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

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Figure S1. 1D RISM radial site-site distribution functions of benzene for various closure approximations and the Amber/OPLS force field.

Figure S2. 1D RISM radial site-site distribution functions of benzene for various closure approximations and the Cornell force field.

Figure S3. 1D RISM radial site-site distribution functions of hexafluorobenzene for various closure approximations and the Amber/OPLS force field.

Figure S4. 1D RISM radial site-site distribution functions of uncharged benzene (q_0 -C₆H₆) for various closure approximations and the Amber/OPLS Lennard-Jones force field.

Figure S5. 1D RISM radial site-site distribution functions of uncharged benzene (q_0 -C₆H₆) for various closure approximations and the Cornell Lennard-Jones force field.

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Figure S7. 1D RISM radial site-site distribution functions of reversed-charge benzene ($q_{\text{rev}}\text{-C}_6\text{H}_6$) for various closure approximations and the Amber/OPLS Lennard-Jones force field.

Figure S8. 1D RISM radial site-site distribution functions of charge-reversed benzene ($q_{rev}\text{-C}_6\text{H}_6$) for various closure approximations and the Cornell Lennard-Jones force field.

Figure S9. 1D RISM radial site-site distribution functions of charge-reversed hexafluorobenzene ($q_{\text{rev}}\text{-C}_6\text{F}_6$) for various closure approximations and the Amber/OPLS Lennard-Jones force field.

Figure S10. RMSD (kJ mol^{-1}) between experimental and pure 3D RISM, EC-RISM^q and EC-RISM^p results with the Cornell (upper three panels) and Amber/OPLS (q_{rev} only) solvent models averaged over all molecules and distinguished by the quantum-chemical level of theory.

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	-273371.665
6-311G**	-1794.613	-80649.113	-330576.122	-68381.052	-93913.104	-70764.176	-117776.791	-25231.584	-273446.430
6-311+G**	-1794.613	-80651.672	-330576.310	-68382.390	-93915.714	-70765.154	-117779.321	-25231.632	-273450.515
aug-cc-pVDZ	-1791.984	-80632.670	-330572.574	-68374.712	-93904.489	-70755.388	-117762.135	-25225.702	-273403.363
aug-cc-pVTZ	-1795.422	-80655.840	-330580.343	-68390.957	-93927.184	-70772.607	-117792.073	-25234.531	-273483.673
aug-cc-pVQZ	-1795.634	-80662.418	-330582.509	-68395.437	-93933.838	-70777.541	-117800.279	-25236.189	-273503.081
B3LYP									
6-31G*	-1824.202	-80882.425	-331021.977	-68727.535	-94327.267	-71102.945	-118336.995	-25425.717	-274520.589
6-311G**	-1827.955	-80917.905	-331044.609	-68747.521	-94355.372	-71126.029	-118374.822	-25435.360	-274606.852
6-311+G**	-1827.955	-80923.867	-331045.034	-68749.876	-94358.911	-71127.809	-118378.518	-25435.478	-274614.924
aug-cc-pVDZ	-1825.489	-80903.531	-331039.703	-68739.256	-94345.901	-71116.013	-118357.911	-25427.125	-274563.348
aug-cc-pVTZ	-1829.002	-80927.560	-331048.873	-68756.681	-94367.794	-71133.924	-118388.753	-25438.297	-274641.781
aug-cc-pVQZ	-1829.232	-80934.372	-331051.179	-68761.352	-94374.748	-71139.176	-118397.593	-25440.302	-274662.716
PBE0									
6-31G*	-1812.055	-80816.893	-330911.143	-68649.814	-94232.116	-71022.689	-118212.533	-25387.128	-274266.755
6-311G**	-1815.449	-80850.293	-330932.642	-68667.951	-94258.100	-71043.531	-118247.262	-25395.706	-274347.367
6-311+G**	-1815.449	-80855.390	-330932.973	-68669.937	-94261.190	-71045.024	-118250.466	-25395.849	-274354.188
aug-cc-pVDZ	-1813.104	-80836.101	-330928.413	-68661.239	-94249.748	-71034.690	-118232.342	-25389.166	-274306.391
aug-cc-pVTZ	-1816.446	-80859.131	-330936.949	-68676.784	-94270.866	-71051.211	-118260.853	-25398.249	-274381.567
aug-cc-pVQZ	-1816.658	-80865.904	-330939.154	-68681.415	-94277.799	-71056.404	-118269.600	-25400.140	-274402.272
MP2									
6-31G*	-1798.670	-80713.225	-330641.650	-68558.847	-94094.887	-70921.944	-118039.960	-25309.107	-273875.062
6-311G**	-1810.102	-80780.274	-330668.567	-68585.059	-94141.439	-70955.550	-118097.322	-25338.401	-274037.758
6-311+G**	-1810.102	-80785.039	-330669.022	-68587.906	-94145.208	-70957.699	-118102.053	-25338.586	-274048.710
aug-cc-pVDZ	-1808.903	-80762.485	-330669.416	-68574.734	-94129.118	-70943.129	-118078.848	-25331.186	-273991.860
aug-cc-pVTZ	-1816.520	-80826.848	-330712.704	-68627.548	-94202.322	-70998.002	-118174.157	-25360.515	-274221.512
aug-cc-pVQZ	-1818.052	-80848.941	-330728.184	-68645.681	-94227.106	-71017.154	-118206.907	-25368.640	-274297.534

