

Polarizable Atomic Multipole-Based Force Field for Molecular Dynamics Simulations of Anionic Lipids

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Table S1 Comparison of torsional conformation energies predict by AMOEBA and QM (MP2/6-31G(d,p)) (kcal/mol) .

	R2	Intercept	Slope	Min/ Max	STD error	Average error
PS-AMOEBA	0.92	-0.16	0.88	0.00/8.78	7.12	1.19
PG-AMOEBA	0.87	-1.61	0.88	0.00/5.56	2.27	1.27

```
#####
##                               ##
##  Force Field Definition  ##
##                               ##
#####
```

```
forcefield      AMOEBA-DMPG
```

```
bond-cubic      -2.55
bond-quartic    3.793125
angle-cubic     -0.014
angle-quartic   0.000056
angle-pentic    -0.0000007
angle-sextic    0.000000022
torsionunit     0.5
vdwtype         BUFFERED-14-7
opbendunit      0.02191418
radiusrule      CUBIC-MEAN
radiustype      R-MIN
radiussize      DIAMETER
epsilonrule     HHG
dielectric      1.0
polarization    MUTUAL
vdw-12-scale    0.0
vdw-13-scale    0.0
vdw-14-scale    1.0
vdw-15-scale    1.0
mpole-12-scale  0.0
mpole-13-scale  0.0
mpole-14-scale  0.4
mpole-15-scale  0.8
polar-12-scale  0.0
polar-13-scale  0.0
polar-14-scale  1.0
polar-15-scale  1.0
polar-14-intra  0.5
direct-11-scale 0.0
direct-12-scale 1.0
direct-13-scale 1.0
direct-14-scale 1.0
mutual-11-scale 1.0
mutual-12-scale 1.0
mutual-13-scale 1.0
mutual-14-scale 1.0
```

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#####
##                               ##
```

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## Atom Type Definitions ##
##                               ##
#####

```

atom	601	601	C1	"DMPG glycerol1 C1	"	6	12.011	4
atom	602	602	H1	"DMPG glycerol1 H1	"	1	1.008	1
atom	603	603	OH1	"DMPG glycerol1 OH1	"	8	15.999	2
atom	604	604	HO1	"DMPG glycerol1 HO1	"	1	1.008	1
atom	605	605	C2	"DMPG glycerol1 C2	"	6	12.011	4
atom	606	606	H2	"DMPG glycerol1 H2	"	1	1.008	1
atom	607	603	OH2	"DMPG glycerol1 OH2	"	8	15.999	2
atom	608	604	HO2	"DMPG glycerol1 HO2	"	1	1.008	1
atom	609	630	C3	"DMPG glycerol1 C3	"	6	12.011	4
atom	610	608	H3	"DMPG glycerol1 H3	"	1	1.008	1
atom	611	609	P1	"DMPG phosphate P1	"	15	30.974	4
atom	612	610	O3	"DMPG phosphate O3	"	8	15.999	1
atom	613	611	O2	"DMPG phosphate O2	"	8	15.999	2
atom	614	611	O4	"DMPG phosphate O4	"	8	15.999	2
atom	615	607	C4	"DMPG glycerol2 C4	"	6	12.011	4
atom	616	608	H4	"DMPG glycerol2 H4	"	1	1.008	1
atom	617	612	C5	"DMPG glycerol2 C5	"	6	12.011	4
atom	618	613	H5	"DMPG glycerol2 H5	"	1	1.008	1
atom	619	614	OG1	"DMPG glycerol2 OG1	"	8	15.999	2
atom	620	615	C1b	"DMPG acyl chainb C1 "	"	6	12.011	3
atom	621	616	O1b	"DMPG sn-2 O1b	"	8	15.999	1
atom	622	617	C2b	"DMPG acyl chainb C2 "	"	6	12.011	4
atom	623	618	H2b	"DMPG acyl chainb H2 "	"	1	1.008	1
atom	624	631	C6	"DMPG glycerol2 C6	"	6	12.011	4
atom	625	608	H6	"DMPG glycerol2 H6	"	1	1.008	1
atom	626	614	OG2	"DMPG glycerol2 OG2	"	8	15.999	2
atom	627	615	C1a	"DMPG acyl chaina C1 "	"	6	12.011	3
atom	628	616	O1a	"DMPG sn-2 O1a	"	8	15.999	1
atom	629	617	C2a	"DMPG acyl chaina C2 "	"	6	12.011	4
atom	630	618	H2a	"DMPG acyl chaina H2 "	"	1	1.008	1
atom	631	619	C3t	"DMPG acyl chainab C3"	"	6	12.011	4
atom	632	620	H3t	"DMPG acyl chainab H3"	"	1	1.008	1
atom	633	619	C4t	"DMPG acyl chainab C4"	"	6	12.011	4
atom	634	620	H4t	"DMPG acyl chainab H4"	"	1	1.008	1
atom	635	619	C5t	"DMPG acyl chainab C5"	"	6	12.011	4
atom	636	620	H5t	"DMPG acyl chainab H5"	"	1	1.008	1
atom	637	619	C6t	"DMPG acyl chainab C6"	"	6	12.011	4
atom	638	620	H6t	"DMPG acyl chainab H6"	"	1	1.008	1
atom	639	619	C7t	"DMPG acyl chainab C7"	"	6	12.011	4
atom	640	620	H7t	"DMPG acyl chainab H7"	"	1	1.008	1
atom	641	619	C8t	"DMPG acyl chainab C8"	"	6	12.011	4
atom	642	620	H8t	"DMPG acyl chainab H8"	"	1	1.008	1
atom	643	619	C9t	"DMPG acyl chainab C9"	"	6	12.011	4
atom	644	620	H9t	"DMPG acyl chainab H9"	"	1	1.008	1
atom	645	619	C10	"DMPG acyl chainab C10"	"	6	12.011	4

```
#####
##                                     ##
##   Van der Waals Parameters   ##
##                                     ##
#####
```

[illegible]

```
##
#####
```

bond	601	605	323.0000	1.5170
bond	601	603	465.1000	1.4024
bond	601	602	341.0000	1.0836
bond	603	604	615.9000	0.9509
bond	605	603	465.1000	1.4129
bond	605	606	341.0000	1.0840
bond	630	605	323.0000	1.5201
bond	630	611	465.1000	1.4011
bond	630	608	341.0000	1.0824
bond	607	612	323.0000	1.5169
bond	607	611	465.1000	1.3921
bond	607	614	465.1000	1.4234
bond	607	608	341.0000	1.0842
bond	609	611	450.0000	1.6479
bond	609	610	775.0000	1.4679
bond	612	614	465.1000	1.4284
bond	612	613	341.0000	1.0800
bond	615	614	465.1000	1.3199
bond	615	616	601.8000	1.1906
bond	617	615	345.3000	1.5107
bond	617	618	341.0000	1.0857
bond	619	617	323.0000	1.5233
bond	619	620	341.0000	1.0837
bond	631	612	323.0000	1.5151
bond	631	614	465.1000	1.4234
bond	631	608	341.0000	1.0792
bond	619	621	323.0000	1.5299
bond	621	622	341.0000	1.0861
bond	619	619	453.0000	1.5312
bond	619	620	341.0000	1.0868

```
#####
##
## Angle Bending Parameters ##
##
#####
```

angle	605	601	603	88.0000	111.3169
angle	605	601	602	42.4400	109.3794
angle	603	601	602	60.9900	110.1884
angle	602	601	602	40.5700	108.1787
angle	601	603	604	64.9600	106.5531

angle	605	603	604	64.9600	106.7288
angle	630	605	601	48.2000	113.3604
angle	630	605	603	88.0000	109.6695
angle	630	605	606	42.4400	108.4718
angle	601	605	603	88.0000	105.8246
angle	601	605	606	42.4400	109.7398
angle	603	605	606	60.9900	109.7272
angle	605	630	611	88.0000	108.9330
angle	605	630	608	42.4400	109.6664
angle	611	630	608	60.9900	107.2293
angle	608	630	608	39.5700	108.8792
angle	612	631	614	88.0000	108.6276
angle	612	607	608	38.0000	110.9853
angle	614	607	608	60.9900	109.4841
angle	608	607	608	39.5700	108.5174
angle	612	607	611	88.0000	107.9292
angle	611	607	608	60.9900	110.5513
angle	611	609	611	65.5800	99.1337
angle	611	609	610	75.8600	108.2462
angle	610	609	610	89.8800	125.6037
angle	630	611	609	80.3000	119.8591
angle	607	611	609	80.3000	118.3962
angle	631	612	607	60.0000	113.6797
angle	631	612	614	88.0000	110.2555
angle	631	612	613	38.0000	107.9899
angle	614	612	613	60.9900	108.4937
angle	607	612	614	88.0000	107.1445
angle	607	612	613	38.0000	109.1704
angle	612	614	615	88.5000	119.5871
angle	607	614	609	80.3000	118.3962
angle	617	615	614	60.0000	111.0471
angle	617	615	616	60.0000	125.0470
angle	614	615	616	50.0000	123.9059
angle	631	614	615	88.5000	118.0991
angle	619	617	615	48.2000	113.1056
angle	619	617	618	38.0000	111.3844
angle	615	617	618	38.0000	107.3072
angle	618	617	618	45.5700	105.7941
angle	617	619	620	42.4400	111.1182
angle	620	619	620	39.5700	107.6064
angle	612	631	608	38.0000	110.9853
angle	614	631	608	60.9900	109.4841
angle	608	631	608	39.5700	108.5174
angle	619	619	619	48.2500	113.3100
angle	619	619	620	37.9900	109.4700
angle	620	619	621	37.9900	109.3700
angle	617	619	619	48.2000	112.2989
angle	622	621	622	39.5100	107.6500
angle	620	619	620	39.6600	106.2700

