

# Supporting Information

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**Table S1. Fitting parameters to the power-law and the Arrhenius equation of the viscosity data of 80 liquids; the melting ( $T_M$ ), glass transition temperature ( $T_g$ ), the references, and temperature range of the experimental data are also reported**

System	Full name	$T_M$ , K	$T_g$ , K	T range, K	$\eta_0$ , P	$T_x$ , K	$\theta$	$T_M/T_x$	$T_x/T_g$	$\ln(\eta_{0A})$ , P	$E/k_B$ , kK	Ref. $\eta$
AC	Acetic acid	289.6	150	304–389	3.97E–03	177	1.856	1.64	1.18			(1)
AMM	Ammonia	195	30	198–240	2.37E–03	122.55	1.655	1.59	4.09			(2)
An			1,160	1,085–2,458	5.70E–02	1742	1.915		1.50	–93.12	139.56	(3)
ANIL	Aniline	266.9	161	274–392	2.73E–03	235.66	1.960	1.13	1.46			(4, 5)
ANOR	Anorthite	1,830	870	1,190–2,426	1.67E–01	1575	3.2	1.16	1.81	–75.45	120.44	(6)
B2O3	Boron Oxide	723	541	536–1675	5.64E+01	702.7	2.900	1.03	1.30	–53.16	45.60	(7)
BAS	Basalt	1,500	973	995–1918	2.27E+00	1,250	3.96	1.2	1.28	–58.62	86.93	(6)
BEZ	Benzene	279	125	266–353	6.48E–03	145	2.130	1.92	1.16	–5.30	1.40	(8)
BRP3	3-bromopentane	146.9	108	107–127	4.60E–02	141	2.290	1.04	1.31	–89.10	12.22	(9)
BSC	Borosilicate Glass		825	807–1611	1.21E+01	993	2.500		1.20	–59.62	75.19	(7)
Ca1244			1,122	1,104–2,073	2.40E–01	1,300	3.260		1.16	–144.98	199.42	(3)
Ca7611			1,199	1,153–2,458	4.36E–01	1,777	3.350		1.48	–54.20	97.39	(3)
CaKNO3	Ca-K-NO <sub>3</sub>		333	354–473	6.08E–03	390	2.080		1.17	–180.80	70.40	(10)
CDF	1-chloro-1,1-difluoroethane	142	27	143–264	8.29E–03	100.65	1.830	1.41	3.73			(2)
CN60.0	Soda lime Silicate G0		1,030	1,012–1,810	6.30E–01	1,211	2.110		1.18	–103.30	136.92	(11)
CN60.2	Soda lime Silicate G2		820	803–1653	1.67E+00	1,221	2.607		1.49	–76.20	86.91	(11)
CN60.4	Soda lime Silicate G4		700	684–1563	5.40E+00	1,094	2.090		1.56	–64.62	66.12	(11)
CTFM	Chlorotrifluoromethane	91.2	18	92–191	9.00E–03	67.034	1.820	1.36	3.72			(2)
CTTC	Carbon tetrachloride	250	60	273–373	4.86E–03	175	1.734	1.43	2.92			(1)
Cum	Isopropylbenzene	177	124.8	136–304	5.07E–03	172	2.020	1.03	1.38	–89.00	14.82	(12)
D2O	Deuterium oxide	276.97	160	277–374	1.35E–03	238.14	1.480	1.16	1.49			(2)
DBP	Dibutyl phthalate	238	170	180–330	7.30E–03	220	2.720	1.08	1.29	–102.44	22.50	(12)
DCDFM	Dichlorodifluoromethane	115.5	18	116–243	5.50E–03	101.66	1.660	1.14	5.65			(2)
DEC	Decane	243.5	54	244–447	4.20E–03	175.477	1.830	1.39	3.25			(2)
DFE	1,1-dichloro-1-fluoroethane	169.7	41	171–305	7.89E–03	123.9	1.930	1.37	3.02			(2)
Di			1,005	962–2312	3.16E–01	1,248	2.999		1.24	–112.34	141.78	(3)
DIOP	Diopside	1,664	990	959–2,065	2.6E–01	1,382	2.37	1.2	1.19	–96.61	126.02	(13, 14)
