Supporting Information

**Structure and Thermodynamics of Nondipolar Molecular Liquids and Solutions from Integral Equation Theory**

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Table S1. IEF-PCM results (electrostatic and apolar contribution to solvation free energy) in kcal mol\(^{-1}\) for the Gibbs energies of gas molecules in benzene solution.

|       | He   | Ne   | Ar   | N\(_2\) | O\(_2\) | CO   | CO\(_2\) | CH\(_4\) | CF\(_4\) |
|-------|------|------|------|---------|--------|------|---------|---------|---------|
| HF    |      |      |      |         |        |      |         |         |         |
| 6-31G*| -1791.641 | -80618.900 | -330555.488 | -68363.457 | -93886.676 | -70744.364 | -117743.261 | -25222.894 | -27337.665 |
| 6-311G** | -1794.613 | -80649.113 | -330576.122 | -68381.052 | -93913.104 | -70764.176 | -117776.791 | -25231.584 | -27346.430 |
| 6-311+G** | -1794.613 | -80651.672 | -330576.310 | -68382.390 | -93915.714 | -70765.154 | -117779.321 | -25231.632 | -27345.515 |
| aug-cc-pVDZ | -1791.984 | -80632.670 | -330572.574 | -68374.712 | -93904.489 | -70755.388 | -117762.135 | -25225.702 | -27340.363 |
| aug-cc-pVTZ | -1795.422 | -80655.840 | -330580.343 | -68390.957 | -93927.184 | -70772.607 | -117792.073 | -25234.531 | -27348.673 |
| aug-cc-pVQZ | -1795.634 | -80662.418 | -330582.509 | -68395.437 | -93933.838 | -70777.541 | -117800.279 | -25236.189 | -27350.081 |
| B3LYP  |      |      |      |         |        |      |         |         |         |
| 6-31G* | -1824.202 | -80882.425 | -331021.977 | -68727.535 | -94327.267 | -71102.945 | -118336.995 | -25425.717 | -27452.589 |
| 6-311G** | -1827.955 | -80917.905 | -331044.609 | -68747.521 | -94355.372 | -71126.029 | -118374.822 | -25435.360 | -27460.852 |
| 6-311+G** | -1827.955 | -80923.867 | -331045.034 | -68749.876 | -94358.911 | -71127.809 | -118378.518 | -25435.478 | -27461.924 |
| aug-cc-pVDZ | -1825.489 | -80903.531 | -331039.703 | -68739.256 | -94345.901 | -71116.013 | -118357.911 | -25427.125 | -27456.348 |
| aug-cc-pVTZ | -1829.002 | -80927.560 | -331048.873 | -68756.681 | -94367.794 | -71133.924 | -118388.753 | -25438.297 | -27461.781 |
| aug-cc-pVQZ | -1829.232 | -80934.372 | -331051.179 | -68761.352 | -94374.748 | -71139.176 | -118397.593 | -25440.302 | -27462.716 |
| PBE0   |      |      |      |         |        |      |         |         |         |
| 6-31G* | -1812.055 | -80816.893 | -330911.143 | -68649.814 | -94232.116 | -71022.689 | -118212.533 | -25387.128 | -27426.755 |
| 6-311G** | -1815.449 | -80850.293 | -330932.642 | -68667.951 | -94258.100 | -71043.531 | -118247.262 | -25395.706 | -27434.367 |
| 6-311+G** | -1815.449 | -80855.390 | -330932.973 | -68669.937 | -94261.190 | -71045.024 | -118250.466 | -25395.849 | -27435.188 |
| aug-cc-pVDZ | -1813.104 | -80836.101 | -330928.413 | -68661.239 | -94249.748 | -71034.690 | -118232.342 | -25389.166 | -27430.391 |
| aug-cc-pVTZ | -1816.446 | -80859.131 | -330936.949 | -68676.784 | -94270.866 | -71051.211 | -118260.853 | -25398.249 | -27438.567 |
| aug-cc-pVQZ | -1816.658 | -80865.904 | -330939.154 | -68681.415 | -94277.799 | -71056.404 | -118269.600 | -25400.140 | -27440.272 |
| MP2    |      |      |      |         |        |      |         |         |         |
| 6-31G* | -1798.670 | -80713.225 | -330641.650 | -68558.847 | -94094.887 | -70921.944 | -118039.960 | -25309.107 | -27387.062 |
| 6-311G** | -1810.102 | -80780.274 | -330668.567 | -68585.059 | -94141.439 | -70955.550 | -118097.322 | -25338.401 | -27403.758 |
| 6-311+G** | -1810.102 | -80785.039 | -330669.022 | -68587.906 | -94145.208 | -70957.699 | -118102.053 | -25338.586 | -27408.710 |
| aug-cc-pVDZ | -1808.903 | -80762.485 | -330669.416 | -68574.734 | -94129.118 | -70943.129 | -118078.848 | -25331.186 | -27399.180 |
| aug-cc-pVTZ | -1816.520 | -80826.848 | -330712.704 | -68627.548 | -94202.322 | -70998.002 | -118174.157 | -25360.515 | -27422.512 |
| aug-cc-pVQZ | -1818.052 | -80848.941 | -330728.184 | -68645.681 | -94227.106 | -71017.154 | -118206.907 | -25368.640 | -27429.534 |
Table S2. IEF-PCM results (electrostatic and apolar contribution to solvation free energy) in kcal mol⁻¹ for the Gibbs energies of gas molecules in hexafluorobenzene solution.

|        | He       | Ne       | Ar       | N₂       | O₂       | CO       | CO₂      | CH₄      | CF₄      |
|--------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| HF     |          |          |          |          |          |          |          |          |          |
| 6-31G* | -1791.641| -80618.900 | -330555.488 | -68363.445 | -93886.672 | -70744.331 | -117743.139 | -25222.889 | -273371.640 |
| 6-311G** | -1794.613 | -80649.113 | -330576.122 | -68381.037 | -93913.098 | -70784.145 | -117776.668 | -25231.578 | -273446.399 |
| 6-311+G** | -1794.613 | -80651.672 | -330576.310 | -68382.375 | -93915.707 | -70765.120 | -117779.193 | -25231.626 | -273450.473 |
| aug-cc-pVDZ | -1791.983 | -80632.670 | -330572.574 | -68374.703 | -93904.487 | -70755.357 | -117762.020 | -25225.696 | -273403.337 |
| aug-cc-pVTZ | -1795.422 | -80655.840 | -330580.343 | -68390.946 | -93927.181 | -70772.578 | -117791.963 | -25234.525 | -273483.646 |
| aug-cc-pVQZ | -1795.634 | -80662.418 | -330582.509 | -68395.427 | -93933.835 | -70777.512 | -117800.170 | -25236.183 | -273503.053 |
| B3LYP  |          |          |          |          |          |          |          |          |          |
| 6-31G* | -1824.202 | -80882.425 | -331021.977 | -68727.521 | -94327.264 | -71102.922 | -118336.916 | -25425.711 | -274520.596 |
| 6-311G** | -1827.955 | -80917.905 | -331044.609 | -68747.504 | -94355.386 | -71126.006 | -118374.737 | -25435.353 | -274606.818 |
| 6-311+G** | -1827.955 | -80923.866 | -331045.034 | -68749.860 | -94358.904 | -71127.764 | -118378.424 | -25435.472 | -274614.877 |
| aug-cc-pVDZ | -1825.488 | -80903.531 | -331039.703 | -68739.244 | -94345.898 | -71115.990 | -118357.827 | -25427.119 | -274563.335 |
| aug-cc-pVTZ | -1829.001 | -80927.560 | -331048.873 | -68756.668 | -94367.791 | -71133.901 | -118388.671 | -25438.289 | -274641.761 |
| aug-cc-pVQZ | -1829.231 | -80934.372 | -331051.179 | -68761.339 | -94374.744 | -71139.154 | -118397.511 | -25440.296 | -274662.689 |
| PBEO   |          |          |          |          |          |          |          |          |          |
| 6-31G* | -1812.055 | -80816.893 | -330911.143 | -68649.801 | -94232.113 | -71022.667 | -118212.455 | -25387.120 | -274266.743 |
| 6-311G** | -1815.449 | -80850.293 | -330932.642 | -68667.935 | -94258.094 | -71043.508 | -118247.179 | -25395.698 | -274347.354 |
| 6-311+G** | -1815.449 | -80855.390 | -330932.973 | -68669.922 | -94261.183 | -71045.000 | -118250.376 | -25395.841 | -274354.165 |
| aug-cc-pVDZ | -1813.103 | -80836.101 | -330928.413 | -68661.228 | -94249.745 | -71034.667 | -118232.262 | -25389.159 | -274306.361 |
| aug-cc-pVTZ | -1816.445 | -80859.131 | -330936.948 | -68676.772 | -94270.863 | -71051.189 | -118260.775 | -25398.242 | -274381.549 |
| aug-cc-pVQZ | -1816.657 | -80865.904 | -330939.153 | -68681.403 | -94277.796 | -71056.382 | -118269.523 | -25400.132 | -274402.250 |
| MP2    |          |          |          |          |          |          |          |          |          |
| 6-31G* | -1798.669 | -80713.225 | -330641.650 | -68558.831 | -94094.885 | -70921.935 | -118039.893 | -25309.101 | -273875.046 |
| 6-311G** | -1810.102 | -80780.274 | -330668.567 | -68585.040 | -94141.434 | -70955.541 | -118097.253 | -25338.395 | -274037.731 |
| 6-311+G** | -1810.102 | -80785.039 | -330669.022 | -68587.888 | -94145.202 | -70957.689 | -118101.975 | -25338.580 | -274048.685 |
| aug-cc-pVDZ | -1808.903 | -80762.485 | -330669.415 | -68574.722 | -94129.117 | -70943.120 | -118078.779 | -25331.180 | -273991.842 |
| aug-cc-pVTZ | -1816.519 | -80826.848 | -330712.704 | -68627.535 | -94202.319 | -70997.993 | -118174.093 | -25360.508 | -274221.490 |
| aug-cc-pVQZ | -1818.051 | -80848.941 | -330728.184 | -68645.668 | -94227.103 | -71017.144 | -118206.842 | -25368.632 | -274297.515 |
Table S3. EC-RISM\(^9\) results (in kcal mol\(^{-1}\)) for the Gibbs energies of gas molecules in Amber/OPLS benzene solution.