angle	619	619	621	48.2900	112.8700
angle	619	621	622	42.4200	111.2700
angle	619	619	623	48.2000	112.8390
angle	619	623	623	60.0000	125.4116
angle	619	623	624	32.0000	115.6966
angle	623	623	624	32.0000	118.8892
angle	620	619	623	38.0000	108.7346

```
#####
##                                     ##
##  Stretch-Bend Parameters  ##
##                                     ##
#####
```

strbnd	605	601	603	18.7000	18.7000
strbnd	605	601	602	11.5000	11.5000
strbnd	603	601	602	-4.5000	38.0000
strbnd	605	603	604	-4.5000	38.0000
strbnd	601	603	604	-4.5000	38.0000
strbnd	630	605	601	38.0000	38.0000
strbnd	630	605	603	18.7000	18.7000
strbnd	630	605	606	-4.5000	38.0000
strbnd	601	605	603	18.7000	18.7000
strbnd	601	605	606	-4.5000	38.0000
strbnd	607	605	606	-4.5000	38.0000
strbnd	612	607	614	18.7000	18.7000
strbnd	612	607	608	11.5000	18.7000
strbnd	614	607	608	-4.5000	38.0000
strbnd	612	631	614	18.7000	18.7000
strbnd	612	631	608	11.5000	18.7000
strbnd	614	631	608	-4.5000	38.0000
strbnd	612	607	611	18.7000	18.7000
strbnd	611	607	608	-4.5000	38.0000
strbnd	611	609	611	14.4000	14.4000
strbnd	611	609	610	14.4000	14.4000
strbnd	607	611	609	38.0000	38.0000
strbnd	607	612	607	18.7000	18.7000
strbnd	607	612	614	18.7000	18.7000
strbnd	607	612	613	11.5000	18.7000
strbnd	614	612	613	-4.5000	38.0000
strbnd	612	614	620	38.0000	38.0000
strbnd	607	614	615	38.0000	38.0000
strbnd	631	614	615	38.0000	38.0000
strbnd	617	615	614	18.7000	18.7000
strbnd	619	617	615	18.7000	18.7000
strbnd	619	617	618	11.5000	18.7000

strbnd	615	617	618	11.5000	18.7000
strbnd	617	620	614	18.7000	18.7000
strbnd	617	621	620	11.5000	11.5000
strbnd	605	630	611	18.7000	18.7000
strbnd	605	630	608	11.5000	11.5000
strbnd	611	630	608	-4.5000	38.0000
strbnd	615	620	619	38.0000	38.0000
strbnd	609	620	619	38.0000	38.0000
strbnd	617	619	620	11.5000	11.5000
strbnd	619	619	619	18.7000	18.7000
strbnd	619	619	620	11.5000	18.7000
strbnd	621	619	620	11.5000	18.7000
strbnd	623	619	624	11.5000	11.5000
strbnd	617	619	619	18.7000	18.7000
strbnd	619	617	618	11.5000	18.7000
strbnd	619	619	623	18.7000	18.7000
strbnd	620	619	623	11.5000	18.7000
strbnd	619	621	622	11.5000	11.5000
strbnd	617	619	620	11.5000	18.7000
strbnd	619	623	624	11.5000	18.7000
strbnd	623	619	623	18.7000	18.7000
strbnd	623	619	624	11.5000	18.7000
strbnd	624	623	623	11.5000	18.7000

```
#####
##                                     ##
##  Out-of-Plane Bend Parameters  ##
##                                     ##
#####
```

opbend	617	615	0	0	0.2002
opbend	614	615	0	0	0.2002
opbend	616	615	0	0	0.6500

```
#####
##                                     ##
##  Torsional Parameters  ##
##                                     ##
#####
```

torsion	603	601	605	630	-0.253 0.0 1	0.007 180.0 2	1.585 0.0 3
torsion	603	601	605	603	0.567 0.0 1	-0.739 180.0 2	1.585 0.0 3

torsion	603	601	605	606	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	602	601	605	630	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	602	601	605	603	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	602	601	605	606	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	605	601	603	604	-1.447 0.0 1	0.531 180.0 2	0.317 0.0 3
torsion	602	601	603	604	0.000 0.0 1	0.000 180.0 2	0.274 0.0 3
torsion	630	605	603	604	-1.372 0.0 1	0.232 180.0 2	0.400 0.0 3
torsion	601	605	603	604	-1.372 0.0 1	0.232 180.0 2	0.400 0.0 3
torsion	606	605	603	604	0.000 0.0 1	0.000 180.0 2	0.266 0.0 3
torsion	605	630	611	609	-5.690 0.0 1	-0.340 180.0 2	-1.004 0.0 3
torsion	608	607	612	631	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	608	607	612	614	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	608	631	612	607	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	608	631	612	614	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	608	630	612	607	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	608	630	605	601	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	608	630	605	603	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	608	630	605	606	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	608	607	611	609	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	608	631	612	613	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	608	607	612	613	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	608	631	614	615	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	608	630	611	609	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	611	630	605	601	-10.510 0.0 1	-1.120 180.0 2	-0.145 0.0 3
torsion	611	630	605	603	-10.337 0.0 1	-2.220 180.0 2	1.661 0.0 3
torsion	611	630	605	606	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	611	607	612	631	2.061 0.0 1	-0.273 180.0 2	0.000 0.0 3
torsion	611	607	612	614	2.473 0.0 1	-0.641 180.0 2	0.000 0.0 3
torsion	611	607	612	613	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	612	631	614	615	0.950 0.0 1	-0.615 180.0 2	-0.900 0.0 3
torsion	612	607	611	609	-3.099 0.0 1	-1.371 180.0 2	-0.640 0.0 3
torsion	614	631	612	607	0.756 0.0 1	-0.023 180.0 2	0.788 0.0 3
torsion	614	631	612	614	0.220 0.0 1	-0.592 180.0 2	0.788 0.0 3
torsion	614	631	612	613	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	611	609	611	630	3.996 0.0 1	-2.322 180.0 2	0.547 0.0 3
torsion	610	609	611	630	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	611	609	611	607	0.000 0.0 1	0.000 180.0 2	4.835 0.0 3
torsion	610	609	611	607	0.000 0.0 1	0.000 180.0 2	-2.217 0.0 3
torsion	631	612	614	615	5.257 0.0 1	-0.267 180.0 2	-3.761 0.0 3
torsion	607	612	614	615	3.413 0.0 1	-1.059 180.0 2	2.755 0.0 3
torsion	613	612	614	615	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	617	615	614	631	0.000 0.0 1	5.965 180.0 2	0.000 0.0 3
torsion	616	615	614	631	0.000 0.0 1	5.965 180.0 2	0.000 0.0 3
torsion	617	615	614	612	0.000 0.0 1	5.294 180.0 2	0.000 0.0 3
torsion	616	615	614	612	0.000 0.0 1	5.294 180.0 2	0.000 0.0 3
torsion	619	617	615	614	1.231 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	619	617	615	616	0.000 0.0 1	-0.039 180.0 2	0.000 0.0 3
torsion	618	617	615	614	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	618	617	615	616	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3

torsion	615	617	619	620	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	615	617	619	619	1.532 0.0 1	-1.981 180.0 2	1.641 0.0 3
torsion	618	617	619	619	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	615	617	619	620	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	618	617	619	620	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	614	615	617	619	0.000 0.0 1	-0.039 180.0 2	0.000 0.0 3
torsion	622	621	619	620	0.000 0.0 1	0.000 180.0 2	0.299 0.0 3
torsion	620	619	623	623	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	620	619	623	624	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	617	619	619	619	2.818 0.0 1	-0.410 180.0 2	2.472 0.0 3
torsion	619	619	619	620	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	617	619	619	620	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	620	619	619	620	0.000 0.0 1	0.000 180.0 2	0.299 0.0 3
torsion	619	619	619	619	0.568 0.0 1	-0.375 180.0 2	2.302 0.0 3
torsion	619	623	623	619	0.000 0.0 1	8.000 180.0 2	0.000 0.0 3
torsion	619	619	623	623	2.775 0.0 1	-0.695 180.0 2	-1.271 0.0 3
torsion	619	623	623	624	0.000 0.0 1	6.100 180.0 2	0.000 0.0 3
torsion	624	623	623	624	0.000 0.0 1	4.070 180.0 2	0.000 0.0 3
torsion	619	619	623	624	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	620	619	619	623	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	619	619	619	623	0.649 0.0 1	0.419 180.0 2	2.472 0.0 3
torsion	619	619	619	621	0.717 0.0 1	-0.133 180.0 2	1.123 0.0 3
torsion	620	619	619	621	0.000 0.0 1	0.000 180.0 2	0.341 0.0 3
torsion	622	621	619	619	0.000 0.0 1	0.000 180.0 2	0.341 0.0 3

```
#####
##                                     ##
##  Atomic Multipole Parameters  ##
##                                     ##
#####
```

