Examining Structure-Property Relationships in Lubricating Monolayer Films through Molecular Dynamics Screening

Andrew Z. Summers,[†,‡] Christopher R. Iacovella,[†,‡] Peter T. Cummings,[†,‡] and Clare McCabe[*,†,‡,¶]

†*Department of Chemical and Biomolecular Engineering, Vanderbilt University, Nashville, TN*

‡*Center for Multiscale Modeling and Simulation, Vanderbilt University, Nashville, TN*

¶*Department of Chemistry, Vanderbilt University, Nashville, TN*

E-mail: c.mccabe@vanderbilt.edu

Additional force field details

The OPLS force field uses the following contributions to the total potential:[1]

$$E_{\text{non-bonded}} = \sum_i \sum_{j>i} \left[\frac{q_i q_j e^2}{r_{ij}} + 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right] \right] \tag{1}$$

$$E_{\text{bond}} = \sum_{\text{bonds}} K_r (r - r_0)^2 \tag{2}$$

$$E_{\text{angle}} = \sum_{\text{angles}} K_\theta (\theta - \theta_0)^2 \tag{3}$$

$$E_{\text{torsion}} = \sum_{\text{torsions}} \frac{1}{2} \left[K_1(1 + \cos\phi) + K_2(1 - \cos 2\phi) + K_3(1 + \cos 3\phi) - K_4(1 - \cos 4\phi) \right] \tag{4}$$

where q_i and q_j are the partial charges on particles i and j, e is Coulomb's constant, r_{ij} is the inter-particle separation, ϵ and σ are interaction-specific Lennard-Jones parameters, K_r, K_θ, and $K_{1,2,3,4}$ are force constants, r_0 is the equilibrium bond distance, θ_0 is the equilibrium angle, and ϕ is the torsion angle.

For certain molecules, such as aromatics and alkenes, improper torsions are necessary to enforce planarity. The OPLS force field primarily utilizes improper parameters from the AMBER family of force fields, where

impropers have the following potential form:

$$E_{\text{impropers}} = \sum_{\text{impropers}} \frac{1}{2} K_\phi [1 + \cos(n\phi - \gamma)] \tag{5}$$

where ϕ is the torsion angle, K_ϕ is the force constant, n is the multiplicity, and γ is the phase angle.

OPLS uses geometric mixing rules for cross-interactions:

$$\sigma_{ij} = (\sigma_{ii}\sigma_{jj})^{\frac{1}{2}} \tag{6}$$

$$\epsilon_{ij} = (\epsilon_{ii}\epsilon_{jj})^{\frac{1}{2}} \tag{7}$$

Additionally, non-bonded interactions are excluded for particles separated by one or two bonds. For particles separated by three bonds, non-bonded interactions are scaled by 0.5.

Detailed below are the OPLS parameters utilized in this work. Parameters used for silica surfaces, silane headgroups, and alkane backbones are provided first. Parameters used for each of the sixteen terminal groups are provided next, where they have been separated by terminal group chemistry.

Silica Surfaces and Alkane Backbones

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_135	C	-0.18	0.35	0.066	1	-
opls_136	C	-0.12	0.35	0.066	1	-
opls_140	H	0.06	0.25	0.03	1	-
opls_1001	O	-0.43	0.3	0.17	2	-
opls_1002	Si	0.86	0.4	0.1	2	-
opls_1003	Si	0.745	0.4	0.1	2	-
opls_1004	C	-0.12	0.35	0.066	1	-
opls_1005	O	-0.683	0.312	0.17	1	-
opls_1006	H	0.418	0	0	1	-
opls_1007	O	-0.215	0.3	0.17	2	-
opls_1008	O	-0.215	0.3	0.17	2	-
opls_1009	H	0.215	0.0	0	n/a	1

[1] Parameters for hydroxyl surface caps on silica surfaces are not available in the OPLS force field. We have used the same σ and ϵ values as the standard OPLS hydroxyl parameters and use a charge of 0.215 to maintain charge neutrality in the system.

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_135-opls_136	C-C	268	0.1529	1	-
opls_135-opls_140	C-H	340	0.109	1	-
opls_136-opls_140	C-H	340	0.109	1	-
opls_136-opls_1004	C-C	268	0.1529	1	-
opls_1004-opls_140	C-H	340	0.109	1	-
opls_1004-opls_1003	C-Si	200	1.85	2	-
opls_1003-opls_1005	Si-O	300	1.65	2	-
opls_1005-opls_1006	O-H	553	0.945	1	-
opls_1003-opls_1007	Si-O	300	1.65	2	-
opls_1007-opls_1002	O-Si	300	1.65	2	-
opls_1001-opls_1002	O-Si	300	1.65	2	-
opls_1002-opls_1008	Si-O	300	1.65	2	-
opls_1008-opls_1009	O-H	553	0.945	1	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_135-opls_136-opls_136	C-C-C	58.35	112.7	1	-
opls_136-opls_136-opls_136	C-C-C	58.35	112.7	1	-
opls_136-opls_136-opls_1004	C-C-C	58.35	112.7	1	-
opls_140-opls_135-opls_140	H-C-H	33	107.8	1	-
opls_140-opls_136-opls_140	H-C-H	33	107.8	1	-
opls_140-opls_1004-opls_140	H-C-H	33	107.8	1	-
opls_140-opls_135-opls_136	H-C-C	37.5	110.7	1	-
opls_140-opls_136-opls_136	H-C-C	37.5	110.7	1	-
opls_140-opls_136-opls_1004	H-C-C	37.5	110.7	1	-
opls_136-opls_1004-opls_1003	C-C-Si	30.47	120	2	-
opls_140-opls_1004-opls_1003	H-C-Si	37.5	110.7	n/a	1
opls_1004-opls_1003-opls_1005	C-Si-O	60	100	2	-
opls_1004-opls_1003-opls_1007	C-Si-O	60	100	2	-
opls_1005-opls_1003-opls_1005	O-Si-O	60	110	2	-
opls_1005-opls_1003-opls_1007	O-Si-O	60	110	2	-
opls_1003-opls_1005-opls_1006	Si-O-H	23.7764	122.888	2	-
opls_1003-opls_1007-opls_1002	Si-O-Si	20	145	2	-
opls_1007-opls_1002-opls_1001	O-Si-O	60	110	2	-
opls_1002-opls_1001-opls_1002	Si-O-Si	20	145	2	-
opls_1001-opls_1002-opls_1001	O-Si-O	60	110	2	-
opls_1001-opls_1002-opls_1008	O-Si-O	60	110	2	-
opls_1002-opls_1008-opls_1009	Si-O-H	23.7764	122.888	2	-

[1] H-C-Si parameters do not exist in OPLS. In the work of Lorenz et al.[2] F-C-C angle parameters were also used for F-C-Si angles. Following this approach, H-C-C angle parameters have been used for H-C-Si angles.