|       | He     | Ne     | Ar     | N\(_2\) | O\(_2\) | CO     | CO\(_2\) | CH\(_4\) | CF\(_4\) |
|-------|--------|--------|--------|---------|--------|--------|---------|---------|---------|
| HF    |        |        |        |         |        |        |         |         |         |
| 6-31G*| -1788.939 | -80616.155 | -330552.844 | -68359.922 | -93883.642 | -70740.806 | -117740.434 | -25222.027 | -273367.856 |
| 6-311G**| -1791.910 | -80646.368 | -330573.478 | -68377.503 | -93910.060 | -70760.639 | -117773.989 | -25230.708 | -273442.586 |
| 6-311+G**| -1791.910 | -80646.927 | -330573.665 | -68378.846 | -93912.667 | -70761.605 | -117776.510 | -25230.755 | -273446.646 |
| aug-cc-pVDZ | -1789.280 | -80629.925 | -330569.930 | -68371.202 | -93901.475 | -70751.853 | -117759.346 | -25224.813 | -273399.523 |
| aug-cc-pVTZ | -1792.718 | -80653.094 | -330577.698 | -68387.453 | -93924.167 | -70769.093 | -117789.321 | -25233.663 | -273479.877 |
| aug-cc-pVQZ | -1792.931 | -80659.673 | -330579.865 | -68391.934 | -93930.822 | -70774.032 | -117797.536 | -25235.322 | -273499.295 |
| B3LYP |        |        |        |         |        |        |         |         |         |
| 6-31G*| -1821.499 | -80879.680 | -331019.333 | -68723.949 | -94324.169 | -71099.423 | -118334.466 | -25424.831 | -274516.714 |
| 6-311G**| -1825.251 | -80915.160 | -331041.965 | -68743.919 | -94352.263 | -71122.510 | -118372.280 | -25434.470 | -274602.931 |
| 6-311+G**| -1825.251 | -80921.121 | -331042.389 | -68746.281 | -94355.793 | -71124.284 | -118375.944 | -25434.585 | -274610.940 |
| aug-cc-pVDZ | -1822.784 | -80900.785 | -331037.059 | -68735.683 | -94342.812 | -71112.497 | -118355.325 | -25426.226 | -274559.388 |
| aug-cc-pVTZ | -1826.296 | -80924.814 | -331046.228 | -68753.122 | -94364.705 | -71130.422 | -118386.169 | -25437.413 | -274637.864 |
| aug-cc-pVQZ | -1826.526 | -80931.627 | -331048.534 | -68757.792 | -94371.659 | -71135.676 | -118395.012 | -25439.420 | -274658.805 |
| PBE0  |        |        |        |         |        |        |         |         |         |
| 6-31G*| -1809.352 | -80814.148 | -330908.500 | -68646.237 | -94229.036 | -71019.175 | -118210.019 | -25386.224 | -274262.922 |
| 6-311G**| -1812.745 | -80847.548 | -330929.998 | -68664.360 | -94255.009 | -71040.016 | -118244.743 | -25394.804 | -274343.505 |
| 6-311+G**| -1812.745 | -80852.645 | -330930.328 | -68666.350 | -94258.091 | -71041.505 | -118247.923 | -25394.943 | -274350.278 |
| aug-cc-pVDZ | -1810.399 | -80833.356 | -330925.768 | -68657.678 | -94246.680 | -71031.180 | -118229.793 | -25388.256 | -274302.484 |
| aug-cc-pVTZ | -1813.741 | -80856.386 | -330934.303 | -68673.233 | -94267.795 | -71047.714 | -118258.308 | -25397.352 | -274377.717 |
| aug-cc-pVQZ | -1813.953 | -80863.159 | -330936.509 | -68677.863 | -94274.728 | -71052.909 | -118267.060 | -25399.243 | -274398.422 |
| MP2   |        |        |        |         |        |        |         |         |         |
| 6-31G*| -1795.967 | -80710.480 | -330639.006 | -68555.198 | -94091.748 | -70918.453 | -118037.217 | -25308.228 | -273871.152 |
| 6-311G**| -1807.398 | -80777.529 | -330665.923 | -68581.402 | -94138.309 | -70952.070 | -118094.606 | -25337.502 | -274033.839 |
| 6-311+G**| -1807.398 | -80782.293 | -330666.375 | -68584.251 | -94142.070 | -70954.201 | -118099.316 | -25337.681 | -274044.747 |
| aug-cc-pVDZ | -1806.199 | -80759.737 | -330666.768 | -68571.112 | -94125.999 | -70939.635 | -118076.107 | -25330.259 | -273967.874 |
| aug-cc-pVTZ | -1813.815 | -80824.101 | -330710.058 | -68623.947 | -94199.212 | -70994.532 | -118171.460 | -25359.623 | -274217.622 |
| aug-cc-pVQZ | -1815.348 | -80846.194 | -330725.538 | -68642.083 | -94224.002 | -71013.688 | -118204.222 | -25367.754 | -274293.626 |
Table S4. EC-RISM\(^6\) results (in kcal mol\(^{-1}\)) for the Gibbs energies of gas molecules in Amber/OPLS hexafluorobenzene solution.

