The PLAFF3 Potential and Parameter Set

This document details the form used in PLAFF3, as described in the manuscript “Development of force field parameters for molecular simulation of polylactide” by J.H. McAliley and D.A. Bruce. The force field originated from OPLS as distributed with GROMACS, with added (CHARMM-style) CMAP interactions for reproducing DFT data on the energetic barriers to torsional rotation in PLA.

Overview

Atom Types and Bond Types

Usage of atom types and bond types in PLAFF3 follows the conventions used in GROMACS. In this document, we reference atom types using the symbol Γ, and bond types using the symbol Π. An atom with index i is assigned an atom type Γ_i, and its bond type is determined as a function of its atom type. Thus, $\Pi_i = f(\Gamma_i)$. The following type definitions are used to construct PLA molecules.

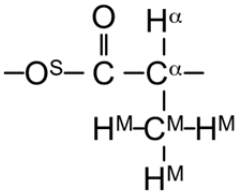
Atom Type, Γ	Bond Type, Π	Mass, m (a.u.)
opls_135	CT	12.011
opls_140	HC	1.008
opls_154	OH	15.9994
opls_155	HO	1.008
opls_180	OS	15.9994
opls_181	CT	12.011
opls_185	HC	1.008
opls_267	C	12.011
opls_268	OH	15.9994
opls_269	O_3	15.9994
opls_270	HO	1.008
opls_282	HC	1.008
opls_465	C_2	12.011
opls_466	O_2	15.9994
opls_467	OS	15.9994
opls_467a	OS	15.9994
opls_468	CT	12.011
opls_469	HC	1.008
opls_491	CT	12.011
opls_491a	CT	12.011

All force field parameters in PLAFF3 are defined as functions of the atom types or bond types of the participating atoms. In the following sections, these are shown using the notation $x_i = f(\Gamma_i)$ or $y_i = f(\Pi_i)$, for example, if x_i is defined by the atom type of i and y_i is defined by the bond type of i.

Residues

The above atom types are arranged as follows in the PLA repeat unit, or residue. The residue has one chiral center, at the α-carbon position. **Note that the tabulated dihedral potentials in PLAFF3 are asymmetric; hence, the proper potential terms must be selected depending on whether the residue has a stereoconfiguration of *R* (dextrorotary, as in PD-LA) or *S* (levorotary, as in PL-LA)**. Additionally, end-group residues are provided as used in parameter fitting.

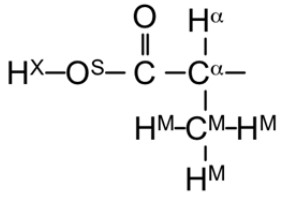
Repeat Unit Residue



Atom	*Γ*
O^S	opls_467a
C	opls_465
C^α	opls_491a
H^α	opls_282

Atom	*Γ*
O	opls_466
C^M	opls_135
H^M	opls_140

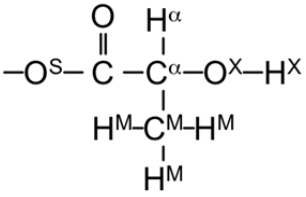
Acid-terminated Residue



Atom	*Γ*
O^S	opls_268
C	opls_267
C^α	opls_491a
H^α	opls_282

Atom	*Γ*
O	opls_269
C^M	opls_135
H^M	opls_140
H^X	opls_270

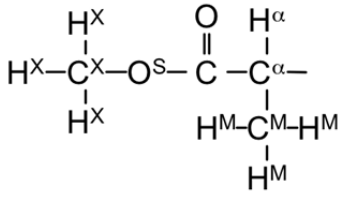
Alcohol-terminated Residue



Atom	*Γ*
O^S	opls_467a
C	opls_465
C^α	opls_491a
H^α	opls_282
O	opls_466

Atom	*Γ*
C^M	opls_135
H^M	opls_140
O^X	opls_154
H^X	opls_155

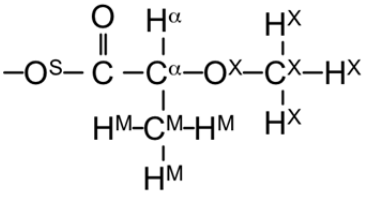
Methyl Ester–terminated Residue



Atom	*Γ*
O^S	opls_467a
C	opls_465
C^α	opls_491a
H^α	opls_282
O	opls_466

Atom	*Γ*
C^M	opls_135
H^M	opls_140
C^X	opls_468
H^X	opls_469

Methoxy-terminated Residue



Atom	*Γ*
O^S	opls_467a
C	opls_465
C^α	opls_491a
H^α	opls_282
O	opls_466

Atom	*Γ*
C^M	opls_135
H^M	opls_140
O^X	opls_180
C^X	opls_181
H^X	opls_185

Atomic Coordinates and Geometries

The functional forms for each component of the potential are dependent on the geometric relationships between pairs or groups of atoms, as defined below. We represent the (three-dimensional) vector coordinates of an atom i in boldface as $\boldsymbol{r}_i$. When two subscripts are specified, a vector difference is implied:

$$\boldsymbol{r}_{ij} = \boldsymbol{r}_j - \boldsymbol{r}_i$$

The corresponding scalar distances are represented in plain-face font:

$$r_{ij} = \left\|\boldsymbol{r}_{ij}\right\|$$

The angle between three atoms i, j, and k is computed as:

$$\theta_{ijk} = \cos^{-1}\left(\boldsymbol{r}_{ji} \cdot \boldsymbol{r}_{jk}\right)$$

