Supporting Information: Shear Viscosity Computed from Finite-Size Effects of Self-Diffusivity in Equilibrium Molecular Dynamics

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S1 Weighted Least-Squares Linear Regression

For a linear model of an independent variable x and dependent variable y, the chi-square merit function (χ^2) is defined as:[1]

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{y_i - y\left(x_i | \, a, b\right)}{\sigma_i} \right)^2 = \sum_{i=1}^{N} \left(\frac{y_i - a - bx_i}{\sigma_i} \right)^2 \tag{S1}$$

in which σ_i is the standard deviation of the i^{th} dependent variable, N indicates the total number of data points (x_i, y_i), a and b are the fitting parameters of the linear regression model. The best fit to the available data can be found when the parameters a and b minimize the chi-square merit function. These values of a and b are:[1]

$$\begin{aligned} a &= \frac{s_{xx} s_y - s_x s_{xy}}{\Delta} \\ b &= \frac{s_{xy} s - s_x s_y}{\Delta} \end{aligned} \tag{S2}$$

where

$$\begin{aligned} s &= \sum_{i=1}^{N} \frac{1}{\sigma_i^2} \\ s_x &= \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2} \\ s_y &= \sum_{i=1}^{N} \frac{y_i}{\sigma_i^2} \\ s_{xx} &= \sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2} \\ s_{xy} &= \sum_{i=1}^{N} \frac{x_i y_i}{\sigma_i^2} \\ \Delta &= s_{xx} s - \left(s_x\right)^2 \end{aligned} \tag{S3}$$

The standard deviation of the parameters a and b are:[1]

$$\sigma_a = \sqrt{\frac{s_{xx}}{\Delta}}$$
$$\sigma_b = \sqrt{\frac{s}{\Delta}} \tag{S4}$$

To calculate the confidence intervals of a and b, the computed standard deviations should be multiplied by a coefficient,[1] which equals 2.0 for 95% confidence intervals.[1] A more detailed explanation of the weighted least-squares linear regression can be found in chapter 15 of the book "Numerical Recipes".[1]

For the D-based method, the independent and dependent variables are the inverse of the system sizes ($x = -\xi k_{\mathrm{B}}T/6\pi L$) and the finite-size self-diffusivities ($y = D_{i,\mathrm{self}}^{\mathrm{MD}}$). Since no knowledge of σ_i for finite-size self-diffusivities is available for a specified system size, this quantity can be estimated from the sample standard deviation, $S_{\mathrm{system},j}$, which is computed from $N_{\mathrm{sim},j}$ independent simulations of the j^{th} system size:

$$S_{\mathrm{system},j} = \sqrt{\frac{\sum_{k=1}^{N_{\mathrm{sim},j}} \left(y_k - \bar{y}_{\mathrm{sim},j}\right)^2}{N_{\mathrm{sim},j} - 1}} \tag{S5}$$

where $\bar{y}_{\mathrm{sim},j} = \sum_{k=1}^{N_{\mathrm{sim},j}} y_k/N_j$ is the average self-diffusivity of the j^{th} system size.

Instead of using all individual data points of a system size in weighted least-squares linear regression analysis (Equations (S3) and (S4)), the data points for each system size can be combined and be represented by only a single data point corresponding to the average self-diffusivity ($\bar{y}_{\mathrm{sim},j}$) and its standard error ($S.E._{\mathrm{system},j} = S_{\mathrm{system},j}/\sqrt{N_{\mathrm{sim},j}}$). This approach does not change the fitted values of a and b as well as the statistical uncertainties in these parameters.

S2 Results

Three sets of simulations were performed in this study: pure water, Lennard-Jones (LJ) systems, and an ionic liquid ([Bmim][Tf_2N]). In Table S1, the computed self-diffusivities of water for the seven system sizes (250, 500, 1000, 2000, 4000, 8000, and 16000 molecules) are listed. In Tables S2 and S3, the self-diffusivities of all species of 250 binary Lennard-Jones (LJ) systems, computed from two system sizes of 500 and 4000 particles, are listed. The shear viscosities computed from the D-based method and the Einstein relation (Equation 1 in the main text) for these binary LJ systems are listed in Table S4. These self-diffusivities and shear viscosities (the Einstein relation) are directly obtained from the Supporting Information of our previous work.[2] Similarly, the self-diffusivities (two system sizes of 500 and 4000 particles) and shear viscosities of 26 ternary LJ systems are provided in Tables S5 to S7. The computed self-diffusivities of the ionic liquid [Bmim][Tf_2N] are listed in Tables S8 to S10 for three temperatures of 300 K, 400 K, and 500 K. The shear viscosities computed from the D-based method and the Einstein relation are listed in Table S11. These values are fitted to the Vogel equation:[3]

$$\ln\left(\eta/[\text{cP}]\ \right) = A + \frac{B}{T+C} \tag{S6}$$

The coefficients of the Vogel equation are provided in Table S12.

S3 Critical properties of the Lennard-Jones Systems

For a LJ fluid, properties such as temperature, pressure, energy, etc. can be specified by the mass (m), size (σ), and interaction (ϵ) parameters of the constituent LJ particles. The relations between these parameters are provided in Appendix B of "Computer Simulation of Liquids".[4] By modifying the size or interaction parameters of the LJ particles, the critical properties of the LJ fluid can be obtained from the theorem of corresponding states:[3]

$$T_{c,2} = \left(\frac{\epsilon_2}{\epsilon_1}\right) T_{c,1} \tag{S7}$$

$$P_{c,2} = \left(\frac{\epsilon_2}{\epsilon_1}\right) \left(\frac{\sigma_1}{\sigma_2}\right)^3 P_{c,1} \tag{S8}$$

where $P_{c,i}$ and $T_{c,i}$ are the critical properties of the i^{th} species. ϵ_2/ϵ_1 and σ_2/σ_1 are the ratios of the modified interaction and size parameters to the initial values. In this study, 250 binary Lennard-Jones systems were investigated by considering various values of ϵ_2/ϵ_1 and σ_2/σ_1. In all these systems, LJ species 1 has $\sigma_1 = \sigma = 1.0$, $\epsilon_1 = \epsilon = 1.0$, and mass = m_1 = 1.0 in reduced units.[4] The critical temperature and pressure of the LJ fluid consisting only of species 1 are obtained from Gibbs ensemble Monte Carlo simulations[4,5] and are equal to 1.24 and 0.113, respectively. In Table S13, the critical properties of the LJ species 2 are listed for the binary systems which show a minimum difference of 10% between the shear viscosities obtained from the D-based method and Einstein relation. In all binary systems listed in Table S13, the mass fraction of species 2 is above 90%. Thus, the critical properties of the mixtures are mainly determined by the critical properties of species 2. For all systems showing high deviations (see Figure 6 of the main text), the critical temperatures are either 0.62 or 0.74. These values are close to the temperature of the MD simulations, i.e., 0.65. This suggests that finite-size self-diffusivities at conditions close to the critical point do not scale with $N^{-1/3}$, where N is the number of molecules in the system. Hence, the finite-size correction proposed by Yeh and Hummer[6] (equation 3 in the main text) and consequently the D-based method cannot be used for systems at near-critical conditions.

S4 Fluctuation of the instantaneous pressure in Molecular Dynamics simulations

As described by Hess,[7] due to large fluctuations in the components of the stress tensor, long MD simulations are required for the use of equilibrium Molecular Dynamics method for the calculation of the shear viscosity. To show this, the standard deviation of the instantaneous pressures of water at 298 K and 1 atm is plotted as a function of the number of water molecules in the simulation box (250 - 16000 molecules) in Figure S1. This figure shows that the fluctuations in pressure scale almost as the square root of the number of molecules ($\sqrt{N}$) and the amplitude of fluctuations is large for conventional MD systems containting hundreds to thousands of molecules.

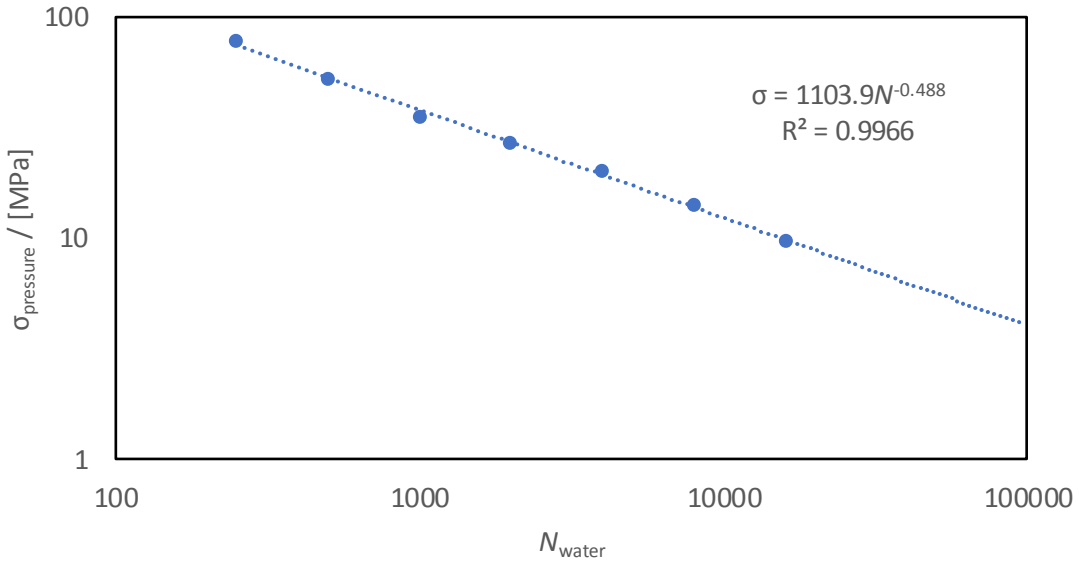

Figure S1: Standard deviation of the instantaneous pressure in water simulations of 250 to 16000 molecules. The SPC/E water model is used. The temperature and pressure are 298 K and 1 atm, respectively.

Table S1: Average ($\bar{D}_{\text{water, self}}$), estimated standard deviations (S_{water}), and standard errors ($S.E._{\text{water}}$) of finite-size self-diffusivities of the SPC/E water model at 298 K and 1 atm. 100 independent simulations of 0.5 ns for each system were carried out. The average self-diffusivities and estimated standard deviations are shown in Figures 1 and 2.

Number of water molecules	$\bar{D}_{\text{water, self}}$ $[10^{-9}\text{m}^2\text{s}^{-1}]$	S_{water} $[10^{-11}\text{m}^2\text{s}^{-1}]$	$S.E._{\text{water}}$ $[10^{-12}\text{m}^2\text{s}^{-1}]$
250	2.420	4.50	4.50
500	2.520	3.94	3.94
1000	2.590	2.73	2.73
2000	2.645	2.39	2.39
4000	2.692	2.06	2.06
8000	2.729	1.42	1.42
16000	2.759	1.35	1.35

Table S2: Average self-diffusion coefficients (D) and corresponding standard errors ($S.E.$) of 250 binary LJ systems of 500 particles at a reduced temperature of 0.65 and a reduced pressure of 0.05. LJ particle type 1 has $\sigma_1 = \sigma = 1.0$, $\epsilon_1 = \epsilon = 1.0$, and mass = $m_1 = 1.0$ in reduced units.[4] k_{12} is a modification factor to the Lorentz-Berthelot mixing rules.[4] L indicates the simulation box length.

ID	x_1	σ_2	ϵ_2	k_{12}	L	$D_{1,\text{self}}$	$S.E._1$	$D_{2,\text{self}}$	$S.E._2$	D_{avg}	$S.E._{\text{avg}}$
1	0.1	1.6	1.0	0.05	13.15	0.050711	0.000064	0.023455	0.000010	0.026180	0.000065
2	0.1	1.6	1.0	0	13.14	0.048806	0.000048	0.023079	0.000013	0.025652	0.000049
3	0.1	1.6	1.0	-0.3	13.09	0.038297	0.000072	0.020755	0.000013	0.022509	0.000073
4	0.1	1.6	1.0	-0.6	13.04	0.030312	0.000034	0.018692	0.000014	0.019854	0.000036
5	0.1	1.6	0.8	0.05	13.53	0.085070	0.000079	0.043870	0.000016	0.047990	0.000081
6	0.1	1.6	0.8	0	13.52	0.081911	0.000028	0.043169	0.000011	0.047043	0.000030
7	0.1	1.6	0.8	-0.3	13.44	0.065829	0.000049	0.039243	0.000008	0.041901	0.000050
8	0.1	1.6	0.8	-0.6	13.36	0.053255	0.000065	0.035687	0.000013	0.037444	0.000066
9	0.1	1.6	0.6	0.05	14.36	0.159102	0.000142	0.090860	0.000035	0.097684	0.000147
10	0.1	1.6	0.6	0	14.33	0.152835	0.000152	0.088901	0.000045	0.095294	0.000158
11	0.1	1.6	0.6	-0.3	14.16	0.122172	0.000181	0.080369	0.000039	0.084549	0.000186
12	0.1	1.6	0.6	-0.6	14.02	0.098924	0.000107	0.072852	0.000030	0.075459	0.000111
13	0.1	1.6	0.5	0.05	15.32	0.242993	0.000273	0.145923	0.000065	0.155630	0.000281
14	0.1	1.6	0.5	0	15.26	0.232973	0.000178	0.143179	0.000076	0.152159	0.000193
15	0.1	1.6	0.5	-0.3	14.97	0.181528	0.000212	0.126619	0.000063	0.132109	0.000222
16	0.1	1.6	0.5	-0.6	14.74	0.144381	0.000089	0.113742	0.000052	0.116806	0.000103
17	0.1	1.4	1.0	0.05	11.52	0.040272	0.000043	0.023543	0.000009	0.025216	0.000044
18	0.1	1.4	1.0	0	11.51	0.038763	0.000044	0.023109	0.000017	0.024674	0.000047
19	0.1	1.4	1.0	-0.3	11.46	0.030363	0.000039	0.020512	0.000011	0.021497	0.000040
20	0.1	1.4	1.0	-0.6	11.41	0.023920	0.000044	0.018085	0.000006	0.018668	0.000045
21	0.1	1.4	0.8	0.05	11.84	0.069303	0.000036	0.044278	0.000020	0.046781	0.000042
22	0.1	1.4	0.8	0	11.82	0.066697	0.000058	0.043344	0.000020	0.045679	0.000061
23	0.1	1.4	0.8	-0.3	11.75	0.053425	0.000044	0.038824	0.000008	0.040284	0.000044
24	0.1	1.4	0.8	-0.6	11.68	0.043094	0.000065	0.034779	0.000013	0.035610	0.000067
25	0.1	1.4	0.6	0.05	12.57	0.134205	0.000166	0.093711	0.000063	0.097760	0.000177
26	0.1	1.4	0.6	0	12.53	0.128893	0.000151	0.091521	0.000045	0.095258	0.000158
27	0.1	1.4	0.6	-0.3	12.37	0.102470	0.000124	0.080777	0.000042	0.082946	0.000131
28	0.1	1.4	0.6	-0.6	12.23	0.082631	0.000078	0.071931	0.000028	0.073001	0.000083
29	0.1	1.4	0.5	0	13.53	0.211723	0.000098	0.159453	0.000094	0.164680	0.000136
30	0.1	1.2	1.0	0.05	9.92	0.031709	0.000029	0.023749	0.000014	0.024545	0.000032
31	0.1	1.2	1.0	0	9.91	0.030414	0.000042	0.023196	0.000012	0.023918	0.000044
32	0.1	1.2	1.0	-0.3	9.86	0.023305	0.000026	0.019929	0.000012	0.020267	0.000029
33	0.1	1.2	1.0	-0.6	9.82	0.017671	0.000024	0.016990	0.000007	0.017058	0.000025
34	0.1	1.2	0.8	0.05	10.19	0.056314	0.000020	0.045226	0.000017	0.046335	0.000026
35	0.1	1.2	0.8	0	10.17	0.054193	0.000016	0.044241	0.000011	0.045237	0.000020

