 121.6 |
| 431.89 | 0.1288 | 54 | 0.002315 | -177.4 | 122.2 |
| 426.89 | 0.0887 | 37 | 0.002343 | -180.5 | 122.6 |
| 421.89 | 0.0582 | 24 | 0.002370 | -184.1 | 122.9 |
| 416.89 | 0.0385 | 16 | 0.002399 | -187.6 | 123.2 |
| 411.89 | 0.0242 | 10 | 0.002428 | -191.5 | 123.5 |

\[
\ln(p_{sat}^*/p_o) = -\frac{78196}{RT_0} - \frac{129904}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right) - \frac{74}{R} \left(\frac{T_0}{T} - 1 - \ln \left(\frac{T}{T_0}\right)\right), \quad T_0 = 435.2 \text{ K}
\]

|   |   |   |   |   |
|---|---|---|---|---|
| 1 |   |   |   |   |
| 456.79 | 0.5574 | 224 | 0.002189 | -165.6 | 128.3 |
| 451.80 | 0.3823 | 153 | 0.002213 | -168.8 | 128.7 |
| 446.81 | 0.2640 | 105 | 0.002238 | -171.9 | 129.0 |
| 441.84 | 0.1798 | 71 | 0.002263 | -175.2 | 129.4 |
| 436.82 | 0.1200 | 47 | 0.002289 | -178.6 | 129.8 |
| 431.85 | 0.08051 | 31 | 0.002316 | -181.9 | 130.2 |
| 426.85 | 0.05213 | 20 | 0.002343 | -185.6 | 130.5 |
| 421.85 | 0.03391 | 13 | 0.002370 | -189.2 | 130.9 |
| 416.85 | 0.02170 | 8.3 | 0.002399 | -193.0 | 131.3 |

\[
\ln(p_{sat}^*/p_o) = -\frac{745196}{RT_0} - \frac{129904}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right) - \frac{74}{R} \left(\frac{T_0}{T} - 1 - \ln \left(\frac{T}{T_0}\right)\right), \quad T_0 = 435.2 \text{ K}
\]

|   |   |   |   |   |
|---|---|---|---|---|
| 2 |   |   |   |   |
| 454.34 | 0.4635 | 185 | 0.002201 | -167.2 | 128.5 |
| 450.31 | 0.3417 | 136 | 0.002221 | -169.7 | 128.8 |
| 444.31 | 0.2159 | 85 | 0.002251 | -173.6 | 129.2 |
| 439.29 | 0.1447 | 57 | 0.002276 | -177.0 | 129.6 |
| 434.32 | 0.09632 | 38 | 0.002302 | -180.4 | 130.0 |
| 429.33 | 0.06477 | 25 | 0.002329 | -183.8 | 130.3 |
| 424.34 | 0.04285 | 17 | 0.002357 | -187.3 | 130.7 |
\[
\ln(p_{sat}^*/p^*) = -\frac{74586}{R} - \frac{124865}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right) - \frac{27}{R} \left(\frac{T_0}{T} - 1 - \ln\left(\frac{T}{T_0}\right)\right), \quad T_0 = 403.9 \text{ K}
\]

