Supplementary Data

Molecular dynamics simulation studies on the structure and the antifouling performance of the gradient polyamide membrane

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Contents

1. Molecular structures of organic foulants used in the Research

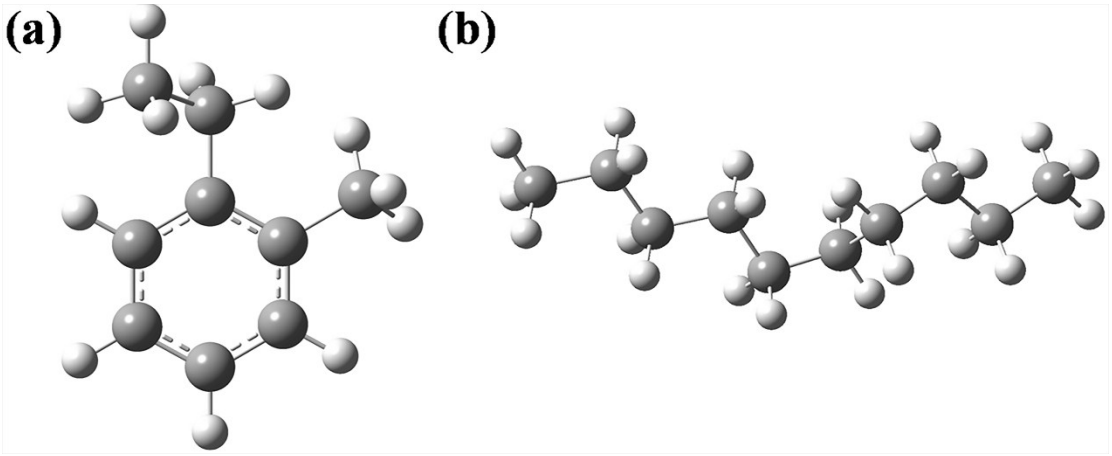
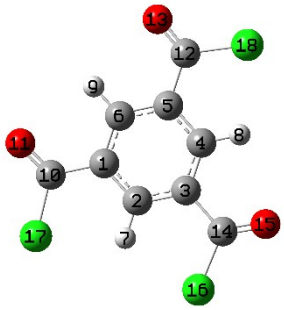


Fig. S1 The molecular structures of (a) 1-ethyl-2-methyl benzene and (b) n-decane, where gray represents carbon atom and white represents hydrogen atom.

2. Force field parameter files



TMC.itp

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ha	ha	0.0000	0.0000	A	2.59964e-01	6.27600e-02
ca	ca	0.0000	0.0000	A	3.39967e-01	3.59824e-01
o	o	0.0000	0.0000	A	2.95992e-01	8.78640e-01

[moleculetype]

; monomer_name	nrexcl
TMC	3

[atoms]

; atom_number	type	resnr	residue	atom	cgnr	charge	mass
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3	ca	1	TMC	C2	3	0.0272	12.000000
4	ca	1	TMC	C3	4	-0.1339	12.000000
5	ca	1	TMC	C4	5	0.0272	12.000000
6	ca	1	TMC	C5	6	-0.1339	12.000000
7	ha	1	TMC	H	7	0.1653	1.000000
8	ha	1	TMC	H1	8	0.1653	1.000000
9	ha	1	TMC	H2	9	0.1653	1.000000
10	c	1	TMC	C6	10	0.4744	12.000000
11	o	1	TMC	O	11	-0.4030	16.000000
12	c	1	TMC	C7	12	0.4744	12.000000
13	o	1	TMC	O1	13	-0.4030	16.000000
14	c	1	TMC	C8	14	0.4744	12.000000
15	o	1	TMC	O2	15	-0.4030	16.000000
16	cl	1	TMC	Cl	16	-0.13	35.500000
17	cl	1	TMC	Cl1	17	-0.13	35.500000
18	cl	1	TMC	Cl2	18	-0.13	35.500000

[bonds]

; at.i	at.j	funct	b0(nm)	kb(kJ mol^{-1} nm^{-2})	at.i:atom_num_i
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4	8	1	1.0870e-01	2.8811e+05	
6	9	1	1.0870e-01	2.8811e+05	
1	2	1	1.3870e-01	4.0033e+05	
1	6	1	1.3870e-01	4.0033e+05	
1	10	1	1.4870e-01	2.9263e+05	
2	3	1	1.3870e-01	4.0033e+05	
3	4	1	1.3870e-01	4.0033e+05	
3	14	1	1.4870e-01	2.9263e+05	
4	5	1	1.3870e-01	4.0033e+05	
5	6	1	1.3870e-01	4.0033e+05	
5	12	1	1.4870e-01	2.9263e+05	
10	11	1	1.2140e-01	5.4225e+05	
10	17	1	1.7660e-01	2.4560e+05	
12	13	1	1.2140e-01	5.4225e+05	
12	18	1	1.7660e-01	2.4560e+05	
14	15	1	1.2140e-01	5.4225e+05	
14	16	1	1.7660e-01	2.4560e+05	

[pairs]

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7	14	1
8	14	1
8	12	1
10	9	1
9	12	1
1	4	1
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2	17	1
2	15	1
2	16	1
6	3	1
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3	12	1
4	15	1
4	16	1
4	13	1
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6	18	1

[angles]

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3	4	8	1	1.2001e+02	4.0551e+02
5	4	8	1	1.2001e+02	4.0551e+02
5	6	9	1	1.2001e+02	4.0551e+02
1	2	3	1	1.1997e+02	5.6216e+02
1	6	5	1	1.1997e+02	5.6216e+02
1	10	11	1	1.2344e+02	5.7463e+02
1	10	17	1	1.1494e+02	5.1891e+02
2	1	6	1	1.1997e+02	5.6216e+02
2	1	10	1	1.2014e+02	5.4091e+02
2	3	4	1	1.1997e+02	5.6216e+02
2	3	14	1	1.2014e+02	5.4091e+02
3	4	5	1	1.1997e+02	5.6216e+02
3	14	15	1	1.2344e+02	5.7463e+02
3	14	16	1	1.1494e+02	5.1891e+02
4	3	14	1	1.2014e+02	5.4091e+02
4	5	6	1	1.1997e+02	5.6216e+02
4	5	12	1	1.2014e+02	5.4091e+02
5	12	13	1	1.2344e+02	5.7463e+02
5	12	18	1	1.1494e+02	5.1891e+02
6	1	10	1	1.2014e+02	5.4091e+02
6	5	12	1	1.2014e+02	5.4091e+02
11	10	17	1	1.2151e+02	5.3790e+02
13	12	18	1	1.2151e+02	5.3790e+02
15	14	16	1	1.2151e+02	5.3790e+02

[dihedrals]

; at.i	at.j	at.k	at.l	funct	C0(kJ mol^{-1})	C1(kJ mol^{-1})	C2(kJ mol^{-1})	C3(kJ mol^{-1})	C4(kJ mol^{-1})	C5(kJ mol^{-1})

2	1	6	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	3	4	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	3	2	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	5	6	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	1	2	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	5	4	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
10	1	2	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
7	2	3	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
8	4	3	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
8	4	5	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
10	1	6	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
9	6	5	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	2	3	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	2	3	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	6	5	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	6	5	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	6	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	10	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	10	17	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	3	4	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	3	14	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	3	14	16	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	1	2	3	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
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3	4	5	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	3	14	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	3	14	16	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	5	12	13	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	5	12	18	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
5	4	3	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
10	1	6	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	1	10	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	1	10	17	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	5	12	13	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	5	12	18	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;

[dihedrals]

; at.i	at.j	at.k	at.l	funct	C0(kJ mol^{-1})	C1(kJ mol^{-1})	C2(kJ mol^{-1})	C3(kJ mol^{-1})	C4(kJ mol^{-1})	C5(kJ mol^{-1})	
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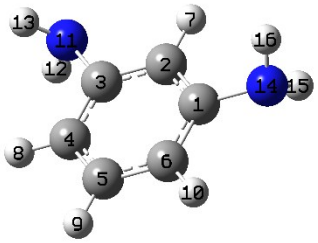
4	3	5	8	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
6	1	5	9	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
1	2	6	10	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
3	2	4	14	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;

5	4	6	12	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
10	1	17	11	3	87.86400	0.00000	-87.86400	0.00000	0.00000	0.00000	;
12	5	13	18	3	87.86400	0.00000	-87.86400	0.00000	0.00000	0.00000	;
14	3	15	16	3	87.86400	0.00000	-87.86400	0.00000	0.00000	0.00000	;



MPD.itp

[atomtypes]

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ha	ha	0.0000	0.0000	A	2.59964e-01	6.27600e-02
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ca	ca	0.0000	0.0000	A	3.39967e-01	3.59824e-01
nh	nh	0.0000	0.0000	A	3.25000e-01	7.11280e-01

[moleculetype]

; monomer_name	nrexcl
mpd	3

[atoms]

; atom_number	type	resnr	residue	atom	cgnr	charge	mass
1	ca	1	mpd	C	1	0.1078	12.000000
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3	ca	1	mpd	C2	3	0.1078	12.000000
4	ca	1	mpd	C3	4	-0.0785	12.000000
5	ca	1	mpd	C4	5	-0.3361	12.000000
6	ca	1	mpd	C5	6	-0.0785	12.000000
7	ha	1	mpd	H	7	0.1305	1.000000
8	ha	1	mpd	H1	8	0.1280	1.000000
9	ha	1	mpd	H2	9	0.1884	1.000000
10	ha	1	mpd	H3	10	0.1280	1.000000
11	nh	1	mpd	N	11	-0.8842	14.000000
12	hn	1	mpd	H4	12	0.3882	1.000000
13	hn	1	mpd	H5	13	0.3882	1.000000
14	nh	1	mpd	N1	14	-0.8842	14.000000
15	hn	1	mpd	H6	15	0.3882	1.000000
16	hn	1	mpd	H7	16	0.3882	1.000000

[bonds]

; at.i	at.j	funct	b0(nm)	kb(kJ mol^{-1} nm^{-2})	at.i:atom_num_i
2	7	1	1.0870e-01	2.8811e+05	
4	8	1	1.0870e-01	2.8811e+05	
5	9	1	1.0870e-01	2.8811e+05	
6	10	1	1.0870e-01	2.8811e+05	
11	12	1	1.0140e-01	3.3572e+05	