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_135-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	3	-
opls_136-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	3	-
opls_136-opls_136-opls_136-opls_1004	C-C-C-C	1.3	-0.05	0.2	0.0	3	-
opls_140-opls_135-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	3	-
opls_140-opls_136-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	3	-
opls_140-opls_136-opls_136-opls_135	H-C-C-C	0.0	0.0	0.3	0.0	3	-
opls_140-opls_136-opls_136-opls_1004	H-C-C-C	0.0	0.0	0.3	0.0	3	-
opls_140-opls_1004-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	3	-
opls_140-opls_135-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	3	-
opls_140-opls_136-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	3	-
opls_140-opls_136-opls_1004-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	3	-
All torsions containing silicon	X-Si-X-X, Si-X-X-X	0	0	0	0	2	1

[1] Any torsion containing a silicon atom is treated as a null torsion.

Methyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_135	C	-0.18	0.35	0.066	1	-
opls_140	H	0.06	0.25	0.03	1	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_135-opls_136	C-C	268	0.1529	1	-
opls_135-opls_140	C-H	340	0.109	1	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_136-opls_136-opls_135	C-C-C	58.35	112.7	1	-
opls_136-opls_135-opls_140	C-C-H	37.5	110.7	1	-
opls_140-opls_135-opls_140	H-C-H	33	107.8	1	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_136-opls_136-opls_136-opls_135	C-C-C-C	1.3	-0.05	0.2	0.0	3	-
opls_136-opls_136-opls_135-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	3	-
opls_140-opls_136-opls_135-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	3	-

Acetyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_135	C	-0.18	0.35	0.066	1	-
opls_282	H	0.06	0.242	0.015	1	-
opls_280	C	0.47	0.375	0.105	1	-
opls_281	O	-0.47	0.296	0.21	1	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_135-opls_282	C-H	340	0.109	1	-
opls_135-opls_280	C-C	317	0.1522	4	-
opls_280-opls_281	C-O	570	0.1229	4	-
opls_280-opls_136	C-C	317	0.1522	4	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_282-opls_135-opls-282	H-C-H	33	107.8	1	-
opls_282-opls_135-opls_280	H-C-C	35	109.5	4	-
opls_135-opls_280-opls_281	C-C-O	80	120.4	4	-
opls_135-opls_280-opls_136	C-C-C	70	116.0	N/A	[1]
opls_281-opls_280-opls_136	O-C-C	80	120.4	4	-
opls_280-opls_136-opls_282	C-C-H	35	109.5	4	-
opls_280-opls_136-opls_136	C-C-C	63	111.1	4	-
opls_282-opls_136-opls_136	H-C-C	37.5	110.7	1	-
opls_136-opls_136-opls_140	C-C-H	37.5	110.7	1	-
opls_136-opls_136-opls_136	C-C-C	58.35	112.7	1	-

[1] No reference found. Parameters used from GROMACS *as is*.

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_282-opls_135-opls_280-opls_281	H-C-C-O	0.0	0.0	0.0	0.0	1	-
opls_282-opls_135-opls_280-opls_136	H-C-C-C	0.0	0.0	0.275	0.0	1	-
opls_135-opls_280-opls_136-opls_136	C-C-C-C	1.454	-0.144	-0.775	0.0	1	-
opls_135-opls_280-opls_136-opls_282	C-C-C-H	0.0	0.0	0.275	0.0	1	-
opls_281-opls_280-opls_136-opls_136	O-C-C-C	-0.277	1.228	-0.694	0.0	1	-
opls_281-opls_280-opls_136-opls_282	O-C-C-H	0.0	0.0	0.0	0.0	1	-
opls_280-opls_136-opls_136-opls_136	C-C-C-C	-1.697	-0.456	0.585	0.0	1	-
opls_280-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	-0.076	0.0	1	-
opls_282-opls_136-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	3	-
opls_282-opls_136-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	3	-

Improper parameters						
Improper	Elements	γ, degrees	K_ϕ, kcal/mol	n	Reference	Notes
opls_281-opls_280-opls_135-opls_136	O-C-C-C	180	21.0	2	4	-

Amino

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_909	H	0.36	0	0	5	-
opls_900	N	-0.9	0.33	0.17	5	-
opls_906	C	0.06	0.35	0.066	5	-
opls_911	H	0.06	0.25	0.015	5	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_909-opls_900	H-N	434	0.101	5	-
opls_900-opls_906	N-C	382	0.1448	5	-
opls_906-opls_911	C-H	340	0.109	5	-
opls_906-opls_136	C-C	268	0.1529	5	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_909-opls_900-opls_909	H-N-H	43.6	106.4	5	-
opls_909-opls_900-opls_906	H-N-C	35	109.5	5	-
opls_900-opls_906-opls_911	N-C-H	35	109.5	5	-
opls_900-opls_906-opls_136	N-C-C	56.2	109.47	5	-
opls_911-opls_906-opls-911	H-C-H	33	107.8	1	-
opls_911-opls_906-opls_136	H-C-C	37.5	110.7	1	-
opls_906-opls_136-opls_140	C-C-H	37.5	110.7	1	-
opls_906-opls_136-opls_136	C-C-C	58.35	112.7	1	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_909-opls_900-opls_906-opls_911	H-N-C-H	0.0	0.0	0.4	0.0	5	-
opls_909-opls_900-opls_906-opls_136	H-N-C-C	-0.19	-0.417	0.418	0.0	5	-
opls_900-opls_906-opls_136-opls_136	N-C-C-C	2.392	-0.674	0.55	0.0	5	-
opls_900-opls_906-opls_136-opls_140	N-C-C-H	-1.013	-0.709	0.473	0.0	5	-
opls_911-opls_906-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	3	-
opls_911-opls_906-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	3	-
opls_906-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	3	-
opls_906-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	3	-

Carboxyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_270	H	0.45	0	0	1	-
opls_268	O	-0.53	0.3	0.17	1	-
opls_267	C	0.52	0.375	0.105	1	-
opls_269	O	-0.44	0.296	0.21	1	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_270-opls_268	H-O	553	0.0945	4	-
opls_268-opls_267	O-C	450	0.1364	4	-
opls_267-opls_269	C-O	570	0.1229	4	-
opls_267-opls_136	C-C	317	0.1522	4	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_270-opls_268-opls_267	H-O-C	35	113	4	-
opls_268-opls_267-opls_269	O-C-O	80	121	6	-
opls_268-opls_267-opls_136	O-C-C	70	108	6	-
opls_269-opls_267-opls_136	O-C-C	80	120.4	4	-
opls_267-opls_136-opls_140	C-C-H	35	109.5	4	-
opls_267-opls_136-opls_136	C-C-C	63	111.1	4	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_270-opls_268-opls_267-opls_269	H-O-C-O	0.0	5.5	0.0	0.0	N/A	1
opls_270-opls_268-opls_267-opls_136	H-O-C-C	1.5	5.5	0.0	0.0	N/A	1
opls_268-opls_267-opls_136-opls_136	O-C-C-C	1.0	0.546	0.45	0.0	6	-
opls_268-opls_267-opls_136-opls_140	O-C-C-H	0.0	0.0	0.0	0.0	6	-
opls_269-opls_267-opls_136-opls_140	O-C-C-H	0.0	0.0	0.0	0.0	6	-
opls_269-opls_267-opls_136-opls_136	O-C-C-C	0.0	0.546	0.0	0.0	6	-
opls_269-opls_267-opls_136-opls_136	C-C-C-C	-2.06	-0.313	0.315	0.0	1	-
opls_267-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	-0.1	0.0	1	-

[1] No reference found. Parameters used from GROMACS *as is*.