| \(p_{sat}^*/p^*\) | \(\ln(p_{sat}^*/p^*)\) | \(R\) | \(\frac{1}{R}\) | \(\text{To}\) |
|----------------|-------------------|-----|---------|-------|
| 427.74         | 0.4085            | 169 | 0.002338| -167.9| 124.0 |
| 422.75         | 0.2910            | 120 | 0.002365| -170.8| 124.2 |
| 417.73         | 0.2006            | 82  | 0.002394| -174.0| 124.4 |
| 412.75         | 0.1326            | 54  | 0.002423| -177.5| 124.5 |
| 407.76         | 0.08151           | 33  | 0.002452| -181.5| 124.7 |
| 402.76         | 0.04971           | 20  | 0.002483| -185.7| 124.9 |
| 397.77         | 0.03122           | 12  | 0.002514| -189.6| 125.1 |
| 392.77         | 0.01941           | 7.7 | 0.002546| -193.6| 125.3 |
| 387.78         | 0.01208           | 4.8 | 0.002579| -197.6| 125.5 |
| 382.78         | 0.007363          | 2.9 | 0.002612| -201.8| 125.6 |
| 425.24         | 0.3257            | 134 | 0.002352| -169.9| 124.1 |
| 420.23         | 0.2227            | 91  | 0.002380| -173.1| 124.3 |
| 415.23         | 0.1534            | 62  | 0.002408| -176.2| 124.4 |
| 410.27         | 0.1020            | 41  | 0.002437| -179.7| 124.6 |
| 405.30         | 0.06620           | 27  | 0.002467| -183.3| 124.8 |
| 400.32         | 0.04145           | 17  | 0.002498| -187.2| 125.0 |
| 395.33         | 0.02583           | 10  | 0.002530| -191.2| 125.2 |
| 390.33         | 0.01572           | 6.2 | 0.002562| -195.4| 125.4 |
| 385.33         | 0.009758          | 3.8 | 0.002595| -199.4| 125.6 |
| 380.33         | 0.005939          | 2.3 | 0.002629| -203.6| 125.7 |
| 427.77         | 0.4372            | 181 | 0.002338| -167.4| 124.0 |
| 422.76         | 0.3076            | 126 | 0.002365| -170.4| 124.2 |
| 417.74         | 0.2114            | 86  | 0.002394| -173.5| 124.4 |
| 412.71         | 0.1379            | 56  | 0.002423| -177.1| 124.5 |
| 407.69         | 0.08929           | 36  | 0.002453| -180.8| 124.7 |
| 402.67         | 0.05332           | 21  | 0.002483| -185.1| 124.9 |
| 397.65         | 0.03454           | 14  | 0.002515| -188.8| 125.1 |
| 392.63         | 0.02083           | 8.2 | 0.002547| -193.1| 125.3 |
| 387.61         | 0.01169           | 4.6 | 0.002580| -197.9| 125.5 |
| 382.60         | 0.007601          | 3.0 | 0.002614| -201.5| 125.7 |

\[
\ln(p_{sat}^*/p^*) = -\frac{75773}{R} - \frac{142145}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right) - \frac{62}{R} \left(\frac{T_0}{T} - 1 - \ln\left(\frac{T}{T_0}\right)\right), \quad T_0 = 413.2 \text{ K}
\]
\[
\ln\left(\frac{\rho_{\text{sat}}}{\rho_o}\right) = -\frac{80852}{R} - \frac{143623}{R} \left(\frac{T}{T_0} - 1\right) - 73 \left(\frac{T}{T_0} - 1 - \ln\left(\frac{T}{T_0}\right)\right), \quad T_0 = 421.2 \text{ K}
\]

|    |    |    |    |    |    |    |
|----|----|----|----|----|----|----|
| 1  | 2  | 3  | 4  | 5  | 6  | 7  |
| 434.90 | 0.4186 | 202 | 0.002299 | -166.5 | 140.8 |
| 429.90 | 0.2750 | 132 | 0.002326 | -170.0 | 141.1 |
| 424.89 | 0.1747 | 83  | 0.002354 | -173.8 | 141.4 |
| 419.88 | 0.1083 | 51  | 0.002382 | -177.9 | 141.7 |
| 414.86 | 0.06644 | 31  | 0.002410 | -182.0 | 142.0 |
| 409.86 | 0.03989 | 19  | 0.002440 | -186.3 | 142.4 |
| 404.85 | 0.02443 | 11  | 0.002470 | -190.4 | 142.7 |
| 399.85 | 0.01436 | 6.6 | 0.002501 | -194.9 | 143.0 |
| 394.85 | 0.006275 | 3.8 | 0.002533 | -199.5 | 143.3 |
| 432.33 | 0.3577 | 172 | 0.002313 | -167.8 | 141.0 |
| 427.35 | 0.2155 | 103 | 0.002340 | -172.1 | 141.3 |
| 422.33 | 0.1318 | 63  | 0.002368 | -176.2 | 141.6 |
| 417.33 | 0.08196 | 39  | 0.002396 | -180.2 | 141.9 |
| 412.33 | 0.05079 | 24  | 0.002425 | -184.2 | 142.2 |
| 407.33 | 0.03176 | 15  | 0.002455 | -188.2 | 142.5 |
| 402.32 | 0.01868 | 8.7 | 0.002486 | -192.7 | 142.8 |
| 397.31 | 0.01071 | 4.9 | 0.002517 | -197.3 | 143.1 |
| 392.30 | 0.006427 | 2.9 | 0.002549 | -201.6 | 143.4 |
| 437.74 | 0.1086 | 44  | 0.002284 | -179.1 | 147.8 |
| 434.95 | 0.08459 | 34  | 0.002299 | -181.2 | 148.0 |
| 431.39 | 0.06076 | 25  | 0.002318 | -183.9 | 148.2 |
| 426.45 | 0.03863 | 16  | 0.002345 | -187.8 | 148.6 |
| 421.45 | 0.02399 | 10  | 0.002373 | -191.8 | 149.0 |
\[
\ln(p_{sat}/p) = -\frac{80351}{R} - \frac{135155}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right) - \frac{65}{R} \left(\frac{T}{T_0} - 1 - \ln\left(\frac{T}{T_0}\right)\right), T_0 = 442.0 \text{ K}
\]