multipole	601	605	603	0.14321		
				0.32240	0.00000	0.09462
				0.23810		
				0.00000	-0.37250	
multipole	602	601	605	-0.36896	0.00000	0.13440
				0.00784		
				-0.02351	0.00000	-0.15975
				0.07822		
multipole	603	601	604	0.00000	0.11571	
				-0.04421	0.00000	-0.19393
				-0.39070		
				0.18127	0.00000	0.29036
				0.30351		
				0.00000	-0.95004	
				-0.71221	0.00000	0.64653

multipole	604	603	601	0.22528		
				-0.03855	0.00000	-0.03655
				-0.07847		
				0.00000	-0.11637	
multipole	605	609	601	-0.23815	0.00000	0.19484
				0.06538		
				0.01518	0.00000	0.02809
				0.00730		
multipole	606	605	609	0.00000	-0.00349	
				0.16576	0.00000	-0.00381
				0.03496		
				0.03145	0.00000	-0.00998
multipole	607	605	608	-0.04100		
				0.00000	0.11430	
				0.05911	0.00000	-0.07330
				-0.34019		
multipole	608	607	605	0.17501	0.00000	0.32600
				0.28616		
				0.00000	-0.85046	
				-0.52577	0.00000	0.56430
multipole	609	605	613	0.21690		
				-0.08046	0.00000	-0.03557
				-0.08494		
				0.00000	-0.02354	
multipole	610	609	605	-0.08847	0.00000	0.10848
				0.12717		
				0.39300	0.00000	0.04872
				0.42188		
multipole	611	612	-612	0.00000	-0.43739	
				-0.47076	0.00000	0.01551
				0.02153		
				-0.01988	0.00000	-0.04884
multipole	612	611	612	-0.04385		
				0.00000	-0.00397	
				0.01708	0.00000	0.04782
				1.75436		
multipole	613	609	611	0.00000	0.00000	-0.02762
				0.11169		
				0.00000	0.13248	
				0.00000	0.00000	-0.24417
multipole	612	611	612	-0.94669		
				0.00000	0.00000	-0.04937
				-0.20908		
				0.00000	-0.25330	
multipole	613	609	611	0.00000	0.00000	0.46238
				-0.53817		
				0.10997	0.00000	0.35554
				-0.36722		
				0.00000	-0.82584	

multipole	614	615	611	-0.21989	0.00000	1.19306
				-0.53817		
				-0.03340	0.00000	0.43339
				-0.44704		
multipole	615	617	614	0.00000	-0.62023	
				-0.16194	0.00000	1.06727
				0.12717		
				0.36195	0.00000	0.06164
multipole	616	615	617	0.26076		
				0.00000	-0.49801	
				-0.09726	0.00000	0.23725
				0.02153		
multipole	617	624	615	0.00104	0.00000	-0.06459
				-0.04854		
				0.00000	0.01303	
				-0.09648	0.00000	0.03551
multipole	618	617	624	0.02657		
				0.04187	0.00000	0.22345
				0.15487		
				0.00000	-0.02748	
multipole	619	617	620	-0.17760	0.00000	-0.12739
				0.08536		
				0.01608	0.00000	0.01881
				-0.09901		
multipole	620	622	619	0.00000	0.07857	
				0.03773	0.00000	0.02044
				-0.29195		
				0.09319	0.00000	0.43233
multipole	621	620	622	-0.15745		
				0.00000	-0.33908	
				-0.17964	0.00000	0.49653
				0.78665		
multipole	622	631	620	0.02327	0.00000	-0.21575
				0.35613		
				0.00000	-0.07671	
				-0.18339	0.00000	-0.27942
multipole	623	622	631	-0.62869		
				0.07600	0.00000	-0.00665
				-0.50354		
				0.00000	0.18185	
multipole	623	622	631	0.20943	0.00000	0.32169
				-0.15650		
				0.13286	0.00000	0.20347
				0.25455		
multipole	623	622	631	0.00000	-0.51114	
				-0.12848	0.00000	0.25659
				0.08635		
				0.04592	0.00000	-0.08127
				0.02657		

multipole	624	617	626	0.00000	-0.01148	
				0.13451	0.00000	-0.01509
				0.08356		
				0.36212	0.00000	0.14124
				0.53656		
multipole	625	624	617	0.00000	-0.37503	
				-0.48187	0.00000	-0.16153
				0.03662		
				-0.07375	0.00000	-0.09505
				0.01557		
multipole	626	624	627	0.00000	0.06592	
				-0.06368	0.00000	-0.08149
				-0.36542		
				0.10786	0.00000	0.28569
				-0.27399		
multipole	627	629	626	0.00000	-0.62678	
				-0.36403	0.00000	0.90077
				0.96543		
				-0.15609	0.00000	0.00907
				0.47252		
multipole	628	627	629	0.00000	-0.19153	
				-0.32984	0.00000	-0.28099
				-0.67403		
				-0.08121	0.00000	-0.08123
				-0.31575		
multipole	629	631	627	0.00000	0.19743	
				0.04400	0.00000	0.11832
				-0.33818		
				-0.09050	0.00000	0.28717
				-0.15732		
multipole	630	629	631	0.00000	-0.14994	
				0.24675	0.00000	0.30726
				0.08282		
				0.05263	0.00000	-0.10003
				0.04780		
multipole	631	633	629	0.00000	0.07340	
				0.12940	0.00000	-0.12120
				-0.12028		
				0.00000	0.00000	0.08920
				-0.45259		
multipole	631	633	622	0.00000	0.22212	
				0.00000	0.00000	0.23047
				-0.12028		
				0.00000	0.00000	0.08920
				-0.45259		
multipole	632	631	633	0.00000	0.22212	
				0.00000	0.00000	0.23047
				0.06014		
				-0.02503	0.00000	0.07942

				-0.13076		
				0.00000	-0.05780	
				-0.05505	0.00000	0.18856
multipole	633	635	631	-0.12028		
				0.00000	0.00000	0.33839
				-0.68115		
				0.00000	0.10340	
				0.00000	0.00000	0.57775
multipole	634	633	635	0.06014		
				0.00661	0.00000	0.11930
				-0.16797		
				0.00000	-0.07505	
				0.12169	0.00000	0.24302
multipole	635	633	637	-0.12028		
				0.00000	0.00000	0.14448
				-0.28128		
				0.00000	-0.00441	
				0.00000	0.00000	0.28569
multipole	636	635	633	0.06014		
				0.01615	0.00000	0.22955
				-0.21643		
				0.00000	-0.20428	
				0.02788	0.00000	0.42071
multipole	637	635	639	-0.12028		
				0.00000	0.00000	-0.01354
				-0.04975		
				0.00000	0.10300	
				0.00000	0.00000	-0.05325
multipole	638	637	635	0.06014		
				0.04578	0.00000	0.17404
				-0.16537		
				0.00000	-0.18492	
				0.07403	0.00000	0.35029
multipole	639	637	641	-0.12028		
				0.00000	0.00000	-0.05085
				-0.30712		
				0.00000	0.15148	
				0.00000	0.00000	0.15564
multipole	640	639	637	0.06014		
				0.08671	0.00000	0.09820
				-0.08927		
				0.00000	-0.11428	
				0.11609	0.00000	0.20355
multipole	641	639	-643	-0.12028		
				0.00000	0.00000	-0.02523
				0.11672		
				0.00000	0.26467	
				0.00000	0.00000	-0.38139
multipole	642	641	639	0.06014		