Improper parameters						
Improper	Elements	γ, degrees	K_ϕ, kcal/mol	n	Reference	Notes
opls_269-opls_267-opls_268-opls_136	O-C-O-C	180	21.0	2	4	-

Nitrile

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_753	N	-0.56	0.32	0.17	3	-
opls_754	C	0.46	0.33	0.066	3	-
opls_756	C	-0.02	0.33	0.066	3	-
opls_759	H	0.06	0.25	0.15	3	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_753-opls_754	N-C	650	0.1157	3	-
opls_754-opls_756	C-C	385	0.1458	3	1
opls_756-opls_759	C-H	340	0.109	1	-
opls_756-opls_136	C-C	268	0.1529	1	-

[1] GROMACS parameters differ from the literature. Parameters from Ref. 3 have been used.

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_753-opls_754-opls_756	N-C-C	150	180	3	-
opls_754-opls_756-opls_759	C-C-H	35	108.5	3	-
opls_754-opls_756-opls_136	C-C-C	58.35	112.7	3	-
opls_759-opls_756-opls_759	H-C-H	33	107.8	1	-
opls_759-opls_756-opls_136	H-C-C	37.5	110.7	1	-
opls_756-opls_136-opls_140	C-C-H	37.5	110.7	1	-
opls_756-opls_136-opls_136	C-C-C	58.35	112.7	1	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_753-opls_754-opls_756-opls_136	N-C-C-C	0.0	0.0	0.0	0.0	3	-
opls_753-opls_754-opls_756-opls_759	N-C-C-H	0.0	0.0	0.0	0.0	3	-
opls_754-opls_756-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	1
opls_754-opls_756-opls_136-opls_140	C-C-C-H	0.0	0.0	0.366	0.0	3	-
opls_759-opls_756-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	3	-
opls_759-opls_756-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	3	-
opls_756-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	3	-
opls_756-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	3	-

[1] Parameters don't exist in GROMACS or the literature. Parameters for alkane C-C-C-C dihedrals have been used.

Cyclopropyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_140	H	0.06	0.25	0.03	N/A	1
opls_711	C	-0.12	0.35	0.066	N/A	1
opls_712	C	-0.06	0.35	0.066	N/A	1

[1] No reference found. Parameters used from GROMACS *as is*.

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_711-opls_140	C-H	340	0.1088	N/A	1
opls_711-opls_712	C-C	260	0.1509	N/A	1
opls_712-opls_140	C-H	340	0.1088	N/A	1
opls_712-opls_136	C-C	280	0.151	N/A	1

[1] No reference found. Parameters used from GROMACS *as is*.

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_140-opls_711-opls_140	H-C-H	35	114.3	N/A	1
opls_140-opls_711-opls_711	H-C-C	37.5	117.2	N/A	1
opls_140-opls_711-opls_712	H-C-C	37.5	117.2	N/A	1
opls_711-opls_711-opls_712	C-C-C	30	60	N/A	1
opls_711-opls_712-opls_711	C-C-C	30	60	N/A	1
opls_711-opls_711-opls_140	C-C-H	37.5	117.2	N/A	1
opls_711-opls_712-opls_140	C-C-H	37.5	117.2	N/A	1
opls_711-opls_712-opls_136	C-C-C	37.5	117.2	N/A	1
opls_140-opls_712-opls_136	H-C-C	35	114.3	N/A	1
opls_712-opls_136-opls_136	C-C-C	58.35	112.7	N/A	2
opls_712-opls_136-opls_140	C-C-H	37.5	110.7	N/A	1

[1] No reference found. Parameters used from GROMACS *as is*.
[2] Parameters not found in GROMACS or the literature. Alkane C-C-C parameters have been used.

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_140-opls_711-opls_711-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	N/A	1
opls_140-opls_711-opls_711-opls_712	H-C-C-C	0.0	0.0	0.3	0.0	N/A	1
opls_140-opls_711-opls_712-opls_711	H-C-C-C	0.0	0.0	0.3	0.0	N/A	1
opls_140-opls_711-opls_712-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	N/A	1
opls_140-opls_711-opls_712-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	N/A	1
opls_711-opls_711-opls_712-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	N/A	1
opls_711-opls_711-opls_712-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	1
opls_711-opls_712-opls_711-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	N/A	1
opls_711-opls_712-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	2
opls_711-opls_712-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	N/A	1
opls_140-opls_712-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	N/A	3
opls_140-opls_712-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	N/A	4
opls_712-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	2
opls_712-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	N/A	3

[1] No reference found. Parameters used from GROMACS *as is*.
[2] Parameters not found in GROMACS or the literature. Parameters for alkane C-C-C-C dihedrals have been used.
[3] Parameters not found in GROMACS or the literature. Parameters for alkane C-C-C-H dihedrals have been used.
[4] Parameters not found in GROMACS or the literature. Parameters for alkane H-C-C-H dihedrals have been used.

Vinyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_144	H	0.115	0.242	0.03	1	-
opls_143	C	-0.23	0.355	0.076	1	-
opls_142	C	-0.115	0.355	0.076	1	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_144-opls_143	C-H	340	0.108	4	-
opls_143-opls_142	C-C	549	0.134	4	-
opls_142-opls_144	C-H	340	0.108	4	-
opls_142-opls_136	C-C	317	0.151	4	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_144-opls_143-opls_144	H-C-H	35	117	N/A	1
opls_144-opls_143-opls_142	H-C-C	35	120	7	
opls_143-opls_142-opls_136	C-C-C	70	124	N/A	1
opls_143-opls_142-opls_144	C-C-H	35	120	7	
opls_144-opls_142-opls_136	H-C-C	35	117	N/A	1
opls_142-opls_136-opls_136	C-C-C	63	111.1	4	
opls_142-opls_136-opls_140	C-C-H	35	109.5	4	

[1] No reference found. Parameters used from GROMACS *as is*.