|          |          |          |          |          |          |
|----------|----------|----------|----------|----------|----------|
| $p_{sat}$ | $p$      | $T$      | $T_0$    |
| 457.25   | 0.25611  | 110      | 0.002187 | -171.5   | 134.2    |
| 452.23   | 0.17013  | 73       | 0.002211 | -174.9   | 134.5    |
| 447.23   | 0.11302  | 48       | 0.002236 | -178.4   | 134.8    |
| 442.21   | 0.07569  | 32       | 0.002261 | -181.8   | 135.1    |
| 437.21   | 0.05036  | 21       | 0.002287 | -185.2   | 135.5    |
| 432.19   | 0.03307  | 14       | 0.002314 | -188.7   | 135.8    |
| 427.17   | 0.02143  | 8.9      | 0.002341 | -192.4   | 136.1    |
| 422.15   | 0.01371  | 5.7      | 0.002369 | -196.2   | 136.4    |
| 464.79   | 0.44427  | 193      | 0.002152 | -166.8   | 133.7    |
| 459.76   | 0.30388  | 131      | 0.002175 | -170.0   | 134.0    |
| 454.75   | 0.20727  | 89       | 0.002199 | -173.3   | 134.3    |
| 449.79   | 0.14146  | 60       | 0.002223 | -176.5   | 134.7    |
| 444.78   | 0.09447  | 40       | 0.002248 | -179.9   | 135.0    |
| 439.76   | 0.06265  | 26       | 0.002274 | -183.4   | 135.3    |
| 434.74   | 0.04127  | 17       | 0.002300 | -186.9   | 135.6    |
| 429.71   | 0.02651  | 11       | 0.002327 | -190.6   | 136.0    |
| 424.73   | 0.01706  | 7.1      | 0.002354 | -194.3   | 136.3    |

\[
\ln(p_{sat}/p) = -\frac{79781}{R} - \frac{144369}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right) - \frac{83}{R} \left(\frac{T}{T_0} - 1 - \ln\left(\frac{T}{T_0}\right)\right), T_0 = 437.9 \text{ K}
\]

