SUPPLEMENTARY MATERIAL

Self-Diffusion Coefficient of Bulk and Confined Water: A Critical Review of Classical Molecular Simulation Studies

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Contents

TABLE SI-1. Available MD simulation data of the self-diffusion coefficient of water at ambient conditions. "**Ref #**" corresponds to the reference (see Reference list at page 71) of the study reporting the self-diffusion coefficient value. "T", "P", and "ρ" correspond to the conditions at which the simulations are performed. "**SSE correction**" indicates if the data are corrected for system size effects (see ref [76]). "**H_2O Ref #**" lists the original H_2O model development papers.

Ref #	Authors	Year	T (K)	P (bar)	ρ (g/cm³)	D (m²/s) (x 10^9)	Statistical Error	SSE correction	Number of H_2O molecules	H_2O force field	H_2O Ref #
3	Rahman et al.	1975	295.15		1	0.73	N/A	No	216	CF	3
4	Stillinger & Rahman	1978	302.65	1.01325		1.1	N/A	No	216	CF modified	4
5	Impey et al.	1982	294		1	2.3	0.2	No	125	MCY	175
6	Jorgensen et al.	1983	294.15	1.01325		4.3	10%	No	125	BF	176
	"----//----"	1983	293.15	1.01325		3.2	10%	No	125	TIPS2	177
9	Lie & Clementi	1986	300		0.998	1.8	N/A	No	343	MCYL	9
	"----//----"	1986	299		0.998	1.9	N/A	No	343	MCYL	9
	"----//----"	1986	300.6		0.998	1.9	N/A	No	343	MCYL	9
	"----//----"	1986	300.6		0.998	2.1	N/A	No	343	MCYL	9
10	Neumann	1986	293		1.0	2.8	N/A	No	256	TIP4P	6
11	Wojcik & Clementi	1986	296		1	2.25	N/A	No	512	MCY	175
	"----//----"	1986	304		1	1.3	N/A	No	512	MCY + *ab initio* 3 body	11
12	Anderson et al.	1987	300		1	2.54	N/A	No	125	SPC modified (flex.)	12
13	Berendsen et al.	1987	306		0.998	2.50	N/A	No	216	SPC/E	13
	"----//----"	1987	308		0.97	4.30	N/A	No	217	SPC	178
14	Reddy & Berkowitz	1987	268		0.999	1.36	N/A	No	216	TIP4P	6
	"----//----"	1987	298		0.999	2.96	N/A	No	216	TIP4P	6
15	Teleman et al.	1987	301			4.4	0.1	No	216	SPC-type; R1 (rigid)	15

	"----//----"	1987	301			2.6	0.1	No	216	SPC-type; R2 (rigid)	15
	"----//----"	1987	301			6.10	0.2	No	216	SPC-type; F (flexible)	15
16	Ahlstrom et al.	1989	303			8.9	N/A	No	216	PSPC - GD	16
	"----//----"	1989	301			0.80	N/A	No	216	PSPC - P(P)	16
	"----//----"	1989	300			0.77	N/A	No	216	PSPC - P(I)	16
	"----//----"	1989	302			0.04	N/A	No	216	PSPC - LD	16
	"----//----"	1989	302			2.0	N/A	No	216	PSPC	16
17	Watanabe & Klein	1989	298		0.997	2.4	0.4	No	216	SPC/E	13
	"----//----"	1989	298		0.997	3.6	0.5	No	216	SPC	178
	"----//----"	1989	298		0.997	3.3	0.5	No	216	TIP4P	6
	"----//----"	1989	298		0.997	1.1	0.3	No	216	WK	17
18	Caldwell et al.	1990	303		0.991	3.1	0.5	No	216	POL1	179
	"----//----"	1990	300		0.998	2.5	N/A	No	216	SPC/E	13
19	Wallqvist et al.	1990			1.0	1.3	0.1	No	216	NEMO	19
20	Ruff & Diestler	1990	298	1		2.2	N/A	No	256	BJH	203
21	Sprik et al.	1990	295	0		1.5	0.4	No	216	Pol	21
22	Straatsma & McCammon	1990	303.6	1.7	0.994	3.1	N/A	No	216	STR/1	22
26	Sprik	1991	300	600	1	2.4	N/A	No	216	Pol.	26
27	Zhu et al.	1991	298		0.997	1.6	N/A	No	256	MST-FP	27
28	Zhu et al.	1991	298	1.01325	0.997	7.1	N/A	No	256	SPC-FP	28
29	Wallqvist & Teleman	1991	300			3.6	0.2	No	216	SPC-flex (harmonic)	29
	"----//----"	1991	300			3.1	0.2	No	216	SPC-flex (unharmonic)	182
	"----//----"	1991	300			4.2	0.2	No	216	SPC-rigid	178
30	Smith & Haymet	1992	298		1	1.44	0.06	No	216	CF	4
	"----//----"	1992	298		1	1.16	0.06	No	216	RCF (rigid)	30
	"----//----"	1992	298		1	3.7	0.1	No	216	SPC	178
31	van Belle et al.	1992	300		1	4.6	0.2	No	216	SPC	178
	"----//----"	1992	300		1	2.4	0.2	No	216	PSPC	16
	"----//----"	1992	300		1	2.7	0.3	No	216	PSPC-PPD	31
34	Rick et al.	1994	298		1	1.9	0.1	No	256	TIP4P-FQ	34
	"----//----"	1994	298		1	1.7	0.1	No	256	SPC-FQ	34
35	Smith & Dang	1994	298		0.997	2.4	0.3	No	216	RPOL	180

#	Author	Year	T		ρ				N	Model	Ref
	"----//----"	1994	298		0.997	2.4	0.4	No	216	SPC/E	13
36	Svishchev & Kusalik	1994	298.15		0.998	2.15	N/A	No	108	SPC/E	13
	"----//----"	1994	298.15		0.998	2.24	N/A	No	256	SPC/E	13
37	Padro et al.	1994	298		1	2.5	N/A	No	216	SPC (flex)	178
39	Astrand et al.	1995	300			1.0	N/A	No	216	NEMO modified	39
40	Soetens & Millot	1995	298.15		1	1.7	N/A	No	216	SPEP/SPEP	40
	"----//----"	1995	298.15		1	1.4	N/A	No	216	SPEP/TPEP	40
	"----//----"	1995	298.15		1	6.1	N/A	No	216	TPEP/TPEP	40
	"----//----"	1995	298.15		1	4.4	N/A	No	216	SPEP/1SITE	40
41	Duan et al.	1995	307.15	1		3.06	N/A	No	256	RWK2	181
42	Mountain	1995	303		0.997	2.7	N/A	No	216	RPOL	180
43	Brodholt et al.	1995	298.15		1	2.3	N/A	No	256	TIP4P-Polarizable	43
44	Svishchev et al.	1996	298		0.997	2.6	2%	No	256	PPC	44
47	Taylor et al.	1996	298		1	3.02	N/A	No	526	SPC/E	13
49	Dang & Chang	1997	298		0.995	2.1	0.1	No	550	TIP4P-type (Polarizable)	49
50	Levitt et al.	1997	273		0.999	1.6	N/A	(see ref)	216	F3C	50
	"----//----"	1997	298		0.997	2.4	0.23	(see ref)	216	F3C	50
51	Lobaugh & Voth	1997	300		0.996	4.2	N/A	No	125	Quantum SPC/F	51
	"----//----"	1997	300		0.996	3.0	0.2	No	125	Classical SPC/F	182
	"----//----"	1997	300		0.996	3.8	N/A	No	125	Quantum SPC/F$_2$	51
	"----//----"	1997	300		0.996	2.2	0.2	No	125	Classical SPC/F$_2$	51
52	de Leeuw & Parker	1998	300		1.15	1.15	N/A	No	256	SW	52
55	Nymand & Linse	2000	303.15		Exp. Dens.	0.786	0.002	No	216	NEMO (SC)	39
	"----//----"	2000	303.15		Exp. Dens.	0.813	0.002	No	216	NEMO (ES)	39
	"----//----"	2000	303.15		Exp. Dens.	0.837	0.002	No	512	NEMO (ES)	39
	"----//----"	2000	303.15		Exp. Dens.	1.20	0.002	No	216	NEMO (RF)	39
	"----//----"	2000	303.15		Exp. Dens.	1.00	0.002	No	512	NEMO (RF)	39
	"----//----"	2000	303.15		Exp. Dens.	1.17	0.002	No	216	NEMO (RF)	39
	"----//----"	2000	303.15		Exp. Dens.	2.75	0.002	No	216	SPC/E (RF)	13
	"----//----"	2000	303.15		Exp. Dens.	3.13	0.002	No	216	SPC/E (RF)	13
	"----//----"	2000	303.15		Exp. Dens.	0.799	0.002	No	216	NEMO (SC)	39
	"----//----"	2000	303.15		Exp. Dens.	0.820	0.002	No	216	NEMO (ES)	39

		Year	Temp	Press	Dens	Val	Err		N	Model	Ref
	"----//----"	2000	303.15		Exp. Dens.	0.855	0.002	No	512	NEMO (ES)	39
	"----//----"	2000	303.15		Exp. Dens.	1.20	0.002	No	216	NEMO (RF)	39
	"----//----"	2000	303.15		Exp. Dens.	1.00	0.002	No	512	NEMO (RF)	39
	"----//----"	2000	303.15		Exp. Dens.	1.16	0.002	No	216	NEMO (RF)	39
	"----//----"	2000	304.15		Exp. Dens.	2.77	0.002	No	216	SPC/E (RF)	13
	"----//----"	2000	305.15		Exp. Dens.	3.13	0.002	No	216	SPC/E (RF)	13
56	Guo & Zhang	2001	303		0.999	2.63	0.06	No	256	SPC/E	13
57	Mahoney & Jorgensen	2001	298.15	1.01325		3.85	0.09	No	267	SPC	178
	"----//----"	2001	298.15	1.01325		2.49	0.05	No	267	SPC/E	13
	"----//----"	2001	298.15	1.01325		5.19	0.08	No	267	TIP3P	6
	"----//----"	2001	298.15	1.01325		3.31	0.08	No	267	TIP4P	6
	"----//----"	2001	298.15		0.993	5.06	0.09	No	267	TIP3P	6
	"----//----"	2001	298.15		0.990	3.29	0.05	No	267	TIP4P	6
	"----//----"	2001	298.15		0.999	2.62	0.04	No	267	TIP5P	183
58	Stern et al.	2001	298.15	1.01325		1.81	0.06	No	256	POL5/TZ	58
	"----//----"	2001	298.15	1.01325		1.25	0.05	No	256	POL5/QZ	58
59	van Maaren & van der Spoel	2001	300		0.997	3.66	0.19	No	820	SWFLEX-AI	59
	"----//----"	2001	300		0.997	3.58	0.02	No	820	SWFLEX-ISO	59
	"----//----"	2001	300		0.996	3.22	0.15	No	820	SWRIGID-AI	59
	"----//----"	2001	300		0.993	3.30	0.34	No	820	SWRIGID-ISO	59
60	Lefohn et al.	2001	300		1.0	1.5	N/A	No	256	2S-PF (Two-State PolarFlex)	60
	"----//----"	2001	300		1.0	1.9	N/A	No	256	3S-PF (Three-State PolarFlex)	60
63	Burnham & Xantheas	2002	300		1.046	2.23	N/A	No	64	TTM2-R	63
64	Guo et al.	2002	303.8		0.999	2.63	0.06	No	256	SPC/E	13
	"----//----"	2002	273.5		1.011	1.27	0.03	No	256	SPC/E	13
65	English & MacElroy	2002	298.15		0.997	2.3	0.1	No	256	SPC/F (flexible)	182
	"----//----"	2002	298.15		0.997	3.4	0.1	No	256	TIP4P	6
	"----//----"	2002	298.15		0.997	2.0	0.1	No	256	TIP4P-FQ	34
68	Tan et al.	2003	298	668.745	0.997	2.24	N/A	No	256	SSD0 (original)	184
	"----//----"	2003	298	1.01325	0.958	2.37	N/A	No	256	SSD0 (original)	184
	"----//----"	2003	298	1.01325	0.99	2.13	N/A	No	256	SSD1 (optimized)	68
69	Yu et al.	2003	300	1.01325		4.3	N/A	No	1331	SPC	69

#	Author	Year	T	P	ρ				N	Model	Ref
	"----//----"	2003	300	1.01325		4.0	N/A	No	1331	STR/1	22
	"----//----"	2003	300	1.01325		3.5	N/A	No	1331	STR/RF	69
	"----//----"	2003	300	1.01325		2.7	N/A	No	1331	COS/B1	69
	"----//----"	2003	300	1.01325		2.6	N/A	No	1331	COS/B2	69
70	Jeon et al.	2003	300		0.997	2.44	0.04	No	256	PRG (PolarFlex Rigid Gausian)	70
	"----//----"	2003	300		0.997	2.40	0.03	No	256	PRG (PolarFlex Rigid Gausian)	70
	"----//----"	2003	300		0.997	2.29	0.07	No	256	PFG (PolarFlex Flexible Gausian)	70
	"----//----"	2003	300		0.997	2.28	0.04	No	256	PFG (PolarFlex Flexible Gausian)	70
	"----//----"	2003	300		0.997	3.0	N/A	No	256	SPC/F (flexible)	182
71	English & MacElroy	2003	260		1.002	0.83	N/A	No	500	F-SPC	182
	"----//----"	2003	298		0.997	2.3	N/A	No	500	F-SPC	182
	"----//----"	2003	298		0.996	2.1	N/A	No	502	TIP4P-FQ	182
72	Ren & Ponder	2003	298		1.0004	2.02	0.05	No	216	AMOEBA	72
73	Spangberg & Hermansson	2003	298		0.998	2.32	0.10		128	SPC/E	13
	"----//----"	2003	298		0.998	2.43	0.03		256	SPC/E	13
	"----//----"	2003	298		0.997	2.57	0.03		512	SPC/E	13
	"----//----"	2003	298		0.998	2.58	0.03		1024	SPC/E	13
	"----//----"	2003	298		0.978	4.08	0.05		512	SPC	178
74	Amira et al.	2004	300		1.000	2.55	N/A	No	512	SPC+CCL	74
	"----//----"	2004	300		1.000	2.57	N/A	No	512	F-SPC	182
75	Horn et al.	2004	272.2	1.01325	0.9996	1.2	0.02	No	512	TIP4P-Ew	75
	"----//----"	2004	297.4	1.01325	0.9954	2.4	0.06	No	512	TIP4P-Ew	75
76	Yeh & Hummer	2004	298	1		6.05	N/A	YES		TIP3P	6
77	Yu & Gunsteren	2004	302.8		0.9972	2.3	N/A	No	1000	COS/G2	77
	"----//----"	2004	302.0		1.0000	2.6	N/A	No	1000	COS/G3	77
79	Saint-Martin et al.	2005	298.15	1.01325		1.16	N/A	No	1000	MCDHO$_{fc}$	185
	"----//----"	2005	298.15	1.01325		1.09	N/A	No	1000	MCDHO$_{ff}$	186
	"----//----"	2005	298.15	1.01325		0.92	N/A	No	1000	MCDHO$_r$	79
	"----//----"	2005	298.15	1.01325		0.9	N/A	No	1000	MCD	79
80	Abascal & Vega	2005	298.15	1	0.9979	2.08	N/A	No	530	TIP4P/2005	80

82	Lamoureux et al.	2006	298.15	1.01325		2.33	0.02	No	250	SWM4-NDP	82
83	Wu et al.	2006	298.16	1.01325	0.977	4.02	0.01	No	216	SPC	178
	"----//----"	2006	298.16	1.01325	0.999	2.41	0.08	No	216	SPC/E	13
	"----//----"	2006	298.16	1.01325	0.986	5.3	0.07	No	216	TIP3P	6
	"----//----"	2006	298.16	1.01325	1.01	2.76	0.07	No	216	SPC/Fd	187
	"----//----"	2006	298.16	1.01325	1.004	2.62	0.01	No	216	F3C	50
	"----//----"	2006	298.16	1.01325	1.034	3.53	0.11	No	216	TIP3P/Fs	188
	"----//----"	2006	298.16	1.01325	1.012	2.32	0.05	No	216	SPC/Fw	83
84	Paesani et al.	2006	298.15	1.01325	0.999	2.4	0.1	No	216	q-SPC/Fw	84
	"----//----"	2006	298.15	1.01325	0.991	3.2	0.1	No	216	SPC/Fw	83
85	Fanourgakis et al.	2006	300	1.01325		1.4	N/A	No	256	TTM2.1-F	85
86	Donchev et al.	2006	298.15	1.01325		1.2	N/A	No	256	QMPFF2	86
	"----//----"	2006	298.15	1.01325		1.9	N/A	No	256	QMPFF2	86
	"----//----"	2006	298.15	1.01325		2.6	N/A	No	256	NCC	189
	"----//----"	2006	298.15	1.01325		1.3	N/A	No	256	NEMO	19
	"----//----"	2006	298.15	1.01325		2.2	N/A	No	256	TTM2-R	63
89	Hofmann et al.	2007	298	1	1.06	1.42	N/A	No		Hofmann et al.	89
90	De Fusco et al.	2007	300	1.01325	1.105	2.63	N/A	No	216	DPP	90
93	Kolafa	2008	298.15	-0.97	0.997048	2.52	0.05	No	1000	POL3	190
	"----//----"	2008	298.15	1	0.997048	2.51	0.05	No	1000	IPOL-0.13	93
	"----//----"	2008	298.15	1	0.997048	3.01	0.06	No	1000	IPOL-0.16	93
	"----//----"	2008	298.15	1	0.997048	2.04	0.04	No	1000	IPOL-0.13-0.1	93
	"----//----"	2008	298.15	1	0.997048	2.37	0.04	No	1000	IPOL-0.16-0.1	93
	"----//----"	2008	298.15	1	0.997048	2.14	0.02	No	1000	APOL-0.13	93
	"----//----"	2008	298.15	1	0.997048	2.61	0.05	No	1000	APOL-0.16	93
94	Mankoo & Keyes	2008	300		0.997	2.38	N/A	No	256	POLIR	94
95	Liem & Popelier	2008	300	1.01325	0.996	1.44	N/A	No	216	QCT	95
96	Kumar & Skinner	2008	298			2.49	0.04	No	256	SPC/E	13
	"----//----"	2008	298			3.44	0.07	No	256	TIP4P	191
	"----//----"	2008	298			2.36	0.05	No	256	Kumar et al.	96
97	Akin-Ojo et al.	2008	298		0.997	2.8	0.2	No	216	MP2f	97
	"----//----"	2008	298		0.997	2.6	0.3	No	216	BLYPf	97

#	Author	Year	Temp	Press	Density			Polar	N	Model	Ref
	"----//----"	2008	298		0.997	1.9	0.1	No	216	B3LYPf	97
99	Vega et al.	2009	298	1		5.51	N/A	No	360	TIP3P	6
	"----//----"	2009	298	1		3.22	N/A	No	360	TIP4P	191
	"----//----"	2009	298	1		2.77	N/A	No	360	TIP5P	183
	"----//----"	2009	298	1		2.07	N/A	No	360	TIP4P/2005	80
100	Walsh & Liang	2009	298		1.0004	2.02	N/A	No	512	AMOEBA	78
	"----//----"	2009	298		0.98	2.52	N/A	No	512	DMIP	100
101	Bauer et al.	2009	298	1.01325		2.15	N/A	Yes	216	TIP4P-FQ	34
	"----//----"	2009	298	1.01325		2.46	N/A	Yes	216	TIP4P-QDP	101
	"----//----"	2009	298	1.01325		2.04	N/A	Yes	216	QDP-P1	101
102	Bauer & Patel	2009	298	1.01325	0.998	2.3	0.04	Yes	216	TIP4P-QDP-LJ	102
103	Liu et al.	2009	298.15	1.01325		1.8	0.1	No	216	q-SPC/Fw	84
	"----//----"	2009	298.15	1.01325		5	0.1	No	216	q-SPC/Fw	84
	"----//----"	2009	298.15	1.01325		2.5	0.1	No	216	q-SPC/Fw	84
104	Kunz & van Gunsteren	2009	298.15	1.01325		2.5	N/A	No	1000	COS/D	104
105	Akin-Ojo & Wang	2009	298.15			3.7	N/A	Yes	216	MP2$_f$_hb	104
106	Molinero & Moore	2009	298			6.50	N/A	No		mW	106
108	Te & Ichiye	2010	298	1		2.22	N/A	No	256	SSDQO1	108
109	Shaik et al.	2010	298	1.01325		2.27	N/A	No	216	Optimized QCT	109
	"----//----"	2010	298	1.01325		2.62	N/A	No	216	TIP5P	183
110	Chiu et al.	2010	298		0.998	4.3	N/A	No	400/3200	CSJ W4	110
	"----//----"	2010	298		1.005	1.6	N/A	No	400/3200	MARTINI W	192
	"----//----"	2010	298		0.993	6.6	N/A	No	400/3200	SSRBK W	193
111	Karamertzanis et al.	2010	298.15	1.01325		1.4	N/A	No	542	Karamertzanis et al.	111
112	Daree et al.	2010	300	1	1.0001	2.23	N/A	No	497	WT4	112
113	Fuhrmans et al.	2010	298	1		1.26	0.05	No	1068	Model 1 Fuhrmans et al.	113
	"----//----"	2010	298	1		1.24	0.07	No	1068	Model 2 Fuhrmans et al.	113
	"----//----"	2010	298	1		1.92	0.03	No	1068	MARTINI W	192
	"----//----"	2010	298	1		4.21	0.19	No	1068	SPC	178
115	Guevara-Carrion et al.	2011	298.15	1		4.34	N/A	No	2048	SPC	178
	"----//----"	2011	298.15	1		2.72	N/A	No	2048	SPC/E	13
	"----//----"	2011	298.15	1		3.69	N/A	No	2048	TIP4P	191