11	13	1	1.0140e-01	3.3572e+05
14	15	1	1.0140e-01	3.3572e+05
14	16	1	1.0140e-01	3.3572e+05
1	2	1	1.3870e-01	4.0033e+05
1	6	1	1.3870e-01	4.0033e+05
1	14	1	1.3640e-01	3.7572e+05
2	3	1	1.3870e-01	4.0033e+05
3	4	1	1.3870e-01	4.0033e+05
3	11	1	1.3640e-01	3.7572e+05
4	5	1	1.3870e-01	4.0033e+05
5	6	1	1.3870e-01	4.0033e+05

[pairs]

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14	5	1

[angles]

; at.i	at.j	at.k	funct	theta(deg)	cth(kJ mol^{-1}rad^{-2})
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1	6	10	1	1.2001e+02	4.0551e+02
1	14	15	1	1.1613e+02	4.1070e+02
1	14	16	1	1.1613e+02	4.1070e+02
3	2	7	1	1.2001e+02	4.0551e+02
3	4	8	1	1.2001e+02	4.0551e+02
3	11	12	1	1.1613e+02	4.1070e+02
3	11	13	1	1.1613e+02	4.1070e+02
4	5	9	1	1.2001e+02	4.0551e+02
5	4	8	1	1.2001e+02	4.0551e+02
5	6	10	1	1.2001e+02	4.0551e+02
6	5	9	1	1.2001e+02	4.0551e+02
12	11	13	1	1.1485e+02	3.3514e+02
15	14	16	1	1.1485e+02	3.3514e+02
1	2	3	1	1.1997e+02	5.6216e+02
1	6	5	1	1.1997e+02	5.6216e+02
2	1	6	1	1.1997e+02	5.6216e+02
2	1	14	1	1.2013e+02	5.8024e+02
2	3	4	1	1.1997e+02	5.6216e+02
2	3	11	1	1.2013e+02	5.8024e+02
3	4	5	1	1.1997e+02	5.6216e+02
4	3	11	1	1.2013e+02	5.8024e+02
4	5	6	1	1.1997e+02	5.6216e+02
6	1	14	1	1.2013e+02	5.8024e+02

[dihedrals]

; at.i	at.j	at.k	at.l	funct	C0(kJ mol^{-1})	C1(kJ mol^{-1})	C2(kJ mol^{-1})	C3(kJ mol^{-1})	C4(kJ mol^{-1})	C5(kJ mol^{-1})	
1	6	5	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	6	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	14	15	3	8.78640	0.00000	-8.78640	0.00000	0.00000	0.00000	;
2	1	14	16	3	8.78640	0.00000	-8.78640	0.00000	0.00000	0.00000	;
2	3	4	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	3	11	12	3	8.78640	0.00000	-8.78640	0.00000	0.00000	0.00000	;
2	3	11	13	3	8.78640	0.00000	-8.78640	0.00000	0.00000	0.00000	;
3	4	5	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	3	2	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	3	11	12	3	8.78640	0.00000	-8.78640	0.00000	0.00000	0.00000	;
4	3	11	13	3	8.78640	0.00000	-8.78640	0.00000	0.00000	0.00000	;
4	5	6	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	1	2	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	1	14	15	3	8.78640	0.00000	-8.78640	0.00000	0.00000	0.00000	;
6	1	14	16	3	8.78640	0.00000	-8.78640	0.00000	0.00000	0.00000	;

6	5	4	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
14	1	2	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
7	2	3	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
8	4	3	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
8	4	5	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
9	5	6	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
14	1	6	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	2	3	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	2	3	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	6	5	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	6	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
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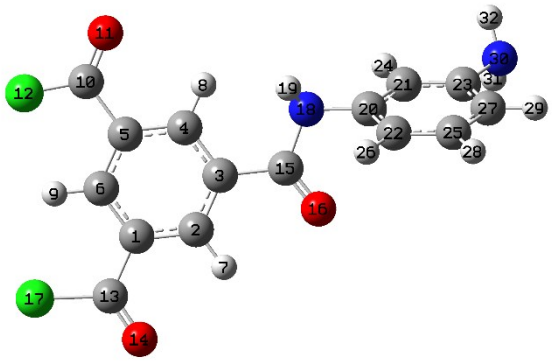
6	1	2	3	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
14	1	2	3	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
3	4	5	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
5	4	3	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
14	1	6	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;

[dihedrals]

; at.i	at.j	at.k	at.l	funct	C0(kJ mol^{-1})	C1(kJ mol^{-1})	C2(kJ mol^{-1})	C3(kJ mol^{-1})	C4(kJ mol^{-1})	C5(kJ mol^{-1})	
2	1	3	7	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
4	3	5	8	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
5	4	6	9	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
6	1	5	10	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
1	2	6	14	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
3	2	4	11	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
11	3	12	13	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
14	1	15	16	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;



TMC-MPD.itp

[atomtypes]

;name	bond_type	mass	charge	ptype	sigma	epsilon
n	n	0.0000	0.0000	A	3.25000e-01	7.11280e-01
cl	cl	0.0000	0.0000	A	3.47094e-01	1.10876e+00
ha	ha	0.0000	0.0000	A	2.59964e-01	6.27600e-02
ca	ca	0.0000	0.0000	A	3.39967e-01	3.59824e-01
hn	hn	0.0000	0.0000	A	1.06908e-01	6.56888e-02
nh	nh	0.0000	0.0000	A	3.25000e-01	7.11280e-01
c	c	0.0000	0.0000	A	3.39967e-01	3.59824e-01
o	o	0.0000	0.0000	A	2.95992e-01	8.78640e-01
cAmide	cAmide	0.0000	0.0000	A	3.39967e-01	3.59824e-01
n	n	0.0000	0.0000	A	3.25000e-01	7.11280e-01

[moleculetype]

; monomer_name	nrexcl
solute	3

[atoms]

; atom_number	type	resnr	residue	atom	cgnr	charge	mass
1	ca	1	mer	C	1	0.0272	12.000000
2	ca	1	mer	C1	2	-0.1339	12.000000
3	ca	1	mer	C2	3	-0.2263	12.000000
4	ca	1	mer	C3	4	-0.0332	12.000000
5	ca	1	mer	C4	5	0.0272	12.000000
6	ca	1	mer	C5	6	-0.1339	12.000000
7	ha	1	mer	H	7	0.1653	1.000000
8	ha	1	mer	H1	8	0.1619	1.000000
9	ha	1	mer	H2	9	0.1653	1.000000
10	c	1	mer	C6	10	0.4744	12.000000
11	o	1	mer	O	11	-0.4030	16.000000
12	cl	1	mer	Cl	12	-0.13	35.500000
13	c	1	mer	C7	13	0.4744	12.000000
14	o	1	mer	O1	14	-0.4030	16.000000

15	cAmide1	mer	C8	15	0.6638	12.000000	
16	o	1	mer	O2	16	-0.544	16.000000
17	cl	1	mer	Cl1	17	-0.13	35.500000
18	n	1	mer	N	18	-0.3872	14.000000
19	hn	1	mer	H3	19	0.2666	1.000000
20	ca	1	mer	C9	20	0.0984	12.000000
21	ca	1	mer	C10	21	-0.0818	12.000000
22	ca	1	mer	C11	22	-0.0785	12.000000
23	ca	1	mer	C12	23	0.1078	12.000000
24	ha	1	mer	H4	24	0.1305	1.000000
25	ca	1	mer	C13	25	-0.3361	12.000000
26	ha	1	mer	H5	26	0.1280	1.000000
27	ca	1	mer	C14	27	-0.0785	12.000000
28	ha	1	mer	H6	28	0.1884	1.000000
29	ha	1	mer	H7	29	0.1280	1.000000
30	nh	1	mer	N1	30	-0.8842	14.000000
31	hn	1	mer	H8	31	0.3882	1.000000
32	hn	1	mer	H9	32	0.3882	1.000000

[bonds]

; at.i	at.j	funct	b0(nm)	kb(kJ mol^{-1} nm^{-2})	at.i:atom_num_i
2	7	1	1.0870e-01	2.8811e+05	
4	8	1	1.0870e-01	2.8811e+05	
6	9	1	1.0870e-01	2.8811e+05	
18	19	1	1.0090e-01	3.4326e+05	
21	24	1	1.0870e-01	2.8811e+05	
22	26	1	1.0870e-01	2.8811e+05	
25	28	1	1.0870e-01	2.8811e+05	
27	29	1	1.0870e-01	2.8811e+05	
30	31	1	1.0140e-01	3.3572e+05	
30	32	1	1.0140e-01	3.3572e+05	
1	2	1	1.3870e-01	4.0033e+05	
1	6	1	1.3870e-01	4.0033e+05	
1	13	1	1.4870e-01	2.9263e+05	
2	3	1	1.3870e-01	4.0033e+05	
3	4	1	1.3870e-01	4.0033e+05	
3	15	1	1.4870e-01	2.9263e+05	
4	5	1	1.3870e-01	4.0033e+05	
5	6	1	1.3870e-01	4.0033e+05	
5	10	1	1.4870e-01	2.9263e+05	
10	11	1	1.2140e-01	5.4225e+05	
10	12	1	1.7660e-01	2.4560e+05	
13	14	1	1.2140e-01	5.4225e+05	
13	17	1	1.7660e-01	2.4560e+05	

15	16	1	1.2140e-01	5.4225e+05
15	18	1	1.3450e-01	4.0016e+05
18	20	1	1.4220e-01	3.1154e+05
20	21	1	1.3870e-01	4.0033e+05
20	22	1	1.3870e-01	4.0033e+05
21	23	1	1.3870e-01	4.0033e+05
22	25	1	1.3870e-01	4.0033e+05
23	27	1	1.3870e-01	4.0033e+05
23	30	1	1.3640e-01	3.7572e+05
25	27	1	1.3870e-01	4.0033e+05

[pairs]

; at.i	at.j	funct
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4	7	1
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6	8	1
13	7	1
7	15	1
8	15	1
8	10	1
13	9	1
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6	17	1
6	11	1
6	12	1
15	21	1
15	22	1
16	20	1
18	23	1
18	25	1
20	27	1
20	30	1
21	25	1
22	23	1
25	30	1

[angles]