|          |          |          |          |          |          |
|----------|----------|----------|----------|----------|----------|
| $p_{sat}$ | $p$      | $T$      | $T_0$    |
| 459.79   | 0.508955 | 202      | 0.002175 | -166.5   | 142.6    |
| 454.80   | 0.335185 | 132      | 0.002199 | -170.0   | 143.0    |
| 449.78   | 0.219541 | 86       | 0.002223 | -173.6   | 143.4    |
| 444.76   | 0.143206 | 56       | 0.002248 | -177.2   | 143.8    |
| 439.75   | 0.092342 | 36       | 0.002274 | -180.8   | 144.2    |
| 434.72   | 0.058632 | 23       | 0.002300 | -184.7   | 144.6    |
| 429.72   | 0.037376 | 14       | 0.002327 | -188.5   | 145.0    |
| 424.64   | 0.022847 | 8.7      | 0.002355 | -192.6   | 145.5    |
| 419.63   | 0.014198 | 5.4      | 0.002383 | -196.6   | 145.9    |
| 462.31   | 0.614672 | 244      | 0.002163 | -164.9   | 142.3    |
| 457.32   | 0.409215 | 162      | 0.002187 | -168.3   | 142.8    |
| 452.32   | 0.271785 | 107      | 0.002211 | -171.8   | 143.2    |
| T (K) | $\ln(p_{sat}^*/p)$ | a | b | c |
|-------|----------------|---|---|---|
| 447.29 | 0.177676 | 69 | 0.002236 | -175.3 | 143.6 |
| 442.31 | 0.116201 | 45 | 0.002261 | -178.9 | 144.0 |
| 437.23 | 0.074952 | 29 | 0.002287 | -182.6 | 144.4 |
| 432.20 | 0.047748 | 18 | 0.002314 | -186.4 | 144.8 |
| 427.21 | 0.030756 | 12 | 0.002341 | -190.1 | 145.3 |
| 422.17 | 0.018083 | 6.9 | 0.002369 | -194.6 | 145.7 |
| 417.16 | 0.010804 | 4.1 | 0.002397 | -198.9 | 146.1 |
| 412.16 | 0.006773 | 2.5 | 0.002426 | -202.8 | 146.5 |

$\ln(p_{sat}^*/p) = -\frac{62288}{n} - \frac{15693}{n^2} \left( \frac{1}{T} - \frac{1}{T_0} \right) \left( \frac{T_0}{T} - 1 - \ln \left( \frac{T}{T_0} \right) \right), T_0 = 447.8 K$

| T (K) | $\ln(p_{sat}^*/p)$ | a | b | c |
|-------|----------------|---|---|---|
| 467.50 | 0.406055 | 147 | 0.002139 | -169.1 | 155.0 |
| 462.28 | 0.260072 | 94 | 0.002163 | -172.8 | 155.5 |
| 457.26 | 0.1666 | 60 | 0.002187 | -176.6 | 156.0 |
| 452.27 | 0.1066 | 38 | 0.002211 | -180.3 | 156.5 |
| 447.24 | 0.0674 | 24 | 0.002236 | -184.2 | 157.0 |
| 442.22 | 0.0422 | 15 | 0.002261 | -188.1 | 157.5 |
| 437.18 | 0.02610 | 9.2 | 0.002287 | -192.2 | 158.0 |
| 432.17 | 0.01550 | 5.4 | 0.002314 | -196.6 | 158.5 |
| 427.16 | 0.00930 | 3.2 | 0.002341 | -200.9 | 159.0 |
| 420.54 | 0.00476 | 1.6 | 0.002378 | -206.5 | 159.6 |

$\ln(p_{sat}^*/p) = \frac{70697}{n} - \frac{118278}{n^2} \left( \frac{1}{T} - \frac{1}{T_0} \right) \left( \frac{T_0}{T} - 1 - \ln \left( \frac{T}{T_0} \right) \right), T_0 = 373.4 K$

| T (K) | $\ln(p_{sat}^*/p)$ | a | b | c |
|-------|----------------|---|---|---|
| 397.59 | 0.4835 | 123 | 0.00252 | -170.6 | 115.6 |
| 392.60 | 0.3171 | 80 | 0.00255 | -174.2 | 116.2 |
| 387.61 | 0.2077 | 52 | 0.00258 | -177.7 | 116.7 |
| 382.62 | 0.1320 | 33 | 0.00261 | -181.5 | 117.3 |
| 377.66 | 0.08199 | 20 | 0.00265 | -185.6 | 117.8 |
\[
\ln(p_{sat}/p) = -\frac{70893}{R} - \frac{136589}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right) - \frac{81}{R} \left(\frac{T_0}{T} - 1 - \ln\left(\frac{T}{T_0}\right)\right), \quad T_0 = 392.9 \text{ K}
\]