#	Author	Year	T	P	ρ				N	Model	Ref
	"----//----"	2011	298.15	1		2.25	N/A	No	2048	TIP4P/2005	80
116	Tainter et al.	2011	298	1.01325	993.5	2.3	0.02	Yes	500	E3B	116
117	Gonzalez & Abascal	2011	298	1	0.9977	1.93	N/A	No	500	TIP4P/2005f	117
	"----//----"	2011	298	1	0.9979	2.08	N/A	No	500	TIP4P/2005	80
118	Hasegawa & Tanimura	2011	298	1	0.9932	1.83	0.02	No	216	Hasegawa & Tanimura	118
119	Alejandre et al.	2011	300	1	0.9947	2.2	N/A	No	500	TIP4Q	119
120	Viererblova & Kolafa	2011	298.15	1.01325		2.461	0.015	Yes	360	POL4D	120
121	Orsi & Essex	2011	298.15	1.01325		2.5	1%	No	4000	ELBA	121
122	Wang & Hou	2011	298			2.984	0.005	No	624	TIP3P	6
	"----//----"	2011	298			3.097	N/A	No	928	TIP3P	6
124	Raabe & Sadus	2012	298.15	1		2.432	0.023	No	400	SPC/E	13
	"----//----"	2012	298.15	1		2.359	0.035	No	400	SPC/Fw	83
	"----//----"	2012	298.15	1		3.861	0.03	No	400	SPC	178
125	Leontyev & Stuchebrukhov	2012	298.15	1.01325	0.9986	6.1	0.1	Yes	2048	MFP/TIP3P	125
	"----//----"	2012	298.15	1.01325	0.9986	6.1	0.1	Yes	2048	TIP3P	6
126	Daree et al.	2012	300	1		4.3	N/A	No	2002	SPC	178
	"----//----"	2012	300	1		2.9	N/A	No	2002/182	Hybrid SPC/WT4	126
	"----//----"	2012	300	1		2.23	N/A	No	182	WT4	112
127	Babin et al.	2012	298.15		0.997	2.3	5	No	256	HBB2-pol	127
128	Tazi et al.	2012	300		0.998	2.97	0.05	Yes	64-4096	SPC/E	13
	"----//----"	2012	300		0.998	2.49	0.06	Yes	2048	TIP4P/2005	80
	"----//----"	2012	300		0.998	2.72	0.09	Yes	512	Dang-Chang	49
132	Lee	2013	300		0.9965	2.78	0.06	No	1024	SPC/E	13
133	Chen et al.	2013	298.15	1.01325		5.06	N/A	No	256	TIP3P	6
	"----//----"	2013	298.15	1.01325		3.29	N/A	No	256	TIP4P	191
	"----//----"	2013	298.15	1.01325		2.62	N/A	No	256	TIP5P	183
	"----//----"	2013	298.15	1.01325		2.4	N/A	No	256	TIP4P-Ew	75
	"----//----"	2013	298.15	1.01325		2.49	N/A	No	256	SPC/E	13
	"----//----"	2013	298.15	1.01325		2.52	N/A	No	256	TIP4P(M)	133
134	Akin-Ojo & Szalewicz	2013	298.15			2.4	N/A	Yes	256	CC-pol-8s'	134
	"----//----"	2013	298.15			2.6	N/A	Yes	256	CC-dpol-8s'	134
135	Yu et al.	2013	298.15	1.01325		3.92	N/A	Yes	267	TIP4P	191

#	Author	Year	T	P	ρ				Size	Model	Ref
	"----//----"	2013	298.15	1.01325		2.74	N/A	Yes	512	TIP4P-Ew	75
	"----//----"	2013	298.15	1.01325		2.49	0.09	Yes	average of 360 and 530	TIP4P/2005	80
	"----//----"	2013	298.15	1.01325		3.06	N/A	Yes	267	TIP5P	183
	"----//----"	2013	298.15	1.01325		2.8	0.1	No	256/512	TIP5P-Ew	194
	"----//----"	2013	298.15	1.01325		2.97	0.05	Yes	216	SPC/E	13
	"----//----"	2013	298.15	1.01325		2.14	0.19	Yes	1000	SWM6	135
	"----//----"	2013	298.15	1.01325		2.14	N/A	Yes	512	AMOEBA	78
	"----//----"	2013	298.15	1.01325		2.3	N/A	No	1000	COS/G2	77
	"----//----"	2013	298.15	1.01325		2.23	N/A	No	64	TTM2-R	195
	"----//----"	2013	298.15	1.01325		2.37	N/A	No	256	TTM3-F	196
	"----//----"	2013	298.15	1.01325		2.26	N/A	No	256	GCPM	197
	"----//----"	2013	298.15	1.01325		2.461	0.012	Yes	360	POL4D	120
	"----//----"	2013	298.15	1.01325		2.43	N/A	No	300/432	BKd3	198
	"----//----"	2013	298.15	1.01325		6.14	0.06	Yes	256	TIP3P	6
	"----//----"	2013	298.15	1.01325		2.85	0.28	Yes	1000	SWM4-NDP	82
136	Kiss & Baranay	2013	298.15	1.01325		2.28	0.04	Yes		BK3	136
137	Corsetti et al.	2013	300		1	1.92	Yes (Fig. 12)	No	200	TIP4P	191
138	Han et al.	2013	298.15	1.01325		2.7	N/A	No	267	XP3P	138
139	Baker & Best	2013	298.15	1.01325		2.81	0.03	No		SWM4A-OPT	139
140	Nagarajan et al.	2013	300			1.24	0.0376	No		Bundled water model	140
141	Stukan et al.	2013	298.15	1.01325		2.4	N/A	No	1024	SWM4-NDP	82
142	Troster et al.	2013	300		0.9965	3.4	N/A	Yes	728/1500/3374	TL3P	142
	"----//----"	2013	300		0.9965	3	N/A	Yes	728/1500/3375	TL4P	142
	"----//----"	2013	300		0.9965	2.8	N/A	Yes	728/1500/3376	TL5P	142
143	Wang et al.	2013	298	1.01325		2.53	N/A	Yes	216/512/1000	iAMOEBA	143
	"----//----"	2013	298	1.01325		1.93	N/A	Yes	216/512/1001	AMOEBA	78
144	Arismendi-Arrieta et al.	2014	298.15		1	2.35	N/A	No	256	NCC(Q)	144
145	Braun et al.	2014	300		1.008	5.81	0.02	No	2100	TIP3P	6
	"----//----"	2014	300		0.995	2.64	0.02	No	2100	SPC/E	13
	"----//----"	2014	300		1.040	0.72	0.02	No	525	BMW	199
146	Bachmann & van Gunsteren	2014	298.15	1.01325	0.972	4.2	N/A	No	1000	SPC	178

	"----//----"	2014	298.15	1.01325	0.999	2	N/A	No	1000	COS/G2	77
	"----//----"	2014	298.15	1.01325	0.996	0.8	N/A	No	1000	COS/D	104
	"----//----"	2014	298.15	1.01325	0.999	2.2	N/A	No	1000	COS/D2	146
147	Fuentes-Azcatl & Alejandre	2014	300	1	0.9967	2.1048	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	300	1	0.9958	2.0963	N/A	No	500	TIP4P/ε	147
148	Troster et al.	2014	300	1		2.3	N/A	Yes		TL6P	148
	"----//----"	2014	300	1		2.2	N/A	Yes		TL6PSk	148
149	Moultos et al.	2014	298.15	1		3.6	0.5	No	2000	SPC	178
	"----//----"	2014	298.15	1		2.6	0.1	No	2000	SPC/E	13
	"----//----"	2014	298.15	1		2.1	0.1	No	2000	TIP4P/2005	80
150	Izadi et al.	2014	298.15	1	0.995	2.44	N/A	No		TIP4P-Ew	75
	"----//----"	2014	298.15	1	0.994	2.54	N/A	No		SPC/E	13
	"----//----"	2014	298.15	1	0.98	5.5	N/A	No		TIP3P	6
	"----//----"	2014	298.15	1	0.979	2.78	N/A	No		TIP5P	183
	"----//----"	2014	298.15	1	0.997	2.3	0.02	No		OPC	150
151	Spura et al.	2014	298.15	1.01325		2.88	N/A	Yes	125/216/343	fm-TIP4P/F-TPSS-D3	151
152	Orsi	2014	298.15	1.01325	0.99945	2.16	0.01	No		ELBA	121
	"----//----"	2014	298.15	1.01325	0.9769	4.42	0.03	No		SPC	178
	"----//----"	2014	298.15	1.01325	0.9984	2.78	0.02	No		SPC/E	13
	"----//----"	2014	298.15	1.01325	0.99586	4.3	0.02	No		TIP3P-Ew	200
	"----//----"	2014	298.15	1.01325	0.99714	2.53	0.01	No		TIP4P-Ew	75
	"----//----"	2014	298.15	1.01325	0.99846	2.28	0.02	No		TIP4P/2005	80
153	Bachmann & van Gunsteren	2014	298.15	1.01325	0.972	4.1	N/A	No	1000	SPC	178
	"----//----"	2014	298.15	1.01325	0.999	2	N/A	No	1000	COS/G2	195
	"----//----"	2014	298.15	1.01325	0.996	0.8	N/A	No	1000	COS/D	104
154	Medders et al.	2014	298.15	1.01325		1.2	0.1	No	256	MB-pol	201
	"----//----"	2014	298.15	1.01325		2.2	0.3	No	256	MB-pol	201
159	Tainter et al.	2015	298.15	1.01325		2.27	N/A	Yes	500	E3B2	202
	"----//----"	2015	298.15	1.01325		2.32	N/A	Yes	500	TIP4P/2005	80
	"----//----"	2015	298.15	1.01325		1.98	N/A	Yes	500	E3B3	159
160	Lobanova et al.	2015	298	1.01325	0.997	1.7	N/A	No		Mie (8-6) CGW1-vle	160

	"----//----"	2015	298	1.01325	0.998	7.4	N/A	No		Mie (8-6) CGW1-ift	160
	"----//----"	2015	298	1.01325	0.999	3.8	N/A	No		CGW2	160
	"----//----"	2015	298	1.01325	1	5.8	N/A	No		Mie (9-6)	160
165	Tran et al.	2016	300	1.01325	0.995	2.24	Yes (Fig. 5)	Yes	512	SSMP	165
166	Jiang et al.	2016	298.15	1		2.42	0.01	Yes	512	HBP	166
	"----//----"	2016	298.15	1		2.04	0.05	Yes	512	BK3	136
	"----//----"	2016	298.15	1		2.1	0.01	Yes	512	TIP4P/2005	80
172	Abbaspour et al.	2018	300	1.01325	0.9966	2.61	N/A	No	500	HFD-Like potential	172

TABLE SI-2. Available MD simulation data of the self-diffusion coefficient of water at other conditions. "**Ref #**" corresponds to the reference (see Reference list at page 71) of the study reporting the self-diffusion coefficient value. "**T**", "**P**", and "**ρ**" correspond to the conditions at which the simulations are performed. "**SSE correction**" indicates if the data are corrected for system size effects (see ref [76]). "**H_2O Ref #**" lists the original H_2O model development papers.

Ref #	Authors	Year	T (K)	P (bar)	ρ (g/cm^3)	D (m^2/s) (x 10^9)	Statistical Error	SSE correction	Number of H_2O molecules	H_2O force field	H_2O Ref #
1	Rahman & Stillinger	1971	307.5		1	4.2	N/A	No	216	BNS (modified)	1
	"----//----"	1971	265			1.50	N/A	No	216	BNS (modified)	1
2	Stillinger & Rahman	1974	270.15		1	1.3	N/A	No	216	ST2	2
	"----//----"	1974	283.15		1	1.9	N/A	No	216	ST2	2
	"----//----"	1974	314.15		1	4.3	N/A	No	216	ST2	2
	"----//----"	1974	391.15		1	8.4	N/A	No	216	ST2	2
5	Impey et al.	1982	242		1	0.50	0.08	No	125	MCY	175
	"----//----"	1982	282		1	1.81	0.07	No	125	MCY	175
	"----//----"	1982	286		1	2.12	0.15	No	125	MCY	175
	"----//----"	1982	294		1	2.3	0.2	No	125	MCY	175
	"----//----"	1982	360		1	5.1	0.2	No	125	MCY	175
7	Jansco et al.	1984	336.15		0.9718	2.4	0.15	No	200	BJH	203
	"----//----"	1984	350.15		1.346	2.7	0.2	No	200	BJH	203
8	Ferrario & Tani	1985	243.15	60	0.985	0.8	N/A	No	343	TIP4P	6
	"----//----"	1985	298.15	370	0.983	45	N/A	No	343	TIP4P	6
	"----//----"	1985	348.15	1030	0.978	7.6	N/A	No	343	TIP4P	6

12	Anderson et al.	1987	259		1	0.76	N/A	No	125	SPC modif. (flex.)	12
	"----//----"	1987	300		1	2.54	N/A	No	125	SPC modif. (flex.)	12
	"----//----"	1987	350		1	5.60	N/A	No	125	SPC modif. (flex.)	12
14	Reddy & Berkowitz	1987	268		0.999	1.36	N/A	No	216	TIP4P	6
	"----//----"	1987	268		1.083	1.47	N/A	No	216	TIP4P	6
	"----//----"	1987	268		1.149	1.27	N/A	No	216	TIP4P	6
	"----//----"	1987	298		0.999	2.96	N/A	No	216	TIP4P	6
	"----//----"	1987	298		1.083	2.88	N/A	No	216	TIP4P	6
	"----//----"	1987	298		1.149	2.38	N/A	No	216	TIP4P	6
23	Barrat & McDonald	1990	270	1500		2.3	0.2	No	N/A	SPC-type; R1 (rigid)	23
	"----//----"	1990	270	1000		1.1	0.1	No	N/A	SPC-type; R2 (rigid)	23
	"----//----"	1990	270	-200		1.7	0.2	No	N/A	SPC-type; F (flex)	23
	"----//----"	1990	300	2000		4.5	0.5	No	N/A	SPC-type; R1 (rigid)	23
	"----//----"	1990	300	1500		2.4	0.2	No	N/A	SPC-type; R2 (rigid)	23
	"----//----"	1990	300	200		3.0	0.3	No	N/A	SPC-type; F (flex)	23
24	Brodholt & Wood	1990	300.91	470	1	3.2	N/A	No	108	TIP4P	6
	"----//----"	1990	338.70	1240	1	4.63	N/A	No	108	TIP4P	6
	"----//----"	1990	373.60	1610	1	7.86	N/A	No	108	TIP4P	6
	"----//----"	1990	436.74	3000	1	11.9	N/A	No	108	TIP4P	6
	"----//----"	1990	498.99	4070	1	15.8	N/A	No	108	TIP4P	6
	"----//----"	1990	670.94	7780	1	20.8	N/A	No	108	TIP4P	6
	"----//----"	1990	717.70	9020	1	22.3	N/A	No	108	TIP4P	6
	"----//----"	1990	862.12	11800	1	28.8	N/A	No	108	TIP4P	6
	"----//----"	1990	1250.00	20000	1	38.9	N/A	No	108	TIP4P	6
	"----//----"	1990	1849.40	30900	1	44.2	N/A	No	108	TIP4P	6
	"----//----"	1990	2344.10	38200	1	69.5	N/A	No	108	TIP4P	6
	"----//----"	1990	1996.00	302600	1.9	3.79	N/A	No	108	TIP4P	6

25	Frattini et al.	1990	256			1.09	N/A	No	108	TIP4P	6
	"----//----"	1990	275			1.85	N/A	No	108	TIP4P	6
	"----//----"	1990	310			3.92	N/A	No	256	TIP4P	6
	"----//----"	1990	347			6.83	N/A	No	108	TIP4P	6
	"----//----"	1990	383			8.71	N/A	No	108	TIP4P	6
32	Sciortino et al.	1992	273		0.75	0.281	N/A	No	216	ST2	2
	"----//----"	1992	273		0.80	0.212	N/A	No	216	ST2	2
	"----//----"	1992	273		0.85	0.331	N/A	No	216	ST2	2
	"----//----"	1992	273		0.90	0.843	N/A	No	216	ST2	2
	"----//----"	1992	273		0.95	1.146	N/A	No	216	ST2	2
	"----//----"	1992	273		1.00	1.647	N/A	No	216	ST2	2
	"----//----"	1992	235		0.835	0.007	N/A	No	216	ST2	2
	"----//----"	1992	235		0.886	0.008	N/A	No	216	ST2	2
	"----//----"	1992	235		0.950	0.054	N/A	No	216	ST2	2
	"----//----"	1992	235		1.00	0.145	N/A	No	216	ST2	2
33	Guissani & Guillot	1993	300		VLE	2.6	0.1	No	256	SPC/E	13
	"----//----"	1993	373		VLE	7.9	N/A	No	256	SPC/E	13
	"----//----"	1993	473		VLE	19.6	N/A	No	256	SPC/E	13
	"----//----"	1993	570		VLE	34.7	N/A	No	256	SPC/E	13
	"----//----"	1993	610		VLE	53.6	N/A	No	256	SPC/E	13
	"----//----"	1993	620		VLE	54.1	N/A	No	256	SPC/E	13
	"----//----"	1993	630		VLE	65.6	N/A	No	256	SPC/E	13
	"----//----"	1993	640		VLE	71.7	N/A	No	256	SPC/E	13
	"----//----"	1993	652		VLE	106.0	N/A	No	256	SPC/E	13
37	Padro et al.	1994	298		1	2.5	N/A	No	216	SPC (flex)	178
	"----//----"	1994	523		0.75	2.6	N/A	No	216	SPC (flex)	178
38	Baez & Clancy	1994	328.3	1	0.9872	3.57	2.9E-01	No	360	SPC/E	13
	"----//----"	1994	307.4	1	1.0013	2.51	2.2E-01	No	360	SPC/E	13

	"----//----"	1994	282.2	1	1.0160	1.51	1.1E-01	No	360	SPC/E	13
	"----//----"	1994	261.2	1	1.0217	1.08	1.9E-01	No	360	SPC/E	13
	"----//----"	1994	250.2	1	1.0251	0.586	7.6E-02	No	360	SPC/E	13
	"----//----"	1994	240.4	1	1.0262	0.501	6.9E-02	No	360	SPC/E	13
	"----//----"	1994	229.9	1	1.0267	0.311	4.8E-02	No	360	SPC/E	13
	"----//----"	1994	220.6	1	1.0251	0.164	3.2E-02	No	360	SPC/E	13
	"----//----"	1994	209.5	1	1.0237	5.50E-02	2.1E-03	No	360	SPC/E	13
	"----//----"	1994	200.2	1	1.0185	1.65E-02	7.2E-04	No	360	SPC/E	13
	"----//----"	1994	190.3	1	1.0097	1.14E-03	2.1E-05	No	360	SPC/E	13
41	Duan et al.	1995	307.15	1		3.06	N/A	No	256	RWK2	181
	"----//----"	1995	373.15	21		7.66	N/A	No	256	RWK2	181
	"----//----"	1995	473.15	2083		12.7	N/A	No	256	RWK2	181
	"----//----"	1995	513.15	3109		14.5	N/A	No	256	RWK2	181
42	Mountain	1995	303		0.997	2.7	N/A	No	216	RPOL	180
	"----//----"	1995	579		0.720	34	N/A	No	216	RPOL	180
	"----//----"	1995	678		0.660	46	N/A	No	216	RPOL	180
	"----//----"	1995	297	490		2.5	N/A	No	216	ST2	2
	"----//----"	1995	575	890		34	N/A	No	216	ST2	2
	"----//----"	1995	667	1400		45	N/A	No	216	ST2	2
43	Brodholt et al.	1995	298.15		1	2.3	N/A	No	256	TIP4P-Polarizable	43
	"----//----"	1995	573.15		0.712	23.3	N/A	No	256	TIP4P-Polarizable	43
	"----//----"	1995	573.15		0.921	12.5	N/A	No	256	TIP4P-Polarizable	43
	"----//----"	1995	298.15		1	2.3	N/A	No	256	SPC/E	13
	"----//----"	1995	573.15		0.712	19.5	N/A	No	256	SPC/E	13
	"----//----"	1995	573.15		0.921	11.8	N/A	No	256	SPC/E	13
44	Svishchev et al.	1996	263		0.9981	0.95	2%	No	256	PPC	44