DMP	Dimethyl phthalate	279	206	243–369	3.60E–03	249.75	2.23	1.12	1.21	–41.77	11.09	(15)
DOD	Dodecane	263.5	76	264–489	4.20E–03	196	1.810	1.34	2.58			(2)
ECT	Ethane, 1-chloro-1,2,2,2-tetrafluoro-	156	36	122–261	1.39E–02	93.39	2.220	1.67	2.59			(2)
EDT	Ethane, 2,2-dichloro-1,1,1-trifluoro-	166	59	166–301	8.30E–03	120	1.870	1.38	2.03			(2)
ETF	Ethane, 1,1,1,2-tetrafluoro-	169.9	71	170–247	3.08E–03	131.2	1.568	1.29	1.85			(2)
ETZ	Ethyl benzene	178.2	111.8	160–303	5.90E–03	149.22	2.02	1.19	1.33			(15)
FM	Fluoromethane	131.4		177–195	4.60E–03	87.7	1.764	1.50				(2)
GEO	GeO2	1,388	810	755–1,787	4.54E+01	1,255	2.99	1.1	1.55	–11.98	34.49	(3)
Gly	Glycerol	291	190	192–343	6.70E–03	277	2.990	1.05	1.46	–66.64	17.75	(16)
H2O	Water	273.15	160	243–340	1.37E–03	225	1.677	1.21	1.41			(17)
HFPA	1,1,1,2,3,3,3-heptafluoropropane	146	47	146–256	6.99E–03	68.133	2.300	2.14	1.45			(2)
HFPB	1,1,1,2,3,3-hexafluoropropane	179	95	243–279	2.90E–03	160	1.788	1.12	1.68			(2)
HFPC	1,1,1,3,3,3-hexafluoropropane	179	98	180–271	2.82E–03	152.72	1.516	1.17	1.56			(2)
HPT	Heptane	182.6	44	180–373	5.00E–03	138	1.809	1.32	3.14			(2)
HXA	Hexane	178	23	175–341	5.60E–03	121.2	1.870	1.47	5.27			(2)
ISB	Isobutane	113	20	116–261	1.13E–02	82.6	2.150	1.37	4.13			(2)
METH	Methanol	175.3	100	178–337	1.05E–02	126	2.270	1.39	1.26	–10.87	1.55	(18)
MTP2	2-methylpentane	120	78	80.5–333	6.46E–03	112.26	1.716	1.07	1.44	–65.37	7.80	(2)
NBB	Butylbenzene	185	125	136–304	5.22E–03	175	1.960	1.06	1.40	–90.44	15.02	(12)
NBS 711	NBS711 glass		705	670–1,622	3.76E+01	881.3	2.230		1.25	–42.57	51.75	(7)
NBS 710	NBS710 glass		830	827–1,776	5.84E+00	1,263	2.190		1.52	–57.43	72.34	(11)
NON	Nonane	219.5	122	220–423	2.94E–03	189.7	1.417	1.16	1.55			(2)
nPBZ	n-propyl benzene	173.7	124	151–303	4.30E–03	164	2.27	1.06	1.32	–50.28	8.59	(15)
nProp	Propanol	147	96.2	103–368	9.00E–03	139	2.900	1.06	1.44	–53.87	7.97	(19)
NS4			784	703–1,725	1.54E+01	1,154	2.998		1.47	–53.01	62.56	(3)
NS66			726	719–1,805	3.86E+00	1,005	2.500		1.38	–70.21	72.77	(11)
NS80			758	718–1,759	9.85E+00	1,209	2.770		1.59	–49.51	39.90	(11)
OCT	Octane	216.3	54	216–398	4.04E–03	159.39	1.684	1.36	2.95			(2)
OTP	o-terphenyl	328.5	246	239–383	3.00E–03	306	1.800	1.07	1.24	–184.12	51.30	(20, 21)
PDE	phenolphthalein dimethyl ether	373	294	296–511	1.79E–03	343.51	2.99	1.08	1.17	–118.00	42.00	(13)
PEN	Pentane	143.4	52	143–309	4.30E–03	115.7	1.520	1.24	2.23			(2)
PHN	Phenol	314.6	197.6	297–343	2.10E–03	236.39	2.78	1.33	1.20			(22)
POC	$\alpha$ -phenyl-o-cresol	323	220	207–285	1.38E–02	266	1.620	1.21	1.21	–135.46	34.64	(20)
POLYS	Polystyrene		332	335–489	1.74E–03	375	2.999		1.05	–165.40	63.50	(23)