|       | He    | Ne    | Ar    | N\(_2\) | O\(_2\) | CO    | CO\(_2\) | CH\(_4\) | CF\(_4\) |
|-------|-------|-------|-------|---------|--------|-------|---------|---------|---------|
| **HF** |       |       |       |         |        |       |         |         |         |
| 6-31G* | -1789.308 | -80616.574 | -330553.386 | -68360.584 | -93884.234 | -70741.476 | -117741.398 | -25222.151 | -273388.882 |
| 6-311G** | -1792.279 | -80646.787 | -330574.019 | -68378.164 | -93910.650 | -70761.303 | -117774.952 | -25230.834 | -273443.636 |
| 6-311+G** | -1792.279 | -80649.346 | -330574.207 | -68379.507 | -93913.257 | -70762.272 | -117777.483 | -25230.881 | -273447.705 |
| aug-cc-pVDZ | -1789.650 | -80630.344 | -330570.471 | -68371.864 | -93902.066 | -70752.521 | -117760.301 | -25224.938 | -273400.560 |
| aug-cc-pVTZ | -1793.088 | -80653.514 | -330578.240 | -68388.113 | -93924.757 | -70769.758 | -117790.265 | -25233.783 | -273480.909 |
| aug-cc-pVQZ | -1793.300 | -80660.092 | -330580.406 | -68392.593 | -93931.412 | -70774.695 | -117798.477 | -25235.443 | -273500.325 |
| **B3LYP** |       |       |       |         |        |       |         |         |         |
| 6-31G* | -1821.869 | -80880.099 | -331019.874 | -68724.617 | -94324.771 | -71100.087 | -118335.398 | -25424.950 | -274517.731 |
| 6-311G** | -1825.621 | -80915.579 | -331042.506 | -68744.586 | -94352.863 | -71123.168 | -118373.216 | -25434.595 | -274603.981 |
| 6-311+G** | -1825.621 | -80921.540 | -331042.931 | -68746.947 | -94356.393 | -71124.947 | -118376.899 | -25434.710 | -274612.009 |
| aug-cc-pVDZ | -1823.153 | -80901.205 | -331037.600 | -68736.351 | -94343.413 | -71113.162 | -118356.263 | -25426.356 | -274560.435 |
| aug-cc-pVTZ | -1826.666 | -80925.233 | -331046.769 | -68753.788 | -94365.305 | -71131.083 | -118387.096 | -25437.542 | -274638.908 |
| aug-cc-pVQZ | -1826.896 | -80932.046 | -331049.075 | -68758.457 | -94372.258 | -71136.336 | -118395.937 | -25439.549 | -274659.847 |
| **PBE0** |       |       |       |         |        |       |         |         |         |
| 6-31G* | -1809.722 | -80814.567 | -330909.041 | -68646.905 | -94229.636 | -71019.838 | -118210.946 | -25386.330 | -274263.929 |
| 6-311G** | -1813.115 | -80847.967 | -330930.539 | -68665.025 | -94255.606 | -71040.673 | -118245.674 | -25394.916 | -274544.542 |
| 6-311+G** | -1813.115 | -80853.064 | -330930.869 | -68667.016 | -94258.688 | -71042.166 | -118248.868 | -25395.054 | -274531.330 |
| aug-cc-pVDZ | -1810.769 | -80833.775 | -330926.310 | -68658.346 | -94247.278 | -71031.842 | -118230.724 | -25388.371 | -274503.515 |
| aug-cc-pVTZ | -1814.110 | -80856.805 | -330934.845 | -68673.898 | -94268.393 | -71048.373 | -118259.228 | -25397.466 | -274378.745 |
| aug-cc-pVQZ | -1814.323 | -80863.578 | -330937.050 | -68678.528 | -94275.325 | -71053.567 | -118267.977 | -25399.357 | -274399.449 |
| **MP2** |       |       |       |         |        |       |         |         |         |
| 6-31G* | -1796.336 | -80710.899 | -330639.548 | -68555.883 | -94092.359 | -70919.098 | -118038.114 | -25308.353 | -273872.175 |
| 6-311G** | -1807.768 | -80777.948 | -330666.465 | -68582.083 | -94138.916 | -70952.709 | -118095.502 | -25337.648 | -274034.885 |
| 6-311+G** | -1807.768 | -80782.714 | -330666.919 | -68584.938 | -94142.680 | -70954.850 | -118100.239 | -25337.837 | -274045.613 |
| aug-cc-pVDZ | -1806.569 | -80760.160 | -330667.314 | -68571.807 | -94126.614 | -70940.288 | -118077.020 | -25330.421 | -273988.922 |
| aug-cc-pVTZ | -1814.185 | -80824.522 | -330710.602 | -68624.632 | -94199.822 | -70995.181 | -118172.358 | -25359.767 | -274218.654 |
| aug-cc-pVQZ | -1815.717 | -80846.615 | -330726.081 | -68642.766 | -94224.612 | -71014.337 | -118205.117 | -25367.894 | -274294.656 |
Table S5. EC-RISM\(^6\) results (in kcal mol\(^{-1}\)) for the Gibbs energies of gas molecules in Cornell benzene solution.

|       | He    | Ne    | Ar    | N\(_2\) | O\(_2\) | CO   | CO\(_2\) | CH\(_4\) | CF\(_4\) |
|-------|-------|-------|-------|---------|--------|------|---------|---------|---------|
| HF    |       |       |       |         |        |      |         |         |         |
| 6-31G*| -1788.973 | -80616.174 | -330552.813 | -68359.886 | -93883.598 | -70740.754 | -117740.247 | -25221.932 | -273367.699 |
| 6-311G**| -1791.944 | -80646.387 | -330573.446 | -68377.468 | -93910.016 | -70760.589 | -117773.799 | -25230.614 | -273442.426 |
| 6-311+G**| -1791.944 | -80646.946 | -330573.634 | -68378.810 | -93912.623 | -70761.554 | -117776.317 | -25230.661 | -273446.486 |
| aug-cc-pVDZ | -1789.315 | -80629.944 | -330569.898 | -68371.166 | -93901.431 | -70751.802 | -117759.162 | -25224.719 | -273399.366 |
| aug-cc-pVTZ | -1792.752 | -80653.113 | -330577.667 | -68387.417 | -93924.124 | -70769.043 | -117789.139 | -25233.568 | -273479.719 |
| aug-cc-pVQZ | -1792.965 | -80659.692 | -330579.833 | -68391.888 | -93930.779 | -70773.982 | -117797.355 | -25235.227 | -273499.137 |
| B3LYP  |       |       |       |         |        |      |         |         |         |
| 6-31G*| -1821.534 | -80879.699 | -331019.302 | -68723.913 | -94324.126 | -71099.378 | -118334.279 | -25424.736 | -274516.557 |
| 6-311G**| -1825.285 | -80915.179 | -331041.933 | -68743.884 | -94352.220 | -71122.467 | -118372.091 | -25434.376 | -274602.772 |
| 6-311+G**| -1825.285 | -80921.140 | -331042.358 | -68746.246 | -94355.750 | -71124.238 | -118375.750 | -25434.491 | -274610.779 |
| aug-cc-pVDZ | -1822.818 | -80900.804 | -331037.027 | -68735.648 | -94342.769 | -71112.451 | -118355.140 | -25426.131 | -274559.231 |
| aug-cc-pVTZ | -1826.331 | -80924.833 | -331046.197 | -68753.087 | -94364.662 | -71130.377 | -118385.987 | -25437.319 | -274637.706 |
| aug-cc-pVQZ | -1826.561 | -80931.646 | -331048.502 | -68757.757 | -94371.616 | -71135.632 | -118394.831 | -25439.326 | -274658.648 |
| PBE0   |       |       |       |         |        |      |         |         |         |
| 6-31G*| -1809.387 | -80814.167 | -330908.468 | -68646.202 | -94228.993 | -71019.130 | -118209.831 | -25386.131 | -274262.766 |
| 6-311G**| -1812.780 | -80847.567 | -330929.966 | -68664.324 | -94254.965 | -71039.973 | -118244.554 | -25394.711 | -274343.345 |
| 6-311+G**| -1812.780 | -80852.664 | -330930.297 | -68666.315 | -94258.048 | -71041.460 | -118247.730 | -25394.850 | -274350.117 |
| aug-cc-pVDZ | -1810.433 | -80833.375 | -330925.737 | -68657.643 | -94246.637 | -71031.135 | -118229.609 | -25388.162 | -274302.327 |
| aug-cc-pVTZ | -1813.775 | -80856.405 | -330934.272 | -68673.198 | -94267.752 | -71047.670 | -118258.127 | -25397.258 | -274377.560 |
| aug-cc-pVQZ | -1813.987 | -80863.178 | -330936.477 | -68677.828 | -94274.685 | -71052.865 | -118266.879 | -25399.149 | -274398.265 |
| MP2    |       |       |       |         |        |      |         |         |         |
| 6-31G*| -1796.001 | -80710.499 | -330638.975 | -68555.164 | -94091.706 | -70918.420 | -118037.063 | -25308.133 | -273870.999 |
| 6-311G**| -1807.433 | -80777.548 | -330665.892 | -68581.368 | -94138.267 | -70952.039 | -118094.449 | -25337.411 | -274033.883 |
| 6-311+G**| -1807.433 | -80782.312 | -330666.344 | -68584.218 | -94142.028 | -70954.170 | -118099.154 | -25337.590 | -274044.591 |
| aug-cc-pVDZ | -1806.234 | -80759.757 | -330666.737 | -68671.079 | -94125.957 | -70939.602 | -118075.951 | -25330.169 | -273987.721 |
| aug-cc-pVTZ | -1813.850 | -80824.120 | -330710.027 | -68623.913 | -94199.170 | -70994.498 | -118171.306 | -25359.530 | -274217.469 |
| aug-cc-pVQZ | -1815.382 | -80846.214 | -330725.507 | -68642.049 | -94223.960 | -71013.654 | -118204.068 | -25367.660 | -274293.473 |
Table S6. EC-RISM<sup>t</sup> results (in kcal mol<sup>-1</sup>) for the Gibbs energies of gas molecules in Amber/OPLS benzene solution.