	"----//----"	1996	298		0.9970	2.6	2%	No	256	PPC	44
	"----//----"	1996	373		0.9583	9.6	2%	No	256	PPC	44
	"----//----"	1996	473		0.8647	18.8	2%	No	256	PPC	44
	"----//----"	1996	573		0.7123	33.2	2%	No	256	PPC	44
45	Gallo et al.	1996	284.5		0.984	1.3000	0.1	No	216	SPC/E	13
46	"----//----"	1996	258.5		0.986	0.5200	5.0E-02	No	216	SPC/E	13
	"----//----"	1996	238.2		0.987	0.1400	1.0E-02	No	216	SPC/E	13
	"----//----"	1996	224.0		0.984	0.0440	4.0E-03	No	216	SPC/E	13
	"----//----"	1996	213.6		0.977	0.0110	4.0E-03	No	216	SPC/E	13
	"----//----"	1996	209.3		0.970	0.0051	9.0E-04	No	216	SPC/E	13
	"----//----"	1996	206.3		0.966	0.0018	1.1E-03	No	216	SPC/E	13
47	Taylor et al.	1996	268		1	1.69	N/A	No	526	SPC/E	13
	"----//----"	1996	283		1	2.17	N/A	No	526	SPC/E	13
	"----//----"	1996	298		1	3.02	N/A	No	526	SPC/E	13
	"----//----"	1996	323		1	4.56	N/A	No	526	SPC/E	13
	"----//----"	1996	348		1	5.64	N/A	No	526	SPC/E	13
	"----//----"	1996	373		1	7.74	N/A	No	526	SPC/E	13
48	Bagchi et al.	1997	277.2	-5		1.60	0.08	No	512	SPC/E	13
	"----//----"	1997	277.2	1209		1.63	0.07	No	512	SPC/E	13
	"----//----"	1997	277.2	2428		1.64	0.08	No	512	SPC/E	13
	"----//----"	1997	277.2	3236		1.55	0.03	No	512	SPC/E	13
	"----//----"	1997	277.2	3993		1.57	0.08	No	512	SPC/E	13
	"----//----"	1997	277.2	6574		1.42	0.05	No	512	SPC/E	13
	"----//----"	1997	277.2	8637		1.23	0.05	No	512	SPC/E	13
	"----//----"	1997	277.2	12156		1.01	0.04	No	512	SPC/E	13
50	Levitt et al.	1997	273		0.999	1.6	N/A	(see ref)	216	F3C	50
	"----//----"	1997	298		0.997	2.4	0.23	(see ref)	216	F3C	50
	"----//----"	1997	323		0.988	3.2	N/A	(see ref)	216	F3C	50

	"----//----"	1997	348	0.975	4.2	N/A	(see ref)	216	F3C	50
	"----//----"	1997	373	0.958	6.6	N/A	(see ref)	216	F3C	50
	"----//----"	1997	398	0.939	7.1	N/A	(see ref)	216	F3C	50
	"----//----"	1997	423	0.916	9.8	N/A	(see ref)	216	F3C	50
	"----//----"	1997	448	0.890	12.4	N/A	(see ref)	216	F3C	50
	"----//----"	1997	473	0.861	16.1	N/A	(see ref)	216	F3C	50
	"----//----"	1997	498	0.829	19.1	N/A	(see ref)	216	F3C	50
	"----//----"	1997	573	0.717	33.8	N/A	(see ref)	216	F3C	50
53	Starr et al.	1999	190	1.00	2.40E-04	4E-06	No	216	SPC/E	13
	"----//----"	1999	200	1.00	1.50E-03	4E-05	No	216	SPC/E	13
	"----//----"	1999	210	0.90	2.92E-03	4E-05	No	216	SPC/E	13
	"----//----"	1999	210	0.95	1.93E-03	4E-05	No	216	SPC/E	13
	"----//----"	1999	210	1.00	1.03E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	210	1.05	2.27E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	210	1.10	3.17E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	210	1.20	3.04E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	210	1.30	8.71E-03	4E-05	No	216	SPC/E	13
	"----//----"	1999	210	1.40	4.90E-04	4E-06	No	216	SPC/E	13
	"----//----"	1999	220	0.95	1.68E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	220	1.00	3.89E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	220	1.05	5.58E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	220	1.10	8.47E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	220	1.15	9.18E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	220	1.20	8.01E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	220	1.25	5.94E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	220	1.30	2.63E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	220	1.40	1.69E-03	4E-05	No	216	SPC/E	13
	"----//----"	1999	230	0.95	6.25E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	230	1.00	0.103	4E-03	No	216	SPC/E	13
	"----//----"	1999	230	1.05	0.134	4E-03	No	216	SPC/E	13
	"----//----"	1999	230	1.10	0.177	4E-03	No	216	SPC/E	13

"----//----"	1999	230	1.20	0.159	4E-03	No	216	SPC/E	13
"----//----"	1999	230	1.30	6.72E-02	4E-04	No	216	SPC/E	13
"----//----"	1999	230	1.40	1.12E-02	4E-04	No	216	SPC/E	13
"----//----"	1999	240	0.95	0.141	4E-03	No	216	SPC/E	13
"----//----"	1999	240	1.00	0.187	4E-03	No	216	SPC/E	13
"----//----"	1999	240	1.05	0.244	4E-03	No	216	SPC/E	13
"----//----"	1999	240	1.10	0.270	4E-03	No	216	SPC/E	13
"----//----"	1999	240	1.20	0.237	4E-03	No	216	SPC/E	13
"----//----"	1999	240	1.30	0.135	4E-03	No	216	SPC/E	13
"----//----"	1999	240	1.40	2.49E-02	4E-04	No	216	SPC/E	13
"----//----"	1999	260	0.95	0.504	4E-03	No	216	SPC/E	13
"----//----"	1999	260	1.00	0.608	4E-03	No	216	SPC/E	13
"----//----"	1999	260	1.05	0.591	4E-03	No	216	SPC/E	13
"----//----"	1999	260	1.10	0.588	4E-03	No	216	SPC/E	13
"----//----"	1999	260	1.20	0.574	4E-03	No	216	SPC/E	13
"----//----"	1999	260	1.30	0.354	4E-03	No	216	SPC/E	13
"----//----"	1999	260	1.40	0.139	4E-03	No	216	SPC/E	13
"----//----"	1999	300	0.95	1.99	4E-02	No	216	SPC/E	13
"----//----"	1999	300	1.00	2.00	4E-02	No	216	SPC/E	13
"----//----"	1999	300	1.05	1.83	4E-02	No	216	SPC/E	13
"----//----"	1999	300	1.10	1.82	4E-02	No	216	SPC/E	13
"----//----"	1999	300	1.20	1.53	4E-02	No	216	SPC/E	13
"----//----"	1999	300	1.30	1.12	4E-02	No	216	SPC/E	13
"----//----"	1999	300	1.40	0.495	4E-03	No	216	SPC/E	13
"----//----"	1999	350	0.90	6.11	4E-02	No	216	SPC/E	13
"----//----"	1999	350	1.00	4.97	4E-02	No	216	SPC/E	13
"----//----"	1999	350	1.10	3.81	4E-02	No	216	SPC/E	13
"----//----"	1999	350	1.20	2.70	4E-02	No	216	SPC/E	13
"----//----"	1999	350	1.30	1.80	4E-02	No	216	SPC/E	13
"----//----"	1999	350	1.40	1.39	4E-02	No	216	SPC/E	13
"----//----"	1999	190	1.00	2.40E-04	4E-06	No	216	SPC/E	13

	"----//----"	1999	200		1.00	1.50E-03	4E-05	No	216	SPC/E	13
	"----//----"	1999	210		1.00	1.03E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	220		1.00	3.89E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	230		1.00	0.103	4E-03	No	216	SPC/E	13
	"----//----"	1999	240		1.00	0.187	4E-03	No	216	SPC/E	13
	"----//----"	1999	260		1.00	0.608	4E-03	No	216	SPC/E	13
	"----//----"	1999	300		1.00	2.00	4E-02	No	216	SPC/E	13
	"----//----"	1999	350		1.00	4.97	4E-02	No	216	SPC/E	13
54	Svishchev & Zassetsky	2000	238			0.24	N/A	No	256	PPC	44
	"----//----"	2000	263			0.72	N/A	No	256	PPC	44
	"----//----"	2000	298			2.15	N/A	No	256	PPC	44
	"----//----"	2000	473			21.7	N/A	No	256	PPC	44
61	Guillot & Guissani	2001	254.61		0.997	0.59	N/A	No	256	DEC	61
	"----//----"	2001	297.09		0.997	2.52	N/A	No	256	DEC	61
	"----//----"	2001	304.37		0.997	2.90	N/A	No	256	DEC	61
	"----//----"	2001	377.18		0.997	6.93	N/A	No	256	DEC	61
	"----//----"	2001	481.55		0.997	13.62	N/A	No	256	DEC	61
	"----//----"	2001	678.16		0.997	22.39	N/A	No	256	DEC	61
	"----//----"	2001	673		0.10	291.18	N/A	No	256	DEC	61
	"----//----"	2001	673		0.30	109.41	N/A	No	256	DEC	61
	"----//----"	2001	673		0.66	45.88	N/A	No	256	DEC	61
	"----//----"	2001	673		0.99	21.18	N/A	No	256	DEC	61
57	Mahoney & Jorgensen	2001	298.15	1.01325	0.999	2.62	0.04	No	267	TIP5P	183
	"----//----"	2001	298.15	506.625	1.026	2.65	0.05	No	267	TIP5P	183
	"----//----"	2001	298.15	1013.25	1.053	2.66	0.05	No	267	TIP5P	183
	"----//----"	2001	298.15	1519.875	1.072	2.60	0.04	No	267	TIP5P	183
	"----//----"	2001	298.15	2026.5	1.092	2.63	0.05	No	267	TIP5P	183
	"----//----"	2001	298.15	3039.75	1.128	2.67	0.05	No	267	TIP5P	183

	"----//----"	2001	348.15	1.01325	0.951	6.78	0.10	No	267	TIP5P	183
	"----//----"	2001	348.15	506.625	0.985	6.97	0.14	No	267	TIP5P	183
	"----//----"	2001	348.15	1013.25	1.011	6.71	0.09	No	267	TIP5P	183
	"----//----"	2001	348.15	1519.875	1.034	6.38	0.09	No	267	TIP5P	183
	"----//----"	2001	348.15	2026.5	1.055	6.33	0.12	No	267	TIP5P	183
	"----//----"	2001	348.15	3039.75	1.091	5.89	0.11	No	267	TIP5P	183
	"----//----"	2001	248.15	1.01325	0.981	0.14	0.02	No	267	TIP5P	183
	"----//----"	2001	260.65	1.01325	0.988	0.43	0.03	No	267	TIP5P	183
	"----//----"	2001	273.15	1.01325	1.007	1.01	0.02	No	267	TIP5P	183
	"----//----"	2001	285.65	1.01325	1.005	1.87	0.08	No	267	TIP5P	183
	"----//----"	2001	298.15	1.01325	0.999	2.62	0.04	No	267	TIP5P	183
	"----//----"	2001	310.65	1.01325	0.989	3.70	0.09	No	267	TIP5P	183
	"----//----"	2001	323.15	1.01325	0.978	4.74	0.08	No	267	TIP5P	183
	"----//----"	2001	335.65	1.01325	0.967	6.33	0.07	No	267	TIP5P	183
	"----//----"	2001	348.15	1.01325	0.951	6.78	0.10	No	267	TIP5P	183
62	Errington & Debenedetti	2001	400		0.85	12.085	N/A	No	256	SPC/E	13
	"----//----"	2001	400		0.90	9.561	N/A	No	256	SPC/E	13
	"----//----"	2001	400		0.95	9.515	N/A	No	256	SPC/E	13
	"----//----"	2001	400		1.00	8.519	N/A	No	256	SPC/E	13
	"----//----"	2001	400		1.05	7.361	N/A	No	256	SPC/E	13
	"----//----"	2001	400		1.10	7.072	N/A	No	256	SPC/E	13
	"----//----"	2001	400		1.15	6.444	N/A	No	256	SPC/E	13
	"----//----"	2001	400		1.20	5.375	N/A	No	256	SPC/E	13
	"----//----"	2001	400		1.25	4.728	N/A	No	256	SPC/E	13
	"----//----"	2001	400		1.30	3.808	N/A	No	256	SPC/E	13
	"----//----"	2001	350		0.85	6.871	N/A	No	256	SPC/E	13
	"----//----"	2001	350		0.90	6.260	N/A	No	256	SPC/E	13
	"----//----"	2001	350		0.95	5.704	N/A	No	256	SPC/E	13
	"----//----"	2001	350		1.00	5.778	N/A	No	256	SPC/E	13
	"----//----"	2001	350		1.05	4.906	N/A	No	256	SPC/E	13

"----//----"	2001	350	1.10	4.165	N/A	No	256	SPC/E	13
"----//----"	2001	350	1.15	3.932	N/A	No	256	SPC/E	13
"----//----"	2001	350	1.20	3.583	N/A	No	256	SPC/E	13
"----//----"	2001	350	1.25	3.042	N/A	No	256	SPC/E	13
"----//----"	2001	350	1.30	2.493	N/A	No	256	SPC/E	13
"----//----"	2001	320	0.85	4.341	N/A	No	256	SPC/E	13
"----//----"	2001	320	0.90	4.397	N/A	No	256	SPC/E	13
"----//----"	2001	320	0.95	3.604	N/A	No	256	SPC/E	13
"----//----"	2001	320	1.00	3.525	N/A	No	256	SPC/E	13
"----//----"	2001	320	1.05	3.327	N/A	No	256	SPC/E	13
"----//----"	2001	320	1.10	3.140	N/A	No	256	SPC/E	13
"----//----"	2001	320	1.15	2.861	N/A	No	256	SPC/E	13
"----//----"	2001	320	1.20	2.749	N/A	No	256	SPC/E	13
"----//----"	2001	320	1.25	2.175	N/A	No	256	SPC/E	13
"----//----"	2001	320	1.30	1.751	N/A	No	256	SPC/E	13
"----//----"	2001	300	0.85	3.217	N/A	No	256	SPC/E	13
"----//----"	2001	300	0.90	2.830	N/A	No	256	SPC/E	13
"----//----"	2001	300	0.95	2.489	N/A	No	256	SPC/E	13
"----//----"	2001	300	1.00	2.350	N/A	No	256	SPC/E	13
"----//----"	2001	300	1.05	2.465	N/A	No	256	SPC/E	13
"----//----"	2001	300	1.10	2.453	N/A	No	256	SPC/E	13
"----//----"	2001	300	1.15	2.047	N/A	No	256	SPC/E	13
"----//----"	2001	300	1.20	1.832	N/A	No	256	SPC/E	13
"----//----"	2001	300	1.25	1.583	N/A	No	256	SPC/E	13
"----//----"	2001	300	1.30	1.418	N/A	No	256	SPC/E	13
"----//----"	2001	280	0.85	1.766	N/A	No	256	SPC/E	13
"----//----"	2001	280	0.90	1.473	N/A	No	256	SPC/E	13
"----//----"	2001	280	0.95	1.466	N/A	No	256	SPC/E	13
"----//----"	2001	280	1.00	1.539	N/A	No	256	SPC/E	13

"----//----"	2001	280	1.05	1.614	N/A	No	256	SPC/E	13
"----//----"	2001	280	1.10	1.471	N/A	No	256	SPC/E	13
"----//----"	2001	280	1.15	1.438	N/A	No	256	SPC/E	13
"----//----"	2001	280	1.20	1.200	N/A	No	256	SPC/E	13
"----//----"	2001	280	1.25	1.113	N/A	No	256	SPC/E	13
"----//----"	2001	280	1.30	0.880	N/A	No	256	SPC/E	13
"----//----"	2001	260	0.85	0.872	N/A	No	256	SPC/E	13
"----//----"	2001	260	0.90	0.754	N/A	No	256	SPC/E	13
"----//----"	2001	260	0.95	0.750	N/A	No	256	SPC/E	13
"----//----"	2001	260	1.00	0.844	N/A	No	256	SPC/E	13
"----//----"	2001	260	1.05	0.902	N/A	No	256	SPC/E	13
"----//----"	2001	260	1.10	0.980	N/A	No	256	SPC/E	13
"----//----"	2001	260	1.15	1.047	N/A	No	256	SPC/E	13
"----//----"	2001	260	1.20	0.874	N/A	No	256	SPC/E	13
"----//----"	2001	260	1.25	0.691	N/A	No	256	SPC/E	13
"----//----"	2001	260	1.30	0.537	N/A	No	256	SPC/E	13
"----//----"	2001	240	0.85	0.287	N/A	No	256	SPC/E	13
"----//----"	2001	240	0.90	0.231	N/A	No	256	SPC/E	13
"----//----"	2001	240	0.95	0.247	N/A	No	256	SPC/E	13
"----//----"	2001	240	1.00	0.369	N/A	No	256	SPC/E	13
"----//----"	2001	240	1.05	0.478	N/A	No	256	SPC/E	13
"----//----"	2001	240	1.10	0.493	N/A	No	256	SPC/E	13
"----//----"	2001	240	1.15	0.465	N/A	No	256	SPC/E	13
"----//----"	2001	240	1.20	0.447	N/A	No	256	SPC/E	13
"----//----"	2001	240	1.25	0.366	N/A	No	256	SPC/E	13
"----//----"	2001	240	1.30	0.285	N/A	No	256	SPC/E	13
"----//----"	2001	220	0.85	0.043	N/A	No	256	SPC/E	13
"----//----"	2001	220	0.90	0.032	N/A	No	256	SPC/E	13
"----//----"	2001	220	0.95	0.045	N/A	No	256	SPC/E	13

	"----//----"	2001	220	1.00	0.096	N/A	No	256	SPC/E	13
	"----//----"	2001	220	1.05	0.163	N/A	No	256	SPC/E	13
	"----//----"	2001	220	1.10	0.180	N/A	No	256	SPC/E	13
	"----//----"	2001	220	1.15	0.222	N/A	No	256	SPC/E	13
	"----//----"	2001	220	1.20	0.206	N/A	No	256	SPC/E	13
	"----//----"	2001	220	1.25	0.154	N/A	No	256	SPC/E	13
	"----//----"	2001	220	1.30	0.102	N/A	No	256	SPC/E	13
64	Guo et al.	2002	303.8	0.999	2.63	6E-02	No	256	SPC/E	13
	"----//----"	2002	273.5	1.011	1.27	3E-02	No	256	SPC/E	13
	"----//----"	2002	253.5	1.015	0.668	2E-02	No	256	SPC/E	13
	"----//----"	2002	232.5	1.014	0.235	8E-03	No	256	SPC/E	13
	"----//----"	2002	212.5	1.004	0.049	4E-03	No	256	SPC/E	13
71	English & MacElroy	2003	260	1.002	0.83	N/A	No	500	F-SPC	182
	"----//----"	2003	298	0.997	2.3	N/A	No	500	F-SPC	182
	"----//----"	2003	350	0.965	6.1	N/A	No	500	F-SPC	182
	"----//----"	2003	400	0.920	10.5	N/A	No	500	F-SPC	182
	"----//----"	2003	260	0.999	0.34	N/A	No	500	TIP4P-FQ	34
	"----//----"	2003	298	0.996	2.1	N/A	No	500	TIP4P-FQ	34
	"----//----"	2003	350	0.961	6.3	N/A	No	500	TIP4P-FQ	34
	"----//----"	2003	400	0.912	13.3	N/A	No	500	TIP4P-FQ	34
66	Nieto-Draghi et al.	2003	275.05	0.995	1.8903	N/A	No	256	TIP5P	183
	"----//----"	2003	447.75	0.995	16.0616	N/A	No	256	TIP5P	183
	"----//----"	2003	673.97	0.995	24.6765	N/A	No	256	TIP5P	183
	"----//----"	2003	951.79	0.995	32.2135	N/A	No	256	TIP5P	183
	"----//----"	2003	1251.41	0.995	38.7636	N/A	No	256	TIP5P	183
	"----//----"	2003	275.12	0.995	2.5231	N/A	No	256	TIP4P	191
	"----//----"	2003	298.12	0.995	3.0361	N/A	No	256	TIP4P	191

"----//----"	2003	448.87	0.995	14.4801	N/A	No	256	TIP4P	191
"----//----"	2003	673.95	0.995	23.0858	N/A	No	256	TIP4P	191
"----//----"	2003	954.07	0.995	30.1370	N/A	No	256	TIP4P	191
"----//----"	2003	1251.40	0.995	36.8058	N/A	No	256	TIP4P	191
"----//----"	2003	274.99	0.995	1.5138	N/A	No	256	DEC	61
"----//----"	2003	299.22	0.995	2.5231	N/A	No	256	DEC	61
"----//----"	2003	447.66	0.995	11.1746	N/A	No	256	DEC	61
"----//----"	2003	673.93	0.995	21.2801	N/A	No	256	DEC	61
"----//----"	2003	951.77	0.995	29.6940	N/A	No	256	DEC	61
"----//----"	2003	448.83	0.995	12.4871	N/A	No	256	DEC	61
"----//----"	2003	673	0.1005	32.7354	N/A	No	256	TIP5P	183
"----//----"	2003	673	0.2007	17.6682	N/A	No	256	TIP5P	183
"----//----"	2003	673	0.2990	12.2422	N/A	No	256	TIP5P	183
"----//----"	2003	673	0.5002	7.3543	N/A	No	256	TIP5P	183
"----//----"	2003	673	0.6612	5.3363	N/A	No	256	TIP5P	183
"----//----"	2003	673	0.9956	2.4664	N/A	No	256	TIP5P	183
"----//----"	2003	673	0.1005	34.7982	N/A	No	256	TIP4P	191
"----//----"	2003	673	0.2007	18.1166	N/A	No	256	TIP4P	191
"----//----"	2003	673	0.2990	12.6457	N/A	No	256	TIP4P	191
"----//----"	2003	673	0.5002	7.5785	N/A	No	256	TIP4P	191
"----//----"	2003	673	0.6612	5.6951	N/A	No	256	TIP4P	191
"----//----"	2003	673	0.9956	2.2870	N/A	No	256	TIP4P	191
"----//----"	2003	673	0.1005	30.9417	N/A	No	256	SPC/E	13
"----//----"	2003	673	0.2007	16.5022	N/A	No	256	SPC/E	13
"----//----"	2003	673	0.2990	11.7040	N/A	No	256	SPC/E	13
"----//----"	2003	673	0.5002	7.3543	N/A	No	256	SPC/E	13
"----//----"	2003	673	0.6612	5.3812	N/A	No	256	SPC/E	13
"----//----"	2003	673	0.9956	2.3767	N/A	No	256	SPC/E	13