(continued)

Table S1. (Continued)

System	Full name	T <sub>M</sub> , K	T <sub>g</sub> , K	T range, K	η <sub>0</sub> , P	T <sub>x</sub> , K	θ	T <sub>M</sub> /T <sub>x</sub>	T <sub>x</sub> /T <sub>g</sub>	ln(η <sub>0A</sub> ), P	E/k <sub>B</sub> , kK	Ref. η
PPCA	Propylene carbonate	218	159.5	157–342	1.40E–02	161	2.070	1.35	1.01	–161.19	29.32	(1)
PRPA	Propane	85.5	30	86–280	6.30E–03	68	1.800	1.26	2.27			(2)
PRPE	Propene	88	29	100–225	5.30E–03	78.47	1.613	1.12	2.71			(2)
PS1	Ti-bearing Na silicate melt 1		796	785–1,683	9.24E+00	1,162	2.150		1.46	–40.06	51.59	(24)
PS2	Ti-bearing Na silicate melt 2		746	784–1,679	5.80E+00	1,206	2.050		1.62	–42.65	54.32	(24)
PS3	Ti-bearing Na silicate melt 3		765	815–1,676	8.88E+00	1,210	2.320		1.58	–42.21	55.31	(24)
PS4	Ti-bearing Na silicate melt 4		809	837–1,591	8.17E+00	1,208	2.050		1.49	–45.22	59.88	(24)
PS5	Ti-bearing Na silicate melt 5		827	884–1,565	6.32E+00	1,220	2.200		1.48	–54.57	77.83	(24)
PS6	Ti-bearing Na silicate melt 6		857	864–1,565	8.77E+00	1,206	2.130		1.41	–48.96	65.04	(24)
Sal	Salol	318	220	213–333	5.00E–03	262	1.350	1.21	1.19	–129.50	33.87	(20)
SBB	Sec-butylbenzene	197.5	127	159–219	4.00E–03	162	2.770	1.22	1.28	–40.70	7.55	(12)
SIO	SiO <sub>2</sub>	1,923	1,480	1276–2,517	5.40E+01	1,612	2.700	1.19	1.09	–28.97	86.19	(3)
TANAB	Tri-α-naphthylbenzene	442	340	330–680	3.40E–03	424	2.170	1.04	1.25	–126.20	51.94	(20)
tBT	t-butanol	298.82		290–315	4.30E–04	248.85	2.85	1.2				(22)
TCFM	Trichlorofluoromethane	162.5	40	163–296	5.20E–03	136.4	1.588	1.19	3.41			(2)
TCTF	1,1,2-trichloro-1,2,2-trifluoroethane	238	120	237–320	2.80E–03	191	1.437	1.25	1.59			(2)
Tol	Toluene	180	113	157–380	4.24E–03	161	1.720	1.12	1.42	–10.08	3.08	(12)
TPE	Triphenyl ethene	341	248	253–570	3.40E–03	297	2.4	1.15	1.20	–134.84	40.83	(6)
TPP	Triphenyl phosphite	295	200	208–424	3.30E–03	215	1.34	1.37	1.08	–9.10	1.39	(25)