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_144-opls_143-opls_142-opls_136	H-C-C-C	0.0	14.0	0.0	0.0	N/A	1
opls_144-opls_143-opls_142-opls_144	H-C-C-H	0.0	14.0	0.0	0.0	N/A	1
opls_143-opls_142-opls_136-opls_136	C-C-C-C	0.346	0.405	-0.904	0.0	N/A	1
opls_143-opls_142-opls_136-opls_140	C-C-C-H	0.0	0.0	-0.372	0.0	1	-
opls_144-opls_142-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	N/A	2
opls_144-opls_142-opls_136-opls_140	H-C-C-H	0.0	0.0	0.318	0.0	N/A	1
opls_142-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	1
opls_142-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.366	0.0	N/A	1

[1] No reference found. Parameters used from GROMACS *as is*.
[2] Parameters not found in GROMACS or the literature. Parameters for alkane C-C-C-H dihedrals have been used.

Improper parameters						
Improper	Elements	γ, degrees	K_ϕ, kcal/mol	n	Reference	Notes
opls_142-opls_143-opls_144-opls_144	C-C-H-H	180	21.0	2	N/A	1
opls_143-opls_142-opls_144-opls_136	C-C-H-C	180	30.0	2	N/A	1

[1] No reference found. Parameters used from GROMACS *as is*.

Fluorophenyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_719	F	-0.22	0.285	0.061	8	-
opls_718	C	0.22	0.355	0.07	8	-
opls_145	C	-0.115	0.355	0.07	1	-
opls_146	H	0.115	0.242	0.03	1	-
opls_149	C	-0.005	0.35	0.066	1	-
opls_140	H	0.06	0.25	0.03	1	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_719-opls_718	F-C	420	0.1354	9	-
opls_718-opls_145	C-C	469	0.14	4	-
opls_145-opls_146	C-H	367	0.108	10	-
opls_145-opls_145	C-C	469	0.14	4	-
opls_145-opls_149	C-C	317	0.151	4	-
opls_149-opls_140	C-H	340	0.109	1	-
opls_149-opls_136	C-C	268	0.1529	1	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_719-opls_718-opls_145	F-C-C	80	120	9	-
opls_718-opls_145-opls_146	C-C-H	35	120	4	-
opls_718-opls_145-opls_145	C-C-C	63	120	5	-
opls_146-opls_145-opls_145	H-C-C	35	120	4	-
opls_145-opls_718-opls_145	C-C-C	63	120	5	-
opls_145-opls_145-opls_145	C-C-C	63	120	5	-
opls_145-opls_145-opls_149	C-C-C	70	120	4	-
opls_145-opls_149-opls_136	C-C-C	63	114	4	-
opls_145-opls_149-opls_140	C-C-H	35	109.5	4	-
opls_149-opls_136-opls_136	C-C-C	58.35	112.7	1	-
opls_149-opls_136-opls_140	C-C-H	37.5	110.7	1	-
opls_140-opls_149-opls_140	H-C-H	33	107.8	1	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_719-opls_718-opls_145-opls_145	F-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_719-opls_718-opls_145-opls_146	F-C-C-H	0.0	7.25	0.0	0.0	5	-
opls_718-opls_145-opls_145-opls_145	C-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_718-opls_145-opls_145-opls_146	C-C-C-H	0.0	7.25	0.0	0.0	5	-
opls_146-opls_145-opls_718-opls_145	H-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_146-opls_145-opls_145-opls_146	H-C-C-H	0.0	7.25	0.0	0.0	5	-
opls_146-opls_145-opls_145-opls_145	H-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_146-opls_145-opls_145-opls_149	H-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_145-opls_145-opls_145-opls_145	C-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_145-opls_145-opls_145-opls_149	C-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_145-opls_718-opls_145-opls_145	C-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_145-opls_145-opls_149-opls_136	C-C-C-C	0.0	0.0	0.0	0.0	1	-
opls_145-opls_145-opls_149-opls_140	C-C-C-H	0.0	0.0	0.0	0.0	1	-
opls_145-opls_149-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	1
opls_145-opls_149-opls_136-opls_140	C-C-C-H	0.0	0.0	0.462	0.0	1	-

[1] No reference found. Parameters used from GROMACS *as is*. GROMACS uses same parameters as alkane C-C-C-C.

Improper parameters						
Improper	Elements	γ, degrees	K_ϕ, kcal/mol	n	Reference	Notes
opls_719-opls_718-opls_145-opls_145	F-C-C-C	180	2.2	2	5	-
opls_146-opls_145-opls_718-opls_145	H-C-C-C	180	2.2	2	5	-
opls_146-opls_145-opls_145-opls_145	H-C-C-C	180	2.2	2	5	-
opls_149-opls_145-opls_145-opls_145	C-C-C-C	180	2.2	2	5	-

Hydroxyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_155	H	0.418	0	0	1	-
opls_154	O	-0.683	0.312	0.17	1	-
opls_157	C	0.145	0.35	0.066	1	-
opls_140	H	0.06	0.25	0.03	1	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_155-opls_154	H-O	553	0.0945	4	-
opls_154-opls_157	O-C	320	0.141	4	-
opls_157-opls_140	C-H	340	0.109	1	-
opls_157-opls_136	C-C	268	0.1529	1	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_155-opls_154-opls_157	H-O-C	55	108.5	4	-
opls_154-opls_157-opls_136	O-C-C	50	109.5	4	-
opls_154-opls_157-opls_140	O-C-H	35	109.5	4	-
opls_140-opls_157-opls_140	H-C-H	33	107.8	1	-
opls_140-opls_157-opls_136	H-C-C	37.5	110.7	1	-
opls_157-opls_136-opls_136	C-C-C	58.35	112.7	1	-
opls_157-opls_136-opls_140	C-C-H	37.5	110.7	1	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_155-opls_154-opls_157-opls_136	H-O-C-C	-0.356	-0.174	0.492	0.0	1	-
opls_155-opls_154-opls_157-opls_140	H-O-C-H	0.0	0.0	0.45	0.0	1	-
opls_154-opls_157-opls_136-opls_136	O-C-C-C	1.711	-0.5	0.663	0.0	1	-
opls_154-opls_157-opls_136-opls_140	O-C-C-H	0.0	0.0	0.468	0.0	1	-
opls_140-opls_157-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	3	-
opls_140-opls_157-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	3	-
opls_157-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	3	-
opls_157-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	3	-

Isopropyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_140	H	0.06	0.25	0.03	1	-
opls_135	C	-0.18	0.35	0.066	1	-
opls_137	C	-0.06	0.35	0.066	1	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_140-opls_135	H-C	340	0.109	1	-
opls_135-opls_137	C-C	268	0.1529	1	-
opls_137-opls_140	C-H	340	0.109	1	-
opls_137-opls_136	C-C	268	0.1529	1	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_140-opls_135-opls_140	H-C-H	33	107.8	1	-
opls_140-opls_135-opls_137	H-C-C	37.5	110.7	1	-
opls_135-opls_137-opls_135	C-C-C	58.35	112.7	1	-
opls_135-opls_137-opls_140	C-C-H	37.5	110.7	1	-
opls_135-opls_137-opls_136	C-C-C	58.35	112.7	1	-
opls_140-opls_137-opls_136	H-C-C	37.5	110.7	1	-
opls_137-opls_136-opls_136	C-C-C	58.35	112.7	1	-
opls_137-opls_136-opls_140	C-C-H	37.5	110.7	1	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_140-opls_135-opls_137-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	3	-
opls_140-opls_135-opls_137-opls_135	H-C-C-C	0.0	0.0	0.3	0.0	3	-
opls_140-opls_135-opls_137-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	3	-
opls_140-opls_137-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	3	-
opls_140-opls_137-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	3	-
opls_135-opls_137-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	3	-
opls_135-opls_137-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	3	-
opls_137-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	3	-
opls_137-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	3	-

Methoxy

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_185	H	0.03	0.25	0.03	1	-
opls_181	C	0.11	0.35	0.066	1	-
opls_180	O	-0.4	0.29	0.14	1	-
opls_182	C	0.14	0.35	0.066	1	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_185-opls_181	H-C	340	0.109	1	-
opls_181-opls_180	C-O	320	0.141	4	-
opls_180-opls_182	O-C	320	0.141	4	-
opls_182-opls_185	C-H	340	0.109	1	-
opls_182-opls_136	C-C	268	0.1529	1	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_185-opls_181-opls_185	H-C-H	33	107.8	1	-
opls_185-opls_181-opls_180	H-C-O	35	109.5	4	-
opls_181-opls_180-opls_182	C-O-C	60	109.5	4	-
opls_180-opls_182-opls_136	O-C-C	50	109.5	4	-
opls_180-opls_182-opls_185	O-C-H	35	109.5	4	-
opls_185-opls_182-opls_185	H-C-H	33	107.8	1	-
opls_185-opls_182-opls_136	H-C-C	37.5	110.7	1	-
opls_182-opls_136-opls_136	C-C-C	58.35	112.7	1	-
opls_182-opls_136-opls_140	C-C-H	37.5	110.7	1	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_185-opls_181-opls_180-opls_182	H-C-O-C	0.0	0.0	0.76	0.0	1	-
opls_181-opls_180-opls_182-opls_136	C-O-C-C	0.65	-0.25	0.67	0.0	1	-
opls_181-opls_180-opls_182-opls_185	C-O-C-H	0.0	0.0	0.76	0.0	1	-
opls_180-opls_182-opls_136-opls_136	O-C-C-C	1.711	-0.5	0.663	0.0	1	-
opls_180-opls_182-opls_136-opls_140	O-C-C-H	0.0	0.0	0.468	0.0	1	-
opls_185-opls_182-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	3	-
opls_185-opls_182-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	3	-
opls_182-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	3	-
opls_182-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	3	-

Nitro

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_761	O	-0.37	0.296	0.17	3	-
opls_760	N	0.54	0.325	0.12	3	-
opls_764	C	0.08	0.35	0.066	3	-
opls_763	H	0.06	0.25	0.015	3	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_761-opls_760	O-N	550	0.1225	3	-
opls_760-opls_764	N-C	375	0.149	3	-
opls_764-opls_763	C-H	340	0.109	1	-
opls_764-opls_136	C-C	268	0.1529	1	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_761-opls_760-opls_761	O-N-O	80	125	3	-
opls_761-opls_760-opls_764	O-N-C	80	117.5	3	-
opls_760-opls_764-opls_763	N-C-H	35	105	3	-
opls_760-opls_764-opls_136	N-C-C	63	111.1	3	-
opls_763-opls_764-opls_763	H-C-H	33	107.8	1	-
opls_763-opls_764-opls_136	H-C-C	37.5	110.7	1	-
opls_764-opls_136-opls_136	C-C-C	58.35	112.7	1	-
opls_764-opls_136-opls_140	C-C-H	37.5	110.7	1	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_761-opls_760-opls_764-opls_136	O-N-C-C	0.0	0.4	0.0	0.0	3	-
opls_761-opls_760-opls_764-opls_763	O-N-C-H	0.0	0.0	0.0	0.0	3	-
opls_760-opls_764-opls_136-opls_136	N-C-C-C	-1.54	-0.214	0.0	0.0	3	1
opls_760-opls_764-opls_136-opls_140	N-C-C-H	0.0	0.0	-0.225	0.0	3	-
opls_763-opls_764-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	3	-
opls_763-opls_764-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	3	-
opls_764-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	3	-
opls_764-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	3	-

[1] Parameters did not exist in GROMACS. Parameters from Ref. 3 have been used.

Nitrophenyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_761	O	-0.37	0.296	0.17	3	-
opls_767	N	0.65	0.325	0.12	3	-
opls_768	C	0.09	0.355	0.07	3	-
opls_145	C	-0.115	0.355	0.07	1	-
opls_146	H	0.115	0.242	0.03	1	-
opls_149	C	-0.005	0.35	0.066	1	-
opls_140	H	0.06	0.25	0.03	1	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_761-opls_767	O-N	550	0.1225	3	-
opls_767-opls_768	N-C	400	0.146	3	-
opls_768-opls_145	C-C	469	0.14	5	-
opls_145-opls_146	C-H	367	0.108	10	-
opls_145-opls_149	C-C	317	0.151	4	-
opls_149-opls_140	C-H	340	0.109	1	-
opls_149-opls_136	C-C	268	0.1529	1	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_761-opls_767-opls_761	O-N-O	80	125	3	-
opls_761-opls_767-opls_768	O-N-C	80	117.5	3	-
opls_767-opls_768-opls_145	N-C-C	85	120	3	-
opls_768-opls_145-opls_145	C-C-C	63	120	5	-
opls_768-opls_145-opls_146	C-C-H	35	120	4	-
opls_145-opls_768-opls_145	C-C-C	63	120	4	-
opls_146-opls_145-opls_768	H-C-C	35	120	4	-
opls_146-opls_145-opls_145	H-C-C	35	120	4	-
opls_145-opls_145-opls_145	C-C-C	63	120	5	-
opls_145-opls_145-opls_149	C-C-C	70	120	4	-
opls_145-opls_149-opls_136	C-C-C	63	114	4	-
opls_145-opls_149-opls_140	C-C-H	35	109.5	4	-
opls_140-opls_149-opls_140	H-C-H	33	107.8	1	-
opls_140-opls_149-opls_136	H-C-C	37.5	110.7	1	-
opls_149-opls_136-opls_136	C-C-C	58.35	112.7	1	-
opls_149-opls_136-opls_140	C-C-H	37.5	110.7	1	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_761-opls_767-opls_768-opls_145	O-N-C-C	0.0	1.15	0.0	0.0	3	-
opls_767-opls_768-opls_145-opls_145	N-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_767-opls_768-opls_145-opls_146	N-C-C-H	0.0	7.25	0.0	0.0	5	-
opls_768-opls_145-opls_145-opls_145	C-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_768-opls_145-opls_145-opls_146	C-C-C-H	0.0	7.25	0.0	0.0	5	-
opls_146-opls_145-opls_768-opls_145	H-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_146-opls_145-opls_145-opls_146	H-C-C-H	0.0	7.25	0.0	0.0	5	-
opls_146-opls_145-opls_145-opls_145	H-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_146-opls_145-opls_145-opls_149	H-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_145-opls_145-opls_145-opls_145	C-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_145-opls_145-opls_145-opls_149	C-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_145-opls_768-opls_145-opls_145	C-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_145-opls_145-opls_149-opls_136	C-C-C-C	0.0	0.0	0.0	0.0	1	-
opls_145-opls_145-opls_149-opls_140	C-C-C-H	0.0	0.0	0.0	0.0	1	-
opls_145-opls_149-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	1
opls_145-opls_149-opls_136-opls_140	C-C-C-H	0.0	0.0	0.462	0.0	1	-