67	Yamaguchi et al.	2003	273	0.90	0.024	N/A	No	512	SPC/E	13
	"----//----"	2003	273	0.96	0.030	N/A	No	512	SPC/E	13
	"----//----"	2003	273	1.00	0.030	N/A	No	512	SPC/E	13
	"----//----"	2003	273	1.04	0.027	N/A	No	512	SPC/E	13
	"----//----"	2003	273	1.10	0.020	N/A	No	512	SPC/E	13
	"----//----"	2003	273	1.14	0.014	N/A	No	512	SPC/E	13
	"----//----"	2003	273	1.20	0.007	N/A	No	512	SPC/E	13
	"----//----"	2003	298	0.90	0.132	N/A	No	512	SPC/E	13
	"----//----"	2003	298	0.96	0.130	N/A	No	512	SPC/E	13
	"----//----"	2003	298	1.00	0.121	N/A	No	512	SPC/E	13
	"----//----"	2003	298	1.04	0.107	N/A	No	512	SPC/E	13
	"----//----"	2003	298	1.10	0.080	N/A	No	512	SPC/E	13
	"----//----"	2003	298	1.14	0.061	N/A	No	512	SPC/E	13
	"----//----"	2003	298	1.20	0.036	N/A	No	512	SPC/E	13
	"----//----"	2003	323	0.90	0.302	N/A	No	512	SPC/E	13
	"----//----"	2003	323	0.96	0.285	N/A	No	512	SPC/E	13
	"----//----"	2003	323	1.00	0.262	N/A	No	512	SPC/E	13
	"----//----"	2003	323	1.04	0.225	N/A	No	512	SPC/E	13
	"----//----"	2003	323	1.10	0.174	N/A	No	512	SPC/E	13
	"----//----"	2003	323	1.14	0.137	N/A	No	512	SPC/E	13
	"----//----"	2003	323	1.20	0.089	N/A	No	512	SPC/E	13
	"----//----"	2003	373	0.90	0.887	N/A	No	512	SPC/E	13
	"----//----"	2003	373	0.96	0.793	N/A	No	512	SPC/E	13
	"----//----"	2003	373	1.00	0.692	N/A	No	512	SPC/E	13
	"----//----"	2003	373	1.04	0.596	N/A	No	512	SPC/E	13
	"----//----"	2003	373	1.10	0.466	N/A	No	512	SPC/E	13
	"----//----"	2003	373	1.14	0.386	N/A	No	512	SPC/E	13
	"----//----"	2003	373	1.20	0.275	N/A	No	512	SPC/E	13

78	Ren & Ponder	2004	255.912			0.218	N/A	No	512	AMOEBA	78
	"----//----"	2004	260.685			0.322	N/A	No	512	AMOEBA	78
	"----//----"	2004	260.685			0.322	N/A	No	512	AMOEBA	78
	"----//----"	2004	265.061			0.541	N/A	No	512	AMOEBA	78
	"----//----"	2004	273.547			0.792	N/A	No	512	AMOEBA	78
	"----//----"	2004	277.26			0.854	N/A	No	512	AMOEBA	78
	"----//----"	2004	285.481			1.292	N/A	No	512	AMOEBA	78
	"----//----"	2004	298.343			1.939	N/A	No	512	AMOEBA	78
	"----//----"	2004	323.138			3.380	N/A	No	512	AMOEBA	78
	"----//----"	2004	348.199			5.228	N/A	No	512	AMOEBA	78
	"----//----"	2004	248.221			0.198	N/A	No	512	AMOEBA-v	78
	"----//----"	2004	260.685			0.510	N/A	No	512	AMOEBA-v	78
	"----//----"	2004	273.68			0.959	N/A	No	512	AMOEBA-v	78
	"----//----"	2004	277.26			1.105	N/A	No	512	AMOEBA-v	78
	"----//----"	2004	298.343			2.106	N/A	No	512	AMOEBA-v	78
	"----//----"	2004	323.271			3.599	N/A	No	512	AMOEBA-v	78
	"----//----"	2004	348.066			5.688	N/A	No	512	AMOEBA-v	78
	"----//----"	2004	298	1		1.9194	N/A	No	512	AMOEBA	78
	"----//----"	2004	298	1000		1.628	N/A	No	512	AMOEBA	78
	"----//----"	2004	298	2000		1.6493	N/A	No	512	AMOEBA	78
	"----//----"	2004	348	1		5.1753	N/A	No	512	AMOEBA	78
	"----//----"	2004	348	1000		5.0403	N/A	No	512	AMOEBA	78
	"----//----"	2004	348	2000		4.6493	N/A	No	512	AMOEBA	78
75	Horn et al.	2004	235.1	1.01325	0.9845	0.17	0.01	No	512	TIP4P-Ew	75
	"----//----"	2004	272.2	1.01325	0.9996	1.2	0.02	No	512	TIP4P-Ew	75
	"----//----"	2004	297.4	1.01325	0.9954	2.4	0.06	No	512	TIP4P-Ew	75
	"----//----"	2004	321.6	1.01325	0.9843	3.9	0.06	No	512	TIP4P-Ew	75

	"----//----"	2004	346.9	1.01325	0.9688	5.7	0.04	No	512	TIP4P-Ew	75
	"----//----"	2004	371.6	1.01325	0.9492	7.8	0.1	No	512	TIP4P-Ew	75
	"----//----"	2004	398.4	1.01325	0.9254	10.3	0.1	No	512	TIP4P-Ew	75
77	Yu & Gunsteren	2004	247.07	1.01325		0.201	N/A	No	1000	COS/G2	77
	"----//----"	2004	257.69	1.01325		0.463	N/A	No	1000	COS/G2	77
	"----//----"	2004	278.21	1.01325		1.125	N/A	No	1000	COS/G2	77
	"----//----"	2004	288.46	1.01325		1.661	N/A	No	1000	COS/G2	77
	"----//----"	2004	300.18	1.01325		2.222	N/A	No	1000	COS/G2	77
	"----//----"	2004	329.30	1.01325		4.241	N/A	No	1000	COS/G2	77
	"----//----"	2004	359.16	1.01325		6.845	N/A	No	1000	COS/G2	77
	"----//----"	2004	379.12	1.01325		9.100	N/A	No	1000	COS/G2	77
	"----//----"	2004	247.44	1.01325		0.525	N/A	No	1000	COS/B2	69
	"----//----"	2004	259.71	1.01325		0.899	N/A	No	1000	COS/B2	69
	"----//----"	2004	282.78	1.01325		1.698	N/A	No	1000	COS/B2	69
	"----//----"	2004	292.67	1.01325		2.433	N/A	No	1000	COS/B2	69
	"----//----"	2004	322.71	1.01325		4.303	N/A	No	1000	COS/B2	69
	"----//----"	2004	353.11	1.01325		6.733	N/A	No	1000	COS/B2	69
	"----//----"	2004	372.53	1.01325		8.527	N/A	No	1000	COS/B2	69
	"----//----"	2004	250.7326	1.01325		1.247	N/A	No	1000	SPC	178
	"----//----"	2004	262.6374	1.01325		1.796	N/A	No	1000	SPC	178
	"----//----"	2004	285.7143	1.01325		3.042	N/A	No	1000	SPC	178
	"----//----"	2004	295.6044	1.01325		3.678	N/A	No	1000	SPC	178
	"----//----"	2004	325.2747	1.01325		5.921	N/A	No	1000	SPC	178
	"----//----"	2004	355.3114	1.01325		8.849	N/A	No	1000	SPC	178
	"----//----"	2004	375.2747	1.01325		10.593	N/A	No	1000	SPC	178
81	Xu et al.	2005	239.72	4000		1.63E-01	N/A	No	512	TIP5P	183
	"----//----"	2005	249.44	4000		3.17E-01	N/A	No	512	TIP5P	183
	"----//----"	2005	259.97	4000		5.12E-01	N/A	No	512	TIP5P	183

"----//----"	2005	279.66	4000	1.05E+00	N/A	No	512	TIP5P	183
"----//----"	2005	299.62	4000	1.80E+00	N/A	No	512	TIP5P	183
"----//----"	2005	319.31	4000	2.91E+00	N/A	No	512	TIP5P	183
"----//----"	2005	219.75	2000	5.82E-03	N/A	No	512	TIP5P	183
"----//----"	2005	229.88	2000	3.12E-02	N/A	No	512	TIP5P	183
"----//----"	2005	234.25	2000	5.46E-02	N/A	No	512	TIP5P	183
"----//----"	2005	239.72	2000	1.25E-01	N/A	No	512	TIP5P	183
"----//----"	2005	249.44	2000	2.63E-01	N/A	No	512	TIP5P	183
"----//----"	2005	259.61	2000	5.55E-01	N/A	No	512	TIP5P	183
"----//----"	2005	280.08	2000	1.17E+00	N/A	No	512	TIP5P	183
"----//----"	2005	299.62	2000	2.00E+00	N/A	No	512	TIP5P	183
"----//----"	2005	319.86	2000	3.32E+00	N/A	No	512	TIP5P	183
"----//----"	2005	349.53	2000	5.67E+00	N/A	No	512	TIP5P	183
"----//----"	2005	219.75	1000	1.28E-03	N/A	No	512	TIP5P	183
"----//----"	2005	229.88	1000	8.24E-03	N/A	No	512	TIP5P	183
"----//----"	2005	239.41	1000	3.21E-02	N/A	No	512	TIP5P	183
"----//----"	2005	245.79	1000	9.06E-02	N/A	No	512	TIP5P	183
"----//----"	2005	249.77	1000	1.96E-01	N/A	No	512	TIP5P	183
"----//----"	2005	259.61	1000	4.37E-01	N/A	No	512	TIP5P	183
"----//----"	2005	278.81	1000	1.30E+00	N/A	No	512	TIP5P	183
"----//----"	2005	298.17	1000	2.11E+00	N/A	No	512	TIP5P	183
"----//----"	2005	319.86	1000	3.60E+00	N/A	No	512	TIP5P	183
"----//----"	2005	350.19	1000	5.67E+00	N/A	No	512	TIP5P	183
"----//----"	2005		4000	see Fig. 4b	N/A	No	1728	ST2	2
"----//----"	2005		3000	see Fig. 4b	N/A	No	1728	ST2	2
"----//----"	2005		2000	see Fig. 4b	N/A	No	1728	ST2	2
"----//----"	2005		1000	see Fig. 4b	N/A	No	1728	ST2	2
"----//----"	2005		0	see Fig. 4b	N/A	No	1728	ST2	2

88	Yoshida et al.	2006	473.15	0.001	2.31E-02	2E-03	No	256	TIP4P-FQ	34
	"----//----"	2006	473.15	0.002	1.09E-02	6E-04	No	256	TIP4P-FQ	34
	"----//----"	2006	473.15	0.005	4.43E-03	2E-04	No	256	TIP4P-FQ	34
	"----//----"	2006	473.15	0.01	2.19E-03	6E-05	No	256	TIP4P-FQ	34
	"----//----"	2006	573.15	0.001	2.91E-02	2E-03	No	256	TIP4P-FQ	34
	"----//----"	2006	573.15	0.002	1.36E-02	4E-04	No	256	TIP4P-FQ	34
	"----//----"	2006	573.15	0.005	5.40E-03	1E-04	No	256	TIP4P-FQ	34
	"----//----"	2006	573.15	0.01	2.82E-03	9E-05	No	256	TIP4P-FQ	34
	"----//----"	2006	573.15	0.05	5.52E-04	2E-05	No	256	TIP4P-FQ	34
	"----//----"	2006	573.15	0.1	2.73E-04	4E-06	No	256	TIP4P-FQ	34
	"----//----"	2006	673.15	0.001	3.48E-02	1E-03	No	256	TIP4P-FQ	34
	"----//----"	2006	673.15	0.002	1.74E-02	3E-04	No	256	TIP4P-FQ	34
	"----//----"	2006	673.15	0.005	6.72E-03	2E-04	No	256	TIP4P-FQ	34
	"----//----"	2006	673.15	0.01	3.40E-03	2E-04	No	256	TIP4P-FQ	34
	"----//----"	2006	673.15	0.05	6.64E-04	1E-05	No	256	TIP4P-FQ	34
	"----//----"	2006	673.15	0.1	3.38E-04	7E-06	No	256	TIP4P-FQ	34
86	Donchev et al.	2006	250		0.1387	N/A	No	256	QMPFF2	86
	"----//----"	2006	260		0.2709	N/A	No	256	QMPFF2	86
	"----//----"	2006	273		0.4656	N/A	No	256	QMPFF2	86
	"----//----"	2006	280		0.7085	N/A	No	256	QMPFF2	86
	"----//----"	2006	290		0.9238	N/A	No	256	QMPFF2	86
	"----//----"	2006	298		1.1875	N/A	No	256	QMPFF2	86
	"----//----"	2006	310		1.6940	N/A	No	256	QMPFF2	86
	"----//----"	2006	320		2.0617	N/A	No	256	QMPFF2	86
	"----//----"	2006	363		4.1980	N/A	No	256	QMPFF2	86
	"----//----"	2006	250		0.4366	N/A	No	256	QMPFF2	86
	"----//----"	2006	260		0.7212	N/A	No	256	QMPFF2	86
	"----//----"	2006	273		1.0406	N/A	No	256	QMPFF2	86
	"----//----"	2006	280		1.2766	N/A	No	256	QMPFF2	86
	"----//----"	2006	290		1.5959	N/A	No	256	QMPFF2	86

	"----//----"	2006	298		1.8457	N/A	No	256	QMPFF2	86
	"----//----"	2006	310		2.4838	N/A	No	256	QMPFF2	86
	"----//----"	2006	320		2.8931	N/A	No	256	QMPFF2	86
	"----//----"	2006	363		5.2165	N/A	No	256	QMPFF2	86
87	Mittal et al.	2006	300	0.85	2.941	N/A	No	500	SPC/E	13
	"----//----"	2006	300	0.90	2.786	N/A	No	500	SPC/E	13
	"----//----"	2006	300	0.95	2.770	N/A	No	500	SPC/E	13
	"----//----"	2006	300	1.00	2.561	N/A	No	500	SPC/E	13
	"----//----"	2006	300	1.05	2.485	N/A	No	500	SPC/E	13
	"----//----"	2006	300	1.10	2.470	N/A	No	500	SPC/E	13
	"----//----"	2006	300	1.15	2.176	N/A	No	500	SPC/E	13
	"----//----"	2006	300	1.20	1.872	N/A	No	500	SPC/E	13
	"----//----"	2006	300	1.25	1.690	N/A	No	500	SPC/E	13
	"----//----"	2006	300	1.30	1.385	N/A	No	500	SPC/E	13
	"----//----"	2006	280	0.85	1.730	N/A	No	500	SPC/E	13
	"----//----"	2006	280	0.90	1.453	N/A	No	500	SPC/E	13
	"----//----"	2006	280	0.95	1.629	N/A	No	500	SPC/E	13
	"----//----"	2006	280	1.00	1.659	N/A	No	500	SPC/E	13
	"----//----"	2006	280	1.05	1.731	N/A	No	500	SPC/E	13
	"----//----"	2006	280	1.10	1.721	N/A	No	500	SPC/E	13
	"----//----"	2006	280	1.15	1.445	N/A	No	500	SPC/E	13
	"----//----"	2006	280	1.20	1.273	N/A	No	500	SPC/E	13
	"----//----"	2006	280	1.25	1.095	N/A	No	500	SPC/E	13
	"----//----"	2006	280	1.30	0.898	N/A	No	500	SPC/E	13
	"----//----"	2006	260	0.85	0.839	N/A	No	500	SPC/E	13
	"----//----"	2006	260	0.90	0.705	N/A	No	500	SPC/E	13
	"----//----"	2006	260	0.95	0.772	N/A	No	500	SPC/E	13
	"----//----"	2006	260	1.00	0.805	N/A	No	500	SPC/E	13
	"----//----"	2006	260	1.05	0.925	N/A	No	500	SPC/E	13

	"----//----"	2006	260		1.10	1.012	N/A	No	500	SPC/E	13
	"----//----"	2006	260		1.15	0.936	N/A	No	500	SPC/E	13
	"----//----"	2006	260		1.20	0.931	N/A	No	500	SPC/E	13
	"----//----"	2006	260		1.25	0.709	N/A	No	500	SPC/E	13
	"----//----"	2006	260		1.30	0.554	N/A	No	500	SPC/E	13
	"----//----"	2006	240		0.85	0.284	N/A	No	500	SPC/E	13
	"----//----"	2006	240		0.90	0.222	N/A	No	500	SPC/E	13
	"----//----"	2006	240		0.95	0.267	N/A	No	500	SPC/E	13
	"----//----"	2006	240		1.00	0.322	N/A	No	500	SPC/E	13
	"----//----"	2006	240		1.05	0.438	N/A	No	500	SPC/E	13
	"----//----"	2006	240		1.10	0.479	N/A	No	500	SPC/E	13
	"----//----"	2006	240		1.15	0.538	N/A	No	500	SPC/E	13
	"----//----"	2006	240		1.20	0.400	N/A	No	500	SPC/E	13
	"----//----"	2006	240		1.25	0.370	N/A	No	500	SPC/E	13
	"----//----"	2006	240		1.30	0.303	N/A	No	500	SPC/E	13
	"----//----"	2006	220		0.85	0.047	N/A	No	500	SPC/E	13
	"----//----"	2006	220		0.90	0.024	N/A	No	500	SPC/E	13
	"----//----"	2006	220		0.95	0.041	N/A	No	500	SPC/E	13
	"----//----"	2006	220		1.00	0.076	N/A	No	500	SPC/E	13
	"----//----"	2006	220		1.05	0.163	N/A	No	500	SPC/E	13
	"----//----"	2006	220		1.10	0.162	N/A	No	500	SPC/E	13
	"----//----"	2006	220		1.15	0.186	N/A	No	500	SPC/E	13
	"----//----"	2006	220		1.20	0.168	N/A	No	500	SPC/E	13
	"----//----"	2006	220		1.25	0.125	N/A	No	500	SPC/E	13
	"----//----"	2006	220		1.30	0.089	N/A	No	500	SPC/E	13
89	Hofmann et al.	2007	268	270	1.09	0.61	N/A	No		Hofmann et al.	89
	"----//----"	2007	298	1	1.06	1.42	N/A	No		Hofmann et al.	89
	"----//----"	2007	298	2100	1.12	1.31	N/A	No		Hofmann et al.	89
	"----//----"	2007	423	100	0.92	9.97	N/A	No		Hofmann et al.	89

91	Yoshida et al	2007	673.15	SC	0.01	2523.56	N/A	No	1000	TIP4P	191
	"----//----"	2007	673.15	SC	0.00	6608.27	N/A	No	1000	TIP4P	191
	"----//----"	2007	673.15	SC	0.04	731.62	N/A	No	1000	TIP4P	191
	"----//----"	2007	673.15	SC	0.09	347.48	N/A	No	1000	TIP4P	191
	"----//----"	2007	673.15	SC	0.19	181.13	N/A	No	1000	TIP4P	191
	"----//----"	2007	673.15	SC	0.39	92.44	N/A	No	1000	TIP4P	191
	"----//----"	2007	673.15	SC	0.59	58.12	N/A	No	1000	TIP4P	191
	"----//----"	2007	673.15	SC	0.99	26.96	N/A	No	1000	TIP4P	191
	"----//----"	2007	673.15	SC	1.19	14.52	N/A	No	1000	TIP4P	191
	"----//----"	2007	673.15	SC	1.49	4.60	N/A	No	1000	TIP4P	191
92	Kumar et al.	2007	220	2000		5.95E-03	N/A	No	512	TIP5P	183
	"----//----"	2007	230	2000		3.28E-02	N/A	No	512	TIP5P	183
	"----//----"	2007	240	2000		1.45E-01	N/A	No	512	TIP5P	183
	"----//----"	2007	250	2000		2.83E-01	N/A	No	512	TIP5P	183
	"----//----"	2007	260	2000		5.52E-01	N/A	No	512	TIP5P	183
	"----//----"	2007	270	2000		6.90E-01	N/A	No	512	TIP5P	183
	"----//----"	2007	280	2000		1.35E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	290	2000		1.68E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	300	2000		2.10E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	320	2000		4.10E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	230	1000		5.12E-03	N/A	No	512	TIP5P	183
	"----//----"	2007	240	1000		4.10E-02	N/A	No	512	TIP5P	183
	"----//----"	2007	250	1000		1.81E-01	N/A	No	512	TIP5P	183
	"----//----"	2007	260	1000		4.42E-01	N/A	No	512	TIP5P	183
	"----//----"	2007	270	1000		6.90E-01	N/A	No	512	TIP5P	183
	"----//----"	2007	280	1000		1.16E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	290	1000		1.68E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	300	1000		2.10E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	320	1000		3.81E+00	N/A	No	512	TIP5P	183