; at.i	at.j	at.k	funct	theta(deg)	cth(kJ mol^{-1}rad^{-2})
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1	6	9	1	1.2001e+02	4.0551e+02
3	2	7	1	1.2001e+02	4.0551e+02
3	4	8	1	1.2001e+02	4.0551e+02
5	4	8	1	1.2001e+02	4.0551e+02
5	6	9	1	1.2001e+02	4.0551e+02

15	18	19	1	1.1846e+02	4.1179e+02
19	18	20	1	1.1594e+02	3.9631e+02
20	21	24	1	1.2001e+02	4.0551e+02
20	22	26	1	1.2001e+02	4.0551e+02
22	25	28	1	1.2001e+02	4.0551e+02
23	21	24	1	1.2001e+02	4.0551e+02
23	27	29	1	1.2001e+02	4.0551e+02
23	30	31	1	1.1613e+02	4.1070e+02
23	30	32	1	1.1613e+02	4.1070e+02
25	22	26	1	1.2001e+02	4.0551e+02
25	27	29	1	1.2001e+02	4.0551e+02
27	25	28	1	1.2001e+02	4.0551e+02
31	30	32	1	1.1485e+02	3.3514e+02
1	2	3	1	1.1997e+02	5.6216e+02
1	6	5	1	1.1997e+02	5.6216e+02
1	13	14	1	1.2344e+02	5.7463e+02
1	13	17	1	1.1494e+02	5.1891e+02
2	1	6	1	1.1997e+02	5.6216e+02
2	1	13	1	1.2014e+02	5.4091e+02
2	3	4	1	1.1997e+02	5.6216e+02
2	3	15	1	1.2014e+02	5.4091e+02
3	4	5	1	1.1997e+02	5.6216e+02
3	15	16	1	1.2344e+02	5.7463e+02
3	15	18	1	1.1514e+02	5.7296e+02
4	3	15	1	1.2014e+02	5.4091e+02
4	5	6	1	1.1997e+02	5.6216e+02
4	5	10	1	1.2014e+02	5.4091e+02
5	10	11	1	1.2344e+02	5.7463e+02
5	10	12	1	1.1494e+02	5.1891e+02
6	1	13	1	1.2014e+02	5.4091e+02
6	5	10	1	1.2014e+02	5.4091e+02
11	10	12	1	1.2151e+02	5.3790e+02
14	13	17	1	1.2151e+02	5.3790e+02
15	18	20	1	1.2371e+02	5.3798e+02
16	15	18	1	1.2203e+02	6.3455e+02
18	20	21	1	1.1989e+02	5.6877e+02
18	20	22	1	1.1989e+02	5.6877e+02
20	21	23	1	1.1997e+02	5.6216e+02
20	22	25	1	1.1997e+02	5.6216e+02
21	20	22	1	1.1997e+02	5.6216e+02
21	23	27	1	1.1997e+02	5.6216e+02
21	23	30	1	1.2013e+02	5.8024e+02
22	25	27	1	1.1997e+02	5.6216e+02
23	27	25	1	1.1997e+02	5.6216e+02

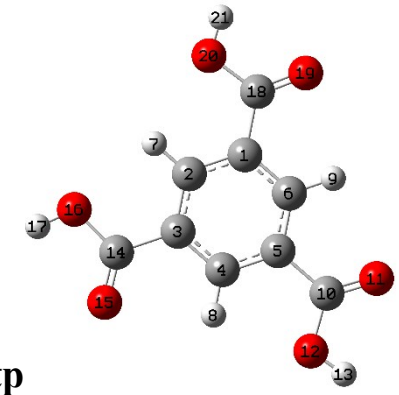
27 23 30 1 1.2013e+02 5.8024e+02

[dihedrals]

; at.i	at.j	at.k	at.l	funct	C0(kJ mol^{-1})	C1(kJ mol^{-1})	C2(kJ mol^{-1})	C3(kJ mol^{-1})	C4(kJ mol^{-1})	C5(kJ mol^{-1})	
2	1	6	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	3	4	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
3	15	18	19	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;
4	3	2	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	5	6	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	1	2	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	5	4	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
13	1	2	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
7	2	3	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
8	4	3	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
8	4	5	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
13	1	6	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
9	6	5	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
16	15	18	19	3	29.28800	-8.36800	-20.92000	0.00000	0.00000	0.00000	;
18	20	21	24	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
18	20	22	26	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
19	18	20	21	3	3.76560	0.00000	-3.76560	0.00000	0.00000	0.00000	;
19	18	20	22	3	3.76560	0.00000	-3.76560	0.00000	0.00000	0.00000	;
20	22	25	28	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
21	20	22	26	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
21	23	27	29	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
21	23	30	31	3	8.78640	0.00000	-8.78640	0.00000	0.00000	0.00000	;
21	23	30	32	3	8.78640	0.00000	-8.78640	0.00000	0.00000	0.00000	;
22	20	21	24	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
22	25	27	29	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
23	27	25	28	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
24	21	23	27	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
24	21	23	30	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
26	22	25	27	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
26	22	25	28	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
27	23	30	31	3	8.78640	0.00000	-8.78640	0.00000	0.00000	0.00000	;
27	23	30	32	3	8.78640	0.00000	-8.78640	0.00000	0.00000	0.00000	;
28	25	27	29	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
29	27	23	30	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	3	2	7	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
3	5	4	8	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
1	5	6	9	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
15	20	18	19	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
20	23	21	24	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
20	25	22	26	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;

22	27	25	28	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
23	25	27	29	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
23	31	30	32	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
1	2	3	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	2	3	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	6	5	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	6	5	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	6	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	13	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	13	17	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	3	4	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	3	15	16	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	3	15	18	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	1	2	3	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
13	1	2	3	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
3	4	5	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
3	4	5	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
3	15	18	20	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;
4	3	15	16	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	3	15	18	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	5	10	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	5	10	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
5	4	3	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
13	1	6	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	1	13	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	1	13	17	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	5	10	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	5	10	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
15	18	20	21	3	3.76560	0.00000	-3.76560	0.00000	0.00000	0.00000	;
15	18	20	22	3	3.76560	0.00000	-3.76560	0.00000	0.00000	0.00000	;
16	15	18	20	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;
18	20	21	23	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
18	20	22	25	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
20	21	23	27	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
20	21	23	30	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
20	22	25	27	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
21	20	22	25	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
21	23	27	25	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
22	20	21	23	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
22	25	27	23	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
25	27	23	30	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	1	2	13	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
15	2	3	4	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
10	4	5	6	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;

5	12	10	11	3	87.86400	0.00000	-87.86400	0.00000	0.00000	0.00000	;
1	17	13	14	3	87.86400	0.00000	-87.86400	0.00000	0.00000	0.00000	;
3	18	15	16	3	87.86400	0.00000	-87.86400	0.00000	0.00000	0.00000	;
21	22	20	18	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
21	27	23	30	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;



TMCOOH.itp

[atomtypes]

;name	bond_type	mass	charge	ptype	sigma	epsilon
oh	oh	0.0000	0.0000	A	3.06647e-01	8.80314e-01
ha	ha	0.0000	0.0000	A	2.59964e-01	6.27600e-02
ca	ca	0.0000	0.0000	A	3.39967e-01	3.59824e-01
ho	ho	0.0000	0.0000	A	0.00000e+00	0.00000e+00
o	o	0.0000	0.0000	A	2.95992e-01	8.78640e-01
cCOOH	cCOOH	0.0000	0.0000	A	3.39967e-01	3.59824e-01

[moleculetype]

; monomer_name	nrexcl
solute	3

[atoms]

; atom_number	type	resnr	residue	atom	cgnr	charge	mass
1	ca	1	trc	C	1	-0.0545	12.000000
2	ca	1	trc	C1	2	-0.1121	12.000000
3	ca	1	trc	C2	3	-0.0545	12.000000
4	ca	1	trc	C3	4	-0.1121	12.000000
5	ca	1	trc	C4	5	-0.0545	12.000000
6	ca	1	trc	C5	6	-0.1121	12.000000
7	ha	1	trc	H	7	0.18700	1.000000
8	ha	1	trc	H1	8	0.18700	1.000000
9	ha	1	trc	H2	9	0.18700	1.000000
10	cCOOH1	trc	C6	10	0.7412	12.000000	
11	o	1	trc	O	11	-0.5747	16.000000
12	oh	1	trc	O1	12	-0.6306	16.000000
13	ho	1	trc	H3	13	0.4568	1.000000
14	cCOOH 1	trc	C7	14	0.7412	12.000000	
15	o	1	trc	O2	15	-0.5747	16.000000
16	oh	1	trc	O3	16	-0.6306	16.000000
17	ho	1	trc	H4	17	0.4568	1.000000
18cCOOH	1	trc	C8	18	0.7412	12.000000	
19	o	1	trc	O4	19	-0.5747	16.000000

20	oh	1	trc	O5	20	-0.6306	16.000000
21	ho	1	trc	H5	21	0.4568	1.000000

[bonds]

; at.i	at.j	funct	b0(nm)	kb(kJ mol^{-1} nm^{-2})	at.i:atom_num_i
2	7	1	1.0870e-01	2.8811e+05	
4	8	1	1.0870e-01	2.8811e+05	
6	9	1	1.0870e-01	2.8811e+05	
12	13	1	9.7400e-02	3.0928e+05	
16	17	1	9.7400e-02	3.0928e+05	
20	21	1	9.7400e-02	3.0928e+05	
1	2	1	1.3870e-01	4.0033e+05	
1	6	1	1.3870e-01	4.0033e+05	
1	18	1	1.4870e-01	2.9263e+05	
2	3	1	1.3870e-01	4.0033e+05	
3	4	1	1.3870e-01	4.0033e+05	
3	14	1	1.4870e-01	2.9263e+05	
4	5	1	1.3870e-01	4.0033e+05	
5	6	1	1.3870e-01	4.0033e+05	
5	10	1	1.4870e-01	2.9263e+05	
10	11	1	1.2140e-01	5.4225e+05	
10	12	1	1.3060e-01	3.9028e+05	
14	15	1	1.2140e-01	5.4225e+05	
14	16	1	1.3060e-01	3.9028e+05	
18	19	1	1.2140e-01	5.4225e+05	
18	20	1	1.3060e-01	3.9028e+05	

[pairs]

; at.i	at.j	funct
1	21	1
2	9	1
2	8	1
3	17	1
4	7	1
4	9	1
5	13	1
6	7	1
6	8	1
18	7	1
7	14	1
8	14	1
8	10	1
18	9	1
9	10	1