- 1 Lide DR (2003) *CRC Handbook of Chemistry and Physics* (CRC, Boca Raton, FL), 84th Ed.
- 2 NIST Chemistry WebBook (2008) <http://webbook.nist.gov/chemistry/fluid/>.
- 3 Sipp A, Bottinga Y, Richet P (2001) New high viscosity data for 3D network liquids and new correlations between old parameters. *J Non-Cryst Solids* 288:166–174.
- 4 Bock E, Czubryt J, Tomchuk E (1970) Proton spin-lattice relaxation time of aniline-d, in deuterated benzene and deuterated aniline solution. *Can J Chem* 48:2814–2818.
- 5 Steiner LA (1938) Viscosity of aniline between 20° and 100° C. *Ind Eng Chem Anal* 10:582–584.
- 6 Mauro JC, Yue Y, Ellison AJ, Gupta PK, Allan DC (2009) Viscosity of glass-forming liquids. *Proc Natl Acad Sci USA* 106:19780–19784.
- 7 Tweer H, Simmons JH, Macedo PB (1971) Application of the environmental application model to the temperature dependence of the viscosity. *J Chem Phys* 54:1952–1959.
- 8 Hu PM, Parsons RW (1958) The viscosity and density of benzene near its freezing point. *Proc Phys Soc* 72:454–457.
- 9 Wilson WL, Mellon PF, Berberian JG (1982) The steady-state shear viscosities of some bromopentanes. *J Chem Phys* 76:2602–2605.
- 10 Weiler R, Blaser S, Macedo PB (1969) Viscosity of a vitreous potassium nitrate-calcium nitrate mixture. *J Phys Chem* 73:4147–4151.
- 11 Neuville DR (2006) Viscosity, structure and mixing in (Ca, Na) silicate melts. *Chem Geo* 229:28–41.
- 12 Rossler E (1990) Corresponding states analysis for viscosity and nuclear magnetic resonance data in the glass transition regime. *J Chem Phys* 92:3725–3735.
- 13 Rha K (2007) Generalized excluded volume and the diffusivity and viscosity of supercooled liquids and glasses over the entire fragility spectrum. *Physica A* 378:167–182.
- 14 Nascimento MLF, Ferreira EB, Zanotto ED (2004) Kinetics and mechanisms of crystal growth and diffusion in a glass-forming liquid. *J Chem Phys*. 121:8924–8928.
- 15 Barlow AJ, Lamb J, Matheson AJ (1966) Viscous behaviour of supercooled liquids. *Proc R Soc London A* 292:322–342.
- 16 Schroter K, Donth E (2000) Viscosity and shear response at the dynamic glass transition of glycerol. *J Chem Phys* 113:9101–9108.
- 17 Cho CH, Urquidi J, Singh S, Wilse Robinson G (1999) Thermal offset viscosities of liquid H<sub>2</sub>O, D<sub>2</sub>O, and T<sub>2</sub>O. *J Phys Chem B* 103:1991–1994.
- 18 Xiang HW, Laescke A, Huber ML (2006) A new reference correlation for the viscosity of methanol. *J Phys Chem Ref Data* 35:1597–1620.
- 19 Ling AC, Willard JE (1968) Viscosities of some organic glasses used as trapping matrices. *J Phys Chem* 72:1918–1923.
- 20 Laughlin WT, Uhlmann DR (1972) Viscous flow in simple organic liquids. *J Phys Chem* 76:2317–2325.
- 21 Rha K, Eu BC (2003) Theory of the viscosity of supercooled liquids and the glass transition: Fragile liquids. *Phys Rev E* 68:051204.
- 22 Hughes JA, Byers CH (1986) Viscosity behavior in supercooled pure liquids and mixtures. ORNL/TM-9998, Oak Ridge National Laboratory, Oak Ridge, TN, December.
- 23 Urakawa O, Swallen SF, Ediger MD, von Meerwall ED (2004) Self-diffusion and viscosity of low molecular weight polystyrene over a wide temperature range. *Macromolecules* 37:1558–1564.
- 24 Liska M, Simurka P, Antalík J, Perichta P (1996) Viscosity of titania-bearing sodium silicate melts. *Chem Geo* 128:199–206.
- 25 Zhao X, Kivelson D (1995) Light-scattering studies of simple molecular supercooled liquids: Structural considerations. *J Phys Chem* 99:6721–6732.