	"----//----"	2007	230	0		3.54E-04	N/A	No	512	TIP5P	183
	"----//----"	2007	240	0		5.12E-03	N/A	No	512	TIP5P	183
	"----//----"	2007	250	0		7.43E-02	N/A	No	512	TIP5P	183
	"----//----"	2007	260	0		2.83E-01	N/A	No	512	TIP5P	183
	"----//----"	2007	270	0		5.12E-01	N/A	No	512	TIP5P	183
	"----//----"	2007	280	0		1.25E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	290	0		1.45E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	300	0		2.10E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	320	0		3.28E+00	N/A	No	512	TIP5P	183
98	Yoshida et al	2008	303.15	VLE	0.99	3.75	N/A	No	256	TIP4P	191
	"----//----"	2008	373.15	VLE	0.96	10.56	N/A	No	256	TIP4P	191
	"----//----"	2008	473.15	VLE	0.86	21.26	N/A	No	256	TIP4P	191
	"----//----"	2008	573.15	VLE	0.70	39.00	N/A	No	256	TIP4P	191
	"----//----"	2008	673.15	VLE	0.59	58.04	N/A	No	256	TIP4P	191
98	Yoshida et al.	2008	303.15	VLE	1	2.61	0.12	No	256	TIP4P	191
	"----//----"	2008	313.15		0.997	3.2	0.04	No	256	TIP4P	191
	"----//----"	2008	323.15		0.992	3.89	0.06	No	256	TIP4P	191
	"----//----"	2008	333.15		0.988	4.62	0.03	No	256	TIP4P	191
	"----//----"	2008	343.15		0.982	5.6	0.08	No	256	TIP4P	191
	"----//----"	2008	353.15		0.976	6.25	0.07	No	256	TIP4P	191
	"----//----"	2008	363.15		0.97	7.22	0.06	No	256	TIP4P	191
	"----//----"	2008	373.15		0.963	8.36	0.3	No	256	TIP4P	191
	"----//----"	2008	383.15		0.955	9.57	0.08	No	256	TIP4P	191
	"----//----"	2008	393.15		0.947	10.4	0.1	No	256	TIP4P	191
	"----//----"	2008	403.15		0.939	11.5	0.3	No	256	TIP4P	191
	"----//----"	2008	413.15		0.93	12.7	0.2	No	256	TIP4P	191
	"----//----"	2008	423.15		0.921	14.2	0.2	No	256	TIP4P	191
	"----//----"	2008	433.15		0.911	15.4	0.1	No	256	TIP4P	191
	"----//----"	2008	443.15		0.901	16.7	0.2	No	256	TIP4P	191

	"----//----"	2008	453.15		0.891	18.4	0.2	No	256	TIP4P	191
	"----//----"	2008	463.15		0.88	19.2	0.1	No	256	TIP4P	191
	"----//----"	2008	473.15		0.869	21.5	0.4	No	256	TIP4P	191
	"----//----"	2008	483.15		0.856	23.5	0.2	No	256	TIP4P	191
	"----//----"	2008	493.15		0.844	24.7	0.1	No	256	TIP4P	191
	"----//----"	2008	503.15		0.831	26.7	0.1	No	256	TIP4P	191
	"----//----"	2008	513.15		0.817	27.9	0.2	No	256	TIP4P	191
	"----//----"	2008	523.15		0.802	30.4	0.2	No	256	TIP4P	191
	"----//----"	2008	533.15		0.787	32.4	0.3	No	256	TIP4P	191
	"----//----"	2008	543.15		0.771	33.8	0.1	No	256	TIP4P	191
	"----//----"	2008	553.15		0.754	36.3	1.5	No	256	TIP4P	191
	"----//----"	2008	563.15		0.735	38.6	0.9	No	256	TIP4P	191
	"----//----"	2008	573.15		0.715	40.4	0.8	No	256	TIP4P	191
	"----//----"	2008	583.15		0.694	43.6	1.1	No	256	TIP4P	191
	"----//----"	2008	593.15		0.67	46.5	1.2	No	256	TIP4P	191
	"----//----"	2008	603.15		0.644	48.9	0.6	No	256	TIP4P	191
	"----//----"	2008	613.15		0.613	52.7	1.4	No	256	TIP4P	191
	"----//----"	2008	623.15		0.577	57.5	0.6	No	256	TIP4P	191
95	Liem & Popelier	2008	300	1.01325	0.996	1.44	N/A	No	216	QCT	95
	"----//----"	2008	300	1.01325	0.996	1.44	N/A	No	216	QCT	95
	"----//----"	2008	300	1013.25	1.045	1.53	N/A	No	216	QCT	95
	"----//----"	2008	300	2026.5	1.086	1.42	N/A	No	216	QCT	95
	"----//----"	2008	300	4053	1.149	1.11	N/A	No	216	QCT	95
	"----//----"	2008	300	6079.5	1.2	0.88	N/A	No	216	QCT	95
	"----//----"	2008	300	8106	1.242	0.7	N/A	No	216	QCT	95
	"----//----"	2008	300	10132.5	1.274	0.58	N/A	No	216	QCT	95
99	Vega et al.	2009	278	1		3.71	N/A	No	360	TIP3P	6
	"----//----"	2009	288	1		4.34	N/A	No	360	TIP3P	6
	"----//----"	2009	298	1		5.51	N/A	No	360	TIP3P	6
	"----//----"	2009	308	1		6.21	N/A	No	360	TIP3P	6

		Year	Temp			Value				Model	
	"----//----"	2009	318	1		6.32	N/A	No	360	TIP3P	6
	"----//----"	2009	278	1		2.08	N/A	No	360	TIP4P	191
	"----//----"	2009	288	1		2.71	N/A	No	360	TIP4P	191
	"----//----"	2009	298	1		3.22	N/A	No	360	TIP4P	191
	"----//----"	2009	308	1		4.12	N/A	No	360	TIP4P	191
	"----//----"	2009	318	1		4.9	N/A	No	360	TIP4P	191
	"----//----"	2009	278	1		1.11	N/A	No	360	TIP5P	183
	"----//----"	2009	288	1		1.74	N/A	No	360	TIP5P	183
	"----//----"	2009	298	1		2.77	N/A	No	360	TIP5P	183
	"----//----"	2009	308	1		3.68	N/A	No	360	TIP5P	183
	"----//----"	2009	318	1		4.81	N/A	No	360	TIP5P	183
	"----//----"	2009	278	1		1.27	N/A	No	360	TIP4P/2005	80
	"----//----"	2009	288	1		1.57	N/A	No	360	TIP4P/2005	80
	"----//----"	2009	298	1		2.07	N/A	No	360	TIP4P/2005	80
	"----//----"	2009	308	1		2.6	N/A	No	360	TIP4P/2005	80
	"----//----"	2009	318	1		3.07	N/A	No	360	TIP4P/2005	80
101	Bauer & Patel	2009	298		VLE	2.3	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	325		VLE	4.12	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	350		VLE	6.26	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	375		VLE	8.08	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	400		VLE	11.04	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	425		VLE	13.68	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	450		VLE	16.32	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	475		VLE	20.60	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	500		VLE	24.40	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	525		VLE	28.85	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	550		VLE	33.79	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	575		VLE	40.05	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	600		VLE	49.95	N/A	Yes	217	TIP4P-QDP-LJ	101

106	Molinero & Moore	2009	361.05	1		10.95	N/A	No	4096	mW	106
	"----//----"	2009	341.00	1		9.67	N/A	No	4096	mW	106
	"----//----"	2009	320.42	1		8.12	N/A	No	4096	mW	106
	"----//----"	2009	298.00	1		6.50	N/A	No	4096	mW	106
	"----//----"	2009	280.21	1		5.45	N/A	No	4096	mW	106
	"----//----"	2009	260.52	1		4.04	N/A	No	4096	mW	106
	"----//----"	2009	240.15	1		2.70	N/A	No	4096	mW	106
	"----//----"	2009	219.98	1		1.44	N/A	No	4096	mW	106
107	Pi et al.	2009	224.72	1		0.039	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	233.62	1		0.113	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	242.65	1		0.253	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	252.09	1		0.382	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	261.80	1		0.592	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	272.04	1		0.871	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	282.97	1		1.438	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	215.82	1500		0.058	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	224.58	1500		0.117	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	233.48	1500		0.214	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	242.65	1500		0.368	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	252.09	1500		0.488	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	261.93	1500		0.796	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	272.31	1500		1.126	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	282.97	1500		1.419	N/A	No	256	TIP4P/2005	80
114	Chopra et al.	2010	500		0.85	19.04	N/A	No	368	SPC/E	13
	"----//----"	2010	500		0.90	18.22	N/A	No	368	SPC/E	13
	"----//----"	2010	500		0.95	17.43	N/A	No	368	SPC/E	13
	"----//----"	2010	500		1.00	14.46	N/A	No	368	SPC/E	13
	"----//----"	2010	500		1.10	11.76	N/A	No	368	SPC/E	13
	"----//----"	2010	500		1.20	9.11	N/A	No	368	SPC/E	13
	"----//----"	2010	500		1.30	6.58	N/A	No	368	SPC/E	13

"----//----"	2010	400	0.85	11.30	N/A	No	368	SPC/E	13
"----//----"	2010	400	0.90	9.83	N/A	No	368	SPC/E	13
"----//----"	2010	400	0.95	9.40	N/A	No	368	SPC/E	13
"----//----"	2010	400	1.00	9.21	N/A	No	368	SPC/E	13
"----//----"	2010	400	1.10	7.49	N/A	No	368	SPC/E	13
"----//----"	2010	400	1.20	5.67	N/A	No	368	SPC/E	13
"----//----"	2010	400	1.30	4.09	N/A	No	368	SPC/E	13
"----//----"	2010	350	0.85	6.39	N/A	No	368	SPC/E	13
"----//----"	2010	350	0.90	5.97	N/A	No	368	SPC/E	13
"----//----"	2010	350	0.95	5.85	N/A	No	368	SPC/E	13
"----//----"	2010	350	1.00	5.46	N/A	No	368	SPC/E	13
"----//----"	2010	350	1.10	4.77	N/A	No	368	SPC/E	13
"----//----"	2010	350	1.20	3.88	N/A	No	368	SPC/E	13
"----//----"	2010	350	1.30	2.80	N/A	No	368	SPC/E	13
"----//----"	2010	300	0.85	2.72	N/A	No	368	SPC/E	13
"----//----"	2010	300	0.90	2.86	N/A	No	368	SPC/E	13
"----//----"	2010	300	0.95	2.61	N/A	No	368	SPC/E	13
"----//----"	2010	300	1.00	2.62	N/A	No	368	SPC/E	13
"----//----"	2010	300	1.10	2.40	N/A	No	368	SPC/E	13
"----//----"	2010	300	1.20	2.04	N/A	No	368	SPC/E	13
"----//----"	2010	300	1.30	1.44	N/A	No	368	SPC/E	13
"----//----"	2010	280	0.85	1.61	N/A	No	368	SPC/E	13
"----//----"	2010	280	0.90	1.58	N/A	No	368	SPC/E	13
"----//----"	2010	280	0.95	1.41	N/A	No	368	SPC/E	13
"----//----"	2010	280	1.00	1.63	N/A	No	368	SPC/E	13
"----//----"	2010	280	1.10	1.60	N/A	No	368	SPC/E	13
"----//----"	2010	280	1.20	1.43	N/A	No	368	SPC/E	13
"----//----"	2010	280	1.30	0.94	N/A	No	368	SPC/E	13
"----//----"	2010	260	0.85	0.79	N/A	No	368	SPC/E	13
"----//----"	2010	260	0.90	0.74	N/A	No	368	SPC/E	13

"----//----"	2010	260	0.95	0.78	N/A	No	368	SPC/E	13
"----//----"	2010	260	1.00	0.86	N/A	No	368	SPC/E	13
"----//----"	2010	260	1.10	1.00	N/A	No	368	SPC/E	13
"----//----"	2010	260	1.20	0.89	N/A	No	368	SPC/E	13
"----//----"	2010	260	1.30	0.60	N/A	No	368	SPC/E	13
"----//----"	2010	250	0.85	0.52	N/A	No	368	SPC/E	13
"----//----"	2010	250	0.90	0.43	N/A	No	368	SPC/E	13
"----//----"	2010	250	0.95	0.51	N/A	No	368	SPC/E	13
"----//----"	2010	250	1.00	0.57	N/A	No	368	SPC/E	13
"----//----"	2010	250	1.10	0.77	N/A	No	368	SPC/E	13
"----//----"	2010	250	1.20	0.67	N/A	No	368	SPC/E	13
"----//----"	2010	250	1.30	0.44	N/A	No	368	SPC/E	13
"----//----"	2010	240	0.85	0.27	N/A	No	368	SPC/E	13
"----//----"	2010	240	0.90	0.21	N/A	No	368	SPC/E	13
"----//----"	2010	240	0.95	0.27	N/A	No	368	SPC/E	13
"----//----"	2010	240	1.00	0.35	N/A	No	368	SPC/E	13
"----//----"	2010	240	1.10	0.52	N/A	No	368	SPC/E	13
"----//----"	2010	240	1.20	0.47	N/A	No	368	SPC/E	13
"----//----"	2010	240	1.30	0.30	N/A	No	368	SPC/E	13
"----//----"	2010	230	0.85	0.13	N/A	No	368	SPC/E	13
"----//----"	2010	230	0.90	0.08	N/A	No	368	SPC/E	13
"----//----"	2010	230	0.95	0.13	N/A	No	368	SPC/E	13
"----//----"	2010	230	1.00	0.19	N/A	No	368	SPC/E	13
"----//----"	2010	230	1.10	0.31	N/A	No	368	SPC/E	13
"----//----"	2010	230	1.20	0.31	N/A	No	368	SPC/E	13
"----//----"	2010	230	1.30	0.20	N/A	No	368	SPC/E	13
"----//----"	2010	220	0.85	0.04	N/A	No	368	SPC/E	13
"----//----"	2010	220	0.90	0.03	N/A	No	368	SPC/E	13
"----//----"	2010	220	0.95	0.04	N/A	No	368	SPC/E	13
"----//----"	2010	220	1.00	0.09	N/A	No	368	SPC/E	13

	"----//----"	2010	220		1.10	0.19	N/A	No	368	SPC/E	13
	"----//----"	2010	220		1.20	0.19	N/A	No	368	SPC/E	13
	"----//----"	2010	220		1.30	0.11	N/A	No	368	SPC/E	13
113	Fuhrmans et al.	2010	323	1		1.8	0.11	No	1068	Model 1 Fuhrmans	113
	"----//----"	2010	323	1		1.81	0.1	No	1068	Model 2 Fuhrmans	113
	"----//----"	2010	323	1		6.19	0.29	No	1068	SPC	178
	"----//----"	2010	323	1		1.97	0.04	No	1068	MARTINI W	192
115	Guevara-Carrion et al.	2011	280	1		3.11	0.02	No	2048	SPC	178
	"----//----"	2011	298.15	1		4.34	0.03	No	2048	SPC	178
	"----//----"	2011	328.15	1		6.80	0.04	No	2048	SPC	178
	"----//----"	2011	280	1		1.79	0.01	No	2048	SPC/E	13
	"----//----"	2011	288.15	1		2.17	0.01	No	2048	SPC/E	13
	"----//----"	2011	298.15	1		2.72	0.02	No	2048	SPC/E	13
	"----//----"	2011	313.15	1		3.60	0.02	No	2048	SPC/E	13
	"----//----"	2011	328.15	1		4.66	0.03	No	2048	SPC/E	13
	"----//----"	2011	343.15	1		5.74	0.04	No	2048	SPC/E	13
	"----//----"	2011	363.15	1		7.39	0.04	No	2048	SPC/E	13
	"----//----"	2011	373.15	1		8.21	0.04	No	2048	SPC/E	13
	"----//----"	2011	280	1		2.49	0.02	No	2048	TIP4P	191
	"----//----"	2011	288.15	1		3.00	0.02	No	2048	TIP4P	191
	"----//----"	2011	298.15	1		3.69	0.02	No	2048	TIP4P	191
	"----//----"	2011	313.15	1		4.84	0.02	No	2048	TIP4P	191
	"----//----"	2011	328.15	1		5.72	0.03	No	2048	TIP4P	191
	"----//----"	2011	343.15	1		7.56	0.04	No	2048	TIP4P	191
	"----//----"	2011	363.15	1		9.69	0.05	No	2048	TIP4P	191
	"----//----"	2011	273.15	1		1.11	0.01	No	2048	TIP4P/2005	80
	"----//----"	2011	280	1		1.38	0.01	No	2048	TIP4P/2005	80

"----//----"	2011	288.15	1	1.75	0.01	No	2048	TIP4P/2005	80
"----//----"	2011	298.15	1	2.26	0.02	No	2048	TIP4P/2005	80
"----//----"	2011	313.15	1	3.05	0.02	No	2048	TIP4P/2005	80
"----//----"	2011	333.15	1	4.42	0.03	No	2048	TIP4P/2005	80
"----//----"	2011	353.15	1	5.94	0.03	No	2048	TIP4P/2005	80
"----//----"	2011	363.15	1	6.93	0.04	No	2048	TIP4P/2005	80
"----//----"	2011	260.00	500	0.77	0.07	No	2048	TIP4P/2005	80
"----//----"	2011	273.15	500	1.22	0.01	No	2048	TIP4P/2005	80
"----//----"	2011	280.00	500	1.47	0.01	No	2048	TIP4P/2005	80
"----//----"	2011	288.15	500	1.77	0.01	No	2048	TIP4P/2005	80
"----//----"	2011	298.15	500	2.3	0.02	No	2048	TIP4P/2005	80
"----//----"	2011	313.15	500	3.1	0.02	No	2048	TIP4P/2005	80
"----//----"	2011	333.15	500	4.34	0.03	No	2048	TIP4P/2005	80
"----//----"	2011	343.15	500	5.04	0.03	No	2048	TIP4P/2005	80
"----//----"	2011	363.15	500	6.62	0.04	No	2048	TIP4P/2005	80
"----//----"	2011	380.00	500	3.49	0.06	No	2048	TIP4P/2005	80
"----//----"	2011	260.00	1000	0.837	0.07	No	2048	TIP4P/2005	80
"----//----"	2011	273.15	1000	1.261	0.09	No	2048	TIP4P/2005	80
"----//----"	2011	280.00	1000	1.52	0.01	No	2048	TIP4P/2005	80
"----//----"	2011	288.15	1000	1.86	0.01	No	2048	TIP4P/2005	80
"----//----"	2011	298.15	1000	2.3	0.02	No	2048	TIP4P/2005	80
"----//----"	2011	313.15	1000	3.09	0.02	No	2048	TIP4P/2005	80
"----//----"	2011	333.15	1000	4.32	0.03	No	2048	TIP4P/2005	80
"----//----"	2011	343.15	1000	4.97	0.03	No	2048	TIP4P/2005	80
"----//----"	2011	363.15	1000	6.49	0.04	No	2048	TIP4P/2005	80
"----//----"	2011	380.00	1000	7.77	0.04	No	2048	TIP4P/2005	80
"----//----"	2011	400.00	1000	7.77	0.04	No	2048	TIP4P/2005	80
"----//----"	2011	260.00	2000	0.89	0.008	No	2048	TIP4P/2005	80
"----//----"	2011	273.15	2000	1.30	0.009	No	2048	TIP4P/2005	80
"----//----"	2011	280.00	2000	1.55	0.001	No	2048	TIP4P/2005	80
"----//----"	2011	288.15	2000	1.90	0.001	No	2048	TIP4P/2005	80
"----//----"	2011	298.15	2000	2.30	0.001	No	2048	TIP4P/2005	80

	"----//----"	2011	313.15	2000		3.06	0.002	No	2048	TIP4P/2005	80
	"----//----"	2011	333.15	2000		4.20	0.002	No	2048	TIP4P/2005	80
	"----//----"	2011	343.15	2000		4.78	0.003	No	2048	TIP4P/2005	80
	"----//----"	2011	363.15	2000		6.10	0.003	No	2048	TIP4P/2005	80
	"----//----"	2011	380.00	2000		7.38	0.004	No	2048	TIP4P/2005	80
	"----//----"	2011	400.00	2000		8.94	0.004	No	2048	TIP4P/2005	80
	"----//----"	2011	260.00	3000		0.90	0.009	No	2048	TIP4P/2005	80
	"----//----"	2011	273.15	3000		1.30	0.001	No	2048	TIP4P/2005	80
	"----//----"	2011	280.00	3000		1.54	0.001	No	2048	TIP4P/2005	80
	"----//----"	2011	288.15	3000		1.86	0.001	No	2048	TIP4P/2005	80
	"----//----"	2011	298.15	3000		2.28	0.001	No	2048	TIP4P/2005	80
	"----//----"	2011	313.15	3000		2.97	0.002	No	2048	TIP4P/2005	80
	"----//----"	2011	333.15	3000		4.05	0.002	No	2048	TIP4P/2005	80
	"----//----"	2011	343.15	3000		5.86	0.003	No	2048	TIP4P/2005	80
	"----//----"	2011	363.15	3000		6.47	0.004	No	2048	TIP4P/2005	80
	"----//----"	2011	400.00	3000		8.38	0.005	No	2048	TIP4P/2005	80
119	Alejandre et al.	2011	280	1	0.9984	1.27	N/A	No	500	TIP4Q	119
	"----//----"	2011	300	1	0.9984	2.2	N/A	No	500	TIP4Q	119
	"----//----"	2011	320	1	0.9872	3.26	N/A	No	500	TIP4Q	119
	"----//----"	2011	340	1	0.9774	4.67	N/A	No	500	TIP4Q	119
120	Viererblova & Kolafa	2011	263.005	1.01325		0.700	0.004	Yes	360	POL4D	120
	"----//----"	2011	272.995	1.01325		1.089	0.007	Yes	360	POL4D	120
	"----//----"	2011	273.150	1.01325		1.086	0.012	Yes	360	POL4D	120
	"----//----"	2011	273.001	1.01325		1.174	0.006	Yes	360	POL4D	120
	"----//----"	2011	282.998	1.01325		1.547	0.009	Yes	360	POL4D	120
	"----//----"	2011	297.981	1.01325		2.423	0.013	Yes	360	POL4D	120
	"----//----"	2011	298.150	1.01325		2.461	0.015	Yes	360	POL4D	120
	"----//----"	2011	298.116	1.01325		2.458	0.028	Yes	360	POL4D	120
	"----//----"	2011	319.964	1.01325		4.054	0.015	Yes	360	POL4D	120
	"----//----"	2011	349.802	1.01325		6.924	0.022	Yes	360	POL4D	120