11	13	1
15	17	1
19	21	1
1	4	1
1	14	1
1	10	1
2	5	1
2	19	1
2	20	1
2	15	1
2	16	1
6	3	1
18	3	1
3	10	1
4	15	1
4	16	1
4	11	1
4	12	1
5	14	1
18	5	1
6	19	1
6	20	1
6	11	1
6	12	1

[angles]

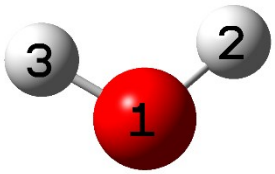
; at.i	at.j	at.k	funct	theta(deg)	cth(kJ mol^{-1}rad^{-2})
1	2	7	1	1.2001e+02	4.0551e+02
1	6	9	1	1.2001e+02	4.0551e+02
3	2	7	1	1.2001e+02	4.0551e+02
3	4	8	1	1.2001e+02	4.0551e+02
5	4	8	1	1.2001e+02	4.0551e+02
5	6	9	1	1.2001e+02	4.0551e+02
10	12	13	1	1.0737e+02	4.2836e+02
14	16	17	1	1.0737e+02	4.2836e+02
18	20	21	1	1.0737e+02	4.2836e+02
1	2	3	1	1.1997e+02	5.6216e+02
1	6	5	1	1.1997e+02	5.6216e+02
1	18	19	1	1.2344e+02	5.7463e+02
1	18	20	1	1.1344e+02	5.8668e+02
2	1	6	1	1.1997e+02	5.6216e+02
2	1	18	1	1.2014e+02	5.4091e+02
2	3	4	1	1.1997e+02	5.6216e+02
2	3	14	1	1.2014e+02	5.4091e+02

3	4	5	1	1.1997e+02	5.6216e+02
3	14	15	1	1.2344e+02	5.7463e+02
3	14	16	1	1.1344e+02	5.8668e+02
4	3	14	1	1.2014e+02	5.4091e+02
4	5	6	1	1.1997e+02	5.6216e+02
4	5	10	1	1.2014e+02	5.4091e+02
5	10	11	1	1.2344e+02	5.7463e+02
5	10	12	1	1.1344e+02	5.8668e+02
6	1	18	1	1.2014e+02	5.4091e+02
6	5	10	1	1.2014e+02	5.4091e+02
11	10	12	1	1.2288e+02	6.4752e+02
15	14	16	1	1.2288e+02	6.4752e+02
19	18	20	1	1.2288e+02	6.4752e+02

[dihedrals]

; at.i	at.j	at.k	at.l	funct	C0(kJ mol^{-1})	C1(kJ mol^{-1})	C2(kJ mol^{-1})	C3(kJ mol^{-1})	C4(kJ mol^{-1})	C5(kJ mol^{-1})	
1	18	20	21	3	19.24640	0.00000	-19.24640	0.00000	0.00000	0.00000	;
2	1	6	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	3	4	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
3	14	16	17	3	19.24640	0.00000	-19.24640	0.00000	0.00000	0.00000	;
4	3	2	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	5	6	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
5	10	12	13	3	19.24640	0.00000	-19.24640	0.00000	0.00000	0.00000	;
6	1	2	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	5	4	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
18	1	2	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
7	2	3	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
8	4	3	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
8	4	5	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
18	1	6	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
9	6	5	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
11	10	12	13	3	27.19600	-7.94960	-19.24640	0.00000	0.00000	0.00000	;
15	14	16	17	3	27.19600	-7.94960	-19.24640	0.00000	0.00000	0.00000	;
19	18	20	21	3	27.19600	-7.94960	-19.24640	0.00000	0.00000	0.00000	;
1	3	2	7	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
3	5	4	8	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
1	5	6	9	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
1	2	3	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	2	3	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	6	5	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	6	5	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	6	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	18	19	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	18	20	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;

2	3	4	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	3	14	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	3	14	16	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	1	2	3	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
18	1	2	3	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
3	4	5	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
3	4	5	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	3	14	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	3	14	16	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	5	10	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	5	10	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
5	4	3	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
18	1	6	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	1	18	19	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	1	18	20	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	5	10	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	5	10	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	1	2	18	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
14	2	3	4	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
10	4	5	6	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
5	11	10	12	3	87.86400	0.00000	-87.86400	0.00000	0.00000	0.00000	;
3	15	14	16	3	87.86400	0.00000	-87.86400	0.00000	0.00000	0.00000	;
1	19	18	20	3	87.86400	0.00000	-87.86400	0.00000	0.00000	0.00000	;