The dihedral angle between four atoms i, j, k, and l is defined as the angle between the planes formed by atoms i, j, and k and atoms j, k, and l:

$$\tau_{ijkl} = \cos^{-1}\left(\left(\boldsymbol{r}_{ij} \times \boldsymbol{r}_{jk}\right) \cdot \left(\boldsymbol{r}_{jk} \times \boldsymbol{r}_{kl}\right)\right)$$

Thus, when i, j, k, and l are consecutively bonded atoms, a value of $\tau_{ijkl} = 0$ is the *cis* arrangement and $\tau_{ijkl} = 180°$ is *trans*. When a dihedral angle is defined between non-consecutively bonded atoms, it is referred to as an *improper* dihedral χ_{ijkl}. The improper dihedral angle, however, is computed using the same formula as a proper dihedral:

$$\chi_{ijkl} = \cos^{-1}\left(\left(\boldsymbol{r}_{ij} \times \boldsymbol{r}_{jk}\right) \cdot \left(\boldsymbol{r}_{jk} \times \boldsymbol{r}_{kl}\right)\right)$$

Nonbonded Interactions

Electrostatic

Functional Form

$$V_q(i,j) = Q_{ij}\frac{q_i q_j}{4\pi\epsilon_0 r_{ij}}$$

$$Q_{ij} = \begin{cases} 0 & \text{when } i = j \text{ or when } i,j \text{ are 1,2 or 1,3 neighbors} \\ 0.5 & \text{when } i,j \text{ are 1,4 neighbors} \\ 1 & \text{otherwise} \end{cases}$$

$$q_i = f(\Gamma_i)$$

Parameters

Γ_i	q_i [e]				
	Repeat Unit Residue	Acid-terminated Residue	Alcohol-terminated Residue	Methyl Ester–terminated Residue	Methoxy-terminated Residue
opls_135	-0.18	-0.18	-0.18	-0.18	-0.18
opls_140	0.06	0.06	0.06	0.06	0.06
opls_154			-0.683		
opls_155			0.418		
opls_180					-0.2
opls_181					0.11
opls_185					0.03
opls_267		0.52			
opls_268		-0.53			
opls_269		-0.44			
opls_270		0.31			
opls_282	0.03	0.03	0.09	0.03	0.03
opls_465	0.52		0.52	0.52	0.52
opls_466	-0.43		-0.44	-0.43	-0.43
opls_467a	-0.34		-0.33	-0.34	-0.34
opls_468				-0.09	
opls_469				0.03	
opls_491a	0.22	0.11	0.425	0.22	0.22

Lennard-Jones

Functional Form

$$V_{LJ}(i,j) = 4Q_{ij}\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right]$$

$$Q_{ij} = \begin{cases} 0 & \text{when } i = j \text{ or when } i,j \text{ are 1,2 or 1,3 neighbors} \\ 0.5 & \text{when } i,j \text{ are 1,4 neighbors} \\ 1 & \text{otherwise} \end{cases}$$

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j}$$

$$\sigma_{ij} = \sqrt{\sigma_i \sigma_j}$$

$$\varepsilon_i = f(\Gamma_i)$$

$$\sigma_i = f(\Gamma_i)$$

Parameters

Γ_i	σ_i [nm]	ε_i [kJ/mol]
opls_135	0.350000	0.276144
opls_140	0.250000	0.125520
opls_154	0.312000	0.711280
opls_155	0.000000	0.000000
opls_180	0.290000	0.585760
opls_181	0.350000	0.276144
opls_185	0.250000	0.125520
opls_267	0.375000	0.439320
opls_268	0.300000	0.711280
opls_269	0.296000	0.878640
opls_270	0.000000	0.000000
opls_282	0.242000	0.062760
opls_465	0.375000	0.439320
opls_466	0.296000	0.878640
opls_467	0.300000	0.711280
opls_467a	0.315378	0.636386
opls_468	0.350000	0.276144
opls_469	0.242000	0.062760
opls_491	0.350000	0.276144
opls_491a	0.405359	0.083680

Bonded Interactions

Bond Stretching

Functional Form

$$V_b(i,j) = k_{ij}^b \left(b_{ij} - r_{ij}\right)^2$$
$$b_{ij} = f\left(\Pi_i, \Pi_j\right)$$