121	Orsi & Essex	2011	303	1.01325	2.6	1%	No	4000	ELBA	121
123	Qvist et al.	2011	230.75	0.9756	0.165	0.001	Yes	2048	SPC/E	13
	"----//----"	2011	246.54	0.9935	0.509	0.004	Yes	2048	SPC/E	13
	"----//----"	2011	253.35	0.9963	0.705	0.006	Yes	2048	SPC/E	13
	"----//----"	2011	259.28	0.9982	0.909	0.007	Yes	2048	SPC/E	13
	"----//----"	2011	266.08	0.9998	1.20	0.01	Yes	2048	SPC/E	13
	"----//----"	2011	276.03	0.9997	1.58	0.02	Yes	2048	SPC/E	13
	"----//----"	2011	290.29	0.9982	2.34	0.02	Yes	2048	SPC/E	13
122	Wang & Hou	2011	235.47		1.059	0.001	No	624	TIP3P	6
	"----//----"	2011	247.96		1.374	0.001	No	624	TIP3P	6
	"----//----"	2011	260.49		1.734	0.009	No	624	TIP3P	6
	"----//----"	2011	273.16		2.085	0.014	No	624	TIP3P	6
	"----//----"	2011	285.49		2.717	0.020	No	624	TIP3P	6
	"----//----"	2011	298.13		2.984	0.005	No	624	TIP3P	6
	"----//----"	2011	310.45		3.667	0.016	No	624	TIP3P	6
	"----//----"	2011	322.85		3.667	0.012	No	624	TIP3P	6
	"----//----"	2011	335.42		4.629	0.008	No	624	TIP3P	6
	"----//----"	2011	347.87		5.056	0.014	No	624	TIP3P	6
	"----//----"	2011	360.43		5.527	0.014	No	624	TIP3P	6
	"----//----"	2011	373.04		6.268	0.007	No	624	TIP3P	6
	"----//----"	2011	400.00		8.073	0.056	No	624	TIP3P	6
124	Raabe & Sadus	2012	277.15	1	1.502	0.06	No	400	SPC/E	13
	"----//----"	2012	298.15	1	2.432	0.023	No	400	SPC/E	13
	"----//----"	2012	323.15	1	3.878	0.169	No	400	SPC/E	13
	"----//----"	2012	353.15	1	5.77	0.277	No	400	SPC/E	13
	"----//----"	2012	277.15	1	1.410	0.047	No	400	SPC/Fw	83
	"----//----"	2012	298.15	1	2.359	0.035	No	400	SPC/Fw	83

"----//----"	2012	313.15	1	3.229	0.158	No	400	SPC/Fw	83
"----//----"	2012	318.15	1	3.431	0.134	No	400	SPC/Fw	83
"----//----"	2012	323.15	1	3.797	0.15	No	400	SPC/Fw	83
"----//----"	2012	333.15	1	4.5	0.094	No	400	SPC/Fw	83
"----//----"	2012	343.15	1	5.218	0.302	No	400	SPC/Fw	83
"----//----"	2012	353.15	1	5.927	0.22	No	400	SPC/Fw	83
"----//----"	2012	363.15	1	6.720	0.205	No	400	SPC/Fw	83
"----//----"	2012	277.15	1	2.659	0.103	No	400	SPC	178
"----//----"	2012	298.15	1	3.861	0.03	No	400	SPC	178
"----//----"	2012	333.15	1	6.675	0.275	No	400	SPC	178
"----//----"	2012	353.15	1	8.281	0.276	No	400	SPC	178
"----//----"	2012	298.15	1	2.359	0.035	No	400	SPC/Fw	83
"----//----"	2012	298.15	500	2.378	0.027	No	400	SPC/Fw	83
"----//----"	2012	298.15	1000	2.328	0.045	No	400	SPC/Fw	83
"----//----"	2012	298.15	1500	2.344	0.041	No	400	SPC/Fw	83
"----//----"	2012	298.15	2000	2.269	0.011	No	400	SPC/Fw	83
"----//----"	2012	318.15	1	3.432	0.134	No	400	SPC/Fw	83
"----//----"	2012	318.15	100	3.502	0.160	No	400	SPC/Fw	83
"----//----"	2012	318.15	1000	3.468	0.187	No	400	SPC/Fw	83
"----//----"	2012	333.15	1	4.499	0.094	No	400	SPC/Fw	83
"----//----"	2012	333.15	100	4.584	0.177	No	400	SPC/Fw	83
"----//----"	2012	333.15	500	4.472	0.193	No	400	SPC/Fw	83
"----//----"	2012	333.15	1000	4.29	0.208	No	400	SPC/Fw	83
"----//----"	2012	673.15	500	60.086	1222	No	400	SPC/Fw	83
"----//----"	2012	673.15	1000	47.297	0.531	No	400	SPC/Fw	83
"----//----"	2012	673.15	2000	37.9	0.412	No	400	SPC/Fw	83
"----//----"	2012	298.15	1	1.43	0.06	No	400	SPC/E	13
"----//----"	2012	298.15	500	1.42	N/A	No	400	SPC/E	13
"----//----"	2012	298.15	1000	1.39	N/A	No	400	SPC/E	13

	"----//----"	2012	298.15	1500		1.35	N/A	No	400	SPC/E	13
	"----//----"	2012	673.15	500		6.06	N/A	No	400	SPC/E	13
	"----//----"	2012	673.15	1000		4.67	N/A	No	400	SPC/E	13
129	Gallo & Rovere	2012	300		1.00	3.77	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	280		1.00	2.13	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	260		1.00	1.22	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	250		1.00	0.797	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	240		1.00	0.539	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	230		1.00	0.337	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	220		1.00	0.169	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	210		1.00	7.10E-02	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	200		1.00	2.60E-02	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	195		1.00	1.20E-02	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	190		1.00	6.40E-03	N/A	No	256 (?)	TIP4P	191
130	Rozmanov & Kusalik	2012	210			2.52E-03	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	215			7.90E-03	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	220			1.99E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	225			4.19E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	230			7.70E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	235			1.28E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	240			1.95E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	245			2.81E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	250			3.84E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	255			5.05E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	260			6.43E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	265			7.96E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	270			9.64E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	275			1.14E+00	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	280			1.34E+00	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	285			1.54E+00	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	290			1.75E+00	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	295			1.96E+00	N/A	No	1000	TIP4P/2005	80

	"----//----"	2012	298			2.10E+00	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	300			2.19E+00	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	305			2.42E+00	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	310			2.65E+00	N/A	No	1000	TIP4P/2005	80
131	Zlenko	2012	273.15	-14.12		1.00	N/A	No	11337	TIP4P	191
	"----//----"	2012	277.15	14.63		1.02	N/A	No	11337	TIP4P	191
	"----//----"	2012	283.15	53.89		1.20	N/A	No	11337	TIP4P	191
	"----//----"	2012	293.15	119.46		1.48	N/A	No	11337	TIP4P	191
	"----//----"	2012	298.15	143.68		1.59	N/A	No	11337	TIP4P	191
	"----//----"	2012	303.15	176.10		1.73	N/A	No	11337	TIP4P	191
	"----//----"	2012	313.15	233.86		2.02	N/A	No	11337	TIP4P	191
	"----//----"	2012	323.15	287.26		2.28	N/A	No	11337	TIP4P	191
	"----//----"	2012	333.15	341.97		2.57	N/A	No	11337	TIP4P	191
	"----//----"	2012	343.15	391.72		2.86	N/A	No	11337	TIP4P	191
	"----//----"	2012	348.15	416.65		3.06	N/A	No	11337	TIP4P	191
	"----//----"	2012	353.15	441.47		3.10	N/A	No	11337	TIP4P	191
	"----//----"	2012	363.15	487.07		3.50	N/A	No	11337	TIP4P	191
	"----//----"	2012	373.15	529.42		3.79	N/A	No	11337	TIP4P	191
132	Lee	2013	300		0.9965	2.78	0.06	No	1024	SPC/E	13
	"----//----"	2013	350		0.9737	6.02	0.09	No	1024	SPC/E	13
	"----//----"	2013	400		0.9375	10.3	0.02	No	1024	SPC/E	13
	"----//----"	2013	450		0.8903	15.3	0.01	No	1024	SPC/E	13
	"----//----"	2013	500		0.8313	21.8	0.03	No	1024	SPC/E	13
	"----//----"	2013	550		0.7558	30.1	0.03	No	1024	SPC/E	13
143	Wang et al.	2013	260	1.01325		0.74	N/A	Yes	216/512/1000	iAMOEBA	143
	"----//----"	2013	273	1.01325		1.23	N/A	Yes	216/512/1000	iAMOEBA	143
	"----//----"	2013	285	1.01325		1.79	N/A	Yes	216/512/1000	iAMOEBA	143
	"----//----"	2013	298	1.01325		2.54	N/A	Yes	216/512/1000	iAMOEBA	143
	"----//----"	2013	310	1.01325		3.25	N/A	Yes	216/512/1000	iAMOEBA	143
	"----//----"	2013	323	1.01325		4.03	N/A	Yes	216/512/1000	iAMOEBA	143

	"----//----"	2013	255	1.01325		0.2	N/A	Yes	216/512/1000	AMOEBA	78
	"----//----"	2013	260	1.01325		0.31	N/A	Yes	216/512/1000	AMOEBA	78
	"----//----"	2013	265	1.01325		0.51	N/A	Yes	216/512/1000	AMOEBA	78
	"----//----"	2013	273	1.01325		0.78	N/A	Yes	216/512/1000	AMOEBA	78
	"----//----"	2013	278	1.01325		0.84	N/A	Yes	216/512/1000	AMOEBA	78
	"----//----"	2013	285	1.01325		1.26	N/A	Yes	216/512/1000	AMOEBA	78
	"----//----"	2013	298	1.01325		1.92	N/A	Yes	216/512/1000	AMOEBA	78
	"----//----"	2013	323	1.01325		3.38	N/A	Yes	216/512/1000	AMOEBA	78
141	Stukan et al.	2013	298.15	1.01325		2.4	N/A	No	1024	SWM4-NDP	82
	"----//----"	2013	323	1.01325		4	N/A	No	1024	SWM4-NDP	82
	"----//----"	2013	348	1.01325		6.1	N/A	No	1024	SWM4-NDP	82
	"----//----"	2013	363	1.01325		7.2	N/A	No	1024	SWM4-NDP	82
137	Corsetti et al.	2013	300		1	1.92	Yes (Fig. 12)	No	200	TIP4P	191
	"----//----"	2013	300		1.05	2.09	Yes (Fig. 12)	No	200	TIP4P	191
	"----//----"	2013	300		1.1	1.54	Yes (Fig. 12)	No	200	TIP4P	191
	"----//----"	2013	300		1.15	1.21	Yes (Fig. 12)	No	200	TIP4P	191
	"----//----"	2013	300		1.2	1.06	Yes (Fig. 12)	No	200	TIP4P	191
144	Arismendi-Arrieta et al.	2014	273			1.34	N/A	No	256	NCC(Q)	144
	"----//----"	2014	283			1.67	N/A	No	256	NCC(Q)	144
	"----//----"	2014	303			2.5	N/A	No	256	NCC(Q)	144
	"----//----"	2014	333			3.8	N/A	No	256	NCC(Q)	144
	"----//----"	2014	373			5.93	N/A	No	256	NCC(Q)	144
150	Kiss & Baranyai	2014	225	1		0.0615	N/A	Yes	432	BK3	136
	"----//----"	2014	230	1		0.0954	N/A	Yes	432	BK3	136
	"----//----"	2014	235	1		0.1417	N/A	Yes	432	BK3	136
	"----//----"	2014	238	1		0.1750	N/A	Yes	432	BK3	136
	"----//----"	2014	243	1		0.2472	N/A	Yes	432	BK3	136

"----//----"	2014	248	1	0.3434	N/A	Yes	432	BK3	136
"----//----"	2014	253	1	0.4498	N/A	Yes	432	BK3	136
"----//----"	2014	258	1	0.5841	N/A	Yes	432	BK3	136
"----//----"	2014	263	1	0.7210	N/A	Yes	432	BK3	136
"----//----"	2014	268	1	0.8902	N/A	Yes	432	BK3	136
"----//----"	2014	273	1	1.0806	N/A	Yes	432	BK3	136
"----//----"	2014	278	1	1.2898	N/A	Yes	432	BK3	136
"----//----"	2014	283	1	1.4885	N/A	Yes	432	BK3	136
"----//----"	2014	288	1	1.7470	N/A	Yes	432	BK3	136
"----//----"	2014	293	1	2.0332	N/A	Yes	432	BK3	136
"----//----"	2014	298	1	2.3268	N/A	Yes	432	BK3	136
"----//----"	2014	303	1	2.6627	N/A	Yes	432	BK3	136
"----//----"	2014	308	1	2.9962	N/A	Yes	432	BK3	136
"----//----"	2014	313	1	3.2872	N/A	Yes	432	BK3	136
"----//----"	2014	323	1	4.0583	N/A	Yes	432	BK3	136
"----//----"	2014	333	1	4.7631	N/A	Yes	432	BK3	136
"----//----"	2014	343	1	5.5903	N/A	Yes	432	BK3	136
"----//----"	2014	353	1	6.5612	N/A	Yes	432	BK3	136
"----//----"	2014	363	1	7.3829	N/A	Yes	432	BK3	136
"----//----"	2014	373	1	8.3075	N/A	Yes	432	BK3	136
"----//----"	2014	223	1500	0.13821	N/A	Yes	432	BK3	136
"----//----"	2014	228	1500	0.18563	N/A	Yes	432	BK3	136
"----//----"	2014	233	1500	0.24309	N/A	Yes	432	BK3	136
"----//----"	2014	238	1500	0.31303	N/A	Yes	432	BK3	136
"----//----"	2014	243	1500	0.39302	N/A	Yes	432	BK3	136
"----//----"	2014	248	1500	0.48931	N/A	Yes	432	BK3	136
"----//----"	2014	253	1500	0.60408	N/A	Yes	432	BK3	136
"----//----"	2014	258	1500	0.71499	N/A	Yes	432	BK3	136
"----//----"	2014	263	1500	0.86794	N/A	Yes	432	BK3	136
"----//----"	2014	268	1500	1.01868	N/A	Yes	432	BK3	136
"----//----"	2014	273	1500	1.18556	N/A	Yes	432	BK3	136
"----//----"	2014	283	1500	1.57898	N/A	Yes	432	BK3	136

		Year									
	"----//----"	2014	298	1500		2.24964	N/A	Yes	432	BK3	136
	"----//----"	2014	313	1500		3.04710	N/A	Yes	432	BK3	136
	"----//----"	2014	333	1500		4.26876	N/A	Yes	432	BK3	136
	"----//----"	2014	353	1500		5.63760	N/A	Yes	432	BK3	136
	"----//----"	2014	373	1500		7.19855	N/A	Yes	432	BK3	136
147	Fuentes-Azcatl & Alejandre	2014	240	1	0.9851	0.1852	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	250	1	0.9929	0.3423	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	260	1	0.9978	0.601	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	270	1	1	0.8644	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	280	1	1.0002	1.1682	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	290	1	0.999	1.643	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	300	1	0.9967	2.1048	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	310	1	0.9935	2.8515	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	320	1	0.9894	3.3919	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	330	1	0.9843	3.9504	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	340	1	0.9789	4.7134	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	240	1	0.9867	0.2141	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	250	1	0.9945	0.3739	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	260	1	0.998	0.6578	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	270	1	0.9997	0.9235	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	280	1	0.9993	1.1939	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	290	1	0 0.998	1.7265	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	300	1	0.9958	2.0963	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	310	1	0.9926	2.6428	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	320	1	0.9885	3.3458	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	330	1	0.9837	3.7811	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	340	1	0.9786	4.3345	N/A	No	500	TIP4P/ε	147
149	Moultos et al.	2014	298.15	1		3.6	0.5	No	2000	SPC	178
	"----//----"	2014	323.15	1		6.2	0.5	No	2000	SPC	178

"----//----"	2014	348.15	1	8.8	0.3	No	2000	SPC	178
"----//----"	2014	373.15	480	10.7	0.2	No	2000	SPC	178
"----//----"	2014	298.15	1	2.6	0.1	No	2000	SPC/E	13
"----//----"	2014	323.15	1	4.3	0.2	No	2000	SPC/E	13
"----//----"	2014	323.15	200	4.2	0.1	No	2000	SPC/E	13
"----//----"	2014	323.15	480	4.2	0.2	No	2000	SPC/E	13
"----//----"	2014	348.15	1	6.2	0.2	No	2000	SPC/E	13
"----//----"	2014	348.15	200	6.2	0.2	No	2000	SPC/E	13
"----//----"	2014	373.15	15	8.4	0.2	No	2000	SPC/E	13
"----//----"	2014	373.15	200	8.2	0.1	No	2000	SPC/E	13
"----//----"	2014	373.15	480	7.8	0.3	No	2000	SPC/E	13
"----//----"	2014	398.15	200	10.8	0.3	No	2000	SPC/E	13
"----//----"	2014	423.15	200	13.6	0.5	No	2000	SPC/E	13
"----//----"	2014	448.15	200	16.7	0.5	No	2000	SPC/E	13
"----//----"	2014	473.15	200	19.9	0.4	No	2000	SPC/E	13
"----//----"	2014	473.15	480	19.4	0.4	No	2000	SPC/E	13
"----//----"	2014	473.15	1000	17.8	0.3	No	2000	SPC/E	13
"----//----"	2014	523.15	200	28.2	0.8	No	2000	SPC/E	13
"----//----"	2014	523.15	480	26.4	0.5	No	2000	SPC/E	13
"----//----"	2014	523.15	1000	24.2	0.7	No	2000	SPC/E	13
"----//----"	2014	573.15	480	35.7	0.8	No	2000	SPC/E	13
"----//----"	2014	623.15	200	60	2	No	2000	SPC/E	13
"----//----"	2014	623.15	480	48	2	No	2000	SPC/E	13
"----//----"	2014	623.15	1000	39.9	0.8	No	2000	SPC/E	13
"----//----"	2014	298.15	1	2.1	0.1	No	2000	TIP4P/2005	80
"----//----"	2014	323.15	1	3.6	0.1	No	2000	TIP4P/2005	80
"----//----"	2014	323.15	200	3.6	0.1	No	2000	TIP4P/2005	80
"----//----"	2014	323.15	480	3.6	0.1	No	2000	TIP4P/2005	80
"----//----"	2014	348.15	1	5.4	0.2	No	2000	TIP4P/2005	80
"----//----"	2014	348.15	200	5.3	0.1	No	2000	TIP4P/2005	80

	"----//----"	2014	373.15	15	7.5	0.1	No	2000	TIP4P/2005	80
	"----//----"	2014	373.15	200	7.4	0.2	No	2000	TIP4P/2005	80
	"----//----"	2014	373.15	480	7.4	0.2	No	2000	TIP4P/2005	80
	"----//----"	2014	398.15	200	9.7	0.2	No	2000	TIP4P/2005	80
	"----//----"	2014	423.15	200	12.6	0.3	No	2000	TIP4P/2005	80
	"----//----"	2014	448.15	200	15.4	0.3	No	2000	TIP4P/2005	80
	"----//----"	2014	473.15	200	18.7	0.6	No	2000	TIP4P/2005	80
	"----//----"	2014	473.15	480	17.6	0.5	No	2000	TIP4P/2005	80
	"----//----"	2014	473.15	1000	17	0.5	No	2000	TIP4P/2005	80
	"----//----"	2014	523.15	200	25.9	0.9	No	2000	TIP4P/2005	80
	"----//----"	2014	523.15	480	24.9	0.8	No	2000	TIP4P/2005	80
	"----//----"	2014	523.15	1000	22.7	0.5	No	2000	TIP4P/2005	80
	"----//----"	2014	573.15	480	32.3	0.7	No	2000	TIP4P/2005	80
	"----//----"	2014	623.15	200	51	2	No	2000	TIP4P/2005	80
	"----//----"	2014	623.15	480	43	1	No	2000	TIP4P/2005	80
	"----//----"	2014	623.15	1000	38	3	No	2000	TIP4P/2005	80
156	Espinosa et al.	2014	170		0.00035	N/A	No		TIP4P	191
	"----//----"	2014	180		0.00059	N/A	No		TIP4P	191
	"----//----"	2014	190		0.00237	N/A	No		TIP4P	191
	"----//----"	2014	200		0.01032	N/A	No		TIP4P	191
	"----//----"	2014	210		0.04893	N/A	No		TIP4P	191
	"----//----"	2014	220		0.15063	N/A	No		TIP4P	191
	"----//----"	2014	230		0.30088	N/A	No		TIP4P	191
	"----//----"	2014	191		0.00040	N/A	No		TIP4P/2005	80
	"----//----"	2014	199		0.00062	N/A	No		TIP4P/2005	80
	"----//----"	2014	207		0.00129	N/A	No		TIP4P/2005	80
	"----//----"	2014	216		0.00796	N/A	No		TIP4P/2005	80
	"----//----"	2014	225		0.03942	N/A	No		TIP4P/2005	80
	"----//----"	2014	234		0.11620	N/A	No		TIP4P/2005	80
	"----//----"	2014	243		0.27595	N/A	No		TIP4P/2005	80