| Temperature (K) | Molarity | Viscosity (cP) | Density (g/mL) | Osmotic Coefficient (mol/L) |
|-----------------|-----------|----------------|---------------|----------------------------|
| 372.69          | 0.04959   | 12             | 0.00268       | -189.8                     | 118.4 |
| 367.71          | 0.02975   | 7.3            | 0.00272       | -194.1                     | 118.9 |
| 362.71          | 0.01715   | 4.2            | 0.00276       | -198.7                     | 119.4 |
| 357.72          | 0.00996   | 2.4            | 0.00280       | -203.3                     | 120.0 |
| 352.73          | 0.005333  | 1.3            | 0.00284       | -208.3                     | 120.5 |
| 395.08          | 0.3996    | 101            | 0.00253       | -172.2                     | 115.9 |
| 390.11          | 0.2586    | 65             | 0.00256       | -175.9                     | 116.5 |
| 385.14          | 0.1638    | 41             | 0.00260       | -179.7                     | 117.0 |
| 380.20          | 0.1036    | 26             | 0.00263       | -183.6                     | 117.5 |
| 375.23          | 0.06385   | 16             | 0.00267       | -187.7                     | 118.1 |
| 370.25          | 0.03843   | 9.4            | 0.00270       | -191.9                     | 118.6 |
| 365.26          | 0.02281   | 5.6            | 0.00274       | -196.3                     | 119.2 |
| 360.27          | 0.01325   | 3.2            | 0.00278       | -200.9                     | 119.7 |
| 355.28          | 0.007454  | 1.8            | 0.00281       | -205.8                     | 120.3 |
| 350.29          | 0.004186  | 1.0            | 0.00285       | -210.6                     | 120.8 |

\[
\ln(p_{sat}/p) = -\frac{82263}{R} - \frac{149823}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right) - \frac{91}{R} \left(\frac{T_0}{T} - 1 - \ln\left(\frac{T}{T_0}\right)\right), \quad T_0 = 360.5 \text{ K}
\]

| Temperature (K) | Molarity | Viscosity (cP) | Density (g/mL) | Osmotic Coefficient (mol/L) |
|-----------------|-----------|----------------|---------------|----------------------------|
| 409.51          | 0.5334    | 199            | 0.002442      | -166.6                     | 135.2 |
| 404.47          | 0.3406    | 127            | 0.002472      | -170.3                     | 135.7 |
| 399.50          | 0.2064    | 76             | 0.002503      | -174.6                     | 136.1 |
| 394.49          | 0.1210    | 44             | 0.002535      | -179.1                     | 136.5 |
| 389.51          | 0.0697    | 25             | 0.002567      | -183.7                     | 136.9 |
| 384.56          | 0.0411    | 15             | 0.002600      | -188.1                     | 137.3 |
| 379.55          | 0.02328   | 8.4            | 0.002635      | -192.9                     | 137.7 |
| 374.57          | 0.01382   | 4.9            | 0.002670      | -197.3                     | 138.1 |
| 412.02          | 0.6925    | 260            | 0.002427      | -164.4                     | 135.0 |
| 407.00          | 0.4249    | 158            | 0.002457      | -168.5                     | 135.5 |
| 402.01          | 0.2590    | 96             | 0.002488      | -172.6                     | 135.9 |
| 397.00          | 0.1573    | 58             | 0.002519      | -176.8                     | 136.3 |
| 392.01          | 0.09372   | 34             | 0.002551      | -181.2                     | 136.7 |
| 387.04          | 0.05466   | 20             | 0.002584      | -185.7                     | 137.1 |
| 382.04          | 0.03152   | 11             | 0.002618      | -190.4                     | 137.5 |
| 377.05          | 0.01800   | 6.5            | 0.002652      | -195.1                     | 137.9 |

\[
\ln(p_{sat}/p) = -\frac{82263}{R} - \frac{149823}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right) - \frac{91}{R} \left(\frac{T_0}{T} - 1 - \ln\left(\frac{T}{T_0}\right)\right), \quad T_0 = 360.5 \text{ K}
\]