ID	x_1	σ_2	ϵ_2	k_{12}	L	$D_{1,\mathrm{self}}$	$S.E._{\cdot 1}$	$D_{2,\mathrm{self}}$	$S.E._{\cdot 2}$	D_{avg}	$S.E._{\cdot \mathrm{avg}}$
36	0.1	1.2	0.8	-0.3	10.10	0.042863	0.000052	0.038653	0.000021	0.039074	0.000056
37	0.1	1.2	0.8	-0.6	10.03	0.033811	0.000031	0.033698	0.000014	0.033709	0.000034
38	0.1	1.2	0.6	0.05	10.80	0.112518	0.000119	0.097136	0.000044	0.098674	0.000127
39	0.1	1.2	0.6	0	10.77	0.108345	0.000096	0.095009	0.000033	0.096343	0.000102
40	0.1	1.2	0.6	-0.3	10.61	0.085006	0.000076	0.081625	0.000031	0.081963	0.000082
41	0.1	1.2	0.6	-0.6	10.47	0.067693	0.000057	0.070688	0.000036	0.070388	0.000067
42	0.1	1.0	1.0	0.05	8.37	0.025586	0.000016	0.025109	0.000015	0.025157	0.000021
43	0.1	1.0	1.0	0	8.36	0.024287	0.000036	0.024301	0.000013	0.024300	0.000038
44	0.1	1.0	1.0	-0.3	8.32	0.017965	0.000022	0.020091	0.000016	0.019878	0.000027
45	0.1	1.0	1.0	-0.6	8.27	0.013083	0.000007	0.016423	0.000009	0.016089	0.000012
46	0.1	1.0	0.8	0.05	8.59	0.046453	0.000026	0.047955	0.000011	0.047805	0.000028
47	0.1	1.0	0.8	0	8.58	0.044575	0.000026	0.046605	0.000015	0.046402	0.000030
48	0.1	1.0	0.8	-0.3	8.50	0.034204	0.000028	0.039239	0.000024	0.038735	0.000037
49	0.1	1.0	0.8	-0.6	8.44	0.025875	0.000035	0.032867	0.000011	0.032167	0.000036
50	0.1	1.0	0.6	0.05	9.09	0.093931	0.000105	0.102748	0.000028	0.101866	0.000109
51	0.1	1.0	0.6	0	9.05	0.089744	0.000073	0.099285	0.000028	0.098331	0.000078
52	0.1	1.0	0.6	-0.3	8.90	0.069196	0.000087	0.082427	0.000022	0.081104	0.000090
53	0.1	1.0	0.6	-0.6	8.77	0.053717	0.000014	0.069047	0.000019	0.067514	0.000024
54	0.3	1.6	1.0	0.05	12.35	0.047747	0.000049	0.022702	0.000020	0.030215	0.000053
55	0.3	1.6	1.0	0	12.33	0.045061	0.000043	0.021674	0.000013	0.028690	0.000045
56	0.3	1.6	1.0	-0.3	12.20	0.030804	0.000037	0.015990	0.000009	0.020434	0.000038
57	0.3	1.6	1.0	-0.6	12.08	0.020269	0.000015	0.011303	0.000012	0.013993	0.000019
58	0.3	1.6	0.8	0.05	12.64	0.073659	0.000057	0.038836	0.000014	0.049283	0.000059
59	0.3	1.6	0.8	0	12.61	0.070158	0.000029	0.037277	0.000021	0.047141	0.000036
60	0.3	1.6	0.8	-0.3	12.42	0.050466	0.000037	0.028478	0.000029	0.035074	0.000047
61	0.3	1.6	0.8	-0.6	12.27	0.035594	0.000021	0.021369	0.000013	0.025636	0.000025
62	0.3	1.6	0.6	0	13.16	0.116505	0.000084	0.069555	0.000042	0.083640	0.000094
63	0.3	1.6	0.6	-0.3	12.85	0.086047	0.000066	0.053065	0.000036	0.062960	0.000076
64	0.3	1.6	0.6	-0.6	12.61	0.063168	0.000032	0.040791	0.000011	0.047504	0.000034
65	0.3	1.6	0.5	-0.6	12.91	0.086671	0.000059	0.058940	0.000054	0.067259	0.000080
66	0.3	1.4	1.0	0.05	10.95	0.038751	0.000039	0.023185	0.000019	0.027855	0.000043
67	0.3	1.4	1.0	0	10.93	0.036547	0.000026	0.022062	0.000014	0.026407	0.000029
68	0.3	1.4	1.0	-0.3	10.82	0.024123	0.000015	0.015703	0.000012	0.018229	0.000019
69	0.3	1.4	1.0	-0.6	10.71	0.015124	0.000010	0.010541	0.000008	0.011916	0.000013
70	0.3	1.4	0.8	0.05	11.20	0.060553	0.000022	0.039465	0.000014	0.045791	0.000026
71	0.3	1.4	0.8	0	11.17	0.057552	0.000034	0.037702	0.000019	0.043657	0.000039
72	0.3	1.4	0.8	-0.3	11.00	0.040372	0.000032	0.027845	0.000019	0.031603	0.000038
73	0.3	1.4	0.8	-0.6	10.86	0.027371	0.000028	0.020038	0.000014	0.022238	0.000031
74	0.3	1.4	0.6	0	11.63	0.096486	0.000071	0.070019	0.000050	0.077959	0.000087
75	0.3	1.4	0.6	-0.3	11.34	0.069881	0.000050	0.051681	0.000037	0.057141	0.000063

ID	x_1	σ_2	ϵ_2	k_{12}	L	$D_{1,\mathrm{self}}$	$S.E._{\cdot 1}$	$D_{2,\mathrm{self}}$	$S.E._{\cdot 2}$	D_{avg}	$S.E._{\cdot \mathrm{avg}}$
76	0.3	1.4	0.6	-0.6	11.13	0.050026	0.000037	0.038514	0.000010	0.041968	0.000038
77	0.3	1.4	0.5	-0.3	11.67	0.096691	0.000077	0.075152	0.000041	0.081614	0.000087
78	0.3	1.4	0.5	-0.6	11.37	0.069448	0.000031	0.055298	0.000033	0.059543	0.000045
79	0.3	1.2	1.0	0.05	9.62	0.031566	0.000016	0.024022	0.000018	0.026285	0.000024
80	0.3	1.2	1.0	0	9.60	0.029307	0.000021	0.022552	0.000015	0.024579	0.000026
81	0.3	1.2	1.0	-0.3	9.49	0.018076	0.000022	0.014896	0.000013	0.015850	0.000025
82	0.3	1.2	1.0	-0.6	9.40	0.010235	0.000010	0.009027	0.000006	0.009390	0.000012
83	0.3	1.2	0.8	0.05	9.82	0.049998	0.000025	0.040802	0.000014	0.043561	0.000029
84	0.3	1.2	0.8	0	9.80	0.047175	0.000010	0.038606	0.000019	0.041176	0.000022
85	0.3	1.2	0.8	-0.3	9.64	0.031397	0.000023	0.026987	0.000013	0.028310	0.000026
86	0.3	1.2	0.8	-0.6	9.52	0.019968	0.000022	0.018122	0.000016	0.018676	0.000027
87	0.3	1.2	0.6	0.05	10.22	0.083902	0.000033	0.075178	0.000042	0.077795	0.000053
88	0.3	1.2	0.6	0	10.17	0.079967	0.000067	0.070991	0.000051	0.073684	0.000084
89	0.3	1.2	0.6	-0.3	9.91	0.055719	0.000027	0.050086	0.000017	0.051776	0.000032
90	0.3	1.2	0.6	-0.6	9.73	0.037938	0.000036	0.035459	0.000017	0.036203	0.000039
91	0.3	1.2	0.5	-0.3	10.16	0.077535	0.000060	0.072138	0.000038	0.073757	0.000071
92	0.3	1.2	0.5	-0.6	9.90	0.053588	0.000029	0.051064	0.000018	0.051821	0.000035
93	0.3	1.0	1.0	0.05	8.38	0.026236	0.000015	0.026038	0.000015	0.026097	0.000021
94	0.3	1.0	1.0	0	8.36	0.024335	0.000019	0.024341	0.000013	0.024339	0.000023
95	0.3	1.0	1.0	-0.3	8.26	0.014161	0.000015	0.015048	0.000011	0.014782	0.000018
96	0.3	1.0	0.8	0.05	8.55	0.041801	0.000014	0.043634	0.000015	0.043084	0.000021
97	0.3	1.0	0.8	0	8.52	0.039067	0.000032	0.040857	0.000014	0.040320	0.000035
98	0.3	1.0	0.8	-0.3	8.38	0.024562	0.000015	0.026768	0.000014	0.026106	0.000021
99	0.3	1.0	0.8	-0.6	8.28	0.014755	0.000014	0.016933	0.000010	0.016280	0.000017
100	0.3	1.0	0.6	0.05	8.85	0.069799	0.000033	0.077940	0.000033	0.075498	0.000047
101	0.3	1.0	0.6	0	8.80	0.065805	0.000033	0.072962	0.000015	0.070815	0.000036
102	0.3	1.0	0.6	-0.3	8.58	0.043784	0.000021	0.049174	0.000014	0.047557	0.000025
103	0.3	1.0	0.6	-0.6	8.43	0.028326	0.000017	0.033038	0.000014	0.031625	0.000022
104	0.3	1.0	0.5	-0.3	8.76	0.060386	0.000037	0.069243	0.000029	0.066586	0.000047
105	0.3	1.0	0.5	-0.6	8.55	0.040093	0.000025	0.047119	0.000017	0.045011	0.000030
106	0.5	1.6	1.0	0.05	11.44	0.043449	0.000045	0.021365	0.000011	0.032407	0.000046
107	0.5	1.6	1.0	0	11.41	0.040754	0.000022	0.019982	0.000012	0.030368	0.000025
108	0.5	1.6	1.0	-0.3	11.25	0.025050	0.000018	0.012485	0.000009	0.018768	0.000020
109	0.5	1.6	1.0	-0.6	11.12	0.013999	0.000015	0.007003	0.000005	0.010501	0.000016
110	0.5	1.6	0.8	0.05	11.64	0.060384	0.000033	0.033121	0.000011	0.046752	0.000035
111	0.5	1.6	0.8	0	11.60	0.057519	0.000048	0.031135	0.000012	0.044327	0.000049
112	0.5	1.6	0.8	-0.3	11.39	0.038637	0.000034	0.020724	0.000016	0.029681	0.000038
113	0.5	1.6	0.8	-0.6	11.23	0.024180	0.000019	0.013162	0.000011	0.018671	0.000022
114	0.5	1.6	0.6	-0.3	11.63	0.060517	0.000025	0.035275	0.000011	0.047896	0.000027
115	0.5	1.6	0.6	-0.6	11.41	0.041092	0.000032	0.023998	0.000016	0.032545	0.000036

ID	x_1	σ_2	ϵ_2	k_{12}	L	$D_{1,\mathrm{self}}$	$S.E._{\cdot 1}$	$D_{2,\mathrm{self}}$	$S.E._{\cdot 2}$	D_{avg}	$S.E._{\cdot \mathrm{avg}}$
116	0.5	1.6	0.5	-0.3	11.83	0.077310	0.000044	0.047785	0.000034	0.062548	0.000055
117	0.5	1.6	0.5	-0.6	11.55	0.054281	0.000041	0.032998	0.000018	0.043640	0.000045
118	0.5	1.4	1.0	0.05	10.33	0.036209	0.000027	0.022208	0.000022	0.029208	0.000035
119	0.5	1.4	1.0	0	10.30	0.033664	0.000022	0.020679	0.000017	0.027172	0.000028
120	0.5	1.4	1.0	-0.3	10.16	0.019817	0.000013	0.012334	0.000011	0.016075	0.000017
121	0.5	1.4	1.0	-0.6	10.04	0.010314	0.000008	0.006485	0.000005	0.008400	0.000009
122	0.5	1.4	0.8	0.05	10.50	0.050680	0.000032	0.033950	0.000021	0.042315	0.000039
123	0.5	1.4	0.8	0	10.46	0.048140	0.000026	0.031856	0.000015	0.039998	0.000030
124	0.5	1.4	0.8	-0.3	10.28	0.030987	0.000025	0.020401	0.000017	0.025694	0.000030
125	0.5	1.4	0.8	-0.6	10.14	0.018536	0.000015	0.012357	0.000010	0.015446	0.000018
126	0.5	1.4	0.6	-0.3	10.47	0.049213	0.000032	0.034516	0.000011	0.041865	0.000034
127	0.5	1.4	0.6	-0.6	10.28	0.032239	0.000015	0.022656	0.000015	0.027447	0.000021
128	0.5	1.4	0.5	-0.3	10.62	0.063272	0.000014	0.046301	0.000018	0.054786	0.000023
129	0.5	1.4	0.5	-0.6	10.39	0.043056	0.000025	0.031178	0.000023	0.037117	0.000034
130	0.5	1.2	1.0	0.05	9.30	0.030266	0.000017	0.023468	0.000023	0.026867	0.000029
131	0.5	1.2	1.0	0	9.27	0.027957	0.000024	0.021650	0.000022	0.024804	0.000032
132	0.5	1.2	1.0	-0.3	9.14	0.015125	0.000011	0.011851	0.000009	0.013488	0.000014
133	0.5	1.2	0.8	0.05	9.44	0.042863	0.000030	0.035510	0.000016	0.039187	0.000034
134	0.5	1.2	0.8	0	9.41	0.040276	0.000018	0.033051	0.000025	0.036663	0.000031
135	0.5	1.2	0.8	-0.3	9.24	0.024453	0.000016	0.019955	0.000011	0.022204	0.000020
136	0.5	1.2	0.8	-0.6	9.12	0.013348	0.000008	0.010931	0.000009	0.012139	0.000012
137	0.5	1.2	0.6	0	9.62	0.058946	0.000023	0.052736	0.000006	0.055841	0.000024
138	0.5	1.2	0.6	-0.3	9.40	0.039427	0.000029	0.033743	0.000019	0.036585	0.000035
139	0.5	1.2	0.6	-0.6	9.25	0.024740	0.000010	0.021116	0.000015	0.022928	0.000018
140	0.5	1.2	0.5	-0.3	9.52	0.050876	0.000012	0.044925	0.000023	0.047901	0.000026
141	0.5	1.2	0.5	-0.6	9.33	0.033523	0.000026	0.029285	0.000023	0.031404	0.000035
142	0.5	1.0	1.0	0.05	8.38	0.026466	0.000020	0.026501	0.000018	0.026484	0.000027
143	0.5	1.0	1.0	0	8.36	0.024288	0.000014	0.024280	0.000020	0.024284	0.000024
144	0.5	1.0	0.8	0.05	8.50	0.036858	0.000019	0.038813	0.000023	0.037835	0.000030
145	0.5	1.0	0.8	0	8.47	0.034298	0.000015	0.035903	0.000020	0.035101	0.000025
146	0.5	1.0	0.8	-0.3	8.33	0.020509	0.000017	0.021146	0.000017	0.020827	0.000024
147	0.5	1.0	0.6	0	8.63	0.049516	0.000019	0.055043	0.000009	0.052279	0.000021
148	0.5	1.0	0.6	-0.3	8.45	0.032094	0.000011	0.034369	0.000014	0.033231	0.000018
149	0.5	1.0	0.6	-0.6	8.33	0.019976	0.000015	0.021175	0.000014	0.020575	0.000020
150	0.5	1.0	0.5	-0.3	8.54	0.040820	0.000024	0.044871	0.000018	0.042846	0.000030
151	0.5	1.0	0.5	-0.6	8.39	0.026698	0.000021	0.028882	0.000019	0.027790	0.000028
152	0.7	1.6	1.0	0.05	10.39	0.037510	0.000025	0.019251	0.000017	0.032032	0.000030
153	0.7	1.6	1.0	0	10.36	0.035284	0.000018	0.017872	0.000013	0.030061	0.000023
154	0.7	1.6	1.0	-0.3	10.21	0.021870	0.000015	0.010518	0.000015	0.018464	0.000021
155	0.7	1.6	1.0	-0.6	10.10	0.012208	0.000011	0.005457	0.000004	0.010183	0.000011