multipole	643	645	641	-0.00822	0.00000	0.09256
				-0.12801		
				0.00000	-0.10497	
				-0.03016	0.00000	0.23298
				-0.12028		
				0.00000	0.00000	0.04373
multipole	644	643	645	-0.11409		
				0.00000	0.25407	
				0.00000	0.00000	-0.13998
				0.06014		
				0.03147	0.00000	0.10815
				-0.04700		
multipole	645	647	643	0.00000	-0.16314	
				0.06910	0.00000	0.21014
				-0.12028		
				0.00000	0.00000	0.04534
				0.03346		
				0.00000	0.20973	
multipole	646	645	647	0.00000	0.00000	-0.24319
				0.06014		
				0.02363	0.00000	0.17973
				-0.11928		
				0.00000	-0.23560	
				0.06988	0.00000	0.35488
multipole	647	649	645	-0.12028		
				0.00000	0.00000	0.19090
				-0.13792		
				0.00000	0.13912	
				0.00000	0.00000	-0.00120
				0.06014		
multipole	648	647	649	-0.00563	0.00000	0.24246
				-0.19465		
				0.00000	-0.25447	
				0.03243	0.00000	0.44912
				-0.12028		
				0.00000	0.00000	0.17802
multipole	649	647	651	-0.14130		
				0.00000	-0.03152	
				0.00000	0.00000	0.17282
				0.06014		
				0.01343	0.00000	0.22793
				-0.19168		
multipole	650	649	647	0.00000	-0.23346	
				0.05530	0.00000	0.42514
				-0.12028		
				0.00000	0.00000	-0.04785
				-0.24581		
				0.00000	-0.05659	
multipole	651	649	653	0.00000	0.00000	0.30240

multipole	652	651	649	0.06014		
				0.10189	0.00000	0.12283
				-0.11650		
				0.00000	-0.13166	
				0.14624	0.00000	0.24816
multipole	653	651	654	-0.16638		
				0.00000	0.00000	0.13817
				0.23776		
				0.00000	0.30333	
				0.00000	0.00000	-0.54109
multipole	654	653	651	0.05546		
				-0.02203	0.00000	0.07426
				-0.02038		
				0.00000	-0.17435	
				-0.01461	0.00000	0.19473

```
#####
##                                     ##
##  Dipole Polarizability Parameters  ##
##                                     ##
#####
```

polarize	601	1.334	0.390	602 603
polarize	602	0.496	0.390	601
polarize	603	0.837	0.390	601 604
polarize	604	0.496	0.390	603
polarize	605	1.334	0.390	606 607
polarize	606	0.496	0.390	605
polarize	607	0.837	0.390	605 608
polarize	608	0.496	0.390	607
polarize	609	1.334	0.390	610 613
polarize	610	0.496	0.390	609
polarize	611	1.828	0.390	612 613 614
polarize	612	0.837	0.390	611
polarize	613	0.837	0.390	609 611
polarize	614	0.837	0.390	611 615
polarize	615	1.334	0.390	614 616
polarize	616	0.496	0.390	615
polarize	617	1.334	0.390	618 619
polarize	618	0.496	0.390	617
polarize	619	0.837	0.390	617 620
polarize	620	1.334	0.390	619 621 622
polarize	621	0.837	0.390	620
polarize	622	1.334	0.390	620 623
polarize	623	0.496	0.390	622
polarize	624	1.334	0.390	608 626
polarize	625	0.496	0.390	624

polarize	626	0.837	0.390	624 627
polarize	627	1.334	0.390	626 628 629
polarize	628	0.837	0.390	627
polarize	629	1.334	0.390	627 630
polarize	630	0.496	0.390	629
polarize	631	1.334	0.390	633 632
polarize	632	0.496	0.390	631
polarize	633	1.334	0.390	631 634
polarize	634	0.496	0.390	633
polarize	635	1.334	0.390	637 636
polarize	636	0.496	0.390	635
polarize	637	1.334	0.390	635 638
polarize	638	0.496	0.390	637
polarize	639	1.334	0.390	640 641
polarize	640	0.496	0.390	639
polarize	641	1.334	0.390	642 639
polarize	642	0.496	0.390	641
polarize	643	1.334	0.390	645 644
polarize	644	0.496	0.390	643
polarize	645	1.334	0.390	643 646
polarize	646	0.496	0.390	645
polarize	647	1.334	0.390	648
polarize	648	0.496	0.390	647
polarize	649	1.334	0.390	650 651
polarize	650	0.496	0.390	649
polarize	651	1.334	0.390	649 652
polarize	652	0.496	0.390	651
polarize	653	1.334	0.390	654
polarize	654	0.496	0.390	653

```
#####
##                               ##
##  Force Field Definition  ##
##                               ##
#####
```

forcefield	AMOEBA-POPS
bond-cubic	-2.55
bond-quartic	3.793125
angle-cubic	-0.014
angle-quartic	0.000056
angle-pentic	-0.0000007
angle-sextic	0.000000022
torsionunit	0.5
vdwtype	BUFFERED-14-7
opbendunit	0.02191418
radiusrule	CUBIC-MEAN
radiustype	R-MIN
radiussize	DIAMETER
epsilonrule	HHG
dielectric	1.0
polarization	MUTUAL
vdw-12-scale	0.0
vdw-13-scale	0.0
vdw-14-scale	1.0
vdw-15-scale	1.0
mpole-12-scale	0.0
mpole-13-scale	0.0
mpole-14-scale	0.4
mpole-15-scale	0.8
polar-12-scale	0.0
polar-13-scale	0.0
polar-14-scale	1.0
polar-15-scale	1.0
polar-14-intra	0.5
direct-11-scale	0.0
direct-12-scale	1.0
direct-13-scale	1.0
direct-14-scale	1.0
mutual-11-scale	1.0
mutual-12-scale	1.0
mutual-13-scale	1.0
mutual-14-scale	1.0

```
#####
##                               ##
```

Atom Type Definitions

##

#####

atom	801	801	N	"POPS serine N+	"	7	14.007	4
atom	802	802	H1	"POPS serine HN	"	1	1.008	1
atom	803	803	CA	"POPS serine CA	"	6	12.011	4
atom	804	804	HA	"POPS serine HA	"	1	1.008	1
atom	805	805	CO	"POPS serine COO-	"	6	12.011	3
atom	806	806	OC	"POPS serine O-	"	8	15.999	1
atom	807	807	CB	"POPS serine CB	"	6	12.011	4
atom	808	808	HB	"POPS serine HB	"	1	1.008	1
atom	809	809	P1	"POPS phosphate P1	"	15	30.974	4
atom	810	810	O3	"POPS phosphate O3	"	8	15.999	1
atom	811	811	O2	"POPS phosphate O2	"	8	15.999	2
atom	812	811	O4	"POPS phosphate O4	"	8	15.999	2
atom	813	812	C1	"POPS glycerol C1	"	6	12.011	4
atom	814	813	H1	"POPS glycerol H1	"	1	1.008	1
atom	815	814	C2	"POPS glycerol C2	"	6	12.011	4
atom	816	815	H2	"POPS glycerol H2	"	1	1.008	1
atom	817	816	OG1	"POPS glycerol OG1	"	8	15.999	2
atom	818	817	C1B	"POPS acyl chainb C1 "	"	6	12.011	3
atom	819	818	O1B	"POPS sn-2 O1b	"	8	15.999	1
atom	820	819	C2B	"POPS acyl chainb C2 "	"	6	12.011	4
atom	821	820	H2B	"POPS acyl chainb H2 "	"	1	1.008	1
atom	822	821	C3	"DLPG glycerol C3	"	6	12.011	4
atom	823	822	H3	"DLPG glycerol H3	"	1	1.008	1
atom	824	816	OG2	"POPS glycerol OG2	"	8	15.999	2
atom	825	817	C1A	"POPS acyl chaina C1 "	"	6	12.011	3
atom	826	818	O1A	"POPS sn-2 O1a	"	8	15.999	1
atom	827	819	C2A	"POPS acyl chaina C2 "	"	6	12.011	4
atom	828	820	H2A	"POPS acyl chaina H2 "	"	1	1.008	1
atom	829	823	C3T	"POPS acyl chainab C3"	"	6	12.011	4
atom	830	824	H3T	"POPS acyl chainab H3"	"	1	1.008	1
atom	831	823	C4t	"POPS acyl chainab C4"	"	6	12.011	4
atom	832	824	H4t	"POPS acyl chainab H4"	"	1	1.008	1
atom	833	823	C5t	"POPS acyl chainab C5"	"	6	12.011	4
atom	834	824	H5t	"POPS acyl chainab H5"	"	1	1.008	1
atom	835	823	C6t	"POPS acyl chainab C6"	"	6	12.011	4
atom	836	824	H6t	"POPS acyl chainab H6"	"	1	1.008	1
atom	837	823	C7t	"POPS acyl chainab C7"	"	6	12.011	4
atom	838	824	H7t	"POPS acyl chainab H7"	"	1	1.008	1
atom	839	823	C8t	"POPS acyl chainab C8"	"	6	12.011	4
atom	840	824	H8t	"POPS acyl chainab H8"	"	1	1.008	1
atom	841	823	C9t	"POPS acyl chainab C9"	"	6	12.011	4
atom	842	824	H9t	"POPS acyl chainab H9"	"	1	1.008	1
atom	843	823	C10	"POPS acyl chainab C10"	"	6	12.011	4
atom	844	824	H10	"POPS acyl chainab H10"	"	1	1.008	1
atom	845	823	C11	"POPS acyl chainab C11"	"	6	12.011	4

