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Supporting Information

Development and Testing of the OPLS All-Atom Force Field on Conformational Energetics and Properties of Organic Liquids

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The following tables contain the available non-bonded and torsional parameters for the OPLS-AA force field. These and the bond-stretching and angle-bending parameters are available by ftp after contacting W. L. Jorgensen by email at bill@adrik.chem.yale.edu.

Form of the Force Field

Bond stretching: $$E_{bond} = \sum_{bonds} K_r (r - r_{eq})^2$$

Angle bending: $$E_{angle} = \sum_{angles} K_\theta (\theta - \theta_{eq})^2$$

Torsion: $$E(\phi) = \frac{V_1}{2}\left[1 + \cos(\phi + f1)\right] + \frac{V_2}{2}\left[1 - \cos(2\phi + f2)\right] + \frac{V_3}{2}\left[1 + \cos(3\phi + f3)\right]$$

Non-bonded: $$E_{ab} = \sum_{i}^{on\,a} \sum_{j}^{on\,b} [q_i q_j e^2 / r_{ij} + 4\varepsilon_{ij}(\sigma_{ij}^{12} / r_{ij}^{12} - \sigma_{ij}^{6} / r_{ij}^{6})] f_{ij}$$

f_{ij} = 0.5 if i, j are 1,4; otherwise, f_{ij} = 1.0

Table 1. OPLS-AA Non-Bonded Parameters for Hydrocarbons and Alcohols

atom or group	q, e⁻	σ, Å	ε, kcal mol^{-1}
C, CH_4	-0.240	3.500	0.066
C, RCH_3	-0.180	3.500	0.066
C, R_2CH_2	-0.120	3.500	0.066
C, R_3CH	-0.060	3.500	0.066
C, R_4C	0.000	3.500	0.066
H, RH, alkanes	0.060	2.500	0.030
C, Benzene	-0.115	3.550	0.070
H, Benzene	0.115	2.420	0.030
C, CH_3 of toluene	-0.065	3.500	0.066
C, CH_2 of ethyl benzene	-0.005	3.500	0.066
C, $R_2C=$	0.000	3.550	0.076
C, RHC=	-0.115	3.550	0.076
C, $H_2C=$	-0.230	3.550	0.076
H, HC=	0.115	2.420	0.030
O, ROH	-0.683	3.120	0.170
H(O), ROH	0.418	0.000	0.000
H(C), CH_3OH	0.040	2.500	0.030
C, CH_3OH and RCH_2OH	0.145	3.500	0.066
C, R_2CHOH	0.205	3.500	0.066
C, R_3COH	0.265	3.500	0.066
C, COH phenol	0.150	3.550	0.070
O, phenol	-0.585	3.070	0.170
H, phenol	0.435	0.000	0.000

Table 2. OPLS-AA Non-Bonded Parameters for Sulfur Compounds and Amines

atom or group	q, e⁻	σ, Å	ε, kcal mol^{-1}
S, RSH	-0.435	3.550	0.250
H(S), RSH	0.255	0.000	0.000
C, CH_3SH	0.000	3.500	0.066
C, RCH_2SH	0.060	3.500	0.066
C, R_2CHSH	0.120	3.500	0.066
C, R_3CSH	0.180	3.500	0.066
S, RSR	-0.435	3.550	0.250
C, CH_3SR	0.0375	3.500	0.066
C, RCH_2SR	0.0975	3.500	0.066
C, R_2CHSR	0.1575	3.500	0.066
C, R_3CSR	0.2175	3.500	0.066
S, RSSR	-0.2175	3.550	0.250
C, CH_3SSR	0.0375	3.500	0.066
C, RCH_2SSR	0.0975	3.500	0.066
C, R_2CHSSR	0.1575	3.500	0.066
C, R_3CSSR	0.2175	3.500	0.066
N, RNH_2	-0.900	3.250	0.170
H, RNH_2	0.350	0.000	0.000
C, CH_3NH_2	0.020	3.500	0.066
C, RCH_2NH_2	0.080	3.500	0.066
C, R_2CHNH_2	0.140	3.500	0.066
C, R_3CNH2	0.200	3.500	0.066