ID	x_1	σ_2	ϵ_2	k_{12}	L	$D_{1,\mathrm{self}}$	$S.E._{\cdot 1}$	$D_{2,\mathrm{self}}$	$S.E._{\cdot 2}$	D_{avg}	$S.E._{\cdot \mathrm{avg}}$
156	0.7	1.6	0.8	0	10.47	0.044665	0.000031	0.024688	0.000016	0.038672	0.000035
157	0.7	1.6	0.8	-0.3	10.30	0.030175	0.000018	0.015533	0.000016	0.025782	0.000024
158	0.7	1.6	0.8	-0.6	10.17	0.018735	0.000015	0.009153	0.000006	0.015860	0.000016
159	0.7	1.6	0.6	-0.3	10.42	0.042254	0.000014	0.023567	0.000010	0.036648	0.000017
160	0.7	1.6	0.6	-0.6	10.27	0.028651	0.000015	0.015202	0.000010	0.024616	0.000018
161	0.7	1.6	0.5	-0.3	10.50	0.050580	0.000033	0.029723	0.000020	0.044323	0.000039
162	0.7	1.6	0.5	-0.6	10.33	0.035829	0.000018	0.019924	0.000017	0.031058	0.000025
163	0.7	1.4	1.0	0.05	9.62	0.032307	0.000018	0.020360	0.000020	0.028723	0.000027
164	0.7	1.4	1.0	0	9.60	0.030251	0.000023	0.018854	0.000020	0.026832	0.000030
165	0.7	1.4	1.0	-0.3	9.47	0.017725	0.000012	0.010511	0.000007	0.015561	0.000014
166	0.7	1.4	1.0	-0.6	9.37	0.008821	0.000005	0.004803	0.000006	0.007615	0.000008
167	0.7	1.4	0.8	0	9.69	0.038552	0.000019	0.025738	0.000015	0.034708	0.000024
168	0.7	1.4	0.8	-0.3	9.54	0.024977	0.000013	0.015633	0.000013	0.022174	0.000018
169	0.7	1.4	0.8	-0.6	9.43	0.014609	0.000008	0.008639	0.000008	0.012818	0.000011
170	0.7	1.4	0.6	-0.3	9.65	0.035471	0.000020	0.023735	0.000017	0.031950	0.000027
171	0.7	1.4	0.6	-0.6	9.52	0.023262	0.000011	0.014800	0.000013	0.020723	0.000018
172	0.7	1.4	0.5	-0.3	9.72	0.042662	0.000020	0.029788	0.000029	0.038800	0.000035
173	0.7	1.4	0.5	-0.6	9.58	0.029507	0.000016	0.019544	0.000015	0.026518	0.000022
174	0.7	1.2	1.0	0.05	8.95	0.028324	0.000014	0.022215	0.000017	0.026491	0.000022
175	0.7	1.2	1.0	0	8.93	0.026291	0.000019	0.020470	0.000030	0.024545	0.000035
176	0.7	1.2	1.0	-0.3	8.81	0.014587	0.000007	0.010655	0.000011	0.013407	0.000013
177	0.7	1.2	0.8	0.05	9.03	0.035456	0.000009	0.029527	0.000019	0.033677	0.000021
178	0.7	1.2	0.8	0	9.00	0.033404	0.000013	0.027375	0.000021	0.031596	0.000025
179	0.7	1.2	0.8	-0.3	8.87	0.021032	0.000014	0.016214	0.000012	0.019586	0.000018
180	0.7	1.2	0.8	-0.6	8.77	0.011252	0.000010	0.008063	0.000010	0.010296	0.000014
181	0.7	1.2	0.6	-0.3	8.96	0.029905	0.000011	0.024403	0.000026	0.028255	0.000028
182	0.7	1.2	0.6	-0.6	8.85	0.019182	0.000011	0.014800	0.000011	0.017867	0.000015
183	0.7	1.2	0.5	-0.3	9.02	0.035862	0.000011	0.030339	0.000026	0.034205	0.000028
184	0.7	1.2	0.5	-0.6	8.91	0.024514	0.000017	0.019599	0.000020	0.023039	0.000026
185	0.7	1.0	1.0	0.05	8.38	0.026076	0.000012	0.026271	0.000015	0.026135	0.000020
186	0.7	1.0	1.0	0	8.36	0.024280	0.000015	0.024280	0.000020	0.024280	0.000025
187	0.7	1.0	0.8	0.05	8.44	0.031766	0.000015	0.033721	0.000016	0.032353	0.000022
188	0.7	1.0	0.8	0	8.42	0.029927	0.000016	0.031341	0.000020	0.030351	0.000026
189	0.7	1.0	0.8	-0.3	8.32	0.019838	0.000010	0.019416	0.000013	0.019711	0.000016
190	0.7	1.0	0.6	0.05	8.52	0.039350	0.000011	0.044445	0.000035	0.040879	0.000037
191	0.7	1.0	0.6	0	8.50	0.037491	0.000012	0.041643	0.000025	0.038737	0.000028
192	0.7	1.0	0.6	-0.3	8.39	0.026574	0.000015	0.027322	0.000019	0.026798	0.000025
193	0.7	1.0	0.6	-0.6	8.30	0.018158	0.000008	0.017547	0.000012	0.017975	0.000015
194	0.7	1.0	0.5	0	8.55	0.042324	0.000013	0.048941	0.000032	0.044309	0.000035
195	0.7	1.0	0.5	-0.3	8.43	0.031106	0.000012	0.033083	0.000018	0.031699	0.000022

ID	x_1	σ_2	ϵ_2	k_{12}	L	$D_{1,\mathrm{self}}$	$S.E._{\cdot 1}$	$D_{2,\mathrm{self}}$	$S.E._{\cdot 2}$	D_{avg}	$S.E._{\cdot \mathrm{avg}}$
196	0.7	1.0	0.5	-0.6	8.34	0.022198	0.000018	0.022158	0.000015	0.022186	0.000023
197	0.9	1.6	1.0	0.05	9.12	0.029218	0.000016	0.015712	0.000027	0.027867	0.000032
198	0.9	1.6	1.0	0	9.10	0.028073	0.000012	0.014907	0.000021	0.026757	0.000024
199	0.9	1.6	1.0	-0.3	9.03	0.020649	0.000010	0.009508	0.000013	0.019535	0.000017
200	0.9	1.6	1.0	-0.6	8.96	0.014242	0.000006	0.005472	0.000006	0.013365	0.000008
201	0.9	1.6	0.8	0	9.14	0.031234	0.000015	0.017482	0.000021	0.029859	0.000026
202	0.9	1.6	0.8	-0.3	9.06	0.024288	0.000012	0.011992	0.000017	0.023058	0.000021
203	0.9	1.6	0.8	-0.6	9.00	0.017954	0.000011	0.007626	0.000011	0.016921	0.000015
204	0.9	1.6	0.6	-0.3	9.10	0.028765	0.000017	0.015417	0.000027	0.027430	0.000032
205	0.9	1.6	0.6	-0.6	9.04	0.022615	0.000010	0.010757	0.000018	0.021429	0.000021
206	0.9	1.6	0.5	-0.3	9.13	0.031394	0.000015	0.017707	0.000015	0.030025	0.000022
207	0.9	1.6	0.5	-0.6	9.07	0.025558	0.000012	0.012864	0.000018	0.024289	0.000021
208	0.9	1.4	1.0	0.05	8.81	0.027104	0.000022	0.017514	0.000020	0.026145	0.000029
209	0.9	1.4	1.0	0	8.80	0.026010	0.000012	0.016539	0.000016	0.025063	0.000020
210	0.9	1.4	1.0	-0.3	8.74	0.019375	0.000008	0.010720	0.000017	0.018510	0.000019
211	0.9	1.4	1.0	-0.6	8.67	0.013436	0.000008	0.006255	0.000010	0.012718	0.000013
212	0.9	1.4	0.8	0.05	8.84	0.029699	0.000008	0.019996	0.000018	0.028728	0.000020
213	0.9	1.4	0.8	0	8.83	0.028768	0.000018	0.019213	0.000026	0.027812	0.000032
214	0.9	1.4	0.8	-0.3	8.77	0.022533	0.000015	0.013301	0.000014	0.021610	0.000021
215	0.9	1.4	0.8	-0.6	8.71	0.016809	0.000008	0.008580	0.000011	0.015986	0.000013
216	0.9	1.4	0.6	-0.3	8.81	0.026428	0.000015	0.016898	0.000015	0.025475	0.000022
217	0.9	1.4	0.6	-0.6	8.75	0.020964	0.000010	0.011824	0.000028	0.020050	0.000029
218	0.9	1.4	0.5	-0.3	8.83	0.028824	0.000023	0.019269	0.000026	0.027868	0.000034
219	0.9	1.4	0.5	-0.6	8.78	0.023522	0.000014	0.014078	0.000018	0.022577	0.000023
220	0.9	1.2	1.0	0.05	8.57	0.025705	0.000010	0.020349	0.000023	0.025170	0.000025
221	0.9	1.2	1.0	0	8.56	0.024796	0.000020	0.019323	0.000009	0.024249	0.000022
222	0.9	1.2	1.0	-0.3	8.50	0.019249	0.000013	0.013207	0.000016	0.018645	0.000021
223	0.9	1.2	1.0	-0.6	8.44	0.014342	0.000011	0.008507	0.000013	0.013758	0.000017
224	0.9	1.2	0.8	0.05	8.59	0.028003	0.000022	0.023264	0.000034	0.027529	0.000041
225	0.9	1.2	0.8	0	8.58	0.027135	0.000011	0.022190	0.000028	0.026640	0.000030
226	0.9	1.2	0.8	-0.3	8.53	0.021824	0.000006	0.015827	0.000029	0.021225	0.000029
227	0.9	1.2	0.8	-0.6	8.48	0.017077	0.000009	0.010897	0.000018	0.016459	0.000020
228	0.9	1.2	0.6	0.05	8.62	0.030557	0.000019	0.026789	0.000037	0.030180	0.000042
229	0.9	1.2	0.6	0	8.61	0.029860	0.000023	0.025869	0.000036	0.029461	0.000043
230	0.9	1.2	0.6	-0.3	8.56	0.025065	0.000011	0.019544	0.000016	0.024513	0.000020
231	0.9	1.2	0.6	-0.6	8.51	0.020530	0.000009	0.014330	0.000016	0.019910	0.000018
232	0.9	1.2	0.5	0	8.63	0.031381	0.000013	0.027994	0.000032	0.031042	0.000034
233	0.9	1.2	0.5	-0.3	8.58	0.027022	0.000014	0.021983	0.000021	0.026518	0.000025
234	0.9	1.2	0.5	-0.6	8.53	0.022672	0.000010	0.016627	0.000025	0.022068	0.000027
235	0.9	1.0	1.0	0.05	8.37	0.025056	0.000014	0.025523	0.000035	0.025103	0.000038

ID	x_1	σ_2	ϵ_2	k_{12}	L	$D_{1,\mathrm{self}}$	$S.E._{\cdot 1}$	$D_{2,\mathrm{self}}$	$S.E._{\cdot 2}$	D_{avg}	$S.E._{\cdot \mathrm{avg}}$
236	0.9	1.0	1.0	0	8.36	0.024383	0.000016	0.024372	0.000021	0.024382	0.000027
237	0.9	1.0	1.0	-0.3	8.32	0.020070	0.000009	0.017917	0.000029	0.019855	0.000031
238	0.9	1.0	1.0	-0.6	8.27	0.016382	0.000007	0.013022	0.000014	0.016046	0.000016
239	0.9	1.0	0.8	0.05	8.39	0.026797	0.000015	0.028646	0.000029	0.026982	0.000033
240	0.9	1.0	0.8	0	8.38	0.026166	0.000009	0.027455	0.000021	0.026295	0.000023
241	0.9	1.0	0.8	-0.3	8.34	0.022087	0.000020	0.020696	0.000040	0.021947	0.000045
242	0.9	1.0	0.8	-0.6	8.30	0.018449	0.000008	0.015525	0.000017	0.018157	0.000019
243	0.9	1.0	0.6	0.05	8.41	0.028865	0.000016	0.032641	0.000023	0.029243	0.000028
244	0.9	1.0	0.6	0	8.40	0.028201	0.000014	0.031316	0.000042	0.028512	0.000045
245	0.9	1.0	0.6	-0.3	8.36	0.024472	0.000015	0.024445	0.000030	0.024469	0.000034
246	0.9	1.0	0.6	-0.6	8.33	0.021002	0.000013	0.018994	0.000027	0.020801	0.000030
247	0.9	1.0	0.5	0.05	8.42	0.029966	0.000017	0.034892	0.000037	0.030459	0.000041
248	0.9	1.0	0.5	0	8.41	0.029396	0.000011	0.033804	0.000024	0.029837	0.000027
249	0.9	1.0	0.5	-0.3	8.38	0.025904	0.000019	0.026853	0.000036	0.025999	0.000041
250	0.9	1.0	0.5	-0.6	8.34	0.022590	0.000005	0.021287	0.000032	0.022460	0.000033

Table S3: Average self-diffusion coefficients (D) and corresponding standard errors ($S.E.$) of 250 binary LJ systems of 4000 particles at a reduced temperature of 0.65 and a reduced pressure of 0.05. LJ particle type 1 has $\sigma_1 = \sigma = 1.0$, $\epsilon_1 = \epsilon = 1.0$, and mass = $m_1 = 1.0$ in reduced units.[4] k_{12} is a modification factor to the Lorentz-Berthelot mixing rules.[4] L indicates the simulation box length.

ID	x_1	σ_2	ϵ_2	k_{12}	L	$D_{1,\text{self}}$	$S.E._1$	$D_{2,\text{self}}$	$S.E._2$	D_{avg}	$S.E._{\text{avg}}$
1	0.1	1.6	1.0	0.05	26.30	0.052232	0.000041	0.024965	0.000010	0.027692	0.000042
2	0.1	1.6	1.0	0	26.28	0.050197	0.000039	0.024536	0.000008	0.027102	0.000039
3	0.1	1.6	1.0	-0.3	26.18	0.039612	0.000014	0.022089	0.000006	0.023842	0.000015
4	0.1	1.6	1.0	-0.6	26.08	0.031521	0.000017	0.019869	0.000013	0.021034	0.000021
5	0.1	1.6	0.8	0.05	27.06	0.087815	0.000096	0.046708	0.000012	0.050819	0.000096
6	0.1	1.6	0.8	0	27.03	0.084478	0.000039	0.045933	0.000010	0.049787	0.000040
7	0.1	1.6	0.8	-0.3	26.87	0.068121	0.000057	0.041722	0.000018	0.044362	0.000060
8	0.1	1.6	0.8	-0.6	26.72	0.055136	0.000026	0.037925	0.000013	0.039646	0.000029
9	0.1	1.6	0.6	0.05	28.72	0.163870	0.000121	0.096284	0.000038	0.103042	0.000127
10	0.1	1.6	0.6	0	28.66	0.157347	0.000052	0.094088	0.000029	0.100414	0.000060
11	0.1	1.6	0.6	-0.3	28.33	0.126450	0.000118	0.084991	0.000019	0.089137	0.000120
12	0.1	1.6	0.6	-0.6	28.05	0.102756	0.000118	0.077161	0.000047	0.079720	0.000127
13	0.1	1.6	0.5	0.05	30.63	0.249398	0.000243	0.153023	0.000035	0.162660	0.000245
14	0.1	1.6	0.5	0	30.53	0.239700	0.000246	0.150809	0.000076	0.159698	0.000258
15	0.1	1.6	0.5	-0.3	29.94	0.187152	0.000143	0.133251	0.000040	0.138641	0.000148
16	0.1	1.6	0.5	-0.6	29.48	0.149815	0.000121	0.120318	0.000036	0.123267	0.000126
17	0.1	1.4	1.0	0.05	23.04	0.041790	0.000046	0.025046	0.000006	0.026720	0.000047
18	0.1	1.4	1.0	0	23.02	0.040149	0.000050	0.024579	0.000006	0.026136	0.000050
19	0.1	1.4	1.0	-0.3	22.92	0.031622	0.000031	0.021820	0.000007	0.022800	0.000031
20	0.1	1.4	1.0	-0.6	22.83	0.024948	0.000025	0.019211	0.000009	0.019784	0.000027
21	0.1	1.4	0.8	0.05	23.68	0.072024	0.000035	0.047079	0.000013	0.049574	0.000037
22	0.1	1.4	0.8	0	23.65	0.069212	0.000067	0.046089	0.000020	0.048402	0.000070
23	0.1	1.4	0.8	-0.3	23.49	0.055795	0.000030	0.041279	0.000011	0.042730	0.000032
24	0.1	1.4	0.8	-0.6	23.35	0.045138	0.000008	0.036974	0.000013	0.037790	0.000016
25	0.1	1.4	0.6	0.05	25.14	0.139257	0.000087	0.099119	0.000065	0.103133	0.000108
26	0.1	1.4	0.6	0	25.07	0.133877	0.000122	0.096828	0.000023	0.100532	0.000124
27	0.1	1.4	0.6	-0.3	24.73	0.107166	0.000087	0.085613	0.000018	0.087768	0.000089
28	0.1	1.4	0.6	-0.6	24.46	0.086733	0.000035	0.076278	0.000020	0.077324	0.000040
29	0.1	1.4	0.5	0	27.06	0.218870	0.000340	0.168005	0.000043	0.173091	0.000343
30	0.1	1.2	1.0	0.05	19.84	0.033235	0.000026	0.025229	0.000008	0.026029	0.000028
31	0.1	1.2	1.0	0	19.82	0.031810	0.000012	0.024643	0.000014	0.025359	0.000019
32	0.1	1.2	1.0	-0.3	19.72	0.024426	0.000021	0.021163	0.000005	0.021490	0.000022
33	0.1	1.2	1.0	-0.6	19.63	0.018696	0.000005	0.018023	0.000004	0.018091	0.000006
34	0.1	1.2	0.8	0.05	20.37	0.059095	0.000045	0.048067	0.000015	0.049170	0.000047
35	0.1	1.2	0.8	0	20.35	0.056917	0.000067	0.047043	0.000012	0.048031	0.000068