	"----//----"	2014	252			0.39000	N/A	No		TIP4P/2005	80
	"----//----"	2014	202			0.00080	N/A	No		TIP4P/ICE	204
	"----//----"	2014	212			0.00119	N/A	No		TIP4P/ICE	204
	"----//----"	2014	232			0.01032	N/A	No		TIP4P/ICE	204
	"----//----"	2014	242			0.04298	N/A	No		TIP4P/ICE	204
	"----//----"	2014	252			0.08222	N/A	No		TIP4P/ICE	204
	"----//----"	2014	252			0.09775	N/A	No		TIP4P/ICE	204
	"----//----"	2014	258			0.17907	N/A	No		TIP4P/ICE	204
	"----//----"	2014	210			0.71448	N/A	No		mW	106
	"----//----"	2014	220			1.30893	N/A	No		mW	106
	"----//----"	2014	230			1.84995	N/A	No		mW	106
	"----//----"	2014	240			2.61458	N/A	No		mW	106
	"----//----"	2014	254			3.38910	N/A	No		mW	106
	"----//----"	2014	260			4.39304	N/A	No		mW	106
157	Shvab & Sadus	2014	277.70		0.998	1.63	N/A	No	500	SPC/E	13
	"----//----"	2014	296.91		0.998	2.45	N/A	No	500	SPC/E	13
	"----//----"	2014	323.82		0.998	4.02	N/A	No	500	SPC/E	13
	"----//----"	2014	343.04		0.998	5.28	N/A	No	500	SPC/E	13
	"----//----"	2014	379.96		0.998	8.06	N/A	No	500	SPC/E	13
	"----//----"	2014	399.95		0.998	9.38	N/A	No	500	SPC/E	13
	"----//----"	2014	420.71		0.998	10.77	N/A	No	500	SPC/E	13
	"----//----"	2014	450.69		0.998	12.34	N/A	No	500	SPC/E	13
	"----//----"	2014	500.65		0.998	14.99	N/A	No	500	SPC/E	13
	"----//----"	2014	550.61		0.998	17.26	N/A	No	500	SPC/E	13
	"----//----"	2014	600.58		0.998	20.09	N/A	No	500	SPC/E	13
	"----//----"	2014	649.79		0.998	23.31	N/A	No	500	SPC/E	13
158	Gallo et al.	2014	SC	SC	SC	see Fig. 1b	N/A	No	4096	TIP4P/2005	80
161	Park et al.	2015	550			29.67148	N/A	No	1024	SPC/E	13

	"----//----"	2015	499		21.56	N/A	No	1024	SPC/E	13
	"----//----"	2015	449		15.33	N/A	No	1024	SPC/E	13
	"----//----"	2015	399		10.20	N/A	No	1024	SPC/E	13
	"----//----"	2015	350		5.95	N/A	No	1024	SPC/E	13
	"----//----"	2015	300		2.80	N/A	No	1024	SPC/E	13
	"----//----"	2015	273	0.9980	1.53	N/A	No	1024	SPC/E	13
	"----//----"	2015	268	0.9993	1.33	N/A	No	1024	SPC/E	13
	"----//----"	2015	263	0.9981	1.13	N/A	No	1024	SPC/E	13
	"----//----"	2015	258	0.9963	0.94	N/A	No	1024	SPC/E	13
	"----//----"	2015	253	0.9935	0.79	N/A	No	1024	SPC/E	13
	"----//----"	2015	248	0.9896	0.65	N/A	No	1024	SPC/E	13
	"----//----"	2015	243	0.9839	0.50	N/A	No	1024	SPC/E	13
159	Tainter et al.	2015	673	0.0995	284.70	Yes (Fig. 13)	Yes	500	E3B3	159
	"----//----"	2015	673	0.1990	154.99	Yes (Fig. 13)	Yes	500	E3B3	159
	"----//----"	2015	673	0.2998	118.40	Yes (Fig. 13)	Yes	500	E3B3	159
	"----//----"	2015	673	0.4006	88.47	Yes (Fig. 13)	Yes	500	E3B3	159
	"----//----"	2015	673	0.5002	69.84	Yes (Fig. 13)	Yes	500	E3B3	159
	"----//----"	2015	673	0.5997	58.54	Yes (Fig. 13)	Yes	500	E3B3	159
	"----//----"	2015	673	0.7005	47.89	Yes (Fig. 13)	Yes	500	E3B3	159
	"----//----"	2015	673	0.0995	280.04	Yes (Fig. 13)	Yes	500	TIP4P/2005	80
	"----//----"	2015	673	0.1990	143.02	Yes (Fig. 13)	Yes	500	TIP4P/2005	80
	"----//----"	2015	673	0.2998	108.43	Yes (Fig. 13)	Yes	500	TIP4P/2005	80
	"----//----"	2015	673	0.4006	89.80	Yes (Fig. 13)	Yes	500	TIP4P/2005	80
	"----//----"	2015	673	0.5002	73.17	Yes (Fig. 13)	Yes	500	TIP4P/2005	80
	"----//----"	2015	673	0.5997	57.87	Yes (Fig. 13)	Yes	500	TIP4P/2005	80
	"----//----"	2015	673	0.7005	49.22	Yes (Fig. 13)	Yes	500	TIP4P/2005	80
160	Lobanova et al.	2015	432.9	VLE	8.65	N/A	No		Mie (8-6) CGW1-vle	160
	"----//----"	2015	412.9	VLE	7.29	N/A	No		Mie (8-6) CGW1-vle	160
	"----//----"	2015	392.9	VLE	6.02	N/A	No		Mie (8-6) CGW1-vle	160
	"----//----"	2015	362.9	VLE	4.56	N/A	No		Mie (8-6) CGW1-vle	160
	"----//----"	2015	343.0	VLE	3.50	N/A	No		Mie (8-6) CGW1-vle	160

	"----//----"	2015	432.9	VLE	14.19	N/A	No		Mie (8-6) CGW1-ift	160
	"----//----"	2015	392.9	VLE	13.91	N/A	No		Mie (8-6) CGW1-ift	160
	"----//----"	2015	372.8	VLE	12.11	N/A	No		Mie (8-6) CGW1-ift	160
	"----//----"	2015	343.0	VLE	11.34	N/A	No		Mie (8-6) CGW1-ift	160
	"----//----"	2015	313.0	VLE	8.82	N/A	No		Mie (8-6) CGW1-ift	160
	"----//----"	2015	298.0	VLE	7.53	N/A	No		Mie (8-6) CGW1-ift	160
	"----//----"	2015	293.0	VLE	7.38	N/A	No		Mie (8-6) CGW1-ift	160
162	Fuentes-Azcatl et al.	2015	240		0.10	N/A	No	500	SPC/ε	162
	"----//----"	2015	250		0.21	N/A	No	500	SPC/ε	162
	"----//----"	2015	260		0.38	N/A	No	500	SPC/ε	162
	"----//----"	2015	270		0.56	N/A	No	500	SPC/ε	162
	"----//----"	2015	280		0.82	N/A	No	500	SPC/ε	162
	"----//----"	2015	290		1.12	N/A	No	500	SPC/ε	162
	"----//----"	2015	300		1.62	N/A	No	500	SPC/ε	162
	"----//----"	2015	310		1.91	N/A	No	500	SPC/ε	162
	"----//----"	2015	320		2.31	N/A	No	500	SPC/ε	162
	"----//----"	2015	330		3.12	N/A	No	500	SPC/ε	162
	"----//----"	2015	340		3.68	N/A	No	500	SPC/ε	162
	"----//----"	2015	350		4.71	N/A	No	500	SPC/ε	162
	"----//----"	2015	240		0.28	N/A	No	500	SPC/ε1	162
	"----//----"	2015	250		0.44	N/A	No	500	SPC/ε1	162
	"----//----"	2015	260		0.70	N/A	No	500	SPC/ε1	162
	"----//----"	2015	270		1.03	N/A	No	500	SPC/ε1	162
	"----//----"	2015	280		1.25	N/A	No	500	SPC/ε1	162
	"----//----"	2015	290		1.60	N/A	No	500	SPC/ε1	162
	"----//----"	2015	300		2.01	N/A	No	500	SPC/ε1	162
	"----//----"	2015	310		2.56	N/A	No	500	SPC/ε1	162
	"----//----"	2015	320		2.95	N/A	No	500	SPC/ε1	162
	"----//----"	2015	330		3.74	N/A	No	500	SPC/ε1	162
	"----//----"	2015	340		4.24	N/A	No	500	SPC/ε1	162
	"----//----"	2015	350		5.09	N/A	No	500	SPC/ε1	162

	"----//----"	2015	240		0.21	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	250		0.37	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	260		0.65	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	270		0.91	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	280		1.18	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	290		1.73	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	300		2.12	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	310		2.66	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	320		3.36	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	330		3.80	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	340		4.36	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	350		5.15	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	240		0.20	N/A	No	500	SPC/E	13
	"----//----"	2015	250		0.36	N/A	No	500	SPC/E	13
	"----//----"	2015	260		0.88	N/A	No	500	SPC/E	13
	"----//----"	2015	270		1.18	N/A	No	500	SPC/E	13
	"----//----"	2015	280		1.57	N/A	No	500	SPC/E	13
	"----//----"	2015	290		2.03	N/A	No	500	SPC/E	13
	"----//----"	2015	300		2.44	N/A	No	500	SPC/E	13
	"----//----"	2015	310		3.22	N/A	No	500	SPC/E	13
	"----//----"	2015	320		3.87	N/A	No	500	SPC/E	13
	"----//----"	2015	330		4.33	N/A	No	500	SPC/E	13
163	Shvab & Sadus	2015	670	0.100	289.47	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670	0.152	200.00	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670	0.203	152.05	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670	0.247	125.15	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670	0.298	112.57	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670	0.322	101.75	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670	0.333	101.75	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670	0.346	98.25	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670	0.400	86.26	N/A	No	1728	TIP4P/2005f	117

	"----//----"	2015	670		0.450	76.61	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670		0.500	67.84	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670		0.550	59.94	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670		0.600	55.85	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670		0.700	45.61	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670		0.800	35.96	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670		0.900	28.65	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670		1.000	23.39	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670		0.100	274.27	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.152	183.04	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.203	144.44	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.247	118.13	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.298	104.68	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.322	100.58	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.333	97.95	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.346	95.32	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.400	81.87	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.450	74.56	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.500	65.50	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.550	61.70	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.600	53.22	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.700	45.32	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.800	37.13	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.900	29.53	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		1.000	23.10	N/A	No	1728	TIP4P/2005	80
164	Corradini et al.	2015	SC	SC	SC	see Fig. 6	N/A	No	4096	TIP4P/2005	80
	"----//----"	2015	SC	SC	SC	see Fig. 6	N/A	No	4096	TIP4P	191
	"----//----"	2015	SC	SC	SC	see Fig. 6	N/A	No	4096	SPC/E	13
	"----//----"	2015	SC	SC	SC	see Fig. 6	N/A	No	4096	TIP5P	183
	"----//----"	2015	SC	SC	SC	see Fig. 6	N/A	No	4096	TIP3P	6

165	Tran et al.	2016	238	1.01325	0.09	Yes (Fig. 5)	Yes	512	SSMP	165
	"----//----"	2016	258	1.01325	0.53	Yes (Fig. 5)	Yes	512	SSMP	165
	"----//----"	2016	268	1.01325	0.85	Yes (Fig. 5)	Yes	512	SSMP	165
	"----//----"	2016	278	1.01325	1.22	Yes (Fig. 5)	Yes	512	SSMP	165
	"----//----"	2016	298	1.01325	2.24	Yes (Fig. 5)	Yes	512	SSMP	165
	"----//----"	2016	318	1.01325	3.49	Yes (Fig. 5)	Yes	512	SSMP	165
	"----//----"	2016	338	1.01325	4.95	Yes (Fig. 5)	Yes	512	SSMP	165
	"----//----"	2016	298	1.01325	2.60	Yes (Fig. 9)	Yes	512	TIP4P-Ew	75
	"----//----"	2016	298	506.625	2.66	Yes (Fig. 9)	Yes	512	TIP4P-Ew	75
	"----//----"	2016	298	1013.25	2.70	Yes (Fig. 9)	Yes	512	TIP4P-Ew	75
	"----//----"	2016	298	5066.25	2.57	Yes (Fig. 9)	Yes	512	TIP4P-Ew	75
	"----//----"	2016	298	10132.5	2.09	Yes (Fig. 9)	Yes	512	TIP4P-Ew	75
	"----//----"	2016	298	1.01325	2.24	Yes (Fig. 9)	Yes	512	SSMP	165
	"----//----"	2016	298	506.625	2.24	Yes (Fig. 9)	Yes	512	SSMP	165
	"----//----"	2016	298	1013.25	2.27	Yes (Fig. 9)	Yes	512	SSMP	165
	"----//----"	2016	298	5066.25	1.83	Yes (Fig. 9)	Yes	512	SSMP	165
	"----//----"	2016	298	10132.5	1.26	Yes (Fig. 9)	Yes	512	SSMP	165
167	Franco et al.	2016	288	1	2.05	Yes (Fig. 1)	No	1000	SPC/E	13
	"----//----"	2016	298	1	2.44	Yes (Fig. 1)	No	1000	SPC/E	13
	"----//----"	2016	308	1	3.02	Yes (Fig. 1)	No	1000	SPC/E	13
	"----//----"	2016	318	1	3.54	Yes (Fig. 1)	No	1000	SPC/E	13
	"----//----"	2016	329	1	4.26	Yes (Fig. 1)	No	1000	SPC/E	13
	"----//----"	2016	288	1	2.03	Yes (Fig. 1)	No	1000	SPC/E	13
	"----//----"	2016	298	1	2.49	Yes (Fig. 1)	No	1000	SPC/E	13
	"----//----"	2016	308	1	3.05	Yes (Fig. 1)	No	1000	SPC/E	13
	"----//----"	2016	318	1	3.65	Yes (Fig. 1)	No	1000	SPC/E	13
	"----//----"	2016	329	1	4.37	Yes (Fig. 1)	No	1000	SPC/E	13
166	Jiang et al.	2016	298.15	1	2.42	0.01	Yes	512	HBP	166

	"----//----"	2016	298.15	200	2.45	0.04	Yes	512	HBP	166
	"----//----"	2016	298.15	480	2.47	0.02	Yes	512	HBP	166
	"----//----"	2016	298.15	1000	2.55	0.04	Yes	512	HBP	166
	"----//----"	2016	373.15	15	7.74	0.01	Yes	512	HBP	166
	"----//----"	2016	373.15	200	7.32	0.04	Yes	512	HBP	166
	"----//----"	2016	373.15	480	7.52	0.02	Yes	512	HBP	166
	"----//----"	2016	373.15	1000	7.17	0.04	Yes	512	HBP	166
	"----//----"	2016	523.15	200	25.1	0.6	Yes	512	HBP	166
	"----//----"	2016	523.15	480	25.3	0.3	Yes	512	HBP	166
	"----//----"	2016	523.15	1000	24.2	0.6	Yes	512	HBP	166
	"----//----"	2016	298.15	1	2.04	0.05	Yes	512	BK3	136
	"----//----"	2016	298.15	200	1.91	0.06	Yes	512	BK3	136
	"----//----"	2016	298.15	480	1.93	0.05	Yes	512	BK3	136
	"----//----"	2016	298.15	1000	1.9	0.1	Yes	512	BK3	136
	"----//----"	2016	373.15	15	7.2	0.1	Yes	512	BK3	136
	"----//----"	2016	373.15	200	7.1	0.1	Yes	512	BK3	136
	"----//----"	2016	373.15	480	6.9	0.2	Yes	512	BK3	136
	"----//----"	2016	373.15	1000	6.8	0.2	Yes	512	BK3	136
	"----//----"	2016	523.15	200	28	2	Yes	512	BK3	136
	"----//----"	2016	523.15	480	24.8	0.08	Yes	512	BK3	136
	"----//----"	2016	523.15	1000	22.8	0.04	Yes	512	BK3	136
	"----//----"	2016	298.15	1	2.1	0.1	Yes	512	TIP4P/2005	80
	"----//----"	2016	373.15	15	7.5	0.1	Yes	512	TIP4P/2005	80
	"----//----"	2016	373.15	200	7.4	0.2	Yes	512	TIP4P/2005	80
	"----//----"	2016	373.15	480	7.4	0.2	Yes	512	TIP4P/2005	80
	"----//----"	2016	523.15	200	25.9	0.9	Yes	512	TIP4P/2005	80
	"----//----"	2016	523.15	480	24.9	0.8	Yes	512	TIP4P/2005	80
	"----//----"	2016	523.15	1000	22.7	0.5	Yes	512	TIP4P/2005	80
168	Ding et al.	2016	268	1.01325	1.38	No	No		ELBA	121

	"----//----"	2016	278	1.01325	1.65	No	No		ELBA	121
	"----//----"	2016	288	1.01325	1.89	No	No		ELBA	121
	"----//----"	2016	298	1.01325	2.21	No	No		ELBA	121
	"----//----"	2016	308	1.01325	2.50	No	No		ELBA	121
	"----//----"	2016	318	1.01325	2.77	No	No		ELBA	121
	"----//----"	2016	328	1.01325	3.13	No	No		ELBA	121
	"----//----"	2016	338	1.01325	3.47	No	No		ELBA	121
	"----//----"	2016	348	1.01325	3.81	No	No		ELBA	121
	"----//----"	2016	358	1.01325	4.32	No	No		ELBA	121
	"----//----"	2016	368	1.01325	4.66	No	No		ELBA	121
	"----//----"	2016	378	1.01325	5.17	No	No		ELBA	121
169	Koster et al.	2016	280	1	1.36	No	No	3000	TIP4P/2005	80
	"----//----"	2016	300	1	2.33	No	No	3000	TIP4P/2005	80
	"----//----"	2016	320	1	3.46	No	No	3000	TIP4P/2005	80
	"----//----"	2016	340	1	4.85	No	No	3000	TIP4P/2005	80
	"----//----"	2016	280	1	2.28	No	No	3000	TIP4P-TPSS	151
	"----//----"	2016	300	1	3.70	No	No	3000	TIP4P-TPSS	151
	"----//----"	2016	320	1	5.47	No	No	3000	TIP4P-TPSS	151
	"----//----"	2016	340	1	7.54	No	No	3000	TIP4P-TPSS	151
	"----//----"	2016	280	1	2.92	No	No	3000	TIP4P-TPSS-D3	151
	"----//----"	2016	300	1	4.37	No	No	3000	TIP4P-TPSS-D3	151
	"----//----"	2016	320	1	6.11	No	No	3000	TIP4P-TPSS-D3	151
	"----//----"	2016	340	1	8.11	No	No	3000	TIP4P-TPSS-D3	151
	"----//----"	2016	280	1	2.97	No	No	3000	Huang et al.	205
	"----//----"	2016	300	1	4.00	No	No	3000	Huang et al.	205
	"----//----"	2016	320	1	5.19	No	No	3000	Huang et al.	205
	"----//----"	2016	340	1	6.48	No	No	3000	Huang et al.	205

170	Dhabal et al.	2016	see Fig. 4a		see Fig. 4a	see Fig. 4a	N/A	No	4096	mW	106
171	Guillaud et al.	2017	228	1.01325		0.065	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	231	1.01325		0.077	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	234	1.01325		0.083	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	237	1.01325		0.13	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	240	1.01325		0.181	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	243	1.01325		0.211	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	246	1.01325		0.277	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	249	1.01325		0.327	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	252	1.01325		0.454	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	255	1.01325		0.443	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	258	1.01325		0.536	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	261	1.01325		0.644	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	264	1.01325		0.715	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	267	1.01325		0.836	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	270	1.01325		0.896	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	273	1.01325		1.094	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	276	1.01325		1.215	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	279	1.01325		1.384	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	282	1.01325		1.471	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	285	1.01325		1.55	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	288	1.01325		1.706	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	291	1.01325		1.927	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	294	1.01325		2.103	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	297	1.01325		2.216	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	300	1.01325		2.481	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	303	1.01325		2.683	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	306	1.01325		2.979	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	309	1.01325		2.903	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	312	1.01325		3.032	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	315	1.01325		3.485	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117

	"----//----"	2017	318	1.01325	3.704	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	321	1.01325	3.803	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	324	1.01325	4.149	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	327	1.01325	4.487	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	330	1.01325	4.566	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	333	1.01325	4.812	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	336	1.01325	5.026	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	339	1.01325	5.205	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	342	1.01325	5.629	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	345	1.01325	5.83	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	348	1.01325	6.25	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	351	1.01325	6.251	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	354	1.01325	6.474	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	357	1.01325	7.063	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	360	1.01325	7.378	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
173	Gabrieli et al.	2018	251.154734	1	0.5029	N/A	No	343	OPC	150
	"----//----"	2018	258.62069	1	0.7076	N/A	No	343	OPC	150
	"----//----"	2018	270.354257	1	1.0295	N/A	No	343	OPC	150
	"----//----"	2018	278.31094	1	1.2841	N/A	No	343	OPC	150
	"----//----"	2018	289.421158	1	1.7357	N/A	No	343	OPC	150
	"----//----"	2018	299.793246	1	2.1941	N/A	No	343	OPC	150
	"----//----"	2018	310.714286	1	2.7003	N/A	No	343	OPC	150
	"----//----"	2018	319.38326	1	3.1289	N/A	No	343	OPC	150
	"----//----"	2018	329.295988	1	3.6991	N/A	No	343	OPC	150
	"----//----"	2018	340.109461	1	4.4026	N/A	No	343	OPC	150
	"----//----"	2018	220.073598	1	0.0289	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	230.08449	1	0.0886	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	233.895706	1	0.1394	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	254.060808	1	0.4568	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	261.914985	1	0.7383	N/A	No	343	TIP4P-Ew	75

	"----//----"	2018	272.662256	1		1.1014	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	281.963576	1		1.4380	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	293.947571	1		2.0612	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	307.832055	1		2.7638	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	311.510571	1		2.8766	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	318.537859	1		3.5606	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	324.952056	1		3.6568	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	338.249972	1		4.7744	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	347.261756	1		5.5286	N/A	No	343	TIP4P-Ew	75
174	Handle & Sciortino	2018	270		0.90	5.87E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		0.94	7.51E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		0.98	8.60E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.02	9.85E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.06	1.13E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.10	1.13E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.14	1.16E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.18	1.04E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.22	9.29E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.26	7.79E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.30	6.53E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.34	4.79E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.38	3.43E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.42	1.97E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	250		0.90	1.18E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	250		0.94	2.21E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	250		0.98	3.23E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	250		1.02	4.62E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	250		1.06	5.29E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	250		1.10	5.66E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	250		1.14	5.93E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	250		1.18	5.55E-02	N/A	No	1000	TIP4P/2005	80

"----//----"	2018	250	1.22	5.09E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	250	1.26	4.27E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	250	1.30	3.13E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	250	1.34	2.24E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	250	1.38	1.23E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	250	1.42	6.46E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	0.90	4.33E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	0.94	9.67E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	0.98	1.73E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.02	2.83E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.06	3.54E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.10	3.79E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.14	3.71E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.18	3.72E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.22	3.26E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.26	2.56E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.30	1.87E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.34	1.29E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.38	6.75E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.42	2.59E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	0.90	1.09E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	0.94	3.63E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	0.98	8.86E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	1.02	1.48E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	1.06	2.07E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	1.10	2.43E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	1.14	2.43E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	1.18	2.28E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	1.22	2.13E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	1.26	1.53E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	1.30	1.10E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	1.34	6.44E-03	N/A	No	1000	TIP4P/2005	80

"----//----"	2018	230	1.38	2.71E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	0.90	1.79E-04	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	0.94	1.11E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	0.98	3.18E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.02	7.43E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.06	1.11E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.10	1.27E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.14	1.27E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.18	1.28E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.22	1.12E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.26	8.20E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.30	4.81E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.34	2.42E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.38	8.88E-04	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	0.94	2.92E-04	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	0.98	1.17E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	1.02	3.05E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	1.06	4.98E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	1.10	6.38E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	1.14	6.68E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	1.18	6.69E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	1.22	4.59E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	1.26	3.44E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	1.30	1.77E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	1.34	5.19E-04	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	200	0.98	2.86E-04	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	200	1.02	1.17E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	200	1.06	1.91E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	200	1.10	2.50E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	200	1.14	2.45E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	200	1.18	2.30E-03	N/A	No	1000	TIP4P/2005	80

"----//----"	2018	200	1.22	1.80E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	200	1.26	1.06E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	200	1.30	4.85E-04	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	200	1.34	7.31E-05	N/A	No	1000	TIP4P/2005	80

TABLE SI-3. Studies in which the self-diffusion coefficient of water confined by various materials has been calculated using MD simulations. D_{par} stands for the parallel component of the self-diffusion coefficient, D_{perp} stands for the perpendicular component of the self-diffusion coefficient, D_{eff} stands for the effective self-diffusion coefficient, D_{bulk} stands for the bulk self-diffusion coefficient, and η stands for viscosity.