Tip3P.itp

```
[ atomtypes ]
;name        bond_type     mass     charge   ptype      sigma          epsilon
OW             OW          0.0000   0.0000    A      3.15061e-01    6.36386e-01
HW             HW          0.0000   0.0000    A      0.00000e+00    0.00000e+00

[ moleculetype ]
; monomer_name          nrexcl
      SOL                    2

[ atoms ]
; atom_number       type         resnr        residue      atom      cgnr       charge      mass
   1                  OW           1           SOL          OW          1         -0.834      16.00000
   2                  HW           1           SOL          HW1         1          0.417       1.00800
   3                  HW           1           SOL          HW2         1          0.417       1.00800

#ifndef FLEXIBLE

[ settles ]
; OW       funct     doh         dhh
1           1          0.09572 0.15139

[ exclusions ]
1       2       3
2       1       3
3       1       2

#else

[ bonds ]
;at.i     at.j        funct          b0(nm)     kb(kJ mol-1 nm-2)          at.i:atom_num_i
1           2           1           0.09572    502416.0
1           3           1           0.09572    502416.0

[ angles ]
; at.i        at.j       at.k       funct           theta(deg)    cth(kJ mol-1rad-2)
2           1           3           1           104.52              628.02
#endif
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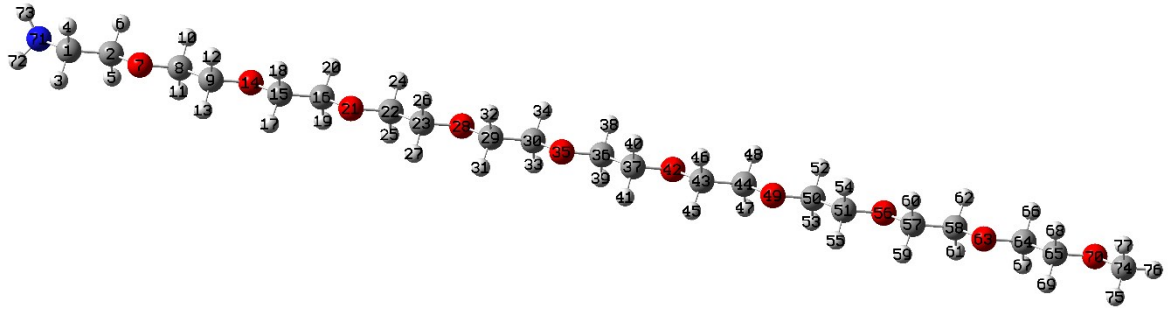
PEG.itp



[atomtypes]

;name	bond_type	mass	charge	ptype	sigma	epsilon
c3	c3	0.0000	0.0000	A	3.39967e-01	4.57730e-01
h1	h1	0.0000	0.0000	A	2.47135e-01	6.56888e-02
hn	hn	0.0000	0.0000	A	1.06908e-01	6.56888e-02
n3	n3	0.0000	0.0000	A	3.25000e-01	7.11280e-01
os	os	0.0000	0.0000	A	3.00001e-01	7.11280e-01

[moleculetype]

; monomer_name	nrexcl
PEG	3

[atoms]

; atom_number	type	resnr	residue	atom	cgnr	charge	mass
1	c3	1	PEG	C	1	0.31160	12.000000
2	c3	1	PEG	C1	2	0.16230	12.000000
3	h1	1	PEG	H	3	-0.03150	1.000000
4	h1	1	PEG	H1	4	0.04050	1.000000
5	h1	1	PEG	H2	5	0.03990	1.000000
6	h1	1	PEG	H3	6	0.03640	1.000000
7	os	1	PEG	O	7	-0.52310	16.000000
8	c3	1	PEG	C2	8	0.23020	12.000000
9	c3	1	PEG	C3	9	0.19350	12.000000
10	h1	1	PEG	H4	10	0.01540	1.000000
11	h1	1	PEG	H5	11	0.00760	1.000000
12	h1	1	PEG	H6	12	0.02690	1.000000
13	h1	1	PEG	H7	13	0.02690	1.000000
14	os	1	PEG	O1	14	-0.47420	16.000000
15	c3	1	PEG	C4	15	0.14310	12.000000
16	c3	1	PEG	C5	16	0.17330	12.000000
17	h1	1	PEG	H8	17	0.03760	1.000000
18	h1	1	PEG	H9	18	0.03760	1.000000

19	h1	1	PEG	H10	19	0.03520	1.000000
20	h1	1	PEG	H11	20	0.03520	1.000000
21	os	1	PEG	O2	21	-0.46080	16.000000
22	c3	1	PEG	C6	22	0.14520	12.000000
23	c3	1	PEG	C7	23	0.16650	12.000000
24	h1	1	PEG	H12	24	0.03750	1.000000
25	h1	1	PEG	H13	25	0.03750	1.000000
26	h1	1	PEG	H14	26	0.03590	1.000000
27	h1	1	PEG	H15	27	0.03590	1.000000
28	os	1	PEG	O3	28	-0.45840	16.000000
29	c3	1	PEG	C8	29	0.14250	12.000000
30	c3	1	PEG	C9	30	0.16720	12.000000
31	h1	1	PEG	H16	31	0.03840	1.000000
32	h1	1	PEG	H17	32	0.03840	1.000000
33	h1	1	PEG	H18	33	0.03580	1.000000
34	h1	1	PEG	H19	34	0.03580	1.000000
35	os	1	PEG	O4	35	-0.45880	16.000000
36	c3	1	PEG	C10	36	0.14520	12.000000
37	c3	1	PEG	C11	37	0.16490	12.000000
38	h1	1	PEG	H20	38	0.03820	1.000000
39	h1	1	PEG	H21	39	0.03820	1.000000
40	h1	1	PEG	H22	40	0.03620	1.000000
41	h1	1	PEG	H23	41	0.03620	1.000000
42	os	1	PEG	O5	42	-0.45930	16.000000
43	c3	1	PEG	C12	43	0.14480	12.000000
44	c3	1	PEG	C13	44	0.16820	12.000000
45	h1	1	PEG	H24	45	0.03810	1.000000
46	h1	1	PEG	H25	46	0.03810	1.000000
47	h1	1	PEG	H26	47	0.03550	1.000000
48	h1	1	PEG	H27	48	0.03550	1.000000
49	os	1	PEG	O6	49	-0.46090	16.000000
50	c3	1	PEG	C14	50	0.14640	12.000000
51	c3	1	PEG	C15	51	0.17050	12.000000
52	h1	1	PEG	H28	52	0.03790	1.000000
53	h1	1	PEG	H29	53	0.03790	1.000000
54	h1	1	PEG	H30	54	0.03470	1.000000
55	h1	1	PEG	H31	55	0.03470	1.000000
56	os	1	PEG	O7	56	-0.46270	16.000000
57	c3	1	PEG	C16	57	0.14840	12.000000
58	c3	1	PEG	C17	58	0.16780	12.000000
59	h1	1	PEG	H32	59	0.03660	1.000000
60	h1	1	PEG	H33	60	0.03660	1.000000
61	h1	1	PEG	H34	61	0.03510	1.000000
62	h1	1	PEG	H35	62	0.03510	1.000000

63	os	1	PEG	O8	63	-0.45850	16.000000
64	c3	1	PEG	C18	64	0.16550	12.000000
65	c3	1	PEG	C19	65	0.12040	12.000000
66	h1	1	PEG	H36	66	0.03320	1.000000
67	h1	1	PEG	H37	67	0.03320	1.000000
68	h1	1	PEG	H38	68	0.04170	1.000000
69	h1	1	PEG	H39	69	0.04170	1.000000
70	os	1	PEG	O9	70	-0.40190	16.000000
71	n3	1	PEG	N	71	-1.06590	14.000000
72	hn	1	PEG	H40	72	0.38830	1.000000
73	hn	1	PEG	H41	73	0.38830	1.000000
74	c3	1	PEG	C20	74	0.03110	12.000000
75	h1	1	PEG	H42	75	0.05400	1.000000
76	h1	1	PEG	H43	76	0.05400	1.000000
77	h1	1	PEG	H44	77	0.05400	1.000000

[bonds]

; at.i	at.j	funct	b0(nm)	kb(kJ mol^{-1} nm^{-2})	at.i:atom_num_i
1	3	1	1.0930e-01	2.8108e+05	
1	4	1	1.0930e-01	2.8108e+05	
2	5	1	1.0930e-01	2.8108e+05	
2	6	1	1.0930e-01	2.8108e+05	
8	10	1	1.0930e-01	2.8108e+05	
8	11	1	1.0930e-01	2.8108e+05	
9	12	1	1.0930e-01	2.8108e+05	
9	13	1	1.0930e-01	2.8108e+05	
15	17	1	1.0930e-01	2.8108e+05	
15	18	1	1.0930e-01	2.8108e+05	
16	19	1	1.0930e-01	2.8108e+05	
16	20	1	1.0930e-01	2.8108e+05	
22	24	1	1.0930e-01	2.8108e+05	
22	25	1	1.0930e-01	2.8108e+05	
23	26	1	1.0930e-01	2.8108e+05	
23	27	1	1.0930e-01	2.8108e+05	
29	31	1	1.0930e-01	2.8108e+05	
29	32	1	1.0930e-01	2.8108e+05	
30	33	1	1.0930e-01	2.8108e+05	
30	34	1	1.0930e-01	2.8108e+05	
36	38	1	1.0930e-01	2.8108e+05	
36	39	1	1.0930e-01	2.8108e+05	
37	40	1	1.0930e-01	2.8108e+05	
37	41	1	1.0930e-01	2.8108e+05	
43	45	1	1.0930e-01	2.8108e+05	
43	46	1	1.0930e-01	2.8108e+05	

44	47	1	1.0930e-01	2.8108e+05
44	48	1	1.0930e-01	2.8108e+05
50	52	1	1.0930e-01	2.8108e+05
50	53	1	1.0930e-01	2.8108e+05
51	54	1	1.0930e-01	2.8108e+05
51	55	1	1.0930e-01	2.8108e+05
57	59	1	1.0930e-01	2.8108e+05
57	60	1	1.0930e-01	2.8108e+05
58	61	1	1.0930e-01	2.8108e+05
58	62	1	1.0930e-01	2.8108e+05
64	66	1	1.0930e-01	2.8108e+05
64	67	1	1.0930e-01	2.8108e+05
65	68	1	1.0930e-01	2.8108e+05
65	69	1	1.0930e-01	2.8108e+05
71	72	1	1.0180e-01	3.2978e+05
71	73	1	1.0180e-01	3.2978e+05
74	75	1	1.0930e-01	2.8108e+05
74	76	1	1.0930e-01	2.8108e+05
74	77	1	1.0930e-01	2.8108e+05
1	2	1	1.5350e-01	2.5363e+05
1	71	1	1.4700e-01	2.6828e+05
2	7	1	1.4390e-01	2.5230e+05
7	8	1	1.4390e-01	2.5230e+05
8	9	1	1.5350e-01	2.5363e+05
9	14	1	1.4390e-01	2.5230e+05
14	15	1	1.4390e-01	2.5230e+05
15	16	1	1.5350e-01	2.5363e+05
16	21	1	1.4390e-01	2.5230e+05
21	22	1	1.4390e-01	2.5230e+05
22	23	1	1.5350e-01	2.5363e+05
23	28	1	1.4390e-01	2.5230e+05
28	29	1	1.4390e-01	2.5230e+05
29	30	1	1.5350e-01	2.5363e+05
30	35	1	1.4390e-01	2.5230e+05
35	36	1	1.4390e-01	2.5230e+05
36	37	1	1.5350e-01	2.5363e+05
37	42	1	1.4390e-01	2.5230e+05
42	43	1	1.4390e-01	2.5230e+05
43	44	1	1.5350e-01	2.5363e+05
44	49	1	1.4390e-01	2.5230e+05
49	50	1	1.4390e-01	2.5230e+05
50	51	1	1.5350e-01	2.5363e+05
51	56	1	1.4390e-01	2.5230e+05
56	57	1	1.4390e-01	2.5230e+05

57	58	1	1.5350e-01	2.5363e+05
58	63	1	1.4390e-01	2.5230e+05
63	64	1	1.4390e-01	2.5230e+05
64	65	1	1.5350e-01	2.5363e+05
65	70	1	1.4390e-01	2.5230e+05
70	74	1	1.4390e-01	2.5230e+05

[pairs]

; at.i	at.j	funct
2	72	1
2	73	1
2	10	1
2	11	1
3	5	1
3	6	1
3	7	1
3	72	1
3	73	1
4	5	1
4	6	1
4	7	1
4	72	1
4	73	1
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5	8	1
71	6	1
6	8	1
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9	18	1
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11	14	1
12	15	1
13	15	1
14	19	1
14	20	1
16	24	1
16	25	1
17	19	1

17	20	1
17	21	1
18	19	1
18	20	1
18	21	1
19	22	1
20	22	1
21	26	1
21	27	1
23	31	1
23	32	1
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38	41	1
38	42	1
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39	41	1
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40	43	1
41	43	1
42	47	1

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63	69	1
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65	76	1
65	77	1
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66	69	1
66	70	1
67	68	1

67	69	1
67	70	1
68	74	1
69	74	1
1	8	1
2	9	1
71	7	1
7	14	1
8	15	1
9	16	1
14	21	1
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30	37	1
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37	44	1
42	49	1
43	50	1
44	51	1
49	56	1
50	57	1
51	58	1
56	63	1
57	64	1
58	65	1
63	70	1
64	74	1

[angles]

; at.i	at.j	at.k	funct	theta(deg)	cth(kJ mol^{-1}rad^{-2})
1	2	5	1	1.1007e+02	3.8794e+02
1	2	6	1	1.1007e+02	3.8794e+02
1	71	72	1	1.0992e+02	3.9438e+02
1	71	73	1	1.0992e+02	3.9438e+02
2	1	3	1	1.1007e+02	3.8794e+02
2	1	4	1	1.1007e+02	3.8794e+02
3	1	4	1	1.0955e+02	3.2786e+02
3	1	71	1	1.0992e+02	4.1330e+02

4	1	71	1	1.0992e+02	4.1330e+02
5	2	6	1	1.0955e+02	3.2786e+02
5	2	7	1	1.0882e+02	4.2543e+02
6	2	7	1	1.0882e+02	4.2543e+02
7	8	10	1	1.0882e+02	4.2543e+02
7	8	11	1	1.0882e+02	4.2543e+02
8	9	12	1	1.1007e+02	3.8794e+02
8	9	13	1	1.1007e+02	3.8794e+02
9	8	10	1	1.1007e+02	3.8794e+02
9	8	11	1	1.1007e+02	3.8794e+02
10	8	11	1	1.0955e+02	3.2786e+02
12	9	13	1	1.0955e+02	3.2786e+02
12	9	14	1	1.0882e+02	4.2543e+02
13	9	14	1	1.0882e+02	4.2543e+02
14	15	17	1	1.0882e+02	4.2543e+02
14	15	18	1	1.0882e+02	4.2543e+02
15	16	19	1	1.1007e+02	3.8794e+02
15	16	20	1	1.1007e+02	3.8794e+02
16	15	17	1	1.1007e+02	3.8794e+02
16	15	18	1	1.1007e+02	3.8794e+02
17	15	18	1	1.0955e+02	3.2786e+02
19	16	20	1	1.0955e+02	3.2786e+02
19	16	21	1	1.0882e+02	4.2543e+02
20	16	21	1	1.0882e+02	4.2543e+02
21	22	24	1	1.0882e+02	4.2543e+02
21	22	25	1	1.0882e+02	4.2543e+02
22	23	26	1	1.1007e+02	3.8794e+02
22	23	27	1	1.1007e+02	3.8794e+02
23	22	24	1	1.1007e+02	3.8794e+02
23	22	25	1	1.1007e+02	3.8794e+02
24	22	25	1	1.0955e+02	3.2786e+02
26	23	27	1	1.0955e+02	3.2786e+02
26	23	28	1	1.0882e+02	4.2543e+02
27	23	28	1	1.0882e+02	4.2543e+02
28	29	31	1	1.0882e+02	4.2543e+02
28	29	32	1	1.0882e+02	4.2543e+02
29	30	33	1	1.1007e+02	3.8794e+02
29	30	34	1	1.1007e+02	3.8794e+02
30	29	31	1	1.1007e+02	3.8794e+02
30	29	32	1	1.1007e+02	3.8794e+02
31	29	32	1	1.0955e+02	3.2786e+02
33	30	34	1	1.0955e+02	3.2786e+02
33	30	35	1	1.0882e+02	4.2543e+02
34	30	35	1	1.0882e+02	4.2543e+02

35	36	38	1	1.0882e+02	4.2543e+02
35	36	39	1	1.0882e+02	4.2543e+02
36	37	40	1	1.1007e+02	3.8794e+02