ID	x_1	σ_2	ϵ_2	k_{12}	L	$D_{1,\mathrm{self}}$	$S.E._{\cdot 1}$	$D_{2,\mathrm{self}}$	$S.E._{\cdot 2}$	D_{avg}	$S.E._{\cdot \mathrm{avg}}$
36	0.1	1.2	0.8	-0.3	20.20	0.045139	0.000014	0.041086	0.000018	0.041492	0.000023
37	0.1	1.2	0.8	-0.6	20.06	0.035811	0.000036	0.035795	0.000006	0.035797	0.000036
38	0.1	1.2	0.6	0.05	21.60	0.117815	0.000044	0.102927	0.000031	0.104416	0.000054
39	0.1	1.2	0.6	0	21.55	0.113538	0.000080	0.100659	0.000027	0.101947	0.000085
40	0.1	1.2	0.6	-0.3	21.22	0.089771	0.000094	0.086503	0.000032	0.086830	0.000099
41	0.1	1.2	0.6	-0.6	20.95	0.071719	0.000062	0.075052	0.000029	0.074719	0.000068
42	0.1	1.0	1.0	0.05	16.74	0.027074	0.000013	0.026638	0.000013	0.026682	0.000019
43	0.1	1.0	1.0	0	16.72	0.025786	0.000027	0.025779	0.000016	0.025780	0.000031
44	0.1	1.0	1.0	-0.3	16.63	0.019130	0.000013	0.021323	0.000003	0.021104	0.000014
45	0.1	1.0	1.0	-0.6	16.55	0.014001	0.000014	0.017414	0.000006	0.017073	0.000015
46	0.1	1.0	0.8	0.05	17.18	0.049406	0.000014	0.050894	0.000009	0.050745	0.000016
47	0.1	1.0	0.8	0	17.15	0.047387	0.000024	0.049479	0.000012	0.049270	0.000027
48	0.1	1.0	0.8	-0.3	17.00	0.036473	0.000027	0.041612	0.000009	0.041098	0.000028
49	0.1	1.0	0.8	-0.6	16.87	0.027847	0.000023	0.034860	0.000011	0.034158	0.000025
50	0.1	1.0	0.6	0.05	18.17	0.099836	0.000080	0.108662	0.000031	0.107779	0.000086
51	0.1	1.0	0.6	0	18.11	0.095420	0.000070	0.105095	0.000027	0.104128	0.000075
52	0.1	1.0	0.6	-0.3	17.79	0.073898	0.000046	0.087352	0.000009	0.086007	0.000047
53	0.1	1.0	0.6	-0.6	17.54	0.057555	0.000036	0.073202	0.000021	0.071637	0.000042
54	0.3	1.6	1.0	0.05	24.70	0.049276	0.000023	0.024305	0.000004	0.031796	0.000023
55	0.3	1.6	1.0	0	24.65	0.046576	0.000018	0.023232	0.000018	0.030235	0.000025
56	0.3	1.6	1.0	-0.3	24.40	0.031883	0.000012	0.017133	0.000010	0.021558	0.000016
57	0.3	1.6	1.0	-0.6	24.17	0.021012	0.000008	0.012090	0.000006	0.014767	0.000010
58	0.3	1.6	0.8	0.05	25.28	0.076060	0.000050	0.041592	0.000017	0.051933	0.000053
59	0.3	1.6	0.8	0	25.21	0.072401	0.000046	0.039852	0.000017	0.049617	0.000049
60	0.3	1.6	0.8	-0.3	24.85	0.052295	0.000016	0.030433	0.000013	0.036992	0.000021
61	0.3	1.6	0.8	-0.6	24.54	0.036958	0.000020	0.022849	0.000006	0.027082	0.000021
62	0.3	1.6	0.6	0	26.32	0.120312	0.000051	0.074293	0.000032	0.088099	0.000060
63	0.3	1.6	0.6	-0.3	25.69	0.089356	0.000050	0.056720	0.000022	0.066510	0.000054
64	0.3	1.6	0.6	-0.6	25.21	0.065653	0.000010	0.043670	0.000003	0.050265	0.000010
65	0.3	1.6	0.5	-0.6	25.83	0.090280	0.000057	0.062988	0.000030	0.071175	0.000065
66	0.3	1.4	1.0	0.05	21.91	0.040312	0.000005	0.024787	0.000014	0.029444	0.000015
67	0.3	1.4	1.0	0	21.87	0.037992	0.000029	0.023578	0.000013	0.027902	0.000031
68	0.3	1.4	1.0	-0.3	21.63	0.025145	0.000014	0.016754	0.000005	0.019271	0.000014
69	0.3	1.4	1.0	-0.6	21.43	0.015840	0.000005	0.011272	0.000004	0.012642	0.000006
70	0.3	1.4	0.8	0.05	22.39	0.063045	0.000023	0.042182	0.000015	0.048441	0.000027
71	0.3	1.4	0.8	0	22.33	0.059955	0.000042	0.040293	0.000011	0.046192	0.000043
72	0.3	1.4	0.8	-0.3	22.00	0.042147	0.000019	0.029746	0.000002	0.033466	0.000019
73	0.3	1.4	0.8	-0.6	21.73	0.028670	0.000008	0.021412	0.000008	0.023589	0.000012
74	0.3	1.4	0.6	0	23.26	0.100713	0.000036	0.074701	0.000059	0.082505	0.000069
75	0.3	1.4	0.6	-0.3	22.68	0.073171	0.000035	0.055150	0.000023	0.060556	0.000042

ID	x_1	σ_2	ϵ_2	k_{12}	L	$D_{1,\mathrm{self}}$	$S.E._{\cdot 1}$	$D_{2,\mathrm{self}}$	$S.E._{\cdot 2}$	D_{avg}	$S.E._{\cdot \mathrm{avg}}$
76	0.3	1.4	0.6	-0.6	22.26	0.052407	0.000017	0.041151	0.000012	0.044528	0.000021
77	0.3	1.4	0.5	-0.3	23.34	0.101133	0.000084	0.080099	0.000021	0.086410	0.000087
78	0.3	1.4	0.5	-0.6	22.73	0.072902	0.000036	0.058981	0.000011	0.063158	0.000038
79	0.3	1.2	1.0	0.05	19.24	0.033083	0.000017	0.025597	0.000012	0.027843	0.000021
80	0.3	1.2	1.0	0	19.20	0.030780	0.000016	0.024054	0.000006	0.026072	0.000017
81	0.3	1.2	1.0	-0.3	18.99	0.019031	0.000014	0.015862	0.000007	0.016813	0.000015
82	0.3	1.2	1.0	-0.6	18.81	0.010816	0.000005	0.009611	0.000005	0.009972	0.000007
83	0.3	1.2	0.8	0.05	19.65	0.052513	0.000013	0.043512	0.000021	0.046212	0.000024
84	0.3	1.2	0.8	0	19.59	0.049583	0.000026	0.041097	0.000011	0.043643	0.000029
85	0.3	1.2	0.8	-0.3	19.29	0.033124	0.000017	0.028722	0.000013	0.030043	0.000022
86	0.3	1.2	0.8	-0.6	19.05	0.021061	0.000011	0.019258	0.000005	0.019799	0.000013
87	0.3	1.2	0.6	0.05	20.44	0.088223	0.000034	0.080119	0.000031	0.082550	0.000046
88	0.3	1.2	0.6	0	20.33	0.084021	0.000041	0.075459	0.000033	0.078028	0.000053
89	0.3	1.2	0.6	-0.3	19.82	0.058776	0.000030	0.053327	0.000013	0.054962	0.000032
90	0.3	1.2	0.6	-0.6	19.45	0.040142	0.000029	0.037745	0.000020	0.038464	0.000035
91	0.3	1.2	0.5	-0.3	20.32	0.081783	0.000024	0.076765	0.000050	0.078271	0.000056
92	0.3	1.2	0.5	-0.6	19.80	0.056703	0.000022	0.054345	0.000022	0.055052	0.000031
93	0.3	1.0	1.0	0.05	16.76	0.027878	0.000012	0.027664	0.000010	0.027728	0.000015
94	0.3	1.0	1.0	0	16.72	0.025847	0.000013	0.025843	0.000015	0.025844	0.000020
95	0.3	1.0	1.0	-0.3	16.53	0.015047	0.000007	0.015977	0.000009	0.015698	0.000012
96	0.3	1.0	0.8	0.05	17.09	0.044385	0.000019	0.046319	0.000014	0.045739	0.000024
97	0.3	1.0	0.8	0	17.04	0.041528	0.000026	0.043374	0.000014	0.042821	0.000029
98	0.3	1.0	0.8	-0.3	16.76	0.026139	0.000008	0.028398	0.000009	0.027721	0.000012
99	0.3	1.0	0.8	-0.6	16.56	0.015730	0.000005	0.017952	0.000004	0.017285	0.000007
100	0.3	1.0	0.6	0.05	17.70	0.074204	0.000042	0.082785	0.000033	0.080211	0.000053
101	0.3	1.0	0.6	0	17.60	0.069950	0.000033	0.077390	0.000026	0.075158	0.000042
102	0.3	1.0	0.6	-0.3	17.17	0.046615	0.000013	0.052069	0.000022	0.050433	0.000026
103	0.3	1.0	0.6	-0.6	16.86	0.030247	0.000016	0.034985	0.000015	0.033564	0.000022
104	0.3	1.0	0.5	-0.3	17.51	0.064306	0.000026	0.073446	0.000024	0.070704	0.000036
105	0.3	1.0	0.5	-0.6	17.10	0.042793	0.000014	0.049897	0.000009	0.047766	0.000017
106	0.5	1.6	1.0	0.05	22.88	0.045033	0.000017	0.023043	0.000014	0.034038	0.000022
107	0.5	1.6	1.0	0	22.82	0.042192	0.000023	0.021555	0.000010	0.031873	0.000025
108	0.5	1.6	1.0	-0.3	22.50	0.026006	0.000006	0.013471	0.000005	0.019739	0.000008
109	0.5	1.6	1.0	-0.6	22.24	0.014493	0.000009	0.007540	0.000006	0.011016	0.000011
110	0.5	1.6	0.8	0.05	23.29	0.062807	0.000022	0.035738	0.000010	0.049272	0.000024
111	0.5	1.6	0.8	0	23.20	0.059809	0.000012	0.033562	0.000014	0.046686	0.000019
112	0.5	1.6	0.8	-0.3	22.78	0.040204	0.000017	0.022388	0.000006	0.031296	0.000018
113	0.5	1.6	0.8	-0.6	22.46	0.025170	0.000010	0.014173	0.000007	0.019671	0.000012
114	0.5	1.6	0.6	-0.3	23.25	0.063029	0.000017	0.038038	0.000016	0.050533	0.000024
115	0.5	1.6	0.6	-0.6	22.82	0.042839	0.000023	0.025863	0.000008	0.034351	0.000024

ID	x_1	σ_2	ϵ_2	k_{12}	L	$D_{1,\mathrm{self}}$	$S.E._{\cdot 1}$	$D_{2,\mathrm{self}}$	$S.E._{\cdot 2}$	D_{avg}	$S.E._{\cdot \mathrm{avg}}$
116	0.5	1.6	0.5	-0.3	23.65	0.080680	0.000032	0.051567	0.000010	0.066123	0.000034
117	0.5	1.6	0.5	-0.6	23.09	0.056644	0.000030	0.035539	0.000016	0.046091	0.000034
118	0.5	1.4	1.0	0.05	20.66	0.037801	0.000018	0.023871	0.000016	0.030836	0.000024
119	0.5	1.4	1.0	0	20.60	0.035190	0.000007	0.022201	0.000007	0.028696	0.000010
120	0.5	1.4	1.0	-0.3	20.31	0.020682	0.000008	0.013260	0.000007	0.016971	0.000011
121	0.5	1.4	1.0	-0.6	20.09	0.010785	0.000004	0.006967	0.000005	0.008876	0.000006
122	0.5	1.4	0.8	0.05	20.99	0.053094	0.000007	0.036492	0.000012	0.044793	0.000013
123	0.5	1.4	0.8	0	20.92	0.050376	0.000022	0.034229	0.000017	0.042302	0.000028
124	0.5	1.4	0.8	-0.3	20.55	0.032435	0.000015	0.021921	0.000009	0.027178	0.000018
125	0.5	1.4	0.8	-0.6	20.28	0.019402	0.000006	0.013261	0.000007	0.016332	0.000010
126	0.5	1.4	0.6	-0.3	20.93	0.051538	0.000010	0.037023	0.000019	0.044281	0.000021
127	0.5	1.4	0.6	-0.6	20.56	0.033801	0.000006	0.024291	0.000014	0.029046	0.000015
128	0.5	1.4	0.5	-0.3	21.24	0.066470	0.000027	0.049696	0.000026	0.058083	0.000038
129	0.5	1.4	0.5	-0.6	20.79	0.045226	0.000014	0.033412	0.000021	0.039319	0.000025
130	0.5	1.2	1.0	0.05	18.60	0.031907	0.000013	0.025094	0.000009	0.028500	0.000016
131	0.5	1.2	1.0	0	18.55	0.029446	0.000012	0.023169	0.000008	0.026308	0.000014
132	0.5	1.2	1.0	-0.3	18.29	0.015928	0.000004	0.012643	0.000003	0.014285	0.000005
133	0.5	1.2	0.8	0.05	18.88	0.045173	0.000019	0.037974	0.000033	0.041573	0.000038
134	0.5	1.2	0.8	0	18.82	0.042462	0.000006	0.035355	0.000006	0.038909	0.000009
135	0.5	1.2	0.8	-0.3	18.49	0.025773	0.000008	0.021300	0.000011	0.023537	0.000014
136	0.5	1.2	0.8	-0.6	18.25	0.014071	0.000005	0.011652	0.000003	0.012862	0.000006
137	0.5	1.2	0.6	0	19.25	0.062179	0.000007	0.056452	0.000019	0.059315	0.000021
138	0.5	1.2	0.6	-0.3	18.80	0.041662	0.000006	0.036006	0.000020	0.038834	0.000021
139	0.5	1.2	0.6	-0.6	18.49	0.026067	0.000017	0.022477	0.000009	0.024272	0.000019
140	0.5	1.2	0.5	-0.3	19.04	0.053744	0.000045	0.047949	0.000038	0.050847	0.000059
141	0.5	1.2	0.5	-0.6	18.67	0.035438	0.000023	0.031221	0.000020	0.033329	0.000030
142	0.5	1.0	1.0	0.05	16.77	0.028146	0.000020	0.028155	0.000016	0.028151	0.000026
143	0.5	1.0	1.0	0	16.72	0.025797	0.000007	0.025798	0.000012	0.025797	0.000014
144	0.5	1.0	0.8	0.05	16.99	0.039183	0.000012	0.041251	0.000010	0.040217	0.000016
145	0.5	1.0	0.8	0	16.94	0.036424	0.000016	0.038103	0.000009	0.037264	0.000018
146	0.5	1.0	0.8	-0.3	16.66	0.021786	0.000004	0.022446	0.000008	0.022116	0.000009
147	0.5	1.0	0.6	0	17.26	0.052705	0.000019	0.058393	0.000021	0.055549	0.000029
148	0.5	1.0	0.6	-0.3	16.90	0.034062	0.000015	0.036398	0.000020	0.035230	0.000025
149	0.5	1.0	0.6	-0.6	16.65	0.021221	0.000005	0.022445	0.000009	0.021833	0.000011
150	0.5	1.0	0.5	-0.3	17.07	0.043425	0.000016	0.047560	0.000016	0.045493	0.000022
151	0.5	1.0	0.5	-0.6	16.79	0.028359	0.000003	0.030558	0.000008	0.029458	0.000009
152	0.7	1.6	1.0	0.05	20.78	0.039130	0.000010	0.020949	0.000009	0.033676	0.000014
153	0.7	1.6	1.0	0	20.72	0.036840	0.000015	0.019468	0.000011	0.031629	0.000018
154	0.7	1.6	1.0	-0.3	20.43	0.022758	0.000006	0.011453	0.000004	0.019367	0.000007
155	0.7	1.6	1.0	-0.6	20.21	0.012719	0.000005	0.005954	0.000003	0.010690	0.000006