Table 3. OPLS-AA Non-Bonded Parameters for Ammonium Ions, Imidazoles, and Carboxylate Ions[a]

atom or group	q, e$^-$	σ, Å	ε, kcal mol^{-1}
N, RNH_3^+	-0.300	3.250	0.170
H, RNH_3^+	0.330	0.000	0.000
C, $CH_3NH_3^+$	0.130	3.500	0.066
C, $RCH_2NH_3^+$	0.190	3.500	0.066
C, $R_2CHNH_3^+$	0.250	3.500	0.066
C, $R_3CNH_3^+$	0.310	3.500	0.066
C, $C_{\varepsilon 1}$ in HID, HIE	0.295	3.550	0.070
C, $C_{\delta 2}$ in HID, C_γ in HIE	-0.015	3.550	0.070
C, C_γ in HID, $C_{\delta 2}$ in HIE	0.015	3.550	0.070
C, $C_{\varepsilon 1}$ in HIP	0.385	3.550	0.070
C, C_γ, $C_{\delta 2}$ in HIP	0.215	3.550	0.070
H, H on C_δ or C_ε in HID, HIE, HIP	0.115	2.420	0.030
N, N_δ in HID or N_ε in HIE	-0.570	3.250	0.170
H, H(N_δ) in HID or H(N_ε) in HIE	0.420	0.000	0.000
N, N_ε in HID or N_δ in HIE	-0.490	3.250	0.170
N, in HIP	-0.540	3.250	0.170
H(N), in HIP	0.460	0.000	0.000
C, CH_3- in 5-methylimidazole	-0.065	3.500	0.066
C, RCH_2- in 5-ethylimidazole	-0.005	3.500	0.066
C, $RCOO^-$	0.700	3.750	0.105
O, $RCOO^-$	-0.800	2.960	0.210
C, CH_3COO^-	-0.280	3.500	0.066
C, RCH_2COO^-	-0.220	3.500	0.066
C, R_2CHCOO^-	-0.160	3.500	0.066
C, R_3CCOO^-	-0.100	3.500	0.066

[a] HID, HIE, and HIP refer to unprotonated histidine (imidazole) with hydrogens on N_δ or N_ε, and protonated histidine (imidazole), respectively.

Table 4. OPLS-AA Non-Bonded Parameters for Guanidinium Ions, Tryptophan, and Amides[a]

atom or group	q, e⁻	σ, Å	ε, kcal mol⁻¹
N, NH_2 in guanidinium	-0.800	3.250	0.170
H, NH_2 in guanidinium	0.460	0.000	0.000
C, guanidinium	0.640	2.250	0.050
N, NHR in alkylguanidinium	-0.700	3.250	0.170
H, NHR in alkylguanidinium	0.440	0.000	0.000
C, CH_3 in methylguanidinium	0.200	3.500	0.066
C, CH_3 in ethylguanidinium (EG)	-0.110	3.500	0.066
C, $CH_2(\delta)$ in Arg, EG	0.190	3.500	0.066
C, $CH_2(\gamma)$ in Arg	-0.050	3.500	0.066
N, N_ε in Trp	-0.570	3.250	0.170
H, H_ε(N) in Trp	0.420	0.000	0.000
C, C_γ in Trp	0.075	3.550	0.070
C, $CH_{\delta,\varepsilon,\zeta,\eta}$ in Trp	-0.115	3.550	0.070
H, $H_{\delta,\varepsilon,\zeta,\eta}$ (C) in Trp	0.115	2.420	0.030
C, C_δ in Trp	-0.055	3.750	0.145
C, C_ε in Trp	0.130	3.750	0.145
C, C=O in amide	0.500	3.750	0.105
O, C=O in amide	-0.500	2.960	0.210
H, HCONRR'	0.000	2.420	0.015
N, 1° amide	-0.760	3.250	0.170
N, 2° amide	-0.500	3.250	0.170
N, 3° amide	-0.140	3.250	0.170
H(N), 1° amide	0.380	0.000	0.000
H(N), 2° amide	0.300	0.000	0.000
C, CH_3N- 2° amide	0.020	3.500	0.066
C, CH_3N- 3° amide	-0.110	3.500	0.066
C, R CH_2N - 3° amide (Cδ in Pro)	-0.050	3.500	0.066
C, R $_2$CHN - 3° amide (Cα in Pro)	0.010	3.500	0.066
C, $CH_2(\alpha)$ in Gly	0.080	3.500	0.066
C, CHR(α) in Ala	0.140	3.500	0.066

C, CRR'(α) in Aib	0.200	3.500	0.066

[a] R in RCONR'R" is neutral and uses alkane parameters.