atom	846	824	H11	"POPS acyl chainab H11"	1	1.008	1
atom	847	823	C12	"POPS acyl chainab C12"	6	12.011	4
atom	848	824	H12	"POPS acyl chainab H12"	1	1.008	1
atom	849	823	C13	"POPS acyl chainab C13"	6	12.011	4
atom	850	824	H13	"POPS acyl chainab H13"	1	1.008	1
atom	851	823	C14	"POPS acyl chainab C14"	6	12.011	4
atom	852	824	H14	"POPS acyl chainab H14"	1	1.008	1
atom	853	823	C15	"POPS acyl chainab C15"	6	12.011	4
atom	854	824	H15	"POPS acyl chainab H15"	1	1.008	1
atom	855	825	C16	"POPS acyl chainab C16"	6	12.011	4
atom	856	826	H16	"POPS acyl chainab H16"	1	1.008	1
atom	857	823	C3b	"POPS acyl chainb C3"	6	12.011	4
atom	858	824	H3b	"POPS acyl chainb H3"	1	1.008	1
atom	859	823	C4b	"POPS acyl chainb C4"	6	12.011	4
atom	860	824	H4b	"POPS acyl chainb H4"	1	1.008	1
atom	861	823	C5b	"POPS acyl chainb C5"	6	12.011	4
atom	862	824	H5b	"POPS acyl chainb H5"	1	1.008	1
atom	863	823	C6b	"POPS acyl chainb C6"	6	12.011	4
atom	864	824	H6b	"POPS acyl chainb H6"	1	1.008	1
atom	865	823	C7b	"POPS acyl chainb C7"	6	12.011	4
atom	866	824	H7b	"POPS acyl chainb H7"	1	1.008	1
atom	867	823	C8b	"POPS acyl chainb C8"	6	12.011	4
atom	868	824	H8b	"POPS acyl chainb H8"	1	1.008	1
atom	869	827	C9b	"POPS acyl chainb C9"	6	12.011	3
atom	870	828	H9b	"POPS acyl chainb H9"	1	1.008	1
atom	871	827	C10	"POPS acyl chainb C10"	6	12.011	3
atom	872	828	H10	"POPS acyl chainb H10"	1	1.008	1
atom	873	823	C11	"POPS acyl chainb C11"	6	12.011	4
atom	874	824	H11	"POPS acyl chainb H11"	1	1.008	1
atom	875	823	C12	"POPS acyl chainb C12"	6	12.011	4
atom	876	824	H12	"POPS acyl chainb H12"	1	1.008	1
atom	877	823	C13	"POPS acyl chainb C13"	6	12.011	4
atom	878	824	H13	"POPS acyl chainb H13"	1	1.008	1
atom	879	823	C14	"POPS acyl chainb C14"	6	12.011	4
atom	880	824	H14	"POPS acyl chainb H14"	1	1.008	1
atom	881	823	C15	"POPS acyl chainb C15"	6	12.011	4
atom	882	824	H15	"POPS acyl chainb H15"	1	1.008	1
atom	883	823	C16	"POPS acyl chainb C16"	6	12.011	4
atom	884	824	H16	"POPS acyl chainb H16"	1	1.008	1
atom	885	823	C17	"POPS acyl chainb C17"	6	12.011	4
atom	886	824	H17	"POPS acyl chainb H17"	1	1.008	1
atom	887	825	C18	"POPS acyl chainb C18"	6	12.011	4
atom	888	826	H18	"POPS acyl chainb H18"	1	1.008	1

```
#####
##                                     ##
##  Van der Waals Parameters  ##
##                                     ##
#####
```

vdw	801	3.7100	0.1050
vdw	802	2.4800	0.0115 0.900
vdw	803	3.6500	0.1010
vdw	804	2.9800	0.0240 0.940
vdw	805	3.8200	0.1060
vdw	806	3.4500	0.1120
vdw	807	3.8200	0.1010
vdw	808	2.9800	0.0240 0.940
vdw	809	4.4500	0.3900
vdw	810	3.6300	0.1120
vdw	811	3.4050	0.1100
vdw	812	3.8200	0.1010
vdw	813	2.9800	0.0240 0.940
vdw	814	3.6500	0.1010
vdw	815	2.9800	0.0240 0.940
vdw	816	3.4050	0.1100
vdw	817	3.8200	0.1060
vdw	818	3.3000	0.1120
vdw	819	3.8200	0.1010
vdw	820	2.9800	0.0240 0.940
vdw	821	3.8200	0.1010
vdw	822	2.9800	0.0240 0.940
vdw	823	3.8200	0.1010
vdw	824	2.9600	0.0240 0.920
vdw	825	3.8200	0.1010
vdw	825	2.9600	0.0240 0.920
vdw	827	3.6500	0.1010
vdw	828	2.5830	0.0260 0.920

```
#####
##                                     ##
##  Bond Stretching Parameters  ##
##                                     ##
#####
```

bond	801	803	381.3	1.4911
bond	801	802	461.9	1.0133
bond	803	805	323.0	1.5570
bond	803	804	341.0	1.0811

bond	805	806	601.8	1.2196
bond	807	803	323.0	1.5251
bond	807	811	465.1	1.4088
bond	807	808	341.0	1.0821
bond	809	811	450.0	1.6343
bond	809	810	775.0	1.4860
bond	812	811	465.1	1.4016
bond	812	813	341.0	1.0808
bond	814	812	323.0	1.5197
bond	814	821	323.0	1.5141
bond	814	816	465.1	1.4302
bond	814	815	341.0	1.0779
bond	817	816	465.1	1.3201
bond	817	818	601.8	1.1909
bond	819	823	323.0	1.5233
bond	819	817	345.3	1.5113
bond	819	820	341.0	1.0858
bond	821	816	465.1	1.4270
bond	821	822	341.0	1.0783
bond	819	823	323.0000	1.5231
bond	823	824	341.0000	1.0832
bond	823	825	323.0000	1.5299
bond	823	823	453.0000	1.5247
bond	825	826	341.0000	1.0861
bond	823	827	323.0000	1.5053
bond	827	827	680.0000	1.3201
bond	827	828	341.0000	1.0810

```
#####
##                                     ##
##  Angle Bending Parameters  ##
##                                     ##
#####
```

angle	803	801	802	35.0000	110.9636
angle	802	801	802	34.5000	107.7790
angle	807	803	801	80.0000	109.9757
angle	807	803	805	60.0000	114.3450
angle	807	803	804	38.0000	110.0352
angle	801	803	805	80.0000	107.7150
angle	801	803	804	50.6000	105.0679
angle	805	803	804	38.0000	109.2687
angle	803	805	806	60.0000	113.4509
angle	806	805	806	57.6000	131.7978
angle	803	807	811	88.0000	113.6748
angle	803	807	808	38.0000	109.6972
angle	811	807	808	60.9900	105.8027
angle	808	807	808	39.5700	107.7343

angle	811	809	811	65.5800	100.9105
angle	811	809	810	75.8600	107.4376
angle	810	809	810	89.8800	123.0639
angle	807	811	809	80.3000	125.5126
angle	812	811	809	80.3000	119.2241
angle	814	812	811	88.0000	111.0121
angle	814	812	813	38.0000	108.9565
angle	811	812	813	60.9900	111.1250
angle	813	812	813	39.5700	108.7747
angle	812	814	821	60.0000	113.1399
angle	812	814	816	88.0000	106.2392
angle	812	814	815	38.0000	109.1733
angle	821	814	816	88.0000	110.6641
angle	821	814	815	38.0000	108.2292
angle	816	814	815	60.9900	109.3395
angle	821	816	817	88.5000	118.1296
angle	814	816	817	88.5000	119.4902
angle	819	817	816	60.0000	111.0770
angle	819	817	818	60.0000	124.9245
angle	816	817	818	50.0000	123.9986
angle	823	819	817	48.2000	113.1038
angle	823	819	820	38.0000	111.3933
angle	817	819	820	38.0000	107.4530
angle	820	819	820	45.5700	105.8127
angle	814	821	816	88.0000	108.5232
angle	814	821	822	38.0000	111.0377
angle	816	821	822	60.9900	109.5067
angle	822	821	822	39.5700	108.6681
angle	819	823	824	38.0000	107.9848
angle	823	823	824	37.9900	109.4700
angle	824	823	825	37.9900	109.3700
angle	819	823	823	48.2000	112.2989
angle	823	823	825	48.2900	112.8700
angle	824	823	824	39.6600	106.2700
angle	823	825	826	42.4200	111.2700
angle	826	825	826	39.5100	107.6500
angle	823	823	827	48.2000	112.8390
angle	823	827	827	60.0000	125.4116
angle	823	827	828	32.0000	115.6966
angle	827	827	828	32.0000	118.8892
angle	824	823	827	38.0000	108.7346
angle	823	823	823	48.2500	113.3100