ID	x_1	σ_2	ϵ_2	k_{12}	L	$D_{1,\mathrm{self}}$	$S.E._{\cdot 1}$	$D_{2,\mathrm{self}}$	$S.E._{\cdot 2}$	D_{avg}	$S.E._{\cdot \mathrm{avg}}$
156	0.7	1.6	0.8	0	20.94	0.046692	0.000017	0.026847	0.000014	0.040739	0.000022
157	0.7	1.6	0.8	-0.3	20.59	0.031469	0.000011	0.016899	0.000011	0.027098	0.000016
158	0.7	1.6	0.8	-0.6	20.34	0.019542	0.000005	0.009969	0.000004	0.016670	0.000006
159	0.7	1.6	0.6	-0.3	20.83	0.044248	0.000016	0.025619	0.000008	0.038659	0.000018
160	0.7	1.6	0.6	-0.6	20.54	0.029946	0.000008	0.016561	0.000010	0.025931	0.000013
161	0.7	1.6	0.5	-0.3	21.01	0.052975	0.000012	0.032331	0.000016	0.046782	0.000020
162	0.7	1.6	0.5	-0.6	20.67	0.037486	0.000025	0.021640	0.000021	0.032733	0.000033
163	0.7	1.4	1.0	0.05	19.25	0.033922	0.000011	0.022050	0.000012	0.030361	0.000016
164	0.7	1.4	1.0	0	19.20	0.031733	0.000012	0.020419	0.000008	0.028339	0.000015
165	0.7	1.4	1.0	-0.3	18.93	0.018575	0.000007	0.011367	0.000005	0.016413	0.000008
166	0.7	1.4	1.0	-0.6	18.73	0.009214	0.000004	0.005199	0.000005	0.008010	0.000006
167	0.7	1.4	0.8	0	19.38	0.040512	0.000009	0.027835	0.000010	0.036709	0.000013
168	0.7	1.4	0.8	-0.3	19.08	0.026213	0.000006	0.016913	0.000010	0.023423	0.000012
169	0.7	1.4	0.8	-0.6	18.86	0.015300	0.000004	0.009346	0.000005	0.013514	0.000006
170	0.7	1.4	0.6	-0.3	19.29	0.037283	0.000014	0.025615	0.000016	0.033782	0.000022
171	0.7	1.4	0.6	-0.6	19.04	0.024428	0.000008	0.015989	0.000010	0.021896	0.000013
172	0.7	1.4	0.5	-0.3	19.43	0.044869	0.000017	0.032142	0.000025	0.041051	0.000030
173	0.7	1.4	0.5	-0.6	19.16	0.031004	0.000015	0.021090	0.000011	0.028030	0.000019
174	0.7	1.2	1.0	0.05	17.90	0.029939	0.000007	0.023846	0.000008	0.028111	0.000011
175	0.7	1.2	1.0	0	17.85	0.027757	0.000009	0.021934	0.000010	0.026010	0.000014
176	0.7	1.2	1.0	-0.3	17.61	0.015358	0.000007	0.011432	0.000006	0.014180	0.000009
177	0.7	1.2	0.8	0.05	18.05	0.037497	0.000004	0.031705	0.000020	0.035759	0.000020
178	0.7	1.2	0.8	0	18.00	0.035333	0.000017	0.029445	0.000011	0.033566	0.000021
179	0.7	1.2	0.8	-0.3	17.75	0.022207	0.000004	0.017346	0.000009	0.020748	0.000010
180	0.7	1.2	0.8	-0.6	17.55	0.011840	0.000004	0.008639	0.000003	0.010880	0.000005
181	0.7	1.2	0.6	-0.3	17.93	0.031582	0.000011	0.026107	0.000012	0.029940	0.000016
182	0.7	1.2	0.6	-0.6	17.71	0.020242	0.000007	0.015835	0.000012	0.018920	0.000014
183	0.7	1.2	0.5	-0.3	18.04	0.037917	0.000008	0.032484	0.000008	0.036287	0.000011
184	0.7	1.2	0.5	-0.6	17.81	0.025878	0.000011	0.020982	0.000018	0.024409	0.000021
185	0.7	1.0	1.0	0.05	16.76	0.027683	0.000009	0.027903	0.000017	0.027749	0.000019
186	0.7	1.0	1.0	0	16.72	0.025769	0.000009	0.025775	0.000017	0.025771	0.000019
187	0.7	1.0	0.8	0.05	16.88	0.033761	0.000005	0.035744	0.000025	0.034356	0.000025
188	0.7	1.0	0.8	0	16.84	0.031803	0.000003	0.033270	0.000020	0.032243	0.000020
189	0.7	1.0	0.8	-0.3	16.64	0.021048	0.000009	0.020610	0.000005	0.020917	0.000010
190	0.7	1.0	0.6	0.05	17.05	0.041832	0.000016	0.047203	0.000043	0.043443	0.000046
191	0.7	1.0	0.6	0	17.00	0.039820	0.000005	0.044146	0.000021	0.041118	0.000021
192	0.7	1.0	0.6	-0.3	16.78	0.028206	0.000006	0.028981	0.000013	0.028439	0.000014
193	0.7	1.0	0.6	-0.6	16.60	0.019243	0.000002	0.018647	0.000006	0.019064	0.000007
194	0.7	1.0	0.5	0	17.11	0.045012	0.000014	0.051927	0.000013	0.047087	0.000019
195	0.7	1.0	0.5	-0.3	16.87	0.033060	0.000007	0.035001	0.000013	0.033642	0.000015

ID	x_1	σ_2	ϵ_2	k_{12}	L	$D_{1,\mathrm{self}}$	$S.E._{\cdot 1}$	$D_{2,\mathrm{self}}$	$S.E._{\cdot 2}$	D_{avg}	$S.E._{\cdot \mathrm{avg}}$
196	0.7	1.0	0.5	-0.6	16.69	0.023541	0.000011	0.023509	0.000011	0.023532	0.000016
197	0.9	1.6	1.0	0.05	18.23	0.030767	0.000017	0.017418	0.000023	0.029432	0.000029
198	0.9	1.6	1.0	0	18.21	0.029598	0.000004	0.016489	0.000008	0.028287	0.000009
199	0.9	1.6	1.0	-0.3	18.05	0.021701	0.000009	0.010586	0.000008	0.020589	0.000012
200	0.9	1.6	1.0	-0.6	17.92	0.014900	0.000003	0.006125	0.000009	0.014022	0.000009
201	0.9	1.6	0.8	0	18.28	0.032906	0.000003	0.019325	0.000017	0.031548	0.000017
202	0.9	1.6	0.8	-0.3	18.12	0.025571	0.000004	0.013320	0.000016	0.024346	0.000016
203	0.9	1.6	0.8	-0.6	18.00	0.018830	0.000003	0.008542	0.000008	0.017801	0.000008
204	0.9	1.6	0.6	-0.3	18.21	0.030282	0.000020	0.017047	0.000020	0.028958	0.000028
205	0.9	1.6	0.6	-0.6	18.09	0.023760	0.000013	0.011907	0.000014	0.022575	0.000019
206	0.9	1.6	0.5	-0.3	18.26	0.033090	0.000006	0.019563	0.000008	0.031737	0.000010
207	0.9	1.6	0.5	-0.6	18.14	0.026899	0.000007	0.014266	0.000009	0.025636	0.000012
208	0.9	1.4	1.0	0.05	17.63	0.028678	0.000003	0.019102	0.000011	0.027720	0.000012
209	0.9	1.4	1.0	0	17.61	0.027515	0.000007	0.018051	0.000012	0.026569	0.000014
210	0.9	1.4	1.0	-0.3	17.47	0.020442	0.000007	0.011798	0.000014	0.019578	0.000015
211	0.9	1.4	1.0	-0.6	17.35	0.014124	0.000003	0.006912	0.000007	0.013402	0.000007
212	0.9	1.4	0.8	0.05	17.69	0.031437	0.000002	0.021916	0.000009	0.030485	0.000010
213	0.9	1.4	0.8	0	17.66	0.030476	0.000010	0.020965	0.000022	0.029525	0.000024
214	0.9	1.4	0.8	-0.3	17.53	0.023797	0.000006	0.014562	0.000012	0.022874	0.000013
215	0.9	1.4	0.8	-0.6	17.42	0.017672	0.000002	0.009452	0.000006	0.016850	0.000006
216	0.9	1.4	0.6	-0.3	17.61	0.027927	0.000006	0.018430	0.000016	0.026977	0.000017
217	0.9	1.4	0.6	-0.6	17.50	0.022097	0.000004	0.012995	0.000008	0.021186	0.000009
218	0.9	1.4	0.5	-0.3	17.66	0.030502	0.000009	0.020999	0.000003	0.029552	0.000009
219	0.9	1.4	0.5	-0.6	17.55	0.024820	0.000008	0.015401	0.000012	0.023878	0.000014
220	0.9	1.2	1.0	0.05	17.13	0.027259	0.000014	0.021903	0.000009	0.026724	0.000016
221	0.9	1.2	1.0	0	17.11	0.026257	0.000007	0.020787	0.000015	0.025710	0.000017
222	0.9	1.2	1.0	-0.3	17.00	0.020353	0.000007	0.014271	0.000010	0.019745	0.000012
223	0.9	1.2	1.0	-0.6	16.89	0.015140	0.000003	0.009252	0.000006	0.014551	0.000007
224	0.9	1.2	0.8	0.05	17.18	0.029737	0.000010	0.025003	0.000006	0.029263	0.000012
225	0.9	1.2	0.8	0	17.16	0.028750	0.000011	0.023830	0.000010	0.028258	0.000015
226	0.9	1.2	0.8	-0.3	17.05	0.023106	0.000011	0.017080	0.000010	0.022504	0.000015
227	0.9	1.2	0.8	-0.6	16.95	0.018053	0.000009	0.011835	0.000017	0.017432	0.000019
228	0.9	1.2	0.6	0.05	17.23	0.032417	0.000018	0.028831	0.000009	0.032058	0.000020
229	0.9	1.2	0.6	0	17.22	0.031706	0.000010	0.027873	0.000012	0.031322	0.000016
230	0.9	1.2	0.6	-0.3	17.12	0.026548	0.000006	0.021037	0.000014	0.025997	0.000015
231	0.9	1.2	0.6	-0.6	17.02	0.021725	0.000012	0.015436	0.000018	0.021096	0.000021
232	0.9	1.2	0.5	0	17.25	0.033301	0.000002	0.030250	0.000001	0.032996	0.000002
233	0.9	1.2	0.5	-0.3	17.15	0.028631	0.000008	0.023630	0.000011	0.028131	0.000013
234	0.9	1.2	0.5	-0.6	17.07	0.023991	0.000013	0.017898	0.000018	0.023382	0.000022
235	0.9	1.0	1.0	0.05	16.74	0.026607	0.000012	0.027091	0.000017	0.026655	0.000021

ID	x_1	σ_2	ϵ_2	k_{12}	L	$D_{1,\mathrm{self}}$	$S.E._{\cdot 1}$	$D_{2,\mathrm{self}}$	$S.E._{\cdot 2}$	D_{avg}	$S.E._{\cdot \mathrm{avg}}$
236	0.9	1.0	1.0	0	16.73	0.025861	0.000006	0.025876	0.000021	0.025863	0.000022
237	0.9	1.0	1.0	-0.3	16.63	0.021308	0.000016	0.019124	0.000014	0.021090	0.000021
238	0.9	1.0	1.0	-0.6	16.54	0.017378	0.000005	0.013972	0.000010	0.017038	0.000011
239	0.9	1.0	0.8	0.05	16.78	0.028466	0.000007	0.030288	0.000020	0.028648	0.000021
240	0.9	1.0	0.8	0	16.76	0.027746	0.000010	0.029055	0.000011	0.027877	0.000015
241	0.9	1.0	0.8	-0.3	16.68	0.023433	0.000007	0.022053	0.000022	0.023295	0.000023
242	0.9	1.0	0.8	-0.6	16.59	0.019558	0.000010	0.016601	0.000020	0.019262	0.000022
243	0.9	1.0	0.6	0.05	16.82	0.030639	0.000008	0.034465	0.000031	0.031022	0.000032
244	0.9	1.0	0.6	0	16.81	0.029971	0.000015	0.033143	0.000016	0.030288	0.000022
245	0.9	1.0	0.6	-0.3	16.73	0.025957	0.000007	0.025949	0.000013	0.025956	0.000015
246	0.9	1.0	0.6	-0.6	16.65	0.022270	0.000010	0.020218	0.000021	0.022065	0.000023
247	0.9	1.0	0.5	0.05	16.84	0.031809	0.000008	0.036971	0.000027	0.032326	0.000028
248	0.9	1.0	0.5	0	16.83	0.031207	0.000008	0.035686	0.000024	0.031655	0.000025
249	0.9	1.0	0.5	-0.3	16.76	0.027518	0.000007	0.028527	0.000009	0.027619	0.000011
250	0.9	1.0	0.5	-0.6	16.69	0.023966	0.000003	0.022645	0.000028	0.023834	0.000029

Table S4: Shear viscosities of 250 binary LJ systems at a reduced temperature of 0.65 and a reduced pressure of 0.05. LJ particle type 1 has $\sigma_1 = \sigma = 1.0$, $\epsilon_1 = \epsilon = 1.0$, and mass $= m_1 = 1.0$ in reduced units.[4] k_{12} is a modification factor to the Lorentz-Berthelot mixing rules.[4] η_1, η_2, and η_{avg} are the shear viscosities computed from the D-based method based on the self-diffusivities of species 1, species 2, and the average self-diffusivity, respectively. η_{EMD} represents the shear viscosity computed from the Einstein relation (η_{EMD}).