[1] No reference found. Parameters used from GROMACS *as is*. GROMACS uses same parameters as alkane C-C-C-C.

Improper parameters						
Improper	Elements	γ, degrees	K_ϕ, kcal/mol	n	Reference	Notes
opls_767-opls_768-opls_145-opls_145	N-C-C-C	180	2.2	2	5	-
opls_146-opls_145-opls_768-opls_145	H-C-C-C	180	2.2	2	5	-
opls_146-opls_145-opls_145-opls_145	H-C-C-C	180	2.2	2	5	-
opls_149-opls_145-opls_145-opls_145	C-C-C-C	180	2.2	2	5	-

Perfluoromethyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_965	F	-0.12	0.295	0.053	11	-
opls_961	C	0.36	0.35	0.066	11	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_965-opls_961	F-C	367	0.1332	11	-
opls_961-opls_136	C-C	268	0.1529	11	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_965-opls_961-opls_965	F-C-F	77	109.1	11	-
opls_965-opls_961-opls_136	F-C-C	50	109.5	11	-
opls_961-opls_136-opls_136	C-C-C	58.35	112.7	1	-
opls_961-opls_136-opls_140	C-C-H	37.5	110.7	1	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_965-opls_961-opls_136-opls_136	F-C-C-C	0.0	0.0	0.463	0.0	12	1
opls_965-opls_961-opls_136-opls_140	F-C-C-H	0.0	0.0	0.29	0.0	12	1
opls_961-opls_136-opls_136-opls_136	C-C-C-C	0.104	-0.312	0.048	-0.083	12	1
opls_961-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.133	0.0	12	1

[1] These parameters are not in GROMACS, as the GROMACS parameters do not distinguish between dihedrals for fluorinated and hydrogenated carbons.

Phenyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_145	C	-0.115	0.355	0.07	1	-
opls_146	H	0.115	0.242	0.03	1	-
opls_149	C	-0.005	0.35	0.066	1	-
opls_140	H	0.06	0.25	0.03	1	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_146-opls_145	H-C	367	0.108	10	-
opls_145-opls_149	C-C	317	0.151	4	-
opls_149-opls_140	C-H	340	0.109	1	-
opls_149-opls_136	C-C	268	0.1529	1	-
opls_145-opls_145	C-C	469	0.14	4	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_146-opls_145-opls_145	H-C-C	35	120	4	-
opls_145-opls_145-opls_145	C-C-C	63	120	5	-
opls_145-opls_145-opls_149	C-C-C	70	120	4	-
opls_145-opls_149-opls_136	C-C-C	63	114	4	-
opls_145-opls_149-opls_140	C-C-H	35	109.5	4	-
opls_140-opls_149-opls_140	H-C-H	33	107.8	1	-
opls_140-opls_149-opls_136	H-C-C	37.5	110.7	1	-
opls_149-opls_136-opls_136	C-C-C	58.35	112.7	1	-
opls_149-opls_136-opls_140	C-C-H	37.5	110.7	1	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_146-opls_145-opls_145-opls_146	H-C-C-H	0.0	7.25	0.0	0.0	5	-
opls_146-opls_145-opls_145-opls_145	H-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_146-opls_145-opls_145-opls_149	H-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_145-opls_145-opls_145-opls_145	C-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_145-opls_145-opls_145-opls_149	C-C-C-C	0.0	7.25	0.0	0.0	5	-
opls_145-opls_145-opls_149-opls_136	C-C-C-C	0.0	0.0	0.0	0.0	1	-
opls_145-opls_145-opls_149-opls_140	C-C-C-H	0.0	0.0	0.0	0.0	1	-
opls_145-opls_149-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	1
opls_145-opls_149-opls_136-opls_140	C-C-C-H	0.0	0.0	0.462	0.0	1	-

[1] No reference found. Parameters used from GROMACS *as is*. GROMACS uses same parameters as alkane C-C-C-C.

Improper parameters						
Improper	Elements	γ, degrees	K_ϕ, kcal/mol	n	Reference	Notes
opls_146-opls_145-opls_145-opls_145	H-C-C-C	180	2.2	2	5	-
opls_149-opls_145-opls_145-opls_145	C-C-C-C	180	2.2	2	5	-

Pyrrole

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_547	H	0.118	0.242	0.03	10	-
opls_546	H	0.155	0.242	0.03	10	-
opls_544	C	-0.149	0.355	0.07	10	-
opls_543	C	-0.163	0.355	0.07	10	-
opls_542	N	-0.239	0.325	0.17	10	-
opls_545	H	0.317	0	0	10	-
opls_679	C	0.035	0.35	0.066	N/A	1
opls_140	H	0.06	0.25	0.03	1	-

[1] No reference found. Parameters used from GROMACS *as is*.

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_547-opls_544	H-C	367	0.108	10	-
opls_544-opls_543	C-C	546	0.1367	10	-
opls_546-opls_543	H-C	367	0.108	10	-
opls_543-opls_542	C-N	427	0.1381	10	-
opls_542-opls_545	N-H	434	0.101	10	-
opls_544-opls_544	C-C	469	0.1424	10	-
opls_543-opls_679	C-C	317	0.1504	N/A	1
opls_679-opls_140	C-H	340	0.109	1	-
opls_679-opls_136	C-C	268	0.1529	1	-

[1] No reference found. Parameters used from GROMACS *as is*.