|        | He    | Ne    | Ar    | N<sub>2</sub> | O<sub>2</sub> | CO    | CO<sub>2</sub> | CH<sub>4</sub> | CF<sub>4</sub> |
|--------|-------|-------|-------|-------------|------------| ------|-------------|-------------|-------------|
| **HF** |       |       |       |             |            |       |             |              |             |
| 6-31G* | -1788.938 | -80616.155 | -330552.842 | -86859.962 | -93883.639 | -70740.934 | -117740.376 | -25221.973 | -273367.834 |
| 6-311G** | -1791.909 | -80646.368 | -330573.472 | -86877.556 | -93910.065 | -70760.766 | -117773.929 | -25230.641 | -273442.559 |
| 6-311+G** | -1791.909 | -80648.926 | -330573.857 | -86878.892 | -93912.667 | -70761.728 | -117776.434 | -25230.684 | -273446.607 |
| aug-cc-pVDZ | -1789.279 | -80629.922 | -330599.922 | -86871.219 | -93901.459 | -70751.964 | -117759.266 | -25224.736 | -273399.487 |
| aug-cc-pVTZ | -1792.717 | -80653.093 | -330577.690 | -86837.479 | -93924.156 | -70769.200 | -117789.242 | -25233.579 | -273479.843 |
| aug-cc-pVQZ | -1792.930 | -80659.672 | -330579.854 | -86891.959 | -93930.811 | -70774.137 | -117797.457 | -25235.238 | -273499.262 |
| **B3LYP** |       |       |       |             |            |       |             |              |             |
| 6-31G* | -1821.496 | -80879.680 | -331019.330 | -86723.981 | -94324.161 | -71099.548 | -118334.412 | -25424.781 | -274516.698 |
| 6-311G** | -1825.249 | -80915.160 | -331041.958 | -86743.964 | -94352.260 | -71122.637 | -118372.228 | -25434.378 | -274602.909 |
| 6-311+G** | -1825.249 | -80921.119 | -331042.376 | -86746.313 | -94355.781 | -71124.400 | -118375.865 | -25434.477 | -274610.898 |
| aug-cc-pVDZ | -1822.781 | -80900.777 | -331037.040 | -86735.679 | -94342.779 | -71112.599 | -118355.236 | -25426.099 | -274559.348 |
| aug-cc-pVTZ | -1826.294 | -80924.809 | -331046.214 | -86753.132 | -94364.680 | -71130.522 | -118386.090 | -25437.297 | -274637.827 |
| aug-cc-pVQZ | -1826.524 | -80931.623 | -331048.518 | -86757.801 | -94371.635 | -71135.774 | -118394.935 | -25439.304 | -274658.770 |
| **PBE0** |       |       |       |             |            |       |             |              |             |
| 6-31G* | -1809.350 | -80814.148 | -330908.497 | -86846.270 | -94229.030 | -71019.301 | -118209.965 | -25386.187 | -274262.907 |
| 6-311G** | -1812.744 | -80847.548 | -330929.992 | -86864.405 | -94255.008 | -71040.144 | -118244.691 | -25394.734 | -274343.483 |
| 6-311+G** | -1812.744 | -80852.643 | -330930.316 | -86866.385 | -94258.082 | -71041.624 | -118247.852 | -25394.857 | -274350.238 |
| aug-cc-pVDZ | -1810.396 | -80833.349 | -330925.755 | -86857.681 | -94246.653 | -71031.286 | -118229.708 | -25388.157 | -274302.447 |
| aug-cc-pVTZ | -1813.739 | -80856.381 | -330934.291 | -86873.246 | -94267.774 | -71047.818 | -118258.233 | -25397.257 | -274377.683 |
| aug-cc-pVQZ | -1813.951 | -80863.155 | -330936.494 | -86877.875 | -94274.707 | -71053.010 | -118266.985 | -25399.148 | -274398.390 |
| **MP2** |       |       |       |             |            |       |             |              |             |
| 6-31G* | -1795.966 | -80710.480 | -330639.004 | -86555.257 | -94091.742 | -70918.553 | -118037.159 | -25308.176 | -273871.136 |
| 6-311G** | -1807.396 | -80777.529 | -330665.917 | -86581.473 | -94138.308 | -70952.177 | -118094.545 | -25337.435 | -274033.817 |
| 6-311+G** | -1807.397 | -80782.292 | -330666.366 | -86584.314 | -94142.068 | -70954.308 | -118099.237 | -25337.610 | -274044.713 |
| aug-cc-pVDZ | -1806.198 | -80759.734 | -330666.760 | -86571.143 | -94125.983 | -70939.727 | -118076.022 | -25330.185 | -273987.845 |
| aug-cc-pVTZ | -1813.815 | -80824.100 | -330710.049 | -86623.225 | -94199.200 | -70994.619 | -118171.379 | -25359.550 | -274217.595 |
| aug-cc-pVQZ | -1815.347 | -80846.193 | -330725.527 | -86642.122 | -94223.991 | -71013.773 | -118204.141 | -25367.682 | -274293.600 |
Table S7. EC-RISM\textsuperscript{o} results (in kcal mol\textsuperscript{-1}) for the Gibbs energies of gas molecules in Amber/OPLS hexafluorobenzene solution.

|        | He     | Ne     | Ar     | N\textsubscript{2} | O\textsubscript{2} | CO     | CO\textsubscript{2} | CH\textsubscript{4} | CF\textsubscript{4} |
|--------|--------|--------|--------|---------------------|---------------------|--------|--------------------|---------------------|---------------------|
| HF     |        |        |        |                     |                     |        |                    |                     |                     |
| 6-31G* | -1789.309 | -80616.574 | -330535.386 | -68360.867 | -93884.254 | -70741.656 | -117741.332 | -25222.230 | -273368.844 |
| 6-311G* | -1792.280 | -80648.767 | -330574.021 | -68378.264 | -93910.866 | -70761.486 | -117774.884 | -25230.942 | -273443.593 |
| 6-311+G* | -1792.280 | -80649.347 | -330574.210 | -68379.606 | -93913.293 | -70762.464 | -117777.414 | -25230.999 | -273447.661 |
| aug-cc-pVDZ | -1789.650 | -80630.345 | -330570.475 | -68371.931 | -93902.079 | -70752.697 | -117760.236 | -25225.075 | -273400.518 |
| aug-cc-pVTZ | -1793.088 | -80653.514 | -330578.243 | -68388.185 | -93924.774 | -70769.929 | -117790.193 | -25233.908 | -273480.868 |
| aug-cc-pVQZ | -1793.300 | -80660.092 | -330580.410 | -68392.666 | -93931.429 | -70774.866 | -117798.403 | -25235.566 | -273500.283 |
| B3LYP  |        |        |        |                     |                     |        |                    |                     |                     |
| 6-31G* | -1821.870 | -80880.099 | -331019.875 | -68724.694 | -94324.785 | -71100.260 | -118335.331 | -25425.034 | -274517.698 |
| 6-311G* | -1825.621 | -80915.579 | -331042.508 | -68744.680 | -94352.890 | -71123.349 | -118373.153 | -25434.719 | -274603.941 |
| 6-311+G* | -1825.621 | -80921.541 | -331042.936 | -68747.042 | -94356.422 | -71125.140 | -118376.829 | -25434.853 | -274611.969 |
| aug-cc-pVDZ | -1823.155 | -80901.209 | -331037.610 | -68736.416 | -94343.428 | -71113.338 | -118356.193 | -25426.516 | -274560.398 |
| aug-cc-pVTZ | -1826.667 | -80925.236 | -331046.776 | -68753.856 | -94365.320 | -71131.254 | -118387.033 | -25437.690 | -274638.870 |
| aug-cc-pVQZ | -1826.897 | -80932.048 | -331049.082 | -68758.525 | -94372.273 | -71136.506 | -118395.872 | -25439.696 | -274659.808 |
| PBE0   |        |        |        |                     |                     |        |                    |                     |                     |
| 6-31G* | -1809.723 | -80814.567 | -330909.042 | -68646.982 | -94229.651 | -71020.012 | -118210.880 | -25386.421 | -274263.897 |
| 6-311G* | -1813.116 | -80847.967 | -330930.541 | -68665.120 | -94255.635 | -71040.854 | -118245.612 | -25395.039 | -274344.504 |
| 6-311+G* | -1813.116 | -80853.065 | -330930.874 | -68667.111 | -94258.719 | -71042.359 | -118248.808 | -25395.198 | -274351.293 |
| aug-cc-pVDZ | -1810.770 | -80833.778 | -330926.317 | -68658.410 | -94247.293 | -71032.018 | -118230.656 | -25388.532 | -274303.479 |
| aug-cc-pVTZ | -1814.111 | -80856.807 | -330934.850 | -68673.966 | -94268.408 | -71048.544 | -118259.165 | -25397.616 | -274378.713 |
| aug-cc-pVQZ | -1814.323 | -80863.579 | -330937.057 | -68678.596 | -94275.341 | -71053.737 | -118267.913 | -25399.506 | -274399.412 |
| MP2    |        |        |        |                     |                     |        |                    |                     |                     |
| 6-31G* | -1796.337 | -80710.899 | -330639.548 | -68555.983 | -94092.370 | -70919.251 | -118038.050 | -25308.435 | -273872.142 |
| 6-311G* | -1807.768 | -80777.948 | -330666.466 | -68582.202 | -94138.941 | -70952.876 | -118095.434 | -25337.758 | -274034.846 |
| 6-311+G* | -1807.768 | -80782.714 | -330666.922 | -68585.055 | -94142.708 | -70955.030 | -118100.168 | -25337.958 | -274045.774 |
| aug-cc-pVDZ | -1806.569 | -80760.162 | -330667.318 | -68571.886 | -94126.622 | -70940.449 | -118076.953 | -25330.563 | -273988.889 |
| aug-cc-pVTZ | -1814.185 | -80824.523 | -330710.605 | -68623.951 | -94199.833 | -70995.335 | -118172.286 | -25359.900 | -274216.619 |
| aug-cc-pVQZ | -1815.718 | -80846.615 | -330726.086 | -68642.851 | -94224.623 | -71014.489 | -118205.042 | -25368.026 | -274294.620 |
Table S8. EC-RISM\textsuperscript{a} results (in kcal mol\textsuperscript{-1}) for the Gibbs energies of gas molecules in Cornell benzene solution.