Table 5. OPLS-AA Non-Bonded Parameters for Ethers, Acetals, Aldehydes, Ketones, and Carboxylic Acids.

Atom or group	q, e⁻	σ, Å	ε, kcal mol⁻¹
O, ROR	-0.400	2.900	0.140
C, CH_3OR	0.110	3.500	0.066
C, RCH_2OR	0.140	3.500	0.066
C, R_2CHOR	0.170	3.500	0.066
C, R_3COR	0.200	3.500	0.066
H, CH_nOR	0.030	2.500	0.030
O, acetal	-0.400	2.900	0.140
C, $ROCH_2OR$	0.200	3.500	0.066
H, $ROCH_2OR$	0.100	2.500	0.030
C, ROCHROR	0.300	3.500	0.066
H, ROCHROR	0.100	2.500	0.030
C, $ROCR_2OR$	0.400	3.500	0.066
C, RCHO	0.450	3.750	0.105
O, RCHO	-0.450	2.960	0.210
H, RCHO	0.000	2.420	0.015
C, R_2CO	0.470	3.750	0.105
O, R_2CO	-0.470	2.960	0.210
H, CH_nCOR[a]	0.060	2.420	0.015
C, RCOOH	0.520	3.750	0.105
O(C), RCOOH	-0.440	2.960	0.210
O(H), RCOOH	-0.530	3.000	0.170
H, RCOOH	0.450	0.000	0.000

[a] H on alpha C of aldehyde and ketone. Alpha C uses alkyl C parameters (Table 1).

Table 6. Bond Stretching and Angle Bending Parameters

	AMBER		CHARMM/22	
Type[a]	**r_{eq} or θ_{eq}**	**K**	**r_{eq} or θ_{eq}**	**K**
CT-CT	1.526	310.0	1.529	268.0
HC-CT	1.090	331.0	1.090	340.0
HC-CT-HC	109.5	35.00	107.8	33.00
HC-CT-CT	109.5	35.00	110.7	37.50
CT-CT-CT	109.5	40.00	112.7	58.35

[a] The AMBER atom types are from reference 3.

Table 7. OPLS-AA Fourier Coefficients (kcal/mol) for Torsional Energy Functions[a]

System	Dihedral	V_1	V_2	V_3
alkane	H-C-C-H	0.000	0.000	0.318
	H-C-C-C	0.000	0.000	0.366
	C-C-C-C	1.740	-0.157	0.279
alkene	H-C-C=C	0.000	0.000	-0.372
ethylbenzene	H-C-C_{ar}-C_{ar}	0.000	0.000	0.000
	C-C-C_{ar}-C_{ar}	0.000	0.000	0.000
	H-C-C-C_{ar}	0.000	0.000	0.462
alcohol	H-C-O-H	0.000	0.000	0.450
	C-C-O-H	-0.356	-0.174	0.492
	H-C-C-O	0.000	0.000	0.468
	C-C-C-O	1.711	-0.500	0.663
phenol	H-O-C_{ar}-C_{ar}	0.000	1.682	0.000
thiol	H-C-S-H	0.000	0.000	0.451
	C-C-S-H	-0.759	-0.282	0.603
	H-C-C-S	0.000	0.000	0.452
	C-C-C-S	1.876	0.000	0.000
sulfide	H-C-S-C	0.000	0.000	0.647
	C-C-C-S	2.619	-0.620	0.258
	C-C-S-C	0.925	-0.576	0.677
disulfide	C-S-S-C	0.000	-7.414	1.705
	H-C-S-S	0.000	0.000	0.558
	C-C-S-S	1.941	-0.836	0.935
1° amine	H-C-N-H	0.000	0.000	0.400
	H-C-C-N	-1.013	-0.709	0.473
	C-C-N-H	-0.190	-0.417	0.418
	C-C-C-N	2.392	-0.674	0.550
ammonium ion	H-C-N-H	0.000	0.000	0.261
	C-C-N-H	0.000	0.000	0.347
	H-C-C-N	0.000	0.000	0.384
	C-C-C-N	2.732	-0.229	0.485

[a] Those listed with $V_1=V_2=V_3=0$ are shown for completeness.