36	37	41	1	1.1007e+02	3.8794e+02
37	36	38	1	1.1007e+02	3.8794e+02
37	36	39	1	1.1007e+02	3.8794e+02
38	36	39	1	1.0955e+02	3.2786e+02
40	37	41	1	1.0955e+02	3.2786e+02
40	37	42	1	1.0882e+02	4.2543e+02
41	37	42	1	1.0882e+02	4.2543e+02
42	43	45	1	1.0882e+02	4.2543e+02
42	43	46	1	1.0882e+02	4.2543e+02
43	44	47	1	1.1007e+02	3.8794e+02
43	44	48	1	1.1007e+02	3.8794e+02
44	43	45	1	1.1007e+02	3.8794e+02
44	43	46	1	1.1007e+02	3.8794e+02
45	43	46	1	1.0955e+02	3.2786e+02
47	44	48	1	1.0955e+02	3.2786e+02
47	44	49	1	1.0882e+02	4.2543e+02
48	44	49	1	1.0882e+02	4.2543e+02
49	50	52	1	1.0882e+02	4.2543e+02
49	50	53	1	1.0882e+02	4.2543e+02
50	51	54	1	1.1007e+02	3.8794e+02
50	51	55	1	1.1007e+02	3.8794e+02
51	50	52	1	1.1007e+02	3.8794e+02
51	50	53	1	1.1007e+02	3.8794e+02
52	50	53	1	1.0955e+02	3.2786e+02
54	51	55	1	1.0955e+02	3.2786e+02
54	51	56	1	1.0882e+02	4.2543e+02
55	51	56	1	1.0882e+02	4.2543e+02
56	57	59	1	1.0882e+02	4.2543e+02
56	57	60	1	1.0882e+02	4.2543e+02
57	58	61	1	1.1007e+02	3.8794e+02
57	58	62	1	1.1007e+02	3.8794e+02
58	57	59	1	1.1007e+02	3.8794e+02
58	57	60	1	1.1007e+02	3.8794e+02
59	57	60	1	1.0955e+02	3.2786e+02
61	58	62	1	1.0955e+02	3.2786e+02
61	58	63	1	1.0882e+02	4.2543e+02
62	58	63	1	1.0882e+02	4.2543e+02
63	64	66	1	1.0882e+02	4.2543e+02
63	64	67	1	1.0882e+02	4.2543e+02
64	65	68	1	1.1007e+02	3.8794e+02
64	65	69	1	1.1007e+02	3.8794e+02

65	64	66	1	1.1007e+02	3.8794e+02
65	64	67	1	1.1007e+02	3.8794e+02
66	64	67	1	1.0955e+02	3.2786e+02
68	65	69	1	1.0955e+02	3.2786e+02
68	65	70	1	1.0882e+02	4.2543e+02
69	65	70	1	1.0882e+02	4.2543e+02
70	74	75	1	1.0882e+02	4.2543e+02
70	74	76	1	1.0882e+02	4.2543e+02
70	74	77	1	1.0882e+02	4.2543e+02
72	71	73	1	1.0713e+02	3.4560e+02
75	74	76	1	1.0955e+02	3.2786e+02
75	74	77	1	1.0955e+02	3.2786e+02
76	74	77	1	1.0955e+02	3.2786e+02
1	2	7	1	1.0842e+02	5.6718e+02
2	1	71	1	1.1038e+02	5.5379e+02
2	7	8	1	1.1245e+02	5.2208e+02
7	8	9	1	1.0842e+02	5.6718e+02
8	9	14	1	1.0842e+02	5.6718e+02
9	14	15	1	1.1245e+02	5.2208e+02
14	15	16	1	1.0842e+02	5.6718e+02
15	16	21	1	1.0842e+02	5.6718e+02
16	21	22	1	1.1245e+02	5.2208e+02
21	22	23	1	1.0842e+02	5.6718e+02
22	23	28	1	1.0842e+02	5.6718e+02
23	28	29	1	1.1245e+02	5.2208e+02
28	29	30	1	1.0842e+02	5.6718e+02
29	30	35	1	1.0842e+02	5.6718e+02
30	35	36	1	1.1245e+02	5.2208e+02
35	36	37	1	1.0842e+02	5.6718e+02
36	37	42	1	1.0842e+02	5.6718e+02
37	42	43	1	1.1245e+02	5.2208e+02
42	43	44	1	1.0842e+02	5.6718e+02
43	44	49	1	1.0842e+02	5.6718e+02
44	49	50	1	1.1245e+02	5.2208e+02
49	50	51	1	1.0842e+02	5.6718e+02
50	51	56	1	1.0842e+02	5.6718e+02
51	56	57	1	1.1245e+02	5.2208e+02
56	57	58	1	1.0842e+02	5.6718e+02
57	58	63	1	1.0842e+02	5.6718e+02
58	63	64	1	1.1245e+02	5.2208e+02
63	64	65	1	1.0842e+02	5.6718e+02
64	65	70	1	1.0842e+02	5.6718e+02
65	70	74	1	1.1245e+02	5.2208e+02

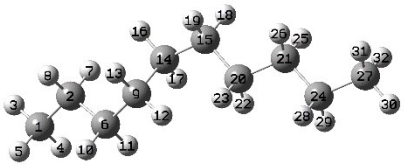
[dihedrals]

; at.i	at.j	at.k	at.l	funct	C0(kJ mol^{-1})	C1(kJ mol^{-1})	C2(kJ mol^{-1})	C3(kJ mol^{-1})	C4(kJ mol^{-1})	C5(kJ mol^{-1})	
2	1	71	72	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
2	1	71	73	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
2	7	8	10	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
2	7	8	11	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
3	1	2	5	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
3	1	2	6	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
3	1	2	7	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
3	1	71	72	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
3	1	71	73	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
4	1	2	5	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
4	1	2	6	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
4	1	2	7	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
4	1	71	72	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
4	1	71	73	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
71	1	2	5	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
5	2	7	8	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
71	1	2	6	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
6	2	7	8	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
7	8	9	12	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
7	8	9	13	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
9	14	15	17	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
9	14	15	18	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
10	8	9	12	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
10	8	9	13	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
10	8	9	14	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
11	8	9	12	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
11	8	9	13	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
11	8	9	14	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
12	9	14	15	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
13	9	14	15	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
14	15	16	19	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
14	15	16	20	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
16	21	22	24	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
16	21	22	25	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
17	15	16	19	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
17	15	16	20	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
17	15	16	21	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
18	15	16	19	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
18	15	16	20	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
18	15	16	21	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
19	16	21	22	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
20	16	21	22	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;

21	22	23	26	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
21	22	23	27	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
23	28	29	31	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
23	28	29	32	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
24	22	23	26	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
24	22	23	27	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
24	22	23	28	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
25	22	23	26	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
25	22	23	27	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
25	22	23	28	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
26	23	28	29	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
27	23	28	29	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
28	29	30	33	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
28	29	30	34	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
30	35	36	38	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
30	35	36	39	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
31	29	30	33	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
31	29	30	34	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
31	29	30	35	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
32	29	30	33	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
32	29	30	34	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
32	29	30	35	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
33	30	35	36	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
34	30	35	36	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
35	36	37	40	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
35	36	37	41	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
37	42	43	45	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
37	42	43	46	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
38	36	37	40	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
38	36	37	41	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
38	36	37	42	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
39	36	37	40	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
39	36	37	41	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
39	36	37	42	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
40	37	42	43	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
41	37	42	43	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
42	43	44	47	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
42	43	44	48	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
44	49	50	52	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
44	49	50	53	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
45	43	44	47	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
45	43	44	48	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
45	43	44	49	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
46	43	44	47	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;

46	43	44	48	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
46	43	44	49	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
47	44	49	50	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
48	44	49	50	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
49	50	51	54	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
49	50	51	55	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
51	56	57	59	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
51	56	57	60	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
52	50	51	54	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
52	50	51	55	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
52	50	51	56	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
53	50	51	54	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
53	50	51	55	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
53	50	51	56	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
54	51	56	57	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
55	51	56	57	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
56	57	58	61	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
56	57	58	62	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
58	63	64	66	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
58	63	64	67	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
59	57	58	61	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
59	57	58	62	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