| Temperature (K) | Molarity | Viscosity (cP) | Density (g/mL) | Osmotic Coefficient (mol/L) |
|-----------------|-----------|----------------|---------------|----------------------------|
| 479.65          | 0.5649    | 221            | 0.002085      | -165.7                     | 148.1 |
\[
\ln(p_{\text{sat}}/p) = -\frac{77427}{R} - \frac{126027}{R} \left( \frac{1}{T} - \frac{1}{T_0} \right) - \frac{56}{P} \left( \frac{T}{T} - 1 - \ln \left( \frac{T}{T_0} \right) \right), T_0 = 423.2 \, \text{K}
\]
\[
\ln\left(\frac{\mu}{\mu_0}\right) = -\frac{70118}{R} - \frac{118558}{R} \left(\frac{1 - 1}{T_0}\right) - \frac{56}{R} \left(\frac{T}{T_0} - 1 - \ln\left(\frac{T}{T_0}\right)\right), T_0 = 378.2 \text{ K}
\]

| T   | \(\mu\) | \(\mu_0\) | \(\Delta\mu\) | \(\Delta T\) |
|-----|--------|--------|-------------|-----------|
| 392.24 | 0.2723 | 82     | 0.002549    | -174.0    | 117.8 |
| 387.24 | 0.1718 | 51     | 0.002582    | -177.8    | 118.1 |
| 382.23 | 0.1069 | 32     | 0.002616    | -181.8    | 118.3 |
| 377.24 | 0.06569 | 19    | 0.002651    | -185.9    | 118.6 |
| 372.24 | 0.03977 | 12    | 0.002686    | -190.2    | 118.9 |
| 367.24 | 0.02374 | 6.9   | 0.002723    | -194.5    | 119.2 |
| 362.25 | 0.01399 | 4.0   | 0.002761    | -199.0    | 119.5 |
| 394.67 | 0.3400 | 103    | 0.002534    | -172.1    | 117.6 |
| 389.72 | 0.2163 | 65     | 0.002566    | -175.9    | 117.9 |
| 384.78 | 0.1365 | 41     | 0.002599    | -179.8    | 118.2 |
| 379.76 | 0.08408 | 25    | 0.002633    | -183.9    | 118.5 |
| 374.77 | 0.05148 | 15    | 0.002668    | -188.0    | 118.8 |
| 369.76 | 0.03082 | 9.0   | 0.002704    | -192.3    | 119.0 |
| 364.75 | 0.01823 | 5.3   | 0.002742    | -196.7    | 119.3 |

\* The combined expanded uncertainties are \(U_e(T) = 0.02\) K, \(U_e(df/dt) = 0.01\) for confidence level = 0.95, \(k = 2\).
\* From reference 1
\* Calculated in this work from the primary data on the frequency shift velocities \(df/dt\)
Table S2: PC-SAFT results for the correlation of LLE, VLE or IDAC data of binary mixture containing the [C$_2$ mim]-IL systems under investigation, and the respective binary interaction parameters. ARD% and AAD for the correlations are given for the two parameter sets of the [C$_2$ mim]-ILs in Table 4 (use of vapor pressure and liquid density) and Table 5 (liquid density only).