#####

##

Stretch-Bend Parameters

##

#####

strbnd	803	801	802	4.3000	14.4000
strbnd	807	803	801	18.7000	18.7000
strbnd	807	803	805	18.7000	18.7000
strbnd	807	803	804	11.5000	18.7000
strbnd	801	803	805	18.7000	18.7000
strbnd	801	803	804	11.5000	11.5000
strbnd	805	803	804	11.5000	18.7000
strbnd	803	805	806	18.7000	18.7000
strbnd	803	807	811	18.7000	18.7000
strbnd	803	807	805	11.5000	18.7000
strbnd	811	807	805	-4.5000	38.0000
strbnd	811	809	811	14.4000	14.4000
strbnd	811	809	810	14.4000	14.4000
strbnd	812	811	809	38.0000	38.0000
strbnd	807	811	809	38.0000	38.0000
strbnd	814	812	811	18.7000	18.7000
strbnd	814	812	813	11.5000	18.7000
strbnd	811	812	813	-4.5000	38.0000
strbnd	812	814	821	18.7000	18.7000
strbnd	812	814	816	18.7000	18.7000
strbnd	812	814	815	11.5000	18.7000
strbnd	821	814	816	18.7000	18.7000
strbnd	821	814	815	11.5000	18.7000
strbnd	816	814	815	-4.5000	38.0000
strbnd	821	816	817	38.0000	38.0000
strbnd	814	816	817	38.0000	38.0000
strbnd	819	817	816	18.7000	18.7000
strbnd	823	819	817	18.7000	18.7000
strbnd	823	819	820	11.5000	18.7000
strbnd	817	819	820	11.5000	18.7000
strbnd	814	821	816	18.7000	18.7000
strbnd	814	821	822	11.5000	18.7000
strbnd	816	821	822	-4.5000	38.0000
strbnd	819	823	824	11.5000	11.5000
strbnd	823	823	823	18.70	18.70
strbnd	823	823	824	11.50	18.70
strbnd	825	823	824	11.50	18.70
strbnd	819	823	823	18.70	18.70
strbnd	823	823	825	18.70	18.70
strbnd	823	825	826	11.50	11.50

#####

##

Out-of-Plane Bend Parameters

##

#####

opbend	803	805	0	0	0.2002
opbend	806	805	0	0	0.2002
opbend	816	817	0	0	0.2002
opbend	818	817	0	0	0.6500
opbend	819	817	0	0	0.2002

```
#####
##                               ##
##  Torsional Parameters  ##
##                               ##
#####
```

torsion	802	801	803	807	0.000 0.0 1	1.000 180.0 2	0.500 0.0 3
torsion	802	801	803	805	0.000 0.0 1	1.000 180.0 2	0.500 0.0 3
torsion	802	801	803	804	0.000 0.0 1	0.661 180.0 2	0.288 0.0 3
torsion	807	803	805	806	0.649 0.0 1	3.076 180.0 2	4.783 0.0 3
torsion	801	803	805	806	-1.896 0.0 1	5.784 180.0 2	-4.176 0.0 3
torsion	804	803	805	806	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	811	807	803	801	0.000 0.0 1	-1.400 180.0 2	9.613 0.0 3
torsion	811	807	803	805	-1.717 0.0 1	0.000 180.0 2	-7.740 0.0 3
torsion	811	807	803	804	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	808	807	803	801	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	808	807	803	805	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	808	807	803	804	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	803	807	811	809	4.989 0.0 1	1.184 180.0 2	1.523 0.0 3
torsion	808	807	811	809	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	811	809	811	807	8.083 0.0 1	-1.836 180.0 2	2.637 0.0 3
torsion	810	809	811	807	0.000 0.0 1	0.000 180.0 2	0.061 0.0 3
torsion	811	809	811	812	8.083 0.0 1	-1.836 180.0 2	2.637 0.0 3
torsion	810	809	811	812	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	814	812	811	809	1.011 0.0 1	0.081 180.0 2	-0.532 0.0 3
torsion	813	812	811	809	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	821	814	812	811	-2.039 0.0 1	4.842 180.0 2	0.000 0.0 3
torsion	821	814	812	813	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	816	814	812	811	-0.776 0.0 1	1.983 180.0 2	0.000 0.0 3
torsion	816	814	812	813	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	815	814	812	811	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	815	814	812	813	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	812	814	821	816	-1.784 0.0 1	0.170 180.0 2	0.000 0.0 3
torsion	812	814	821	822	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	816	814	821	816	-2.407 0.0 1	-0.682 180.0 2	0.000 0.0 3
torsion	816	814	821	822	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	815	814	821	816	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	815	814	821	822	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	812	814	816	817	3.811 0.0 1	-1.403 180.0 2	0.000 0.0 3
torsion	821	814	816	817	4.577 0.0 1	-1.750 180.0 2	0.000 0.0 3
torsion	815	814	816	817	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3

torsion	819	817	816	821	0.000 0.0 1	5.989 180.0 2	0.000 0.0 3
torsion	818	817	816	821	0.000 0.0 1	5.989 180.0 2	0.000 0.0 3
torsion	819	817	816	814	0.000 0.0 1	5.789 180.0 2	0.000 0.0 3
torsion	818	817	816	814	0.000 0.0 1	5.789 180.0 2	0.000 0.0 3
torsion	820	819	817	816	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	820	819	817	818	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	814	821	816	817	-0.118 0.0 1	-0.259 180.0 2	-0.230 0.0 3
torsion	822	821	816	817	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	816	817	819	823	1.231 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	818	817	819	823	0.000 0.0 1	-0.039 180.0 2	0.000 0.0 3
torsion	816	817	816	823	0.000 0.0 1	-0.039 180.0 2	0.000 0.0 3
torsion	817	819	823	823	1.532 0.0 1	-1.981 180.0 2	1.641 0.0 3
torsion	820	819	823	823	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	817	819	823	824	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	820	819	823	824	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	819	823	823	823	2.818 0.0 1	-0.410 180.0 2	2.472 0.0 3
torsion	819	823	823	824	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	823	823	823	824	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	823	823	823	823	0.568 0.0 1	-0.375 180.0 2	2.302 0.0 3
torsion	823	823	823	825	0.717 0.0 1	-0.133 180.0 2	1.123 0.0 3
torsion	824	823	823	824	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	826	825	823	823	0.000 0.0 1	0.000 180.0 2	0.341 0.0 3
torsion	826	825	823	824	0.000 0.0 1	0.000 180.0 2	0.299 0.0 3
torsion	824	823	823	825	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	823	827	827	823	0.000 0.0 1	8.000 180.0 2	0.000 0.0 3
torsion	823	823	827	827	2.775 0.0 1	-0.695 180.0 2	-1.271 0.0 3
torsion	823	827	827	828	0.000 0.0 1	6.100 180.0 2	0.000 0.0 3
torsion	828	827	827	828	0.000 0.0 1	4.070 180.0 2	0.000 0.0 3
torsion	823	823	827	828	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	824	823	823	827	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	823	823	823	827	0.649 0.0 1	0.419 180.0 2	2.472 0.0 3
torsion	824	823	827	827	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3
torsion	824	823	827	828	0.000 0.0 1	0.000 180.0 2	0.000 0.0 3

```
#####
##                                     ##
##  Atomic Multipole Parameters  ##
##                                     ##
#####
```

multipole	801	803	802	0.15009		
				0.00000	0.00000	0.39088
				-0.31903		
				0.00000	-0.46883	
				0.00000	0.00000	0.78786

multipole	802	801	803	0.19148		
				0.00205	0.00000	-0.11665
				-0.12490		
				0.00000	0.00289	
multipole	803	807	801	0.00403	0.00000	0.12201
				-0.33444		
				0.10140	0.00000	0.26744
				0.69333		
multipole	804	803	807	0.00000	-0.87872	
				-0.46582	0.00000	0.18539
				0.07315		
				-0.04502	0.00000	-0.15377
multipole	805	806	-806	0.06032		
				0.00000	0.12156	
				-0.11208	0.00000	-0.18188
				1.09754		
multipole	806	805	806	0.00000	0.00000	-0.06279
				-0.56105		
				0.00000	-0.33758	
				0.00000	0.00000	0.89863
multipole	807	803	811	-0.80443		
				0.00000	0.00000	-0.07425
				-0.31203		
				0.00000	0.04975	
multipole	808	807	803	0.00000	0.00000	0.26228
				0.12827		
				0.37502	0.00000	0.06061
				0.20110		
multipole	809	810	-810	0.00000	-0.48816	
				-0.36209	0.00000	0.28706
				0.02153		
				0.01173	0.00000	-0.07125
multipole	810	809	810	0.00617		
				0.00000	0.00959	
				-0.04033	0.00000	-0.01576
				1.75597		
multipole	811	807	809	0.00000	0.00000	-0.03715
				0.41622		
				0.00000	0.35763	
				0.00000	0.00000	-0.77385
multipole	811	807	809	-0.94589		
				0.00000	0.00000	-0.03105
				-0.08297		
				0.00000	-0.26637	
multipole	811	807	809	0.00000	0.00000	0.34934
				-0.53707		
				0.01649	0.00000	0.42047
				-0.42634		
				0.00000	-0.64972	