59	57	58	63	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
60	57	58	61	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
60	57	58	62	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
60	57	58	63	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
61	58	63	64	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
62	58	63	64	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
63	64	65	68	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
63	64	65	69	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
65	70	74	75	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
65	70	74	76	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
65	70	74	77	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
66	64	65	68	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
66	64	65	69	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
66	64	65	70	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
67	64	65	68	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
67	64	65	69	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
67	64	65	70	3	1.04600	-1.04600	0.00000	0.00000	0.00000	0.00000	;
68	65	70	74	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
69	65	70	74	3	1.60247	4.80742	0.00000	-6.40989	0.00000	0.00000	;
1	2	7	8	3	2.43927	4.80742	-0.83680	-6.40989	0.00000	0.00000	;
2	7	8	9	3	2.43927	4.80742	-0.83680	-6.40989	0.00000	0.00000	;
71	1	2	7	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;

7	8	9	14	3	0.60250	1.80749	9.83240	-2.40998	0.00000	0.00000	;
8	9	14	15	3	2.43927	4.80742	-0.83680	-6.40989	0.00000	0.00000	;
9	14	15	16	3	2.43927	4.80742	-0.83680	-6.40989	0.00000	0.00000	;
14	15	16	21	3	0.60250	1.80749	9.83240	-2.40998	0.00000	0.00000	;
15	16	21	22	3	2.43927	4.80742	-0.83680	-6.40989	0.00000	0.00000	;
16	21	22	23	3	2.43927	4.80742	-0.83680	-6.40989	0.00000	0.00000	;
21	22	23	28	3	0.60250	1.80749	9.83240	-2.40998	0.00000	0.00000	;
22	23	28	29	3	2.43927	4.80742	-0.83680	-6.40989	0.00000	0.00000	;
23	28	29	30	3	2.43927	4.80742	-0.83680	-6.40989	0.00000	0.00000	;
28	29	30	35	3	0.60250	1.80749	9.83240	-2.40998	0.00000	0.00000	;
29	30	35	36	3	2.43927	4.80742	-0.83680	-6.40989	0.00000	0.00000	;
30	35	36	37	3	2.43927	4.80742	-0.83680	-6.40989	0.00000	0.00000	;
35	36	37	42	3	0.60250	1.80749	9.83240	-2.40998	0.00000	0.00000	;
36	37	42	43	3	2.43927	4.80742	-0.83680	-6.40989	0.00000	0.00000	;
37	42	43	44	3	2.43927	4.80742	-0.83680	-6.40989	0.00000	0.00000	;
42	43	44	49	3	0.60250	1.80749	9.83240	-2.40998	0.00000	0.00000	;
43	44	49	50	3	2.43927	4.80742	-0.83680	-6.40989	0.00000	0.00000	;
44	49	50	51	3	2.43927	4.80742	-0.83680	-6.40989	0.00000	0.00000	;
49	50	51	56	3	0.60250	1.80749	9.83240	-2.40998	0.00000	0.00000	;
50	51	56	57	3	2.43927	4.80742	-0.83680	-6.40989	0.00000	0.00000	;
51	56	57	58	3	2.43927	4.80742	-0.83680	-6.40989	0.00000	0.00000	;
56	57	58	63	3	0.60250	1.80749	9.83240	-2.40998	0.00000	0.00000	;
57	58	63	64	3	2.43927	4.80742	-0.83680	-6.40989	0.00000	0.00000	;
58	63	64	65	3	2.43927	4.80742	-0.83680	-6.40989	0.00000	0.00000	;
63	64	65	70	3	0.60250	1.80749	9.83240	-2.40998	0.00000	0.00000	;
64	65	70	74	3	2.43927	4.80742	-0.83680	-6.40989	0.00000	0.00000	;



n-decane.itp

[atomtypes]

;name	bond_type	mass	charge	ptype	sigma	epsilon
c3	c3	0.0000	0.0000	A	3.39967e-01	4.57730e-01
hc	hc	0.0000	0.0000	A	2.64953e-01	6.56888e-02

[moleculetype]

; monomer_name	nrexcl
ECA	3

[atoms]

; atom_number	type	resnr	residue	atom	cgnr	charge	mass
1	c3	1	ECA	C	1	-0.09750	12.000000
2	c3	1	ECA	C1	2	0.03990	12.000000
3	hc	1	ECA	H	3	0.01940	1.000000
4	hc	1	ECA	H1	4	0.01940	1.000000
5	hc	1	ECA	H2	5	0.01940	1.000000
6	c3	1	ECA	C2	6	-0.02160	12.000000
7	hc	1	ECA	H3	7	0.00390	1.000000
8	hc	1	ECA	H4	8	0.00390	1.000000
9	c3	1	ECA	C3	9	-0.03450	12.000000
10	hc	1	ECA	H5	10	0.01090	1.000000
11	hc	1	ECA	H6	11	0.01090	1.000000
12	hc	1	ECA	H7	12	0.01080	1.000000
13	hc	1	ECA	H8	13	0.01080	1.000000
14	c3	1	ECA	C4	14	-0.00450	12.000000
15	c3	1	ECA	C5	15	-0.01930	12.000000
16	hc	1	ECA	H9	16	0.00460	1.000000
17	hc	1	ECA	H10	17	0.00460	1.000000
18	hc	1	ECA	H11	18	0.00310	1.000000
19	hc	1	ECA	H12	19	0.00310	1.000000
20	c3	1	ECA	C6	20	0.00370	12.000000
21	c3	1	ECA	C7	21	-0.00750	12.000000
22	hc	1	ECA	H13	22	0.00460	1.000000
23	hc	1	ECA	H14	23	0.00460	1.000000
24	c3	1	ECA	C8	24	0.04530	12.000000
25	hc	1	ECA	H15	25	0.00390	1.000000
26	hc	1	ECA	H16	26	0.00390	1.000000
27	c3	1	ECA	C9	27	-0.06900	12.000000
28	hc	1	ECA	H17	28	-0.00730	1.000000

29	hc	1	ECA	H18	29	-0.00730	1.000000
30	hc	1	ECA	H19	30	0.01260	1.000000
31	hc	1	ECA	H20	31	0.01260	1.000000
32	hc	1	ECA	H21	32	0.01260	1.000000

[bonds]

; at.i	at.j	funct	b0(nm)	kb(kJ mol^{-1} nm^{-2})	at.i:atom_num_i
1	3	1	1.0920e-01	2.8225e+05	
1	4	1	1.0920e-01	2.8225e+05	
1	5	1	1.0920e-01	2.8225e+05	
2	7	1	1.0920e-01	2.8225e+05	
2	8	1	1.0920e-01	2.8225e+05	
6	10	1	1.0920e-01	2.8225e+05	
6	11	1	1.0920e-01	2.8225e+05	
9	12	1	1.0920e-01	2.8225e+05	
9	13	1	1.0920e-01	2.8225e+05	
14	16	1	1.0920e-01	2.8225e+05	
14	17	1	1.0920e-01	2.8225e+05	
15	18	1	1.0920e-01	2.8225e+05	
15	19	1	1.0920e-01	2.8225e+05	
20	22	1	1.0920e-01	2.8225e+05	
20	23	1	1.0920e-01	2.8225e+05	
21	25	1	1.0920e-01	2.8225e+05	
21	26	1	1.0920e-01	2.8225e+05	
24	28	1	1.0920e-01	2.8225e+05	
24	29	1	1.0920e-01	2.8225e+05	
27	30	1	1.0920e-01	2.8225e+05	
27	31	1	1.0920e-01	2.8225e+05	
27	32	1	1.0920e-01	2.8225e+05	
1	2	1	1.5350e-01	2.5363e+05	
2	6	1	1.5350e-01	2.5363e+05	
6	9	1	1.5350e-01	2.5363e+05	
9	14	1	1.5350e-01	2.5363e+05	
14	15	1	1.5350e-01	2.5363e+05	
15	20	1	1.5350e-01	2.5363e+05	
20	21	1	1.5350e-01	2.5363e+05	
21	24	1	1.5350e-01	2.5363e+05	
24	27	1	1.5350e-01	2.5363e+05	

[pairs]

1	10	1
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2	13	1

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29	30	1
29	31	1
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1	9	1
2	14	1
6	15	1
9	20	1
14	21	1
15	24	1
20	27	1

[angles]

; at.i	at.j	at.k	funct	theta(deg)	cth(kJ mol^{-1}rad^{-2})
1	2	7	1	1.1005e+02	3.8802e+02
1	2	8	1	1.1005e+02	3.8802e+02
2	1	3	1	1.1005e+02	3.8802e+02
2	1	4	1	1.1005e+02	3.8802e+02
2	1	5	1	1.1005e+02	3.8802e+02
2	6	10	1	1.1005e+02	3.8802e+02
2	6	11	1	1.1005e+02	3.8802e+02
3	1	4	1	1.0835e+02	3.2995e+02

3	1	5	1	1.0835e+02	3.2995e+02
4	1	5	1	1.0835e+02	3.2995e+02
6	2	7	1	1.1005e+02	3.8802e+02
6	2	8	1	1.1005e+02	3.8802e+02
6	9	12	1	1.1005e+02	3.8802e+02
6	9	13	1	1.1005e+02	3.8802e+02
7	2	8	1	1.0835e+02	3.2995e+02
9	6	10	1	1.1005e+02	3.8802e+02
9	6	11	1	1.1005e+02	3.8802e+02
9	14	16	1	1.1005e+02	3.8802e+02
9	14	17	1	1.1005e+02	3.8802e+02
10	6	11	1	1.0835e+02	3.2995e+02
12	9	13	1	1.0835e+02	3.2995e+02
12	9	14	1	1.1005e+02	3.8802e+02
13	9	14	1	1.1005e+02	3.8802e+02
14	15	18	1	1.1005e+02	3.8802e+02
14	15	19	1	1.1005e+02	3.8802e+02
15	14	16	1	1.1005e+02	3.8802e+02
15	14	17	1	1.1005e+02	3.8802e+02
15	20	22	1	1.1005e+02	3.8802e+02
15	20	23	1	1.1005e+02	3.8802e+02
16	14	17	1	1.0835e+02	3.2995e+02
18	15	19	1	1.0835e+02	3.2995e+02
18	15	20	1	1.1005e+02	3.8802e+02
19	15	20	1	1.1005e+02	3.8802e+02
20	21	25	1	1.1005e+02	3.8802e+02
20	21	26	1	1.1005e+02	3.8802e+02
21	20	22	1	1.1005e+02	3.8802e+02
21	20	23	1	1.1005e+02	3.8802e+02
21	24	28	1	1.1005e+02	3.8802e+02
21	24	29	1	1.1005e+02	3.8802e+02
22	20	23	1	1.0835e+02	3.2995e+02
24	21	25	1	1.1005e+02	3.8802e+02
24	21	26	1	1.1005e+02	3.8802e+02
24	27	30	1	1.1005e+02	3.8802e+02
24	27	31	1	1.1005e+02	3.8802e+02
24	27	32	1	1.1005e+02	3.8802e+02
25	21	26	1	1.0835e+02	3.2995e+02
27	24	28	1	1.1005e+02	3.8802e+02
27	24	29	1	1.1005e+02	3.8802e+02
28	24	29	1	1.0835e+02	3.2995e+02
30	27	31	1	1.0835e+02	3.2995e+02
30	27	32	1	1.0835e+02	3.2995e+02
31	27	32	1	1.0835e+02	3.2995e+02

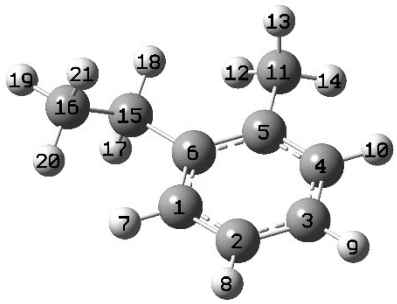
1	2	6	1	1.1063e+02	5.2894e+02
2	6	9	1	1.1063e+02	5.2894e+02
6	9	14	1	1.1063e+02	5.2894e+02
9	14	15	1	1.1063e+02	5.2894e+02
14	15	20	1	1.1063e+02	5.2894e+02
15	20	21	1	1.1063e+02	5.2894e+02
20	21	24	1	1.1063e+02	5.2894e+02
21	24	27	1	1.1063e+02	5.2894e+02

[dihedrals]

; at.i	at.j	at.k	at.l	funct	C0(kJ mol^{-1})	C1(kJ mol^{-1})	C2(kJ mol^{-1})	C3(kJ mol^{-1})	C4(kJ mol^{-1})	C5(kJ mol^{-1})
1	2	6	10	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
1	2	6	11	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
2	6	9	12	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
2	6	9	13	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
3	1	2	6	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
3	1	2	7	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
3	1	2	8	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
4	1	2	6	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
4	1	2	7	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
4	1	2	8	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
5	1	2	6	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
5	1	2	7	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
5	1	2	8	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
6	9	14	16	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
6	9	14	17	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
7	2	6	9	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
7	2	6	10	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
7	2	6	11	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
8	2	6	9	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
8	2	6	10	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
8	2	6	11	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
9	14	15	18	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
9	14	15	19	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
10	6	9	12	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
10	6	9	13	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
10	6	9	14	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
11	6	9	12	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
11	6	9	13	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
11	6	9	14	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
12	9	14	15	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
12	9	14	16	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