|       | He    | Ne     | Ar     | N\textsubscript{2} | O\textsubscript{2} | CO     | CO\textsubscript{2} | CH\textsubscript{4} | CF\textsubscript{4} |
|-------|-------|--------|--------|------------------|------------------|--------|------------------|------------------|------------------|
| HF    |       |        |        |                  |                  |        |                  |                  |                  |
| 6-31G*| -1788.972 | -80616.174 | -330552.811 | -883599.915 | -938833.590 | -70740.866 | -117740.194 | -25221.896 | -273367.670 |
| 6-311G**| -1791.944 | -80646.387 | -330573.441 | -883777.508 | -93910.015 | -70760.701 | -117773.745 | -25230.567 | -273442.392 |
| 6-311+G**| -1791.944 | -80648.946 | -330573.827 | -883878.844 | -93912.618 | -70761.662 | -117776.249 | 25230.611 | -273446.441 |
| aug-cc-pVDZ | -1789.314 | -80629.941 | -330569.891 | -88371.175 | -93901.412 | -70751.899 | -117759.090 | -25224.665 | -273399.324 |
| aug-cc-pVQZ | -1792.752 | -80653.112 | -330577.659 | -88387.433 | -93924.108 | -70769.137 | -117789.068 | -25233.507 | -273479.679 |
| aug-cc-pVQZ | -1792.964 | -80659.691 | -330579.824 | -88391.914 | -93930.763 | -70774.075 | -117797.283 | -25235.166 | -273499.098 |
| B3LYP |       |        |        |                  |                  |        |                  |                  |                  |
| 6-31G*| -1821.531 | -80879.699 | -331019.300 | -88723.935 | -94324.113 | -71099.489 | -118334.230 | -25424.704 | -274516.533 |
| 6-311G**| -1825.284 | -80915.179 | -331041.928 | -88743.916 | -94352.211 | -71122.580 | -118372.044 | -25434.309 | -274602.742 |
| 6-311+G**| -1825.284 | -80921.138 | -331042.347 | -88746.267 | -94355.733 | -71124.342 | -118375.679 | -25434.411 | -274610.732 |
| aug-cc-pVDZ | -1822.815 | -80900.797 | -331037.011 | -88735.637 | -94342.734 | -71112.542 | -118355.061 | -25426.038 | -274559.186 |
| aug-cc-pVQZ | -1826.329 | -80924.829 | -331046.184 | -88753.089 | -94364.634 | -71130.466 | -118385.917 | -25437.232 | -274637.663 |
| aug-cc-pVQZ | -1826.559 | -80931.642 | -331048.488 | -88757.758 | -94371.589 | -71135.719 | -118394.762 | -25439.239 | -274658.607 |
| PBE0  |       |        |        |                  |                  |        |                  |                  |                  |
| 6-31G*| -1809.385 | -80814.167 | -330908.466 | -88646.224 | -94228.981 | -71019.242 | -118209.783 | -25386.108 | -274262.742 |
| 6-311G**| -1812.778 | -80847.567 | -330929.961 | -88664.357 | -94254.959 | -71040.087 | -118244.508 | -25394.662 | -274343.316 |
| 6-311+G**| -1812.778 | -80852.662 | -330930.286 | -88666.339 | -94258.034 | -71041.566 | -118247.667 | -25394.788 | -274350.072 |
| aug-cc-pVDZ | -1810.431 | -80833.369 | -330925.725 | -88657.638 | -94246.607 | -71031.229 | -118229.533 | -25388.090 | -274302.285 |
| aug-cc-pVQZ | -1813.773 | -80856.401 | -330934.261 | -88673.202 | -94267.727 | -71047.762 | -118258.060 | -25397.188 | -274377.520 |
| aug-cc-pVQZ | -1813.986 | -80863.175 | -330936.464 | -88677.832 | -94274.660 | -71052.955 | -118266.812 | -25399.079 | -274398.226 |
| MP2   |       |        |        |                  |                  |        |                  |                  |                  |
| 6-31G*| -1796.000 | -80710.499 | -330638.973 | -88555.209 | -94091.694 | -70918.508 | -118037.010 | -25308.099 | -273870.975 |
| 6-311G**| -1807.432 | -80777.548 | -330665.886 | -88581.424 | -94138.260 | -70952.133 | -118094.394 | -25337.364 | -274033.653 |
| 6-311+G**| -1807.432 | -80782.312 | -330666.336 | -88584.266 | -94142.019 | -70954.264 | -118099.082 | -25337.541 | -274044.551 |
| aug-cc-pVDZ | -1806.233 | -80759.754 | -330666.730 | -88671.099 | -94125.937 | -70939.683 | -118075.874 | -25330.117 | -273987.685 |
| aug-cc-pVTZ | -1813.849 | -80824.119 | -330710.019 | -88623.178 | -94199.153 | -70994.575 | -118171.232 | -25359.478 | -274217.435 |
| aug-cc-pVQZ | -1815.381 | -80846.213 | -330725.497 | -88642.076 | -94223.944 | -71013.729 | -118203.994 | -25367.609 | -274293.440 |
Table S9. 3D-RISM results (in kcal mol\(^{-1}\)) for the Gibbs energies (excess chemical potentials) of gas molecules in Amber/OPLS benzene solution with vacuum solute charges. Charges on noble gases are zero, so only their pure Lennard-Jones (LJ) result is reported in the first line.

|        | He     | Ne     | Ar     | N\(_2\) | O\(_2\) | CO     | CO\(_2\) | CH\(_4\) | CF\(_4\) |
|--------|--------|--------|--------|---------|--------|--------|---------|---------|---------|
| **LJ** | 2.702  | 2.763  | 2.717  |         |        |        |         |         |         |
| **HF** |        |        |        |         |        |        |         |         |         |
| 6-31G* | 3.448  | 3.026  | 3.291  | 1.815   | 0.830  | 3.677  |         |         |         |
| 6-311G** | 3.436  | 3.010  | 3.286  | 1.779   | 0.833  | 3.632  |         |         |         |
| 6-311+G** | 3.436  | 3.012  | 3.282  | 1.750   | 0.832  | 3.629  |         |         |         |
| aug-cc-pVDZ | 3.448  | 3.018  | 3.290  | 1.844   | 0.842  | 3.685  |         |         |         |
| aug-cc-pVTZ | 3.431  | 3.014  | 3.283  | 1.852   | 0.821  | 3.637  |         |         |         |
| aug-cc-pVQZ | 3.429  | 3.012  | 3.282  | 1.851   | 0.821  | 3.631  |         |         |         |
| **B3LYP** |        |        |        |         |        |        |         |         |         |
| 6-31G* | 3.490  | 3.094  | 3.310  | 1.865   | 0.844  | 3.832  |         |         |         |
| 6-311G** | 3.474  | 3.081  | 3.306  | 1.833   | 0.842  | 3.799  |         |         |         |
| 6-311+G** | 3.474  | 3.081  | 3.300  | 1.796   | 0.841  | 3.802  |         |         |         |
| aug-cc-pVDZ | 3.488  | 3.085  | 3.310  | 1.898   | 0.853  | 3.853  |         |         |         |
| aug-cc-pVTZ | 3.468  | 3.081  | 3.303  | 1.913   | 0.836  | 3.811  |         |         |         |
| aug-cc-pVQZ | 3.466  | 3.078  | 3.302  | 1.912   | 0.836  | 3.805  |         |         |         |
| **PBE0** |        |        |        |         |        |        |         |         |         |
| 6-31G* | 3.485  | 3.077  | 3.308  | 1.857   | 0.843  | 3.789  |         |         |         |
| 6-311G** | 3.471  | 3.063  | 3.304  | 1.825   | 0.841  | 3.753  |         |         |         |
| 6-311+G** | 3.472  | 3.063  | 3.298  | 1.796   | 0.840  | 3.754  |         |         |         |
| aug-cc-pVDZ | 3.484  | 3.068  | 3.308  | 1.889   | 0.850  | 3.807  |         |         |         |
| aug-cc-pVTZ | 3.466  | 3.064  | 3.301  | 1.905   | 0.836  | 3.766  |         |         |         |
| aug-cc-pVQZ | 3.464  | 3.061  | 3.300  | 1.904   | 0.836  | 3.760  |         |         |         |
| **MP2** |        |        |        |         |        |        |         |         |         |
| 6-31G* | 3.528  | 3.141  | 3.319  | 1.888   | 0.838  | 3.839  |         |         |         |
| 6-311G** | 3.511  | 3.108  | 3.315  | 1.841   | 0.840  | 3.767  |         |         |         |
| 6-311+G** | 3.512  | 3.107  | 3.307  | 1.812   | 0.839  | 3.770  |         |         |         |
| aug-cc-pVDZ | 3.530  | 3.122  | 3.320  | 1.930   | 0.853  | 3.865  |         |         |         |
| aug-cc-pVTZ | 3.503  | 3.109  | 3.312  | 1.926   | 0.832  | 3.779  |         |         |         |
| aug-cc-pVQZ | 3.497  | 3.101  | 3.310  | 1.920   | 0.830  | 3.780  |         |         |         |
Table S10. 3D-RISM results (in kcal mol$^{-1}$) for the Gibbs energies (excess chemical potentials) of gas molecules in Amber/OPLS hexafluorobenzene solution with vacuum solute charges. Charges on noble gases are zero, so only their pure Lennard-Jones (LJ) result is reported in the first line.