**Table S2. Fitting parameters to the power-law and the Arrhenius equation of the inverse of the self-diffusion coefficient data of 12 liquids; the melting ( $T_M$ ), glass transition temperature ( $T_g$ ), the references, and temperature range of the experimental data are also reported**

System	Full name	$T_M$ , K	$T_g$ , K	T range, K	$1/D_0$ , $m^{-2}s$	$T_x$ , K	$\theta$	$T_M/T_g$	$T_x/T_g$	$\ln(1/D_{0A})$ , $m^{-2}s$	$E/k_B$ , kK	Ref. $D_s$
CDE	Cresolphthaleine dimethyl ether	387	310	371–431	2.09E+08	377.4	2.622	1.03	1.22	–36.74	24.92	(1)
DIOP	Diopside	1,664	990	1,666–2,263	8.46E+07	1180	2.650	1.41	1.19			(2)
Gly	Glycerol	291	190	256–459	7.29E+08	238.3	3.930	1.22	1.25	0.17	8.09	(1, 3)
METH	Methanol	175.3	100	154–338	2.24E+08	172.3	2.290	1.02	1.72	11.37	2.07	(4, 5)
OTP	o-terphenyl	328.5	246	246–344	7.93E+08	302	1.470	1.09	1.23	–63.97	26.77	(6, 7)
PDE	phenolphthalein dimethyl ether	373	294	337–428	2.76E+08	362.96	2.380	1.03	1.23	–21.87	17.85	(1, 8)
POLYS	Polystyrene		332	335–581	1.62E+09	375	3.050		1.13	–94.48	47.37	(9)
PP6	PEP-PDMS-6		201	309–433	8.72E+9	260.53	4.000		1.30			(10)
PPCA	Propylene carbonate	218	159.5	179–332	1.33E+09	168	3.050	1.30	1.05	–13.64	8.11	(11)
Sal	Salol	318	220	249–369	2.16E+08	276	1.860	1.15	1.25	–102.50	33.67	(1)
TANAB	Tri- $\alpha$ -naphthylbenzene	442	340	343–476	3.37E+08	424.9	2.120	1.04	1.25	–80.60	43.21	(12)
Tol	Toluene	180	113	135–378	3.41E+08	160.4	1.890	1.12	1.42	–23.65	7.53	(13)

- Chang I, Sillescu H (1997) Heterogeneity at the glass transition: Translational and rotational self-diffusion. *J Phys Chem B* 101:8794–8801.
- Nascimento MLF, Ferreira EB, Zanotto ED (2004) Kinetics and mechanisms of crystal growth and diffusion in a glass-forming liquid. *J Chem Phys* 121:8924–8928.
- Chen B, Sigmund EE, Halperin WP (2006) Stokes-Einstein relation in supercooled aqueous solutions of glycerol. *Phys Rev Lett* 96:145502.
- Karger N, Vardag T, Ludemann H-D (1990) Temperature dependence of self-diffusion in compressed monohydric alcohols. *J Chem Phys* 93:3437–3444.
- Rathbun RE, Babb AL (1961) Self-diffusion in liquids III temperature dependence in pure liquids. *J Phys Chem* 65:1072–1074.
- Rha K, Eu BC (2003) Theory of the viscosity of supercooled liquids and the glass transition: Fragile liquids. *Phys Rev E* 68:051204.
- Mapes MK, Swallen SF, Ediger MD (2006) Self-diffusion of supercooled o-terphenyl near the glass transition temperature. *J Phys Chem B* 110:507–511.
- Rha K (2007) Generalized excluded volume and the diffusivity and viscosity of supercooled liquids and glasses over the entire fragility spectrum. *Physica A* 378:167–182.
- Urakawa O, Swallen SF, Ediger MD, von Meerwall ED (2004) Self-diffusion and viscosity of low molecular weight polystyrene over a wide temperature range. *Macromolecules* 37:1558–1564.
- Fleischer G, Rittig F, Stepanek P, Almdal K, Papadakis CM (1999) Self-diffusion of a symmetric PEP-PDMS diblock copolymer above and below the disorder-to-order transition. *Macromolecules* 32:1956–1961.
- Qi F, et al. (2000) Structural relaxation of the fragile glass-former propylene carbonate studied by nuclear magnetic resonance. *J Chem Phys* 112:9455–9462.
- Swallen SF, Bonvallet PA, McMahon RJ, Ediger MD (2003) Self-diffusion of tris-naphthylbenzene near the glass transition temperature. *Phys Rev Lett* 90:015901.
- NaNagara B, O'Conner RD, Blum FD (1992) Mobility of toluene in polystyrene-toluene solutions. A NMR Study. *J Phys Chem* 96:6417–6423.