12	9	14	17	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
13	9	14	15	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;

13	9	14	16	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
13	9	14	17	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
14	15	20	22	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
14	15	20	23	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
15	20	21	25	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
15	20	21	26	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
16	14	15	18	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
16	14	15	19	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
16	14	15	20	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
17	14	15	18	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
17	14	15	19	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
17	14	15	20	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
18	15	20	21	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
18	15	20	22	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
18	15	20	23	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
19	15	20	21	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
19	15	20	22	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
19	15	20	23	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
20	21	24	28	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
20	21	24	29	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
21	24	27	30	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
21	24	27	31	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
21	24	27	32	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
22	20	21	24	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
22	20	21	25	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
22	20	21	26	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
23	20	21	24	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
23	20	21	25	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
23	20	21	26	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
25	21	24	27	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
25	21	24	28	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
25	21	24	29	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
26	21	24	27	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000 ;
26	21	24	28	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
26	21	24	29	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
28	24	27	30	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
28	24	27	31	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
28	24	27	32	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
29	24	27	30	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
29	24	27	31	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
29	24	27	32	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000 ;
1	2	6	9	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000 ;
2	6	9	14	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000 ;
6	9	14	15	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000 ;

9	14	15	20	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000 ;
14	15	20	21	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000 ;
15	20	21	24	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000 ;
20	21	24	27	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000 ;



MEBE.itp

[atomtypes]

;name	bond_type	mass	charge	ptype	sigma	epsilon
hc	hc	0.0000	0.0000	A	2.64953e-01	6.56888e-02
c3	c3	0.0000	0.0000	A	3.39967e-01	4.57730e-01
ha	ha	0.0000	0.0000	A	2.59964e-01	6.27600e-02
ca	ca	0.0000	0.0000	A	3.39967e-01	3.59824e-01

[moleculetype]

; monomer_name	nrexcl
EBE	3

[atoms]

; atom_number	type	resnr	residue	atom	cgnr	charge	mass
1	ca	1	EBE	C	1	-0.19520	12.000000
2	ca	1	EBE	C1	2	-0.18060	12.000000
3	ca	1	EBE	C2	3	-0.15160	12.000000
4	ca	1	EBE	C3	4	-0.22640	12.000000
5	ca	1	EBE	C4	5	0.07550	12.000000
6	ca	1	EBE	C5	6	0.03990	12.000000
7	ha	1	EBE	H	7	0.14570	1.000000
8	ha	1	EBE	H1	8	0.15100	1.000000
9	ha	1	EBE	H2	9	0.14710	1.000000
10	ha	1	EBE	H3	10	0.15360	1.000000
11	c3	1	EBE	C6	11	-0.16840	12.000000
12	hc	1	EBE	H4	12	0.05460	1.000000
13	hc	1	EBE	H5	13	0.05460	1.000000
14	hc	1	EBE	H6	14	0.05460	1.000000
15	c3	1	EBE	C7	15	-0.01510	12.000000
16	c3	1	EBE	C8	16	-0.07110	12.000000
17	hc	1	EBE	H7	17	0.03530	1.000000
18	hc	1	EBE	H8	18	0.03530	1.000000
19	hc	1	EBE	H9	19	0.02040	1.000000
20	hc	1	EBE	H10	20	0.02040	1.000000
21	hc	1	EBE	H11	21	0.02040	1.000000

[bonds]

; at.i	at.j	funct	b0(nm)	kb(kJ mol^{-1} nm^{-2})	at.i:atom_num_i
1	7	1	1.0870e-01	2.8811e+05	
2	8	1	1.0870e-01	2.8811e+05	
3	9	1	1.0870e-01	2.8811e+05	
4	10	1	1.0870e-01	2.8811e+05	
11	12	1	1.0920e-01	2.8225e+05	
11	13	1	1.0920e-01	2.8225e+05	
11	14	1	1.0920e-01	2.8225e+05	
15	17	1	1.0920e-01	2.8225e+05	
15	18	1	1.0920e-01	2.8225e+05	
16	19	1	1.0920e-01	2.8225e+05	
16	20	1	1.0920e-01	2.8225e+05	
16	21	1	1.0920e-01	2.8225e+05	
1	2	1	1.3870e-01	4.0033e+05	
1	6	1	1.3870e-01	4.0033e+05	
2	3	1	1.3870e-01	4.0033e+05	
3	4	1	1.3870e-01	4.0033e+05	
4	5	1	1.3870e-01	4.0033e+05	
5	6	1	1.3870e-01	4.0033e+05	
5	11	1	1.5130e-01	2.7070e+05	
6	15	1	1.5130e-01	2.7070e+05	
15	16	1	1.5350e-01	2.5363e+05	

[pairs]

; at.i	at.j	funct
1	9	1
1	17	1
1	18	1
2	10	1
7	3	1
4	8	1
4	12	1
4	13	1
4	14	1
5	9	1
7	5	1
5	17	1
5	18	1
6	8	1
6	10	1
6	12	1
6	13	1
6	14	1
6	19	1

6	20	1
6	21	1
7	8	1
7	15	1
8	9	1
9	10	1
10	11	1
17	19	1
17	20	1
17	21	1
18	19	1
18	20	1
18	21	1
1	4	1
1	11	1
1	16	1
2	5	1
2	15	1
6	3	1
3	11	1
4	15	1
5	16	1
11	15	1

[angles]

; at.i	at.j	at.k	funct	theta(deg)	cth(kJ mol^{-1}rad^{-2})
1	2	8	1	1.2001e+02	4.0551e+02
2	1	7	1	1.2001e+02	4.0551e+02
2	3	9	1	1.2001e+02	4.0551e+02
3	2	8	1	1.2001e+02	4.0551e+02
3	4	10	1	1.2001e+02	4.0551e+02
4	3	9	1	1.2001e+02	4.0551e+02
5	4	10	1	1.2001e+02	4.0551e+02
5	11	12	1	1.1015e+02	3.9296e+02
5	11	13	1	1.1015e+02	3.9296e+02
5	11	14	1	1.1015e+02	3.9296e+02
6	1	7	1	1.2001e+02	4.0551e+02
6	15	17	1	1.1015e+02	3.9296e+02
6	15	18	1	1.1015e+02	3.9296e+02
12	11	13	1	1.0835e+02	3.2995e+02
12	11	14	1	1.0835e+02	3.2995e+02
13	11	14	1	1.0835e+02	3.2995e+02
15	16	19	1	1.1005e+02	3.8802e+02
15	16	20	1	1.1005e+02	3.8802e+02

15	16	21	1	1.1005e+02	3.8802e+02
16	15	17	1	1.1005e+02	3.8802e+02
16	15	18	1	1.1005e+02	3.8802e+02
17	15	18	1	1.0835e+02	3.2995e+02
19	16	20	1	1.0835e+02	3.2995e+02
19	16	21	1	1.0835e+02	3.2995e+02
20	16	21	1	1.0835e+02	3.2995e+02
1	2	3	1	1.1997e+02	5.6216e+02
1	6	5	1	1.1997e+02	5.6216e+02
1	6	15	1	1.2063e+02	5.3421e+02
2	1	6	1	1.1997e+02	5.6216e+02
2	3	4	1	1.1997e+02	5.6216e+02
3	4	5	1	1.1997e+02	5.6216e+02
4	5	6	1	1.1997e+02	5.6216e+02
4	5	11	1	1.2063e+02	5.3421e+02
5	6	15	1	1.2063e+02	5.3421e+02
6	5	11	1	1.2063e+02	5.3421e+02
6	15	16	1	1.1209e+02	5.2928e+02

[dihedrals]

; at.i	at.j	at.k	at.l	funct	C0(kJ mol^{-1})	C1(kJ mol^{-1})	C2(kJ mol^{-1})	C3(kJ mol^{-1})	C4(kJ mol^{-1})	C5(kJ mol^{-1})	
1	2	3	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	6	15	17	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
1	6	15	18	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
2	3	4	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
7	1	2	3	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	3	2	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	5	11	12	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
4	5	11	13	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
4	5	11	14	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
5	4	3	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
7	1	6	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
5	6	15	17	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
5	6	15	18	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
6	1	2	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	5	4	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	5	11	12	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
6	5	11	13	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
6	5	11	14	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
6	15	16	19	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
6	15	16	20	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
6	15	16	21	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
7	1	2	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
7	1	6	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;

8	2	3	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
9	3	4	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
10	4	5	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
17	15	16	19	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
17	15	16	20	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
17	15	16	21	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
18	15	16	19	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
18	15	16	20	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
18	15	16	21	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
7	1	6	2	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
1	3	2	8	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
2	4	3	9	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
3	5	4	10	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
1	2	3	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	6	5	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	6	5	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	6	15	16	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
2	1	6	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	6	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	3	4	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	1	2	3	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
3	4	5	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
3	4	5	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	5	6	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
5	6	15	16	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
11	5	6	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	6	5	11	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
15	1	6	5	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;