ID	x_1	σ_2	ϵ_2	k_{12}	η_1	$\eta_{1,95\%}$	η_2	$\eta_{2,95\%}$	η_{avg}	$\eta_{\text{avg},95\%}$	η_{EMD}	$\eta_{\text{EMD},95\%}$
1	0.1	1.6	1.0	0.05	2.45	0.25	2.46	0.05	2.46	0.25	2.39	0.07
2	0.1	1.6	1.0	0	2.68	0.24	2.56	0.05	2.57	0.22	2.45	0.07
3	0.1	1.6	1.0	-0.3	2.84	0.32	2.80	0.06	2.81	0.32	2.75	0.08
4	0.1	1.6	1.0	-0.6	3.10	0.19	3.19	0.10	3.18	0.23	3.04	0.06
5	0.1	1.6	0.8	0.05	1.32	0.12	1.27	0.02	1.28	0.11	1.23	0.02
6	0.1	1.6	0.8	0	1.41	0.05	1.31	0.01	1.32	0.05	1.26	0.01
7	0.1	1.6	0.8	-0.3	1.59	0.10	1.47	0.02	1.48	0.09	1.38	0.03
8	0.1	1.6	0.8	-0.6	1.95	0.14	1.64	0.03	1.66	0.11	1.54	0.02
9	0.1	1.6	0.6	0.05	0.71	0.06	0.63	0.01	0.64	0.05	0.57	0.01
10	0.1	1.6	0.6	0	0.76	0.05	0.66	0.01	0.67	0.04	0.58	0.01
11	0.1	1.6	0.6	-0.3	0.81	0.08	0.75	0.01	0.75	0.07	0.65	0.02
12	0.1	1.6	0.6	-0.6	0.91	0.08	0.81	0.02	0.82	0.06	0.73	0.01
13	0.1	1.6	0.5	0.05	0.50	0.06	0.45	0.01	0.45	0.05	0.35	0.00
14	0.1	1.6	0.5	0	0.48	0.04	0.42	0.01	0.42	0.04	0.35	0.00
15	0.1	1.6	0.5	-0.3	0.58	0.05	0.49	0.01	0.50	0.04	0.40	0.00
16	0.1	1.6	0.5	-0.6	0.61	0.03	0.50	0.01	0.51	0.03	0.45	0.01
17	0.1	1.4	1.0	0.05	2.80	0.23	2.83	0.04	2.83	0.24	2.70	0.06
18	0.1	1.4	1.0	0	3.07	0.29	2.89	0.07	2.91	0.27	2.82	0.07
19	0.1	1.4	1.0	-0.3	3.39	0.27	3.26	0.06	3.28	0.26	3.19	0.04
20	0.1	1.4	1.0	-0.6	4.17	0.41	3.81	0.07	3.84	0.36	3.67	0.02
21	0.1	1.4	0.8	0.05	1.52	0.06	1.48	0.03	1.48	0.06	1.41	0.03
22	0.1	1.4	0.8	0	1.65	0.12	1.51	0.03	1.52	0.10	1.44	0.04
23	0.1	1.4	0.8	-0.3	1.76	0.08	1.70	0.02	1.70	0.08	1.62	0.02
24	0.1	1.4	0.8	-0.6	2.05	0.13	1.91	0.03	1.92	0.12	1.85	0.05
25	0.1	1.4	0.6	0.05	0.77	0.06	0.72	0.02	0.72	0.06	0.63	0.01
26	0.1	1.4	0.6	0	0.78	0.06	0.74	0.01	0.74	0.06	0.65	0.01
27	0.1	1.4	0.6	-0.3	0.84	0.05	0.82	0.02	0.82	0.05	0.74	0.01
28	0.1	1.4	0.6	-0.6	0.97	0.04	0.92	0.01	0.93	0.04	0.84	0.02
29	0.1	1.4	0.5	0	0.51	0.05	0.42	0.01	0.43	0.04	0.36	0.00
30	0.1	1.2	1.0	0.05	3.23	0.17	3.33	0.07	3.32	0.19	3.21	0.05
31	0.1	1.2	1.0	0	3.54	0.22	3.41	0.09	3.42	0.23	3.32	0.05
32	0.1	1.2	1.0	-0.3	4.43	0.27	4.02	0.08	4.06	0.24	3.89	0.04
33	0.1	1.2	1.0	-0.6	4.87	0.24	4.83	0.07	4.83	0.24	4.67	0.11
34	0.1	1.2	0.8	0.05	1.73	0.06	1.69	0.03	1.69	0.06	1.61	0.03

ID	x_1	σ_2	ϵ_2	k_{12}	η_1	$\eta_{1,95\%}$	η_2	$\eta_{2,95\%}$	η_{avg}	$\eta_{\text{avg},95\%}$	η_{EMD}	$\eta_{\text{EMD},95\%}$
35	0.1	1.2	0.8	0	1.77	0.09	1.72	0.02	1.72	0.09	1.65	0.02
36	0.1	1.2	0.8	-0.3	2.13	0.10	1.99	0.05	2.00	0.10	1.96	0.10
37	0.1	1.2	0.8	-0.6	2.44	0.12	2.33	0.03	2.34	0.11	2.22	0.02
38	0.1	1.2	0.6	0.05	0.85	0.04	0.78	0.01	0.79	0.04	0.72	0.02
39	0.1	1.2	0.6	0	0.87	0.04	0.80	0.01	0.81	0.04	0.73	0.01
40	0.1	1.2	0.6	-0.3	0.97	0.05	0.95	0.02	0.95	0.05	0.86	0.01
41	0.1	1.2	0.6	-0.6	1.16	0.05	1.07	0.02	1.08	0.05	1.02	0.01
42	0.1	1.0	1.0	0.05	3.93	0.11	3.82	0.10	3.83	0.14	3.66	0.07
43	0.1	1.0	1.0	0	3.91	0.23	3.96	0.11	3.95	0.26	3.79	0.10
44	0.1	1.0	1.0	-0.3	5.05	0.23	4.78	0.12	4.80	0.24	4.67	0.04
45	0.1	1.0	1.0	-0.6	6.45	0.22	5.97	0.13	6.01	0.23	5.95	0.17
46	0.1	1.0	0.8	0.05	1.93	0.04	1.94	0.02	1.94	0.04	1.85	0.03
47	0.1	1.0	0.8	0	2.03	0.05	1.99	0.03	1.99	0.06	1.91	0.04
48	0.1	1.0	0.8	-0.3	2.54	0.09	2.43	0.05	2.44	0.10	2.31	0.02
49	0.1	1.0	0.8	-0.6	2.94	0.12	2.91	0.05	2.92	0.13	2.87	0.04
50	0.1	1.0	0.6	0.05	0.91	0.04	0.91	0.01	0.91	0.04	0.82	0.01
51	0.1	1.0	0.6	0	0.95	0.03	0.93	0.01	0.93	0.03	0.86	0.01
52	0.1	1.0	0.6	-0.3	1.17	0.05	1.12	0.01	1.12	0.05	1.06	0.02
53	0.1	1.0	0.6	-0.6	1.45	0.03	1.34	0.02	1.35	0.03	1.28	0.02
54	0.3	1.6	1.0	0.05	2.59	0.18	2.47	0.06	2.51	0.18	2.41	0.05
55	0.3	1.6	1.0	0	2.62	0.16	2.55	0.07	2.57	0.17	2.51	0.06
56	0.3	1.6	1.0	-0.3	3.72	0.27	3.51	0.08	3.57	0.26	3.53	0.08
57	0.3	1.6	1.0	-0.6	5.45	0.25	5.15	0.18	5.24	0.30	5.06	0.06
58	0.3	1.6	0.8	0.05	1.61	0.10	1.40	0.02	1.46	0.09	1.37	0.04
59	0.3	1.6	0.8	0	1.73	0.08	1.51	0.03	1.57	0.08	1.45	0.04
60	0.3	1.6	0.8	-0.3	2.15	0.10	2.01	0.07	2.05	0.11	1.92	0.02
61	0.3	1.6	0.8	-0.6	2.92	0.12	2.70	0.05	2.76	0.12	2.63	0.09
62	0.3	1.6	0.6	0	0.98	0.05	0.78	0.02	0.83	0.04	0.75	0.02
63	0.3	1.6	0.6	-0.3	1.15	0.06	1.04	0.02	1.07	0.06	1.00	0.02
64	0.3	1.6	0.6	-0.6	1.56	0.04	1.35	0.01	1.41	0.04	1.33	0.01
65	0.3	1.6	0.5	-0.6	1.05	0.05	0.94	0.03	0.97	0.05	0.89	0.01
66	0.3	1.4	1.0	0.05	2.86	0.14	2.79	0.08	2.81	0.16	2.74	0.02
67	0.3	1.4	1.0	0	3.10	0.16	2.95	0.07	2.99	0.17	2.85	0.06
68	0.3	1.4	1.0	-0.3	4.43	0.17	4.31	0.11	4.34	0.20	4.14	0.09
69	0.3	1.4	1.0	-0.6	6.37	0.20	6.25	0.15	6.28	0.25	6.32	0.09
70	0.3	1.4	0.8	0.05	1.75	0.04	1.61	0.02	1.65	0.05	1.56	0.02
71	0.3	1.4	0.8	0	1.82	0.08	1.69	0.03	1.73	0.08	1.64	0.03
72	0.3	1.4	0.8	-0.3	2.51	0.11	2.34	0.05	2.39	0.11	2.27	0.05
73	0.3	1.4	0.8	-0.6	3.47	0.15	3.28	0.08	3.33	0.16	3.24	0.10
74	0.3	1.4	0.6	0	0.99	0.04	0.90	0.03	0.93	0.05	0.86	0.02

ID	x_1	σ_2	ϵ_2	k_{12}	η_1	$\eta_{1,95\%}$	η_2	$\eta_{2,95\%}$	η_{avg}	$\eta_{\text{avg},95\%}$	η_{EMD}	$\eta_{\text{EMD},95\%}$
75	0.3	1.4	0.6	-0.3	1.31	0.05	1.24	0.03	1.26	0.06	1.18	0.02
76	0.3	1.4	0.6	-0.6	1.85	0.06	1.67	0.02	1.72	0.06	1.62	0.02
77	0.3	1.4	0.5	-0.3	0.94	0.05	0.85	0.02	0.87	0.04	0.80	0.01
78	0.3	1.4	0.5	-0.6	1.25	0.03	1.17	0.02	1.19	0.04	1.11	0.03
79	0.3	1.2	1.0	0.05	3.35	0.11	3.23	0.09	3.26	0.14	3.09	0.08
80	0.3	1.2	1.0	0	3.46	0.12	3.39	0.07	3.41	0.14	3.31	0.02
81	0.3	1.2	1.0	-0.3	5.40	0.29	5.34	0.16	5.36	0.33	5.23	0.11
82	0.3	1.2	1.0	-0.6	8.95	0.36	8.92	0.25	8.93	0.43	9.16	0.30
83	0.3	1.2	0.8	0.05	1.98	0.04	1.84	0.03	1.88	0.05	1.80	0.02
84	0.3	1.2	0.8	0	2.07	0.05	2.00	0.04	2.03	0.06	1.91	0.04
85	0.3	1.2	0.8	-0.3	2.94	0.10	2.92	0.06	2.93	0.11	2.84	0.09
86	0.3	1.2	0.8	-0.6	4.70	0.21	4.52	0.14	4.58	0.24	4.34	0.13
87	0.3	1.2	0.6	0.05	1.11	0.02	0.97	0.02	1.01	0.03	0.95	0.01
88	0.3	1.2	0.6	0	1.19	0.05	1.08	0.03	1.11	0.05	1.02	0.01
89	0.3	1.2	0.6	-0.3	1.62	0.04	1.52	0.02	1.55	0.04	1.47	0.03
90	0.3	1.2	0.6	-0.6	2.28	0.10	2.20	0.05	2.22	0.10	2.13	0.06
91	0.3	1.2	0.5	-0.3	1.13	0.03	1.04	0.03	1.07	0.04	0.99	0.01
92	0.3	1.2	0.5	-0.6	1.59	0.04	1.51	0.03	1.53	0.04	1.46	0.01
93	0.3	1.0	1.0	0.05	3.56	0.08	3.59	0.08	3.58	0.12	3.53	0.08
94	0.3	1.0	1.0	0	3.87	0.12	3.90	0.10	3.89	0.16	3.84	0.09
95	0.3	1.0	1.0	-0.3	6.68	0.25	6.38	0.20	6.47	0.31	6.43	0.08
96	0.3	1.0	0.8	0.05	2.22	0.04	2.13	0.03	2.16	0.05	2.07	0.02
97	0.3	1.0	0.8	0	2.34	0.08	2.28	0.04	2.30	0.08	2.22	0.02
98	0.3	1.0	0.8	-0.3	3.70	0.08	3.58	0.07	3.62	0.11	3.49	0.05
99	0.3	1.0	0.8	-0.6	6.06	0.19	5.81	0.12	5.88	0.21	5.90	0.08
100	0.3	1.0	0.6	0.05	1.25	0.03	1.14	0.02	1.17	0.04	1.14	0.02
101	0.3	1.0	0.6	0	1.34	0.03	1.26	0.02	1.28	0.03	1.22	0.03
102	0.3	1.0	0.6	-0.3	2.01	0.04	1.97	0.04	1.98	0.05	1.88	0.05
103	0.3	1.0	0.6	-0.6	3.02	0.07	2.98	0.06	3.00	0.10	2.89	0.05
104	0.3	1.0	0.5	-0.3	1.43	0.03	1.33	0.02	1.36	0.04	1.31	0.02
105	0.3	1.0	0.5	-0.6	2.12	0.05	2.06	0.03	2.08	0.05	1.99	0.02
106	0.5	1.6	1.0	0.05	2.70	0.16	2.55	0.05	2.62	0.17	2.50	0.03
107	0.5	1.6	1.0	0	2.98	0.13	2.73	0.05	2.85	0.13	2.69	0.02
108	0.5	1.6	1.0	-0.3	4.55	0.19	4.41	0.09	4.48	0.20	4.36	0.03
109	0.5	1.6	1.0	-0.6	8.91	0.62	8.20	0.25	8.54	0.63	8.05	0.18
110	0.5	1.6	0.8	0.05	1.73	0.06	1.60	0.02	1.67	0.06	1.60	0.02
111	0.5	1.6	0.8	0	1.84	0.08	1.74	0.03	1.79	0.08	1.72	0.01
112	0.5	1.6	0.8	-0.3	2.74	0.13	2.58	0.05	2.66	0.14	2.61	0.08
113	0.5	1.6	0.8	-0.6	4.41	0.19	4.31	0.11	4.36	0.22	4.22	0.13
114	0.5	1.6	0.6	-0.3	1.67	0.04	1.52	0.02	1.60	0.04	1.49	0.02

ID	x_1	σ_2	ϵ_2	k_{12}	η_1	$\eta_{1,95\%}$	η_2	$\eta_{2,95\%}$	η_{avg}	$\eta_{\text{avg},95\%}$	η_{EMD}	$\eta_{\text{EMD},95\%}$
115	0.5	1.6	0.6	-0.6	2.46	0.11	2.30	0.04	2.38	0.11	2.27	0.03
116	0.5	1.6	0.5	-0.3	1.23	0.04	1.09	0.02	1.16	0.04	1.12	0.04
117	0.5	1.6	0.5	-0.6	1.79	0.08	1.67	0.03	1.73	0.08	1.65	0.04
118	0.5	1.4	1.0	0.05	2.98	0.12	2.85	0.09	2.91	0.15	2.80	0.06
119	0.5	1.4	1.0	0	3.11	0.10	3.12	0.07	3.12	0.12	3.02	0.08
120	0.5	1.4	1.0	-0.3	5.57	0.20	5.20	0.14	5.38	0.24	5.24	0.12
121	0.5	1.4	1.0	-0.6	10.36	0.39	10.11	0.29	10.23	0.49	10.60	0.32
122	0.5	1.4	0.8	0.05	1.93	0.05	1.83	0.03	1.88	0.06	1.81	0.03
123	0.5	1.4	0.8	0	2.09	0.06	1.97	0.04	2.03	0.07	1.93	0.02
124	0.5	1.4	0.8	-0.3	3.29	0.13	3.13	0.08	3.21	0.15	3.06	0.03
125	0.5	1.4	0.8	-0.6	5.57	0.21	5.34	0.14	5.45	0.25	5.37	0.28
126	0.5	1.4	0.6	-0.3	2.01	0.06	1.87	0.03	1.94	0.06	1.79	0.02
127	0.5	1.4	0.6	-0.6	3.05	0.06	2.91	0.07	2.98	0.10	2.83	0.05
128	0.5	1.4	0.5	-0.3	1.44	0.03	1.36	0.03	1.40	0.04	1.32	0.03
129	0.5	1.4	0.5	-0.6	2.17	0.06	2.11	0.06	2.14	0.08	2.04	0.05
130	0.5	1.2	1.0	0.05	3.21	0.08	3.24	0.10	3.22	0.13	3.19	0.07
131	0.5	1.2	1.0	0	3.54	0.13	3.47	0.11	3.51	0.16	3.45	0.09
132	0.5	1.2	1.0	-0.3	6.67	0.19	6.76	0.16	6.71	0.25	6.67	0.14
133	0.5	1.2	0.8	0.05	2.24	0.07	2.10	0.06	2.17	0.09	2.10	0.05
134	0.5	1.2	0.8	0	2.38	0.04	2.26	0.05	2.32	0.07	2.23	0.04
135	0.5	1.2	0.8	-0.3	4.01	0.11	3.93	0.09	3.97	0.14	3.80	0.06
136	0.5	1.2	0.8	-0.6	7.42	0.18	7.44	0.20	7.43	0.27	7.39	0.35
137	0.5	1.2	0.6	0	1.57	0.02	1.37	0.01	1.46	0.03	1.41	0.04
138	0.5	1.2	0.6	-0.3	2.33	0.06	2.30	0.06	2.31	0.08	2.23	0.06
139	0.5	1.2	0.6	-0.6	3.99	0.12	3.89	0.10	3.94	0.16	3.68	0.08
140	0.5	1.2	0.5	-0.3	1.79	0.06	1.70	0.05	1.74	0.08	1.65	0.02
141	0.5	1.2	0.5	-0.6	2.74	0.10	2.71	0.09	2.72	0.13	2.61	0.06
142	0.5	1.0	1.0	0.05	3.47	0.12	3.53	0.10	3.50	0.16	3.47	0.07
143	0.5	1.0	1.0	0	3.88	0.08	3.86	0.12	3.87	0.14	3.79	0.09
144	0.5	1.0	0.8	0.05	2.48	0.05	2.36	0.05	2.42	0.07	2.36	0.02
145	0.5	1.0	0.8	0	2.72	0.05	2.63	0.05	2.67	0.08	2.62	0.10
146	0.5	1.0	0.8	-0.3	4.60	0.13	4.52	0.13	4.56	0.18	4.46	0.13
147	0.5	1.0	0.6	0	1.78	0.03	1.69	0.02	1.73	0.04	1.68	0.02
148	0.5	1.0	0.6	-0.3	2.94	0.06	2.86	0.07	2.90	0.09	2.74	0.06
149	0.5	1.0	0.6	-0.6	4.72	0.12	4.63	0.12	4.67	0.17	4.51	0.03
150	0.5	1.0	0.5	-0.3	2.20	0.05	2.13	0.04	2.17	0.06	2.11	0.05
151	0.5	1.0	0.5	-0.6	3.51	0.09	3.48	0.08	3.50	0.12	3.29	0.07
152	0.7	1.6	1.0	0.05	2.90	0.10	2.77	0.06	2.86	0.11	2.70	0.08
153	0.7	1.6	1.0	0	3.04	0.09	2.96	0.06	3.01	0.11	2.96	0.07
154	0.7	1.6	1.0	-0.3	5.39	0.20	5.12	0.17	5.31	0.27	5.11	0.12