**Table S3. Fitting parameters to the power-law and the Arrhenius equation of the relaxation time data of 8 liquids; the melting ( $T_M$ ), glass transition temperature ( $T_g$ ), the references, and temperature range of the experimental data are also reported**

System	Full name	$T_M$ , K	$T_g$ , K	T range, K	$\tau_0$ , s	$T_x$ , K	$\theta$	$T_M/T_x$	$T_x/T_g$	$\ln(\tau_{0A})$ , s	$E/k_B$ , kK	Ref. $\tau$
BPH	Benzophenone	321	208	200–434	7.65E–12	255.6	1.960	1.26	1.23	–139.45	29.71	(1)
BRP3	3-bromopentane	146.9	108	111–298	1.70E–11	140	2.300	1.05	1.30	–91.79	10.65	(2)
CaKNO3	Ca-K-NO <sub>3</sub>		333	341–468	2.68E–12	391.7	2.378		1.18	–196.24	69.00	(3)
Gly	Glycerol	291	190	221–270	1.16E–10	231.4	2.999	1.26	1.22	–69.25	13.30	(4)
KDE	cresolphthalein-dimethylether	383	312	308–500	1.29E–11	375	2.650	1.02	1.20	–126.55	40.76	(5)
OTP	o-terphenyl	328.5	246	248–311	9.77E–12	291.3	1.650	1.13	1.18	–135.42	33.94	(5)
PPCA	Propylene carbonate	218	159.5	162–310	8.39E–12	188.9	2.700	1.15	1.18	–137.99	22.46	(5)
Sal	Salol	318	220	219–383	1.11E–11	263	1.817	1.21	1.20	–116.40	25.80	(6)

- Lunkenheimer P, Pardo LC, Kohler M, Loidl, A. (2008) Broadband dielectric spectroscopy on benzophenone:  $\alpha$  relaxation,  $\beta$  relaxation, and mode coupling theory. *Phys Rev E* 77:031506.
- Richert T, Angell CA (1998) Dynamics of glass-forming liquids. V. On the link between molecular dynamics and configurational entropy. *J Chem Phys* 108:9016–9026.
- Yang Y, Nelson KA (1996) Impulsive stimulated thermal scattering study of a relaxation dynamics and the Debye-Waller factor anomaly in Ca<sub>0.4</sub>K<sub>0.6</sub>(NO<sub>3</sub>)<sub>1.4</sub>. *J Chem Phys* 104:5429–5436.
- Paolucci DM, Nelson KA (2000) Impulsive stimulated thermal scattering study of structural relaxation in supercooled glycerol. *J Chem Phys* 112:6725–6732.
- Paluch M, Ngai KL, Hensel-Bielowka S (2001) Pressure and temperature dependences of the relaxation dynamics of cresolphthalein-dimethylether: Evidence of contributions from thermodynamics and molecular interactions. *J Chem Phys* 114:10872–10883.
- Yang Y, Nelson KA (1995) Impulsive stimulated light scattered from glass-forming liquids. II. Salol relaxation dynamics, nonergodicity parameter, and testing of mode coupling theory. *J Chem Phys* 103:7732–7739.