Parameters

Π_i	Π_j	b_{ij} [nm]	k_{ij}^b [kJ/(mol nm^2)]
C_2	CT	128.90[a]	669.44[a]
C_2	O_2	111.10[a]	527.18[a]
OS	C_2	109.50[a]	292.88[a]
CT	CT	110.70[a]	313.80[a]
CT	HC	109.50[a]	418.40[a]
CT	OS	107.80	276.14
CT	OH	109.50	292.88
HO	OH	123.40	694.54
C	OH	108.84	694.54
C	CT	113.04	677.81
C	O_3	105.58	418.40

a. These parameters were altered from the original OPLS parameters to reproduce DFT calculations

Angle Bending

Functional Form

$$V_\theta(i,j,k) = k^\theta_{ijk}\left(\theta^0_{ijk} - \theta_{ijk}\right)^2$$
$$k^\theta_{ijk} = f\left(\Pi_i, \Pi_j, \Pi_k\right)$$
$$\theta^0_{ijk} = f\left(\Pi_i, \Pi_j, \Pi_k\right)$$

Parameters

Π_i	Π_j	Π_k	θ^0_{ijk} [degrees]	k^θ_{ijk} [kJ/(mol rad^2)]
CT	C_2	O_2	128.90[a]	669.44[a]
C_2	CT	CT	111.10	527.18
C_2	CT	HC	109.50	292.88
CT	CT	HC	110.70	313.80
CT	CT	OS	109.50	418.40
HC	CT	HC	107.80	276.14
HC	CT	OS	109.50	292.88
O_2	C_2	OS	123.40	694.54
CT	OS	C_2	108.84[a]	694.54[a]
OS	C_2	CT	113.04[a]	677.81[a]
C_2	CT	OS	105.58[a]	418.40[a]
CT	OS	CT	109.50	502.08
CT	OH	HO	108.50	460.24
C_2	CT	OH	109.50	418.40
CT	C	OH	108.00	585.76
O_3	C	OH	121.00	669.44
C	OH	HO	113.00	292.88
CT	C	O_3	120.40	669.44
C	CT	CT	111.10	527.18
C	CT	HC	109.50	292.88
C	CT	OS	109.50	418.40
CT	CT	OH	109.50	418.40
HC	CT	OH	109.50	292.88

a. These parameters were altered from the original OPLS parameters to reproduce DFT calculations

Proper Torsion (Analytic)

Functional Form

$$V_\tau(i,j,k,l) = \sum_{n=0}^{3} C_{ijkl}^{n}\left[\cos\left(\tau_{ijkl} - 180°\right)\right]^n$$

$$C_{ijkl}^{n} = f\left(\Pi_i, \Pi_j, \Pi_k, \Pi_l, n\right)$$

Parameters

Π_i	Π_j	Π_k	Π_l	C_{ijkl}^{0} [kJ/mol]	C_{ijkl}^{1} [kJ/mol]	C_{ijkl}^{2} [kJ/mol]	C_{ijkl}^{3} [kJ/mol]
C	CT	CT	HC	-0.20920	-0.62760	0.00000	0.83680
C	CT	OS	C_2	1.71544	2.84512	1.04600	-5.60656
C_2	CT	CT	HC	-0.15899	-0.47698	0.00000	0.63596
C_2	CT	OH	HO	-0.44350	3.83255	0.72801	-4.11705
C_2	CT	OS	C_2	1.71544	2.84512	1.04600	-5.60656
C_2	CT	OS	CT	1.71544	2.84512	1.04600	-5.60656
C_2	OS	CT	CT	-2.19660	5.20071	0.52719	-3.53130
C_2	OS	CT	HC	0.41421	1.24265	0.00000	-1.65686
CT	C	OH	HO	26.15000	-3.13800	-23.01200	0.00000
CT	CT	C	O_3	2.28446	0.00000	-2.28446	0.00000
CT	CT	C	OH	5.31786	0.73220	-2.28446	-3.76560
CT	CT	C_2	O_2	3.10662	-3.77606	-5.13795	5.80739
CT	CT	C_2	OS	-1.15688	-3.47063	0.00000	4.62750
CT	CT	OH	HO	-0.44350	3.83255	0.72801	-4.11705
CT	CT	OS	CT	1.71544	2.84512	1.04600	-5.60656
CT	OS	C_2	O_2	21.43881	0.00000	-21.43881	0.00000
CT	OS	CT	HC	1.58992	4.76976	0.00000	-6.35968
HC	CT	C	O_3	0.00000	0.00000	0.00000	0.00000
HC	CT	C	OH	0.00000	0.00000	0.00000	0.00000
HC	CT	C_2	O_2	0.00000	0.00000	0.00000	0.00000
HC	CT	C_2	OS	0.27615	0.82844	0.00000	-1.10458
HC	CT	CT	HC	0.62760	1.88280	0.00000	-2.51040
HC	CT	CT	OH	0.97905	2.93716	0.00000	-3.91622
HC	CT	CT	OS	0.97905	2.93716	0.00000	-3.91622
HC	CT	OH	HO	0.94140	2.82420	0.00000	-3.76560
HO	OH	C	O_3	23.01200	0.00000	-23.01200	0.00000
O_2	C_2	CT	OH	0.00000	0.00000	0.00000	0.00000
O_2	C_2	CT	OS	0.00000	0.00000	0.00000	0.00000
OH	C	CT	OS	0.00000	0.00000	0.00000	0.00000
OH	CT	C_2	OS	-1.15060	1.15060	0.00000	0.00000
OS	CT	C	O_3	0.00000	0.00000	0.00000	0.00000
OS	CT	C_2	OS	-1.15060	1.15060	0.00000	0.00000

Proper Torsion (Tabulated)

Tabulated torsional potentials in PLAFF3 are used *in lieu of* the analytic potentials from OPLS for rotation about the OS–C_2 ester bonds in PLA. For non-correlated torsions, the tabulated potential and its derivative are specified at regular intervals of the dihedral angle. Intermediate values are computed using cubic splines. See the GROMACS user manual for more details.