ID	x_1	σ_2	ϵ_2	k_{12}	η_1	$\eta_{1,95\%}$	η_2	$\eta_{2,95\%}$	η_{avg}	$\eta_{\text{avg},95\%}$	η_{EMD}	$\eta_{\text{EMD},95\%}$
155	0.7	1.6	1.0	-0.6	9.48	0.44	9.74	0.22	9.56	0.49	10.12	0.19
156	0.7	1.6	0.8	0	2.30	0.08	2.16	0.04	2.26	0.09	2.17	0.06
157	0.7	1.6	0.8	-0.3	3.67	0.12	3.48	0.10	3.61	0.16	3.42	0.11
158	0.7	1.6	0.8	-0.6	5.96	0.24	5.90	0.11	5.94	0.26	5.86	0.16
159	0.7	1.6	0.6	-0.3	2.36	0.05	2.29	0.03	2.34	0.06	2.26	0.06
160	0.7	1.6	0.6	-0.6	3.68	0.10	3.51	0.07	3.62	0.12	3.52	0.04
161	0.7	1.6	0.5	-0.3	1.94	0.06	1.79	0.04	1.89	0.07	1.79	0.04
162	0.7	1.6	0.5	-0.6	2.86	0.11	2.76	0.09	2.83	0.14	2.70	0.07
163	0.7	1.4	1.0	0.05	3.15	0.08	3.01	0.08	3.11	0.12	3.01	0.08
164	0.7	1.4	1.0	0	3.44	0.12	3.26	0.09	3.39	0.15	3.22	0.13
165	0.7	1.4	1.0	-0.3	6.09	0.20	6.04	0.12	6.07	0.23	6.00	0.16
166	0.7	1.4	1.0	-0.6	13.28	0.46	13.19	0.53	13.25	0.70	13.71	0.59
167	0.7	1.4	0.8	0	2.58	0.06	2.41	0.04	2.52	0.07	2.46	0.07
168	0.7	1.4	0.8	-0.3	4.15	0.10	4.01	0.10	4.11	0.14	3.96	0.06
169	0.7	1.4	0.8	-0.6	7.51	0.18	7.34	0.20	7.46	0.27	7.30	0.24
170	0.7	1.4	0.6	-0.3	2.80	0.08	2.70	0.07	2.77	0.10	2.63	0.08
171	0.7	1.4	0.6	-0.6	4.41	0.11	4.32	0.12	4.38	0.16	4.28	0.07
172	0.7	1.4	0.5	-0.3	2.28	0.06	2.14	0.07	2.24	0.09	2.11	0.05
173	0.7	1.4	0.5	-0.6	3.41	0.10	3.31	0.08	3.38	0.13	3.20	0.10
174	0.7	1.2	1.0	0.05	3.39	0.06	3.35	0.08	3.38	0.10	3.29	0.05
175	0.7	1.2	1.0	0	3.74	0.11	3.75	0.16	3.74	0.19	3.60	0.10
176	0.7	1.2	1.0	-0.3	7.21	0.18	7.15	0.22	7.19	0.29	7.11	0.12
177	0.7	1.2	0.8	0.05	2.65	0.03	2.49	0.06	2.60	0.07	2.54	0.03
178	0.7	1.2	0.8	0	2.82	0.06	2.63	0.06	2.76	0.09	2.73	0.06
179	0.7	1.2	0.8	-0.3	4.69	0.11	4.87	0.13	4.75	0.17	4.65	0.12
180	0.7	1.2	0.8	-0.6	9.49	0.34	9.68	0.34	9.54	0.47	9.78	0.36
181	0.7	1.2	0.6	-0.3	3.26	0.06	3.20	0.11	3.24	0.12	3.06	0.05
182	0.7	1.2	0.6	-0.6	5.21	0.12	5.34	0.17	5.25	0.20	5.08	0.07
183	0.7	1.2	0.5	-0.3	2.64	0.03	2.53	0.06	2.61	0.08	2.49	0.04
184	0.7	1.2	0.5	-0.6	4.03	0.12	3.97	0.16	4.01	0.20	3.88	0.11
185	0.7	1.0	1.0	0.05	3.64	0.07	3.58	0.10	3.62	0.12	3.52	0.04
186	0.7	1.0	1.0	0	3.93	0.09	3.91	0.14	3.92	0.17	3.85	0.17
187	0.7	1.0	0.8	0.05	2.91	0.05	2.87	0.08	2.89	0.10	2.82	0.08
188	0.7	1.0	0.8	0	3.10	0.05	3.01	0.09	3.07	0.11	3.00	0.08
189	0.7	1.0	0.8	-0.3	4.86	0.11	4.93	0.11	4.88	0.15	4.85	0.21
190	0.7	1.0	0.6	0.05	2.31	0.04	2.08	0.08	2.24	0.10	2.16	0.05
191	0.7	1.0	0.6	0	2.47	0.03	2.30	0.06	2.42	0.07	2.32	0.04
192	0.7	1.0	0.6	-0.3	3.58	0.07	3.52	0.10	3.56	0.12	3.43	0.04
193	0.7	1.0	0.6	-0.6	5.44	0.08	5.36	0.14	5.42	0.16	5.32	0.20
194	0.7	1.0	0.5	0	2.13	0.03	1.92	0.04	2.06	0.06	1.98	0.06

ID	x_1	σ_2	ϵ_2	k_{12}	η_1	$\eta_{1,95\%}$	η_2	$\eta_{2,95\%}$	η_{avg}	$\eta_{\text{avg},95\%}$	η_{EMD}	$\eta_{\text{EMD},95\%}$
195	0.7	1.0	0.5	-0.3	2.97	0.04	3.03	0.07	2.99	0.08	2.87	0.02
196	0.7	1.0	0.5	-0.6	4.37	0.14	4.34	0.12	4.36	0.18	4.21	0.08
197	0.9	1.6	1.0	0.05	3.46	0.10	3.14	0.13	3.43	0.19	3.29	0.08
198	0.9	1.6	1.0	0	3.52	0.06	3.40	0.10	3.51	0.12	3.42	0.05
199	0.9	1.6	1.0	-0.3	5.15	0.14	5.03	0.14	5.14	0.20	5.01	0.03
200	0.9	1.6	1.0	-0.6	8.31	0.17	8.37	0.27	8.32	0.32	8.30	0.10
201	0.9	1.6	0.8	0	3.20	0.06	2.90	0.08	3.17	0.12	3.00	0.03
202	0.9	1.6	0.8	-0.3	4.21	0.08	4.07	0.14	4.20	0.17	4.10	0.08
203	0.9	1.6	0.8	-0.6	6.21	0.16	5.94	0.17	6.18	0.24	5.98	0.07
204	0.9	1.6	0.6	-0.3	3.55	0.12	3.30	0.14	3.52	0.19	3.33	0.09
205	0.9	1.6	0.6	-0.6	4.73	0.14	4.70	0.19	4.72	0.23	4.57	0.17
206	0.9	1.6	0.5	-0.3	3.16	0.06	2.89	0.05	3.13	0.09	2.97	0.03
207	0.9	1.6	0.5	-0.6	4.02	0.09	3.85	0.11	4.01	0.15	3.91	0.08
208	0.9	1.4	1.0	0.05	3.53	0.10	3.50	0.10	3.52	0.14	3.47	0.11
209	0.9	1.4	1.0	0	3.69	0.07	3.68	0.10	3.69	0.12	3.61	0.04
210	0.9	1.4	1.0	-0.3	5.25	0.11	5.20	0.21	5.25	0.24	5.30	0.14
211	0.9	1.4	1.0	-0.6	8.21	0.20	8.60	0.32	8.25	0.36	8.27	0.18
212	0.9	1.4	0.8	0.05	3.18	0.03	2.88	0.06	3.15	0.08	3.12	0.06
213	0.9	1.4	0.8	0	3.24	0.08	3.16	0.12	3.24	0.15	3.24	0.06
214	0.9	1.4	0.8	-0.3	4.42	0.11	4.43	0.13	4.42	0.17	4.29	0.09
215	0.9	1.4	0.8	-0.6	6.51	0.12	6.44	0.18	6.50	0.22	6.35	0.22
216	0.9	1.4	0.6	-0.3	3.71	0.08	3.63	0.10	3.70	0.13	3.55	0.07
217	0.9	1.4	0.6	-0.6	4.94	0.09	4.78	0.23	4.92	0.27	4.79	0.20
218	0.9	1.4	0.5	-0.3	3.30	0.10	3.20	0.10	3.29	0.14	3.20	0.04
219	0.9	1.4	0.5	-0.6	4.29	0.11	4.22	0.14	4.29	0.18	4.10	0.05
220	0.9	1.2	1.0	0.05	3.68	0.08	3.68	0.12	3.68	0.14	3.64	0.06
221	0.9	1.2	1.0	0	3.91	0.12	3.91	0.09	3.91	0.15	3.78	0.11
222	0.9	1.2	1.0	-0.3	5.22	0.14	5.41	0.19	5.23	0.23	5.15	0.18
223	0.9	1.2	1.0	-0.6	7.27	0.21	7.78	0.30	7.31	0.34	7.34	0.34
224	0.9	1.2	0.8	0.05	3.29	0.09	3.28	0.13	3.29	0.16	3.24	0.05
225	0.9	1.2	0.8	0	3.53	0.07	3.48	0.12	3.53	0.15	3.40	0.08
226	0.9	1.2	0.8	-0.3	4.48	0.08	4.58	0.22	4.49	0.23	4.35	0.08
227	0.9	1.2	0.8	-0.6	5.92	0.16	6.16	0.32	5.94	0.34	5.81	0.03
228	0.9	1.2	0.6	0.05	3.05	0.09	2.78	0.10	3.02	0.15	2.94	0.05
229	0.9	1.2	0.6	0	3.08	0.08	2.84	0.11	3.06	0.15	3.03	0.06
230	0.9	1.2	0.6	-0.3	3.86	0.07	3.83	0.11	3.86	0.13	3.75	0.07
231	0.9	1.2	0.6	-0.6	4.81	0.12	5.20	0.22	4.85	0.23	4.71	0.09
232	0.9	1.2	0.5	0	2.95	0.04	2.51	0.07	2.90	0.10	2.86	0.03
233	0.9	1.2	0.5	-0.3	3.55	0.07	3.47	0.10	3.54	0.12	3.43	0.04
234	0.9	1.2	0.5	-0.6	4.35	0.11	4.51	0.22	4.36	0.23	4.14	0.07

ID	x_1	σ_2	ϵ_2	k_{12}	η_1	$\eta_{1,95\%}$	η_2	$\eta_{2,95\%}$	η_{avg}	$\eta_{\text{avg},95\%}$	η_{EMD}	$\eta_{\text{EMD},95\%}$
235	0.9	1.0	1.0	0.05	3.77	0.09	3.73	0.18	3.77	0.21	3.68	0.06
236	0.9	1.0	1.0	0	3.96	0.09	3.89	0.15	3.95	0.18	3.81	0.09
237	0.9	1.0	1.0	-0.3	4.75	0.14	4.87	0.26	4.76	0.29	4.73	0.09
238	0.9	1.0	1.0	-0.6	5.94	0.10	6.23	0.23	5.97	0.23	5.93	0.08
239	0.9	1.0	0.8	0.05	3.50	0.07	3.55	0.15	3.50	0.16	3.41	0.09
240	0.9	1.0	0.8	0	3.70	0.06	3.65	0.11	3.69	0.13	3.56	0.05
241	0.9	1.0	0.8	-0.3	4.36	0.14	4.33	0.29	4.36	0.32	4.26	0.07
242	0.9	1.0	0.8	-0.6	5.33	0.12	5.49	0.27	5.34	0.28	5.26	0.11
243	0.9	1.0	0.6	0.05	3.28	0.07	3.19	0.13	3.27	0.16	3.11	0.05
244	0.9	1.0	0.6	0	3.29	0.08	3.19	0.16	3.28	0.18	3.22	0.05
245	0.9	1.0	0.6	-0.3	3.94	0.09	3.89	0.17	3.94	0.20	3.78	0.11
246	0.9	1.0	0.6	-0.6	4.64	0.12	4.80	0.27	4.65	0.28	4.54	0.07
247	0.9	1.0	0.5	0.05	3.15	0.07	2.80	0.12	3.11	0.17	2.98	0.06
248	0.9	1.0	0.5	0	3.21	0.05	3.09	0.11	3.20	0.13	3.08	0.08
249	0.9	1.0	0.5	-0.3	3.62	0.09	3.49	0.15	3.61	0.19	3.56	0.07
250	0.9	1.0	0.5	-0.6	4.27	0.04	4.32	0.27	4.27	0.27	4.13	0.06

Table S5: Average self-diffusion coefficients (D) and corresponding standard errors ($S.E.$) of 26 ternary LJ systems of 500 particles at a reduced temperature of 0.65 and a reduced pressure of 0.05. LJ particle type 1 has $\sigma_1 = \sigma = 1.0$, $\epsilon_1 = \epsilon = 1.0$, and mass $= m_1 = 1.0$ in reduced units.[4] k_{ij} is a modification factor to the Lorentz-Berthelot mixing rules.[4] L indicates the simulation box length.