multipole	812	813	809	-0.44476	0.00000	1.07606
				-0.53707		
				0.05695	0.00000	0.47693
				0.28714		
multipole	813	815	812	0.00000	-0.72246	
				-0.19766	0.00000	0.43532
				0.12827		
				0.34076	0.00000	0.07223
multipole	814	813	815	0.13762		
				0.00000	-0.55896	
				-0.19291	0.00000	0.42134
				0.02153		
multipole	815	813	822	0.03021	0.00000	-0.06371
				0.05822		
				0.00000	-0.03614	
				-0.10939	0.00000	-0.02208
multipole	816	815	813	0.02757		
				0.12524	0.00000	0.12788
				-0.17310		
				0.00000	0.01627	
multipole	817	815	818	-0.12352	0.00000	0.15683
				0.08536		
				-0.07809	0.00000	0.01361
				0.00564		
multipole	818	820	817	0.00000	-0.05585	
				-0.19930	0.00000	0.05021
				-0.29085		
				0.12793	0.00000	0.43009
multipole	819	818	820	-0.41410		
				0.00000	-0.45847	
				-0.01045	0.00000	0.87257
				0.78775		
multipole	820	857	818	0.00714	0.00000	-0.23085
				0.35926		
				0.00000	-0.09910	
				-0.13018	0.00000	-0.26016
multipole	821	820	857	-0.62759		
				0.07317	0.00000	-0.02732
				-0.38754		
				0.00000	0.12847	
multipole	822	813	809	0.19485	0.00000	0.25907
				-0.15540		
				0.15356	0.00000	0.19795
				0.12509		
multipole	823	815	812	0.00000	-0.37752	
				-0.23203	0.00000	0.25243
				0.08635		
				0.03876	0.00000	-0.07943
multipole	824	813	809	0.01560		

multipole	822	815	824	0.00000	0.05741	
				0.13378	0.00000	-0.07301
				0.08475		
				0.37847	0.00000	0.14032
multipole	823	822	815	0.50696		
				0.00000	-0.25857	
				-0.38564	0.00000	-0.24839
				0.03662		
multipole	824	822	825	-0.07725	0.00000	-0.09404
				-0.06019		
				0.00000	0.10374	
				-0.09173	0.00000	-0.04355
multipole	825	827	824	-0.36432		
				0.09158	0.00000	0.29562
				-0.05455		
				0.00000	-0.48997	
multipole	826	825	827	-0.00432	0.00000	0.54452
				0.96653		
				-0.14867	0.00000	0.00065
				0.62223		
multipole	827	829	825	0.00000	-0.34695	
				-0.41223	0.00000	-0.27528
				-0.67293		
				-0.07701	0.00000	-0.08391
multipole	828	827	829	-0.22330		
				0.00000	0.13331	
				0.00013	0.00000	0.08999
				-0.33708		
multipole	829	831	827	-0.08126	0.00000	0.29167
				-0.14312		
				0.00000	-0.02152	
				0.23449	0.00000	0.16464
multipole	830	829	831	0.08282		
				0.07172	0.00000	-0.10755
				-0.01476		
				0.00000	0.11799	
multipole	831	829	833	0.17685	0.00000	-0.10323
				-0.12028		
				0.00000	0.00000	-0.27624
				-0.28898		
multipole	833	829	835	0.00000	0.27171	
				0.00000	0.00000	0.01727
				0.06014		
				0.02626	0.00000	0.09284
multipole	835	829	837	-0.09440		
				0.00000	-0.11726	
				-0.04794	0.00000	0.21166
				-0.12028		
multipole	837	829	839	0.00000	0.00000	0.02019

				0.23109		
				0.00000	0.51643	
				0.00000	0.00000	-0.74752
multipole	832	831	829	0.06014		
				-0.02225	0.00000	-0.03876
				0.16126		
				0.00000	-0.12762	
multipole	833	835	831	-0.09711	0.00000	-0.03364
				-0.12028		
				0.00000	0.00000	0.38294
				-0.23632		
				0.00000	0.09598	
multipole	834	833	835	0.00000	0.00000	0.14034
				0.06014		
				-0.05338	0.00000	-0.05236
				0.05217		
				0.00000	-0.03071	
multipole	835	833	837	-0.00241	0.00000	-0.02146
				-0.12028		
				0.00000	0.00000	0.08043
				-0.28788		
				0.00000	0.15240	
multipole	836	835	833	0.00000	0.00000	0.13548
				0.06014		
				0.01189	0.00000	0.06548
				-0.04124		
				0.00000	-0.12950	
multipole	837	839	835	0.02846	0.00000	0.17074
				-0.12028		
				0.00000	0.00000	0.19119
				-0.24827		
				0.00000	0.18257	
multipole	838	837	839	0.00000	0.00000	0.06570
				0.06014		
				-0.01631	0.00000	0.07167
				-0.05599		
				0.00000	-0.10649	
multipole	839	837	-841	-0.00219	0.00000	0.16248
				-0.12028		
				0.00000	0.00000	0.16276
				0.40325		
				0.00000	-0.24444	
multipole	840	839	841	0.00000	0.00000	-0.15881
				0.06014		
				0.01220	0.00000	0.06285
				-0.12021		
				0.00000	-0.07078	
multipole	841	843	839	0.02300	0.00000	0.19099
				-0.12028		

				0.00000	0.00000	-0.00371
				-0.27290		
				0.00000	0.24262	
				0.00000	0.00000	0.03028
multipole	842	841	839	0.06014		
				0.00111	0.00000	0.17584
				-0.11309		
				0.00000	-0.19933	
				0.02464	0.00000	0.31242
multipole	843	845	841	-0.12028		
				0.00000	0.00000	-0.03035
				-0.38338		
				0.00000	-0.11244	
				0.00000	0.00000	0.49582
multipole	844	843	845	0.06014		
				0.10649	0.00000	0.17604
				-0.15014		
				0.00000	-0.17048	
				0.15885	0.00000	0.32062
multipole	845	843	-847	-0.12028		
				0.00000	0.00000	0.21358
				0.41809		
				0.00000	-0.33917	
				0.00000	0.00000	-0.07892
multipole	846	845	847	0.06014		
				-0.01053	0.00000	0.17164
				-0.21578		
				0.00000	-0.14027	
				-0.02295	0.00000	0.35605
multipole	847	849	845	-0.12028		
				0.00000	0.00000	0.08114
				-0.43635		
				0.00000	0.13193	
				0.00000	0.00000	0.30442
multipole	848	847	849	0.06014		
				0.01274	0.00000	0.26178
				-0.22740		
				0.00000	-0.24814	
				0.04916	0.00000	0.47554
multipole	849	847	851	-0.12028		
				0.00000	0.00000	0.28031
				0.20634		
				0.00000	-0.50100	
				0.00000	0.00000	0.29466
multipole	850	849	851	0.06014		
				0.04950	0.00000	0.14333
				-0.14948		
				0.00000	-0.16464	
				-0.00394	0.00000	0.31412

multipole	851	849	-853	-0.12028		
				0.00000	0.00000	0.10812
				0.17407		
				0.00000	0.10057	
multipole	852	851	853	0.00000	0.00000	-0.27464
				0.06014		
				-0.00763	0.00000	0.14643
				-0.13955		
multipole	853	851	855	0.00000	-0.13611	
				0.00017	0.00000	0.27566
				-0.12028		
				0.25888	0.00000	-0.07373
multipole	854	853	855	-0.40444		
				0.00000	0.18904	
				-0.17448	0.00000	0.21540
				0.06014		
multipole	855	853	856	-0.11707	0.00000	0.13841
				-0.14215		
				0.00000	-0.15682	
				-0.13312	0.00000	0.29897
multipole	856	855	853	-0.16638		
				0.00000	0.00000	0.17570
				-0.11035		
				0.00000	-0.08951	
multipole	857	859	820	0.00000	0.00000	0.19986
				0.05546		
				0.00839	0.00000	0.05163
				-0.07452		
multipole	858	857	859	0.00000	-0.10058	
				0.02040	0.00000	0.17510
				-0.12028		
				0.00000	0.00000	0.16483
multipole	859	861	857	-0.34157		
				0.00000	0.29032	
				0.00000	0.00000	0.05125
				0.06014		
multipole	860	859	857	-0.09385	0.00000	0.06163
				-0.05752		
				0.00000	-0.11452	
				-0.16015	0.00000	0.17204
multipole	861	859	857	-0.12028		
				0.00000	0.00000	0.21055
				0.06973		
				0.00000	-0.16737	
multipole	862	859	857	0.00000	0.00000	0.09764
				0.06014		
				0.11641	0.00000	-0.06467
				0.17364		
multipole	863	859	857	0.00000	-0.07819	