|       | He   | Ne   | Ar   | N$_2$ | O$_2$ | CO   | CO$_2$ | CH$_4$ | CF$_4$ |
|-------|------|------|------|-------|-------|------|-------|-------|--------|
| HF    |      |      |      |       |       |      |       |       |        |
| 6-31G*| 2.786| 2.434| 2.622| 0.859 | 0.704 | 2.651|
| 6-311G**| 2.775| 2.420| 2.622| 0.823 | 0.706 | 2.582|
| 6-311+G**| 2.776| 2.422| 2.616| 0.785 | 0.705 | 2.571|
| aug-cc-pVDZ| 2.786| 2.427| 2.623| 0.898 | 0.715 | 2.649|
| aug-cc-pVTZ| 2.771| 2.424| 2.619| 0.917 | 0.699 | 2.605|
| aug-cc-pVQZ| 2.769| 2.422| 2.619| 0.918 | 0.698 | 2.602|
| B3LYP |      |      |      |       |       |      |       |       |        |
| 6-31G*| 2.821| 2.492| 2.629| 0.886 | 0.720 | 2.775|
| 6-311G**| 2.808| 2.481| 2.632| 0.857 | 0.717 | 2.714|
| 6-311+G**| 2.808| 2.481| 2.622| 0.809 | 0.717 | 2.708|
| aug-cc-pVDZ| 2.820| 2.485| 2.631| 0.932 | 0.728 | 2.786|
| aug-cc-pVTZ| 2.802| 2.481| 2.628| 0.961 | 0.712 | 2.746|
| aug-cc-pVQZ| 2.801| 2.479| 2.628| 0.963 | 0.711 | 2.743|
| PBE0  |      |      |      |       |       |      |       |       |        |
| 6-31G*| 2.817| 2.477| 2.628| 0.881 | 0.719 | 2.741|
| 6-311G**| 2.806| 2.465| 2.631| 0.852 | 0.716 | 2.678|
| 6-311+G**| 2.806| 2.465| 2.621| 0.814 | 0.716 | 2.670|
| aug-cc-pVDZ| 2.816| 2.470| 2.631| 0.925 | 0.726 | 2.748|
| aug-cc-pVTZ| 2.801| 2.467| 2.628| 0.955 | 0.713 | 2.710|
| aug-cc-pVQZ| 2.799| 2.464| 2.628| 0.956 | 0.712 | 2.707|
| MP2   |      |      |      |       |       |      |       |       |        |
| 6-31G*| 2.854| 2.532| 2.630| 0.902 | 0.714 | 2.781|
| 6-311G**| 2.839| 2.504| 2.635| 0.856 | 0.715 | 2.689|
| 6-311+G**| 2.840| 2.503| 2.623| 0.816 | 0.715 | 2.684|
| aug-cc-pVDZ| 2.855| 2.516| 2.633| 0.956 | 0.729 | 2.797|
| aug-cc-pVTZ| 2.832| 2.504| 2.631| 0.964 | 0.708 | 2.721|
| aug-cc-pVQZ| 2.828| 2.498| 2.632| 0.962 | 0.705 | 2.723|
Table S11. 3D-RISM results (in kcal mol\(^{-1}\)) for the Gibbs energies (excess chemical potentials) of gas molecules in Cornell benzene solution with vacuum solute charges. Charges on noble gases are zero, so only their pure Lennard-Jones (LJ) result is reported in the first line.

|          | He  | Ne  | Ar  | N\(_2\) | O\(_2\) | CO  | CO\(_2\) | CH\(_4\) | CF\(_4\) |
|----------|-----|-----|-----|---------|--------|-----|---------|---------|---------|
| **LJ**   |     |     |     |         |        |     |         |         |         |
| 6-31G*   | 2.667 | 2.744 | 2.748 |         |        |     |         |         |         |
| 6-311G** | 3.484 | 3.069 | 3.342 | 2.001   | 0.924  | 3.834 |         |         |         |
| 6-311+G**| 3.471 | 3.054 | 3.335 | 1.966   | 0.926  | 3.792 |         |         |         |
| aug-cc-pVDZ| 3.483 | 3.062 | 3.341 | 2.026   | 0.936  | 3.842 |         |         |         |
| aug-cc-pVTZ| 3.466 | 3.058 | 3.333 | 2.032   | 0.916  | 3.795 |         |         |         |
| aug-cc-pVQZ| 3.464 | 3.055 | 3.331 | 2.030   | 0.915  | 3.789 |         |         |         |
| **HF**   |     |     |     |         |        |     |         |         |         |
| 6-31G*   | 3.525 | 3.137 | 3.365 | 2.053   | 0.939  | 3.988 |         |         |         |
| 6-311G** | 3.509 | 3.124 | 3.358 | 2.021   | 0.936  | 3.959 |         |         |         |
| 6-311+G**| 3.510 | 3.124 | 3.354 | 1.989   | 0.936  | 3.962 |         |         |         |
| aug-cc-pVDZ| 3.523 | 3.128 | 3.364 | 2.081   | 0.947  | 4.010 |         |         |         |
| aug-cc-pVTZ| 3.503 | 3.124 | 3.355 | 2.092   | 0.931  | 3.968 |         |         |         |
| aug-cc-pVQZ| 3.501 | 3.121 | 3.354 | 2.092   | 0.930  | 3.963 |         |         |         |
| **B3LYP**|     |     |     |         |        |     |         |         |         |
| 6-31G*   | 3.520 | 3.120 | 3.363 | 2.044   | 0.938  | 3.946 |         |         |         |
| 6-311G** | 3.507 | 3.106 | 3.357 | 2.013   | 0.935  | 3.913 |         |         |         |
| 6-311+G**| 3.507 | 3.106 | 3.352 | 1.988   | 0.935  | 3.914 |         |         |         |
| aug-cc-pVDZ| 3.519 | 3.111 | 3.362 | 2.072   | 0.944  | 3.965 |         |         |         |
| aug-cc-pVTZ| 3.501 | 3.107 | 3.354 | 2.085   | 0.931  | 3.923 |         |         |         |
| aug-cc-pVQZ| 3.499 | 3.105 | 3.352 | 2.084   | 0.930  | 3.918 |         |         |         |
| **PBE0** |     |     |     |         |        |     |         |         |         |
| 6-31G*   | 3.563 | 3.184 | 3.376 | 2.076   | 0.932  | 3.995 |         |         |         |
| 6-311G** | 3.546 | 3.151 | 3.369 | 2.031   | 0.934  | 3.927 |         |         |         |
| 6-311+G**| 3.547 | 3.150 | 3.363 | 2.005   | 0.934  | 3.931 |         |         |         |
| aug-cc-pVDZ| 3.564 | 3.165 | 3.377 | 2.114   | 0.948  | 4.022 |         |         |         |
| aug-cc-pVTZ| 3.538 | 3.151 | 3.367 | 2.107   | 0.926  | 3.937 |         |         |         |
| aug-cc-pVQZ| 3.532 | 3.143 | 3.364 | 2.101   | 0.924  | 3.937 |         |         |         |
### Table S12. EC-RISM^q results for the Gibbs energies of gas molecules in uncharged Amber/OPLS benzene (q_0-C_6H_6) solution.

|          | He   | Ne   | Ar   | N_2  | O_2  | CO   | CO_2 | CH_4 | CF_4 |
|----------|------|------|------|------|------|------|------|------|------|
| B3LYP    | -1825.236 | -80915.106 | -331041.816 | -68743.762 | -94352.121 | -71122.352 | -118371.421 | -25434.369 | -274602.643 |
| aug-cc-pVTZ | -1826.267 | -80924.761 | -331046.079 | -68752.965 | -94364.563 | -71130.259 | -118385.381 | -25437.311 | -274637.592 |