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_546-opls_543-opls_544	H-C-C	35	132.1	10	-
opls_546-opls_543-opls_542	H-C-N	35	121.6	10	-
opls_543-opls_544-opls_547	C-C-H	35	125.7	10	-
opls_543-opls_544-opls_544	C-C-C	70	107.3	10	-
opls_543-opls_542-opls_545	C-N-H	35	120	10	-
opls_543-opls_542-opls_543	C-N-C	70	109.8	10	-
opls_547-opls_544-opls_544	H-C-C	35	127.5	10	-
opls_545-opls_542-opls_543	H-N-C	35	120	10	-
opls_542-opls_543-opls_544	N-C-C	70	107.7	10	-
opls_542-opls_543-opls_679	N-C-C	70	121.6	N/A	1
opls_544-opls_543-opls_679	C-C-C	70	132.1	N/A	1
opls_543-opls_679-opls_136	C-C-C	63	114	N/A	1
opls_543-opls_679-opls_140	C-C-H	35	109.5	N/A	1
opls_140-opls_679-opls_140	H-C-H	33	107.8	1	-
opls_140-opls_679-opls_136	H-C-C	37.5	110.7	1	-
opls_679-opls_136-opls_136	C-C-C	58.35	112.7	1	-
opls_679-opls_136-opls_140	C-C-H	37.5	110.7	1	-

[1] No reference found. Parameters used from GROMACS *as is*.

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_546-opls_543-opls_544-opls_547	H-C-C-H	0.0	7.25	0.0	0.0	N/A	1
opls_546-opls_543-opls_544-opls_544	H-C-C-C	0.0	7.25	0.0	0.0	N/A	1
opls_546-opls_543-opls_542-opls_545	H-C-N-H	0.0	3.0	0.0	0.0	N/A	1
opls_546-opls_543-opls_542-opls_543	H-C-N-C	0.0	3.2	0.0	0.0	N/A	1
opls_543-opls_544-opls_544-opls_543	C-C-C-C	0.0	7.25	0.0	0.0	N/A	1
opls_543-opls_544-opls_544-opls_547	C-C-C-H	0.0	7.25	0.0	0.0	N/A	1
opls_543-opls_542-opls_543-opls_544	C-N-C-C	0.0	3.2	0.0	0.0	N/A	1
opls_543-opls_542-opls_543-opls_679	C-N-C-C	0.0	3.2	0.0	0.0	N/A	1
opls_544-opls_543-opls_542-opls_543	C-C-N-C	0.0	3.2	0.0	0.0	N/A	1
opls_544-opls_543-opls_542-opls_545	C-C-N-H	0.0	3.2	0.0	0.0	N/A	1
opls_544-opls_544-opls_543-opls_542	C-C-C-N	0.0	7.25	0.0	0.0	N/A	1
opls_544-opls_544-opls_543-opls_679	C-C-C-C	0.0	7.25	0.0	0.0	N/A	1
opls_547-opls_544-opls_543-opls_542	H-C-C-N	0.0	7.25	0.0	0.0	N/A	1
opls_545-opls_542-opls_543-opls_679	H-N-C-C	0.0	3.2	0.0	0.0	N/A	1
opls_542-opls_543-opls_679-opls_136	N-C-C-C	1.7	-0.6	0.0	0.0	N/A	1
opls_542-opls_543-opls_679-opls_140	N-C-C-H	0.0	0.0	0.42	0.0	N/A	1
opls_547-opls_544-opls_543-opls_679	H-C-C-C	0.0	7.25	0.0	0.0	N/A	1
opls_544-opls_543-opls_679-opls_136	C-C-C-C	0.0	0.0	0.0	0.0	N/A	1
opls_544-opls_543-opls_679-opls_140	C-C-C-H	0.0	0.0	0.0	0.0	N/A	1
opls_543-opls_679-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	2
opls_543-opls_679-opls_136-opls_140	C-C-C-H	0.0	0.0	0.462	0.0	N/A	1
opls_140-opls_679-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	N/A	1
opls_140-opls_679-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	N/A	1
opls_679-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	1
opls_679-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	N/A	1

[1] No reference found. Parameters used from GROMACS *as is*.
[2] Parameters don't exist in GROMACS or the literature. Parameters for C(aromatic)-C-C-C dihedrals have been used.

Improper parameters						
Improper	Elements	γ, degrees	K_ϕ, kcal/mol	n	Reference	Notes
opls_546-opls_543-opls_542-opls_544	H-C-N-C	180	2.2	2	5	-
opls_547-opls_544-opls_543-opls_544	H-C-C-C	180	2.2	2	5	-
opls_679-opls_543-opls_542-opls_544	C-C-N-C	180	2.2	2	5	-
opls_545-opls_542-opls_543-opls_543	H-N-C-C	180	2.0	2	4	-

Additional details on molecular descriptors

Molecular descriptor	Description	Category
Approximate Surface Area	Approximation of molecular surface area using the approach defined by Labute[13]	Size
Asphericity	Measure of molecular shape (from Baumgartner[14]); $A = 0$ for spherical shape, $A = 1$ for highly prolate shapes, and $A = 0.25$ for oblate shapes	Shape
Balaban J	Related to connectivity, degree of branching[15]	Complexity
Bertz C_T	Measure of molecular complexity through connectivity[16]	Complexity
Chi0, Chi1	Connectivity indices[17]	Complexity
Chi0n - Chi4n	Connectivity indices over various molecular fragments (0=atoms, 1=one bond fragments, 2=two bond fragments, etc.)[17]	Complexity
Chi0v - Chi4v	Valence connectivity indices (0=atoms, 1=one bond fragments, 2=two bond fragments, etc.)[17]	Complexity
Eccentricity	Shape descriptor calculated from the inertia matrix (0=spherical, 1=linear), from Arteca[18]	Shape
Hall-Kier alpha	Modifying term for kappa descriptors, related to shape/flexibility[19]	Shape
Hall-Kier kappa1	Alpha-modified topological shape descriptor; related to complexity/number of cycles (rings) in the bond graph[19]	Shape
Hall-Kier kappa2	Alpha-modified topological shape descriptor; related to degree of star-like bond graph vs. linearity[19]	Shape
Hall-Kier kappa3	Alpha-modified topological shape descriptor; related to "centrality" of branching[19]	Shape
Hydrogen bond factor	Developed in this work; related to ability for formation of inter-monolayer hydrogen bonds	Charge distribution, Misc.
IPC	Complexity/connectivity descriptor estimated from adjacency matrix of bond graph[20]	Complexity