| Organic Compound | System | $k_{ij}$ | AAD  | ARD%  | $k_{ij}$ | AAD  | ARD%  |
|------------------|--------|----------|------|-------|----------|------|-------|
|                  |        |          |      |       |          |      |       |
| [C$_2$ mim][NTf$_2$] |        |          |      |       |          |      |       |
| Water            | LLE    | -0.045   | 0.056| 8.122 | 0.005    | 0.050| 7.258 |
| CO$_2$           | VLE    | 0.200    | 38.99| 28.64 | 0.100    | 25.59| 35.85 |
| [C$_2$ mim][SCN] |        |          |      |       |          |      |       |
| Water            | IDAC   | -0.090   | 0.01 | 3.29  | -0.145   | 0.01 | 4.84  |
| CO$_2$           | VLE    | 0.120    | 0.10 | 6.72  | 0.270    | 0.09 | 7.80  |
| [C$_2$ mim][CF$_3$CO$_2$] |        |          |      |       |          |      |       |
| Water            | IDAC   | -0.135   | 0.01 | 6.81  | -0.205   | 0.003| 2.02  |
| CO$_2$           | VLE    | 0.125    | 0.38 | 73.57 | 0.200    | 0.46 | 67.75 |
| [C$_2$ mim][CF$_3$SO$_3$] |        |          |      |       |          |      |       |
| Water            | VLE    | 0.037    | 0.02 | 26.92 | -0.040   | 0.02 | 23.16 |
| Methanol         | IDAC   | -0.103   | 0.03 | 3.75  | -0.160   | 0.06 | 8.45  |
| [C$_2$ mim][C(C$_2$H$_5$O)$_2$PO$_2$] | |          |      |       |          |      |       |
| CO$_2$           | VLE    | 0.360    | 17.03| 59.58 | 0.220    | 1.90 | 4.09  |
| Hexane           | IDAC   | 0.008    | 5.56 | 7.88  | 0.190    | 4.24 | 6.17  |
| Pentane          | IDAC   | 0.030    | 2.38 | 5.80  | 0.193    | 2.16 | 5.19  |
| [C$_2$ mim][PF$_3$] | |          |      |       |          |      |       |
| CO$_2$           | VLE    | 0.088    | 139.21| 39.24 | 0.088    | 181.00| 34.58 |
| H$_2$S           | VLE    | 0.002    | 1.02 | 10.76 | 0.018    | 0.46 | 5.49  |
| [C$_2$ mim][BF$_3$] | |          |      |       |          |      |       |
| Water            | VLE    | 0.030    | 0.10 | 36.68 | -0.067   | 0.05 | 20.21 |
| Water            | IDAC   | 0.030    | 0.003| 0.59  | -0.067   | 0.002| 0.38  |
| Benzene          | VLE    | -0.005   | 0.001| 2.88  | 0.015    | 0.002| 5.92  |
| [C$_2$ mim][B(CN)$_3$] |        |          |      |       |          |      |       |
| Water            | IDAC   | 0.024    | 0.02 | 1.08  | -0.030   | 0.08 | 5.24  |
| CO$_2$           | VLE    | 0.140    | 3.19 | 14.49 | 0.190    | 2.91 | 11.98 |
| [C$_2$ mim][C(CN)$_3$] | |          |      |       |          |      |       |
| Water            | IDAC   | -0.017   | -0.02| 0.07  | -0.050   | 0.04 | 4.76  |
| CO$_2$           | VLE    | 0.075    | 0.08 | 0.21  | 0.235    | 0.17 | 7.39  |
| [C$_2$ mim][CH$_3$SO$_3$] |        |          |      |       |          |      |       |
| Water            | VLE    | -0.070   | 0.002| 35.19 | -0.200   | 0.002| 21.41 |
| Water            | IDAC   | -0.225   | 0.003| 3.15  | -0.340   | 0.002| 3.21  |
| CO$_2$           | VLE    | 0.150    | 4.49 | 16.42 | 0.250    | 4.16 | 14.23 |
| Substance          | IDAC | 0.150 | 0.150 | 0.452 | 0.150 | 8.754 | 0.150 |
|--------------------|------|-------|-------|-------|-------|-------|-------|
| Water              |      |       |       |       |       |       |       |
| CO₂                | VLE  | 0.160 | 0.160 | 0.859 | 0.160 | 12.458| 0.190 |

**[C₂ mim][4-CH₃-Ph-SO₃]**

| Substance          | IDAC | -0.060 | 0.005 | 1.86  | -0.110 | 0.004 | 1.35  |
|--------------------|------|--------|-------|-------|---------|-------|-------|
| Methanol           |      |        |       |       |         |       |       |
| Ethanol            |      | 0.063  | 0.001 | 0.15  | 0.042   | 0.001 | 0.13  |
| 1-Propanol         |      | 0.080  | 0.01  | 2.15  | 0.088   | 0.02  | 2.56  |
| 2-Propanol         |      | 0.105  | 0.02  | 1.77  | 0.097   | 0.02  | 2.42  |
| 1-Butanol          |      | 0.063  | 0.01  | 0.84  | 0.043   | 0.01  | 1.29  |

References

(1) Zaitsau, D. H.; Fumino, K.; Emel’yanenko, V. N.; Yermalayeu, A. V.; Ludwig, R.; Verevkin, S. P. Structure-property relationships in ionic liquids: a study of the anion dependence in vaporization enthalpies of imidazolium-based ionic liquids. *Chemphyschem: a European journal of chemical physics and physical chemistry* **2012**, *13*, 1868–1876.