Functional Form

$$V_\omega(i,j,k,l) = f^{\omega}_{ijkl}(\tau_{ijkl})$$

Parameters

$(\Pi_i, \Pi_j, \Pi_k, \Pi_l) = (\mathrm{CT}, \mathrm{OS}, \mathrm{C\_2}, \mathrm{CT})^*$		
τ_{ijkl} [degrees]	f^{ω}_{ijkl} [kJ/mol]	$\frac{df^{\omega}_{ijkl}}{d\tau_{ijkl}}$ [kJ/(mol degree)]
-180	0.0000000000	0.3779906263
-160	-3.9509145667	-0.2313567527
-140	13.3476743437	-1.1755452574
-120	42.4093730569	-1.7079403383
-100	67.9468372768	-0.8804297622
-80	73.0192727523	0.7303414146
-60	48.7932646983	1.3038332217
-40	24.5218316287	0.9977435561
-20	4.5339569403	0.7191129079
0	-12.2738556584	0.5686108744
20	-15.5887684605	0.2160830556
40	-2.6160371115	-1.1846296261
60	25.1789521997	-1.5097729796
80	53.6850857648	-0.7474595868
100	70.9867982982	0.0531049352
120	63.8977128448	2.0838740428
140	40.7817973310	1.3322976366
160	14.5117511257	1.0331344903

* Potential is listed for CT with *S* stereoconfiguration (levorotary). For the *R* isomer, multiply τ_{ijkl} by (-1)

Correlated Proper Torsion (Tabulated)

CMAP potentials in PLAFF3 are used *in addition to* the analytic (non-correlated) potentials previously listed. The tabulated potential is specified at regular intervals of the dihedral angles. Intermediate values are computed using bicubic splines. The following table lists τ_{ijkl} and τ_{jklm} in degrees; $V_{\phi\psi}$ is given in kJ/mol.

Functional Form

$$V_{\phi\psi}(i,j,k,l,m) = f_{ijkl}^{\phi\psi}(\tau_{ijkl}, \tau_{jklm})$$

Parameters

τ_{ijkl}		$(\Pi_i, \Pi_j, \Pi_k, \Pi_l, \Pi_m) = (\text{C\_2, OS, CT, C\_2, OS})^*$								
-180	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	8.7134	9.5761	10.4451	11.8312	13.571	15.5286	17.5743	19.4594	20.9676
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	21.6616	21.2127	19.5809	17.2102	14.3267	11.1645	8.2648	6.0222	4.6832
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	4.3376	5.0783	6.8393	9.364	12.2601	15.0876	17.3725	18.9012	19.6035
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	19.5111	18.6705	17.2098	15.2613	13.0966	11.2414	9.885	8.8619	8.3605
-170	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	8.4256	8.716	8.8195	10.0027	11.6841	13.5948	15.6038	17.5717	19.1421
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	19.9067	19.5193	18.0041	15.8095	13.096	10.1985	7.4562	5.2802	4.0034
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	3.6604	4.3576	5.9771	8.3212	11.0082	13.5922	15.7301	17.2603	18.4583
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	17.8327	17.3395	16.0222	13.9521	12.43	11.0235	9.5931	8.738	8.5496
-160	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	8.3716	8.4776	8.8075	8.8055	9.7396	11.656	13.6827	15.6724	17.271
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	18.0406	17.5962	16.1602	14.0798	11.5096	8.8277	6.3309	4.2399	2.993
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	2.6399	3.2248	4.6817	6.8838	9.4442	11.9012	13.9849	15.8578	17.2083
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	17.1607	16.3345	15.3226	12.9674	11.0915	8.9981	7.9056	7.5885	7.9092
-150	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	6.6135	6.8608	7.9747	8.6521	9.2958	9.837	11.8795	13.9066	15.5147
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	16.1207	15.5806	14.2243	12.2578	9.7835	7.1342	4.8033	2.9949	1.8121
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	1.3933	1.8864	3.2634	5.3775	7.8479	10.2787	12.3647	14.3534	15.4152
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	15.5201	14.0099	12.2451	10.0727	8.1595	6.7099	5.9346	5.7436	6.2937

* Potential is listed for CT with *S* stereoconfiguration (levorotary). For the *R* isomer, multiply τ_{ijkl} and τ_{jklm} by (-1)