multipole	861	863	859	0.11793	0.00000	-0.09545
				-0.12028		
				0.00000	0.00000	0.22207
				-0.45142		
multipole	862	861	863	0.00000	0.12922	
				0.00000	0.00000	0.32220
				0.06014		
				-0.05716	0.00000	0.04611
multipole	863	861	-865	-0.08401		
				0.00000	-0.02608	
				-0.12239	0.00000	0.11009
				-0.12028		
multipole	864	863	865	0.00000	0.00000	0.24675
				0.81584		
				0.00000	-0.41153	
				0.00000	0.00000	-0.40431
multipole	865	863	867	0.06014		
				0.00068	0.00000	-0.06235
				0.06236		
				0.00000	0.04198	
multipole	866	865	863	0.01631	0.00000	-0.10434
				-0.12028		
				0.00000	0.00000	0.26583
				-0.29207		
multipole	867	865	869	0.00000	-0.09693	
				0.00000	0.00000	0.38900
				0.06014		
				-0.01064	0.00000	-0.01444
multipole	868	867	865	-0.04530		
				0.00000	-0.02924	
				-0.01287	0.00000	0.07454
				-0.08684		
multipole	869	867	871	0.16232	0.00000	0.16012
				0.20689		
				0.00000	0.04491	
				-0.27071	0.00000	-0.25180
multipole	870	869	867	0.06914		
				-0.02374	0.00000	-0.10784
				0.13103		
				0.00000	0.01169	
multipole	870	869	867	0.00244	0.00000	-0.14272
				-0.10494		
				0.01927	0.00000	0.13175
				-0.00325		
multipole	870	869	867	0.00000	-0.10324	
				0.23581	0.00000	0.10649
				0.05350		
				0.01400	0.00000	-0.09671
				0.11469		

multipole	871	873	869	0.00000	-0.06088	
				-0.00053	0.00000	-0.05381
				-0.10494		
				0.01803	0.00000	0.12881
				0.07379		
multipole	872	871	873	0.00000	-0.16541	
				0.22004	0.00000	0.09162
				0.05350		
				0.01945	0.00000	-0.10314
				0.15986		
multipole	873	875	871	0.00000	-0.05584	
				0.01670	0.00000	-0.10402
				-0.08684		
				0.15984	0.00000	0.15576
				0.15285		
multipole	874	873	875	0.00000	-0.00851	
				-0.33188	0.00000	-0.14434
				0.06914		
				-0.02413	0.00000	-0.11505
				0.10858		
multipole	875	877	873	0.00000	0.03784	
				-0.01793	0.00000	-0.14642
				-0.12028		
				0.00000	0.00000	0.26690
				-0.09146		
multipole	876	875	877	0.00000	0.03942	
				0.00000	0.00000	0.05204
				0.06014		
				-0.02429	0.00000	-0.00551
				-0.01934		
multipole	877	875	-879	0.00000	-0.04490	
				-0.01314	0.00000	0.06424
				-0.12028		
				0.00000	0.00000	0.26491
				0.48080		
multipole	878	877	879	0.00000	-0.40857	
				0.00000	0.00000	-0.07223
				0.06014		
				0.00166	0.00000	-0.04633
				0.02742		
multipole	879	877	881	0.00000	0.02210	
				-0.03703	0.00000	-0.04952
				-0.12028		
				0.00000	0.00000	0.25521
				-0.24375		
multipole	880	879	877	0.00000	0.21673	
				0.00000	0.00000	0.02702
				0.06014		
				-0.04480	0.00000	0.03903

multipole	881	879	883	-0.05620		
				0.00000	-0.05569	
				-0.04031	0.00000	0.11189
				-0.12028		
				0.00000	0.00000	0.20623
multipole	882	881	883	0.13103		
				0.00000	-0.20157	
				0.00000	0.00000	0.07054
				0.06014		
				0.12155	0.00000	-0.09278
multipole	883	881	885	0.12585		
				0.00000	0.02360	
				0.18633	0.00000	-0.14945
				-0.12028		
				0.00000	0.00000	0.25000
multipole	884	883	885	0.29752		
				0.00000	-0.37898	
				0.00000	0.00000	0.08146
				0.06014		
				0.02573	0.00000	-0.10674
multipole	885	883	887	0.10417		
				0.00000	0.02370	
				0.02516	0.00000	-0.12787
				-0.12028		
				0.30410	0.00000	0.17140
multipole	886	885	887	0.08329		
				0.00000	-0.50724	
				-0.27934	0.00000	0.42395
				0.06014		
				0.02307	0.00000	-0.14797
multipole	887	885	888	0.11998		
				0.00000	0.08791	
				0.03663	0.00000	-0.20789
				-0.16638		
				0.00000	0.00000	0.25061
multipole	888	887	885	-0.29507		
				0.00000	-0.32451	
				0.00000	0.00000	0.61958
				0.05546		
				0.00780	0.00000	-0.07615
				-0.01142		
				0.00000	0.03391	
				-0.02243	0.00000	-0.02249

```
#####
##                                     ##
```

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##  Dipole Polarizability Parameters  ##
##                                     ##
#####

```

polarize	801	1.073	0.390	802 803
polarize	802	0.496	0.390	801
polarize	803	1.334	0.390	801 804 805
polarize	804	0.496	0.390	803
polarize	805	1.334	0.390	803 806
polarize	806	0.921	0.390	805
polarize	807	1.334	0.390	808 811
polarize	808	0.496	0.390	807
polarize	809	1.828	0.390	810 811 812
polarize	810	0.837	0.390	809
polarize	811	0.837	0.390	807 809
polarize	812	0.837	0.390	809 813
polarize	813	1.334	0.390	812 814
polarize	814	0.496	0.390	813
polarize	815	1.334	0.390	816 817
polarize	816	0.496	0.390	815
polarize	817	0.837	0.390	815 818
polarize	818	1.334	0.390	817 819 820
polarize	819	0.837	0.390	818
polarize	820	1.334	0.390	818 821
polarize	821	0.496	0.390	820
polarize	822	1.334	0.390	823 824
polarize	823	0.496	0.390	822
polarize	824	0.837	0.390	822 825
polarize	825	1.334	0.390	824 826 827
polarize	826	0.837	0.390	825
polarize	827	1.334	0.390	825 828
polarize	828	0.496	0.390	827
polarize	829	1.334	0.390	830 831
polarize	830	0.496	0.390	829
polarize	831	1.334	0.390	829 832
polarize	832	0.496	0.390	831
polarize	833	1.334	0.390	834 835
polarize	834	0.496	0.390	833
polarize	835	1.334	0.390	833 836
polarize	836	0.496	0.390	835
polarize	837	1.334	0.390	838 839
polarize	838	0.496	0.390	837
polarize	839	1.334	0.390	837 840
polarize	840	0.496	0.390	839
polarize	841	1.334	0.390	842 843
polarize	842	0.496	0.390	841
polarize	843	1.334	0.390	841 844
polarize	844	0.496	0.390	843

polarize	845	1.334	0.390	846
polarize	846	0.496	0.390	845
polarize	847	1.334	0.390	848 849
polarize	848	0.496	0.390	847
polarize	849	1.334	0.390	847 850
polarize	850	0.496	0.390	849
polarize	851	1.334	0.390	852
polarize	852	0.496	0.390	851
polarize	853	1.334	0.390	854 855
polarize	854	0.496	0.390	853
polarize	855	1.334	0.390	853 856
polarize	856	0.496	0.390	855
polarize	857	1.334	0.390	858
polarize	858	0.496	0.390	857
polarize	859	1.334	0.390	860 861
polarize	860	0.496	0.390	859
polarize	861	1.334	0.390	859 862
polarize	862	0.496	0.390	861
polarize	863	1.334	0.390	864 865
polarize	864	0.496	0.390	863
polarize	865	1.334	0.390	863 866
polarize	866	0.496	0.390	865
polarize	867	1.334	0.390	868
polarize	868	0.496	0.390	867
polarize	869	1.334	0.390	870 871
polarize	870	0.496	0.390	869
polarize	871	1.334	0.390	869 872
polarize	872	0.496	0.390	871
polarize	873	1.334	0.390	874
polarize	874	0.496	0.390	873
polarize	875	1.334	0.390	876 877
polarize	876	0.496	0.390	875
polarize	877	1.334	0.390	875 878
polarize	878	0.496	0.390	877
polarize	879	1.334	0.390	880 881
polarize	880	0.496	0.390	879
polarize	881	1.334	0.390	879 882
polarize	882	0.496	0.390	881
polarize	883	1.334	0.390	884
polarize	884	0.496	0.390	883
polarize	885	1.334	0.390	886 887
polarize	886	0.496	0.390	885
polarize	887	1.334	0.390	885 888
polarize	888	0.496	0.390	887