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	N ₂	O ₂	CO	CO ₂	CH ₄	CF ₄
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	-70764.145	-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	-94355.366	-71126.006	-118374.737	-25435.353	-274606.818
6-311+G**	-1827.955	-80923.866	-331045.034	-68749.860	-94358.904	-71127.784	-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
PBE0									
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	-94277.795	-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^q 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	-80648.927	-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	-273987.874
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^q 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	-273368.882
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	-274344.542
6-311+G**	-1813.115	-80853.064	-330930.869	-68667.016	-94258.688	-71042.166	-118248.868	-25395.054	-274351.330
aug-cc-pVDZ	-1810.769	-80833.775	-330926.310	-68658.346	-94247.278	-71031.842	-118230.724	-25388.371	-274303.515
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	-274045.813
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^q 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	-80648.946	-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	-68391.898	-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	-274033.683
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	-68571.079	-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^φ 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*	-1788.938	-80616.155	-330552.842	-68359.962	-93883.639	-70740.934	-117740.376	-25221.973	-273367.834
6-311G**	-1791.909	-80646.368	-330573.472	-68377.556	-93910.065	-70760.766	-117773.929	-25230.641	-273442.559
6-311+G**	-1791.909	-80648.926	-330573.657	-68378.892	-93912.667	-70761.728	-117776.434	-25230.684	-273446.607
aug-cc-pVDZ	-1789.279	-80629.922	-330569.922	-68371.219	-93901.459	-70751.964	-117759.266	-25224.736	-273399.487
aug-cc-pVTZ	-1792.717	-80653.093	-330577.690	-68387.479	-93924.156	-70769.200	-117789.242	-25233.579	-273479.843
aug-cc-pVQZ	-1792.930	-80659.672	-330579.854	-68391.959	-93930.811	-70774.137	-117797.457	-25235.238	-273499.262
B3LYP									
6-31G*	-1821.496	-80879.680	-331019.330	-68723.981	-94324.161	-71099.548	-118334.412	-25424.781	-274516.698
6-311G**	-1825.249	-80915.160	-331041.958	-68743.964	-94352.260	-71122.637	-118372.228	-25434.378	-274602.909
6-311+G**	-1825.249	-80921.119	-331042.376	-68746.313	-94355.781	-71124.400	-118375.865	-25434.477	-274610.898
aug-cc-pVDZ	-1822.781	-80900.777	-331037.040	-68735.679	-94342.779	-71112.599	-118355.236	-25426.099	-274559.348
aug-cc-pVTZ	-1826.294	-80924.809	-331046.214	-68753.132	-94364.680	-71130.522	-118386.090	-25437.297	-274637.827
aug-cc-pVQZ	-1826.524	-80931.623	-331048.518	-68757.801	-94371.635	-71135.774	-118394.935	-25439.304	-274658.770
PBE0									
6-31G*	-1809.350	-80814.148	-330908.497	-68646.270	-94229.030	-71019.301	-118209.965	-25386.187	-274262.907
6-311G**	-1812.744	-80847.548	-330929.992	-68664.405	-94255.008	-71040.144	-118244.691	-25394.734	-274343.483
6-311+G**	-1812.744	-80852.643	-330930.316	-68666.385	-94258.082	-71041.624	-118247.852	-25394.857	-274350.238
aug-cc-pVDZ	-1810.396	-80833.349	-330925.755	-68657.681	-94246.653	-71031.286	-118229.708	-25388.157	-274302.447
aug-cc-pVTZ	-1813.739	-80856.381	-330934.291	-68673.246	-94267.774	-71047.818	-118258.233	-25397.257	-274377.683
aug-cc-pVQZ	-1813.951	-80863.155	-330936.494	-68677.875	-94274.707	-71053.010	-118266.985	-25399.148	-274398.390
MP2									
6-31G*	-1795.966	-80710.480	-330639.004	-68555.257	-94091.742	-70918.553	-118037.159	-25308.176	-273871.136
6-311G**	-1807.398	-80777.529	-330665.917	-68581.473	-94138.308	-70952.177	-118094.545	-25337.435	-274033.817
6-311+G**	-1807.397	-80782.292	-330666.366	-68584.314	-94142.068	-70954.308	-118099.237	-25337.610	-274044.713
aug-cc-pVDZ	-1806.198	-80759.734	-330666.760	-68571.143	-94125.983	-70939.727	-118076.022	-25330.185	-273987.845
aug-cc-pVTZ	-1813.815	-80824.100	-330710.049	-68623.225	-94199.200	-70994.619	-118171.379	-25359.550	-274217.595
aug-cc-pVQZ	-1815.347	-80846.193	-330725.527	-68642.122	-94223.991	-71013.773	-118204.141	-25367.682	-274293.600