Molecular descriptor	Description	Category
Inertial shape factor	Characterization of molecular shape from principal moments of inertia ($pm_2/(pm_1 * pm_3)$, where pm1-3 are the three principal moments), from Todeschini and Consoni [19]	Shape
logP	Octanol - water partition coefficient estimated through the method of Wildman and Crippen; [21] measure of hydrophobicity	Charge distribution/Misc.
Molar refractivity	Estimation of molecular polarizability; calculated through the method of Wildman and Crippen [21]	Size
Molecular weight	-	Size
Molecular weight (heavy atoms)	Molecular weight excluding hydrogens	Size
Normalized principal moments ratios (NPR1, NPR2)	Used to characterize molecular shape, from Sauer and Schwarz [22]	Shape
Number of heavy atoms	Number of non-hydrogen atoms	Size
Number of rotatable bonds	-	Size/Shape
Number of valence electrons	-	Size
Plane of best fit	Measure of molecular planarity (0=planar, increasing with less planarity) [23]	Shape
Principal moments of inertia (PMI1, PMI2, PMI3)	Three principal moments of inertia for the molecule (1=smallest, 3=largest)	Shape
Radius of gyration	(From Arteca [18]) Characterizes molecular shape, specifically elongation	Shape/Size
Spherocity	Measure of molecular shape (0=spherical, 1=flat), from Robinson et al. [24]	Shape
Topological polar surface area	Estimation of surface area of only polar atoms, from Ertl et al. [25]	Charge distribution

Molecular descriptor	Description	Category
Total hydrophobic VSA	Sum of SA contributions from atoms with $-0.20 \leq q < 0.20$	Charge distribution
Total negative van der Waals surface area (VSA)	Sum of SA contributions from atoms with $q < 0.0$	Charge distribution
Total negative polar VSA	Sum of SA contributions from atoms with $q < -0.20$	Charge distribution
Total polar VSA	Sum of SA contributions from atoms with $\|q\| > 0.20$	Charge distribution
Total positive VSA	Sum of SA contributions from atoms with $q > 0.0$	Charge distribution
Total positive polar VSA	Sum of SA contributions from atoms with $q \geq 0.20$	Charge distribution
Fractional hydrophobic VSA	Total hydrophobic VSA / Total VSA	Charge distribution
Fractional negative VSA	Total negative VSA / Total VSA	Charge distribution
Fractional negative polar VSA	Total negative polar VSA / Total VSA	Charge distribution
Fractional polar VSA	Total polar VSA / Total VSA	Charge distribution
Fractional positive VSA	Total positive VSA / Total VSA	Charge distribution
Fractional positive polar VSA	Total positive polar VSA / Total VSA	Charge distribution

Mean-based estimation of chemically-dissimilar tribology

As an initial attempt at exploring how the mixing of monolayer chemistries alters tribological response, the COF and adhesion of chemically-dissimilar monolayers was predicted from the results calculated for chemically-identical systems using a simple arithmetic mean. For example, the COF and adhesion of a "hydroxyl-methyl" system is estimated by taking the average of the COF and adhesion calculated for the "hydroxyl-hydroxyl" and "methyl-methyl" systems. If the estimation over-predicts the actual value, that would suggest that the mixing of monolayer chemistries provides an advantageous route to improving monolayer tribological performance. The actual vs. expected values for both COF and adhesion using this ap-

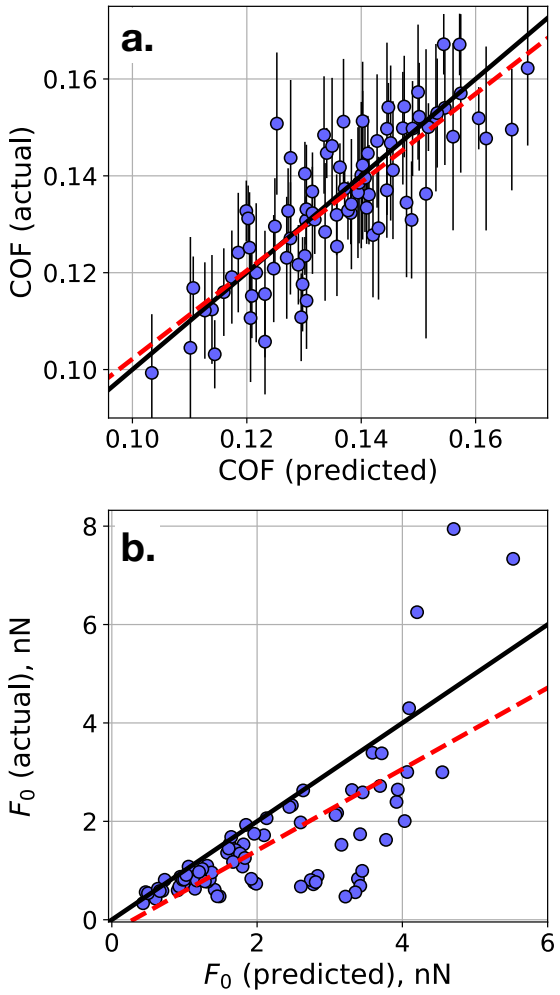

Figure S1: Predicted values of a. COF and b. adhesive force for chemically-dissimilar monolayer systems, as calculated by the mean of the values obtained for chemically identical systems, compared to the actual values. The y=x line is drawn in black for reference, while the dashed red line represents a linear regression of the data. Each unique surface chemistry (averaged over five monolayer surface configurations) is represented by a single point, and errors bars represent a single standard deviation calculated from the estimation of these five configurations.

proach are shown in Fig. S1. Interestingly, from Fig. S1a it is observed that the COF of chemically-dissimilar systems is reasonably-approximated by the averaging of values from the chemically-identical systems, as the COF of nearly all chemically-dissimilar systems is predicted correctly within error of the measurement.

Conversely, Fig. S1b shows that the force of adhesion is not well predicted by this approach. It appears that if one monolayer in a system is terminated by a polar functional group and the other is terminated by a nonpolar functional group, the adhesive force will be most similar to that of the pure nonpolar system, rather than an average of the two. As a result, when predicting the adhesive force for chemically-dissimilar systems featuring a mixture of polar and nonpolar groups using mean data from chemically-identical systems, adhesion values are over-estimated, as evidenced by the high concentration of points below the y=x line in Fig. S1b.

Details on construction of silica surfaces

Silica surfaces are carved from an amorphous silica bulk, as in our previous work.[26] Bulk silica was generated by putting a stoichiometric ratio of Si and O into a 5nm x 5nm x 5nm box at a density of 2.2g/mL. The procedure of Litton and Garofalini[27] was then followed, whereby the system was heated to 10000K, followed by a step-wise annealing through intermediate temperatures of 8000, 6000, 4000, 3000, 2000, and 1000K before ending at 300K. The ReaxFF force field[28] was used to model silicaon and oxygen bonding, and parameters from Fogarty et al. were used.[29] Surfaces were then carved from the amorphous silica bulk using an analytical approach to achieve a hydroxyl density of 5 OH/nm^2 by bridging neighboring surface oxygens,[30,31] using the mBuild package.[32,33] This approach yields amorphous silica surfaces that lack in-plane attachment site order (which is not the case for crystalline surface models) and feature an atomic scale surface roughness of roughly 0.11nm, similar to values obtained in previous work using synthesis mimetic simulations to mimic the "piranha" treatment of surfaces typical in experiment.[34]

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