### Table S13. EC-RISM^q results for the Gibbs energies of gas molecules in uncharged Amber/OPLS hexafluorobenzene (q_0-C_6F_6) solution.

|          | He   | Ne   | Ar   | N_2  | O_2  | CO   | CO_2 | CH_4 | CF_4 |
|----------|------|------|------|------|------|------|------|------|------|
| B3LYP    | -1825.581 | -80915.503 | -331042.323 | -68744.381 | -94352.682 | -71122.964 | -118372.016 | -25434.569 | -274603.489 |
| aug-cc-pVTZ | -1826.618 | -80925.158 | -331046.587 | -68753.583 | -94365.124 | -71130.870 | -118385.976 | -25437.511 | -274638.438 |

### Table S14. 1D RISM/PSE-1 results for the Gibbs energies of gas molecules in Amber/OPLS benzene solution.

|          | He   | Ne   | Ar   | N_2  | O_2  | CO   | CO_2 | CH_4 | CF_4 |
|----------|------|------|------|------|------|------|------|------|------|
| MP2      |       |      |      |      |      |      |      |      |      |
| aug-cc-pVTZ | 2.707 | 2.769 | 2.727 | 4.874 | 4.237 | 4.658 | 4.221 | 2.509 | 9.414 |

### Table S15. 1D RISM/PSE-1 results for the Gibbs energies of gas molecules in Amber/OPLS hexafluorobenzene solution.

|          | He   | Ne   | Ar   | N_2  | O_2  | CO   | CO_2 | CH_4 | CF_4 |
|----------|------|------|------|------|------|------|------|------|------|
| MP2      |       |      |      |      |      |      |      |      |      |
| aug-cc-pVTZ | 2.340 | 2.352 | 2.188 | 4.048 | 3.510 | 3.811 | 3.079 | 2.229 | 7.723 |
### Table S16. EC-RISM $^\text{c}$ results for the Gibbs energies of gas molecules in charge-reversed Amber/OPLS benzene (q_{rev}-C$_6$H$_6$) solution.

|        | He   | Ne   | Ar   | N$_2$ | O$_2$ | CO   | CO$_2$ | CH$_4$ | CF$_4$ |
|--------|------|------|------|-------|-------|------|--------|--------|--------|
| HF     |      |      |      |       |       |      |        |        |        |
| 6-31G* | -1788.995 | -80618.205 | -330552.844 | -68359.958 | -93883.665 | -70740.852 | -117740.790 | -25221.960 | -273367.989 |
| 6-311G** | -1791.966 | -80646.417 | -330573.477 | -68377.538 | -93910.082 | -70760.682 | -117774.347 | -25230.641 | -273442.750 |
| 6-311+G** | -1791.968 | -80648.977 | -330573.686 | -68378.881 | -93912.689 | -70761.650 | -117776.881 | -25230.687 | -273446.819 |
| aug-cc-pVDZ | -1789.337 | -80629.974 | -330569.929 | -68371.237 | -93901.497 | -70751.898 | -117759.690 | -25224.743 | -273399.666 |
| aug-cc-pVTZ | -1792.775 | -80653.144 | -330577.697 | -68387.488 | -93924.189 | -70769.137 | -117789.653 | -25233.591 | -273480.022 |
| aug-cc-pVQZ | -1792.987 | -80659.722 | -330579.864 | -68391.968 | -93930.844 | -70774.075 | -117797.866 | -25235.250 | -273499.438 |

|        |      |      |      |       |       |      |        |        |        |
| B3LYP  |      |      |      |       |       |      |        |        |        |
| 6-31G* | -1821.556 | -80879.730 | -331019.333 | -68723.987 | -94324.195 | -71099.462 | -118334.816 | -25424.758 | -274516.828 |
| 6-311G** | -1825.308 | -80915.209 | -331041.964 | -68743.956 | -94352.288 | -71122.547 | -118372.634 | -25434.401 | -274603.083 |
| 6-311+G** | -1825.308 | -80921.171 | -331042.388 | -68746.317 | -94355.818 | -71124.324 | -118376.319 | -25434.514 | -274611.109 |
| aug-cc-pVDZ | -1822.840 | -80900.835 | -331037.057 | -68735.720 | -94342.836 | -71112.537 | -118355.671 | -25426.161 | -274559.527 |
| aug-cc-pVTZ | -1826.353 | -80924.864 | -331046.227 | -68753.158 | -94364.729 | -71130.461 | -118386.499 | -25437.348 | -274638.005 |
| aug-cc-pVQZ | -1826.563 | -80931.676 | -331048.533 | -68757.828 | -94371.683 | -71135.714 | -118395.341 | -25439.355 | -274658.945 |

|        |      |      |      |       |       |      |        |        |        |
| PBE0   |      |      |      |       |       |      |        |        |        |
| 6-31G* | -1809.409 | -80814.198 | -330908.499 | -68646.274 | -94229.061 | -71019.214 | -118210.365 | -25386.133 | -274263.031 |
| 6-311G** | -1812.802 | -80847.598 | -330929.997 | -68664.396 | -94255.033 | -71040.052 | -118245.093 | -25394.718 | -274343.649 |
| 6-311+G** | -1812.802 | -80852.695 | -330930.327 | -68666.387 | -94258.115 | -71041.544 | -118248.291 | -25394.854 | -274350.436 |
| aug-cc-pVDZ | -1810.455 | -80833.405 | -330925.767 | -68657.715 | -94246.704 | -71031.219 | -118230.135 | -25388.171 | -274302.613 |
| aug-cc-pVTZ | -1813.797 | -80856.435 | -330934.302 | -68673.269 | -94267.819 | -71047.752 | -118258.635 | -25397.268 | -274377.848 |
| aug-cc-pVQZ | -1814.009 | -80863.208 | -330936.507 | -68677.899 | -94274.751 | -71052.947 | -118267.384 | -25399.159 | -274386.552 |

|        |      |      |      |       |       |      |        |        |        |
| MP2    |      |      |      |       |       |      |        |        |        |
| 6-31G* | -1796.023 | -80710.530 | -330639.006 | -68555.248 | -94091.779 | -70918.474 | -118037.437 | -25308.168 | -273871.259 |
| 6-311G** | -1807.455 | -80777.579 | -330665.923 | -68581.450 | -94138.338 | -70952.091 | -118094.831 | -25337.464 | -274033.975 |
| 6-311+G** | -1807.455 | -80782.345 | -330666.379 | -68584.306 | -94142.103 | -70954.233 | -118099.576 | -25337.656 | -274044.907 |
| aug-cc-pVDZ | -1806.256 | -80759.792 | -330666.774 | -68571.174 | -94126.035 | -70939.668 | -118076.355 | -25330.242 | -273988.009 |
| aug-cc-pVTZ | -1813.872 | -80824.154 | -330710.060 | -68624.001 | -94199.245 | -70994.563 | -118171.694 | -25359.588 | -274217.747 |
| aug-cc-pVQZ | -1815.404 | -80846.246 | -330725.540 | -68642.135 | -94224.035 | -71013.719 | -118204.454 | -25367.715 | -274293.748 |
Table S17. EC-RISM$^\circ$ results for the Gibbs energies of gas molecules in charge-reversed Amber/OPLS benzene ($q_{\text{rev}}$-C$_6$F$_{13}$) solution.