Table S7. EC-RISM^φ 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*	-1789.309	-80616.574	-330553.386	-68360.667	-93884.254	-70741.656	-117741.332	-25222.230	-273368.844
6-311G**	-1792.280	-80646.787	-330574.021	-68378.264	-93910.686	-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	-274218.619
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^o 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*	-1788.972	-80616.174	-330552.811	-68359.915	-93883.590	-70740.866	-117740.194	-25221.896	-273367.670
6-311G**	-1791.944	-80646.387	-330573.441	-68377.508	-93910.015	-70760.701	-117773.745	-25230.567	-273442.392
6-311+G**	-1791.944	-80648.946	-330573.627	-68378.844	-93912.618	-70761.662	-117776.249	-25230.611	-273446.441
aug-cc-pVDZ	-1789.314	-80629.941	-330569.891	-68371.175	-93901.412	-70751.899	-117759.090	-25224.665	-273399.324
aug-cc-pVTZ	-1792.752	-80653.112	-330577.659	-68387.433	-93924.108	-70769.137	-117789.068	-25233.507	-273479.679
aug-cc-pVQZ	-1792.964	-80659.691	-330579.824	-68391.914	-93930.763	-70774.075	-117797.283	-25235.166	-273499.098
B3LYP									
6-31G*	-1821.531	-80879.699	-331019.300	-68723.935	-94324.113	-71099.489	-118334.230	-25424.704	-274516.533
6-311G**	-1825.284	-80915.179	-331041.928	-68743.916	-94352.211	-71122.580	-118372.044	-25434.309	-274602.742
6-311+G**	-1825.284	-80921.138	-331042.347	-68746.267	-94355.733	-71124.342	-118375.679	-25434.411	-274610.732
aug-cc-pVDZ	-1822.815	-80900.797	-331037.011	-68735.637	-94342.734	-71112.542	-118355.061	-25426.038	-274559.186
aug-cc-pVTZ	-1826.329	-80924.829	-331046.184	-68753.089	-94364.634	-71130.466	-118385.917	-25437.232	-274637.663
aug-cc-pVQZ	-1826.559	-80931.642	-331048.488	-68757.758	-94371.589	-71135.719	-118394.762	-25439.239	-274658.607
PBE0									
6-31G*	-1809.385	-80814.167	-330908.466	-68646.224	-94228.981	-71019.242	-118209.783	-25386.108	-274262.742
6-311G**	-1812.778	-80847.567	-330929.961	-68664.357	-94254.959	-71040.087	-118244.508	-25394.662	-274343.316
6-311+G**	-1812.778	-80852.662	-330930.286	-68666.339	-94258.034	-71041.566	-118247.667	-25394.788	-274350.072
aug-cc-pVDZ	-1810.431	-80833.369	-330925.725	-68657.638	-94246.607	-71031.229	-118229.533	-25388.090	-274302.285
aug-cc-pVTZ	-1813.773	-80856.401	-330934.261	-68673.202	-94267.727	-71047.762	-118258.060	-25397.188	-274377.520
aug-cc-pVQZ	-1813.986	-80863.175	-330936.464	-68677.832	-94274.660	-71052.955	-118266.812	-25399.079	-274398.226
MP2									
6-31G*	-1796.000	-80710.499	-330638.973	-68555.209	-94091.694	-70918.508	-118037.010	-25308.099	-273870.975
6-311G**	-1807.432	-80777.548	-330665.886	-68581.424	-94138.260	-70952.133	-118094.394	-25337.364	-274033.653
6-311+G**	-1807.432	-80782.312	-330666.336	-68584.266	-94142.019	-70954.264	-118099.082	-25337.541	-274044.551
aug-cc-pVDZ	-1806.233	-80759.754	-330666.730	-68571.099	-94125.937	-70939.683	-118075.874	-25330.117	-273987.685
aug-cc-pVTZ	-1813.849	-80824.119	-330710.019	-68623.178	-94199.153	-70994.575	-118171.232	-25359.478	-274217.435
aug-cc-pVQZ	-1815.381	-80846.213	-330725.497	-68642.076	-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
LJ	2.332	2.344	2.175						
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	2.667	2.744	2.748						
HF									
6-31G*				3.484	3.069	3.342	2.001	0.924	3.834
6-311G**				3.471	3.054	3.335	1.966	0.926	3.792
6-311+G**				3.472	3.056	3.332	1.941	0.926	3.790
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
B3LYP									
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
PBE0									
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
MP2									
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 -C₆H₆) solution.