	References	Year	Journal	vol.	First page	T / K	D_{par}	D_{perp}	D_{eff}	D_{bulk}	η	Confining material	H₂O force field	Method
1	Bellissent-Funel et al.	1995	*Phys. Rev. E*	51	4558	238-298	-	-	Yes	No	No	vycor glass	Lee & Rossky, 1994	EISF
2	Smirnov & Bougeard	1999	*J. Phys. Chem. B*	103	5266	300	-	-	Yes	Yes	No	kaolinite (clay)	SPC (Toukan & Rahman, 1985)	Green-Kubo
3	Spohr et al.	1999	*J. Mol. Liquids*	80	165	298	Yes	No	No	Yes	No	silica	SPC/E	Einstein
4	Ricci et al.	2000	*J. Phys. Condens. Matter*	12	A345	298	Yes	No	No	No	No	vycor glass	SPC/E	MSD
5	Martí & Gordillo	2002	*Chem. Phys. Lett.*	354	227	573, 673, 773	No	No	Yes	Yes	No	carbon nanotubes	Flex. SPC (Martí et al., 2004)	VACF
6	Beckstein & Samsom	2003	*Proc. Nac. Acad. Sci.*	100	7063	300	Yes	Yes	No	Yes	No	L-J	SPC	Einstein
7	Brovchenko et al.	2003	*Eur. Phys. J. E*	12	69	300 – 533	Yes	Yes	Yes	Yes	No	hydrophobic & hydrophilic cylinders	TIP4P	MSD
8	Marañón Di Leo & Marañón	2003	*J. Mol. Structure (Theochem)*	623	159	300	Yes	Yes	No	Yes	No	hydrophobic & hydrophilic nanotubes	SPC/E	MSD
9	Mashl et al.	2003	*Nano Lett.*	3	589	300	Yes	No	No	Yes	No	carbon nanotubes	SPC/E	MSD
10	Liu et al.	2004	*J. Phys. Chem. B*	108	6595	-	Yes	Yes	No	Yes	No	-	-	Liu et al. (2004)
11	Patsahan & Holovko	2004	*Condens. Matter Phys.*	7	3	300, 350	-	-	Yes	-	No	silica gel	SPC/E	Einstein
12	Zangi	2004	*J. Phys. Condens. Matter*	16	55388	300	Yes	No	No	Yes	No	quartz	TIP5P	Zangi, 2003
13	Jensen et al.	2004	*J. Chem. Phys.*	120	9729	300	Yes	No	No	Yes	No	hydrophobic & hydrophilic crystalline structures	TIP3	MSD
14	Choudhury & Pettitt	2005	*J. Phys. Chem. B*	109	6422	298	-	-	Yes	Yes	No	graphite	SPC/E	Green-Kubo/Einstein
15	Liu & Wang	2005	*Phys. Rev. B*	72	85420	298	Yes	Yes	No	Yes	Yes	single-walled carbon nanotube	SPC	Einstein
16	Sega et al.	2005	*Phys. Rev. E*	72	41201	333	Yes	Yes	-	-	No	GME ganglioside bilayers	SPC	Sega et al., 2005
17	Ju et al.	2005	*J. Chem. Phys.*	122	154707	400	Yes	Yes	No	No	No	Au plates	F3C	Green-Kubo
18	Cui	2005	*J. Chem. Phys.*	123	54706	298.15	Yes	Yes	No	Yes	No	cylindrical pores	TIP3P	Einstein
19	Kośmider et al.	2005	*Mat. Sci.-Poland*	23	475	233, 309, 344	No	No	Yes	Yes	No	single-walled carbon nanotube	flexible SPC	Green-Kubo
20	Kumar et al.	2005	*Phys. Rev. E*	72	51503	220-300	Yes	No	No	Yes	No	hydrophobic plates (paraffin)	TIP5P	Einstein
21	Martí et al.	2006	*J. Phys. Chem. B*	110	23987	298	Yes	Yes	-	Yes	No	highly oriented pyrolitc graphite	SPC	Green-Kubo/Einstein
22	Striolo	2006	*Nano Lett.*	6	633	298	Yes	-	-	No	No	carbon nanotubes	SPC/E	-

#	Author	Year	Journal	Vol	Page	T						Substrate	Water model	Method
23	Shirono & Daiguji	2006	*Chem. Phys. Lett.*	417	251	300	No	No	Yes	No	No	Na-LSX zeolites	SPC-FQ	MSD
24	Leng & Cummings	2006	*J. Chem. Phys.*	124	74711	298	No	No	Yes	Yes	No	mica	TIP4P	-
25	Hua et al.	2006	*J. Phys. Chem. B*	110	3704	-	No	Yes	No	Yes	No	BphC enzyme	SPC	Einstein
26	Hirunsit & Balbuena	2007	*J. Phys. Chem. C*	111	1709	298	-	-	Yes	-	No	graphite	SPC/E	Einstein
27	Prědota et al.	2007	*J. Phys. Chem. C*	111	3071	298, 448, 523	Yes	Yes	-	Yes	Yes	Rutile (a-TiO2)	SPC/E	Prědota et al. (2004)
28	Striolo	2007	*Nanotechnol.*	18	475704	300	Yes	-	-	No	No	carbon nanotubes	SPC/E	-
29	Porion et al.	2007	*J. Phys. Chem. C*	111	5441	298	No	No	Yes	No	No	natural clay (montmorillonite)	SPC	Einstein
30	Michot et al.	2007	*J. Phys. Chem. C*	111	9819	298	No	No	Yes	Yes	No	Na saponite clay	SPC	MSD
31	Gordillo & Martí	2007	*Phys. Rev. B*	75	85406	323-398	Yes	Yes	Yes	Yes	No	graphite	flexible SPC	VACF
32	Li et al.	2007	*Phys. Rev. B*	75	115415	300	No	No	Yes	Yes	Yes	mica, glass and graphite	SPC/E	-
33	Lane et al.	2008	*Langmuir*	24	5209	300	-	-	Yes	Yes	No	SAM layers of alkanethiol on Au	SPC/E	Einstein
34	Thomas & McGaughey	2008	*Nano Lett.*	8	2788	298	No	No	No	Yes	Yes	carbon nanotubes	TIP5P	Green-Kubo
35	Stanley et al.	2008	*AIP Conference Proceedings*	982	251	200-300	No	No	Yes	No	No	Protein and DNA	ST2, Jagla, TIP5P	MSD
36	Won & Aluru	2008	*J. Phys. Chem. C*	112	1812	300	Yes	No	No	Yes	No	boron nitride nanotube	SPC/E	Einstein
37	Kerisit & Liu	2009	*Environ. Sci. Technol.*	43	777	300	Yes	Yes	-	Yes	No	Feldspar	SPC/E	Einstein
38	Sendner et al.	2009	*Langmuir*	25	10768	300	No	Yes	-	Yes	Yes	diamond	SPC/E	Time correlation function
39	Zhang et al.	2009	*Mol. Sim.*	5	1215	298.15	-	-	Yes	Yes	No	amorphous silica	SPC/E	Einstein
40	Kumar et al.	2009	*J. Phys. Condens. Matter*	21	504108	220-300	Yes	Yes	No	Yes	No	solid paraffin	TIP5P	MSD
41	Di Napoli & Gamba	2009	*Physica B*	404	2883	300	Yes	No	No	Yes	No	Newton black films	TIP5P	MSD
42	Martí et al.	2009	*Phys. Rev. E*	79	31606	673	No	No	Yes	Yes	No	graphene	flexible SPC	VACF
43	Bonnaud et al.	2010	*J. Phys. Condens. Matter*	22	284110	300	Yes	Yes	No	Yes	No	hydroxylated silica	SPC	Einstein
44	Martí et al.	2010	*J. Mol. Liquids*	153	72	298-673	-	-	Yes	Yes	No	graphene	SPC	Green-Kubo
45	Park & Aluru	2010	*J. Phys. Chem. C*	114	2595	300	Yes	No	-	Yes	No	graphene	SPC/E	Einstein
46	Han et al.	2010	*Nature Phys.*	6	685	240, 250, 270, 300	Yes	No	No	No	No	hydrophobic plates	TIP5P	MSD
47	Farimani & Aluru	2011	*J. Phys. Chem. B*	115	12145	300	Yes	Yes	-	Yes	No	carbon nanotubes	SPC/E	Einstein
48	Lerbret et al.	2011	*Food Biophys.*	6	233	300	-	Yes	Yes	Yes	No	silica (cylindrical pores)	SPC/E	Einstein
49	Wei et al.	2011	*Fluid Phase Equilib.*	302	316	300	Yes	No	No	Yes	No	rutile (TiO2) and graphite	SPC/E	-
50	Boţan et al.	2011	*J. Phys. Chem. C*	115	16109	300	Yes	Yes	No	Yes	Yes	clay (montmorillonite)	SPC/E	Liu et al. (2004)
51	Nguyen & Bhatia	2012	*J. Phys. Chem. C*	116	3667	298	-	-	Yes	Yes	No	disordered carbons	SPC/E	-

#	Author	Year	Journal	Vol	Page	Temp						Material	Water model	Method
52	Zheng et al.	2012	*Phys. Chem. Chem. Phys.*	14	964	298, 325, 350	Yes	-	-	Yes	No	carbon nanotubes	TIP4P-EW	Einstein
53	Mosaddeghi et al.	2012	*J. Chem. Phys.*	137	184703	300	Yes	Yes	Yes	Yes	No	graphite plates	SPC/E	Green-Kubo/Einstein
54	Michot et al.	2012	*J. Phys. Chem. C*	116	16619	300	Yes	Yes	No	Yes	No	clay (synthetic saponite)	SPC/E	MSD/VACF
55	Bai & Zeng	2012	*PNAS*	109	21240	250	No	No	Yes	Yes	No	hydrophobic nanopore	TIP5P	-
56	Bauer et al.	2012	*Phys. Rev. E*	85	51506	300	Yes	Yes	Yes	Yes	No	hydrophobic plates	TIP3P, TIP4P, SPC/E, SWM4-NDP, TIP4P-FQ	Green-Kubo
57	Dickey & Stevens	2012	*Phys. Rev. E*	86	51601	300	Yes	No	No	Yes	No	SiO2	TIP4P/2005	Einstein
58	Choudhury	2013	*Chem. Phys.*	421	68	298	Yes	No	No	Yes	No	paraffin	SPC/E	Einstein
59	Sanghi & Aluru	2013	*J. Chem. Phys.*	138	124109	300	No	No	Yes	Yes	No	graphite	SPC/E	MSD
60	Solveyra et al.	2013	*J. Phys. Chem. C*	117	3330	300	Yes	No	Yes	Yes	No	TiO2	SPC/E	MSD (Lounnas et al. 1994)
61	Rao et al.	2013	*J. Phys. Chem. C*	117	14061	460	Yes	No	No	Yes	No	clay	SPC	MSD
62	Siboulet et al.	2013	*Mol. Phys.*	111	22	300	Yes	Yes	No	Yes	No	amorphous silica	SPC/E	Smoluchowski
63	Xu et al.	2013	*Nanotechnol.*	24	505504	300, 400, 600	Yes	No	No	Yes	No	graphene	SPC/F	MSD
64	Kim et al.	2013	*Scientific Reports*	3	2309	300	No	No	Yes	Yes	No	graphene and mica	SPC/E	Einstein
65	Silva	2014	*J. Nanostruct. Chem.*	4	104	300	Yes	-	-	Yes	No	carbon nanotubes	SPC/E	Einstein
66	Qomi et al.	2014	*J. Chem. Phys.*	140	54515	300	Yes	No	No	Yes	No	Calcium-silicate	SPC/E	Einstein
67	Ding et al.	2014	*J. Membr. Sci.*	458	236	300	No	No	Yes	Yes	No	polyamide RO membrane	TIP4P/2005	MSD
68	Ou et al.	2014	*J. Phys. Chem. C*	118	29887	300	Yes	Yes	Yes	Yes	No	Mg(OH)2	flexible SPC	Einstein
69	Boek	2014	*Mol. Phys.*	112	1472	298	No	No	Yes	Yes	No	clay (montmorillonite)	TIP4P	Einstein
70	Renou et al.	2014	*Mol. Phys.*	112	2275	300	Yes	No	Yes	Yes	No	silica (cylindrical pores)	TIP4P/2005	Einstein
71	Pham et al.	2015	*Theor. Chem. Acc.*	134	59	293-323	-	-	Yes	Yes	Yes	hydroxyapatite	Polarizable core-shell	Einstein
72	Yang et al.	2015	*Chin. J. Chem. Eng.*	23	1587	298.15	Yes	No	No	Yes	No	graphene	SPC/E	MSD
73	Kolokathis et al.	2015	*J. Phys. Chem. C*	119	20074	300	No	No	Yes	Yes	No	iron carboxylate sorbent	SPC/E	Einstein
74	Hou et al.	2015	*Microfluid Nanofluid*	19	1309	300	No	No	Yes	Yes	No	Calcium-silicate	-	Einstein
75	Chiavazzo et al.	2015	*Nature Comm.*	5	3565	300	No	No	Yes	Yes	No	protein, CNT, Fe3O4 & SiO2	SPC/E	Einstein
76	Hou et al.	2015	*Phys. Chem. Chem. Phys.*	17	1411	300	Yes	Yes	Yes	Yes	No	Calcium-silicate	ReaxFF	MSD
77	Diallo et al.	2015	*Phys. Rev. E*	91	22124	220-280	No	No	Yes	Yes	No	activated carbon fibers nanopores	SPC/E	EISF
78	Tahat & Martí	2015	*Phys. Rev. E*	92	32402	298	No	No		Yes	Yes	graphene	TIP3P	MSD
79	Hanot et al.	2016	*Nanoscale*	8	3314	300	-	-	Yes	No	No	ionic surfactant	SPC/E	Einstein
80	Ishikawa et al.	2016	*J. Mineral. Petrol. Sci.*	111	297	298-573	Yes	No	-	Yes	No	quartz	Kawamura, 2008	Green-Kubo

No.	Author	Year	Journal									Description	Model	Method
81	Muscatello et al.	2016	ACS Appl. Mater. Interfaces	8	12330	300	Yes	No	No	No	No	graphene membranes	SPC/E	Green-Kubo
82	Shahbabei & Kim	2016	Coll. & Surf. A	507	190	300	Yes	No	No	No	No	aquaporin-like pores	SPC/E	MSD
83	Chen et al.	2016	J. Phys. Chem. C	120	12924	300	Yes	No	No	No	No	layered double hydroxides	SPC	Einstein/jump model
84	Futera & English	2016	J. Phys. Chem. C	120	19603	300	Yes	No	No	Yes	No	TiO2	flexible SPC	Green-Kubo/Einstein
85	Yamashita & Daiguji	2016	Mol. Phys.	114	884	350	No	No	Yes	Yes	No	hydrophilic nanopores	ELBA	MSD
86	Zhou et al.	2016	Amer. Mineralog.	101	713	298	No	No	Yes	Yes	No	sepiolite (clay mineral)	ClayFF	MSD
87	Nie et al.	2016	Front. Phys.	11	114702	300	Yes	No	No	Yes	No	carbon nanochannels	SPC/E	-
88	Cao et al.	2016	J. Chem. Eng. Data	61	4131	300	Yes	No	No	Yes	No	TiO2 nanotubes & carbon nanotubes	SPC/E	-
89	Hou et al.	2016	Langmuir	32	4153	300 – 1500	No	No	Yes	Yes	No	Calcium-silicate	SPC/E	MSD
90	Köhler & Silva	2016	Chem. Phys. Lett.	645	38	300	Yes	No	No	Yes	Yes	carbon nanotubes	TIP4P/2005	MSD
91	McDonnell et al.	2016	J. Phys. Chem. B	120	8997	300	Yes	No	No	No	No	chitin/chitosan	TIP4P	MSD
92	Mozaffari	2016	Mol. Sim.	42	1475	285 – 390	Yes	No	No	Yes	No	graphene	SPC/E	Einstein
93	Ishikawa et al.	2017	Proc. Earth and Plan. Sci.	17	853	298-573	Yes	No	-	Yes	No	quartz	Kawamura, 2008	Green-Kubo
94	Prakash et al.	2017	Appl. Surf. Sci.	418	296	310	-	-	Yes	Yes	No	hydroxyapatite	CS and SPC/E	Einstein
95	Prakash et al.	2017	Phys. Chem. Miner.	44	509	310	Yes	Yes	-	Yes	No	hydroxyapatite	SPC/E	Green-Kubo
96	Zubeltzu & Artacho	2017	J. Chem. Phys.	147	194509	-	Yes	No	No	No	No	L-J parallel walls	TIP4P/2005	Einstein
97	Han et al.	2017	J. Phys. Chem. C	121	381	300	Yes	Yes	Yes	No	No	zeolites	TIP4P/Ew	Einstein
98	Mutisya et al.	2017	J. Phys. Chem. C	121	6674	300	Yes	No	Yes	Yes	No	calcite slit pore	SPC/Fw (Raiteri et al. 2010)	Liu et al. (2004)
99	Chen et al.	2017	J. Phys. Chem. C	121	23752	300-425	Yes	No	No	No	No	layered double hydroxides	SPC	Einstein/jump model
100	Köhler et al.	2017	Phys. Chem. Chem. Phys.	19	12921	300	Yes	No	No	No	Yes	hydrophobic & hydrophilic nanotubes	TIP4P/2005	Einstein
101	Li et al.	2017	Construction & Building materials	151	563	300	No	No	Yes	Yes	No	Calcium-silicate	ClayFF	MSD
102	Martí et al.	2017	Entropy	19	135	298	Yes	Yes	Yes	Yes	No	carbon nanotube & graphene	Martí & Gordillo, 2001	MSD
103	Sahu & Ali	2017	J. Chem. Eng. Data	62	2307	298-573	Yes	No	No	No	No	carbon nanotubes	SPC	MSD
104	Gavazzoni et al.	2017	J. Chem. Phys.	146	234509	173, 235, 293	Yes	No	No	Yes	No	AlPO4-54 nanotubes	TIP4P/2005	Einstein
105	Jeddi & Castrillón	2017	J. Phys. Chem. B	121	9666	301	Yes	No	No	Yes	No	silica	SPC/E	MSD
106	Bucior et al.	2017	Langmuir	33	11834	298	No	No	Yes	Yes	No	carbon nanotubes	TIP3P	Einstein
107	Jiao et al.	2017	Scientific Reports	7	2646	300	Yes	No	No	Yes	No	graphene	TIP4P/Ew, SPC/E	Einstein
108	Berrod et al.	2017	Scientific Reports	7	8326	-	No	No	Yes	No	No	ionomers and surfactant	Savage & Voth, 2014	MSD
109	Abbaspour et al.	2018	J. Mol. Liquids	250	26	300	-	-	Yes	No	No	graphene, graphite, boron nitride, silicon carbide	SPC/E	Einstein

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Water Force Fields

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