τ_{ijkl}		$(\Pi_i, \Pi_j, \Pi_k, \Pi_l, \Pi_m) = (\text{C\_2, OS, CT, C\_2, OS})^*$								
-140	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	4.6471	4.9697	5.9663	6.8181	8.3189	9.3534	10.3396	11.9627	13.5057
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	13.9426	13.4456	12.2882	10.4956	8.0694	5.3831	3.0223	1.3586	0.2909
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-0.1039	0.381	1.6913	3.7162	6.1296	8.5307	10.6285	12.5574	13.5634
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	13.9	12.5019	10.5493	8.3449	6.3651	4.9416	4.0664	3.8284	4.2753
-130	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	3.3207	4.0785	5.046	6.2404	7.5674	8.1007	9.1222	10.5044	11.8035
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	12.2545	12.0393	11.2086	9.6255	7.2527	4.566	2.1334	0.4555	-0.5042
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-0.9573	-0.5053	0.7736	2.69	5.0453	7.4588	9.5519	11.532	12.6174
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	13.0495	11.774	9.8946	7.6972	5.6365	4.0791	3.1033	2.6715	2.7803
-120	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	3.1947	3.8302	4.7086	5.849	7.1426	7.9849	8.6663	9.8254	11.0904
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	11.7766	12.0125	11.5895	10.2473	7.9566	5.1826	2.6426	0.9449	-0.1419
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-0.7119	-0.2762	0.9738	2.7841	4.9909	7.3413	9.3898	11.4771	12.7492
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	13.406	12.2782	10.4856	8.3224	6.2267	4.6009	3.464	2.8503	2.7946
-110	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	4.2101	4.73	5.4504	6.4669	7.6885	8.4007	8.9882	10.1756	11.6536
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	12.8195	13.6121	13.6345	12.5526	10.2466	7.2913	4.6378	2.7264	1.4774
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	0.9616	1.1699	2.2867	3.8671	5.7541	7.8694	9.9315	12.0404	13.5178
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	14.4649	13.6117	11.9902	9.9272	7.9009	6.1797	4.9004	4.1223	3.8889

* Potential is listed for CT with *S* stereoconfiguration (levorotary). For the *R* isomer, multiply τ_{ijkl} and τ_{jklm} by (-1)

τ_{ijkl}		$(\Pi_i, \Pi_j, \Pi_k, \Pi_l, \Pi_m) =$ (C_2, OS, CT, C_2, OS)*								
-100	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	5.4544	5.8372	6.366	7.1895	8.2776	9.3401	9.9138	11.2664	13.252
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	15.1339	16.5077	16.8501	15.871	13.4443	10.0913	6.9371	4.7336	3.3792
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	2.1872	3.1215	3.9101	4.8514	6.1292	7.8792	9.9419	11.9518	13.6834
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	15.0614	14.7643	13.5218	11.6518	9.7126	7.9632	6.6289	5.7314	5.323
-90	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	5.589	5.6379	5.9481	6.5684	7.4908	8.4674	9.7822	12.1238	15.2391
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	17.8953	19.599	19.9315	18.7179	15.6975	11.5993	7.9031	5.8528	4.807
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	3.2811	3.5807	3.6718	3.8177	4.3722	5.9488	8.1735	9.9213	11.8816
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	13.7846	14.4496	13.875	12.397	10.6073	8.8341	7.3988	6.3524	5.7553
-80	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	3.0728	2.8022	2.9666	3.6097	4.5419	6.0055	8.9341	13.1546	17.0202
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	19.8906	21.3858	21.1111	18.9773	15.2789	10.6826	6.8448	4.4471	2.2271
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	0.0772	-0.2287	-0.0644	-0.1998	0.2906	2.2313	5.0044	6.1004	7.8068
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	9.9037	11.6331	11.9031	10.8475	9.1063	7.2561	5.672	4.4213	3.5645
-70	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	-2.3471	-2.6838	-2.4689	-1.7784	-0.2697	3.0956	8.3704	13.3505	17.7102
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	20.2738	20.7677	19.3014	16.1855	11.7137	6.7848	1.8158	-2.5121	-6.2513
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-6.4711	-6.3929	-6.0959	-5.8883	-5.0454	-2.5409	0.9878	1.279	2.5386
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	4.1336	6.4909	7.1402	6.0931	4.1939	2.1456	0.3741	-1.0606	-1.8512

* Potential is listed for CT with *S* stereoconfiguration (levorotary). For the *R* isomer, multiply τ_{ijkl} and τ_{jklm} by (-1)