ID	k_{12}	k_{13}	k_{23}	L	D_1	$S.E._1$	D_2	$S.E._2$	D_3	$S.E._3$	D_{avg}	$S.E._{\text{avg}}$
1	-0.6	-0.6	-0.3	8.28	0.015250	0.000015	0.015783	0.000013	0.016919	0.000020	0.015570	0.000028
2	-0.6	-0.6	0	8.30	0.017115	0.000021	0.018089	0.000015	0.019627	0.000019	0.017700	0.000032
3	-0.6	-0.6	0.05	8.30	0.017373	0.000021	0.018393	0.000028	0.020003	0.000021	0.017985	0.000040
4	-0.6	-0.3	-0.6	8.29	0.016931	0.000013	0.016432	0.000016	0.018599	0.000026	0.016632	0.000033
5	-0.6	-0.3	-0.3	8.32	0.019214	0.000009	0.019196	0.000019	0.022033	0.000032	0.019203	0.000039
6	-0.6	-0.3	0	8.35	0.021426	0.000032	0.021685	0.000030	0.025711	0.000034	0.021581	0.000055
7	-0.6	0.05	-0.6	8.34	0.021139	0.000017	0.020107	0.000021	0.024428	0.000023	0.020520	0.000036
8	-0.3	-0.6	-0.6	8.30	0.017821	0.000015	0.018296	0.000017	0.018069	0.000025	0.018106	0.000034
9	-0.3	-0.6	-0.3	8.33	0.020187	0.000019	0.021462	0.000017	0.021206	0.000018	0.020952	0.000031
10	-0.3	-0.6	0	8.36	0.022609	0.000017	0.024652	0.000020	0.024423	0.000022	0.023834	0.000034
11	-0.3	-0.6	0.05	8.36	0.022974	0.000027	0.025126	0.000027	0.024840	0.000021	0.024265	0.000044
12	-0.3	-0.3	-0.6	8.35	0.022478	0.000015	0.022138	0.000027	0.023271	0.000017	0.022274	0.000036
13	-0.3	-0.3	-0.3	8.38	0.025510	0.000022	0.026035	0.000021	0.027529	0.000025	0.025825	0.000040
14	-0.3	-0.3	0	8.42	0.028584	0.000027	0.029851	0.000027	0.031936	0.000043	0.029344	0.000058
15	-0.3	-0.3	0.05	8.42	0.029042	0.000025	0.030370	0.000047	0.032618	0.000052	0.029839	0.000075
16	-0.3	0.05	-0.6	8.41	0.028056	0.000010	0.027031	0.000040	0.030055	0.000028	0.027441	0.000050
17	-0.3	0.05	-0.3	8.45	0.031917	0.000038	0.031814	0.000038	0.036123	0.000026	0.031855	0.000059
18	0.05	-0.6	-0.6	8.36	0.023515	0.000014	0.024873	0.000015	0.022933	0.000030	0.024330	0.000036
19	0.05	-0.6	-0.3	8.40	0.026478	0.000023	0.029297	0.000023	0.026738	0.000025	0.028170	0.000041
20	0.05	-0.3	-0.6	8.42	0.029570	0.000030	0.029820	0.000026	0.029273	0.000038	0.029720	0.000055
21	0.05	-0.3	-0.3	8.47	0.033750	0.000024	0.035595	0.000030	0.034789	0.000030	0.034857	0.000049
22	0.05	-0.3	0	8.51	0.037919	0.000026	0.041124	0.000022	0.040260	0.000033	0.039842	0.000048
23	0.05	-0.3	0.05	8.52	0.038483	0.000028	0.041890	0.000035	0.040959	0.000042	0.040527	0.000061
24	0.05	0.05	-0.3	8.55	0.041727	0.000032	0.043052	0.000037	0.044971	0.000028	0.042522	0.000057
25	0.05	0.05	0	8.62	0.048728	0.000047	0.051530	0.000050	0.054344	0.000037	0.050410	0.000078
26	0.05	0.05	0.05	8.63	0.049874	0.000043	0.052700	0.000047	0.055696	0.000050	0.051569	0.000081

Table S6: Average self-diffusion coefficients (D) and corresponding standard errors ($S.E.$) of 26 ternary LJ systems of 4000 particles at a reduced temperature of 0.65 and a reduced pressure of 0.05. LJ particle type 1 has $\sigma_1 = \sigma = 1.0$, $\epsilon_1 = \epsilon = 1.0$, and mass = $m_1 = 1.0$ in reduced units.[4] k_{ij} is a modification factor to the Lorentz-Berthelot mixing rules.[4] L indicates the simulation box length.

ID	k_{12}	k_{13}	k_{23}	L	D_1	$S.E._1$	D_2	$S.E._2$	D_3	$S.E._3$	D_{avg}	$S.E._{\text{avg}}$
1	-0.6	-0.6	-0.3	16.55	0.016236	0.000008	0.016786	0.000008	0.017928	0.000008	0.016566	0.000014
2	-0.6	-0.6	0	16.60	0.018212	0.000007	0.019167	0.000010	0.020759	0.000009	0.018785	0.000016
3	-0.6	-0.6	0.05	16.60	0.018514	0.000007	0.019497	0.000008	0.021177	0.000010	0.019104	0.000015
4	-0.6	-0.3	-0.6	16.58	0.018006	0.000010	0.017497	0.000007	0.019704	0.000009	0.017701	0.000014
5	-0.6	-0.3	-0.3	16.64	0.020440	0.000009	0.020417	0.000012	0.023351	0.000008	0.020426	0.000017
6	-0.6	-0.3	0	16.70	0.022785	0.000006	0.023015	0.000010	0.027218	0.000013	0.022923	0.000017
7	-0.6	0.05	-0.6	16.68	0.022451	0.000008	0.021451	0.000007	0.025864	0.000006	0.021851	0.000012
8	-0.3	-0.6	-0.6	16.60	0.018899	0.000007	0.019398	0.000008	0.019173	0.000007	0.019198	0.000013
9	-0.3	-0.6	-0.3	16.66	0.021461	0.000013	0.022758	0.000010	0.022517	0.000010	0.022239	0.000019
10	-0.3	-0.6	0	16.72	0.024066	0.000010	0.026157	0.000007	0.025879	0.000008	0.025320	0.000015
11	-0.3	-0.6	0.05	16.72	0.024467	0.000007	0.026649	0.000011	0.026375	0.000013	0.025776	0.000019
12	-0.3	-0.3	-0.6	16.70	0.023849	0.000010	0.023566	0.000010	0.024670	0.000009	0.023679	0.000017
13	-0.3	-0.3	-0.3	16.77	0.027091	0.000011	0.027616	0.000011	0.029144	0.000011	0.027406	0.000019
14	-0.3	-0.3	0	16.84	0.030430	0.000014	0.031685	0.000014	0.033821	0.000008	0.031183	0.000021
15	-0.3	-0.3	0.05	16.85	0.030940	0.000015	0.032258	0.000011	0.034568	0.000012	0.031731	0.000022
16	-0.3	0.05	-0.6	16.81	0.029779	0.000009	0.028793	0.000007	0.031870	0.000013	0.029188	0.000018
17	-0.3	0.05	-0.3	16.90	0.033941	0.000015	0.033863	0.000016	0.038267	0.000014	0.033894	0.000026
18	0.05	-0.6	-0.6	16.73	0.024932	0.000012	0.026366	0.000012	0.024380	0.000007	0.025793	0.000019
19	0.05	-0.6	-0.3	16.80	0.028145	0.000013	0.031103	0.000020	0.028423	0.000009	0.029920	0.000026
20	0.05	-0.3	-0.6	16.84	0.031360	0.000013	0.031693	0.000013	0.031133	0.000014	0.031559	0.000022
21	0.05	-0.3	-0.3	16.93	0.035864	0.000010	0.037704	0.000011	0.036917	0.000014	0.036968	0.000021
22	0.05	-0.3	0	17.03	0.040350	0.000015	0.043658	0.000014	0.042644	0.000020	0.042335	0.000029
23	0.05	-0.3	0.05	17.04	0.041000	0.000011	0.044470	0.000026	0.043424	0.000017	0.043082	0.000033
24	0.05	0.05	-0.3	17.11	0.044187	0.000017	0.045881	0.000009	0.047740	0.000016	0.045204	0.000025
25	0.05	0.05	0	17.24	0.051760	0.000022	0.054606	0.000018	0.057544	0.000026	0.053468	0.000039
26	0.05	0.05	0.05	17.27	0.052943	0.000017	0.055991	0.000033	0.059074	0.000032	0.054772	0.000049

Table S7: Shear viscosities of 26 ternary LJ systems at a reduced temperature of 0.65 and a reduced pressure of 0.05. LJ particle type 1 has $\sigma_1 = \sigma = 1.0$, $\epsilon_1 = \epsilon = 1.0$, and mass $= m_1 = 1.0$ in reduced units.[4] k_{ij} is the modification factor to the Lorentz-Berthelot mixing rules.[4] Shear viscosities are obtained from the D-based method (η_i where i represents the three species or the average self-diffusivity, avg) and the Einstein relation (η_{EMD}). $\eta_{i,95\%}$ denotes 95% confidence intervals.

ID	k_{12}	k_{13}	k_{23}	η_1	$\eta_{1,95\%}$	η_2	$\eta_{2,95\%}$	η_3	$\eta_{3,95\%}$	η_{avg}	$\eta_{\mathrm{avg},95\%}$	η_{EMD}	$\eta_{\mathrm{EMD},95\%}$
1	-0.6	-0.6	-0.3	6.00	0.20	5.90	0.18	5.86	0.25	5.94	0.37	5.99	0.10
2	-0.6	-0.6	0	5.38	0.22	5.48	0.19	5.21	0.19	5.44	0.36	5.24	0.14
3	-0.6	-0.6	0.05	5.16	0.20	5.34	0.28	5.02	0.20	5.27	0.40	5.08	0.08
4	-0.6	-0.3	-0.6	5.50	0.17	5.54	0.18	5.35	0.26	5.52	0.37	5.50	0.12
5	-0.6	-0.3	-0.3	4.80	0.10	4.82	0.18	4.46	0.22	4.81	0.33	4.69	0.06
6	-0.6	-0.3	0	4.32	0.21	4.41	0.21	3.89	0.19	4.37	0.38	4.10	0.07
7	-0.6	0.05	-0.6	4.47	0.13	4.37	0.15	4.09	0.14	4.41	0.25	4.29	0.07
8	-0.3	-0.6	-0.6	5.47	0.17	5.35	0.18	5.34	0.25	5.40	0.35	5.25	0.09
9	-0.3	-0.6	-0.3	4.61	0.17	4.53	0.14	4.49	0.14	4.57	0.26	4.42	0.07
10	-0.3	-0.6	0	4.02	0.11	3.89	0.11	4.02	0.13	3.94	0.20	3.91	0.05
11	-0.3	-0.6	0.05	3.92	0.15	3.84	0.15	3.82	0.12	3.88	0.24	3.81	0.10
12	-0.3	-0.3	-0.6	4.28	0.11	4.11	0.16	4.19	0.12	4.17	0.23	4.11	0.10
13	-0.3	-0.3	-0.3	3.69	0.12	3.69	0.11	3.62	0.12	3.69	0.21	3.53	0.06
14	-0.3	-0.3	0	3.15	0.10	3.17	0.10	3.09	0.14	3.16	0.21	3.07	0.04
15	-0.3	-0.3	0.05	3.06	0.09	3.08	0.16	2.98	0.16	3.07	0.25	3.01	0.04
16	-0.3	0.05	-0.6	3.38	0.05	3.30	0.15	3.21	0.11	3.33	0.20	3.24	0.07
17	-0.3	0.05	-0.3	2.86	0.11	2.83	0.11	2.70	0.07	2.84	0.18	2.74	0.06
18	0.05	-0.6	-0.6	4.13	0.11	3.92	0.10	4.05	0.17	4.00	0.22	3.94	0.06
19	0.05	-0.6	-0.3	3.50	0.11	3.23	0.11	3.46	0.11	3.33	0.18	3.34	0.07
20	0.05	-0.3	-0.6	3.25	0.12	3.10	0.09	3.13	0.13	3.16	0.20	3.08	0.06
21	0.05	-0.3	-0.3	2.73	0.07	2.74	0.08	2.72	0.09	2.74	0.14	2.61	0.04
22	0.05	-0.3	0	2.36	0.06	2.27	0.05	2.41	0.08	2.31	0.10	2.26	0.03
23	0.05	-0.3	0.05	2.28	0.05	2.22	0.08	2.33	0.09	2.25	0.12	2.20	0.04
24	0.05	0.05	-0.3	2.32	0.07	2.02	0.05	2.06	0.05	2.13	0.10	2.06	0.03
25	0.05	0.05	0	1.87	0.06	1.84	0.06	1.77	0.05	1.86	0.11	1.73	0.05
26	0.05	0.05	0.05	1.85	0.06	1.72	0.06	1.68	0.06	1.77	0.11	1.68	0.05

Table S8: Finite-size self-diffusion coefficients of [Bmim][Tf_2N] at 300 K and 1 atm. 40 and 8 independent simulations of 50 ns were performed for two system sizes of 150 and 1200 ion pairs, respectively. All average diffusion coefficients (D) and corresponding standard errors ($S.E.$) are reported in units of $10^{-10}m^2s^{-1}$.

N	D_{Tf_2N}	$S.E._{Tf_2N}$	D_{Bmim}	$S.E._{Bmim}$	D_{avg}	$S.E._{avg}$
150	8.071	0.098	12.716	0.104	10.395	0.084
1200	8.782	0.068	13.399	0.107	11.091	0.081

Table S9: Finite-size self-diffusion coefficients of [Bmim][Tf_2N] at 400 K and 1 atm. 40 and 8 independent simulations of 50 ns were performed for two system sizes of 150 and 1200 ion pairs, respectively. All average diffusion coefficients (D) and corresponding standard errors ($S.E.$) are reported in units $10^{-10}m^2s^{-1}$.

N	D_{Tf_2N}	$S.E._{Tf_2N}$	D_{Bmim}	$S.E._{Bmim}$	D_{avg}	$S.E._{avg}$
150	1.627	0.007	2.313	0.010	1.970	0.007
1200	1.780	0.007	2.456	0.010	2.118	0.007

Table S10: Finite-size self-diffusion coefficients of [Bmim][Tf_2N] at 500 K and 1 atm. 40 and 8 independent simulations of 50 ns were performed for two system sizes of 150 and 1200 ion pairs, respectively. All average diffusion coefficients (D) and corresponding standard errors ($S.E.$) are reported in units of $10^{-12}m^2s^{-1}$.

N	D_{Tf_2N}	$S.E._{Tf_2N}$	D_{Bmim}	$S.E._{Bmim}$	D_{avg}	$S.E._{avg}$
150	6.669	0.011	8.865	0.017	7.767	0.011
1200	7.305	0.018	9.418	0.015	8.361	0.016

Table S11: Shear viscosities of [Bmim][Tf_2N] at a pressure of 1 atm and three temperatures (300 K, 400 K, and 500 K). Shear viscosities are obtained from the D-based method (η_i where i represents Tf_2N, Bmim, or the average self-diffusivity, avg) and the Einstein relation (η_{EMD}). The self-diffusivities used for the D-based method are reported in Tables S8 to S10. The simulations computed from the Einstein relation were performed for 200 ns (400 K and 500 K) and 450 ns (300 K). All shear viscosities are reported in cP.

T / K	η_{Tf_2N}	$\eta_{Tf_2N,95\%}$	η_{Bmim}	$\eta_{Bmim,95\%}$	η_{avg}	$\eta_{avg,95\%}$	η_{EMD}	$\eta_{EMD,95\%}$
300	105	35	109	48	107	36	136	20
400	6.4	0.8	6.8	1.3	6.6	0.9	8.2	0.6
500	1.87	0.12	2.15	0.18	2.00	0.13	2.17	0.07

Table S12: Coefficients of the Vogel equation[3] ($\ln(\eta/[\mathrm{cP}]) = A + \frac{B}{T+C}$) used in Figure 8 of the main text.

	A	B	C
Einstein relation	-2.22	1051	-152.1
D-based method	-4.54	2362	-33.5
Green-Kubo relation[8]	-3.85	1908	-67.11

Table S13: Critical temperatures ($T_{c,2}$) and pressures ($P_{c,2}$) of species 2 of binary LJ systems showing large differences between shear viscosities computed from the D-based method and the Einstein relation (see Figure 6 of the main text). LJ interactions are truncated and shifted at 4σ. The critical properties of species 1 with $\sigma_1 = \sigma = 1.0$ and $\epsilon_1 = \epsilon = 1.0$ are: $T_{c,1} = 1.24$ and $P_{c,1} = 0.113$, respectively. x_2 and w_2 represent the mole fraction and mass fraction of the species 2 in the binary LJ system, respectively.

ID	x_2	w_2	ϵ_2/ϵ_1	σ_2/σ_1	k_{12}	deviation	$T_{c,2}$	$P_{c,2}$
1	0.1	0.97	0.5	1.6	0.05	31%	**0.62**	0.014
2	0.1	0.97	0.5	1.6	-0.30	25%	**0.62**	0.014
3	0.1	0.97	0.5	1.6	0.00	21%	**0.62**	0.014
4	0.1	0.96	0.5	1.4	0.00	18%	**0.62**	0.021
5	0.1	0.97	0.6	1.6	0.00	15%	0.74	0.017
6	0.1	0.97	0.6	1.6	-0.30	15%	0.74	0.017
7	0.1	0.97	0.5	1.6	-0.60	14%	0.62	0.014
8	0.1	0.96	0.6	1.4	0.05	14%	0.74	0.025
9	0.1	0.96	0.6	1.4	0.00	14%	0.74	0.025
10	0.1	0.97	0.6	1.6	-0.60	13%	0.74	0.017
11	0.3	0.91	0.6	1.6	0.00	12%	0.74	0.017
12	0.1	0.97	0.6	1.6	0.05	11%	0.74	0.017
13	0.1	0.96	0.6	1.4	-0.30	11%	0.74	0.025
14	0.1	0.90	0.6	1.0	0.05	11%	0.74	0.068
15	0.1	0.94	0.6	1.2	0.00	10%	0.74	0.039

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