	He	Ne	Ar	N ₂	O ₂	CO	CO ₂	CH ₄	CF ₄
B3LYP									
6-311G**	-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 -C₆F₆) solution.

	He	Ne	Ar	N ₂	O ₂	CO	CO ₂	CH ₄	CF ₄
B3LYP									
6-311G**	-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^q results for the Gibbs energies of gas molecules in charge-reversed Amber/OPLS benzene ($q_{\text{rev}}\text{-C}_6\text{H}_6$) solution.

	He	Ne	Ar	N ₂	O ₂	CO	CO ₂	CH ₄	CF ₄
HF									
6-31G*	-1788.995	-80616.205	-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**	-1791.966	-80648.977	-330573.665	-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	-1826.583	-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	-274398.552
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^q results for the Gibbs energies of gas molecules in charge-reversed Amber/OPLS benzene ($q_{\text{rev}}\text{-C}_6\text{F}_6$) 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	-80880.095	-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	-274611.686
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	-118076.563	-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 (γ) distribution functions $g_\gamma(\mathbf{r})$ around benzene and hexafluorobenzene (AMBER/OPLS). Additionally EC-RISM ^{φ} /PSE-1/B3LYP/6-31G(d) data are shown.

Solvent model	γ	C ₆ H ₆	C ₆ F ₆
		max($g_\gamma(\mathbf{r})$)	
C ₆ H ₆	C	1.59	2.54
	H	2.30	1.58
C ₆ F ₆	C	2.28	1.29
	F	1.84	2.83
C ₆ H ₆ (EC-RISM) ^{φ}	C	1.62	2.10
	H	2.04	1.57
C ₆ F ₆ (EC-RISM) ^{φ}	C	2.21	1.70
	F	1.89	2.12
q_{rev} -C ₆ H ₆	C	2.27	1.60
	H	1.55	2.74
q_{rev} -C ₆ F ₆	C	1.40	2.65
	F	2.50	1.89
q_0 -C ₆ H ₆	C	1.77	1.81
	H	1.61	1.55
q_0 -C ₆ F 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.

RMSD	3D RISM ^{qvac} AMBER/OPLS	EC-RISM ^q AMBER/OPLS	EC-RISM ^p AMBER/OPLS	3D RISM ^{qvac} Cornell	EC-RISM ^q Cornell	EC-RISM ^p Cornell	EC-RISM ^q (χ_{qrev})
HF							
6-31G*	0.241	0.243	0.227	0.276	0.279	0.270	0.337
6-311G**	0.236	0.238	0.221	0.268	0.271	0.266	0.338
6-311+G**	0.242	0.236	0.217	0.287	0.277	0.274	0.343
aug-cc-pVDZ	0.243	0.238	0.220	0.282	0.269	0.258	0.318
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
6-311+G**	0.239	0.233	0.216	0.278	0.269	0.269	0.324
aug-cc-pVDZ	0.240	0.235	0.213	0.281	0.270	0.258	0.332
aug-cc-pVTZ	0.236	0.233	0.213	0.271	0.264	0.258	0.322
aug-cc-pVQZ	0.240	0.220	0.210	0.280	0.250	0.251	0.306
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
6-311+G**	0.236	0.231	0.214	0.272	0.265	0.263	0.325
aug-cc-pVDZ	0.242	0.237	0.217	0.285	0.275	0.270	0.340
aug-cc-pVTZ	0.244	0.226	0.209	0.285	0.248	0.239	0.294
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
6-311+G**	0.235	0.231	0.213	0.272	0.265	0.262	0.324
aug-cc-pVDZ	0.239	0.235	0.216	0.277	0.268	0.265	0.322
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