τ_{ijkl}		$(\Pi_i, \Pi_j, \Pi_k, \Pi_l, \Pi_m) =$ (C_2, OS, CT, C_2, OS)*								
-60	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	-10.1277	-10.28	-9.6494	-7.8076	-4.0013	1.3441	6.9542	12.7199	16.9264
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	18.5358	17.648	14.6701	10.1829	4.8188	-1.9294	-8.0904	-12.6709	-13.0383
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-13.0497	-13.7413	-13.2654	-12.8971	-11.4369	-8.1902	-3.79	1.0324	0.9623
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	1.1013	0.2953	0.2222	-1.5073	-3.8378	-6.0411	-7.9748	-9.3657	-9.8191
-50	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	-18.4392	-17.3793	-15.7423	-12.3899	-7.527	-1.5047	5.1571	10.9694	14.1971
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	14.4626	11.8141	7.1266	1.1467	-6.7555	-14.1312	-19.2415	-19.7955	-19.9222
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-21.1286	-21.5411	-21.345	-20.6932	-18.4094	-14.1964	-8.7063	-2.7673	-2.247
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	-2.7786	-5.9474	-7.8399	-10.6429	-13.486	-15.9146	-17.8973	-19.0742	-18.7367
-40	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	-25.1957	-23.7742	-21.1593	-17.251	-11.2682	-3.9328	3.2086	7.9426	9.6804
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	8.0266	3.5009	-3.1368	-11.9514	-19.8732	-25.2321	-26.2323	-26.3479	-27.8381
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-29.1804	-29.7249	-29.6628	-28.5627	-25.0425	-19.2169	-9.4612	-1.2193	0.8184
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	-2.8951	-9.8325	-16.3835	-20.1684	-23.4101	-25.8008	-27.5728	-28.151	-26.673
-30	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	-31.5742	-29.9953	-25.9966	-20.908	-10.8799	-1.3746	4.0073	5.2373	4.0326
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	-0.1377	-7.175	-16.2134	-24.4317	-29.7568	-31.3756	-31.7987	-33.1041	-36.3528
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-38.0629	-37.6115	-37.6063	-34.4795	-24.0802	-12.8036	-4.081	0.4863	-0.8082
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	-7.1205	-16.4421	-24.5326	-28.6956	-31.8687	-33.9567	-35.3648	-34.4001	-32.6759

* Potential is listed for CT with *S* stereoconfiguration (levorotary). For the *R* isomer, multiply τ_{ijkl} and τ_{jklm} by (-1)

τ_{ijkl}		$(\Pi_i, \Pi_j, \Pi_k, \Pi_l, \Pi_m) = (\text{C\_2, OS, CT, C\_2, OS})^*$								
-20	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	-37.8623	-33.5327	-22.5975	-11.8379	-1.5302	3.4284	4.2272	1.8777	-2.8767
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	-9.0853	-16.5357	-24.6607	-30.5805	-33.8907	-35.3425	-36.7644	-40.2783	-43.1365
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-43.2699	-42.8762	-35.7408	-25.1636	-15.1204	-7.0722	-2.8612	-2.0833	-5.1018
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	-11.6014	-20.3902	-30.5639	-34.6511	-37.3981	-37.9021	-37.6629	-38.5077	-39.5496
-10	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	-31.7119	-20.1465	-10.9444	-3.1336	1.1773	1.4629	-0.3094	-4.5581	-9.9329
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	-14.8128	-20.127	-26.3265	-30.875	-34.5817	-37.7564	-41.2857	-44.7338	-42.7415
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-39.1667	-32.7524	-24.4083	-16.3009	-10.3408	-5.5044	-3.4278	-5.3805	-10.5435
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	-16.8442	-22.9269	-28.1818	-32.5132	-35.5855	-38.199	-40.1803	-41.3546	-40.6391
0	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	-14.823	-8.0989	-2.725	0.1723	0.3177	-0.9357	-4.3977	-8.5996	-12.1157
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	-14.6235	-17.3479	-21.7867	-25.9296	-29.3436	-32.5618	-34.3906	-32.9715	-30.7075
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-26.9473	-21.7572	-17.0092	-11.5643	-6.5243	-3.537	-4.1522	-8.4528	-14.143
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	-19.4712	-24.0414	-27.8358	-31.358	-34.6916	-37.0333	-36.8046	-32.8143	-24.3115
10	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	-1.9787	0.4557	1.8895	2.0952	1.2699	-1.6829	-4.9533	-7.1682	-7.9946
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	-7.905	-8.7916	-12.1407	-15.4516	-17.5485	-18.9798	-19.0254	-19.5572	-19.5637
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-18.0961	-15.2441	-10.777	-6.189	-3.0595	-2.4439	-5.1351	-9.8379	-14.232
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	-17.5044	-20.0346	-22.4209	-24.9576	-26.8027	-26.3322	-22.2796	-13.8104	-5.643

* Potential is listed for CT with *S* stereoconfiguration (levorotary). For the *R* isomer, multiply τ_{ijkl} and τ_{jklm} by (-1)