Table 8. OPLS-AA Fourier Coefficients (kcal/mol) for Torsional Energy Functions[a]

System	Dihedral	V_1	V_2	V_3
ether	H-C-O-C	0.000	0.000	0.760
	C-C-O-C	0.650	-0.250	0.670
acetal	C-O-C-O	-0.574	-0.997	0.000
carboxylate ion	H-C-C-O	0.000	0.000	0.000
	C-C-C-O	0.000	0.820	0.000
	H-C-C-C(O)	0.000	0.000	-0.225
	C-C-C-C(O)	-3.185	-0.825	0.493
carboxylic acid	O-C-O-H	0.000	4.830	0.000
	C-C-O-H	0.000	4.830	0.000
aldehyde/ketone	H-C-C-O	0.000	0.000	0.000
aldehyde	H-C-C(O)-H	0.000	0.000	0.360
ketone	H-C-C(O)-C	0.000	0.000	0.275
aldehyde/ketone	C-C-C-O	-0.277	1.228	-0.694
aldehyde	C-C-C(O)-H	0.000	0.000	0.000
ketone	C-C-C(O)-C	1.454	-0.144	-0.775
aldehyde/ketone	H-C-C-C(O)	0.000	0.000	-0.076
aldehyde/ketone	C-C-C-C(O)	-1.697	-0.456	0.585
amide	C(O)-N-C-H	0.000	0.000	-0.139
	C(O)-N-C-C	-1.396	-0.427	0.000
	H-N-C-H	0.000	0.000	0.000
	H-N-C-C	0.000	0.000	0.000
	N-C-C-H	0.000	0.000	0.464
	N-C-C-C	1.964	0.000	0.659
	H-C-C(O)-N	0.000	0.000	0.000
	H-C-C(O)-O	0.000	0.000	0.000
	C-C-C(O)-N	3.250	-0.402	-0.136
	C-C-C(O)-O	0.000	1.166	0.000
	H-C-C-C(O)	0.000	0.000	-0.100
	C-C-C-C(O)	-2.060	-0.313	0.315
	H-C-N3°-C	0.000	0.000	0.000
	H,C-C(O)-N-H	0.000	4.900	0.000

H,C-C(O)-N-C	2.800	6.089	0.000
O-C(O)-N-H	0.000	4.900	0.000
O-C(O)-N-C	0.000	6.089	0.000

[a] Those listed with $V_1=V_2=V_3=0$ are shown for completeness.

Table 9. OPLS-AA Fourier Coefficients (kcal/mol) for Torsional Energy Functions[a]

System	Dihedral	V_1	V_2	V_3
peptide[a] φ	C(O)-N-C-C(O)	-2.365	0.912	-0.850
peptide φ'	C(O)-N-C-C	0.000	0.462	0.000
peptide φ"	C(O)-N-C-H	0.000	0.000	0.000
peptide	H-N-Cα-X	0.000	0.000	0.000
peptide ψ	N-C-C(O)-N	1.816	1.222	1.581
peptide ψ'	C-C-C(O)-N	1.173	0.189	-1.200
peptide ψ"	H-C-C(O)-N	0.000	0.000	0.000
peptide	X-Cα-C(O)-O	0.000	0.000	0.000
peptide χ_1	N-C-C-C	0.845	-0.962	0.713
peptide χ_1	N-C-C-H	0.000	0.000	0.464
peptide χ_1	C(O)-C-C-H	0.000	0.000	-0.076
peptide χ_1[b]	C(O)-C-C-C	-1.697	-0.456	0.585
χ_1, Ser & Thr	N-C-C-O	6.280	-1.467	2.030
Ser & Thr	C(O)-C-C-O	-6.180	0.000	0.000
χ_1, Cys	N-C-C-S	0.583	-1.163	0.141
Cys	C(O)-C-C-S	-4.214	-2.114	0.969
5-ethylimidazole	H-C-C-N	0.000	0.000	0.419
	C-C-C-N	2.366	-0.262	0.505
3-ethylindole	H-C-C3-C2	0.000	0.000	-0.480
	H-C-C3-C	0.000	0.000	0.000
	C-C-C3-C2	-0.714	0.000	0.000
	C-C-C3-C	0.000	0.000	0.000
guanidinium ion	H-N-C-N	0.000	3.900	0.000
	C-N-C-N	0.000	7.936	0.000
	C-C-N-C	1.829	0.243	-0.498
	H-C-C-N	0.000	0.000	-0.582
	H-C-N-H	0.000	0.000	0.000

[a] The ϕ and ψ are used in the standard way. The " and ' denote dihedrals which extend to the C_α hydrogen and C_β carbon, respectively. [b] The remaining dihedral parameters for χ_1 with the C_α hydrogen are the same as for alkanes, alcohols, and thiols.