|       | He   | Ne   | Ar   | N$_2$ | O$_2$ | CO   | CO$_2$ | CH$_4$ | CF$_4$ |
|-------|------|------|------|-------|-------|------|--------|--------|--------|
| HF    |      |      |      |       |       |      |        |        |        |
| 6-31G*| -1789.318 | -80616.569 | -330553.310 | -68360.521 | -93884.174 | -70741.420 | -117740.832 | -25222.185 | -273368.589 |
| 6-311G* | -1792.289 | -80646.782 | -330573.944 | -68378.100 | -93910.590 | -70761.253 | -117774.381 | -25230.867 | -273443.297 |
| 6-311+G* | -1792.289 | -80649.342 | -330574.132 | -68379.443 | -93913.197 | -70762.218 | -117776.897 | -25230.915 | -273447.356 |
| aug-cc-pVDZ | -1789.660 | -80630.339 | -330570.396 | -68371.800 | -93902.006 | -70752.468 | -117759.748 | -25224.974 | -273400.256 |
| aug-cc-pVTZ | -1793.098 | -80653.509 | -330578.165 | -68388.049 | -93924.697 | -70769.707 | -117789.724 | -25233.820 | -273480.596 |
| aug-cc-pVQZ | -1793.310 | -80660.087 | -330580.331 | -68392.529 | -93931.352 | -70774.645 | -117797.939 | -25235.479 | -273500.013 |
| B3LYP  |      |      |      |       |       |      |        |        |        |
| 6-31G* | -1821.879 | -80808.095 | -331019.799 | -68724.554 | -94324.712 | -71100.044 | -118334.882 | -25424.990 | -274517.478 |
| 6-311G* | -1825.630 | -80915.574 | -331042.431 | -68744.523 | -94352.804 | -71123.130 | -118372.689 | -25434.631 | -274603.681 |
| 6-311+G* | -1825.630 | -80921.536 | -331042.856 | -68746.885 | -94356.334 | -71124.903 | -118376.346 | -25434.747 | -274611.688 |
| aug-cc-pVDZ | -1823.163 | -80901.200 | -331037.525 | -68736.289 | -94343.354 | -71113.117 | -118355.742 | -25426.389 | -274560.152 |
| aug-cc-pVTZ | -1826.676 | -80925.229 | -331046.694 | -68753.725 | -94365.246 | -71131.041 | -118386.587 | -25437.574 | -274638.619 |
| aug-cc-pVQZ | -1826.906 | -80932.041 | -331049.000 | -68758.394 | -94372.199 | -71136.295 | -118395.430 | -25439.581 | -274659.560 |
| PBE0   |      |      |      |       |       |      |        |        |        |
| 6-31G* | -1809.732 | -80814.562 | -330908.966 | -68646.842 | -94229.576 | -71019.796 | -118210.433 | -25386.385 | -274263.681 |
| 6-311G* | -1813.125 | -80847.962 | -330930.464 | -68664.963 | -94255.547 | -71040.636 | -118245.151 | -25394.965 | -274344.248 |
| 6-311+G* | -1813.125 | -80853.059 | -330930.794 | -68666.953 | -94258.629 | -71042.123 | -118248.326 | -25395.105 | -274351.018 |
| aug-cc-pVDZ | -1810.778 | -80833.770 | -330926.235 | -68658.283 | -94247.219 | -71031.799 | -118230.210 | -25388.418 | -274303.242 |
| aug-cc-pVTZ | -1814.120 | -80856.800 | -330934.770 | -68673.835 | -94268.333 | -71048.333 | -118258.727 | -25397.513 | -274378.467 |
| aug-cc-pVQZ | -1814.332 | -80863.573 | -330936.975 | -68678.465 | -94275.266 | -71053.528 | -118267.478 | -25399.404 | -274399.171 |
| MP2    |      |      |      |       |       |      |        |        |        |
| 6-31G* | -1796.346 | -80710.894 | -330639.473 | -68555.811 | -94092.299 | -70919.082 | -118037.672 | -25308.387 | -273871.918 |
| 6-311G* | -1807.778 | -80777.943 | -330666.389 | -68582.012 | -94138.855 | -70952.698 | -118095.053 | -25337.670 | -274034.585 |
| 6-311+G* | -1807.778 | -80782.708 | -330666.842 | -68584.864 | -94142.617 | -70954.831 | -118099.758 | -25337.851 | -274045.495 |
| aug-cc-pVDZ | -1806.579 | -80760.153 | -330667.236 | -68571.728 | -94126.547 | -70940.266 | -118076.663 | -25330.434 | -273988.648 |
| aug-cc-pVTZ | -1814.195 | -80824.516 | -330710.525 | -68624.557 | -94199.758 | -70995.160 | -118171.914 | -25359.788 | -274218.379 |
| aug-cc-pVQZ | -1815.727 | -80846.609 | -330726.005 | -68642.692 | -94224.547 | -71014.316 | -118204.674 | -25367.917 | -274294.383 |
**TABLE S18.** Maxima of the 3D RISM/PSE-1 spatial solvent site \((\gamma)\) distribution functions \(g_\gamma(r)\) around benzene and hexafluorobenzene (AMBER/OPLS). Additionally EC-RISM/\(^\phi/PSE-1/B3LYP/6-31G(d)\) data are shown.

| Solvent model | \(C_6H_6\) | \(C_6F_6\) |
|---------------|------------|------------|
| \(C_6H_6\)   | C          | 1.59       | 2.54       |
|               | H          | 2.30       | 1.58       |
| \(C_6F_6\)   | C          | 2.28       | 1.29       |
|               | F          | 1.84       | 2.83       |
| \(C_6H_6\)   | C          | 1.62       | 2.10       |
| \(\text{EC-RISM})^\phi\) | H | 2.04 | 1.57 |
| \(C_6F_6\)   | C          | 2.21       | 1.70       |
| \(\text{EC-RISM})^\phi\) | F | 1.89 | 2.12 |
| \(q_{rev}-C_6H_6\) | C | 2.27 | 1.60 |
|                   | H | 1.55 | 2.74 |
| \(q_{rev}-C_6F_6\) | C | 1.40 | 2.65 |
|                   | F | 2.50 | 1.89 |
| \(q_0-C_6H_6\)  | C | 1.77 | 1.81 |
|                   | H | 1.61 | 1.55 |
| \(q_0-C_6F_6\)  | C | 1.52 | 1.57 |
|                   | F | 1.96 | 1.92 |
**Table S19.** RMSD (kcal mol$^{-1}$) between various 3D/EC-RISM results and experimental data averaged over all gas molecules and divided into the different quantum-chemical levels of theory and solvation models.

|       | 3D RISM$^\text{vac}$ AMBER/OPLS | EC-RISM AMBER/OPLS | EC-RISM$^\phi$ AMBER/OPLS | 3D RISM$^\text{vac}$ Cornell | EC-RISM$^\phi$ Cornell | EC-RISM$^\phi$ Cornell | EC-RISM$^\phi$ ($X_{\text{rev}}$) |
|-------|----------------------------------|--------------------|-----------------------------|-------------------------------|------------------------|------------------------|-----------------------------|
| **HF** |                                 |                    |                             |                               |                        |                        |                             |
| 6-31G* | 0.241                            | 0.243              | 0.227                       | 0.276                         | 0.279                  | 0.279                  | 0.337                       |
| 6-311G** | 0.236                           | 0.238              | 0.221                       | 0.268                         | 0.271                  | 0.266                  | 0.338                       |
| aug-cc-pVDZ | 0.242                       | 0.236              | 0.217                       | 0.287                         | 0.277                  | 0.274                  | 0.343                       |
| aug-cc-pVTZ | 0.236                         | 0.233              | 0.213                       | 0.272                         | 0.264                  | 0.259                  | 0.322                       |
| aug-cc-pVQZ | 0.244                         | 0.223              | 0.209                       | 0.289                         | 0.256                  | 0.252                  | 0.321                       |
| **B3LYP** |                                 |                    |                             |                               |                        |                        |                             |
| 6-31G* | 0.238                            | 0.240              | 0.221                       | 0.276                         | 0.279                  | 0.269                  | 0.351                       |
| 6-311G** | 0.236                           | 0.238              | 0.220                       | 0.267                         | 0.271                  | 0.264                  | 0.337                       |
| aug-cc-pVDZ | 0.239                       | 0.233              | 0.216                       | 0.278                         | 0.269                  | 0.269                  | 0.324                       |
| aug-cc-pVTZ | 0.240                         | 0.235              | 0.213                       | 0.281                         | 0.270                  | 0.258                  | 0.332                       |
| aug-cc-pVQZ | 0.240                         | 0.233              | 0.213                       | 0.271                         | 0.264                  | 0.258                  | 0.322                       |
| **PBE0** |                                 |                    |                             |                               |                        |                        |                             |
| 6-31G* | 0.240                            | 0.242              | 0.225                       | 0.279                         | 0.283                  | 0.278                  | 0.356                       |
| 6-311G** | 0.243                           | 0.236              | 0.218                       | 0.283                         | 0.269                  | 0.258                  | 0.319                       |
| aug-cc-pVDZ | 0.236                       | 0.231              | 0.214                       | 0.272                         | 0.265                  | 0.263                  | 0.325                       |
| aug-cc-pVTZ | 0.242                         | 0.237              | 0.217                       | 0.285                         | 0.275                  | 0.270                  | 0.340                       |
| aug-cc-pVQZ | 0.238                         | 0.222              | 0.207                       | 0.276                         | 0.247                  | 0.243                  | 0.305                       |
| **MP2** |                                 |                    |                             |                               |                        |                        |                             |
| 6-31G* | 0.237                            | 0.239              | 0.224                       | 0.271                         | 0.275                  | 0.272                  | 0.336                       |
| 6-311G** | 0.240                           | 0.233              | 0.212                       | 0.282                         | 0.270                  | 0.260                  | 0.334                       |
| aug-cc-pVDZ | 0.235                       | 0.231              | 0.213                       | 0.272                         | 0.265                  | 0.262                  | 0.324                       |
| aug-cc-pVTZ | 0.242                         | 0.221              | 0.203                       | 0.285                         | 0.247                  | 0.239                  | 0.309                       |
| aug-cc-pVQZ | 0.237                         | 0.222              | 0.206                       | 0.274                         | 0.247                  | 0.242                  | 0.304                       |