τ_{ijkl}		$(\Pi_i, \Pi_j, \Pi_k, \Pi_l, \Pi_m) = (\text{C\_2, OS, CT, C\_2, OS})^*$								
20	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	6.1118	5.7645	5.2909	4.8696	2.8447	0.3461	-0.7766	-0.3959	1.0682
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	2.5182	2.6508	0.9598	-0.5281	-2.35	-5.6629	-8.4405	-11.2446	-12.433
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-11.2957	-8.3665	-4.9529	-2.0851	-0.9132	-2.1278	-5.1836	-8.2515	-10.1401
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	-10.9828	-11.6808	-12.7152	-13.7263	-13.2383	-9.7812	-2.706	4.0282	5.6764
30	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	10.8437	9.2324	8.4088	7.5477	6.025	5.7459	6.7635	8.8407	11.7664
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	14.5716	16.0473	14.762	10.838	5.6401	1.2314	-2.5083	-5.2505	-5.9177
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-4.9246	-3.069	-1.0614	0.1404	-0.2775	-1.7147	-2.9459	-3.2674	-2.6102
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	-1.4961	-0.7353	-0.4196	0.2932	2.6695	6.9322	11.1669	12.1579	11.9868
40	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	13.0581	11.4625	11.0788	10.7657	11.1863	12.7138	14.9646	18.5936	23.0091
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	26.0323	24.8564	19.9834	14.6347	9.9891	5.9466	2.3436	-0.107	-1.1201
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-0.9527	-0.1403	0.6146	0.6018	0.1351	0.4161	1.6606	3.5764	5.9613
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	8.2412	9.9175	11.1052	12.4516	14.3589	16.036	16.3459	16.0482	15.0181
50	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	13.5835	12.8002	13.3951	14.6985	16.8589	19.2764	22.595	27.7041	30.5504
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	29.767	25.9416	21.4552	17.0829	12.8668	8.9068	5.4467	2.6037	1.0213
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	0.6475	0.787	0.7031	0.7644	1.9503	4.2109	6.8835	9.8945	13.0152
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	15.6162	17.3903	18.4629	19.1948	19.5768	19.3774	18.6281	17.1467	15.4323

* Potential is listed for CT with *S* stereoconfiguration (levorotary). For the *R* isomer, multiply τ_{ijkl} and τ_{jklm} by (-1)

τ_{ijkl}		$(\Pi_i, \Pi_j, \Pi_k, \Pi_l, \Pi_m) =$ (C_2, OS, CT, C_2, OS)*								
60	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	13.1774	13.6194	15.9128	18.8032	21.7141	24.6607	27.7404	30.2701	30.2352
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	28.334	25.2927	21.9447	18.2105	14.0906	10.1966	6.0469	2.9449	1.4053
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	0.8245	0.4908	0.6625	2.2275	4.8171	7.6818	10.7738	14.0197	17.0081
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	19.2734	20.6992	21.325	21.3974	20.8529	19.7567	18.0883	16.098	14.3831
70	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	12.1585	13.9782	17.8833	21.8578	24.8842	26.9424	27.883	28.133	27.4635
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	25.7107	23.8	21.4746	17.8898	13.9201	9.262	4.8115	2.0933	0.8452
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	0.1593	0.0629	1.5424	3.99	6.5838	9.3678	12.4883	15.4591	17.9355
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	19.6934	20.7291	21.0039	20.5191	19.3679	17.7086	15.7232	13.7854	12.419
80	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	10.4994	13.3972	17.9741	22.1316	24.7336	25.6628	25.5912	24.7628	23.6681
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	22.7565	21.9335	19.6571	16.1616	11.8369	6.5635	2.6861	0.7842	-0.2871
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-0.6726	0.1654	1.9026	3.9397	6.3764	9.2217	12.1749	14.7669	16.7276
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	17.9813	18.5863	18.523	17.6028	16.0931	14.2969	12.3472	10.6921	9.7903
90	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	7.9077	11.3159	16.0378	19.8294	22.1879	22.8145	21.0979	20.4885	20.6988
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	20.4205	19.5539	16.7262	13.4302	8.3199	3.4507	0.9238	-0.71	-1.6432
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-1.5129	-0.6237	0.6522	2.4868	5.0185	7.8745	10.5589	12.7057	14.2005
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	15.112	15.4729	15.1093	13.9244	12.3208	10.5881	8.8561	7.4431	6.7594

* Potential is listed for CT with *S* stereoconfiguration (levorotary). For the *R* isomer, multiply τ_{ijkl} and τ_{jklm} by (-1)

τ_{ijkl}		$(\Pi_i, \Pi_j, \Pi_k, \Pi_l, \Pi_m) =$ (C_2, OS, CT, C_2, OS)*								
100	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	4.6234	8.2489	12.9271	16.3076	18.3527	18.2314	17.0245	18.3013	18.7383
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	18.5019	16.9118	14.1577	9.8875	4.8275	1.7624	-0.6074	-2.4435	-3.3041
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-3.4034	-2.8948	-1.645	0.4696	3.1936	6.014	8.4738	10.294	11.455
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	12.113	12.1992	11.5717	10.2175	8.5769	6.8853	5.2434	3.9786	3.3707
110	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	1.7044	5.0929	9.3107	12.3514	14.2868	15.144	16.3187	17.4696	17.5258
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	17.0571	15.3127	11.6702	7.2242	3.8078	0.6375	-2.2627	-4.4076	-5.6602
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-6.0111	-5.383	-3.7932	-1.3648	1.5612	4.4593	6.8753	8.6002	9.6188
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	10.0454	9.867	8.9979	7.4783	5.69	3.9063	2.2806	1.0317	0.4222
120	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	-0.2023	2.6829	6.3664	9.2959	11.9047	14.0601	15.9532	17.2394	17.5058
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	16.613	14.238	10.6553	7.3655	3.8266	0.0021	-3.3967	-5.9496	-7.4525
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-7.7227	-6.8262	-4.8848	-2.1312	1.0694	4.2088	6.7797	8.4797	9.3848
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	9.604	9.1499	8.0268	6.2946	4.3089	2.3922	0.7807	-0.4666	-1.1363
130	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	-0.6072	1.6911	4.9203	7.9272	10.8834	13.4802	15.703	17.2343	17.2005
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	16.084	13.8707	11.2444	8.3301	4.6179	0.4889	-3.1507	-5.8386	-7.3723
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-7.6104	-6.601	-4.4575	-1.4289	2.0594	5.3982	8.0229	9.7056	10.4766
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	10.5597	9.9137	8.5699	6.6237	4.4828	2.464	0.8408	-0.2744	-1.1211

* Potential is listed for CT with *S* stereoconfiguration (levorotary). For the *R* isomer, multiply τ_{ijkl} and τ_{jklm} by (-1)

τ_{ijkl}		$(\Pi_i, \Pi_j, \Pi_k, \Pi_l, \Pi_m) =$ (C_2, OS, CT, C_2, OS)*								
140	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	0.6174	2.2017	4.4888	7.5587	10.4932	13.2065	15.5389	16.7522	16.8635
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	16.019	14.6159	12.6707	9.9941	6.3077	2.2476	-1.3262	-4.0081	-5.6383
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-6.0094	-5.0628	-2.8225	0.3741	3.9832	7.4197	10.0943	11.7608	12.5043
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	12.5177	11.7945	10.3178	8.2549	5.9896	3.8792	2.2596	1.204	0.3609
150	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	2.9128	4.0751	5.7462	7.8538	10.4533	13.0375	15.3568	16.9199	17.6277
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	17.5999	16.7838	15.2039	12.493	8.8552	4.9741	1.4866	-1.1527	-2.8144
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	-3.3148	-2.4615	-0.3048	2.8193	6.3968	9.8145	12.5264	14.2513	15.0693
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	15.1096	14.3318	12.801	10.6687	8.3114	6.2091	4.6537	3.6286	2.8338
160	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	5.7293	6.6861	7.9761	9.6265	11.8108	14.1266	16.3741	18.2723	19.4644
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	19.8509	19.3666	17.7751	15.0614	11.6175	7.9838	4.6758	2.1294	0.5357
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	0.0258	0.7674	2.7401	5.664	9.1016	12.4197	15.104	16.8276	17.6437
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	17.677	16.896	15.3652	13.2226	10.8839	8.7968	7.2882	6.3705	5.7036
170	τ_{jklm}	-180	-170	-160	-150	-140	-130	-120	-110	-100
	$V_{\phi\psi}$	8.5664	9.2998	10.4288	11.8422	13.7274	15.8313	17.9465	19.8445	21.2618
	τ_{jklm}	-90	-80	-70	-60	-50	-40	-30	-20	-10
	$V_{\phi\psi}$	21.8533	21.4085	19.7488	17.159	14.031	10.6698	7.5977	5.2139	3.7415
	τ_{jklm}	0	10	20	30	40	50	60	70	80
	$V_{\phi\psi}$	3.319	4.0557	5.9057	8.6374	11.8126	14.9075	17.433	19.0705	19.8051
	τ_{jklm}	90	100	110	120	130	140	150	160	170
	$V_{\phi\psi}$	19.7662	18.9327	17.4002	15.2864	13.0323	11.0323	9.6208	8.8188	8.3407

* Potential is listed for CT with *S* stereoconfiguration (levorotary). For the *R* isomer, multiply τ_{ijkl} and τ_{jklm} by (-1)

Improper Torsion

Functional Form

$$V_\chi(i,j,k,l) = k^\chi_{ijkl}\left[1+\cos\left(n^\chi_{ijkl}\chi_{ijkl}-\chi^0_{ijkl}\right)\right]$$
$$\chi_{ijkl} = \cos^{-1}\left(\left(\boldsymbol{r}_{ij}\times\boldsymbol{r}_{jk}\right)\cdot\left(\boldsymbol{r}_{jk}\times\boldsymbol{r}_{kl}\right)\right)$$
$$\chi^0_{ijkl} = f\left(\Pi_i,\Pi_j,\Pi_k,\Pi_l\right)$$
$$k^\chi_{ijkl} = f\left(\Pi_i,\Pi_j,\Pi_k,\Pi_l\right)$$
$$n^\chi_{ijkl} = f\left(\Pi_i,\Pi_j,\Pi_k,\Pi_l\right)$$

Parameters

Π_i	Π_j	Π_k	Π_l	χ^0_{ijkl}	k^χ_{ijkl}	n^χ_{ijkl}
O	C	CT	OS	180	43.932	2
O_2	C_2	CT	OS	180	43.932	2
O_3	C_2	CT	OS	180	43.932	2